



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 02:26 PM EDT

PDB ID : 6UO1 / pdb_00006uo1
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with mRNA (containing pseudouridine at the first position of the codon) and deacylated A-, P-, and E-site tRNAs at 2.95Å resolution
Authors : Batool, Z.; Dobosz-Bartoszek, M.; Polikanov, Y.S.
Deposited on : 2019-10-14
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

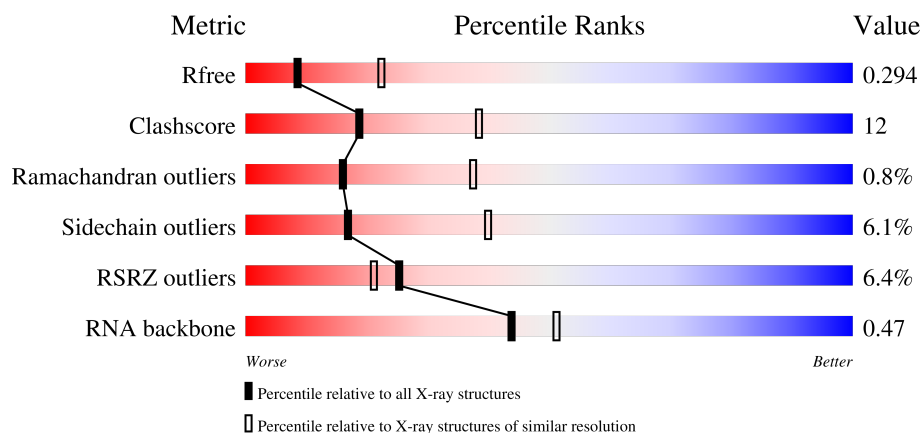
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)
RNA backbone	3983	1046 (3.16-2.76)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	
1	2A	2915	
2	1B	121	
2	2B	121	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	
27	25	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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
54	PSU	2y	55	-	-	X	-
56	MG	1A	3041	-	-	-	X
56	MG	1A	3214	-	-	-	X
56	MG	1A	3234	-	-	-	X
56	MG	1A	3294	-	-	-	X
56	MG	1A	3339	-	-	-	X
56	MG	1A	3429	-	-	-	X
56	MG	1A	3591	-	-	-	X
56	MG	1A	3674	-	-	-	X
56	MG	1a	3031	-	-	-	X
56	MG	1a	3143	-	-	-	X
56	MG	1a	3214	-	-	-	X
56	MG	2a	3082	-	-	-	X
56	MG	2a	3091	-	-	-	X
56	MG	2a	3093	-	-	-	X
56	MG	2a	3096	-	-	-	X
58	SF4	1d	501	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 295398 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 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2871	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	2E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1423	913	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1097	701	191	204	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1064	681	186	196	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
11	2P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	1Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	2Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	2R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			873	550	174	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
15	2T	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	2U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	1W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
18	2W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	1X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	2X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
21	2Z	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	13	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	23	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	16	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	26	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	17	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	27	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	18	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
30	28	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	19	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	29	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1548	973	301	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			810	514	144	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			983	623	193	167			
40	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			709	440	138	131			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	131			

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	1l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
43	2l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	1o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
46	2o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
47	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	1r	68	Total	C	N	O		0	0	0
			555	355	108	92				
49	2r	68	Total	C	N	O		0	0	0
			555	355	108	92				

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
51	2t	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

- Molecule 52 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			277	125	50	89	13			
53	2v	8	Total	C	N	O	P	0	0	0
			167	75	25	59	8			

- Molecule 54 is a RNA chain called A-site and E-site tRNAs.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	71	Total	C	N	O	P	S	0	0
			1530	685	274	498	71	2		
54	1y	74	Total	C	N	O	P	S	0	0
			1585	707	285	518	74	1		
54	2w	69	Total	C	N	O	P	S	0	0
			1482	662	267	482	69	2		
54	2y	73	Total	C	N	O	P	S	0	0
			1565	698	283	510	73	1		

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		
55	2x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	680	Total	Mg	0	0
			680	680		
56	1a	238	Total	Mg	0	0
			238	238		
56	2A	351	Total	Mg	0	0
			351	351		
56	2a	183	Total	Mg	0	0
			183	183		

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

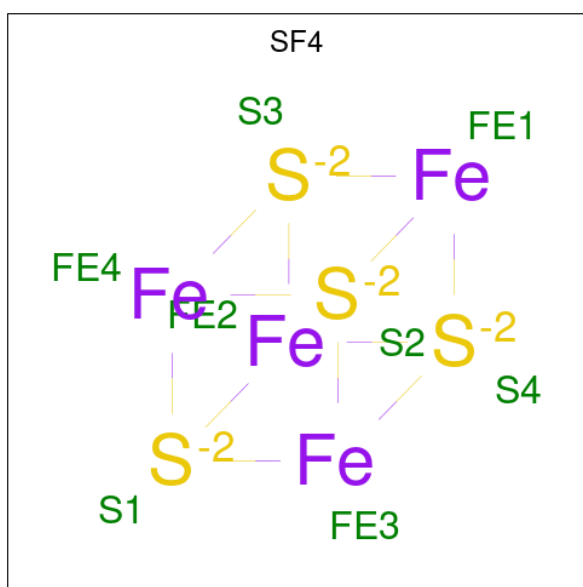
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	14	1	Total 1	Zn 1	0	0
57	15	1	Total 1	Zn 1	0	0
57	16	1	Total 1	Zn 1	0	0
57	19	1	Total 1	Zn 1	0	0
57	1n	1	Total 1	Zn 1	0	0
57	2Y	1	Total 1	Zn 1	0	0
57	24	1	Total 1	Zn 1	0	0
57	25	1	Total 1	Zn 1	0	0
57	26	1	Total 1	Zn 1	0	0
57	29	1	Total 1	Zn 1	0	0
57	2n	1	Total 1	Zn 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	1d	1	Total 8	Fe 4	S 4	0	0
58	2d	1	Total 8	Fe 4	S 4	0	0

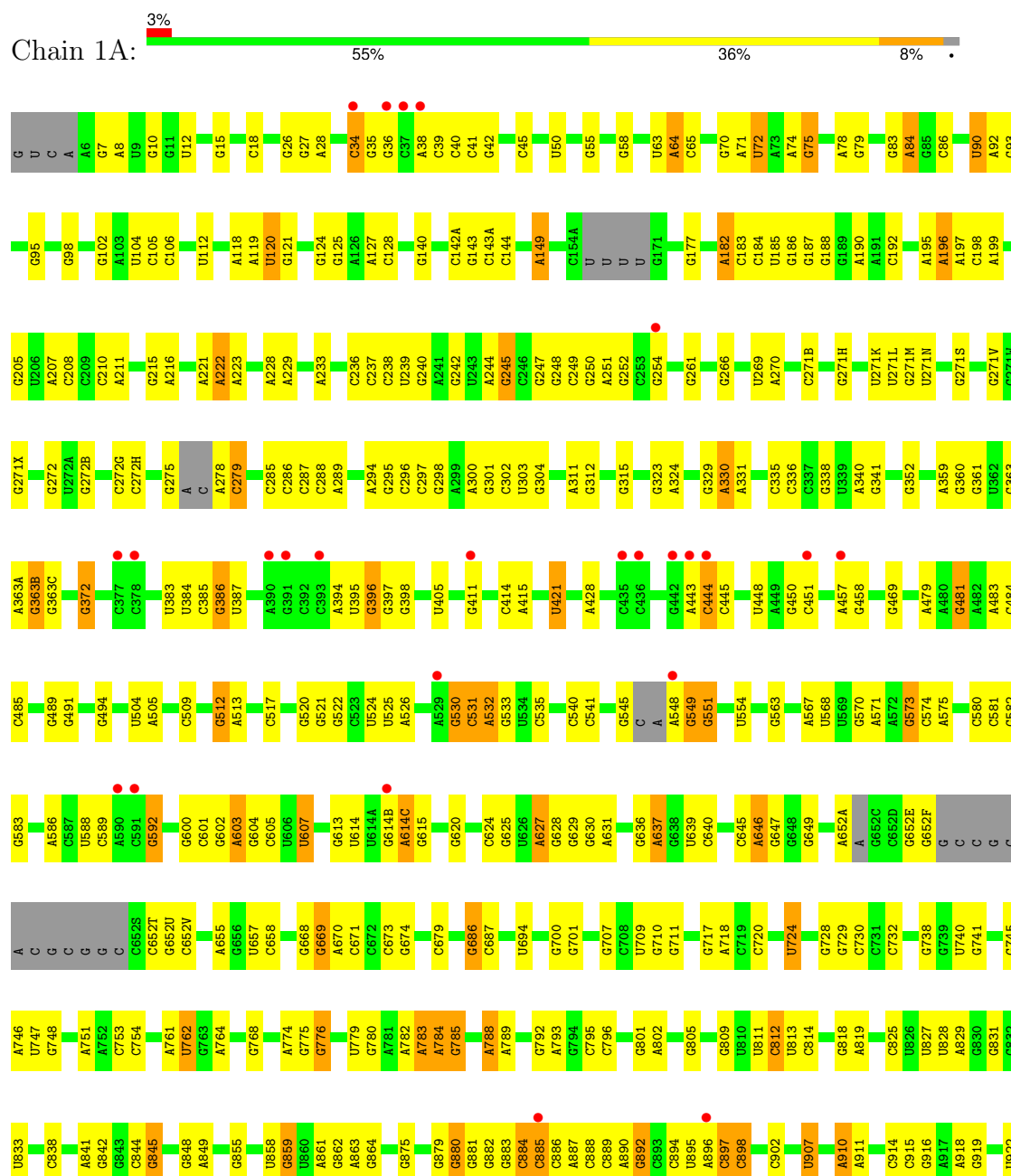
- Molecule 59 is water.

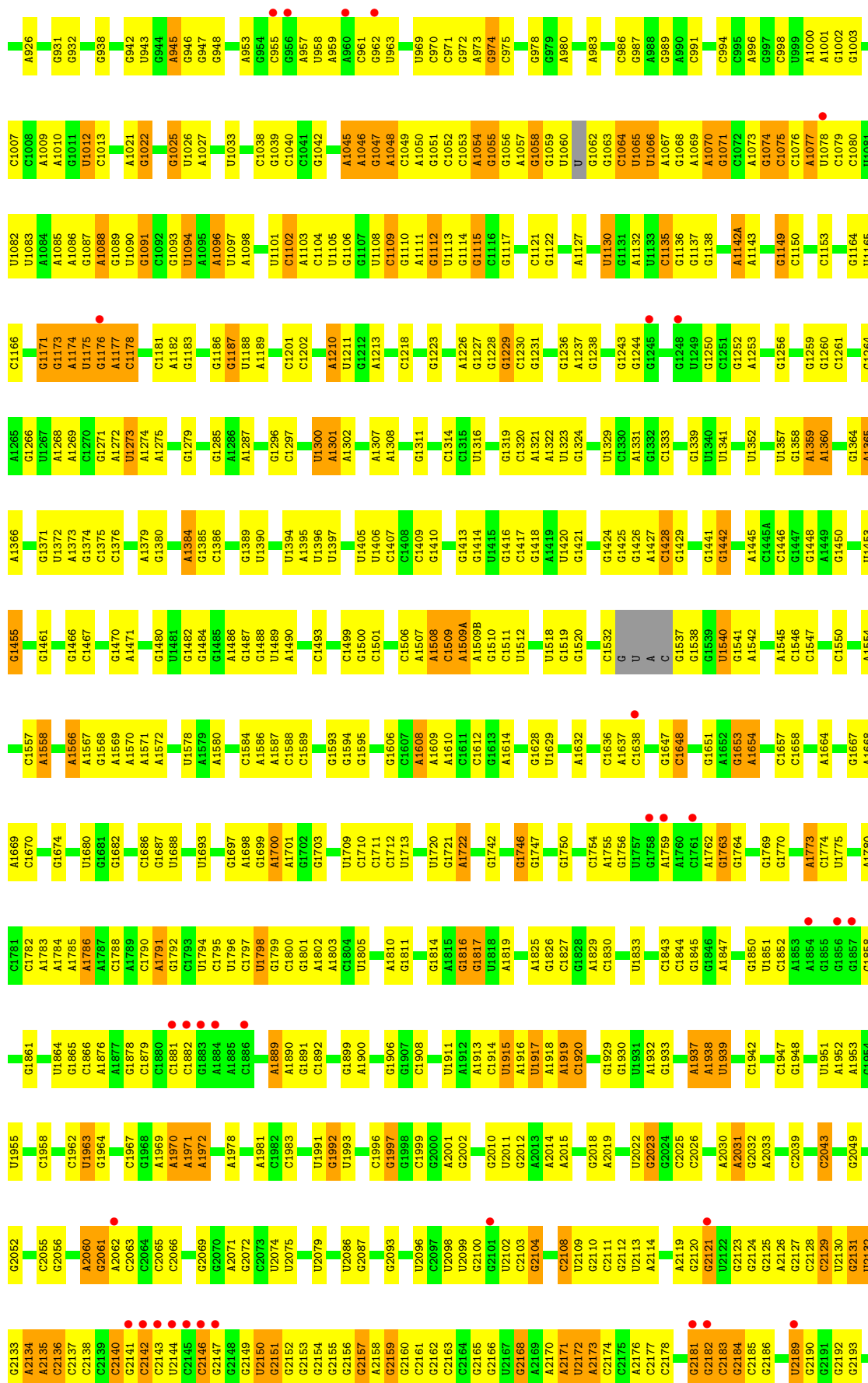
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	585	Total 585	O 585	0	0
59	1a	181	Total 181	O 181	0	0
59	2A	234	Total 234	O 234	0	0
59	2a	167	Total 167	O 167	0	0

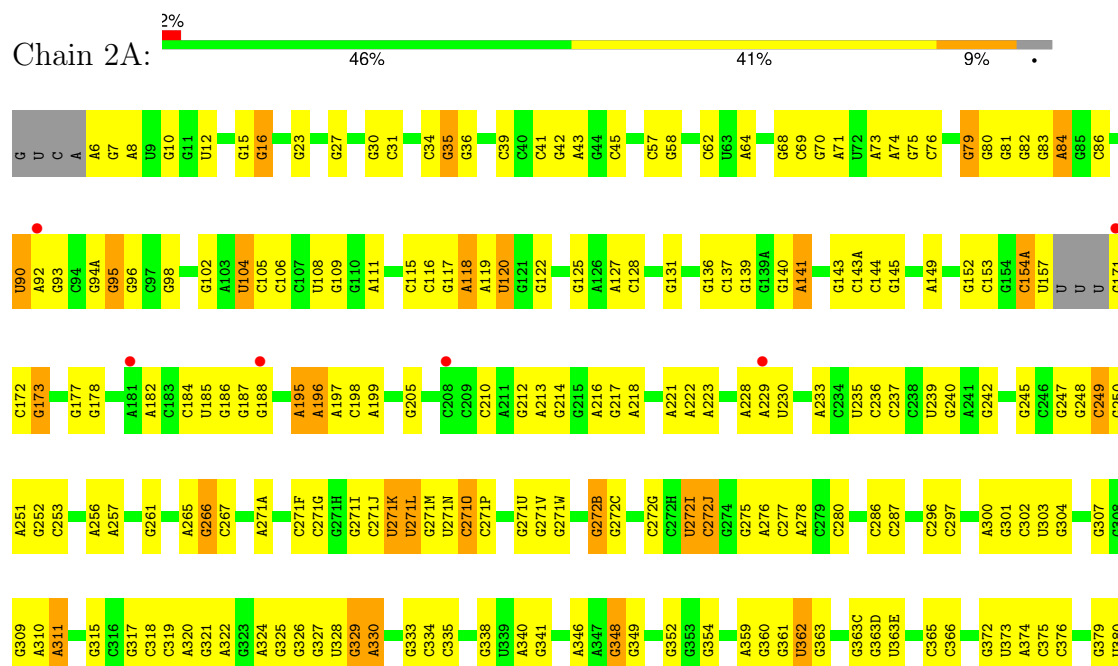
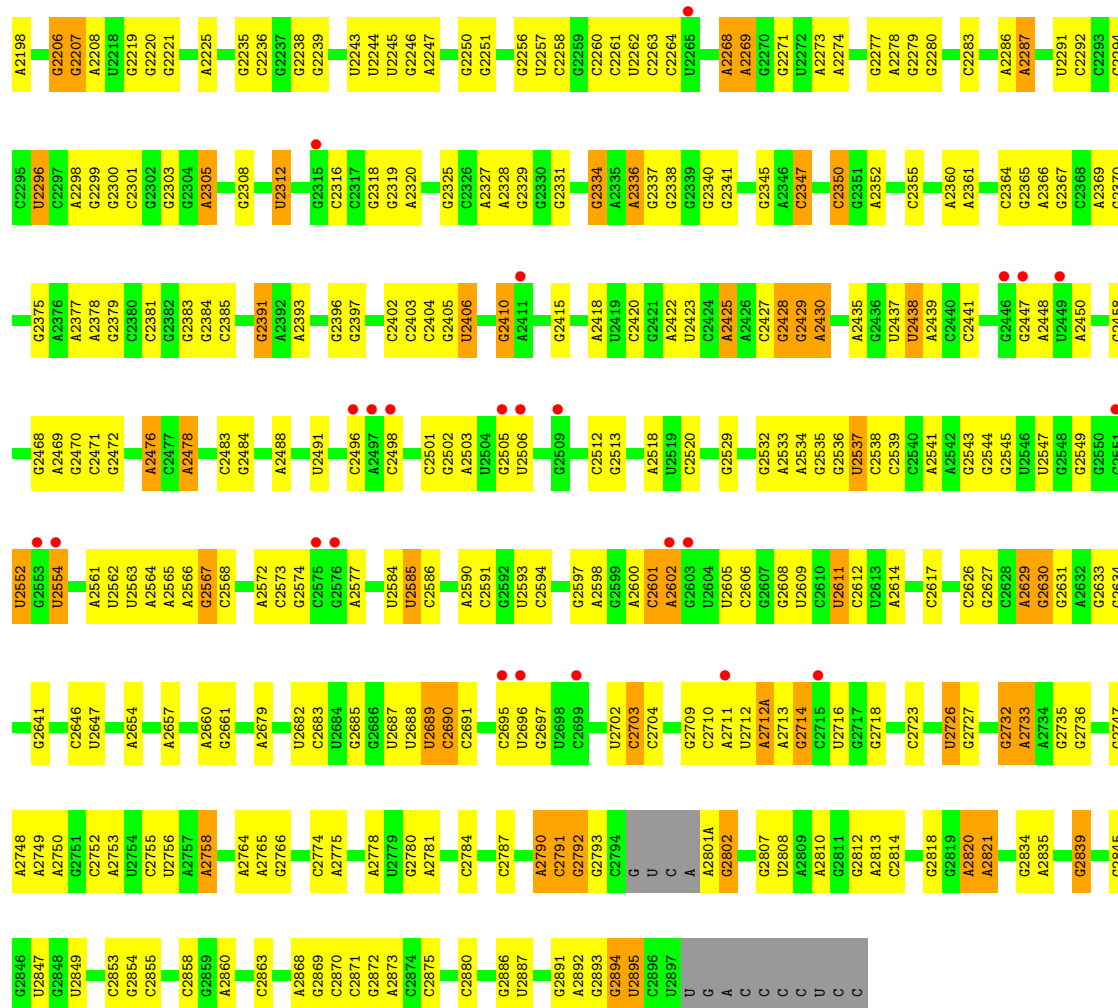
3 Residue-property plots

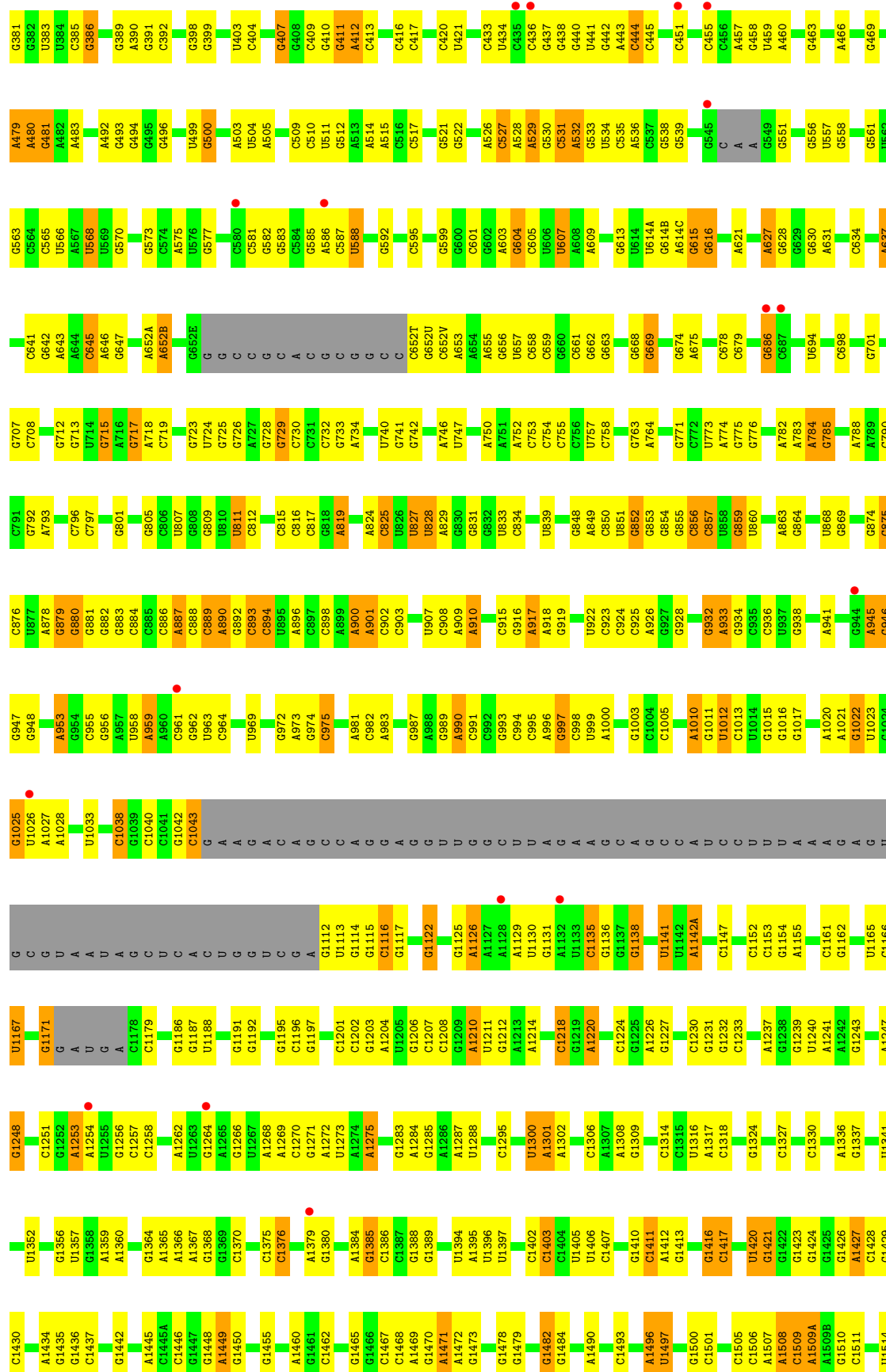
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 23S Ribosomal RNA

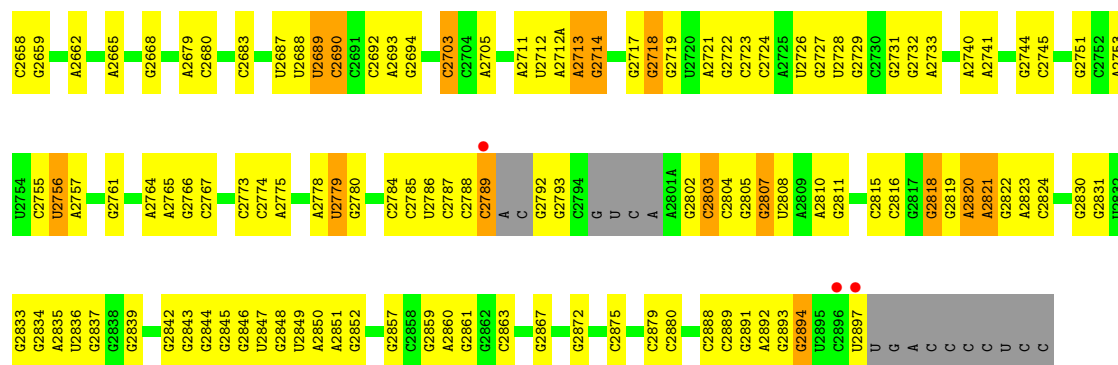




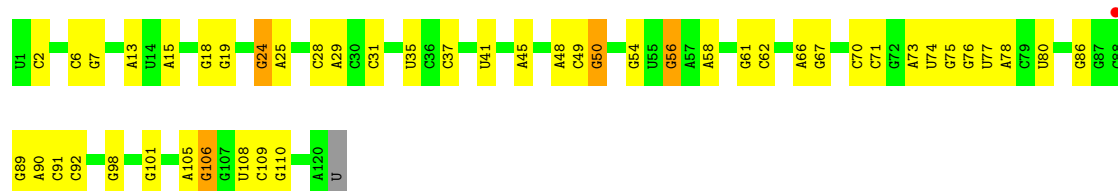




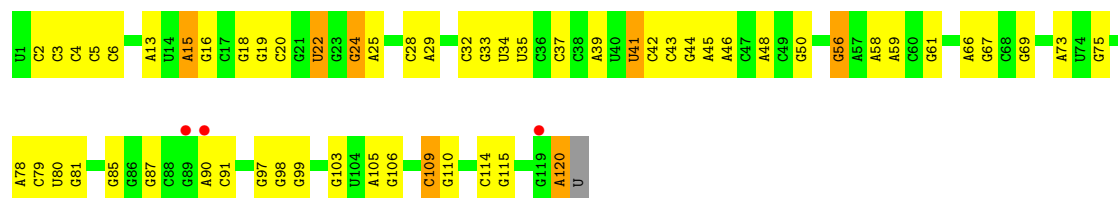
A2577	C2496	A2422	G2361	G2181	G2120	C2043	G1961	A1859	G1781				G1591	G1515
G2578	A2497	A2425	A2351	G2182	G2121	C2050	C1962	G1860	C1782				C1592	C1516
C2579	C2498	G2426	A2352	C2183	U2122	A2051	U1963	G1861	A1783				G1593	U1517
U2580		G2427	G2353	C2184	G2123	G2052	G1964	G1862	A1784				U1518	G1519
C2586	G2502	C2428	G2354	C2185	A2126		C1967	G1863	A1785				G1598	G1520
A2587	A2504	G2429	G2355	G2187	G2127	C2055	G1968	G1865	A1786				U1593	U1523
G2588	G2505	A2430	C2364	C2188	C2128	G2056	A1969	G1866	C1787				G1594	G1524
A2589	U2506	U2431	G2365	U2189	C2129	A2060	A1877	A1877	C1788				G1595	G1525
C2590	C2507	A2432	A2366	G2190	U2130	G2061	G1878	G1878	C1790				G1596	G1526
C2591		A2433	G2367	G2191	G2131	A2062	A1972	G1879	A1791				A1603	G1527
G2592	U2511	A2434	C2368	G2192	U2132		G1973	C1882	G1792				G1605	
	G2512	A2435	A2369	G2193	G2133	C2066	C1974	G1883	G1793				G1606	
U2596	G2513		G2370	G2194	G2134			G1889	U1794				C1607	
G2597	U2514	A2439	G2371	U2197	A2135		C1983	A1889	C1788				A1608	
A2598	C2515	C2440	C2374	A2198	C2136	G2069	G1984	A1890	C1789				C1532	
	G2516	C2441	G2375	G2299	G2137	G2070	A1970	A1890	C1790				G1533	
A2602	G2517	C2442	G2376	G2300	C2138	A2071	A1985	A1891	G1792				U	
G2603	G2518	C2443	A2376	C2301	G2139	G2072	A1986	G1894	G1793				A	
U2604	U2519		A2377	G2302	C2140	C2073	C1990	G1899	C1800				C1536	
U2605	G2520	G2446	A2378	G2303	G2141	G2074	U1991	A1900	A1801				G1537	
		G2447	C2379	G2304	C2142	U2075	G1992	A1900	A1802				G1538	
G2608	C2527	A2448	C2380	A2225	C2143		U1993	G1906	A1803				G1539	
U2609	U2528	U2449	C2381	G2226	U2144	C2078	C1996	G1907	G1804				U1540	
C2610	G2529	A2450	G2382	A2225	U2145	U2079	G1997	G1908	U1805				G1541	
U2611	A2530		G2383	U2232	C2146								A1542	
C2612	A2531	G2454	G2384	U2233	G2147	U2086	G1998	U1911	U1808				A1543	
	G2532	G2455	G2385	G2235	G2148	G2087	C1999	A1809	G1721				A1544	
U2615	A2533	G2456	C2386	U2236	C2149	G2088	G2000	A1913	C1636					
		U2457	A2388	G2237	U2150	U2089	A2001	G1914	A1722				C1637	
G2616	G2536		G2389	G2238	G2151	G2090	G2002	U1915	U1739				C1647	
C2617	U2537	U2462	U2390	G2239	G2152	U2091		A1916	G1740				C1548	
G2618	C2538	C2463	G2391	U2240	G2153	U2092	A2005	U1917	A1812				C1549	
	C2539	G2464	A2392	U2241	G2154	G2093	G2010	A1920	G1814				C1550	
		C2465	A2393	U2242	G2155	G2094	G2010	G1920	A1815				C1556	
G2626	G2544	G2466	C2394	U2243	G2156	C2095	G1921	G1921	G1816				C1557	
C2627	U2545	C2467	C2395	U2244	G2157	U2096	A2014	G1746	C1745A				A1558	
A2628	U2546	G2468	G2396	C2248	A2158	C2097		C1924	G1649				G1559	
G2630	U2547	A2469	G2397	U2249	G2159	U2098	G2018		A1821				G1560	
	G2548		A2399	G2250	G2160	U2099	A2019	A1927	C1827					
C2631	G2549	C2474	U2400	G2251	C2161	G2100		A1928	G1828				A1566	
A2632		G2475	U2401	G2252	G2162	G2101	U2022	G1929	A1829				A1567	
G2633		A2476	C2402	G2253	C2163	U2102	G2023	G1930	G1835				G1568	
G2634	U2552	C2477	C2403	C2258	C2164	C2103	G2024	U1931	G1835				G1569	
	G2553		C2404	C2261	G2165	G2104	C2025						C1657	
G2641	U2554		C2405	C2262	G2166	C2105	C2026	G1935	C1838				C1658	
G2642	C2555	C2480	U2406	C2263	U2167	G2106	G2027	A1936	U1839				U1659	
G2643	G2556	G2481	G2407	G2264	G2168	C2107		A1937	A1762				C1660	
G2644	G2557	C2482	U2408	U2265	A2169	C2108	A2030	U1938	G1763				G1661	
G2645		C2483	G2409	A2266	A2170	U2109	A2031	U1939	G1764				C1662	
G2646	U2562	G2484	G2410	A2267	A2171	G2110	G2032		G1843				C1663	
U2647		G2485	G2411	A2268	U2172	G2111	A2033	C1942	G1846				A1664	
G2648	A2566	A2412	A2412	A2269	A2173	G2112	C2036	U1943	A1847				C1667	
U2649	C2567	G2487	G2413	A2270	C2174	U2113	U1944	U1944	A1848				G1668	
U2650	C2568	A2488	G2414	A2271	C2175	A2114	G1945	G1945	U1851				A1669	
C2651		G2490	G2415	A2272	A2176	G2115	U1955		C1852				C1670	
C2652	U2572			C2275	C2177	G2116	C2038	U1955	A1853				A1586	
U2653	G2573		U2419	C2276	C2178	A2117	C2039		A1854				G1674	
A2654	G2574		C2420	A2278	C2179	U2118	C2040	G1959	A1854				U1680	
A2657	G2576		G2495	G2279	U2180	A2119	A2042	A1960	G1858					



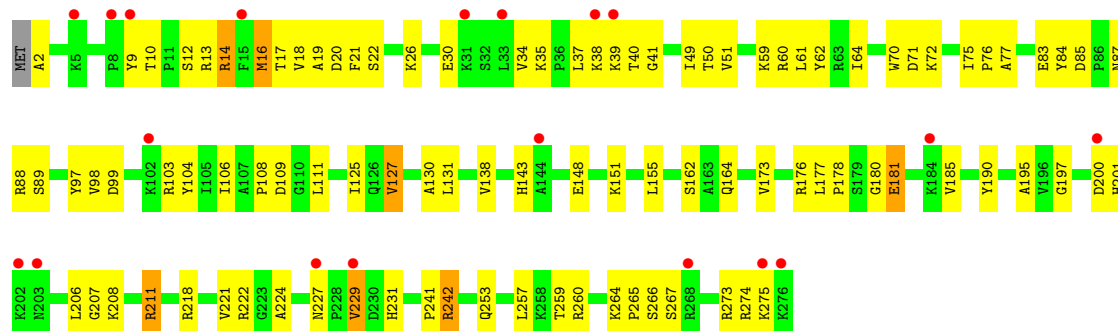
• Molecule 2: 5S Ribosomal RNA



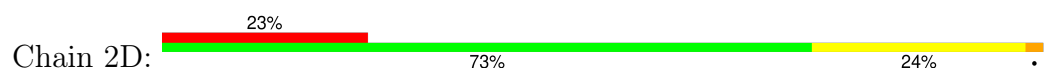
• Molecule 2: 5S Ribosomal RNA

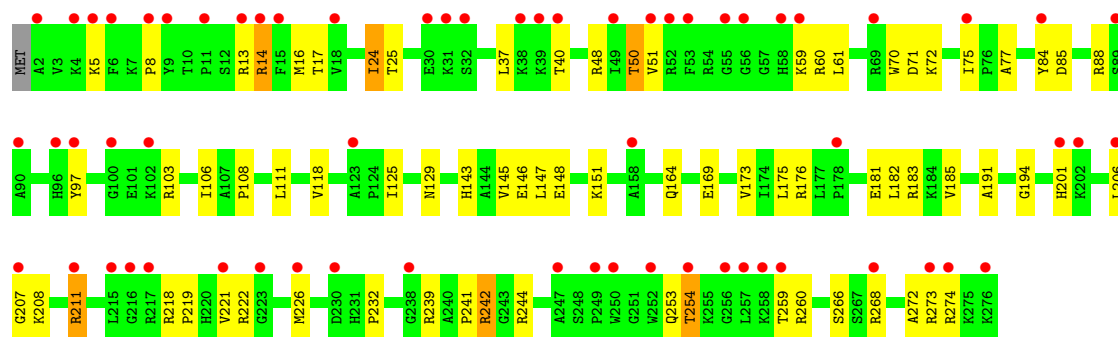


• Molecule 3: 50S ribosomal protein L2

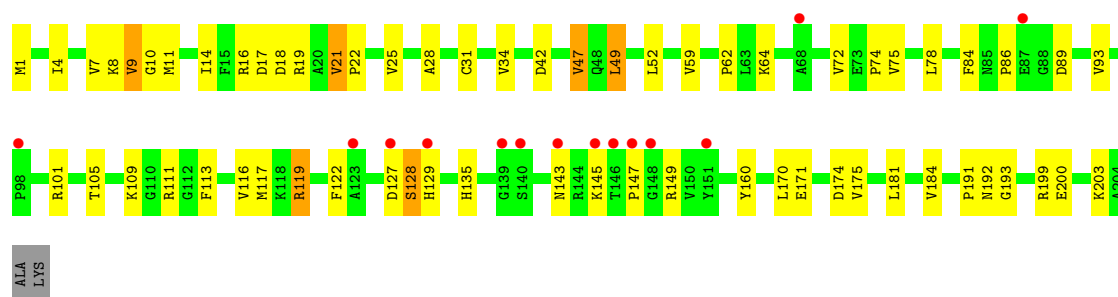


• Molecule 3: 50S ribosomal protein L2

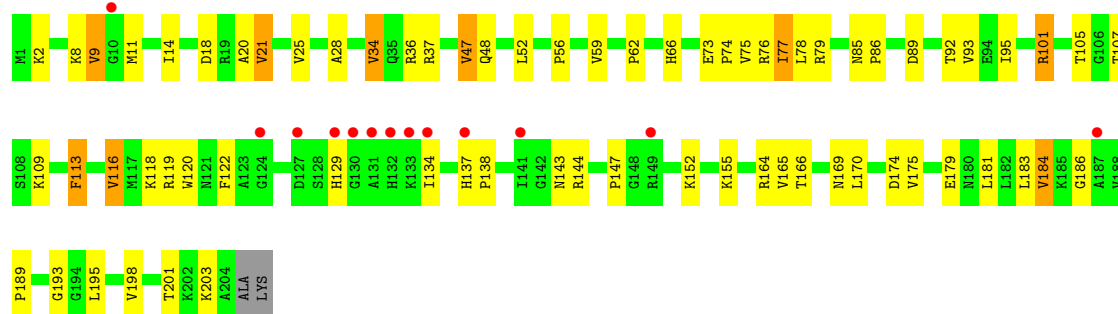




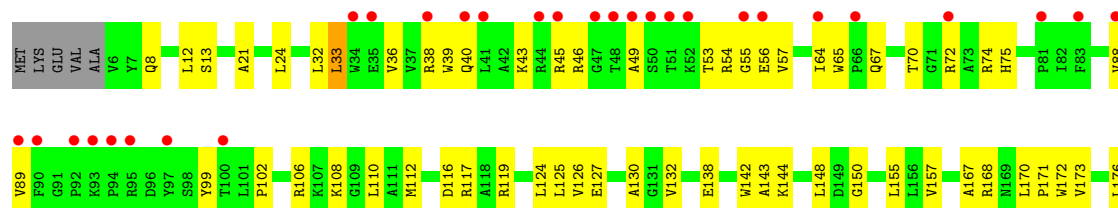
• Molecule 4: 50S ribosomal protein L3

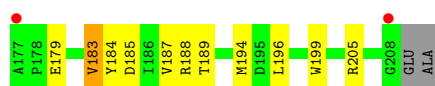


• Molecule 4: 50S ribosomal protein L3

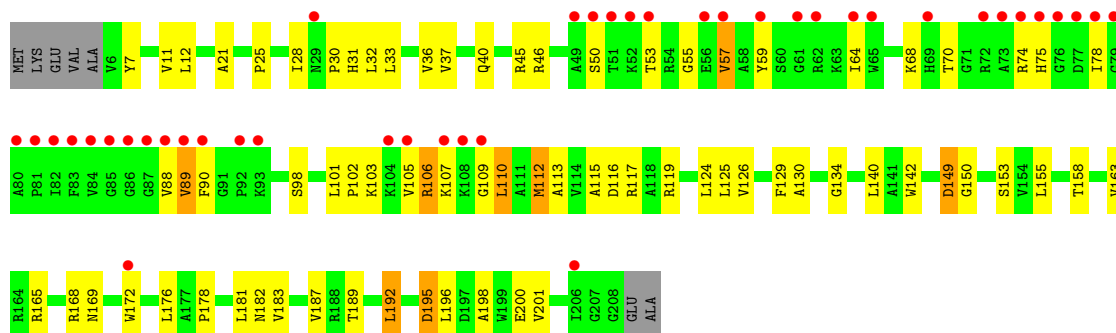


• Molecule 5: 50S ribosomal protein L4

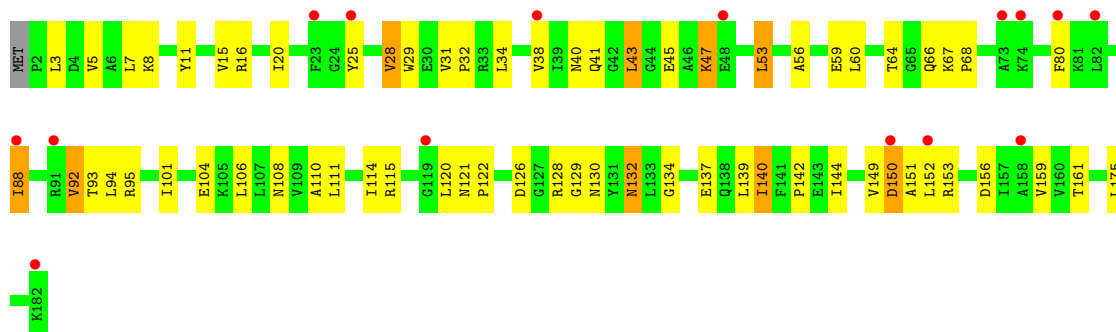




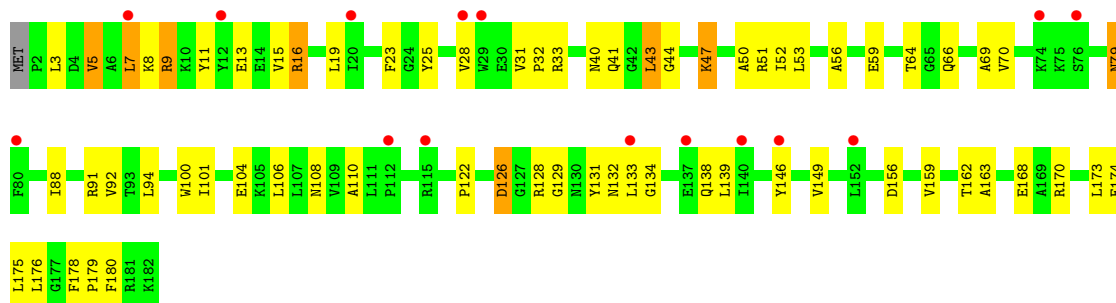
• Molecule 5: 50S ribosomal protein L4



• Molecule 6: 50S ribosomal protein L5

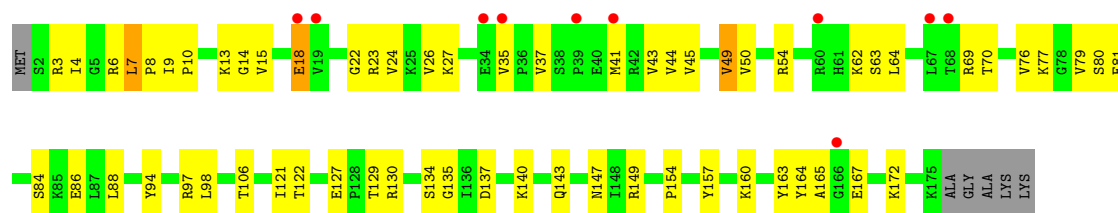


• Molecule 6: 50S ribosomal protein L5

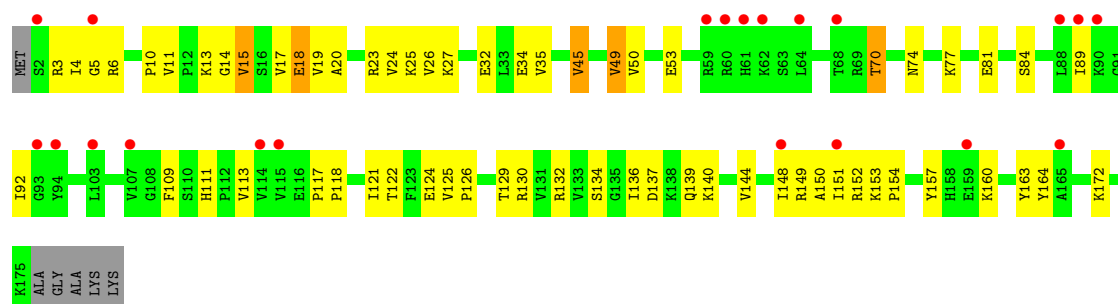


• Molecule 7: 50S ribosomal protein L6

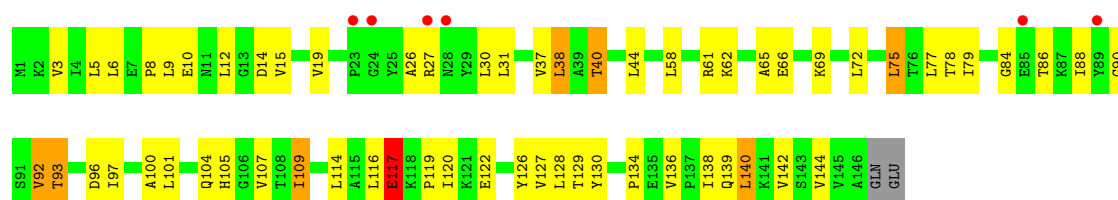




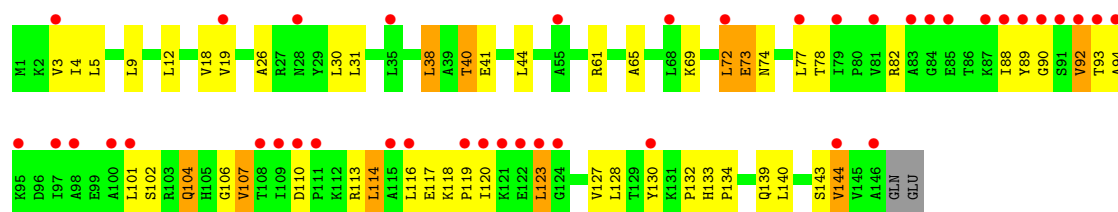
• Molecule 7: 50S ribosomal protein L6



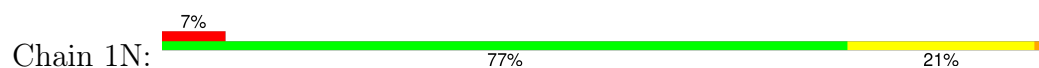
• Molecule 8: 50S ribosomal protein L9



• Molecule 8: 50S ribosomal protein L9

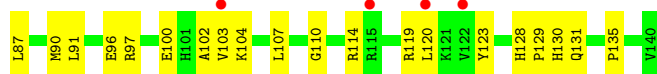
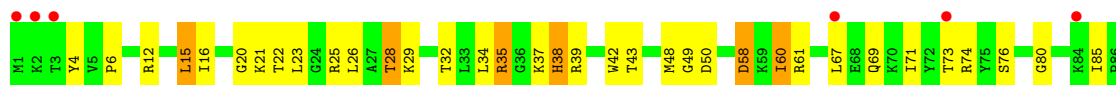


• Molecule 9: 50S ribosomal protein L13





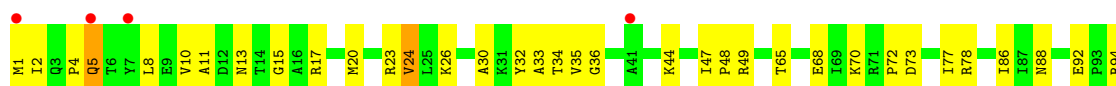
• Molecule 9: 50S ribosomal protein L13



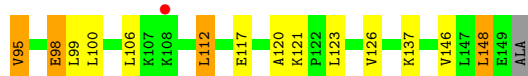
• Molecule 10: 50S ribosomal protein L14



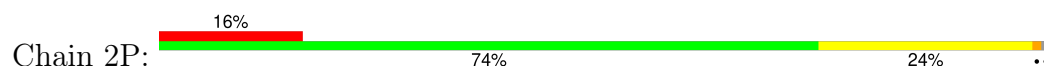
• Molecule 10: 50S ribosomal protein L14

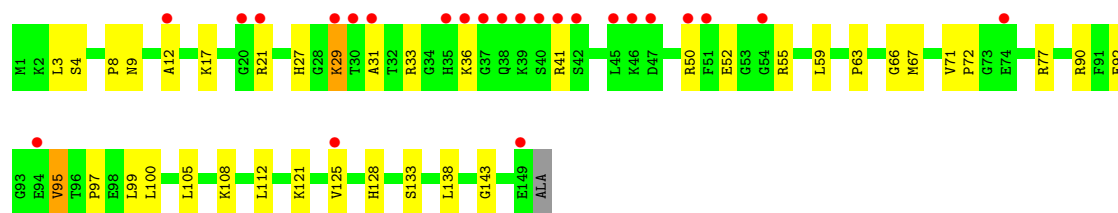


• Molecule 11: 50S ribosomal protein L15

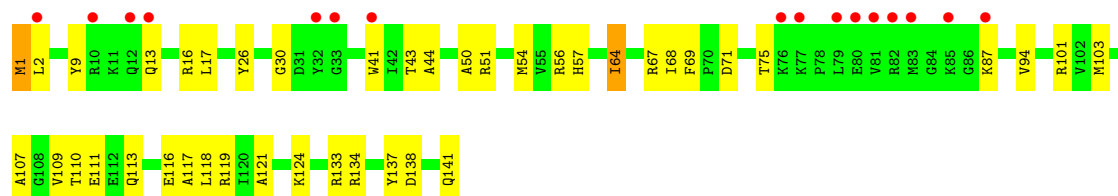
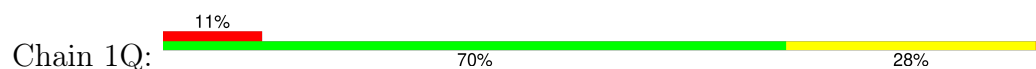


• Molecule 11: 50S ribosomal protein L15

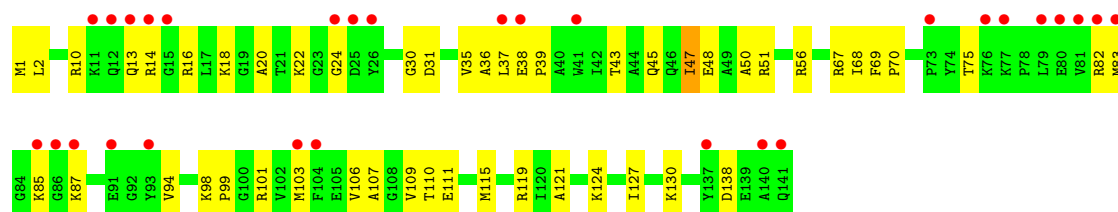




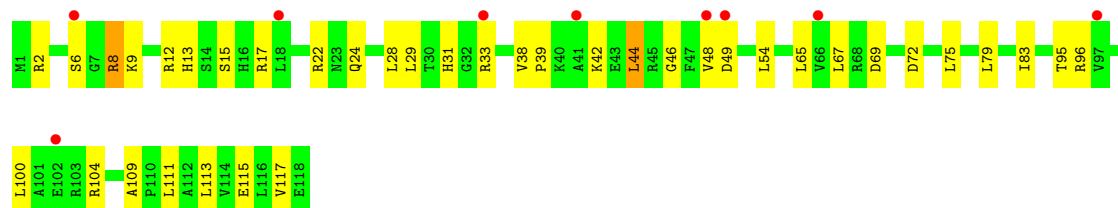
• Molecule 12: 50S ribosomal protein L16



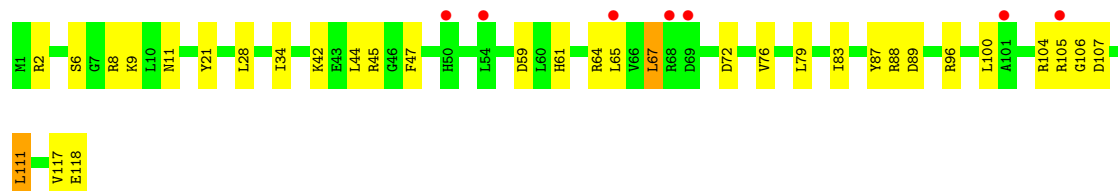
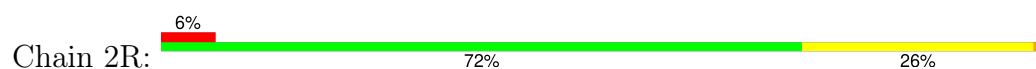
• Molecule 12: 50S ribosomal protein L16



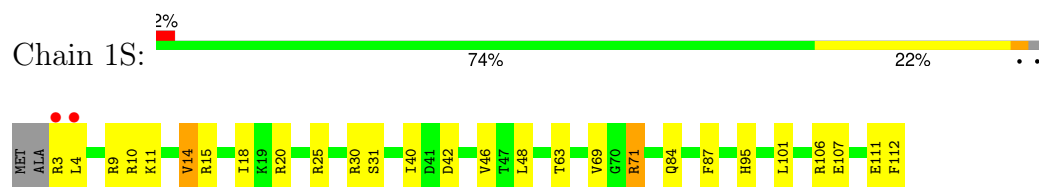
• Molecule 13: 50S ribosomal protein L17



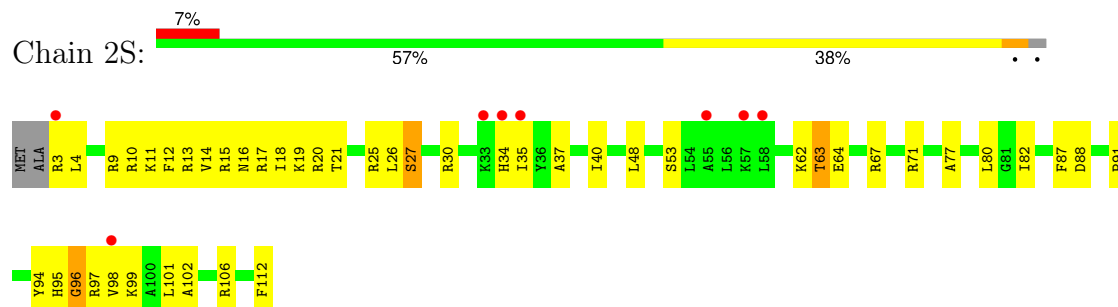
• Molecule 13: 50S ribosomal protein L17



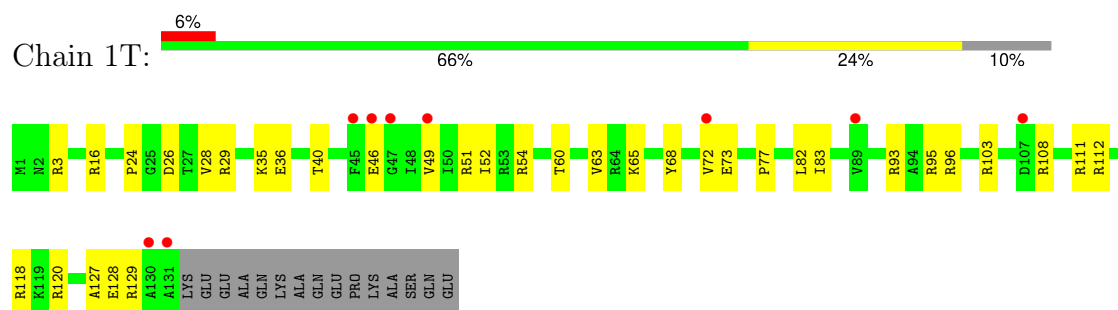
- Molecule 14: 50S ribosomal protein L18



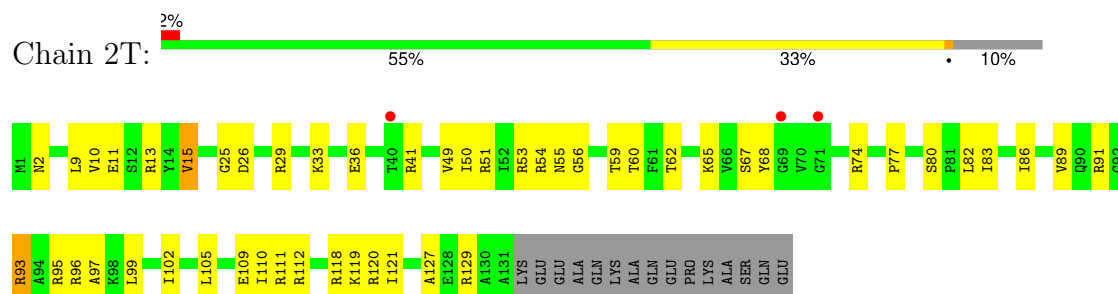
- Molecule 14: 50S ribosomal protein L18



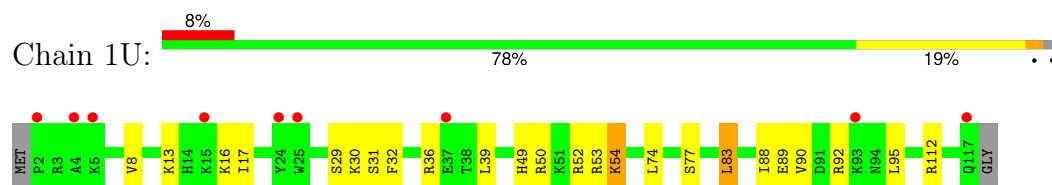
- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



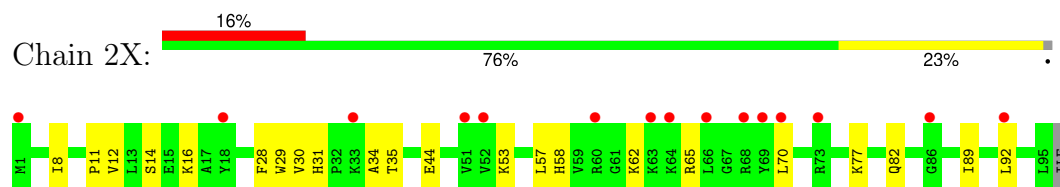
- Molecule 16: 50S ribosomal protein L20



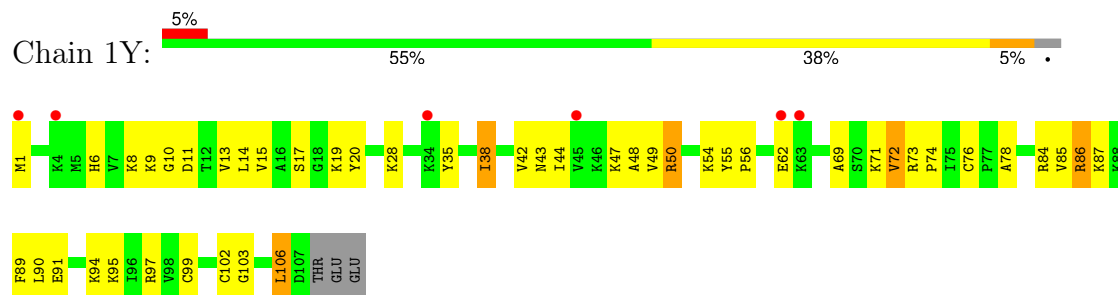
- Molecule 16: 50S ribosomal protein L20



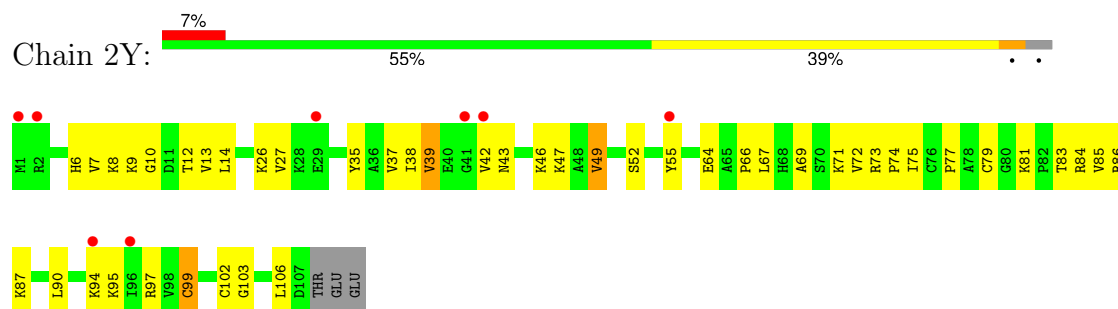
- Molecule 19: 50S ribosomal protein L23



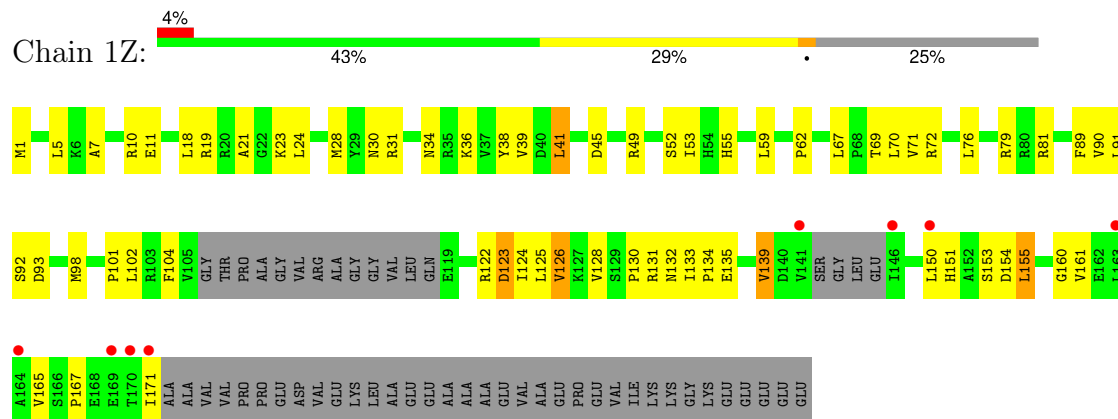
- Molecule 20: 50S ribosomal protein L24



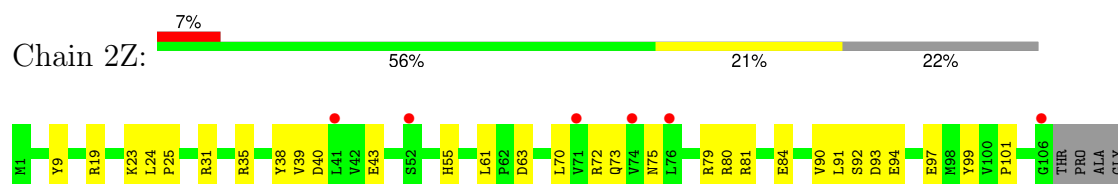
- Molecule 20: 50S ribosomal protein L24

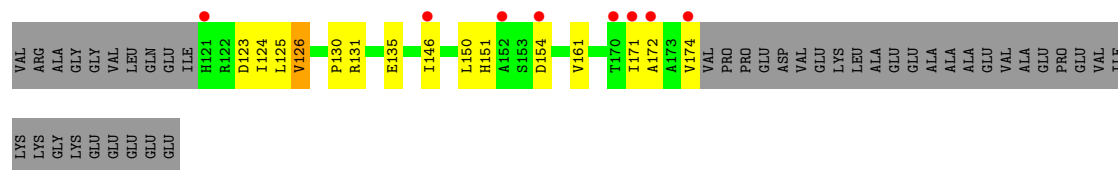


- Molecule 21: 50S ribosomal protein L25

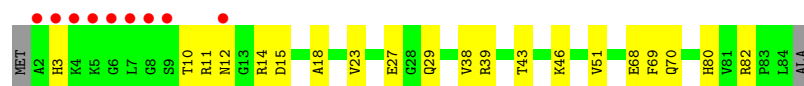
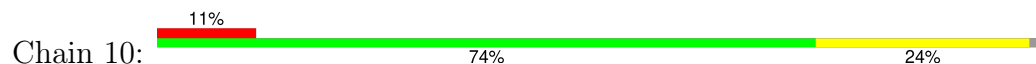


- Molecule 21: 50S ribosomal protein L25

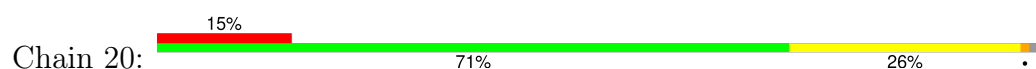




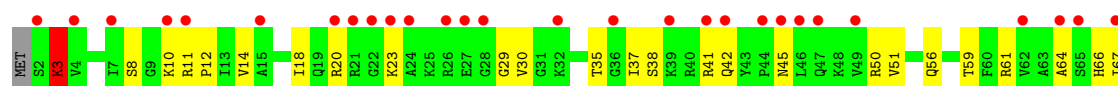
- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27



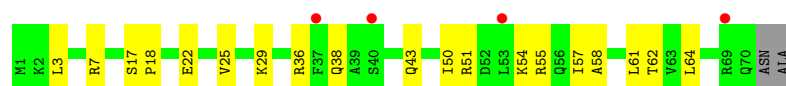
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28

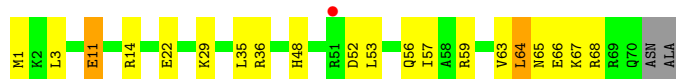


- Molecule 24: 50S ribosomal protein L29

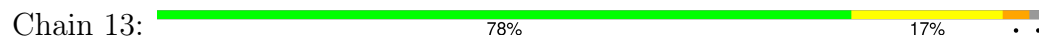


- Molecule 24: 50S ribosomal protein L29

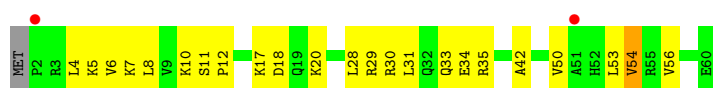




- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30



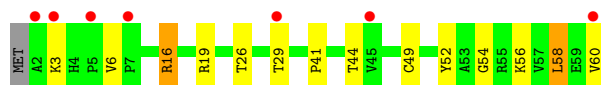
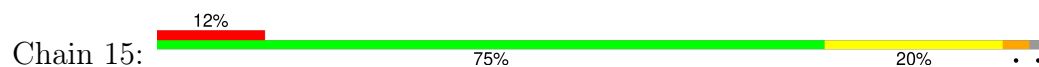
- Molecule 26: 50S ribosomal protein L31



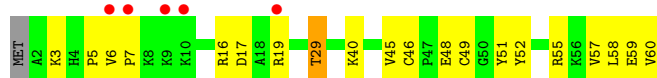
- Molecule 26: 50S ribosomal protein L31



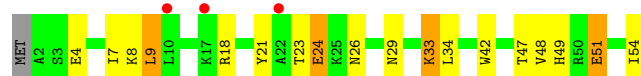
- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



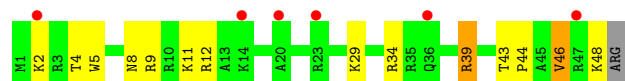
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



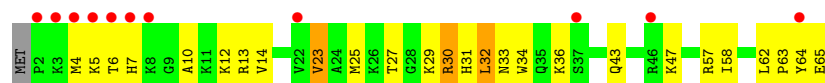
- Molecule 29: 50S ribosomal protein L34



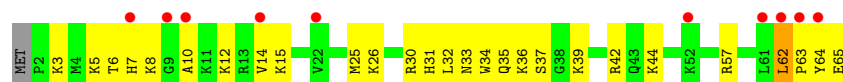
- Molecule 29: 50S ribosomal protein L34



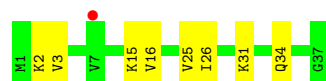
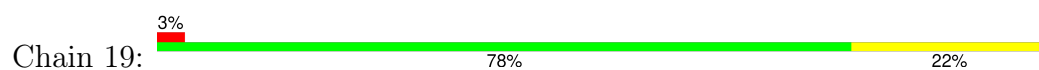
- Molecule 30: 50S ribosomal protein L35



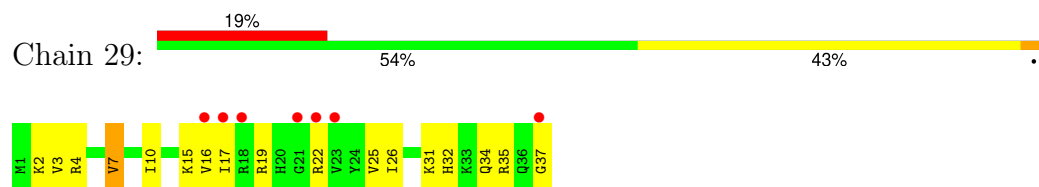
- Molecule 30: 50S ribosomal protein L35



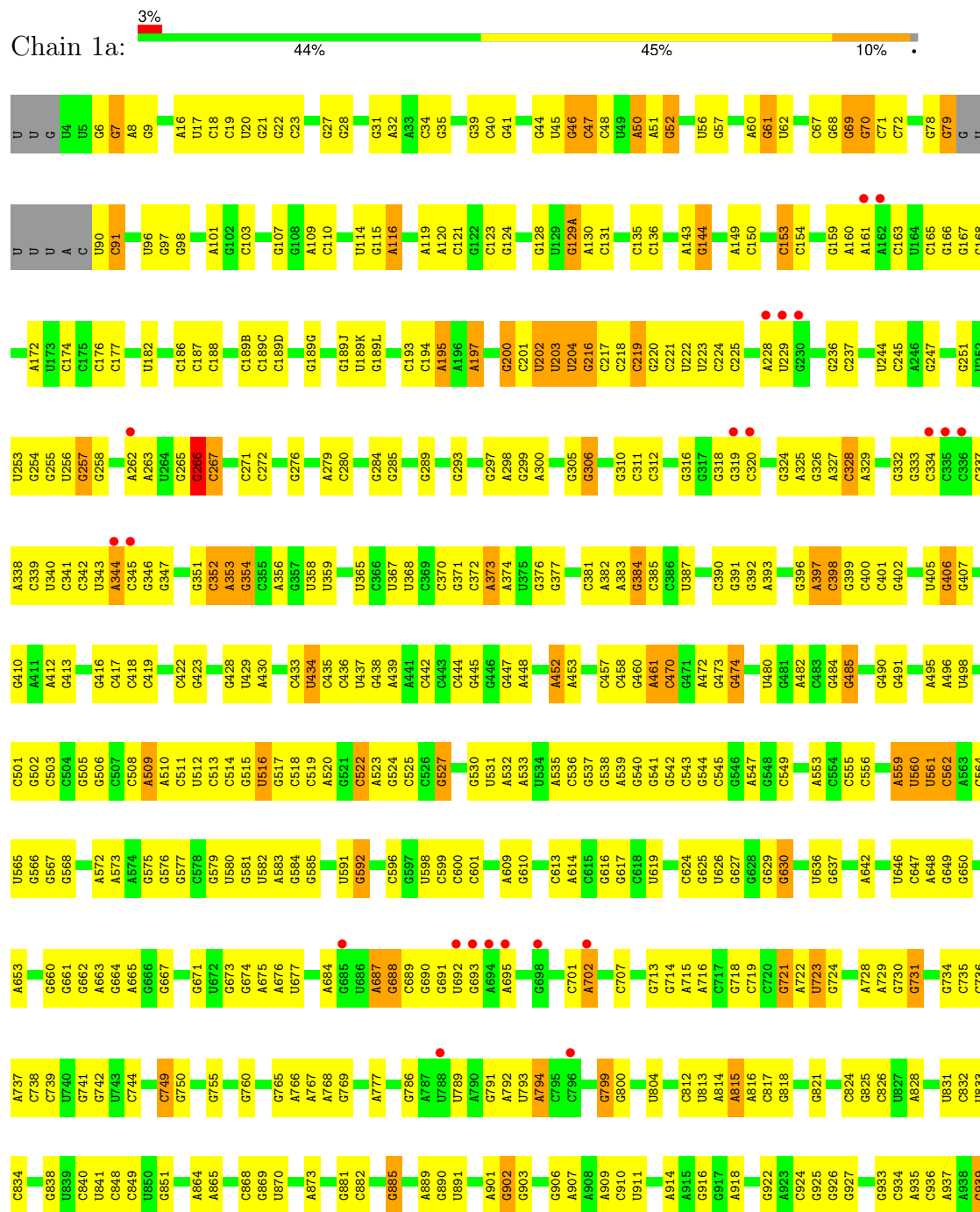
- Molecule 31: 50S ribosomal protein L36



• Molecule 31: 50S ribosomal protein L36

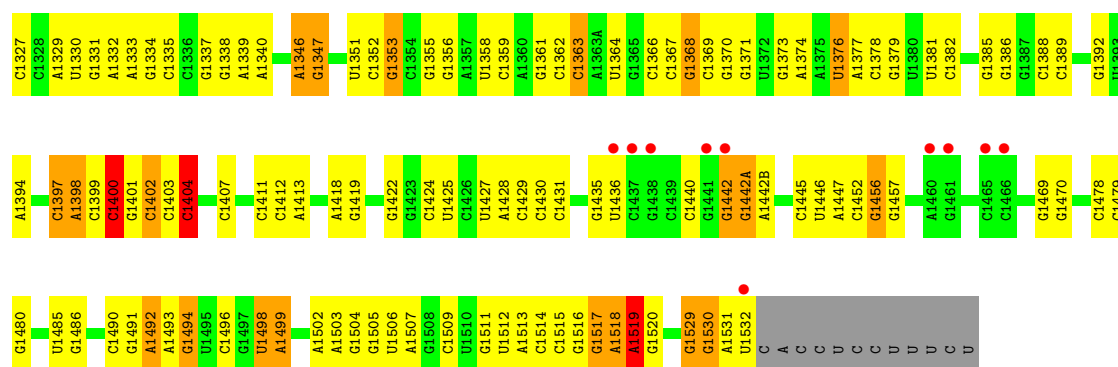


• Molecule 32: 16S Ribosomal RNA

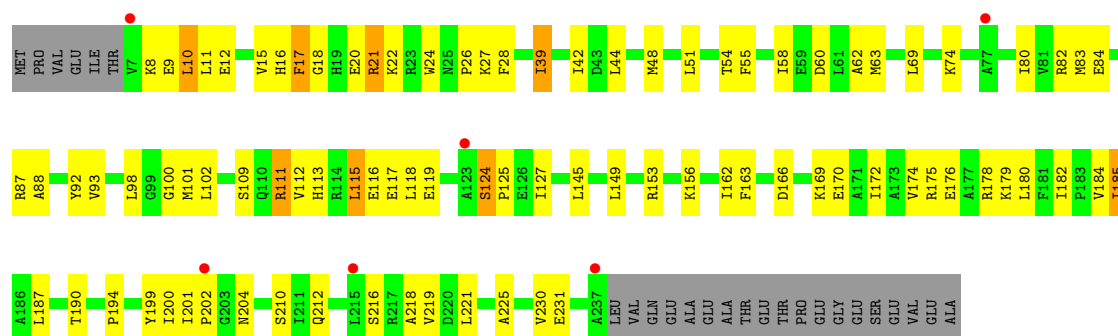




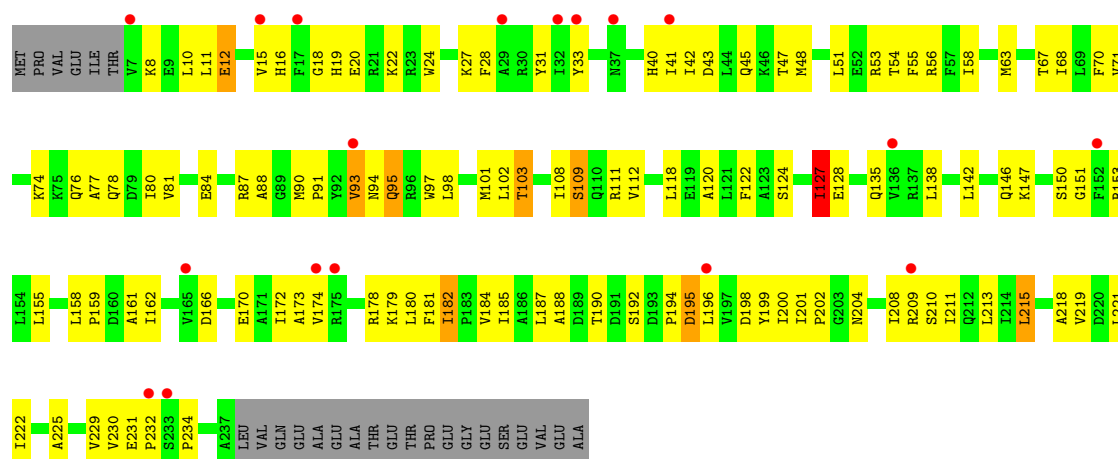
A1261	C1262	C1263	C1264	C1265	G1266	C1267	A1268	A1269	C1270	A1271	C1272	G1273	G1274	A1275	G1276	C1277	C1278	G1279	A1280	U1281	C1284	A1285	A1286	A1287	A1288	A1289	G1290	G1291	U1292	G1293	G1294	G1295	A1299	G1300	U1301	U1302	C1303	G1304	C1305	A1306	G1309	G1310	G1311	G1312	U1313	G1316	C1317	A1318	A1319	C1320	C1321	C1322	G1323	G1326	C1326		
A1191	C1192	C1193	U1194	C1195	C1196	G1197	C1200	A1201	G1202	C1203	A1204	G1273	G1274	A1275	G1276	C1277	C1208	C1209	G1210	U1211	U1212	A1213	C1214	G1215	C1218	U1219	G1220	C1223	G1224	A1225	C1226	A1227	C1228	A1229	U1232	A1236	C1237	A1238	G1239	U1240	G1241	C1242	C1243	C1244	A1245	C1246	A1251	A1252	G1255	A1256	C1321	U1257	G1258	C1322	G1323	C1326	
G1124	U1125	U1126	U1127	G1128	C1129	A1130	G1131	C1132	G1133	C1134	U1135	U1136	C1137	G1138	G1139	C1140	C1141	G1142	G1143	G1144	C1145	A1146	C1147	U1148	C1149	U1150	A1151	A1152	G1153	G1154	G1155	U1156	A1157	C1158	U1159	G1160	G1161	C1162	C1163	G1164	C1165	G1166	A1170	G1171	G1178	A1183	G1184	G1185	G1186	G1187	A1188	C1189	U1192	C1190	A1123		
A1055	U1056	C1060	C1061	G1062	C1063	U1064	U1065	U1066	A1067	G1068	C1071	G1074	C1075	G1076	U1077	U1078	G1079	A1080	G1081	U1082	U1083	U1084	U1085	U1086	G1089	G1094	U1095	C1096	C1097	C1098	G1099	C1100	A1101	A1102	C1103	G1104	A1105	G1106	C1107	G1108	C1109	A1110	A1111	C1112	C1113	G1114	G1117	C1118	C1119	G1120	U1121	U1122	A1123				
G998	C999	U1000	A1001	G1001A	G1002	C1003	A1004	A1005	C1006	C1007	C1008	G1009	G1010	G1011	U1012	G1013	A1014	A1015	A1016	G1017	C1018	U1019	U1020	G1021	G1022	G1023	G1024	U1025	G1026	C1027	C1028	C1029	C1030	G1030A	G1030B	C1030C	A1030D	G1031	G1032	G1033	G1034	A1035	C1036	C1037	C1038	C1039	U1040	A1041	G1042	C1043	A1044	C1045	A1046	G1047	C1051	U1052	G1053
G927	C928	C931	C932	G933	C934	A935	C936	A937	A938	G939	U943	G944	A949	U952	G953	G954	U955	U956	A959	C978	U960	U961	A964	A965	A966	C967	A968	A969	C970	C971	C972	G973	A974	A975	G976	A977	C978	A978	C979	C980	U981	C984	C985	A986	G987	C988	C989	C990	U991	U992	G993	A994	C995	A996	U997		
C848	G851	G852	C853	G854	G855	C856	C857	A859	A864	A865	C868	G869	U870	U871	U872	C877	C878	C879	C880	G881	C882	G883	U884	G885	G886	G887	G890	G894	A901	G902	G903	C904	U905	G906	A909	C910	U911	G923	G924	G925	C926	U927	A928	U929	U931	G938	U939	C924	G925	G926							
G750	A753	C754	G755	C756	U757	G758	G761	A767	A768	G769	G774	A777	G778	C779	A782	U788	U789	A790	G791	A792	U793	A794	C795	C796	A715	A716	A573	A574	C508	A509	A510	C511	U512	C513	C514	G515	U516	U517	A518	C519	A520	G521	C522	G523	C524	C525	C526	G527	G530	U531	A532	A533					
U678	C679	C680	C681	G682	G683	A684	G685	U686	G688	C689	G690	G691	U692	A694	A695	A696	G700	C701	A702	G703	A705	C707	C708	G709	G713	G714	A715	A716	A573	A574	C508	A509	A510	C511	U512	C513	C514	G515	U516	U517	A518	C519	A520	G521	C522	G523	C524	C525	C526	G527	G530	U531	A532	A533			
A602	U605	G606	A607	A608	A609	G610	A614	C615	C618	U619	C620	A621	A622	C623	C624	G627	G628	G629	G630	G631	A632	U636	G637	G638	G639	A640	G644	G645	U646	C647	G650	A653	U656	G657	U658	G659	A660	G661	G662	A663	A665	G666	G670	G671	U672	G673	A675	A676	U677	C749							
C879	C880	C881	G882	G883	A884	G885	U886	A887	C888	C889	G890	G891	U892	A894	A895	G900	C901	A902	G903	A905	C907	C908	G909	G913	G914	A915	A916	A573	A574	C508	A509	A510	C511	U512	C513	C514	G515	U516	U517	A518	C519	A520	G521	C522	G523	C524	C525	C526	G527	G530	U531	A532	A533				
G376	G377	G378	A383	G384	C385	C386	G387	U388	A389	C390	G396	A397	C398	C399	C400	C401	C402	C403	U404	G405	U406	G407	A408	C409	U410	A411	A412	C413	C417	C418	C419	G424	G425	G426	U427	C428	U429	A430	A431	A432	U437	C438	A439	A441	C442	C443	C444	C445	C446	C447	A448	A452					
G305	G306	C311	C314	A315	G319	C320	A321	C322	U323	G324	A325	C326	C327	C328	A329	C330	G331	C332	G333	C336	C337	A338	C339	U340	C341	A344	C345	G346	G347	G348	G351	C352	A353	G354	C355	A356	G357	U358	U359	A360	G361	G362	A363	A364	U365	U366	C370	G371	C372	A373	A374						



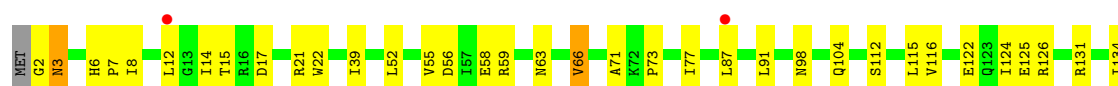
• Molecule 33: 30S ribosomal protein S2

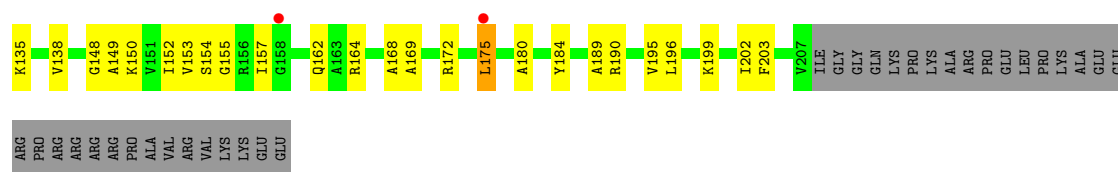


• Molecule 33: 30S ribosomal protein S2

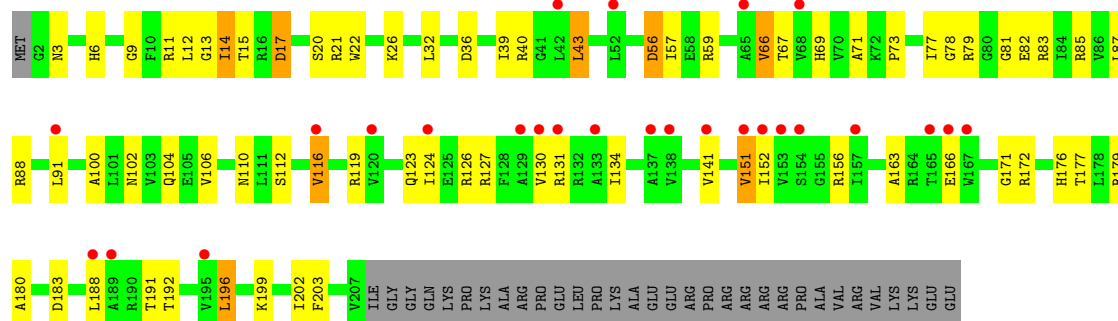


• Molecule 34: 30S ribosomal protein S3

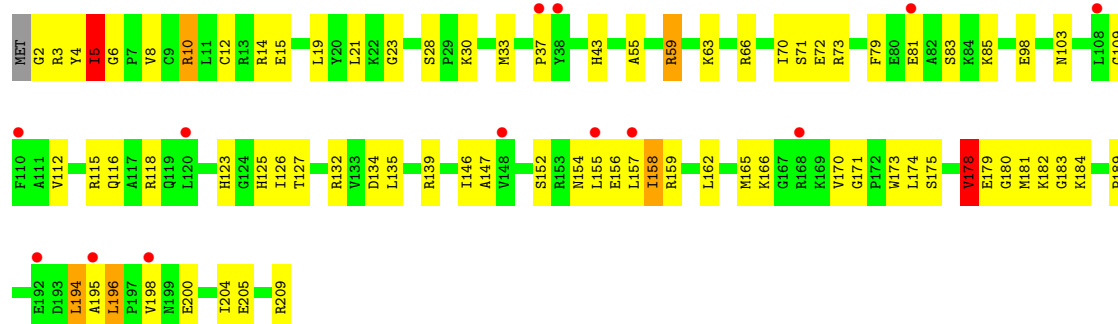




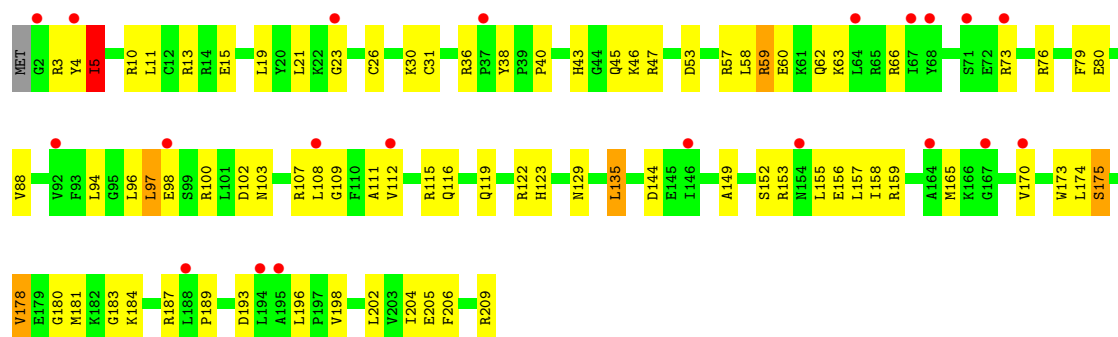
• Molecule 34: 30S ribosomal protein S3



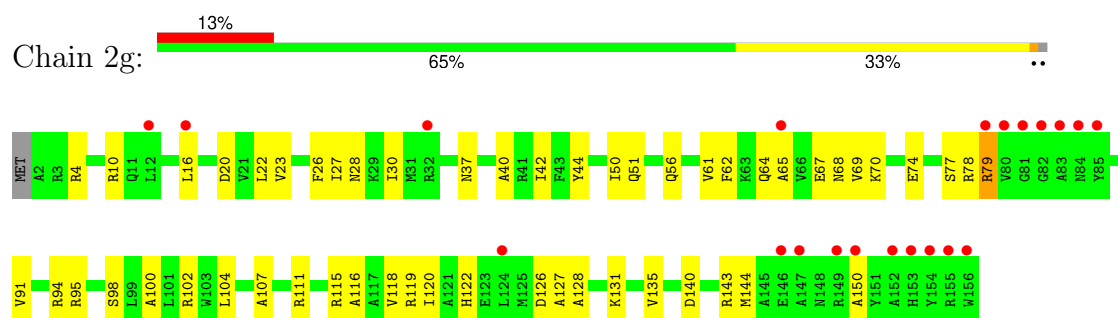
• Molecule 35: 30S ribosomal protein S4



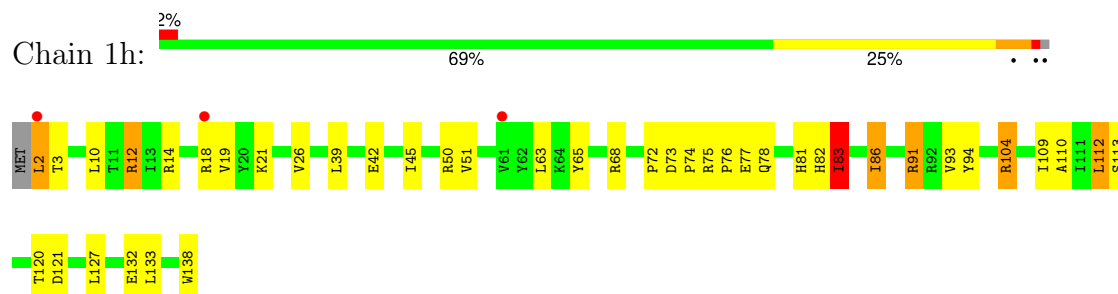
• Molecule 35: 30S ribosomal protein S4



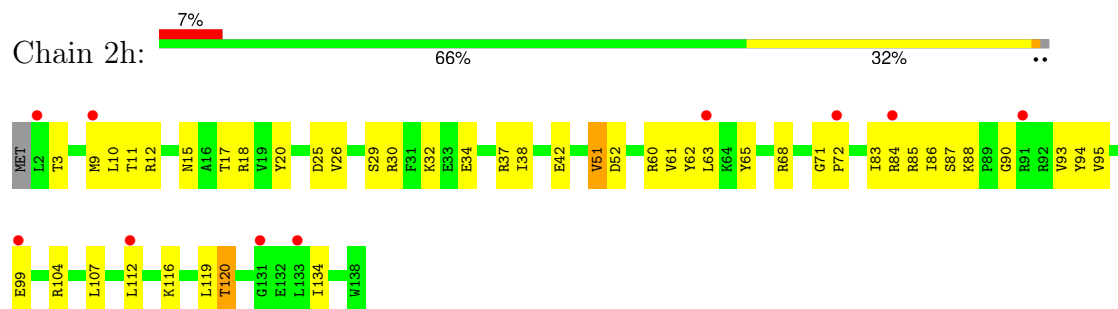
• Molecule 36: 30S ribosomal protein S5



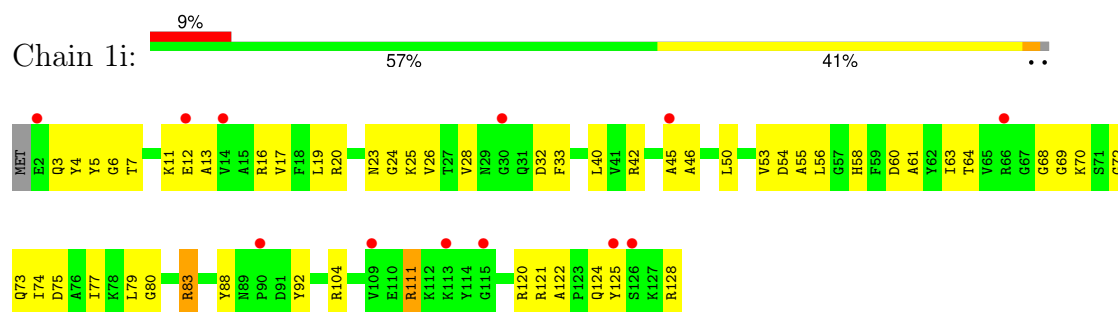
- Molecule 39: 30S ribosomal protein S8



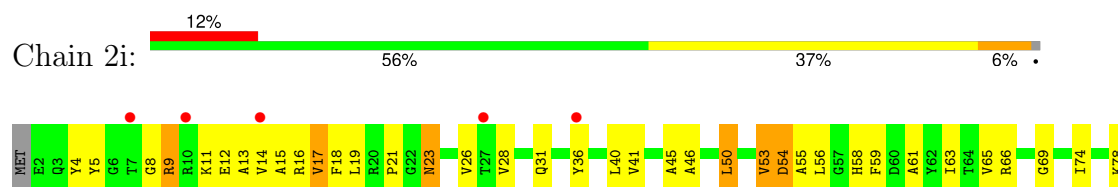
- Molecule 39: 30S ribosomal protein S8

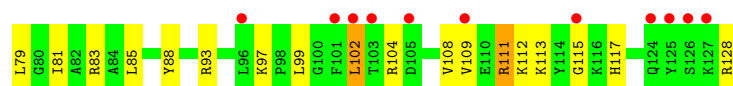


- Molecule 40: 30S ribosomal protein S9

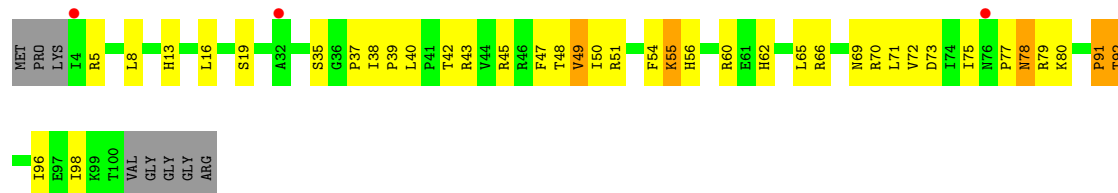


- Molecule 40: 30S ribosomal protein S9

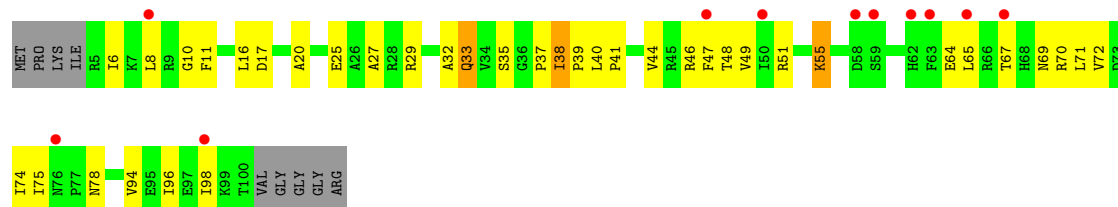




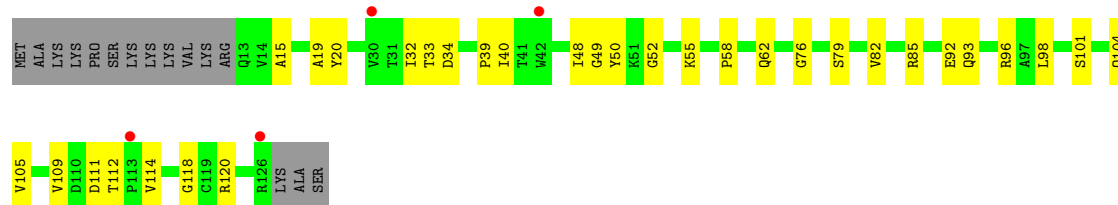
- Molecule 41: 30S ribosomal protein S10



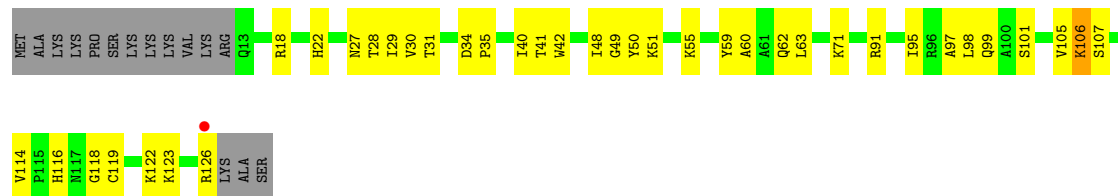
- Molecule 41: 30S ribosomal protein S10



- Molecule 42: 30S ribosomal protein S11

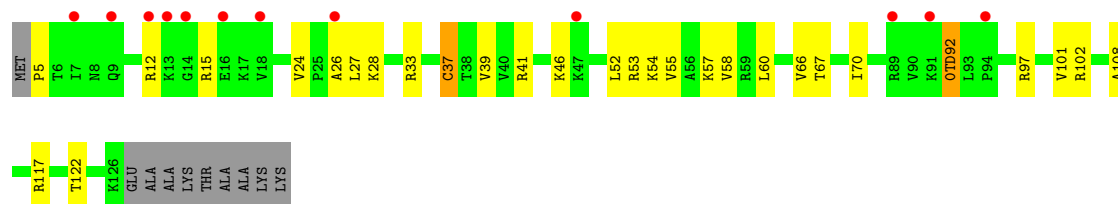


- Molecule 42: 30S ribosomal protein S11

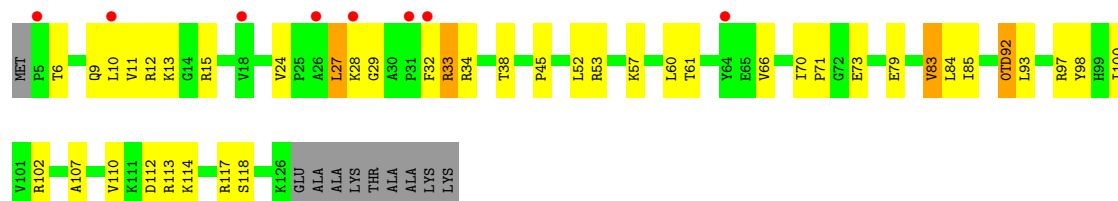


- Molecule 43: 30S ribosomal protein S12

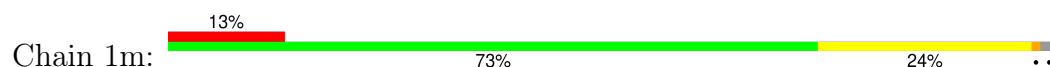




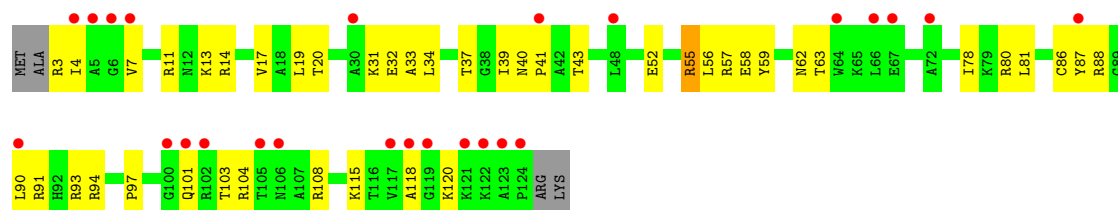
- Molecule 43: 30S ribosomal protein S12



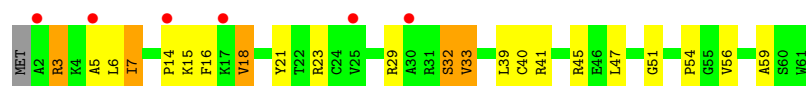
- Molecule 44: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S13

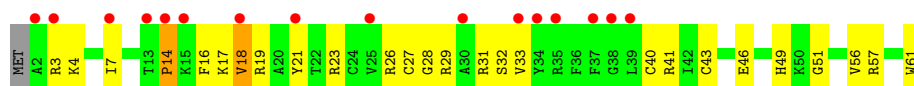


- Molecule 45: 30S ribosomal protein S14 type Z

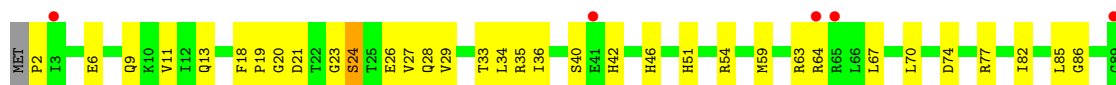


- Molecule 45: 30S ribosomal protein S14 type Z

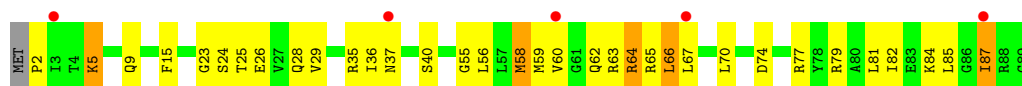




- Molecule 46: 30S ribosomal protein S15



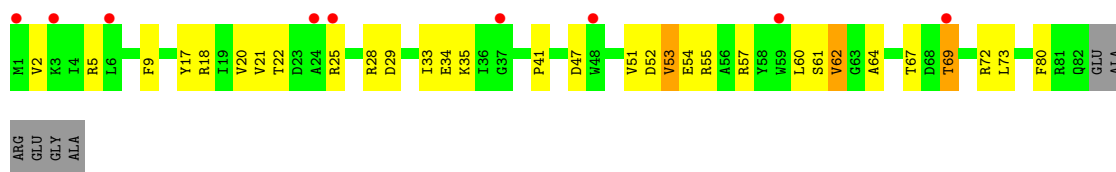
- Molecule 46: 30S ribosomal protein S15



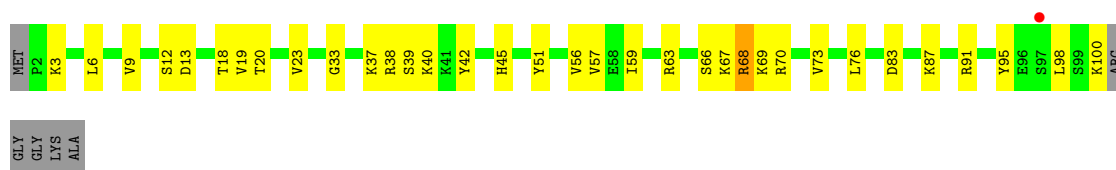
- Molecule 47: 30S ribosomal protein S16



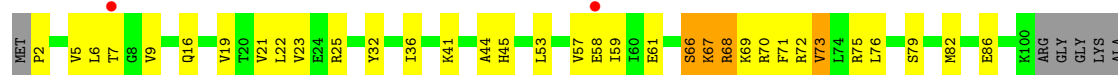
- Molecule 47: 30S ribosomal protein S16



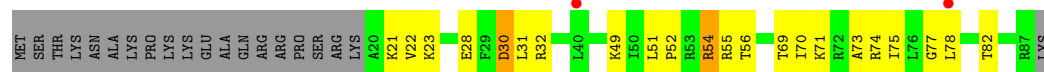
- Molecule 48: 30S ribosomal protein S17



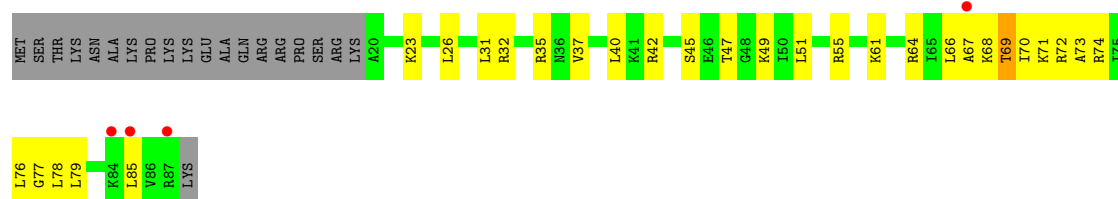
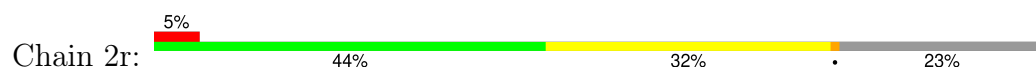
- Molecule 48: 30S ribosomal protein S17



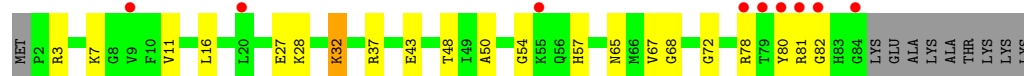
- Molecule 49: 30S ribosomal protein S18



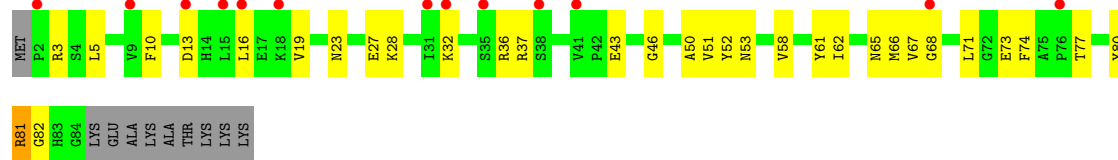
- Molecule 49: 30S ribosomal protein S18



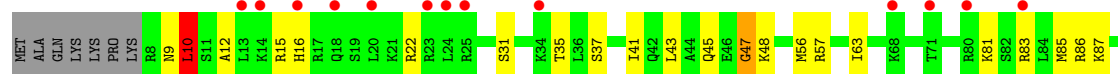
- Molecule 50: 30S ribosomal protein S19

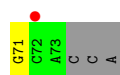


- Molecule 50: 30S ribosomal protein S19



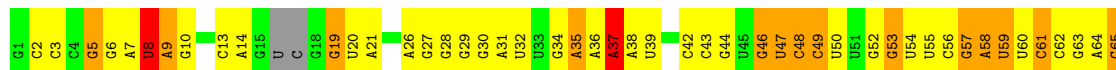
- Molecule 51: 30S ribosomal protein S20





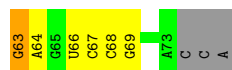
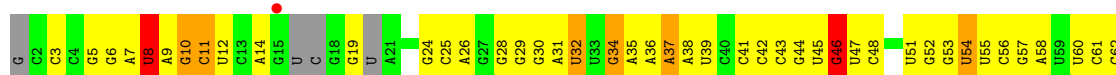
- Molecule 54: A-site and E-site tRNAs

Chain 1y: 25% 49% 21% . .



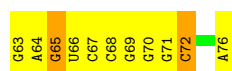
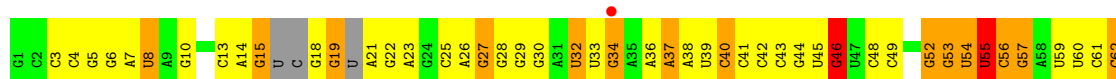
- Molecule 54: A-site and E-site tRNAs

Chain 2w: 25% 54% 9% . 9%



- Molecule 54: A-site and E-site tRNAs

Chain 2y: 20% 53% 21% . .



- Molecule 55: P-site tRNA

Chain 1x: 5% 60% 27% 12% .



- Molecule 55: P-site tRNA

Chain 2x: 48% 43% 8% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.73Å 445.10Å 613.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	360.30 – 2.95 360.30 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (360.30-2.95) 99.7 (360.30-2.95)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.238 , 0.292 0.241 , 0.294	Depositor DCC
R_{free} test set	59210 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	104.3	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 111.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	295398	wwPDB-VP
Average B, all atoms (Å ²)	95.0	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: OMG, MG, 0TD, 5MU, 2MG, 4SU, 2MA, UR3, MA6, 4OC, 5MC, 7MG, MIA, 2MU, PSU, SF4, ZN, M2G

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	1A	0.17	0/69009	0.33	0/107712
1	2A	0.15	0/67293	0.33	0/105034
2	1B	0.14	0/2882	0.29	0/4494
2	2B	0.13	0/2879	0.31	0/4487
3	1D	0.18	0/2186	0.42	1/2944 (0.0%)
3	2D	0.17	0/2186	0.42	0/2944
4	1E	0.18	0/1592	0.41	0/2149
4	2E	0.16	0/1592	0.38	0/2149
5	1F	0.16	0/1619	0.39	0/2193
5	2F	0.15	0/1615	0.36	0/2188
6	1G	0.14	0/1448	0.38	0/1957
6	2G	0.14	0/1453	0.38	0/1963
7	1H	0.16	0/1356	0.35	0/1834
7	2H	0.14	0/1356	0.35	0/1834
8	1I	0.13	0/1112	0.38	0/1514
8	2I	0.19	0/1079	0.40	0/1475
9	1N	0.16	0/1144	0.36	0/1543
9	2N	0.15	0/1144	0.36	0/1543
10	1O	0.19	0/943	0.40	0/1269
10	2O	0.15	0/943	0.41	0/1269
11	1P	0.20	0/1152	0.45	0/1533
11	2P	0.16	0/1152	0.43	0/1533
12	1Q	0.17	0/1143	0.38	0/1527
12	2Q	0.14	0/1143	0.35	0/1527
13	1R	0.19	0/982	0.46	0/1312
13	2R	0.15	0/982	0.40	0/1312
14	1S	0.15	0/883	0.36	0/1176
14	2S	0.16	0/880	0.39	0/1172
15	1T	0.16	0/1105	0.41	0/1477
15	2T	0.16	0/1097	0.43	0/1468
16	1U	0.16	0/977	0.36	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.15	0/977	0.38	0/1301
17	1V	0.18	0/782	0.39	0/1049
17	2V	0.15	0/782	0.37	0/1049
18	1W	0.17	0/897	0.38	0/1205
18	2W	0.15	0/897	0.37	0/1205
19	1X	0.18	0/764	0.44	2/1025 (0.2%)
19	2X	0.14	0/764	0.37	0/1025
20	1Y	0.17	0/819	0.41	0/1095
20	2Y	0.17	0/819	0.37	0/1095
21	1Z	0.15	0/1267	0.39	0/1717
21	2Z	0.15	0/1299	0.40	0/1763
22	10	0.16	0/662	0.42	0/881
22	20	0.14	0/662	0.40	0/881
23	11	0.17	0/762	0.36	0/1014
23	21	0.15	0/762	0.36	0/1014
24	12	0.16	0/590	0.36	0/781
24	22	0.15	0/590	0.33	0/781
25	13	0.18	0/474	0.42	0/635
25	23	0.15	0/469	0.38	0/630
26	14	0.19	0/565	0.54	0/761
26	24	0.22	0/545	0.55	0/737
27	15	0.16	0/469	0.39	0/635
27	25	0.25	0/469	0.43	0/635
28	16	0.18	0/460	0.42	0/613
28	26	0.14	0/456	0.37	0/608
29	17	0.18	0/426	0.41	0/561
29	27	0.16	0/426	0.46	0/561
30	18	0.17	0/525	0.36	0/691
30	28	0.15	0/525	0.35	0/691
31	19	0.19	0/310	0.39	0/407
31	29	0.19	0/310	0.43	0/407
32	1a	0.15	1/35795 (0.0%)	0.33	1/55864 (0.0%)
32	2a	0.15	0/35886	0.34	0/56005
33	1b	0.17	0/1881	0.44	0/2542
33	2b	0.17	0/1860	0.43	0/2518
34	1c	0.18	0/1572	0.36	0/2126
34	2c	0.14	0/1566	0.37	0/2119
35	1d	0.15	0/1685	0.40	0/2262
35	2d	0.15	0/1704	0.40	0/2284
36	1e	0.16	0/1145	0.43	1/1543 (0.1%)
36	2e	0.16	0/1149	0.44	0/1548
37	1f	0.14	0/823	0.35	0/1115
37	2f	0.15	0/829	0.40	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.16	0/1250	0.38	0/1679
38	2g	0.15	0/1254	0.40	1/1683 (0.1%)
39	1h	0.15	0/1108	0.39	0/1494
39	2h	0.14	0/1108	0.37	0/1494
40	1i	0.17	0/1002	0.45	0/1346
40	2i	0.17	0/997	0.46	0/1343
41	1j	0.15	0/722	0.43	0/982
41	2j	0.16	0/727	0.43	0/988
42	1k	0.13	0/844	0.32	0/1145
42	2k	0.22	0/848	0.38	0/1149
43	1l	0.18	0/937	0.39	0/1260
43	2l	0.17	0/937	0.39	0/1260
44	1m	0.15	0/969	0.40	0/1302
44	2m	0.16	0/961	0.40	0/1291
45	1n	0.16	0/501	0.38	0/664
45	2n	0.14	0/501	0.40	0/664
46	1o	0.14	0/739	0.35	0/985
46	2o	0.14	0/739	0.36	0/985
47	1p	0.14	0/697	0.41	0/939
47	2p	0.14	0/693	0.38	0/935
48	1q	0.14	0/836	0.37	0/1117
48	2q	0.14	0/836	0.42	0/1117
49	1r	0.14	0/560	0.40	0/746
49	2r	0.13	0/560	0.36	0/746
50	1s	0.16	0/667	0.45	0/900
50	2s	0.19	0/661	0.45	0/893
51	1t	0.17	0/730	0.53	1/965 (0.1%)
51	2t	0.15	0/729	0.41	0/965
52	1u	0.16	0/203	0.45	0/266
52	2u	0.15	0/203	0.39	0/266
53	1v	0.14	0/288	0.30	0/446
53	2v	0.18	0/163	0.33	0/251
54	1w	0.23	1/1537 (0.1%)	0.36	0/2390
54	1y	0.22	1/1606 (0.1%)	0.38	0/2497
54	2w	0.23	1/1487 (0.1%)	0.39	0/2311
54	2y	0.25	0/1583	0.44	0/2459
55	1x	0.22	0/1725	0.35	0/2689
55	2x	0.21	0/1725	0.36	0/2689
All	All	0.16	4/316379 (0.0%)	0.35	7/473636 (0.0%)

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
26	24	0	1
41	2j	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	8	4SU	O3'-P	5.20	1.61	1.56
54	2w	8	4SU	O3'-P	5.14	1.61	1.56
54	1w	8	4SU	O3'-P	5.13	1.61	1.56
32	1a	1498	UR3	O3'-P	5.02	1.61	1.56

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	1t	99	LEU	CB-CA-C	-8.29	105.95	117.23
38	2g	50	ILE	N-CA-C	-7.20	104.52	112.80
36	1e	103	GLY	N-CA-C	-5.76	105.30	111.93
19	1X	94	GLY	CA-C-N	5.59	131.76	121.70
19	1X	94	GLY	C-N-CA	5.59	131.76	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	24	56	VAL	Peptide
41	2j	32	ALA	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	1A	61852	0	31193	806	0
1	2A	60322	0	30421	980	0
2	1B	2577	0	1305	35	0
2	2B	2575	0	1303	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	1D	2136	0	2218	76	0
3	2D	2136	0	2218	58	0
4	1E	1559	0	1618	45	0
4	2E	1559	0	1618	50	0
5	1F	1584	0	1625	52	0
5	2F	1580	0	1619	55	0
6	1G	1423	0	1436	45	0
6	2G	1428	0	1438	51	0
7	1H	1330	0	1407	36	0
7	2H	1330	0	1407	39	0
8	1I	1097	0	1140	41	0
8	2I	1064	0	1082	42	0
9	1N	1117	0	1184	22	0
9	2N	1117	0	1184	38	0
10	1O	933	0	996	26	0
10	2O	933	0	996	31	0
11	1P	1135	0	1212	43	0
11	2P	1135	0	1212	34	0
12	1Q	1122	0	1179	32	0
12	2Q	1122	0	1179	37	0
13	1R	968	0	1033	25	0
13	2R	968	0	1033	21	0
14	1S	873	0	927	21	0
14	2S	870	0	923	34	0
15	1T	1091	0	1151	24	0
15	2T	1083	0	1136	33	0
16	1U	959	0	1019	17	0
16	2U	959	0	1019	31	0
17	1V	771	0	830	19	0
17	2V	771	0	830	23	0
18	1W	886	0	940	23	0
18	2W	886	0	940	19	0
19	1X	750	0	814	16	0
19	2X	750	0	814	13	0
20	1Y	806	0	881	28	0
20	2Y	806	0	881	33	0
21	1Z	1240	0	1240	39	0
21	2Z	1271	0	1273	32	0
22	10	653	0	674	17	0
22	20	653	0	674	20	0
23	11	755	0	826	24	0
23	21	755	0	826	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	12	588	0	643	15	0
24	22	588	0	643	17	0
25	13	469	0	518	8	0
25	23	464	0	514	18	0
26	14	552	0	533	23	0
26	24	532	0	503	21	0
27	15	455	0	465	7	0
27	25	455	0	465	16	0
28	16	453	0	473	10	0
28	26	449	0	469	17	0
29	17	418	0	467	10	0
29	27	418	0	467	12	0
30	18	517	0	582	24	0
30	28	517	0	582	23	0
31	19	307	0	335	6	0
31	29	307	0	335	15	0
32	1a	32246	0	16295	641	0
32	2a	32327	0	16339	756	0
33	1b	1846	0	1867	64	0
33	2b	1825	0	1828	88	0
34	1c	1548	0	1535	38	0
34	2c	1542	0	1517	51	0
35	1d	1655	0	1672	57	0
35	2d	1674	0	1714	63	0
36	1e	1129	0	1185	42	0
36	2e	1133	0	1191	41	0
37	1f	810	0	804	18	0
37	2f	816	0	808	29	0
38	1g	1231	0	1238	34	0
38	2g	1235	0	1249	39	0
39	1h	1088	0	1126	32	0
39	2h	1088	0	1126	37	0
40	1i	983	0	986	45	0
40	2i	978	0	966	41	0
41	1j	709	0	650	25	0
41	2j	714	0	672	32	0
42	1k	829	0	825	19	0
42	2k	833	0	836	19	0
43	1l	932	0	981	21	0
43	2l	932	0	981	34	0
44	1m	958	0	1002	23	0
44	2m	950	0	988	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	1n	492	0	529	23	0
45	2n	492	0	529	28	0
46	1o	728	0	760	22	0
46	2o	728	0	760	26	0
47	1p	681	0	697	25	0
47	2p	677	0	686	24	0
48	1q	823	0	891	29	0
48	2q	823	0	891	31	0
49	1r	555	0	618	15	0
49	2r	555	0	618	23	0
50	1s	652	0	662	22	0
50	2s	646	0	644	30	0
51	1t	728	0	798	19	0
51	2t	727	0	796	20	0
52	1u	199	0	208	10	0
52	2u	199	0	208	8	0
53	1v	277	0	139	5	0
53	2v	167	0	84	12	0
54	1w	1530	0	786	32	0
54	1y	1585	0	804	42	0
54	2w	1482	0	755	34	0
54	2y	1565	0	795	52	0
55	1x	1625	0	829	21	0
55	2x	1625	0	829	26	0
56	1A	680	0	0	0	0
56	1a	238	0	0	0	0
56	2A	351	0	0	0	0
56	2a	183	0	0	0	0
57	14	1	0	0	0	0
57	15	1	0	0	0	0
57	16	1	0	0	0	0
57	19	1	0	0	0	0
57	1Y	1	0	0	0	0
57	1n	1	0	0	0	0
57	24	1	0	0	0	0
57	25	1	0	0	0	0
57	26	1	0	0	0	0
57	29	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2n	1	0	0	0	0
58	1d	8	0	0	2	0
58	2d	8	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1A	585	0	0	24	0
59	1a	181	0	0	7	0
59	2A	234	0	0	12	0
59	2a	167	0	0	10	0
All	All	295398	0	196565	5467	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 12.

The worst 5 of 5467 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)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.19	1.34
32:2a:997:U:H3	32:2a:1044:A:N6	1.31	1.27
1:2A:2138:C:N4	1:2A:2153:G:H1	1.36	1.24
1:1A:1082:U:O4	1:1A:1086:A:N1	1.89	1.05
32:2a:1244:C:N4	32:2a:1293:G:H1	1.59	1.01

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	
3	1D	273/276 (99%)	262 (96%)	10 (4%)	1 (0%)	30	53
3	2D	273/276 (99%)	259 (95%)	14 (5%)	0	100	100
4	1E	202/206 (98%)	188 (93%)	13 (6%)	1 (0%)	24	49
4	2E	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	12	32
5	1F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	24	49
5	2F	201/210 (96%)	194 (96%)	5 (2%)	2 (1%)	12	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	1G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	21	45
6	2G	179/182 (98%)	166 (93%)	12 (7%)	1 (1%)	21	45
7	1H	172/180 (96%)	159 (92%)	13 (8%)	0	100	100
7	2H	172/180 (96%)	162 (94%)	8 (5%)	2 (1%)	10	28
8	1I	144/148 (97%)	128 (89%)	15 (10%)	1 (1%)	18	40
8	2I	144/148 (97%)	127 (88%)	16 (11%)	1 (1%)	18	40
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	37
11	1P	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
11	2P	147/150 (98%)	139 (95%)	6 (4%)	2 (1%)	9	24
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
14	2S	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	14	34
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
15	2T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	16	37
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	90 (91%)	6 (6%)	3 (3%)	3	9
17	2V	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
19	1X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
19	2X	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	1Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	12	32
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
21	1Z	148/206 (72%)	131 (88%)	16 (11%)	1 (1%)	18	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	2Z	156/206 (76%)	142 (91%)	14 (9%)	0	100	100
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
23	11	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11	29
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	2
26	24	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	2
27	15	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
27	25	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	0	1 (2%)	5	15
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	202 (88%)	23 (10%)	4 (2%)	7	20
33	2b	229/256 (90%)	205 (90%)	20 (9%)	4 (2%)	7	20
34	1c	204/239 (85%)	189 (93%)	14 (7%)	1 (0%)	24	49
34	2c	204/239 (85%)	192 (94%)	10 (5%)	2 (1%)	12	32
35	1d	206/209 (99%)	200 (97%)	4 (2%)	2 (1%)	12	32
35	2d	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	24	49
36	1e	146/162 (90%)	133 (91%)	11 (8%)	2 (1%)	9	24
36	2e	146/162 (90%)	130 (89%)	14 (10%)	2 (1%)	9	24
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	1g	153/156 (98%)	141 (92%)	9 (6%)	3 (2%)	6	16
38	2g	153/156 (98%)	142 (93%)	10 (6%)	1 (1%)	18	40
39	1h	135/138 (98%)	130 (96%)	4 (3%)	1 (1%)	18	40
39	2h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
40	1i	125/128 (98%)	116 (93%)	7 (6%)	2 (2%)	7	21
40	2i	125/128 (98%)	113 (90%)	10 (8%)	2 (2%)	7	21
41	1j	95/105 (90%)	81 (85%)	8 (8%)	6 (6%)	1	2
41	2j	94/105 (90%)	83 (88%)	7 (7%)	4 (4%)	2	4
42	1k	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	6	19
42	2k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	6	19
43	1l	119/132 (90%)	109 (92%)	10 (8%)	0	100	100
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	110 (91%)	11 (9%)	0	100	100
44	2m	120/126 (95%)	110 (92%)	10 (8%)	0	100	100
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7	20
46	1o	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	10	28
46	2o	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
47	1p	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	9	26
47	2p	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	9	26
48	1q	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	12	32
48	2q	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	12	32
49	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
50	2s	81/93 (87%)	72 (89%)	8 (10%)	1 (1%)	10	28
51	1t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2	4
51	2t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	5	16
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
All	All	11370/12128 (94%)	10654 (94%)	629 (6%)	87 (1%)	16	37

5 of 87 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	47	LYS
33	1b	17	PHE
35	1d	5	ILE
40	1i	54	ASP
5	2F	130	ALA

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	
3	1D	215/218 (99%)	201 (94%)	14 (6%)	15	37
3	2D	215/218 (99%)	204 (95%)	11 (5%)	21	47
4	1E	164/166 (99%)	154 (94%)	10 (6%)	17	40
4	2E	164/166 (99%)	148 (90%)	16 (10%)	7	21
5	1F	160/166 (96%)	152 (95%)	8 (5%)	22	47
5	2F	159/166 (96%)	145 (91%)	14 (9%)	9	24
6	1G	143/156 (92%)	132 (92%)	11 (8%)	12	30
6	2G	143/156 (92%)	132 (92%)	11 (8%)	12	30
7	1H	144/148 (97%)	131 (91%)	13 (9%)	9	24
7	2H	144/148 (97%)	134 (93%)	10 (7%)	14	35
8	1I	113/124 (91%)	101 (89%)	12 (11%)	6	19
8	2I	105/124 (85%)	93 (89%)	12 (11%)	5	16
9	1N	118/119 (99%)	112 (95%)	6 (5%)	21	47
9	2N	118/119 (99%)	109 (92%)	9 (8%)	12	31
10	1O	100/100 (100%)	91 (91%)	9 (9%)	9	24
10	2O	100/100 (100%)	95 (95%)	5 (5%)	22	47
11	1P	115/116 (99%)	108 (94%)	7 (6%)	17	40
11	2P	115/116 (99%)	112 (97%)	3 (3%)	40	65
12	1Q	111/111 (100%)	108 (97%)	3 (3%)	39	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	16	38
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9	24
13	2R	101/101 (100%)	93 (92%)	8 (8%)	11	29
14	1S	86/88 (98%)	83 (96%)	3 (4%)	32	57
14	2S	85/88 (97%)	79 (93%)	6 (7%)	13	33
15	1T	115/127 (91%)	111 (96%)	4 (4%)	32	57
15	2T	113/127 (89%)	106 (94%)	7 (6%)	16	39
16	1U	93/94 (99%)	87 (94%)	6 (6%)	15	37
16	2U	93/94 (99%)	87 (94%)	6 (6%)	15	37
17	1V	80/82 (98%)	74 (92%)	6 (8%)	12	31
17	2V	80/82 (98%)	74 (92%)	6 (8%)	12	31
18	1W	90/92 (98%)	87 (97%)	3 (3%)	33	58
18	2W	90/92 (98%)	86 (96%)	4 (4%)	25	51
19	1X	77/78 (99%)	77 (100%)	0	100	100
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28	54
20	1Y	85/91 (93%)	74 (87%)	11 (13%)	4	13
20	2Y	85/91 (93%)	80 (94%)	5 (6%)	18	41
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	11	28
21	2Z	137/179 (76%)	133 (97%)	4 (3%)	37	61
22	10	65/67 (97%)	64 (98%)	1 (2%)	57	76
22	20	65/67 (97%)	63 (97%)	2 (3%)	35	59
23	11	80/83 (96%)	77 (96%)	3 (4%)	29	55
23	21	80/83 (96%)	77 (96%)	3 (4%)	29	55
24	12	65/67 (97%)	64 (98%)	1 (2%)	57	76
24	22	65/67 (97%)	63 (97%)	2 (3%)	35	59
25	13	51/52 (98%)	47 (92%)	4 (8%)	11	30
25	23	50/52 (96%)	48 (96%)	2 (4%)	28	53
26	14	59/63 (94%)	52 (88%)	7 (12%)	5	15
26	24	53/63 (84%)	49 (92%)	4 (8%)	12	31
27	15	50/52 (96%)	44 (88%)	6 (12%)	5	14
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	16	51/52 (98%)	45 (88%)	6 (12%)	5	15
28	26	50/52 (96%)	46 (92%)	4 (8%)	11	28
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	33
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	21
30	18	54/55 (98%)	49 (91%)	5 (9%)	8	23
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	55
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	61
31	29	34/34 (100%)	32 (94%)	2 (6%)	18	41
33	1b	192/220 (87%)	180 (94%)	12 (6%)	16	38
33	2b	187/220 (85%)	171 (91%)	16 (9%)	10	25
34	1c	142/188 (76%)	135 (95%)	7 (5%)	22	48
34	2c	140/188 (74%)	130 (93%)	10 (7%)	13	33
35	1d	169/181 (93%)	157 (93%)	12 (7%)	13	33
35	2d	173/181 (96%)	161 (93%)	12 (7%)	14	35
36	1e	113/123 (92%)	105 (93%)	8 (7%)	13	33
36	2e	114/123 (93%)	108 (95%)	6 (5%)	20	45
37	1f	84/90 (93%)	80 (95%)	4 (5%)	23	48
37	2f	85/90 (94%)	82 (96%)	3 (4%)	32	57
38	1g	119/127 (94%)	116 (98%)	3 (2%)	42	66
38	2g	120/127 (94%)	117 (98%)	3 (2%)	42	66
39	1h	114/119 (96%)	99 (87%)	15 (13%)	4	12
39	2h	114/119 (96%)	108 (95%)	6 (5%)	20	45
40	1i	90/99 (91%)	86 (96%)	4 (4%)	25	51
40	2i	89/99 (90%)	78 (88%)	11 (12%)	4	13
41	1j	66/92 (72%)	63 (96%)	3 (4%)	24	50
41	2j	69/92 (75%)	66 (96%)	3 (4%)	26	52
42	1k	82/99 (83%)	79 (96%)	3 (4%)	30	55
42	2k	83/99 (84%)	78 (94%)	5 (6%)	17	40
43	1l	96/108 (89%)	91 (95%)	5 (5%)	21	46
43	2l	96/108 (89%)	90 (94%)	6 (6%)	16	38
44	1m	93/101 (92%)	92 (99%)	1 (1%)	65	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	2m	92/101 (91%)	90 (98%)	2 (2%)	45	69
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7	20
45	2n	49/50 (98%)	47 (96%)	2 (4%)	27	53
46	1o	78/80 (98%)	74 (95%)	4 (5%)	21	47
46	2o	78/80 (98%)	71 (91%)	7 (9%)	9	24
47	1p	69/74 (93%)	64 (93%)	5 (7%)	13	33
47	2p	68/74 (92%)	64 (94%)	4 (6%)	18	41
48	1q	94/97 (97%)	93 (99%)	1 (1%)	65	80
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13	32
49	1r	59/77 (77%)	56 (95%)	3 (5%)	21	47
49	2r	59/77 (77%)	54 (92%)	5 (8%)	10	25
50	1s	69/80 (86%)	67 (97%)	2 (3%)	37	61
50	2s	67/80 (84%)	64 (96%)	3 (4%)	24	50
51	1t	70/82 (85%)	69 (99%)	1 (1%)	59	77
51	2t	70/82 (85%)	69 (99%)	1 (1%)	59	77
52	1u	18/22 (82%)	16 (89%)	2 (11%)	6	17
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9303/10064 (92%)	8733 (94%)	570 (6%)	17	40

5 of 570 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	2b	93	VAL
34	2c	56	ASP
33	2b	71	VAL
40	2i	83	ARG
33	1b	230	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
41	1j	68	HIS
38	2g	148	ASN
6	2G	66	GLN
38	2g	68	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	2s	83	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	474 (16%)	22 (0%)
1	2A	2791/2915 (95%)	530 (18%)	22 (0%)
2	1B	119/121 (98%)	14 (11%)	0
2	2B	118/121 (97%)	17 (14%)	0
32	1a	1497/1521 (98%)	280 (18%)	0
32	2a	1501/1521 (98%)	313 (20%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	7/24 (29%)	3 (42%)	0
54	1w	69/76 (90%)	15 (21%)	0
54	1y	72/76 (94%)	28 (38%)	0
54	2w	66/76 (86%)	18 (27%)	0
54	2y	70/76 (92%)	25 (35%)	0
55	1x	75/77 (97%)	10 (13%)	0
55	2x	75/77 (97%)	10 (13%)	0
All	All	9335/9620 (97%)	1740 (18%)	44 (0%)

5 of 1740 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	45	C

5 of 44 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	528	A
1	2A	1530	C
1	2A	752	A
1	2A	1210	A
1	2A	1913	A

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

86 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$
54	PSU	1y	39	54	18,21,22	1.32	2 (11%)	21,30,33	2.14	3 (14%)
43	0TD	1l	92	43	8,9,10	4.46	1 (12%)	6,11,13	7.25	2 (33%)
32	M2G	1a	966	32	24,27,28	1.30	4 (16%)	33,40,43	1.87	6 (18%)
1	PSU	2A	2605	1	18,21,22	1.35	2 (11%)	21,30,33	2.04	4 (19%)
1	5MC	1A	1942	1	19,22,23	1.54	3 (15%)	26,32,35	1.16	3 (11%)
1	4OC	1A	1920	1	19,22,24	0.79	0	25,31,35	0.92	1 (4%)
32	UR3	1a	1498	32	19,22,23	1.03	1 (5%)	26,32,35	1.77	4 (15%)
54	4SU	2y	8	54,56	18,21,22	1.76	4 (22%)	25,30,33	2.38	6 (24%)
54	7MG	1y	46	54	23,26,27	1.35	3 (13%)	27,39,42	2.75	6 (22%)
54	PSU	1w	39	54	18,21,22	1.26	1 (5%)	21,30,33	2.28	4 (19%)
54	7MG	1w	46	54	23,26,27	1.32	3 (13%)	27,39,42	2.65	7 (25%)
54	PSU	2w	32	54	18,21,22	1.36	2 (11%)	21,30,33	2.00	3 (14%)
54	PSU	2y	32	54	18,21,22	1.37	2 (11%)	21,30,33	2.00	4 (19%)
55	5MC	2x	32	55	19,22,23	1.74	3 (15%)	26,32,35	1.21	3 (11%)
1	PSU	2A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	2.01	4 (19%)
1	OMG	1A	2251	56,55,1	23,26,27	1.19	3 (13%)	32,38,41	2.03	6 (18%)
32	MA6	1a	1519	32	23,26,27	1.57	4 (17%)	33,38,41	2.33	11 (33%)
1	PSU	1A	1917	1	18,21,22	1.38	2 (11%)	21,30,33	2.05	3 (14%)
55	4SU	1x	8	56,55	18,21,22	2.09	4 (22%)	25,30,33	1.66	5 (20%)
54	MIA	1w	37	54	28,31,32	2.39	6 (21%)	38,44,47	2.77	13 (34%)
54	4SU	2w	8	54	18,21,22	1.79	5 (27%)	25,30,33	2.13	4 (16%)
55	PSU	2x	55	55	18,21,22	1.36	2 (11%)	21,30,33	2.02	4 (19%)
55	4SU	2x	8	56,55	18,21,22	2.02	6 (33%)	25,30,33	1.75	6 (24%)
1	OMG	2A	2251	55,1	23,26,27	1.21	3 (13%)	32,38,41	2.03	6 (18%)
1	PSU	1A	1911	1	18,21,22	1.37	3 (16%)	21,30,33	2.09	4 (19%)
32	MA6	2a	1519	32	23,26,27	1.56	4 (17%)	33,38,41	2.26	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	2A	1915	1	19,22,23	1.46	6 (31%)	27,32,35	2.05	7 (25%)
32	5MC	1a	1407	32	19,22,23	1.59	3 (15%)	26,32,35	1.09	2 (7%)
54	MIA	2y	37	54,32	21,24,32	1.62	4 (19%)	30,35,47	2.00	7 (23%)
1	5MC	1A	1962	56,1	19,22,23	1.67	3 (15%)	26,32,35	1.12	2 (7%)
32	M2G	2a	966	32	24,27,28	1.32	4 (16%)	33,40,43	1.85	6 (18%)
1	5MU	1A	1915	1	19,22,23	1.39	6 (31%)	27,32,35	2.05	7 (25%)
32	MA6	1a	1518	32	23,26,27	1.54	4 (17%)	33,38,41	2.32	14 (42%)
53	PSU	1v	19	53,54	18,21,22	1.46	3 (16%)	21,30,33	1.60	3 (14%)
53	PSU	2v	19	53,54,56	18,21,22	1.40	2 (11%)	21,30,33	1.97	3 (14%)
1	2MA	1A	2503	56,1	22,25,26	1.49	4 (18%)	32,37,40	2.30	9 (28%)
32	4OC	2a	1402	56,32	20,23,24	0.77	0	25,32,35	0.97	0
55	PSU	1x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.14	4 (19%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	21,30,33	1.94	4 (19%)
54	PSU	2w	55	54	18,21,22	1.40	2 (11%)	21,30,33	2.08	3 (14%)
32	MA6	2a	1518	32	23,26,27	1.55	4 (17%)	33,38,41	2.31	12 (36%)
55	5MU	1x	54	55	19,22,23	1.37	5 (26%)	27,32,35	2.02	7 (25%)
54	PSU	2y	55	54	18,21,22	1.37	3 (16%)	21,30,33	1.96	3 (14%)
43	0TD	2l	92	43	8,9,10	4.48	1 (12%)	6,11,13	8.22	2 (33%)
32	5MC	1a	1404	32	19,22,23	1.70	3 (15%)	26,32,35	1.13	2 (7%)
32	5MC	2a	1400	32	19,22,23	1.71	2 (10%)	26,32,35	1.45	6 (23%)
32	UR3	2a	1498	32	19,22,23	1.05	2 (10%)	26,32,35	1.78	3 (11%)
1	2MU	1A	2552	56,1	19,22,24	1.28	3 (15%)	25,31,36	1.95	6 (24%)
55	5MC	1x	32	56,55	19,22,23	1.67	3 (15%)	26,32,35	1.14	3 (11%)
54	PSU	1y	55	54	18,21,22	1.37	2 (11%)	21,30,33	2.10	4 (19%)
32	5MC	2a	1407	56,32	19,22,23	1.65	3 (15%)	26,32,35	1.13	3 (11%)
1	5MU	2A	1939	1	19,22,23	1.39	5 (26%)	27,32,35	2.20	6 (22%)
54	4SU	1w	8	54	18,21,22	1.79	4 (22%)	25,30,33	2.18	5 (20%)
54	PSU	2y	39	54	18,21,22	1.39	2 (11%)	21,30,33	1.85	4 (19%)
32	5MC	2a	1404	32	19,22,23	1.59	2 (10%)	26,32,35	1.18	3 (11%)
54	5MU	1y	54	54	19,22,23	1.37	5 (26%)	27,32,35	2.18	6 (22%)
54	5MU	2w	54	54	19,22,23	1.42	6 (31%)	27,32,35	1.89	6 (22%)
55	5MU	2x	54	55	19,22,23	1.39	5 (26%)	27,32,35	2.13	6 (22%)
54	5MU	2y	54	54	19,22,23	1.44	5 (26%)	27,32,35	2.05	5 (18%)
54	PSU	1w	32	54	18,21,22	1.37	2 (11%)	21,30,33	2.02	3 (14%)
1	PSU	1A	2605	1	18,21,22	1.36	2 (11%)	21,30,33	1.98	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	1A	1939	1	19,22,23	1.44	5 (26%)	27,32,35	2.20	6 (22%)
32	PSU	1a	516	32	18,21,22	1.38	2 (11%)	21,30,33	1.90	3 (14%)
32	5MC	1a	967	32	19,22,23	1.57	3 (15%)	26,32,35	1.11	2 (7%)
54	PSU	1w	55	54	18,21,22	1.44	2 (11%)	21,30,33	2.09	3 (14%)
54	PSU	2w	39	54	18,21,22	1.29	2 (11%)	21,30,33	2.25	5 (23%)
32	7MG	1a	527	56,32	23,26,27	1.33	3 (13%)	27,39,42	2.62	7 (25%)
1	PSU	2A	1917	1	18,21,22	1.40	2 (11%)	21,30,33	2.07	4 (19%)
1	5MC	2A	1942	1	19,22,23	1.61	3 (15%)	26,32,35	1.21	2 (7%)
32	5MC	2a	967	32	19,22,23	1.69	3 (15%)	26,32,35	1.15	3 (11%)
32	5MC	1a	1400	32	19,22,23	1.61	3 (15%)	26,32,35	1.10	2 (7%)
32	7MG	2a	527	32	23,26,27	1.34	3 (13%)	27,39,42	2.62	6 (22%)
1	5MC	2A	1962	1	19,22,23	1.60	3 (15%)	26,32,35	1.18	2 (7%)
1	4OC	2A	1920	1	19,22,24	0.79	0	25,31,35	0.90	1 (4%)
32	2MG	1a	1207	32	23,26,27	1.28	4 (17%)	33,38,41	2.11	5 (15%)
54	4SU	1y	8	54	18,21,22	1.71	4 (22%)	25,30,33	2.18	4 (16%)
54	7MG	2w	46	54	23,26,27	1.34	3 (13%)	27,39,42	2.61	7 (25%)
54	5MU	1w	54	54	19,22,23	1.44	6 (31%)	27,32,35	1.83	9 (33%)
32	2MG	2a	1207	56,32	23,26,27	1.26	4 (17%)	33,38,41	2.13	5 (15%)
54	PSU	1y	32	54	18,21,22	1.34	2 (11%)	21,30,33	2.01	4 (19%)
54	MIA	2w	37	54	24,27,32	2.13	5 (20%)	32,39,47	2.46	11 (34%)
32	4OC	1a	1402	32	20,23,24	0.74	0	25,32,35	0.93	1 (4%)
54	7MG	2y	46	54	23,26,27	1.40	3 (13%)	27,39,42	2.73	6 (22%)
1	2MA	2A	2503	1	22,25,26	1.46	5 (22%)	32,37,40	2.24	9 (28%)
1	2MU	2A	2552	56,1	19,22,24	1.26	4 (21%)	25,31,36	1.89	6 (24%)
54	MIA	1y	37	54	21,24,32	1.60	4 (19%)	30,35,47	1.99	7 (23%)

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
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4OC	1A	1920	1	-	0/9/27/30	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54,56	-	1/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	5/7/37/38	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	0/7/37/38	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	3/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	56,55,1	-	0/9/27/28	0/3/3/3
32	MA6	1a	1519	32	-	4/11/29/30	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	56,55	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	2/15/33/34	0/3/3/3
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	1/7/25/26	0/2/2/2
55	4SU	2x	8	56,55	-	1/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/9/27/28	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	5/11/29/30	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54,32	-	2/7/25/34	0/3/3/3
1	5MC	1A	1962	56,1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	5MU	1A	1915	1	-	1/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	2/11/29/30	0/3/3/3
53	PSU	1v	19	53,54	-	3/7/25/26	0/2/2/2
53	PSU	2v	19	53,54,56	-	2/7/25/26	0/2/2/2
1	2MA	1A	2503	56,1	-	1/7/25/26	0/3/3/3
32	4OC	2a	1402	56,32	-	2/9/29/30	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/11/29/30	0/3/3/3
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	4/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	5/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	56,1	-	0/9/27/28	0/2/2/2
55	5MC	1x	32	56,55	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	1/7/25/26	0/2/2/2
32	5MC	2a	1407	56,32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	56,32	-	3/7/37/38	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	2/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	7MG	2a	527	32	-	3/7/37/38	0/3/3/3
1	5MC	2A	1962	1	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
54	4SU	1y	8	54	-	2/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	2/7/37/38	0/3/3/3
54	5MU	1w	54	54	-	2/7/25/26	0/2/2/2
32	2MG	2a	1207	56,32	-	1/9/27/28	0/3/3/3
54	PSU	1y	32	54	-	2/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
54	7MG	2y	46	54	-	2/7/37/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MA	2A	2503	1	-	1/7/25/26	0/3/3/3
1	2MU	2A	2552	56,1	-	0/9/27/28	0/2/2/2
54	MIA	1y	37	54	-	2/7/25/34	0/3/3/3

The worst 5 of 267 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.32	1.69	1.82
43	1l	92	0TD	CB-SB	-12.24	1.69	1.82
54	1w	37	MIA	C2-S10	-7.23	1.69	1.75
54	2w	37	MIA	C2-S10	-7.10	1.69	1.75
54	1w	37	MIA	C13-C14	6.93	1.53	1.32

The worst 5 of 424 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-19.93	66.54	102.36
43	1l	92	0TD	CSB-SB-CB	-17.51	70.90	102.36
54	2y	46	7MG	N9-C4-N3	9.94	140.03	125.46
54	1y	46	7MG	N9-C4-N3	9.92	139.99	125.46
54	1w	46	7MG	N9-C4-N3	9.05	138.72	125.46

There are no chirality outliers.

5 of 82 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	2l	92	0TD	SB-CB-CG-OD2
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	2a	967	5MC	O4'-C4'-C5'-O5'
32	2a	1207	2MG	N3-C2-N2-CM2
32	2a	1400	5MC	O4'-C1'-N1-C2

There are no ring outliers.

51 monomers are involved in 91 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	1l	92	0TD	3	0
32	1a	966	M2G	1	0
32	1a	1498	UR3	1	0
54	2y	8	4SU	2	0
54	1w	39	PSU	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2w	32	PSU	2	0
54	2y	32	PSU	2	0
55	2x	32	5MC	1	0
32	1a	1519	MA6	2	0
1	1A	1917	PSU	1	0
55	1x	8	4SU	2	0
54	2w	8	4SU	1	0
55	2x	55	PSU	1	0
1	2A	2251	OMG	1	0
32	2a	1519	MA6	5	0
1	2A	1915	5MU	1	0
32	2a	966	M2G	1	0
1	1A	1915	5MU	1	0
32	1a	1518	MA6	2	0
53	2v	19	PSU	3	0
32	2a	1402	4OC	1	0
55	1x	55	PSU	1	0
32	2a	1518	MA6	5	0
55	1x	54	5MU	2	0
54	2y	55	PSU	9	0
43	2l	92	0TD	2	0
32	2a	1400	5MC	3	0
32	2a	1498	UR3	1	0
1	1A	2552	2MU	2	0
1	2A	1939	5MU	1	0
54	1w	8	4SU	1	0
32	2a	1404	5MC	2	0
54	2w	54	5MU	1	0
54	2y	54	5MU	1	0
1	1A	1939	5MU	1	0
32	1a	516	PSU	1	0
32	1a	967	5MC	2	0
1	2A	1942	5MC	1	0
32	2a	967	5MC	3	0
1	2A	1962	5MC	2	0
1	2A	1920	4OC	2	0
32	1a	1207	2MG	3	0
54	1y	8	4SU	1	0
54	2w	46	7MG	1	0
54	1w	54	5MU	2	0
32	2a	1207	2MG	4	0
54	2w	37	MIA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2y	46	7MG	2	0
1	2A	2503	2MA	2	0
1	2A	2552	2MU	2	0
54	1y	37	MIA	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1466 ligands modelled in this entry, 1464 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	$\# Z > 2$
58	SF4	1d	501	35	0,12,12	-	-	-		
58	SF4	2d	501	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	1d	501	35	-	-	0/6/5/5
58	SF4	2d	501	35	-	-	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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	1d	501	SF4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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	1A	2860/2915 (98%)	-0.03	82 (2%)	53	46	67, 83, 117, 127	0
1	2A	2789/2915 (95%)	-0.09	47 (1%)	69	62	79, 94, 115, 128	0
2	1B	120/121 (99%)	-0.51	1 (0%)	82	78	77, 89, 99, 110	0
2	2B	120/121 (99%)	0.15	3 (2%)	58	50	96, 106, 115, 119	0
3	1D	275/276 (99%)	0.81	19 (6%)	23	19	71, 84, 93, 110	0
3	2D	275/276 (99%)	1.30	63 (22%)	2	2	78, 89, 98, 106	0
4	1E	204/206 (99%)	0.59	14 (6%)	23	19	70, 85, 96, 106	0
4	2E	204/206 (99%)	0.51	13 (6%)	25	21	82, 92, 100, 104	0
5	1F	203/210 (96%)	0.88	31 (15%)	5	5	72, 87, 101, 111	0
5	2F	203/210 (96%)	1.12	42 (20%)	2	2	82, 96, 105, 111	0
6	1G	181/182 (99%)	0.70	15 (8%)	17	15	77, 95, 104, 116	0
6	2G	181/182 (99%)	0.75	15 (8%)	17	15	97, 106, 113, 116	0
7	1H	174/180 (96%)	0.44	10 (5%)	29	24	81, 90, 98, 104	0
7	2H	174/180 (96%)	0.71	21 (12%)	8	8	95, 106, 112, 115	0
8	1I	146/148 (98%)	0.38	6 (4%)	41	34	86, 101, 107, 111	0
8	2I	146/148 (98%)	1.48	41 (28%)	1	1	92, 109, 117, 126	0
9	1N	140/140 (100%)	0.82	10 (7%)	22	19	74, 86, 97, 103	0
9	2N	140/140 (100%)	0.73	10 (7%)	22	19	82, 96, 104, 115	0
10	1O	122/122 (100%)	0.58	7 (5%)	29	24	73, 84, 92, 100	0
10	2O	122/122 (100%)	0.32	4 (3%)	49	42	82, 92, 99, 106	0
11	1P	149/150 (99%)	0.93	19 (12%)	7	7	67, 87, 100, 108	0
11	2P	149/150 (99%)	0.93	24 (16%)	4	4	81, 98, 111, 116	0
12	1Q	141/141 (100%)	0.91	16 (11%)	10	9	76, 86, 94, 105	0
12	2Q	141/141 (100%)	1.33	29 (20%)	2	2	85, 97, 105, 111	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.75	9 (7%) 20 18	72, 83, 95, 97	0
13	2R	118/118 (100%)	0.49	7 (5%) 28 23	82, 90, 97, 99	0
14	1S	110/112 (98%)	0.41	2 (1%) 67 59	80, 89, 94, 102	0
14	2S	110/112 (98%)	0.52	8 (7%) 21 18	92, 99, 104, 108	0
15	1T	131/146 (89%)	0.55	9 (6%) 23 19	78, 87, 99, 107	0
15	2T	131/146 (89%)	0.42	3 (2%) 61 53	83, 93, 104, 108	0
16	1U	116/118 (98%)	0.89	9 (7%) 19 17	70, 83, 92, 104	0
16	2U	116/118 (98%)	0.85	16 (13%) 6 6	81, 95, 105, 111	0
17	1V	101/101 (100%)	0.68	11 (10%) 10 9	72, 86, 95, 99	0
17	2V	101/101 (100%)	0.51	11 (10%) 10 9	88, 99, 106, 109	0
18	1W	112/113 (99%)	0.77	9 (8%) 18 16	72, 82, 93, 111	0
18	2W	112/113 (99%)	0.53	11 (9%) 13 12	80, 90, 100, 112	0
19	1X	95/96 (98%)	0.75	9 (9%) 14 12	71, 84, 96, 108	0
19	2X	95/96 (98%)	1.16	15 (15%) 5 4	87, 97, 105, 111	0
20	1Y	107/110 (97%)	0.63	6 (5%) 30 25	79, 89, 102, 106	0
20	2Y	107/110 (97%)	0.90	8 (7%) 20 18	92, 99, 108, 114	0
21	1Z	154/206 (74%)	0.46	8 (5%) 33 28	85, 96, 110, 116	0
21	2Z	160/206 (77%)	0.84	14 (8%) 15 14	95, 105, 112, 120	0
22	10	83/85 (97%)	1.41	9 (10%) 11 10	75, 84, 101, 110	0
22	20	83/85 (97%)	1.13	13 (15%) 5 5	90, 97, 109, 113	0
23	11	97/98 (98%)	1.58	29 (29%) 1 1	75, 86, 102, 108	0
23	21	97/98 (98%)	0.78	10 (10%) 12 11	81, 92, 103, 107	0
24	12	70/72 (97%)	0.33	4 (5%) 29 24	80, 88, 97, 104	0
24	22	70/72 (97%)	0.32	1 (1%) 73 67	90, 100, 106, 110	0
25	13	59/60 (98%)	0.24	0 100 100	75, 85, 94, 97	0
25	23	59/60 (98%)	0.42	2 (3%) 48 41	91, 97, 106, 110	0
26	14	69/71 (97%)	0.43	1 (1%) 73 67	91, 102, 113, 117	0
26	24	69/71 (97%)	0.83	5 (7%) 21 19	98, 110, 116, 121	0
27	15	59/60 (98%)	0.72	7 (11%) 9 8	74, 82, 93, 98	0
27	25	59/60 (98%)	0.56	5 (8%) 16 15	79, 88, 99, 105	0
28	16	53/54 (98%)	0.34	3 (5%) 29 24	76, 85, 92, 95	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.58	4 (7%) 20 18	88, 95, 102, 105	0
29	17	48/49 (97%)	0.93	6 (12%) 8 7	73, 79, 94, 102	0
29	27	48/49 (97%)	0.75	2 (4%) 40 33	80, 86, 97, 107	0
30	18	64/65 (98%)	1.19	11 (17%) 4 3	72, 82, 88, 91	0
30	28	64/65 (98%)	1.05	10 (15%) 5 5	84, 92, 99, 100	0
31	19	37/37 (100%)	0.62	1 (2%) 56 48	78, 84, 92, 94	0
31	29	37/37 (100%)	0.94	7 (18%) 3 3	93, 101, 105, 110	0
32	1a	1488/1521 (97%)	-0.09	47 (3%) 50 43	80, 97, 114, 122	0
32	2a	1491/1521 (98%)	0.08	48 (3%) 50 43	89, 105, 116, 125	0
33	1b	231/256 (90%)	0.40	6 (2%) 57 49	92, 103, 111, 120	0
33	2b	231/256 (90%)	0.71	18 (7%) 19 17	96, 109, 115, 120	0
34	1c	206/239 (86%)	0.26	4 (1%) 66 58	89, 99, 106, 109	0
34	2c	206/239 (86%)	0.78	26 (12%) 8 7	97, 107, 111, 114	0
35	1d	208/209 (99%)	0.75	13 (6%) 26 22	87, 97, 105, 115	0
35	2d	208/209 (99%)	0.90	21 (10%) 12 11	91, 102, 111, 116	0
36	1e	148/162 (91%)	0.43	7 (4%) 36 30	86, 95, 101, 106	0
36	2e	148/162 (91%)	0.67	6 (4%) 41 34	93, 103, 110, 111	0
37	1f	100/101 (99%)	0.41	3 (3%) 52 45	89, 98, 104, 108	0
37	2f	100/101 (99%)	0.46	5 (5%) 34 28	91, 99, 105, 110	0
38	1g	155/156 (99%)	0.61	16 (10%) 12 11	91, 98, 108, 112	0
38	2g	155/156 (99%)	0.85	21 (13%) 7 6	94, 104, 111, 114	0
39	1h	137/138 (99%)	0.46	3 (2%) 62 54	88, 97, 103, 108	0
39	2h	137/138 (99%)	0.75	10 (7%) 21 18	94, 104, 109, 116	0
40	1i	127/128 (99%)	0.75	12 (9%) 14 12	88, 99, 106, 110	0
40	2i	127/128 (99%)	0.98	16 (12%) 8 7	93, 107, 113, 115	0
41	1j	97/105 (92%)	0.59	3 (3%) 51 44	86, 102, 109, 116	0
41	2j	96/105 (91%)	1.08	11 (11%) 9 9	98, 109, 114, 117	0
42	1k	114/129 (88%)	0.52	4 (3%) 47 40	89, 99, 106, 111	0
42	2k	114/129 (88%)	0.58	1 (0%) 81 76	91, 101, 107, 110	0
43	1l	121/132 (91%)	0.58	12 (9%) 13 11	83, 91, 98, 103	0
43	2l	121/132 (91%)	0.82	8 (6%) 24 21	91, 100, 106, 109	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.68	16 (13%) 7 7	86, 99, 107, 117	0
44	2m	122/126 (96%)	1.18	25 (20%) 2 2	97, 107, 115, 120	0
45	1n	60/61 (98%)	0.77	6 (10%) 12 11	88, 95, 101, 102	0
45	2n	60/61 (98%)	1.56	16 (26%) 1 1	96, 108, 113, 115	0
46	1o	88/89 (98%)	0.58	5 (5%) 29 24	83, 96, 104, 109	0
46	2o	88/89 (98%)	0.51	5 (5%) 29 24	94, 102, 109, 111	0
47	1p	82/88 (93%)	1.11	14 (17%) 4 3	92, 100, 106, 108	0
47	2p	82/88 (93%)	0.87	9 (10%) 10 9	90, 99, 104, 109	0
48	1q	99/105 (94%)	0.47	1 (1%) 79 74	88, 97, 103, 107	0
48	2q	99/105 (94%)	0.36	2 (2%) 65 57	91, 99, 107, 111	0
49	1r	68/88 (77%)	0.41	2 (2%) 53 46	88, 97, 104, 106	0
49	2r	68/88 (77%)	0.58	4 (5%) 28 23	91, 101, 106, 111	0
50	1s	83/93 (89%)	0.72	9 (10%) 11 10	93, 99, 106, 113	0
50	2s	83/93 (89%)	1.17	13 (15%) 5 5	102, 107, 112, 114	0
51	1t	96/106 (90%)	0.90	15 (15%) 5 5	90, 100, 105, 108	0
51	2t	96/106 (90%)	1.06	19 (19%) 3 3	91, 99, 107, 111	0
52	1u	23/27 (85%)	0.73	1 (4%) 40 32	93, 98, 101, 102	0
52	2u	23/27 (85%)	1.12	2 (8%) 16 14	102, 106, 109, 112	0
53	1v	12/24 (50%)	0.54	2 (16%) 4 4	88, 98, 119, 119	0
53	2v	7/24 (29%)	1.39	2 (28%) 1 1	100, 103, 118, 118	0
54	1w	64/76 (84%)	0.34	2 (3%) 51 44	94, 117, 124, 127	0
54	1y	67/76 (88%)	0.23	0 100 100	83, 120, 124, 126	0
54	2w	62/76 (81%)	0.49	1 (1%) 70 63	107, 122, 127, 130	0
54	2y	66/76 (86%)	0.64	1 (1%) 72 65	97, 119, 123, 126	0
55	1x	72/77 (93%)	0.04	4 (5%) 30 25	85, 97, 110, 112	0
55	2x	72/77 (93%)	-0.16	0 100 100	95, 108, 115, 119	0
All	All	20862/21748 (95%)	0.40	1334 (6%) 25 21	67, 96, 113, 130	0

The worst 5 of 1334 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	10	6	GLY	14.2
22	10	8	GLY	12.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
22	10	7	LEU	11.7
22	10	4	LYS	11.5
22	10	5	LYS	8.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	5MU	2y	54	21/22	0.45	0.15	101,120,137,154	0
54	PSU	1y	55	20/21	0.56	0.13	119,126,131,138	0
54	5MU	2w	54	21/22	0.58	0.15	103,113,118,121	0
54	7MG	1w	46	24/25	0.62	0.12	105,115,124,133	0
54	4SU	2y	8	20/21	0.62	0.12	115,120,129,132	0
54	PSU	2w	55	20/21	0.62	0.12	105,120,127,131	0
54	4SU	2w	8	20/21	0.63	0.11	122,126,137,146	0
54	PSU	2y	55	20/21	0.65	0.14	114,121,139,154	0
54	4SU	1w	8	20/21	0.67	0.10	112,119,134,134	0
54	7MG	2w	46	24/25	0.68	0.11	113,122,129,141	0
54	PSU	1y	39	20/21	0.70	0.10	107,116,137,143	0
54	PSU	1y	32	20/21	0.70	0.13	105,113,128,129	0
54	5MU	1y	54	21/22	0.72	0.10	114,120,132,137	0
54	7MG	1y	46	24/25	0.73	0.10	109,119,125,130	0
54	7MG	2y	46	24/25	0.73	0.11	114,121,128,137	0
54	MIA	1y	37	22/30	0.75	0.11	108,117,123,134	0
54	PSU	2y	32	20/21	0.75	0.12	109,122,134,138	0
54	4SU	1y	8	20/21	0.76	0.09	115,120,127,132	0
54	PSU	1w	55	20/21	0.77	0.10	102,112,115,117	0
54	MIA	2y	37	22/30	0.77	0.13	107,116,130,143	0
54	PSU	2y	39	20/21	0.79	0.14	110,119,130,143	0
1	5MU	2A	1915	21/22	0.80	0.11	101,107,111,116	0
54	MIA	2w	37	25/30	0.80	0.15	91,115,118,133	0
54	PSU	1w	32	20/21	0.81	0.10	90,101,108,117	0
54	MIA	1w	37	29/30	0.81	0.17	78,99,107,108	0
32	2MG	2a	1207	24/25	0.82	0.11	100,107,116,125	0
55	4SU	2x	8	20/21	0.83	0.08	97,110,116,120	0
55	PSU	2x	55	20/21	0.83	0.08	106,112,122,123	0
54	PSU	2w	39	20/21	0.84	0.14	115,123,126,127	0
53	PSU	1v	19	20/21	0.85	0.13	79,95,102,102	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	5MU	1w	54	21/22	0.86	0.10	104,108,117,119	0
32	PSU	1a	516	20/21	0.86	0.10	84,92,98,104	0
55	PSU	1x	55	20/21	0.86	0.09	94,100,107,116	0
55	5MU	2x	54	21/22	0.86	0.08	103,111,114,124	0
55	4SU	1x	8	20/21	0.87	0.08	93,100,106,110	0
53	PSU	2v	19	20/21	0.87	0.12	105,112,119,120	0
54	PSU	1w	39	20/21	0.88	0.09	97,105,119,120	0
54	PSU	2w	32	20/21	0.88	0.12	108,114,123,126	0
32	PSU	2a	516	20/21	0.89	0.09	92,103,111,114	0
1	5MU	1A	1939	21/22	0.89	0.10	66,78,86,90	0
32	5MC	2a	967	21/22	0.90	0.14	99,102,110,118	0
1	5MC	2A	1962	21/22	0.90	0.12	77,89,95,99	0
1	PSU	2A	1917	20/21	0.90	0.07	86,103,108,111	0
55	5MU	1x	54	21/22	0.90	0.07	86,97,101,105	0
1	4OC	2A	1920	21/23	0.91	0.09	89,98,103,108	0
1	PSU	2A	2605	20/21	0.91	0.12	79,88,93,96	0
55	5MC	2x	32	21/22	0.91	0.12	99,105,110,112	0
1	5MU	2A	1939	21/22	0.91	0.11	75,86,91,95	0
1	PSU	2A	1911	20/21	0.92	0.08	86,98,105,106	0
32	7MG	2a	527	24/25	0.92	0.11	89,95,101,112	0
43	0TD	1l	92	10/11	0.92	0.11	88,91,97,113	0
1	5MC	2A	1942	21/22	0.92	0.10	88,94,99,106	0
32	5MC	2a	1400	21/22	0.92	0.17	87,108,118,120	0
32	2MG	1a	1207	24/25	0.93	0.08	77,95,102,105	0
55	5MC	1x	32	21/22	0.93	0.11	84,95,100,102	0
1	5MU	1A	1915	21/22	0.93	0.07	82,100,104,110	0
32	4OC	2a	1402	22/23	0.93	0.11	97,104,109,114	0
32	5MC	2a	1404	21/22	0.93	0.10	84,99,105,110	0
1	OMG	2A	2251	24/25	0.94	0.14	74,88,94,96	0
32	M2G	2a	966	25/26	0.94	0.12	93,99,106,113	0
1	2MA	2A	2503	23/24	0.94	0.11	70,81,88,92	0
1	PSU	1A	2605	20/21	0.94	0.10	66,79,85,86	0
1	5MC	1A	1942	21/22	0.94	0.10	65,81,86,88	0
32	5MC	1a	1400	21/22	0.94	0.12	81,91,96,104	0
1	PSU	1A	1911	20/21	0.94	0.09	70,90,95,100	0
1	PSU	1A	1917	20/21	0.94	0.07	83,90,95,96	0
32	5MC	1a	1404	21/22	0.94	0.12	74,83,96,97	0
32	7MG	1a	527	24/25	0.94	0.10	78,89,96,98	0
32	5MC	2a	1407	21/22	0.95	0.09	93,98,101,106	0
32	MA6	2a	1519	24/25	0.95	0.15	86,99,103,105	0
1	2MU	1A	2552	21/23	0.95	0.12	58,78,84,92	0
32	4OC	1a	1402	22/23	0.95	0.11	82,92,98,100	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	2MU	2A	2552	21/23	0.95	0.07	74,84,89,91	0
32	M2G	1a	966	25/26	0.95	0.12	81,87,96,98	0
1	OMG	1A	2251	24/25	0.95	0.12	66,80,85,86	0
32	5MC	1a	1407	21/22	0.95	0.08	76,88,93,97	0
32	MA6	1a	1519	24/25	0.96	0.14	82,87,92,99	0
32	5MC	1a	967	21/22	0.96	0.09	77,88,95,101	0
1	2MA	1A	2503	23/24	0.96	0.13	58,74,81,83	0
1	5MC	1A	1962	21/22	0.96	0.07	72,83,91,94	0
1	4OC	1A	1920	21/23	0.96	0.08	76,89,95,96	0
32	UR3	1a	1498	21/22	0.96	0.15	78,85,89,93	0
32	UR3	2a	1498	21/22	0.96	0.11	88,98,102,106	0
32	MA6	2a	1518	24/25	0.96	0.08	90,97,101,102	0
32	MA6	1a	1518	24/25	0.97	0.09	58,85,89,93	0
43	0TD	2l	92	10/11	0.97	0.09	95,101,103,110	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3120	1/1	0.18	0.33	111,111,111,111	0
56	MG	2a	3082	1/1	0.24	0.45	109,109,109,109	0
56	MG	2a	3162	1/1	0.35	0.12	126,126,126,126	0
56	MG	2a	3144	1/1	0.36	0.17	101,101,101,101	0
56	MG	2a	3087	1/1	0.37	0.37	94,94,94,94	0
56	MG	1a	3149	1/1	0.39	0.28	110,110,110,110	0
56	MG	2a	3173	1/1	0.40	0.32	115,115,115,115	0
56	MG	2a	3106	1/1	0.42	0.22	124,124,124,124	0
56	MG	1A	3674	1/1	0.43	0.43	81,81,81,81	0
56	MG	1A	3579	1/1	0.47	0.16	118,118,118,118	0
56	MG	2a	3077	1/1	0.49	0.28	95,95,95,95	0
56	MG	2a	3091	1/1	0.50	0.43	92,92,92,92	0
56	MG	2A	3323	1/1	0.51	0.18	104,104,104,104	0
56	MG	2a	3180	1/1	0.51	0.20	102,102,102,102	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3041	1/1	0.52	0.56	105,105,105,105	0
56	MG	1A	3045	1/1	0.52	0.27	94,94,94,94	0
56	MG	1A	3020	1/1	0.53	0.33	89,89,89,89	0
56	MG	2a	3166	1/1	0.53	0.15	115,115,115,115	0
56	MG	1A	3648	1/1	0.54	0.20	127,127,127,127	0
56	MG	2A	3258	1/1	0.54	0.25	103,103,103,103	0
56	MG	1A	3441	1/1	0.54	0.32	103,103,103,103	0
56	MG	2a	3161	1/1	0.54	0.29	104,104,104,104	0
56	MG	1A	3533	1/1	0.55	0.30	114,114,114,114	0
56	MG	1A	3377	1/1	0.55	0.37	102,102,102,102	0
56	MG	2A	3277	1/1	0.55	0.30	93,93,93,93	0
56	MG	2A	3344	1/1	0.56	0.28	106,106,106,106	0
56	MG	1A	3119	1/1	0.56	0.29	107,107,107,107	0
56	MG	1a	3214	1/1	0.56	0.43	103,103,103,103	0
56	MG	2A	3019	1/1	0.56	0.34	101,101,101,101	0
56	MG	1A	3497	1/1	0.57	0.15	96,96,96,96	0
56	MG	1A	3394	1/1	0.57	0.37	91,91,91,91	0
56	MG	2A	3190	1/1	0.57	0.23	98,98,98,98	0
56	MG	2A	3221	1/1	0.58	0.37	107,107,107,107	0
56	MG	2A	3317	1/1	0.58	0.18	92,92,92,92	0
56	MG	1A	3190	1/1	0.58	0.40	118,118,118,118	0
56	MG	1a	3166	1/1	0.59	0.20	100,100,100,100	0
56	MG	2a	3050	1/1	0.59	0.21	105,105,105,105	0
56	MG	2a	3066	1/1	0.59	0.21	106,106,106,106	0
56	MG	1A	3534	1/1	0.59	0.29	86,86,86,86	0
56	MG	1a	3021	1/1	0.59	0.34	102,102,102,102	0
56	MG	1A	3559	1/1	0.59	0.18	115,115,115,115	0
56	MG	2A	3201	1/1	0.59	0.23	102,102,102,102	0
56	MG	2A	3074	1/1	0.60	0.27	102,102,102,102	0
56	MG	1A	3063	1/1	0.61	0.31	80,80,80,80	0
56	MG	2A	3341	1/1	0.61	0.22	94,94,94,94	0
56	MG	2a	3098	1/1	0.62	0.34	101,101,101,101	0
56	MG	2A	3326	1/1	0.62	0.16	91,91,91,91	0
56	MG	2a	3121	1/1	0.62	0.26	114,114,114,114	0
56	MG	1A	3486	1/1	0.63	0.22	68,68,68,68	0
56	MG	1a	3209	1/1	0.63	0.39	90,90,90,90	0
56	MG	2a	3006	1/1	0.63	0.20	104,104,104,104	0
56	MG	1A	3629	1/1	0.63	0.29	106,106,106,106	0
56	MG	2A	3205	1/1	0.63	0.20	111,111,111,111	0
56	MG	1a	3157	1/1	0.63	0.39	89,89,89,89	0
56	MG	2A	3078	1/1	0.64	0.23	75,75,75,75	0
56	MG	2A	3289	1/1	0.64	0.21	102,102,102,102	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3020	1/1	0.64	0.16	98,98,98,98	0
56	MG	1a	3122	1/1	0.64	0.12	93,93,93,93	0
56	MG	2a	3090	1/1	0.64	0.36	91,91,91,91	0
56	MG	1A	3172	1/1	0.65	0.24	94,94,94,94	0
56	MG	1A	3256	1/1	0.65	0.31	84,84,84,84	0
56	MG	1A	3565	1/1	0.66	0.33	83,83,83,83	0
56	MG	1A	3294	1/1	0.66	0.44	87,87,87,87	0
56	MG	2a	3156	1/1	0.66	0.24	104,104,104,104	0
56	MG	2A	3138	1/1	0.66	0.20	102,102,102,102	0
56	MG	1A	3428	1/1	0.66	0.29	79,79,79,79	0
56	MG	2a	3164	1/1	0.66	0.18	114,114,114,114	0
56	MG	1a	3162	1/1	0.66	0.32	93,93,93,93	0
56	MG	2a	3100	1/1	0.66	0.35	94,94,94,94	0
56	MG	2a	3079	1/1	0.66	0.11	90,90,90,90	0
56	MG	1A	3599	1/1	0.67	0.22	100,100,100,100	0
56	MG	1a	3051	1/1	0.67	0.36	99,99,99,99	0
56	MG	2A	3026	1/1	0.67	0.14	92,92,92,92	0
56	MG	1a	3182	1/1	0.67	0.23	102,102,102,102	0
56	MG	1a	3096	1/1	0.67	0.12	95,95,95,95	0
56	MG	1A	3601	1/1	0.68	0.17	102,102,102,102	0
56	MG	2a	3152	1/1	0.68	0.12	111,111,111,111	0
56	MG	1a	3236	1/1	0.68	0.27	85,85,85,85	0
56	MG	1A	3219	1/1	0.68	0.21	84,84,84,84	0
56	MG	1A	3470	1/1	0.68	0.28	100,100,100,100	0
56	MG	2a	3062	1/1	0.68	0.24	94,94,94,94	0
56	MG	1a	3198	1/1	0.68	0.29	89,89,89,89	0
56	MG	1a	3068	1/1	0.68	0.33	95,95,95,95	0
56	MG	2A	3343	1/1	0.68	0.21	99,99,99,99	0
56	MG	1a	3044	1/1	0.69	0.29	90,90,90,90	0
56	MG	1A	3657	1/1	0.69	0.39	79,79,79,79	0
56	MG	1a	3152	1/1	0.69	0.20	102,102,102,102	0
56	MG	2a	3036	1/1	0.69	0.35	95,95,95,95	0
56	MG	2A	3095	1/1	0.69	0.33	89,89,89,89	0
56	MG	2a	3138	1/1	0.69	0.29	95,95,95,95	0
56	MG	2A	3301	1/1	0.69	0.20	83,83,83,83	0
56	MG	2a	3146	1/1	0.69	0.11	100,100,100,100	0
56	MG	1A	3591	1/1	0.70	0.40	83,83,83,83	0
56	MG	1A	3636	1/1	0.70	0.21	73,73,73,73	0
56	MG	1A	3117	1/1	0.70	0.14	98,98,98,98	0
56	MG	1A	3445	1/1	0.70	0.17	80,80,80,80	0
56	MG	2A	3025	1/1	0.71	0.16	88,88,88,88	0
56	MG	2A	3316	1/1	0.71	0.14	93,93,93,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3359	1/1	0.71	0.15	89,89,89,89	0
56	MG	1A	3623	1/1	0.71	0.21	87,87,87,87	0
56	MG	2A	3210	1/1	0.71	0.18	75,75,75,75	0
56	MG	2A	3330	1/1	0.71	0.19	101,101,101,101	0
56	MG	1a	3197	1/1	0.72	0.26	102,102,102,102	0
56	MG	2a	3139	1/1	0.72	0.25	81,81,81,81	0
56	MG	2A	3139	1/1	0.72	0.28	101,101,101,101	0
56	MG	2A	3184	1/1	0.72	0.25	82,82,82,82	0
56	MG	2a	3150	1/1	0.72	0.25	87,87,87,87	0
56	MG	1A	3376	1/1	0.72	0.28	92,92,92,92	0
56	MG	1A	3053	1/1	0.72	0.35	95,95,95,95	0
56	MG	2a	3092	1/1	0.72	0.27	88,88,88,88	0
56	MG	1A	3457	1/1	0.72	0.28	77,77,77,77	0
56	MG	1A	3592	1/1	0.72	0.22	84,84,84,84	0
56	MG	2A	3090	1/1	0.72	0.20	98,98,98,98	0
56	MG	2a	3113	1/1	0.72	0.19	111,111,111,111	0
56	MG	2A	3003	1/1	0.72	0.25	84,84,84,84	0
56	MG	2a	3015	1/1	0.73	0.34	98,98,98,98	0
56	MG	1a	3191	1/1	0.73	0.27	93,93,93,93	0
56	MG	2A	3261	1/1	0.73	0.18	98,98,98,98	0
56	MG	2A	3084	1/1	0.73	0.21	90,90,90,90	0
56	MG	1A	3339	1/1	0.73	0.42	112,112,112,112	0
56	MG	2A	3094	1/1	0.73	0.15	85,85,85,85	0
56	MG	1A	3414	1/1	0.73	0.31	82,82,82,82	0
56	MG	1a	3121	1/1	0.73	0.10	88,88,88,88	0
56	MG	1A	3340	1/1	0.73	0.30	78,78,78,78	0
56	MG	1A	3266	1/1	0.73	0.28	65,65,65,65	0
56	MG	1a	3009	1/1	0.73	0.19	91,91,91,91	0
56	MG	1A	3290	1/1	0.73	0.34	90,90,90,90	0
56	MG	1a	3031	1/1	0.73	0.41	103,103,103,103	0
56	MG	1A	3456	1/1	0.73	0.20	96,96,96,96	0
56	MG	2a	3099	1/1	0.73	0.23	93,93,93,93	0
56	MG	1A	3165	1/1	0.73	0.29	86,86,86,86	0
56	MG	2a	3115	1/1	0.74	0.18	103,103,103,103	0
56	MG	1A	3646	1/1	0.74	0.20	92,92,92,92	0
56	MG	2a	3122	1/1	0.74	0.36	114,114,114,114	0
56	MG	2a	3134	1/1	0.74	0.23	100,100,100,100	0
56	MG	2a	3076	1/1	0.74	0.26	99,99,99,99	0
56	MG	1A	3479	1/1	0.74	0.21	86,86,86,86	0
56	MG	1a	3077	1/1	0.74	0.19	84,84,84,84	0
56	MG	1A	3239	1/1	0.74	0.23	93,93,93,93	0
56	MG	1a	3036	1/1	0.74	0.35	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3134	1/1	0.74	0.23	91,91,91,91	0
56	MG	1A	3361	1/1	0.74	0.37	71,71,71,71	0
56	MG	2a	3010	1/1	0.74	0.21	86,86,86,86	0
56	MG	1a	3140	1/1	0.74	0.32	84,84,84,84	0
56	MG	2A	3147	1/1	0.74	0.16	84,84,84,84	0
56	MG	2A	3302	1/1	0.74	0.13	82,82,82,82	0
56	MG	1a	3194	1/1	0.74	0.16	102,102,102,102	0
56	MG	2a	3176	1/1	0.74	0.28	83,83,83,83	0
56	MG	1a	3143	1/1	0.74	0.42	91,91,91,91	0
56	MG	1a	3238	1/1	0.75	0.30	99,99,99,99	0
56	MG	1A	3025	1/1	0.75	0.23	87,87,87,87	0
56	MG	2a	3142	1/1	0.75	0.30	103,103,103,103	0
56	MG	1A	3587	1/1	0.75	0.28	80,80,80,80	0
56	MG	2A	3325	1/1	0.75	0.15	91,91,91,91	0
56	MG	2a	3148	1/1	0.75	0.19	92,92,92,92	0
56	MG	2a	3060	1/1	0.75	0.14	101,101,101,101	0
56	MG	1A	3407	1/1	0.75	0.21	91,91,91,91	0
56	MG	1A	3481	1/1	0.75	0.25	83,83,83,83	0
56	MG	2A	3293	1/1	0.75	0.13	95,95,95,95	0
56	MG	2a	3114	1/1	0.75	0.25	92,92,92,92	0
56	MG	2A	3294	1/1	0.75	0.11	104,104,104,104	0
56	MG	2A	3055	1/1	0.75	0.17	92,92,92,92	0
56	MG	2a	3171	1/1	0.75	0.14	115,115,115,115	0
56	MG	1a	3133	1/1	0.75	0.21	90,90,90,90	0
56	MG	2a	3132	1/1	0.75	0.22	83,83,83,83	0
56	MG	2A	3311	1/1	0.75	0.22	106,106,106,106	0
56	MG	1a	3189	1/1	0.76	0.34	85,85,85,85	0
56	MG	1A	3513	1/1	0.76	0.20	88,88,88,88	0
56	MG	1A	3600	1/1	0.76	0.15	77,77,77,77	0
56	MG	1A	3519	1/1	0.76	0.20	88,88,88,88	0
56	MG	1a	3060	1/1	0.76	0.15	83,83,83,83	0
56	MG	1a	3063	1/1	0.76	0.21	89,89,89,89	0
56	MG	2a	3123	1/1	0.76	0.34	79,79,79,79	0
56	MG	1A	3615	1/1	0.76	0.14	95,95,95,95	0
56	MG	1A	3525	1/1	0.76	0.09	101,101,101,101	0
56	MG	1A	3318	1/1	0.76	0.32	99,99,99,99	0
56	MG	2A	3230	1/1	0.76	0.30	82,82,82,82	0
56	MG	1A	3336	1/1	0.76	0.34	81,81,81,81	0
56	MG	1A	3211	1/1	0.76	0.33	88,88,88,88	0
56	MG	1A	3257	1/1	0.76	0.29	80,80,80,80	0
56	MG	2a	3069	1/1	0.76	0.17	103,103,103,103	0
56	MG	1A	3651	1/1	0.76	0.14	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3035	1/1	0.76	0.29	92,92,92,92	0
56	MG	2A	3047	1/1	0.76	0.18	89,89,89,89	0
56	MG	1A	3573	1/1	0.76	0.15	88,88,88,88	0
56	MG	1A	3658	1/1	0.76	0.23	98,98,98,98	0
56	MG	1A	3161	1/1	0.76	0.18	90,90,90,90	0
56	MG	1A	3191	1/1	0.76	0.29	90,90,90,90	0
56	MG	1A	3240	1/1	0.76	0.15	101,101,101,101	0
56	MG	1a	3027	1/1	0.76	0.29	76,76,76,76	0
56	MG	1a	3173	1/1	0.76	0.18	75,75,75,75	0
56	MG	1A	3506	1/1	0.76	0.19	118,118,118,118	0
56	MG	2a	3070	1/1	0.77	0.09	87,87,87,87	0
56	MG	1A	3234	1/1	0.77	0.43	96,96,96,96	0
56	MG	2A	3087	1/1	0.77	0.11	88,88,88,88	0
56	MG	2A	3246	1/1	0.77	0.21	105,105,105,105	0
56	MG	1A	3181	1/1	0.77	0.14	78,78,78,78	0
56	MG	1A	3316	1/1	0.77	0.38	83,83,83,83	0
56	MG	1A	3676	1/1	0.77	0.38	84,84,84,84	0
56	MG	1A	3447	1/1	0.77	0.18	91,91,91,91	0
56	MG	2A	3022	1/1	0.77	0.27	96,96,96,96	0
56	MG	1a	3020	1/1	0.77	0.21	74,74,74,74	0
56	MG	1A	3157	1/1	0.77	0.16	92,92,92,92	0
56	MG	1A	3518	1/1	0.77	0.20	97,97,97,97	0
56	MG	2A	3303	1/1	0.77	0.16	98,98,98,98	0
56	MG	1A	3104	1/1	0.77	0.17	90,90,90,90	0
56	MG	2a	3061	1/1	0.77	0.08	92,92,92,92	0
56	MG	1a	3033	1/1	0.77	0.21	87,87,87,87	0
56	MG	2a	3064	1/1	0.77	0.16	99,99,99,99	0
56	MG	1A	3137	1/1	0.77	0.28	82,82,82,82	0
56	MG	1A	3145	1/1	0.77	0.31	93,93,93,93	0
56	MG	1a	3211	1/1	0.78	0.33	77,77,77,77	0
56	MG	1a	3134	1/1	0.78	0.07	77,77,77,77	0
56	MG	1A	3584	1/1	0.78	0.12	92,92,92,92	0
56	MG	2A	3152	1/1	0.78	0.11	85,85,85,85	0
56	MG	2A	3170	1/1	0.78	0.21	95,95,95,95	0
56	MG	1A	3265	1/1	0.78	0.31	65,65,65,65	0
56	MG	2a	3154	1/1	0.78	0.11	101,101,101,101	0
56	MG	1A	3429	1/1	0.78	0.43	87,87,87,87	0
56	MG	1A	3168	1/1	0.78	0.23	78,78,78,78	0
56	MG	1A	3444	1/1	0.78	0.17	83,83,83,83	0
56	MG	1A	3125	1/1	0.78	0.22	77,77,77,77	0
56	MG	2a	3080	1/1	0.78	0.16	85,85,85,85	0
56	MG	1A	3122	1/1	0.78	0.23	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3026	1/1	0.78	0.22	90,90,90,90	0
56	MG	1a	3210	1/1	0.78	0.28	91,91,91,91	0
56	MG	2A	3244	1/1	0.78	0.15	90,90,90,90	0
56	MG	1A	3123	1/1	0.79	0.10	93,93,93,93	0
56	MG	1A	3540	1/1	0.79	0.19	94,94,94,94	0
56	MG	2a	3107	1/1	0.79	0.08	106,106,106,106	0
56	MG	1a	3187	1/1	0.79	0.31	78,78,78,78	0
56	MG	2A	3068	1/1	0.79	0.21	106,106,106,106	0
56	MG	2a	3024	1/1	0.79	0.17	90,90,90,90	0
56	MG	1A	3214	1/1	0.79	0.44	96,96,96,96	0
56	MG	1a	3018	1/1	0.79	0.19	74,74,74,74	0
56	MG	1A	3618	1/1	0.79	0.17	98,98,98,98	0
56	MG	1a	3126	1/1	0.79	0.16	100,100,100,100	0
56	MG	1a	3130	1/1	0.79	0.26	99,99,99,99	0
56	MG	2a	3136	1/1	0.79	0.19	85,85,85,85	0
56	MG	1A	3242	1/1	0.79	0.25	78,78,78,78	0
56	MG	2a	3063	1/1	0.79	0.15	83,83,83,83	0
56	MG	1A	3248	1/1	0.79	0.25	76,76,76,76	0
56	MG	2A	3119	1/1	0.79	0.28	90,90,90,90	0
56	MG	1A	3250	1/1	0.79	0.34	94,94,94,94	0
56	MG	1A	3170	1/1	0.79	0.27	99,99,99,99	0
56	MG	1a	3223	1/1	0.79	0.34	84,84,84,84	0
56	MG	2A	3313	1/1	0.79	0.23	96,96,96,96	0
56	MG	1A	3319	1/1	0.79	0.32	100,100,100,100	0
56	MG	1A	3401	1/1	0.79	0.31	90,90,90,90	0
56	MG	2A	3153	1/1	0.79	0.27	81,81,81,81	0
56	MG	1A	3144	1/1	0.79	0.16	85,85,85,85	0
56	MG	1A	3409	1/1	0.79	0.33	70,70,70,70	0
56	MG	1A	3663	1/1	0.79	0.28	89,89,89,89	0
56	MG	1a	3168	1/1	0.79	0.10	111,111,111,111	0
56	MG	2a	3093	1/1	0.79	0.42	87,87,87,87	0
56	MG	1a	3172	1/1	0.79	0.23	90,90,90,90	0
56	MG	2A	3209	1/1	0.79	0.32	83,83,83,83	0
56	MG	2a	3096	1/1	0.80	0.41	84,84,84,84	0
56	MG	2a	3097	1/1	0.80	0.23	89,89,89,89	0
56	MG	2A	3017	1/1	0.80	0.20	98,98,98,98	0
56	MG	1A	3042	1/1	0.80	0.21	64,64,64,64	0
56	MG	1A	3378	1/1	0.80	0.37	73,73,73,73	0
56	MG	2a	3105	1/1	0.80	0.36	95,95,95,95	0
56	MG	1a	3010	1/1	0.80	0.28	85,85,85,85	0
56	MG	1a	3083	1/1	0.80	0.24	93,93,93,93	0
56	MG	2a	3012	1/1	0.80	0.10	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3380	1/1	0.80	0.24	67,67,67,67	0
56	MG	2A	3044	1/1	0.80	0.22	78,78,78,78	0
56	MG	1a	3174	1/1	0.80	0.12	87,87,87,87	0
56	MG	2A	3048	1/1	0.80	0.19	83,83,83,83	0
56	MG	1a	3111	1/1	0.80	0.33	103,103,103,103	0
56	MG	1a	3115	1/1	0.80	0.19	89,89,89,89	0
56	MG	1a	3116	1/1	0.80	0.18	90,90,90,90	0
56	MG	2a	3135	1/1	0.80	0.16	108,108,108,108	0
56	MG	1A	3386	1/1	0.80	0.46	68,68,68,68	0
56	MG	2A	3282	1/1	0.80	0.14	87,87,87,87	0
56	MG	1A	3583	1/1	0.80	0.14	88,88,88,88	0
56	MG	1A	3517	1/1	0.80	0.23	77,77,77,77	0
56	MG	1a	3030	1/1	0.80	0.22	105,105,105,105	0
56	MG	2a	3067	1/1	0.80	0.09	112,112,112,112	0
56	MG	1A	3132	1/1	0.80	0.27	82,82,82,82	0
56	MG	1A	3352	1/1	0.80	0.33	95,95,95,95	0
56	MG	1A	3036	1/1	0.80	0.25	99,99,99,99	0
56	MG	1A	3139	1/1	0.80	0.21	79,79,79,79	0
56	MG	1A	3374	1/1	0.80	0.19	63,63,63,63	0
56	MG	1a	3226	1/1	0.80	0.25	89,89,89,89	0
56	MG	1a	3233	1/1	0.80	0.23	76,76,76,76	0
56	MG	2A	3318	1/1	0.80	0.17	87,87,87,87	0
56	MG	2a	3088	1/1	0.80	0.29	97,97,97,97	0
56	MG	1a	3054	1/1	0.80	0.24	85,85,85,85	0
56	MG	1a	3154	1/1	0.80	0.32	78,78,78,78	0
56	MG	2A	3159	1/1	0.80	0.23	91,91,91,91	0
56	MG	1A	3140	1/1	0.80	0.30	89,89,89,89	0
56	MG	2A	3281	1/1	0.81	0.21	88,88,88,88	0
56	MG	1a	3207	1/1	0.81	0.20	96,96,96,96	0
56	MG	2A	3287	1/1	0.81	0.13	83,83,83,83	0
56	MG	2A	3031	1/1	0.81	0.27	100,100,100,100	0
56	MG	2a	3059	1/1	0.81	0.09	79,79,79,79	0
56	MG	1a	3165	1/1	0.81	0.12	87,87,87,87	0
56	MG	2A	3148	1/1	0.81	0.14	96,96,96,96	0
56	MG	2A	3296	1/1	0.81	0.49	102,102,102,102	0
56	MG	1A	3015	1/1	0.81	0.15	86,86,86,86	0
56	MG	1A	3324	1/1	0.81	0.25	67,67,67,67	0
56	MG	1A	3367	1/1	0.81	0.23	104,104,104,104	0
56	MG	2A	3308	1/1	0.81	0.12	103,103,103,103	0
56	MG	2A	3166	1/1	0.81	0.25	79,79,79,79	0
56	MG	1A	3368	1/1	0.81	0.23	99,99,99,99	0
56	MG	1a	3082	1/1	0.81	0.13	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	3180	1/1	0.81	0.16	90,90,90,90	0
56	MG	1a	3016	1/1	0.81	0.14	87,87,87,87	0
56	MG	2A	3079	1/1	0.81	0.13	89,89,89,89	0
56	MG	2A	3080	1/1	0.81	0.17	80,80,80,80	0
56	MG	1a	3039	1/1	0.81	0.28	80,80,80,80	0
56	MG	1a	3098	1/1	0.81	0.13	87,87,87,87	0
56	MG	2A	3226	1/1	0.81	0.15	73,73,73,73	0
56	MG	2A	3012	1/1	0.81	0.11	92,92,92,92	0
56	MG	1a	3040	1/1	0.81	0.15	89,89,89,89	0
56	MG	2a	3002	1/1	0.81	0.22	98,98,98,98	0
56	MG	1A	3528	1/1	0.81	0.23	78,78,78,78	0
56	MG	2A	3249	1/1	0.81	0.10	81,81,81,81	0
56	MG	2A	3100	1/1	0.81	0.23	86,86,86,86	0
56	MG	1A	3626	1/1	0.81	0.20	86,86,86,86	0
56	MG	1A	3254	1/1	0.81	0.32	78,78,78,78	0
56	MG	2a	3178	1/1	0.81	0.36	96,96,96,96	0
56	MG	2a	3101	1/1	0.81	0.18	101,101,101,101	0
56	MG	1A	3261	1/1	0.82	0.19	72,72,72,72	0
56	MG	2A	3092	1/1	0.82	0.22	99,99,99,99	0
56	MG	2a	3007	1/1	0.82	0.17	99,99,99,99	0
56	MG	1A	3330	1/1	0.82	0.39	96,96,96,96	0
56	MG	1a	3050	1/1	0.82	0.11	80,80,80,80	0
56	MG	1A	3241	1/1	0.82	0.25	68,68,68,68	0
56	MG	2a	3018	1/1	0.82	0.13	71,71,71,71	0
56	MG	1A	3612	1/1	0.82	0.15	95,95,95,95	0
56	MG	2A	3125	1/1	0.82	0.28	88,88,88,88	0
56	MG	2A	3280	1/1	0.82	0.15	94,94,94,94	0
56	MG	2A	3130	1/1	0.82	0.30	90,90,90,90	0
56	MG	2A	3024	1/1	0.82	0.17	95,95,95,95	0
56	MG	2A	3137	1/1	0.82	0.13	91,91,91,91	0
56	MG	1A	3549	1/1	0.82	0.24	83,83,83,83	0
56	MG	2a	3127	1/1	0.82	0.14	100,100,100,100	0
56	MG	2a	3129	1/1	0.82	0.16	92,92,92,92	0
56	MG	1A	3552	1/1	0.82	0.19	100,100,100,100	0
56	MG	2A	3142	1/1	0.82	0.14	81,81,81,81	0
56	MG	2A	3143	1/1	0.82	0.15	93,93,93,93	0
56	MG	2A	3027	1/1	0.82	0.11	87,87,87,87	0
56	MG	1A	3016	1/1	0.82	0.27	66,66,66,66	0
56	MG	2A	3034	1/1	0.82	0.21	71,71,71,71	0
56	MG	2a	3068	1/1	0.82	0.08	83,83,83,83	0
56	MG	1A	3019	1/1	0.82	0.14	81,81,81,81	0
56	MG	1a	3080	1/1	0.82	0.32	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3071	1/1	0.82	0.13	88,88,88,88	0
56	MG	2a	3072	1/1	0.82	0.15	107,107,107,107	0
56	MG	1A	3128	1/1	0.82	0.12	75,75,75,75	0
56	MG	1a	3023	1/1	0.82	0.20	87,87,87,87	0
56	MG	1A	3065	1/1	0.82	0.14	71,71,71,71	0
56	MG	2a	3157	1/1	0.82	0.09	114,114,114,114	0
56	MG	1a	3215	1/1	0.82	0.27	84,84,84,84	0
56	MG	1a	3217	1/1	0.82	0.24	85,85,85,85	0
56	MG	2A	3324	1/1	0.82	0.08	83,83,83,83	0
56	MG	2A	3204	1/1	0.82	0.31	90,90,90,90	0
56	MG	1A	3087	1/1	0.82	0.20	79,79,79,79	0
56	MG	1A	3400	1/1	0.82	0.53	90,90,90,90	0
56	MG	1A	3364	1/1	0.82	0.24	96,96,96,96	0
56	MG	1A	3099	1/1	0.82	0.10	77,77,77,77	0
56	MG	1A	3530	1/1	0.82	0.22	79,79,79,79	0
56	MG	1A	3557	1/1	0.83	0.25	89,89,89,89	0
56	MG	1A	3505	1/1	0.83	0.14	70,70,70,70	0
56	MG	1A	3560	1/1	0.83	0.25	88,88,88,88	0
56	MG	1A	3052	1/1	0.83	0.18	77,77,77,77	0
56	MG	1A	3299	1/1	0.83	0.37	90,90,90,90	0
56	MG	2A	3314	1/1	0.83	0.17	94,94,94,94	0
56	MG	1a	3101	1/1	0.83	0.40	88,88,88,88	0
56	MG	2A	3149	1/1	0.83	0.19	84,84,84,84	0
56	MG	1a	3107	1/1	0.83	0.31	84,84,84,84	0
56	MG	2A	3321	1/1	0.83	0.10	101,101,101,101	0
56	MG	1A	3301	1/1	0.83	0.25	85,85,85,85	0
56	MG	2A	3029	1/1	0.83	0.21	94,94,94,94	0
56	MG	1A	3313	1/1	0.83	0.21	72,72,72,72	0
56	MG	2a	3104	1/1	0.83	0.10	100,100,100,100	0
56	MG	2A	3033	1/1	0.83	0.10	81,81,81,81	0
56	MG	2A	3176	1/1	0.83	0.22	89,89,89,89	0
56	MG	1A	3390	1/1	0.83	0.34	87,87,87,87	0
56	MG	1A	3653	1/1	0.83	0.18	95,95,95,95	0
56	MG	1A	3449	1/1	0.83	0.24	76,76,76,76	0
56	MG	1a	3124	1/1	0.83	0.20	70,70,70,70	0
56	MG	2a	3119	1/1	0.83	0.16	107,107,107,107	0
56	MG	2a	3005	1/1	0.83	0.20	96,96,96,96	0
56	MG	1a	3202	1/1	0.83	0.21	89,89,89,89	0
56	MG	1a	3203	1/1	0.83	0.06	105,105,105,105	0
56	MG	1A	3235	1/1	0.83	0.36	73,73,73,73	0
56	MG	2A	3216	1/1	0.83	0.09	87,87,87,87	0
56	MG	2A	3219	1/1	0.83	0.14	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3220	1/1	0.83	0.32	74,74,74,74	0
56	MG	1a	3045	1/1	0.83	0.19	85,85,85,85	0
56	MG	1a	3046	1/1	0.83	0.23	73,73,73,73	0
56	MG	1a	3049	1/1	0.83	0.12	87,87,87,87	0
56	MG	1A	3363	1/1	0.83	0.27	79,79,79,79	0
56	MG	1A	3595	1/1	0.83	0.25	69,69,69,69	0
56	MG	2a	3143	1/1	0.83	0.15	107,107,107,107	0
56	MG	2A	3247	1/1	0.83	0.19	101,101,101,101	0
56	MG	1a	3216	1/1	0.83	0.15	81,81,81,81	0
56	MG	1a	3145	1/1	0.83	0.36	97,97,97,97	0
56	MG	2A	3260	1/1	0.83	0.23	87,87,87,87	0
56	MG	1a	3218	1/1	0.83	0.20	80,80,80,80	0
56	MG	2A	3265	1/1	0.83	0.20	93,93,93,93	0
56	MG	1a	3222	1/1	0.83	0.16	91,91,91,91	0
56	MG	1A	3147	1/1	0.83	0.22	86,86,86,86	0
56	MG	1A	3150	1/1	0.83	0.12	91,91,91,91	0
56	MG	2A	3114	1/1	0.83	0.16	79,79,79,79	0
56	MG	1a	3062	1/1	0.83	0.09	71,71,71,71	0
56	MG	1A	3267	1/1	0.83	0.43	76,76,76,76	0
56	MG	2a	3168	1/1	0.83	0.15	112,112,112,112	0
56	MG	2A	3290	1/1	0.83	0.13	94,94,94,94	0
56	MG	2A	3126	1/1	0.83	0.14	80,80,80,80	0
56	MG	1A	3278	1/1	0.83	0.26	59,59,59,59	0
56	MG	1A	3230	1/1	0.83	0.56	72,72,72,72	0
56	MG	2A	3009	1/1	0.83	0.21	89,89,89,89	0
56	MG	1a	3163	1/1	0.84	0.36	66,66,66,66	0
56	MG	2A	3007	1/1	0.84	0.33	80,80,80,80	0
56	MG	2A	3300	1/1	0.84	0.21	79,79,79,79	0
56	MG	1A	3205	1/1	0.84	0.17	78,78,78,78	0
56	MG	2A	3011	1/1	0.84	0.09	87,87,87,87	0
56	MG	1a	3070	1/1	0.84	0.36	85,85,85,85	0
56	MG	2a	3089	1/1	0.84	0.36	86,86,86,86	0
56	MG	2A	3307	1/1	0.84	0.09	79,79,79,79	0
56	MG	2A	3013	1/1	0.84	0.15	79,79,79,79	0
56	MG	2A	3309	1/1	0.84	0.18	85,85,85,85	0
56	MG	2A	3146	1/1	0.84	0.14	79,79,79,79	0
56	MG	1a	3072	1/1	0.84	0.17	94,94,94,94	0
56	MG	1A	3508	1/1	0.84	0.16	86,86,86,86	0
56	MG	1A	3143	1/1	0.84	0.36	84,84,84,84	0
56	MG	1A	3515	1/1	0.84	0.32	63,63,63,63	0
56	MG	1A	3263	1/1	0.84	0.42	78,78,78,78	0
56	MG	1a	3092	1/1	0.84	0.12	85,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	3184	1/1	0.84	0.24	71,71,71,71	0
56	MG	1a	3019	1/1	0.84	0.16	96,96,96,96	0
56	MG	1A	3431	1/1	0.84	0.23	76,76,76,76	0
56	MG	1A	3044	1/1	0.84	0.12	89,89,89,89	0
56	MG	2A	3187	1/1	0.84	0.16	81,81,81,81	0
56	MG	1A	3520	1/1	0.84	0.18	88,88,88,88	0
56	MG	1A	3322	1/1	0.84	0.19	92,92,92,92	0
56	MG	1A	3058	1/1	0.84	0.18	80,80,80,80	0
56	MG	2a	3120	1/1	0.84	0.13	103,103,103,103	0
56	MG	1a	3201	1/1	0.84	0.09	93,93,93,93	0
56	MG	2a	3004	1/1	0.84	0.42	98,98,98,98	0
56	MG	1A	3244	1/1	0.84	0.20	81,81,81,81	0
56	MG	1A	3531	1/1	0.84	0.20	92,92,92,92	0
56	MG	1A	3246	1/1	0.84	0.32	78,78,78,78	0
56	MG	2A	3070	1/1	0.84	0.10	74,74,74,74	0
56	MG	1a	3208	1/1	0.84	0.19	80,80,80,80	0
56	MG	1A	3283	1/1	0.84	0.34	58,58,58,58	0
56	MG	2A	3222	1/1	0.84	0.27	89,89,89,89	0
56	MG	1a	3125	1/1	0.84	0.19	106,106,106,106	0
56	MG	1A	3285	1/1	0.84	0.26	56,56,56,56	0
56	MG	2a	3140	1/1	0.84	0.16	88,88,88,88	0
56	MG	1A	3464	1/1	0.84	0.18	73,73,73,73	0
56	MG	2A	3086	1/1	0.84	0.16	78,78,78,78	0
56	MG	2a	3037	1/1	0.84	0.12	106,106,106,106	0
56	MG	1A	3469	1/1	0.84	0.17	84,84,84,84	0
56	MG	2a	3055	1/1	0.84	0.18	95,95,95,95	0
56	MG	2a	3057	1/1	0.84	0.21	74,74,74,74	0
56	MG	1A	3222	1/1	0.84	0.29	64,64,64,64	0
56	MG	2A	3254	1/1	0.84	0.15	78,78,78,78	0
56	MG	2A	3091	1/1	0.84	0.14	74,74,74,74	0
56	MG	1A	3160	1/1	0.84	0.26	76,76,76,76	0
56	MG	1A	3360	1/1	0.84	0.32	68,68,68,68	0
56	MG	1a	3220	1/1	0.84	0.40	80,80,80,80	0
56	MG	2A	3099	1/1	0.84	0.14	89,89,89,89	0
56	MG	1A	3192	1/1	0.84	0.19	74,74,74,74	0
56	MG	1A	3572	1/1	0.84	0.10	85,85,85,85	0
56	MG	1a	3058	1/1	0.84	0.11	75,75,75,75	0
56	MG	1A	3408	1/1	0.84	0.19	96,96,96,96	0
56	MG	1A	3670	1/1	0.84	0.25	76,76,76,76	0
56	MG	1A	3198	1/1	0.84	0.12	83,83,83,83	0
56	MG	2A	3131	1/1	0.84	0.29	95,95,95,95	0
56	MG	1A	3134	1/1	0.85	0.19	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3017	1/1	0.85	0.25	89,89,89,89	0
56	MG	1A	3279	1/1	0.85	0.31	82,82,82,82	0
56	MG	1A	3417	1/1	0.85	0.22	79,79,79,79	0
56	MG	1A	3199	1/1	0.85	0.19	70,70,70,70	0
56	MG	1a	3234	1/1	0.85	0.19	85,85,85,85	0
56	MG	2a	3028	1/1	0.85	0.16	85,85,85,85	0
56	MG	2a	3033	1/1	0.85	0.13	86,86,86,86	0
56	MG	2a	3034	1/1	0.85	0.16	79,79,79,79	0
56	MG	1A	3202	1/1	0.85	0.30	73,73,73,73	0
56	MG	1a	3237	1/1	0.85	0.15	106,106,106,106	0
56	MG	2a	3049	1/1	0.85	0.23	79,79,79,79	0
56	MG	1A	3328	1/1	0.85	0.17	94,94,94,94	0
56	MG	1A	3098	1/1	0.85	0.12	80,80,80,80	0
56	MG	2A	3188	1/1	0.85	0.18	92,92,92,92	0
56	MG	1a	3117	1/1	0.85	0.24	83,83,83,83	0
56	MG	2A	3193	1/1	0.85	0.12	86,86,86,86	0
56	MG	1A	3331	1/1	0.85	0.19	75,75,75,75	0
56	MG	1A	3661	1/1	0.85	0.22	87,87,87,87	0
56	MG	1A	3059	1/1	0.85	0.12	81,81,81,81	0
56	MG	1A	3024	1/1	0.85	0.15	83,83,83,83	0
56	MG	1A	3116	1/1	0.85	0.14	113,113,113,113	0
56	MG	1a	3128	1/1	0.85	0.26	98,98,98,98	0
56	MG	2A	3111	1/1	0.85	0.08	81,81,81,81	0
56	MG	1a	3055	1/1	0.85	0.10	83,83,83,83	0
56	MG	1A	3346	1/1	0.85	0.36	92,92,92,92	0
56	MG	1A	3302	1/1	0.85	0.30	59,59,59,59	0
56	MG	1A	3355	1/1	0.85	0.12	68,68,68,68	0
56	MG	2A	3229	1/1	0.85	0.17	90,90,90,90	0
56	MG	1A	3308	1/1	0.85	0.14	80,80,80,80	0
56	MG	2A	3234	1/1	0.85	0.09	84,84,84,84	0
56	MG	1A	3404	1/1	0.85	0.27	62,62,62,62	0
56	MG	1A	3608	1/1	0.85	0.10	87,87,87,87	0
56	MG	2a	3086	1/1	0.85	0.18	87,87,87,87	0
56	MG	1A	3536	1/1	0.85	0.20	74,74,74,74	0
56	MG	1A	3405	1/1	0.85	0.25	78,78,78,78	0
56	MG	2A	3253	1/1	0.85	0.13	74,74,74,74	0
56	MG	1a	3022	1/1	0.85	0.16	89,89,89,89	0
56	MG	2A	3039	1/1	0.85	0.15	88,88,88,88	0
56	MG	2a	3170	1/1	0.85	0.15	80,80,80,80	0
56	MG	1a	3160	1/1	0.85	0.26	76,76,76,76	0
56	MG	1A	3194	1/1	0.85	0.08	72,72,72,72	0
56	MG	1A	3197	1/1	0.85	0.33	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3274	1/1	0.85	0.17	92,92,92,92	0
56	MG	1A	3556	1/1	0.85	0.19	81,81,81,81	0
56	MG	1A	3381	1/1	0.86	0.23	68,68,68,68	0
56	MG	1a	3066	1/1	0.86	0.10	101,101,101,101	0
56	MG	1A	3551	1/1	0.86	0.13	97,97,97,97	0
56	MG	1A	3358	1/1	0.86	0.24	83,83,83,83	0
56	MG	2A	3243	1/1	0.86	0.10	88,88,88,88	0
56	MG	1A	3554	1/1	0.86	0.08	109,109,109,109	0
56	MG	1a	3151	1/1	0.86	0.20	80,80,80,80	0
56	MG	1A	3555	1/1	0.86	0.21	80,80,80,80	0
56	MG	1A	3188	1/1	0.86	0.28	91,91,91,91	0
56	MG	2a	3008	1/1	0.86	0.27	85,85,85,85	0
56	MG	2a	3009	1/1	0.86	0.31	84,84,84,84	0
56	MG	1A	3023	1/1	0.86	0.19	88,88,88,88	0
56	MG	1A	3129	1/1	0.86	0.18	93,93,93,93	0
56	MG	2A	3255	1/1	0.86	0.20	91,91,91,91	0
56	MG	1A	3232	1/1	0.86	0.32	52,52,52,52	0
56	MG	2A	3054	1/1	0.86	0.32	89,89,89,89	0
56	MG	1A	3640	1/1	0.86	0.20	81,81,81,81	0
56	MG	2A	3150	1/1	0.86	0.26	88,88,88,88	0
56	MG	1A	3007	1/1	0.86	0.11	91,91,91,91	0
56	MG	2A	3276	1/1	0.86	0.25	82,82,82,82	0
56	MG	1A	3647	1/1	0.86	0.12	93,93,93,93	0
56	MG	1a	3103	1/1	0.86	0.30	79,79,79,79	0
56	MG	2A	3162	1/1	0.86	0.15	77,77,77,77	0
56	MG	2A	3164	1/1	0.86	0.18	82,82,82,82	0
56	MG	2a	3124	1/1	0.86	0.19	83,83,83,83	0
56	MG	2a	3042	1/1	0.86	0.12	82,82,82,82	0
56	MG	2a	3043	1/1	0.86	0.13	70,70,70,70	0
56	MG	2a	3047	1/1	0.86	0.30	83,83,83,83	0
56	MG	1a	3232	1/1	0.86	0.27	76,76,76,76	0
56	MG	2A	3168	1/1	0.86	0.21	98,98,98,98	0
56	MG	1a	3171	1/1	0.86	0.21	86,86,86,86	0
56	MG	2a	3056	1/1	0.86	0.09	97,97,97,97	0
56	MG	1A	3365	1/1	0.86	0.19	75,75,75,75	0
56	MG	2a	3058	1/1	0.86	0.28	93,93,93,93	0
56	MG	2A	3182	1/1	0.86	0.11	81,81,81,81	0
56	MG	2A	3183	1/1	0.86	0.19	80,80,80,80	0
56	MG	1A	3463	1/1	0.86	0.17	75,75,75,75	0
56	MG	2a	3145	1/1	0.86	0.14	90,90,90,90	0
56	MG	1a	3114	1/1	0.86	0.17	86,86,86,86	0
56	MG	1A	3210	1/1	0.86	0.14	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3581	1/1	0.86	0.12	84,84,84,84	0
56	MG	1A	3268	1/1	0.86	0.19	68,68,68,68	0
56	MG	2A	3196	1/1	0.86	0.34	81,81,81,81	0
56	MG	1A	3269	1/1	0.86	0.27	69,69,69,69	0
56	MG	1A	3277	1/1	0.86	0.41	73,73,73,73	0
56	MG	1A	3314	1/1	0.86	0.26	54,54,54,54	0
56	MG	2A	3098	1/1	0.86	0.27	79,79,79,79	0
56	MG	1A	3056	1/1	0.86	0.17	80,80,80,80	0
56	MG	2a	3073	1/1	0.86	0.23	113,113,113,113	0
56	MG	2A	3215	1/1	0.86	0.22	86,86,86,86	0
56	MG	1A	3126	1/1	0.86	0.17	76,76,76,76	0
56	MG	1A	3678	1/1	0.86	0.25	75,75,75,75	0
56	MG	1a	3200	1/1	0.86	0.26	83,83,83,83	0
56	MG	1A	3504	1/1	0.86	0.24	77,77,77,77	0
56	MG	1A	3545	1/1	0.86	0.13	67,67,67,67	0
56	MG	2A	3225	1/1	0.86	0.36	75,75,75,75	0
56	MG	2a	3011	1/1	0.87	0.20	101,101,101,101	0
56	MG	1A	3262	1/1	0.87	0.30	64,64,64,64	0
56	MG	2a	3013	1/1	0.87	0.28	85,85,85,85	0
56	MG	1A	3659	1/1	0.87	0.28	80,80,80,80	0
56	MG	1A	3108	1/1	0.87	0.16	84,84,84,84	0
56	MG	1A	3152	1/1	0.87	0.16	84,84,84,84	0
56	MG	1A	3370	1/1	0.87	0.22	82,82,82,82	0
56	MG	1a	3085	1/1	0.87	0.40	89,89,89,89	0
56	MG	1a	3146	1/1	0.87	0.30	79,79,79,79	0
56	MG	1a	3205	1/1	0.87	0.10	102,102,102,102	0
56	MG	2A	3194	1/1	0.87	0.12	85,85,85,85	0
56	MG	2A	3108	1/1	0.87	0.11	72,72,72,72	0
56	MG	1A	3673	1/1	0.87	0.22	77,77,77,77	0
56	MG	1a	3093	1/1	0.87	0.17	88,88,88,88	0
56	MG	2A	3298	1/1	0.87	0.09	76,76,76,76	0
56	MG	1A	3062	1/1	0.87	0.14	92,92,92,92	0
56	MG	1A	3303	1/1	0.87	0.30	78,78,78,78	0
56	MG	1a	3099	1/1	0.87	0.13	90,90,90,90	0
56	MG	2A	3213	1/1	0.87	0.16	90,90,90,90	0
56	MG	1a	3213	1/1	0.87	0.16	117,117,117,117	0
56	MG	1a	3100	1/1	0.87	0.23	78,78,78,78	0
56	MG	1A	3218	1/1	0.87	0.23	96,96,96,96	0
56	MG	1A	3350	1/1	0.87	0.35	76,76,76,76	0
56	MG	1a	3105	1/1	0.87	0.12	86,86,86,86	0
56	MG	1A	3022	1/1	0.87	0.09	83,83,83,83	0
56	MG	2A	3315	1/1	0.87	0.13	103,103,103,103	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3182	1/1	0.87	0.14	72,72,72,72	0
56	MG	1A	3225	1/1	0.87	0.27	65,65,65,65	0
56	MG	1a	3057	1/1	0.87	0.26	92,92,92,92	0
56	MG	2a	3141	1/1	0.87	0.08	82,82,82,82	0
56	MG	1a	3224	1/1	0.87	0.26	77,77,77,77	0
56	MG	2A	3232	1/1	0.87	0.22	53,53,53,53	0
56	MG	2A	3062	1/1	0.87	0.17	84,84,84,84	0
56	MG	1A	3642	1/1	0.87	0.24	74,74,74,74	0
56	MG	1A	3227	1/1	0.87	0.19	72,72,72,72	0
56	MG	2A	3329	1/1	0.87	0.14	100,100,100,100	0
56	MG	2A	3245	1/1	0.87	0.12	94,94,94,94	0
56	MG	1A	3588	1/1	0.87	0.20	82,82,82,82	0
56	MG	2a	3153	1/1	0.87	0.10	106,106,106,106	0
56	MG	2A	3076	1/1	0.87	0.11	77,77,77,77	0
56	MG	2A	3156	1/1	0.87	0.16	69,69,69,69	0
56	MG	2A	3347	1/1	0.87	0.41	86,86,86,86	0
56	MG	2A	3348	1/1	0.87	0.18	79,79,79,79	0
56	MG	1A	3034	1/1	0.87	0.10	79,79,79,79	0
56	MG	2a	3083	1/1	0.87	0.08	76,76,76,76	0
56	MG	2a	3085	1/1	0.87	0.33	83,83,83,83	0
56	MG	1a	3235	1/1	0.87	0.08	93,93,93,93	0
56	MG	1A	3189	1/1	0.87	0.09	78,78,78,78	0
56	MG	1a	3067	1/1	0.87	0.15	80,80,80,80	0
56	MG	1A	3203	1/1	0.87	0.29	74,74,74,74	0
56	MG	1A	3083	1/1	0.87	0.21	71,71,71,71	0
56	MG	2A	3264	1/1	0.87	0.07	91,91,91,91	0
56	MG	2a	3179	1/1	0.87	0.14	106,106,106,106	0
56	MG	2A	3173	1/1	0.87	0.20	70,70,70,70	0
56	MG	2A	3285	1/1	0.88	0.20	82,82,82,82	0
56	MG	1a	3053	1/1	0.88	0.11	79,79,79,79	0
56	MG	1A	3176	1/1	0.88	0.31	95,95,95,95	0
56	MG	1A	3229	1/1	0.88	0.21	74,74,74,74	0
56	MG	2A	3291	1/1	0.88	0.16	87,87,87,87	0
56	MG	1A	3297	1/1	0.88	0.23	77,77,77,77	0
56	MG	1A	3343	1/1	0.88	0.20	72,72,72,72	0
56	MG	1A	3466	1/1	0.88	0.09	92,92,92,92	0
56	MG	1A	3389	1/1	0.88	0.34	75,75,75,75	0
56	MG	1A	3054	1/1	0.88	0.18	86,86,86,86	0
56	MG	2A	3160	1/1	0.88	0.19	88,88,88,88	0
56	MG	1a	3065	1/1	0.88	0.14	87,87,87,87	0
56	MG	1A	3471	1/1	0.88	0.10	88,88,88,88	0
56	MG	1A	3300	1/1	0.88	0.22	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3397	1/1	0.88	0.23	83,83,83,83	0
56	MG	2A	3169	1/1	0.88	0.11	79,79,79,79	0
56	MG	2A	3310	1/1	0.88	0.14	91,91,91,91	0
56	MG	1A	3200	1/1	0.88	0.27	63,63,63,63	0
56	MG	2A	3032	1/1	0.88	0.11	78,78,78,78	0
56	MG	1A	3014	1/1	0.88	0.23	93,93,93,93	0
56	MG	2A	3177	1/1	0.88	0.21	74,74,74,74	0
56	MG	1A	3575	1/1	0.88	0.26	83,83,83,83	0
56	MG	1A	3503	1/1	0.88	0.20	90,90,90,90	0
56	MG	1A	3356	1/1	0.88	0.09	61,61,61,61	0
56	MG	2a	3094	1/1	0.88	0.17	89,89,89,89	0
56	MG	1A	3183	1/1	0.88	0.13	74,74,74,74	0
56	MG	1a	3002	1/1	0.88	0.15	83,83,83,83	0
56	MG	2A	3189	1/1	0.88	0.27	89,89,89,89	0
56	MG	1a	3188	1/1	0.88	0.22	81,81,81,81	0
56	MG	1a	3087	1/1	0.88	0.15	100,100,100,100	0
56	MG	2A	3327	1/1	0.88	0.07	96,96,96,96	0
56	MG	2a	3102	1/1	0.88	0.17	90,90,90,90	0
56	MG	1a	3005	1/1	0.88	0.16	80,80,80,80	0
56	MG	1A	3184	1/1	0.88	0.13	73,73,73,73	0
56	MG	2A	3066	1/1	0.88	0.13	92,92,92,92	0
56	MG	1a	3094	1/1	0.88	0.15	96,96,96,96	0
56	MG	1A	3207	1/1	0.88	0.17	74,74,74,74	0
56	MG	1a	3014	1/1	0.88	0.20	78,78,78,78	0
56	MG	2A	3075	1/1	0.88	0.17	83,83,83,83	0
56	MG	2a	3116	1/1	0.88	0.13	82,82,82,82	0
56	MG	1A	3021	1/1	0.88	0.24	55,55,55,55	0
56	MG	1A	3590	1/1	0.88	0.21	68,68,68,68	0
56	MG	1A	3362	1/1	0.88	0.22	53,53,53,53	0
56	MG	1A	3012	1/1	0.88	0.17	78,78,78,78	0
56	MG	1a	3104	1/1	0.88	0.26	74,74,74,74	0
56	MG	1A	3418	1/1	0.88	0.20	75,75,75,75	0
56	MG	1A	3270	1/1	0.88	0.30	75,75,75,75	0
56	MG	1a	3108	1/1	0.88	0.07	93,93,93,93	0
56	MG	1a	3109	1/1	0.88	0.12	103,103,103,103	0
56	MG	1A	3276	1/1	0.88	0.30	64,64,64,64	0
56	MG	1a	3024	1/1	0.88	0.10	83,83,83,83	0
56	MG	1a	3026	1/1	0.88	0.34	80,80,80,80	0
56	MG	1A	3141	1/1	0.88	0.12	70,70,70,70	0
56	MG	2A	3238	1/1	0.88	0.36	93,93,93,93	0
56	MG	2a	3019	1/1	0.88	0.18	95,95,95,95	0
56	MG	1A	3433	1/1	0.88	0.17	97,97,97,97	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	3118	1/1	0.88	0.11	101,101,101,101	0
56	MG	2A	3104	1/1	0.88	0.19	98,98,98,98	0
56	MG	2A	3105	1/1	0.88	0.09	71,71,71,71	0
56	MG	1A	3610	1/1	0.88	0.23	79,79,79,79	0
56	MG	1A	3434	1/1	0.88	0.10	81,81,81,81	0
56	MG	2a	3147	1/1	0.88	0.13	89,89,89,89	0
56	MG	1A	3094	1/1	0.88	0.07	63,63,63,63	0
56	MG	2a	3149	1/1	0.88	0.13	74,74,74,74	0
56	MG	1a	3038	1/1	0.88	0.18	88,88,88,88	0
56	MG	2a	3040	1/1	0.88	0.09	78,78,78,78	0
56	MG	1A	3617	1/1	0.88	0.14	69,69,69,69	0
56	MG	1a	3127	1/1	0.88	0.20	82,82,82,82	0
56	MG	1A	3443	1/1	0.88	0.13	82,82,82,82	0
56	MG	1a	3043	1/1	0.88	0.18	95,95,95,95	0
56	MG	2A	3262	1/1	0.88	0.16	84,84,84,84	0
56	MG	2a	3053	1/1	0.88	0.20	90,90,90,90	0
56	MG	2a	3054	1/1	0.88	0.10	90,90,90,90	0
56	MG	1A	3327	1/1	0.88	0.10	78,78,78,78	0
56	MG	1A	3095	1/1	0.88	0.16	81,81,81,81	0
56	MG	2A	3267	1/1	0.88	0.19	93,93,93,93	0
56	MG	1A	3539	1/1	0.88	0.14	85,85,85,85	0
56	MG	1A	3633	1/1	0.88	0.11	75,75,75,75	0
56	MG	1A	3030	1/1	0.88	0.20	69,69,69,69	0
56	MG	2A	3005	1/1	0.88	0.10	84,84,84,84	0
56	MG	2A	3145	1/1	0.88	0.19	77,77,77,77	0
56	MG	1A	3133	1/1	0.88	0.23	76,76,76,76	0
56	MG	1A	3652	1/1	0.89	0.27	86,86,86,86	0
56	MG	1A	3498	1/1	0.89	0.07	85,85,85,85	0
56	MG	1A	3500	1/1	0.89	0.18	86,86,86,86	0
56	MG	1A	3410	1/1	0.89	0.22	77,77,77,77	0
56	MG	2A	3195	1/1	0.89	0.30	84,84,84,84	0
56	MG	1A	3577	1/1	0.89	0.12	94,94,94,94	0
56	MG	1A	3333	1/1	0.89	0.25	73,73,73,73	0
56	MG	2A	3202	1/1	0.89	0.22	88,88,88,88	0
56	MG	2A	3203	1/1	0.89	0.20	87,87,87,87	0
56	MG	1a	3129	1/1	0.89	0.15	88,88,88,88	0
56	MG	1A	3580	1/1	0.89	0.11	74,74,74,74	0
56	MG	1A	3666	1/1	0.89	0.12	92,92,92,92	0
56	MG	1A	3416	1/1	0.89	0.23	82,82,82,82	0
56	MG	2A	3211	1/1	0.89	0.18	81,81,81,81	0
56	MG	1A	3369	1/1	0.89	0.24	86,86,86,86	0
56	MG	1a	3064	1/1	0.89	0.17	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3334	1/1	0.89	0.19	64,64,64,64	0
56	MG	2a	3095	1/1	0.89	0.28	75,75,75,75	0
56	MG	1a	3227	1/1	0.89	0.22	64,64,64,64	0
56	MG	1A	3585	1/1	0.89	0.24	76,76,76,76	0
56	MG	2A	3346	1/1	0.89	0.17	78,78,78,78	0
56	MG	2A	3101	1/1	0.89	0.09	83,83,83,83	0
56	MG	1A	3420	1/1	0.89	0.34	76,76,76,76	0
56	MG	1A	3680	1/1	0.89	0.28	85,85,85,85	0
56	MG	1A	3373	1/1	0.89	0.23	54,54,54,54	0
56	MG	1A	3009	1/1	0.89	0.09	75,75,75,75	0
56	MG	1A	3100	1/1	0.89	0.27	61,61,61,61	0
56	MG	2A	3231	1/1	0.89	0.19	74,74,74,74	0
56	MG	1A	3027	1/1	0.89	0.33	68,68,68,68	0
56	MG	1A	3167	1/1	0.89	0.13	90,90,90,90	0
56	MG	1A	3131	1/1	0.89	0.09	84,84,84,84	0
56	MG	1A	3442	1/1	0.89	0.10	77,77,77,77	0
56	MG	1A	3091	1/1	0.89	0.24	75,75,75,75	0
56	MG	1A	3385	1/1	0.89	0.14	74,74,74,74	0
56	MG	2a	3014	1/1	0.89	0.25	89,89,89,89	0
56	MG	2A	3135	1/1	0.89	0.24	78,78,78,78	0
56	MG	2A	3136	1/1	0.89	0.10	71,71,71,71	0
56	MG	2A	3248	1/1	0.89	0.16	85,85,85,85	0
56	MG	1A	3252	1/1	0.89	0.14	73,73,73,73	0
56	MG	1A	3112	1/1	0.89	0.11	66,66,66,66	0
56	MG	2a	3023	1/1	0.89	0.16	80,80,80,80	0
56	MG	2a	3130	1/1	0.89	0.08	74,74,74,74	0
56	MG	1A	3614	1/1	0.89	0.10	89,89,89,89	0
56	MG	2A	3140	1/1	0.89	0.14	81,81,81,81	0
56	MG	1A	3114	1/1	0.89	0.05	93,93,93,93	0
56	MG	2a	3031	1/1	0.89	0.13	109,109,109,109	0
56	MG	1A	3393	1/1	0.89	0.25	82,82,82,82	0
56	MG	1a	3181	1/1	0.89	0.30	66,66,66,66	0
56	MG	1A	3213	1/1	0.89	0.25	66,66,66,66	0
56	MG	1a	3183	1/1	0.89	0.24	78,78,78,78	0
56	MG	1A	3622	1/1	0.89	0.24	91,91,91,91	0
56	MG	1a	3186	1/1	0.89	0.12	85,85,85,85	0
56	MG	2A	3030	1/1	0.89	0.24	81,81,81,81	0
56	MG	2A	3275	1/1	0.89	0.24	81,81,81,81	0
56	MG	2a	3048	1/1	0.89	0.23	94,94,94,94	0
56	MG	1A	3396	1/1	0.89	0.19	99,99,99,99	0
56	MG	1A	3237	1/1	0.89	0.08	74,74,74,74	0
56	MG	1A	3399	1/1	0.89	0.27	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3157	1/1	0.89	0.21	70,70,70,70	0
56	MG	1a	3190	1/1	0.89	0.10	95,95,95,95	0
56	MG	1A	3467	1/1	0.89	0.19	73,73,73,73	0
56	MG	1A	3287	1/1	0.89	0.32	80,80,80,80	0
56	MG	1a	3196	1/1	0.89	0.25	85,85,85,85	0
56	MG	1A	3238	1/1	0.89	0.11	60,60,60,60	0
56	MG	1a	3041	1/1	0.89	0.16	81,81,81,81	0
56	MG	1A	3291	1/1	0.89	0.29	79,79,79,79	0
56	MG	1A	3293	1/1	0.89	0.08	78,78,78,78	0
56	MG	1A	3329	1/1	0.89	0.28	77,77,77,77	0
56	MG	2a	3167	1/1	0.89	0.11	101,101,101,101	0
56	MG	1A	3124	1/1	0.89	0.13	86,86,86,86	0
56	MG	1a	3047	1/1	0.89	0.15	82,82,82,82	0
56	MG	2A	3181	1/1	0.89	0.14	90,90,90,90	0
56	MG	1a	3119	1/1	0.89	0.22	88,88,88,88	0
56	MG	2A	3071	1/1	0.89	0.22	75,75,75,75	0
56	MG	2A	3073	1/1	0.89	0.17	85,85,85,85	0
56	MG	1a	3120	1/1	0.89	0.12	87,87,87,87	0
56	MG	1A	3115	1/1	0.89	0.08	87,87,87,87	0
56	MG	2A	3297	1/1	0.90	0.28	93,93,93,93	0
56	MG	1a	3195	1/1	0.90	0.17	80,80,80,80	0
56	MG	2A	3175	1/1	0.90	0.22	65,65,65,65	0
56	MG	1A	3527	1/1	0.90	0.17	74,74,74,74	0
56	MG	2A	3061	1/1	0.90	0.21	76,76,76,76	0
56	MG	1A	3075	1/1	0.90	0.24	78,78,78,78	0
56	MG	2A	3304	1/1	0.90	0.15	92,92,92,92	0
56	MG	1A	3298	1/1	0.90	0.34	83,83,83,83	0
56	MG	2a	3075	1/1	0.90	0.10	98,98,98,98	0
56	MG	1a	3199	1/1	0.90	0.17	93,93,93,93	0
56	MG	1A	3079	1/1	0.90	0.08	96,96,96,96	0
56	MG	2a	3078	1/1	0.90	0.35	85,85,85,85	0
56	MG	1a	3048	1/1	0.90	0.24	73,73,73,73	0
56	MG	1A	3039	1/1	0.90	0.17	70,70,70,70	0
56	MG	1A	3671	1/1	0.90	0.21	79,79,79,79	0
56	MG	1A	3594	1/1	0.90	0.21	77,77,77,77	0
56	MG	2A	3192	1/1	0.90	0.19	77,77,77,77	0
56	MG	1A	3084	1/1	0.90	0.29	71,71,71,71	0
56	MG	1A	3142	1/1	0.90	0.09	73,73,73,73	0
56	MG	1A	3273	1/1	0.90	0.18	62,62,62,62	0
56	MG	1A	3344	1/1	0.90	0.27	79,79,79,79	0
56	MG	2A	3082	1/1	0.90	0.08	85,85,85,85	0
56	MG	1A	3304	1/1	0.90	0.23	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	3003	1/1	0.90	0.18	92,92,92,92	0
56	MG	1a	3004	1/1	0.90	0.12	101,101,101,101	0
56	MG	1A	3029	1/1	0.90	0.21	65,65,65,65	0
56	MG	1a	3008	1/1	0.90	0.09	66,66,66,66	0
56	MG	1A	3485	1/1	0.90	0.20	61,61,61,61	0
56	MG	2A	3332	1/1	0.90	0.12	116,116,116,116	0
56	MG	2A	3333	1/1	0.90	0.09	101,101,101,101	0
56	MG	1A	3422	1/1	0.90	0.21	67,67,67,67	0
56	MG	1a	3138	1/1	0.90	0.41	91,91,91,91	0
56	MG	1a	3221	1/1	0.90	0.19	79,79,79,79	0
56	MG	2A	3345	1/1	0.90	0.13	77,77,77,77	0
56	MG	1a	3139	1/1	0.90	0.24	81,81,81,81	0
56	MG	1A	3424	1/1	0.90	0.27	81,81,81,81	0
56	MG	1A	3005	1/1	0.90	0.11	74,74,74,74	0
56	MG	2a	3001	1/1	0.90	0.15	74,74,74,74	0
56	MG	1a	3017	1/1	0.90	0.11	81,81,81,81	0
56	MG	1a	3071	1/1	0.90	0.15	75,75,75,75	0
56	MG	1a	3148	1/1	0.90	0.11	112,112,112,112	0
56	MG	1A	3031	1/1	0.90	0.13	62,62,62,62	0
56	MG	2A	3113	1/1	0.90	0.23	73,73,73,73	0
56	MG	1a	3076	1/1	0.90	0.20	58,58,58,58	0
56	MG	2A	3115	1/1	0.90	0.09	80,80,80,80	0
56	MG	2A	3118	1/1	0.90	0.15	72,72,72,72	0
56	MG	1A	3619	1/1	0.90	0.14	86,86,86,86	0
56	MG	2A	3121	1/1	0.90	0.19	79,79,79,79	0
56	MG	2a	3126	1/1	0.90	0.11	86,86,86,86	0
56	MG	1a	3078	1/1	0.90	0.28	65,65,65,65	0
56	MG	1a	3156	1/1	0.90	0.28	73,73,73,73	0
56	MG	1A	3501	1/1	0.90	0.19	71,71,71,71	0
56	MG	1A	3387	1/1	0.90	0.28	80,80,80,80	0
56	MG	1A	3033	1/1	0.90	0.11	86,86,86,86	0
56	MG	1a	3084	1/1	0.90	0.17	94,94,94,94	0
56	MG	1A	3148	1/1	0.90	0.25	79,79,79,79	0
56	MG	1A	3437	1/1	0.90	0.17	79,79,79,79	0
56	MG	1a	3167	1/1	0.90	0.19	109,109,109,109	0
56	MG	1a	3089	1/1	0.90	0.25	78,78,78,78	0
56	MG	2A	3257	1/1	0.90	0.10	76,76,76,76	0
56	MG	2a	3029	1/1	0.90	0.15	87,87,87,87	0
56	MG	1a	3091	1/1	0.90	0.17	83,83,83,83	0
56	MG	1a	3025	1/1	0.90	0.07	85,85,85,85	0
56	MG	1A	3284	1/1	0.90	0.36	86,86,86,86	0
56	MG	1A	3204	1/1	0.90	0.21	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3576	1/1	0.90	0.19	76,76,76,76	0
56	MG	1a	3097	1/1	0.90	0.10	95,95,95,95	0
56	MG	2A	3266	1/1	0.90	0.08	88,88,88,88	0
56	MG	1A	3258	1/1	0.90	0.28	95,95,95,95	0
56	MG	1a	3032	1/1	0.90	0.11	76,76,76,76	0
56	MG	1A	3326	1/1	0.90	0.19	83,83,83,83	0
56	MG	1a	3035	1/1	0.90	0.12	81,81,81,81	0
56	MG	1A	3026	1/1	0.90	0.12	77,77,77,77	0
56	MG	2a	3051	1/1	0.90	0.28	79,79,79,79	0
56	MG	2a	3052	1/1	0.90	0.22	95,95,95,95	0
56	MG	2A	3154	1/1	0.90	0.17	74,74,74,74	0
56	MG	1A	3151	1/1	0.90	0.20	64,64,64,64	0
56	MG	1A	3006	1/1	0.90	0.19	69,69,69,69	0
56	MG	1A	3521	1/1	0.90	0.10	64,64,64,64	0
56	MG	2A	3286	1/1	0.90	0.07	93,93,93,93	0
56	MG	2a	3169	1/1	0.90	0.08	78,78,78,78	0
56	MG	2A	3038	1/1	0.90	0.06	65,65,65,65	0
56	MG	1A	3121	1/1	0.90	0.08	76,76,76,76	0
56	MG	1a	3192	1/1	0.90	0.14	85,85,85,85	0
56	MG	2a	3174	1/1	0.90	0.20	101,101,101,101	0
56	MG	2A	3045	1/1	0.90	0.21	76,76,76,76	0
56	MG	1a	3193	1/1	0.90	0.22	88,88,88,88	0
56	MG	1A	3586	1/1	0.90	0.30	71,71,71,71	0
56	MG	2A	3053	1/1	0.90	0.13	77,77,77,77	0
56	MG	1A	3228	1/1	0.91	0.13	59,59,59,59	0
56	MG	1A	3672	1/1	0.91	0.27	68,68,68,68	0
56	MG	2A	3057	1/1	0.91	0.12	89,89,89,89	0
56	MG	2A	3172	1/1	0.91	0.20	80,80,80,80	0
56	MG	1A	3164	1/1	0.91	0.22	72,72,72,72	0
56	MG	2A	3174	1/1	0.91	0.14	79,79,79,79	0
56	MG	1a	3059	1/1	0.91	0.06	82,82,82,82	0
56	MG	2a	3074	1/1	0.91	0.18	98,98,98,98	0
56	MG	2A	3305	1/1	0.91	0.12	85,85,85,85	0
56	MG	1a	3204	1/1	0.91	0.12	80,80,80,80	0
56	MG	1A	3038	1/1	0.91	0.13	74,74,74,74	0
56	MG	1A	3255	1/1	0.91	0.18	59,59,59,59	0
56	MG	1A	3206	1/1	0.91	0.17	76,76,76,76	0
56	MG	2A	3072	1/1	0.91	0.15	74,74,74,74	0
56	MG	1A	3679	1/1	0.91	0.09	83,83,83,83	0
56	MG	1a	3131	1/1	0.91	0.10	107,107,107,107	0
56	MG	1a	3132	1/1	0.91	0.07	101,101,101,101	0
56	MG	1A	3320	1/1	0.91	0.11	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3321	1/1	0.91	0.17	62,62,62,62	0
56	MG	1a	3136	1/1	0.91	0.23	84,84,84,84	0
56	MG	1A	3452	1/1	0.91	0.18	97,97,97,97	0
56	MG	1A	3135	1/1	0.91	0.16	59,59,59,59	0
56	MG	1a	3069	1/1	0.91	0.10	81,81,81,81	0
56	MG	1A	3085	1/1	0.91	0.16	92,92,92,92	0
56	MG	1A	3605	1/1	0.91	0.09	93,93,93,93	0
56	MG	1A	3461	1/1	0.91	0.12	59,59,59,59	0
56	MG	1a	3073	1/1	0.91	0.23	78,78,78,78	0
56	MG	1A	3609	1/1	0.91	0.10	74,74,74,74	0
56	MG	1a	3150	1/1	0.91	0.14	83,83,83,83	0
56	MG	2A	3206	1/1	0.91	0.13	73,73,73,73	0
56	MG	1A	3260	1/1	0.91	0.34	62,62,62,62	0
56	MG	2A	3096	1/1	0.91	0.07	90,90,90,90	0
56	MG	1A	3236	1/1	0.91	0.42	60,60,60,60	0
56	MG	1a	3079	1/1	0.91	0.18	73,73,73,73	0
56	MG	1A	3070	1/1	0.91	0.10	52,52,52,52	0
56	MG	1A	3088	1/1	0.91	0.08	71,71,71,71	0
56	MG	2A	3217	1/1	0.91	0.08	82,82,82,82	0
56	MG	1a	3158	1/1	0.91	0.36	81,81,81,81	0
56	MG	1A	3264	1/1	0.91	0.35	67,67,67,67	0
56	MG	1A	3043	1/1	0.91	0.14	74,74,74,74	0
56	MG	2A	3109	1/1	0.91	0.11	93,93,93,93	0
56	MG	2A	3001	1/1	0.91	0.19	75,75,75,75	0
56	MG	2A	3112	1/1	0.91	0.21	89,89,89,89	0
56	MG	1A	3332	1/1	0.91	0.35	77,77,77,77	0
56	MG	2A	3004	1/1	0.91	0.08	91,91,91,91	0
56	MG	1A	3153	1/1	0.91	0.14	72,72,72,72	0
56	MG	2A	3116	1/1	0.91	0.10	91,91,91,91	0
56	MG	1A	3480	1/1	0.91	0.08	104,104,104,104	0
56	MG	2A	3237	1/1	0.91	0.10	92,92,92,92	0
56	MG	2A	3008	1/1	0.91	0.17	79,79,79,79	0
56	MG	1A	3035	1/1	0.91	0.09	70,70,70,70	0
56	MG	2A	3124	1/1	0.91	0.18	86,86,86,86	0
56	MG	1A	3221	1/1	0.91	0.37	79,79,79,79	0
56	MG	1A	3632	1/1	0.91	0.16	63,63,63,63	0
56	MG	2A	3129	1/1	0.91	0.09	73,73,73,73	0
56	MG	2a	3021	1/1	0.91	0.11	101,101,101,101	0
56	MG	2a	3137	1/1	0.91	0.18	81,81,81,81	0
56	MG	1A	3558	1/1	0.91	0.14	97,97,97,97	0
56	MG	1A	3634	1/1	0.91	0.18	83,83,83,83	0
56	MG	1A	3421	1/1	0.91	0.26	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3637	1/1	0.91	0.14	100,100,100,100	0
56	MG	1A	3493	1/1	0.91	0.08	69,69,69,69	0
56	MG	1A	3113	1/1	0.91	0.10	75,75,75,75	0
56	MG	1A	3645	1/1	0.91	0.22	82,82,82,82	0
56	MG	1A	3566	1/1	0.91	0.07	93,93,93,93	0
56	MG	1A	3423	1/1	0.91	0.19	78,78,78,78	0
56	MG	1A	3002	1/1	0.91	0.07	72,72,72,72	0
56	MG	1A	3650	1/1	0.91	0.13	90,90,90,90	0
56	MG	1A	3426	1/1	0.91	0.33	72,72,72,72	0
56	MG	1A	3272	1/1	0.91	0.20	49,49,49,49	0
56	MG	2a	3044	1/1	0.91	0.19	86,86,86,86	0
56	MG	1A	3383	1/1	0.91	0.25	69,69,69,69	0
56	MG	1A	3654	1/1	0.91	0.13	89,89,89,89	0
56	MG	2a	3155	1/1	0.91	0.14	84,84,84,84	0
56	MG	2A	3037	1/1	0.91	0.09	75,75,75,75	0
56	MG	1A	3430	1/1	0.91	0.17	61,61,61,61	0
56	MG	2a	3158	1/1	0.91	0.08	116,116,116,116	0
56	MG	2A	3151	1/1	0.91	0.05	78,78,78,78	0
56	MG	2A	3278	1/1	0.91	0.15	89,89,89,89	0
56	MG	1A	3185	1/1	0.91	0.10	80,80,80,80	0
56	MG	2A	3040	1/1	0.91	0.17	82,82,82,82	0
56	MG	2A	3042	1/1	0.91	0.15	89,89,89,89	0
56	MG	1A	3274	1/1	0.91	0.14	78,78,78,78	0
56	MG	1A	3347	1/1	0.91	0.22	70,70,70,70	0
56	MG	2A	3158	1/1	0.91	0.18	78,78,78,78	0
56	MG	2A	3046	1/1	0.91	0.21	68,68,68,68	0
56	MG	1A	3514	1/1	0.91	0.09	94,94,94,94	0
56	MG	1A	3311	1/1	0.91	0.30	61,61,61,61	0
56	MG	2A	3050	1/1	0.91	0.13	81,81,81,81	0
56	MG	2a	3177	1/1	0.91	0.26	86,86,86,86	0
56	MG	2A	3165	1/1	0.91	0.13	77,77,77,77	0
56	MG	2A	3295	1/1	0.91	0.08	91,91,91,91	0
56	MG	1A	3440	1/1	0.91	0.20	77,77,77,77	0
56	MG	2a	3181	1/1	0.91	0.22	90,90,90,90	0
56	MG	2a	3183	1/1	0.91	0.06	98,98,98,98	0
56	MG	1A	3082	1/1	0.92	0.13	69,69,69,69	0
56	MG	2A	3197	1/1	0.92	0.12	78,78,78,78	0
56	MG	2A	3199	1/1	0.92	0.23	74,74,74,74	0
56	MG	1A	3532	1/1	0.92	0.10	88,88,88,88	0
56	MG	2A	3002	1/1	0.92	0.23	81,81,81,81	0
56	MG	1A	3451	1/1	0.92	0.06	85,85,85,85	0
56	MG	2a	3081	1/1	0.92	0.06	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3613	1/1	0.92	0.11	64,64,64,64	0
56	MG	1a	3164	1/1	0.92	0.16	81,81,81,81	0
56	MG	2A	3106	1/1	0.92	0.07	73,73,73,73	0
56	MG	1A	3092	1/1	0.92	0.11	70,70,70,70	0
56	MG	1A	3280	1/1	0.92	0.26	77,77,77,77	0
56	MG	2A	3328	1/1	0.92	0.10	90,90,90,90	0
56	MG	1A	3537	1/1	0.92	0.47	113,113,113,113	0
56	MG	1A	3173	1/1	0.92	0.23	74,74,74,74	0
56	MG	1A	3208	1/1	0.92	0.15	74,74,74,74	0
56	MG	1A	3543	1/1	0.92	0.17	86,86,86,86	0
56	MG	1A	3175	1/1	0.92	0.21	75,75,75,75	0
56	MG	1A	3286	1/1	0.92	0.20	96,96,96,96	0
56	MG	1a	3176	1/1	0.92	0.11	84,84,84,84	0
56	MG	2A	3023	1/1	0.92	0.18	71,71,71,71	0
56	MG	1a	3179	1/1	0.92	0.19	90,90,90,90	0
56	MG	2A	3123	1/1	0.92	0.20	81,81,81,81	0
56	MG	1A	3550	1/1	0.92	0.15	101,101,101,101	0
56	MG	1a	3028	1/1	0.92	0.08	76,76,76,76	0
56	MG	1A	3630	1/1	0.92	0.17	77,77,77,77	0
56	MG	2a	3003	1/1	0.92	0.16	69,69,69,69	0
56	MG	2A	3128	1/1	0.92	0.14	54,54,54,54	0
56	MG	1A	3323	1/1	0.92	0.26	81,81,81,81	0
56	MG	1A	3032	1/1	0.92	0.18	75,75,75,75	0
56	MG	1a	3102	1/1	0.92	0.18	72,72,72,72	0
56	MG	2a	3109	1/1	0.92	0.12	82,82,82,82	0
56	MG	1A	3178	1/1	0.92	0.09	82,82,82,82	0
56	MG	1a	3034	1/1	0.92	0.15	73,73,73,73	0
56	MG	1A	3195	1/1	0.92	0.08	78,78,78,78	0
56	MG	1A	3217	1/1	0.92	0.18	60,60,60,60	0
56	MG	2A	3036	1/1	0.92	0.19	87,87,87,87	0
56	MG	1A	3474	1/1	0.92	0.27	74,74,74,74	0
56	MG	1A	3138	1/1	0.92	0.20	82,82,82,82	0
56	MG	1A	3001	1/1	0.92	0.09	70,70,70,70	0
56	MG	1A	3419	1/1	0.92	0.28	87,87,87,87	0
56	MG	1a	3042	1/1	0.92	0.06	74,74,74,74	0
56	MG	2A	3043	1/1	0.92	0.16	82,82,82,82	0
56	MG	1A	3372	1/1	0.92	0.23	63,63,63,63	0
56	MG	2a	3128	1/1	0.92	0.22	74,74,74,74	0
56	MG	1A	3076	1/1	0.92	0.12	54,54,54,54	0
56	MG	2a	3022	1/1	0.92	0.15	83,83,83,83	0
56	MG	1A	3490	1/1	0.92	0.18	79,79,79,79	0
56	MG	2a	3133	1/1	0.92	0.07	92,92,92,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3243	1/1	0.92	0.11	81,81,81,81	0
56	MG	2a	3025	1/1	0.92	0.07	86,86,86,86	0
56	MG	1A	3077	1/1	0.92	0.18	93,93,93,93	0
56	MG	1A	3245	1/1	0.92	0.35	56,56,56,56	0
56	MG	2A	3051	1/1	0.92	0.15	80,80,80,80	0
56	MG	1A	3425	1/1	0.92	0.11	62,62,62,62	0
56	MG	1A	3655	1/1	0.92	0.24	67,67,67,67	0
56	MG	1A	3223	1/1	0.92	0.17	59,59,59,59	0
56	MG	2a	3035	1/1	0.92	0.11	94,94,94,94	0
56	MG	1A	3427	1/1	0.92	0.11	78,78,78,78	0
56	MG	2A	3058	1/1	0.92	0.16	78,78,78,78	0
56	MG	1A	3379	1/1	0.92	0.26	55,55,55,55	0
56	MG	2A	3161	1/1	0.92	0.11	69,69,69,69	0
56	MG	1A	3582	1/1	0.92	0.08	73,73,73,73	0
56	MG	1A	3662	1/1	0.92	0.10	90,90,90,90	0
56	MG	1A	3047	1/1	0.92	0.20	68,68,68,68	0
56	MG	2A	3283	1/1	0.92	0.11	84,84,84,84	0
56	MG	2a	3151	1/1	0.92	0.07	111,111,111,111	0
56	MG	1A	3226	1/1	0.92	0.34	62,62,62,62	0
56	MG	1A	3342	1/1	0.92	0.19	64,64,64,64	0
56	MG	1a	3061	1/1	0.92	0.08	79,79,79,79	0
56	MG	2A	3288	1/1	0.92	0.15	71,71,71,71	0
56	MG	1A	3512	1/1	0.92	0.17	82,82,82,82	0
56	MG	1A	3384	1/1	0.92	0.33	75,75,75,75	0
56	MG	1A	3306	1/1	0.92	0.34	82,82,82,82	0
56	MG	2a	3160	1/1	0.92	0.18	104,104,104,104	0
56	MG	1A	3436	1/1	0.92	0.21	68,68,68,68	0
56	MG	1A	3307	1/1	0.92	0.15	60,60,60,60	0
56	MG	2a	3163	1/1	0.92	0.19	103,103,103,103	0
56	MG	1a	3142	1/1	0.92	0.20	85,85,85,85	0
56	MG	1A	3439	1/1	0.92	0.23	84,84,84,84	0
56	MG	1A	3275	1/1	0.92	0.26	61,61,61,61	0
56	MG	1A	3186	1/1	0.92	0.22	95,95,95,95	0
56	MG	2A	3085	1/1	0.92	0.32	101,101,101,101	0
56	MG	1A	3596	1/1	0.92	0.13	81,81,81,81	0
56	MG	2A	3185	1/1	0.92	0.13	76,76,76,76	0
56	MG	2A	3186	1/1	0.92	0.15	79,79,79,79	0
56	MG	1A	3312	1/1	0.92	0.29	62,62,62,62	0
56	MG	1A	3391	1/1	0.92	0.23	80,80,80,80	0
56	MG	1A	3351	1/1	0.92	0.22	58,58,58,58	0
56	MG	1a	3007	1/1	0.92	0.23	67,67,67,67	0
56	MG	1A	3602	1/1	0.92	0.21	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3187	1/1	0.92	0.22	75,75,75,75	0
56	MG	1A	3353	1/1	0.92	0.13	66,66,66,66	0
56	MG	2A	3097	1/1	0.92	0.23	91,91,91,91	0
56	MG	1A	3669	1/1	0.93	0.11	79,79,79,79	0
56	MG	1A	3496	1/1	0.93	0.22	72,72,72,72	0
56	MG	1A	3180	1/1	0.93	0.27	93,93,93,93	0
56	MG	1A	3067	1/1	0.93	0.14	65,65,65,65	0
56	MG	1a	3110	1/1	0.93	0.12	90,90,90,90	0
56	MG	1A	3146	1/1	0.93	0.06	62,62,62,62	0
56	MG	1A	3078	1/1	0.93	0.12	79,79,79,79	0
56	MG	1A	3048	1/1	0.93	0.14	74,74,74,74	0
56	MG	2A	3171	1/1	0.93	0.08	86,86,86,86	0
56	MG	2A	3010	1/1	0.93	0.07	85,85,85,85	0
56	MG	1A	3411	1/1	0.93	0.28	66,66,66,66	0
56	MG	2A	3273	1/1	0.93	0.14	86,86,86,86	0
56	MG	1A	3412	1/1	0.93	0.22	79,79,79,79	0
56	MG	1a	3185	1/1	0.93	0.08	90,90,90,90	0
56	MG	2A	3015	1/1	0.93	0.09	84,84,84,84	0
56	MG	2A	3016	1/1	0.93	0.07	82,82,82,82	0
56	MG	1A	3616	1/1	0.93	0.16	84,84,84,84	0
56	MG	1A	3149	1/1	0.93	0.25	76,76,76,76	0
56	MG	1A	3448	1/1	0.93	0.11	78,78,78,78	0
56	MG	1A	3510	1/1	0.93	0.19	64,64,64,64	0
56	MG	1A	3563	1/1	0.93	0.11	97,97,97,97	0
56	MG	2A	3284	1/1	0.93	0.11	79,79,79,79	0
56	MG	1a	3123	1/1	0.93	0.05	72,72,72,72	0
56	MG	2a	3027	1/1	0.93	0.06	83,83,83,83	0
56	MG	1A	3511	1/1	0.93	0.11	62,62,62,62	0
56	MG	1A	3625	1/1	0.93	0.21	66,66,66,66	0
56	MG	1A	3415	1/1	0.93	0.18	78,78,78,78	0
56	MG	2a	3032	1/1	0.93	0.05	79,79,79,79	0
56	MG	1A	3074	1/1	0.93	0.09	81,81,81,81	0
56	MG	1A	3055	1/1	0.93	0.09	79,79,79,79	0
56	MG	1A	3382	1/1	0.93	0.28	60,60,60,60	0
56	MG	1A	3066	1/1	0.93	0.13	78,78,78,78	0
56	MG	1A	3110	1/1	0.93	0.17	82,82,82,82	0
56	MG	1A	3281	1/1	0.93	0.16	64,64,64,64	0
56	MG	1A	3282	1/1	0.93	0.28	63,63,63,63	0
56	MG	1A	3639	1/1	0.93	0.20	67,67,67,67	0
56	MG	1a	3135	1/1	0.93	0.13	82,82,82,82	0
56	MG	1a	3074	1/1	0.93	0.14	88,88,88,88	0
56	MG	1A	3174	1/1	0.93	0.08	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3524	1/1	0.93	0.16	84,84,84,84	0
56	MG	1A	3643	1/1	0.93	0.16	86,86,86,86	0
56	MG	1A	3644	1/1	0.93	0.16	65,65,65,65	0
56	MG	1A	3156	1/1	0.93	0.21	66,66,66,66	0
56	MG	1a	3144	1/1	0.93	0.22	71,71,71,71	0
56	MG	2A	3132	1/1	0.93	0.13	97,97,97,97	0
56	MG	2A	3212	1/1	0.93	0.10	83,83,83,83	0
56	MG	1A	3136	1/1	0.93	0.08	78,78,78,78	0
56	MG	1A	3159	1/1	0.93	0.07	69,69,69,69	0
56	MG	2A	3312	1/1	0.93	0.09	74,74,74,74	0
56	MG	1A	3392	1/1	0.93	0.28	80,80,80,80	0
56	MG	1A	3649	1/1	0.93	0.06	86,86,86,86	0
56	MG	2A	3052	1/1	0.93	0.07	72,72,72,72	0
56	MG	1a	3086	1/1	0.93	0.12	76,76,76,76	0
56	MG	1A	3249	1/1	0.93	0.29	77,77,77,77	0
56	MG	1A	3366	1/1	0.93	0.30	72,72,72,72	0
56	MG	2a	3065	1/1	0.93	0.12	83,83,83,83	0
56	MG	2A	3223	1/1	0.93	0.12	72,72,72,72	0
56	MG	1A	3289	1/1	0.93	0.15	92,92,92,92	0
56	MG	2A	3144	1/1	0.93	0.09	75,75,75,75	0
56	MG	1A	3315	1/1	0.93	0.17	57,57,57,57	0
56	MG	2A	3060	1/1	0.93	0.07	79,79,79,79	0
56	MG	1A	3341	1/1	0.93	0.15	70,70,70,70	0
56	MG	1a	3037	1/1	0.93	0.17	82,82,82,82	0
56	MG	1A	3212	1/1	0.93	0.25	54,54,54,54	0
56	MG	1A	3488	1/1	0.93	0.13	80,80,80,80	0
56	MG	2a	3165	1/1	0.93	0.08	116,116,116,116	0
56	MG	2A	3331	1/1	0.93	0.20	67,67,67,67	0
56	MG	1a	3229	1/1	0.93	0.21	85,85,85,85	0
56	MG	2A	3240	1/1	0.93	0.12	84,84,84,84	0
56	MG	2A	3334	1/1	0.93	0.15	105,105,105,105	0
56	MG	2A	3339	1/1	0.93	0.15	92,92,92,92	0
56	MG	2A	3242	1/1	0.93	0.14	70,70,70,70	0
56	MG	1a	3231	1/1	0.93	0.20	82,82,82,82	0
56	MG	1A	3371	1/1	0.93	0.30	52,52,52,52	0
56	MG	1A	3492	1/1	0.93	0.11	77,77,77,77	0
56	MG	2a	3084	1/1	0.93	0.19	78,78,78,78	0
56	MG	1A	3317	1/1	0.93	0.25	56,56,56,56	0
56	MG	1A	3547	1/1	0.93	0.12	71,71,71,71	0
56	MG	1A	3548	1/1	0.93	0.17	91,91,91,91	0
56	MG	1A	3665	1/1	0.93	0.17	74,74,74,74	0
56	MG	1A	3603	1/1	0.93	0.09	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	ZN	24	501	1/1	0.93	0.13	168,168,168,168	0
56	MG	1A	3450	1/1	0.94	0.15	76,76,76,76	0
56	MG	1A	3589	1/1	0.94	0.08	86,86,86,86	0
56	MG	2a	3016	1/1	0.94	0.11	91,91,91,91	0
56	MG	1A	3375	1/1	0.94	0.13	62,62,62,62	0
56	MG	2A	3191	1/1	0.94	0.13	74,74,74,74	0
56	MG	1A	3541	1/1	0.94	0.16	72,72,72,72	0
56	MG	1A	3542	1/1	0.94	0.06	77,77,77,77	0
56	MG	1A	3398	1/1	0.94	0.14	67,67,67,67	0
56	MG	2A	3127	1/1	0.94	0.14	78,78,78,78	0
56	MG	1A	3453	1/1	0.94	0.07	84,84,84,84	0
56	MG	1A	3546	1/1	0.94	0.10	69,69,69,69	0
56	MG	2A	3198	1/1	0.94	0.06	83,83,83,83	0
56	MG	1A	3455	1/1	0.94	0.08	63,63,63,63	0
56	MG	2a	3108	1/1	0.94	0.05	98,98,98,98	0
56	MG	2A	3200	1/1	0.94	0.09	86,86,86,86	0
56	MG	2a	3110	1/1	0.94	0.12	80,80,80,80	0
56	MG	1A	3011	1/1	0.94	0.07	65,65,65,65	0
56	MG	1A	3357	1/1	0.94	0.39	76,76,76,76	0
56	MG	2a	3030	1/1	0.94	0.19	77,77,77,77	0
56	MG	1a	3075	1/1	0.94	0.19	72,72,72,72	0
56	MG	2a	3118	1/1	0.94	0.05	115,115,115,115	0
56	MG	1A	3459	1/1	0.94	0.07	62,62,62,62	0
56	MG	1A	3460	1/1	0.94	0.10	55,55,55,55	0
56	MG	1A	3037	1/1	0.94	0.12	83,83,83,83	0
56	MG	2A	3208	1/1	0.94	0.16	71,71,71,71	0
56	MG	2A	3006	1/1	0.94	0.11	71,71,71,71	0
56	MG	1A	3101	1/1	0.94	0.15	86,86,86,86	0
56	MG	2a	3125	1/1	0.94	0.12	75,75,75,75	0
56	MG	2a	3038	1/1	0.94	0.13	101,101,101,101	0
56	MG	2a	3039	1/1	0.94	0.09	89,89,89,89	0
56	MG	1A	3102	1/1	0.94	0.09	78,78,78,78	0
56	MG	1A	3406	1/1	0.94	0.18	59,59,59,59	0
56	MG	1A	3166	1/1	0.94	0.24	77,77,77,77	0
56	MG	2a	3131	1/1	0.94	0.07	84,84,84,84	0
56	MG	1A	3468	1/1	0.94	0.15	83,83,83,83	0
56	MG	2a	3045	1/1	0.94	0.07	102,102,102,102	0
56	MG	1A	3288	1/1	0.94	0.07	70,70,70,70	0
56	MG	1A	3086	1/1	0.94	0.21	70,70,70,70	0
56	MG	1A	3069	1/1	0.94	0.22	67,67,67,67	0
56	MG	1a	3088	1/1	0.94	0.08	96,96,96,96	0
56	MG	2A	3081	1/1	0.94	0.19	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3473	1/1	0.94	0.09	86,86,86,86	0
56	MG	2A	3018	1/1	0.94	0.07	85,85,85,85	0
56	MG	2A	3224	1/1	0.94	0.20	62,62,62,62	0
56	MG	1A	3325	1/1	0.94	0.14	69,69,69,69	0
56	MG	2A	3021	1/1	0.94	0.10	98,98,98,98	0
56	MG	2A	3228	1/1	0.94	0.13	68,68,68,68	0
56	MG	2A	3320	1/1	0.94	0.07	79,79,79,79	0
56	MG	1A	3522	1/1	0.94	0.10	69,69,69,69	0
56	MG	2A	3155	1/1	0.94	0.20	66,66,66,66	0
56	MG	2A	3089	1/1	0.94	0.05	82,82,82,82	0
56	MG	1A	3621	1/1	0.94	0.13	69,69,69,69	0
56	MG	1A	3523	1/1	0.94	0.10	96,96,96,96	0
56	MG	1A	3574	1/1	0.94	0.18	77,77,77,77	0
56	MG	1A	3624	1/1	0.94	0.17	64,64,64,64	0
56	MG	1a	3206	1/1	0.94	0.06	89,89,89,89	0
56	MG	1A	3169	1/1	0.94	0.30	84,84,84,84	0
56	MG	2A	3163	1/1	0.94	0.15	79,79,79,79	0
56	MG	1A	3292	1/1	0.94	0.07	50,50,50,50	0
56	MG	1A	3388	1/1	0.94	0.40	69,69,69,69	0
56	MG	1A	3482	1/1	0.94	0.17	75,75,75,75	0
56	MG	1A	3349	1/1	0.94	0.09	72,72,72,72	0
56	MG	1A	3224	1/1	0.94	0.17	65,65,65,65	0
56	MG	2A	3102	1/1	0.94	0.06	72,72,72,72	0
56	MG	1A	3118	1/1	0.94	0.11	60,60,60,60	0
56	MG	1a	3159	1/1	0.94	0.21	72,72,72,72	0
56	MG	1a	3056	1/1	0.94	0.15	83,83,83,83	0
56	MG	1A	3296	1/1	0.94	0.16	76,76,76,76	0
56	MG	1A	3127	1/1	0.94	0.24	72,72,72,72	0
56	MG	2A	3350	1/1	0.94	0.17	70,70,70,70	0
56	MG	2A	3110	1/1	0.94	0.12	79,79,79,79	0
56	MG	1A	3638	1/1	0.94	0.10	80,80,80,80	0
56	MG	2A	3178	1/1	0.94	0.16	63,63,63,63	0
56	MG	2a	3172	1/1	0.94	0.11	89,89,89,89	0
56	MG	2A	3263	1/1	0.94	0.07	86,86,86,86	0
56	MG	2A	3179	1/1	0.94	0.13	74,74,74,74	0
56	MG	2A	3180	1/1	0.94	0.08	74,74,74,74	0
56	MG	2A	3041	1/1	0.94	0.08	69,69,69,69	0
56	MG	1a	3012	1/1	0.94	0.07	93,93,93,93	0
56	MG	1A	3354	1/1	0.94	0.11	83,83,83,83	0
56	MG	1a	3112	1/1	0.94	0.18	70,70,70,70	0
56	MG	1A	3060	1/1	0.94	0.17	75,75,75,75	0
56	MG	2A	3117	1/1	0.94	0.12	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3538	1/1	0.94	0.12	87,87,87,87	0
56	MG	1A	3509	1/1	0.95	0.13	75,75,75,75	0
56	MG	1a	3178	1/1	0.95	0.13	81,81,81,81	0
56	MG	1A	3310	1/1	0.95	0.36	76,76,76,76	0
56	MG	1A	3597	1/1	0.95	0.07	87,87,87,87	0
56	MG	2A	3064	1/1	0.95	0.26	82,82,82,82	0
56	MG	1A	3598	1/1	0.95	0.18	74,74,74,74	0
56	MG	1A	3050	1/1	0.95	0.09	76,76,76,76	0
56	MG	1A	3096	1/1	0.95	0.05	90,90,90,90	0
56	MG	1A	3155	1/1	0.95	0.21	65,65,65,65	0
56	MG	2A	3292	1/1	0.95	0.07	91,91,91,91	0
56	MG	2a	3111	1/1	0.95	0.09	86,86,86,86	0
56	MG	2A	3207	1/1	0.95	0.08	68,68,68,68	0
56	MG	1A	3335	1/1	0.95	0.14	66,66,66,66	0
56	MG	1A	3097	1/1	0.95	0.13	94,94,94,94	0
56	MG	1A	3472	1/1	0.95	0.10	72,72,72,72	0
56	MG	2a	3117	1/1	0.95	0.11	92,92,92,92	0
56	MG	1A	3010	1/1	0.95	0.16	65,65,65,65	0
56	MG	1A	3057	1/1	0.95	0.14	79,79,79,79	0
56	MG	2A	3077	1/1	0.95	0.11	77,77,77,77	0
56	MG	2A	3214	1/1	0.95	0.11	92,92,92,92	0
56	MG	1A	3477	1/1	0.95	0.11	56,56,56,56	0
56	MG	1A	3251	1/1	0.95	0.09	69,69,69,69	0
56	MG	1A	3564	1/1	0.95	0.05	97,97,97,97	0
56	MG	2A	3218	1/1	0.95	0.15	83,83,83,83	0
56	MG	1a	3081	1/1	0.95	0.16	81,81,81,81	0
56	MG	1A	3071	1/1	0.95	0.22	74,74,74,74	0
56	MG	1A	3660	1/1	0.95	0.18	65,65,65,65	0
56	MG	1A	3080	1/1	0.95	0.06	66,66,66,66	0
56	MG	1A	3196	1/1	0.95	0.26	81,81,81,81	0
56	MG	1A	3090	1/1	0.95	0.11	84,84,84,84	0
56	MG	2A	3020	1/1	0.95	0.23	69,69,69,69	0
56	MG	1A	3664	1/1	0.95	0.15	82,82,82,82	0
56	MG	2A	3227	1/1	0.95	0.12	81,81,81,81	0
56	MG	1A	3216	1/1	0.95	0.24	50,50,50,50	0
56	MG	1A	3348	1/1	0.95	0.20	74,74,74,74	0
56	MG	2A	3093	1/1	0.95	0.07	71,71,71,71	0
56	MG	1A	3668	1/1	0.95	0.07	82,82,82,82	0
56	MG	1A	3620	1/1	0.95	0.24	91,91,91,91	0
56	MG	2A	3233	1/1	0.95	0.16	71,71,71,71	0
56	MG	1A	3489	1/1	0.95	0.09	78,78,78,78	0
56	MG	1A	3081	1/1	0.95	0.12	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3491	1/1	0.95	0.27	84,84,84,84	0
56	MG	2A	3167	1/1	0.95	0.09	87,87,87,87	0
56	MG	2A	3241	1/1	0.95	0.09	89,89,89,89	0
56	MG	1A	3259	1/1	0.95	0.20	54,54,54,54	0
56	MG	1A	3106	1/1	0.95	0.08	63,63,63,63	0
56	MG	1A	3495	1/1	0.95	0.16	66,66,66,66	0
56	MG	1a	3153	1/1	0.95	0.12	84,84,84,84	0
56	MG	1A	3677	1/1	0.95	0.19	55,55,55,55	0
56	MG	1a	3212	1/1	0.95	0.09	71,71,71,71	0
56	MG	2A	3335	1/1	0.95	0.13	100,100,100,100	0
56	MG	2A	3338	1/1	0.95	0.07	97,97,97,97	0
56	MG	1a	3155	1/1	0.95	0.17	74,74,74,74	0
56	MG	2A	3107	1/1	0.95	0.07	92,92,92,92	0
56	MG	1A	3627	1/1	0.95	0.16	60,60,60,60	0
56	MG	1A	3628	1/1	0.95	0.14	56,56,56,56	0
56	MG	1A	3454	1/1	0.95	0.13	66,66,66,66	0
56	MG	2a	3159	1/1	0.95	0.05	92,92,92,92	0
56	MG	1a	3001	1/1	0.95	0.12	90,90,90,90	0
56	MG	1A	3003	1/1	0.95	0.07	60,60,60,60	0
56	MG	2A	3259	1/1	0.95	0.11	76,76,76,76	0
56	MG	1a	3161	1/1	0.95	0.10	82,82,82,82	0
56	MG	1a	3106	1/1	0.95	0.05	98,98,98,98	0
56	MG	1A	3220	1/1	0.95	0.21	71,71,71,71	0
56	MG	1A	3201	1/1	0.95	0.19	68,68,68,68	0
56	MG	1A	3402	1/1	0.95	0.12	51,51,51,51	0
56	MG	1a	3225	1/1	0.95	0.07	85,85,85,85	0
56	MG	1A	3403	1/1	0.95	0.30	59,59,59,59	0
56	MG	2A	3049	1/1	0.95	0.07	81,81,81,81	0
56	MG	2A	3270	1/1	0.95	0.15	80,80,80,80	0
56	MG	2A	3271	1/1	0.95	0.11	83,83,83,83	0
56	MG	2A	3272	1/1	0.95	0.07	89,89,89,89	0
56	MG	2A	3122	1/1	0.95	0.09	86,86,86,86	0
56	MG	2a	3175	1/1	0.95	0.08	76,76,76,76	0
56	MG	1A	3109	1/1	0.95	0.06	78,78,78,78	0
56	MG	1a	3228	1/1	0.95	0.17	72,72,72,72	0
56	MG	1A	3004	1/1	0.95	0.05	56,56,56,56	0
56	MG	1A	3432	1/1	0.95	0.36	57,57,57,57	0
56	MG	1A	3507	1/1	0.95	0.15	92,92,92,92	0
56	MG	1A	3641	1/1	0.95	0.15	68,68,68,68	0
56	MG	2a	3182	1/1	0.95	0.07	106,106,106,106	0
56	MG	2A	3056	1/1	0.95	0.10	73,73,73,73	0
57	ZN	14	501	1/1	0.95	0.11	162,162,162,162	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3465	1/1	0.95	0.05	80,80,80,80	0
56	MG	2A	3306	1/1	0.96	0.07	74,74,74,74	0
56	MG	2A	3250	1/1	0.96	0.14	65,65,65,65	0
56	MG	2A	3252	1/1	0.96	0.10	73,73,73,73	0
56	MG	1A	3604	1/1	0.96	0.12	67,67,67,67	0
56	MG	1a	3175	1/1	0.96	0.05	87,87,87,87	0
56	MG	1A	3209	1/1	0.96	0.12	56,56,56,56	0
56	MG	2A	3256	1/1	0.96	0.08	98,98,98,98	0
56	MG	1A	3606	1/1	0.96	0.15	71,71,71,71	0
56	MG	1a	3137	1/1	0.96	0.17	79,79,79,79	0
56	MG	2A	3065	1/1	0.96	0.24	88,88,88,88	0
56	MG	1A	3607	1/1	0.96	0.12	58,58,58,58	0
56	MG	2A	3067	1/1	0.96	0.04	82,82,82,82	0
56	MG	1A	3158	1/1	0.96	0.30	67,67,67,67	0
56	MG	2A	3069	1/1	0.96	0.08	82,82,82,82	0
56	MG	1A	3305	1/1	0.96	0.17	65,65,65,65	0
56	MG	1a	3141	1/1	0.96	0.25	59,59,59,59	0
56	MG	1A	3516	1/1	0.96	0.08	81,81,81,81	0
56	MG	2A	3028	1/1	0.96	0.05	68,68,68,68	0
56	MG	2A	3120	1/1	0.96	0.09	94,94,94,94	0
56	MG	1A	3051	1/1	0.96	0.09	68,68,68,68	0
56	MG	1A	3089	1/1	0.96	0.15	59,59,59,59	0
56	MG	1A	3008	1/1	0.96	0.08	74,74,74,74	0
56	MG	1A	3309	1/1	0.96	0.16	67,67,67,67	0
56	MG	1A	3162	1/1	0.96	0.07	83,83,83,83	0
56	MG	1A	3163	1/1	0.96	0.05	46,46,46,46	0
56	MG	1A	3247	1/1	0.96	0.06	55,55,55,55	0
56	MG	1a	3113	1/1	0.96	0.10	86,86,86,86	0
56	MG	1A	3295	1/1	0.96	0.33	66,66,66,66	0
56	MG	2A	3336	1/1	0.96	0.14	77,77,77,77	0
56	MG	2A	3337	1/1	0.96	0.08	78,78,78,78	0
56	MG	1A	3502	1/1	0.96	0.12	61,61,61,61	0
56	MG	1A	3553	1/1	0.96	0.12	89,89,89,89	0
56	MG	1A	3526	1/1	0.96	0.06	76,76,76,76	0
56	MG	2A	3133	1/1	0.96	0.14	65,65,65,65	0
56	MG	1A	3018	1/1	0.96	0.09	84,84,84,84	0
56	MG	1A	3177	1/1	0.96	0.07	89,89,89,89	0
56	MG	1A	3529	1/1	0.96	0.11	71,71,71,71	0
56	MG	1a	3052	1/1	0.96	0.13	84,84,84,84	0
56	MG	2a	3112	1/1	0.96	0.06	87,87,87,87	0
56	MG	1A	3478	1/1	0.96	0.08	83,83,83,83	0
56	MG	1A	3154	1/1	0.96	0.12	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3111	1/1	0.96	0.11	83,83,83,83	0
56	MG	2A	3141	1/1	0.96	0.15	81,81,81,81	0
56	MG	1A	3193	1/1	0.96	0.23	62,62,62,62	0
56	MG	2A	3239	1/1	0.96	0.08	77,77,77,77	0
56	MG	1a	3090	1/1	0.96	0.28	87,87,87,87	0
56	MG	1A	3458	1/1	0.96	0.06	82,82,82,82	0
56	MG	1A	3338	1/1	0.96	0.14	45,45,45,45	0
56	MG	1A	3064	1/1	0.96	0.07	84,84,84,84	0
56	MG	2A	3299	1/1	0.96	0.11	66,66,66,66	0
56	MG	1A	3567	1/1	0.96	0.05	87,87,87,87	0
56	MG	1a	3170	1/1	0.96	0.12	76,76,76,76	0
56	MG	1A	3568	1/1	0.96	0.05	79,79,79,79	0
56	MG	2A	3103	1/1	0.96	0.08	83,83,83,83	0
56	MG	1A	3569	1/1	0.96	0.07	95,95,95,95	0
56	MG	1A	3105	1/1	0.96	0.25	74,74,74,74	0
56	MG	2A	3236	1/1	0.97	0.28	69,69,69,69	0
56	MG	1A	3435	1/1	0.97	0.08	59,59,59,59	0
56	MG	2A	3279	1/1	0.97	0.11	70,70,70,70	0
56	MG	1A	3017	1/1	0.97	0.05	64,64,64,64	0
56	MG	1A	3072	1/1	0.97	0.21	67,67,67,67	0
56	MG	2a	3103	1/1	0.97	0.07	73,73,73,73	0
56	MG	1A	3535	1/1	0.97	0.10	90,90,90,90	0
56	MG	1A	3271	1/1	0.97	0.13	49,49,49,49	0
56	MG	1A	3561	1/1	0.97	0.09	64,64,64,64	0
56	MG	1a	3029	1/1	0.97	0.12	64,64,64,64	0
56	MG	1A	3073	1/1	0.97	0.07	81,81,81,81	0
56	MG	1a	3230	1/1	0.97	0.06	84,84,84,84	0
56	MG	2A	3063	1/1	0.97	0.03	67,67,67,67	0
56	MG	1A	3413	1/1	0.97	0.28	71,71,71,71	0
56	MG	1A	3494	1/1	0.97	0.05	75,75,75,75	0
56	MG	1A	3593	1/1	0.97	0.13	65,65,65,65	0
56	MG	1A	3046	1/1	0.97	0.16	54,54,54,54	0
56	MG	1A	3253	1/1	0.97	0.17	71,71,71,71	0
56	MG	1A	3476	1/1	0.97	0.13	89,89,89,89	0
56	MG	1A	3107	1/1	0.97	0.13	81,81,81,81	0
56	MG	1A	3570	1/1	0.97	0.10	99,99,99,99	0
56	MG	1A	3499	1/1	0.97	0.14	72,72,72,72	0
56	MG	1A	3040	1/1	0.97	0.08	115,115,115,115	0
56	MG	1A	3656	1/1	0.97	0.11	70,70,70,70	0
56	MG	1A	3446	1/1	0.97	0.08	65,65,65,65	0
56	MG	1A	3462	1/1	0.97	0.05	64,64,64,64	0
56	MG	1A	3130	1/1	0.97	0.06	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	3013	1/1	0.97	0.08	77,77,77,77	0
56	MG	1A	3631	1/1	0.97	0.04	82,82,82,82	0
56	MG	2A	3349	1/1	0.97	0.08	81,81,81,81	0
56	MG	2a	3041	1/1	0.97	0.24	69,69,69,69	0
56	MG	1a	3015	1/1	0.97	0.06	90,90,90,90	0
56	MG	1A	3345	1/1	0.97	0.21	66,66,66,66	0
56	MG	1A	3483	1/1	0.97	0.04	77,77,77,77	0
56	MG	2A	3083	1/1	0.97	0.07	80,80,80,80	0
56	MG	2a	3046	1/1	0.97	0.06	85,85,85,85	0
56	MG	2A	3269	1/1	0.97	0.05	74,74,74,74	0
56	MG	1a	3147	1/1	0.97	0.25	71,71,71,71	0
56	MG	1A	3484	1/1	0.97	0.06	80,80,80,80	0
56	MG	1A	3635	1/1	0.97	0.04	78,78,78,78	0
56	MG	1A	3171	1/1	0.97	0.19	77,77,77,77	0
56	MG	1A	3061	1/1	0.97	0.05	77,77,77,77	0
56	MG	1A	3487	1/1	0.97	0.08	81,81,81,81	0
56	MG	2A	3235	1/1	0.97	0.15	69,69,69,69	0
56	MG	1A	3049	1/1	0.98	0.06	61,61,61,61	0
56	MG	1A	3611	1/1	0.98	0.07	75,75,75,75	0
56	MG	1a	3011	1/1	0.98	0.14	94,94,94,94	0
56	MG	1A	3438	1/1	0.98	0.07	71,71,71,71	0
56	MG	1a	3169	1/1	0.98	0.10	80,80,80,80	0
56	MG	1A	3475	1/1	0.98	0.05	88,88,88,88	0
56	MG	2A	3340	1/1	0.98	0.03	67,67,67,67	0
56	MG	1A	3675	1/1	0.98	0.14	47,47,47,47	0
56	MG	2A	3342	1/1	0.98	0.12	78,78,78,78	0
56	MG	1A	3068	1/1	0.98	0.05	74,74,74,74	0
56	MG	1A	3395	1/1	0.98	0.04	72,72,72,72	0
56	MG	1A	3103	1/1	0.98	0.10	68,68,68,68	0
56	MG	1A	3093	1/1	0.98	0.06	73,73,73,73	0
56	MG	1a	3219	1/1	0.98	0.09	74,74,74,74	0
56	MG	1a	3095	1/1	0.98	0.15	62,62,62,62	0
56	MG	1A	3337	1/1	0.98	0.05	57,57,57,57	0
56	MG	2A	3322	1/1	0.98	0.06	86,86,86,86	0
56	MG	2A	3351	1/1	0.98	0.04	84,84,84,84	0
56	MG	1A	3013	1/1	0.98	0.06	69,69,69,69	0
56	MG	1A	3028	1/1	0.98	0.06	68,68,68,68	0
56	MG	1A	3562	1/1	0.98	0.04	60,60,60,60	0
56	MG	1A	3667	1/1	0.98	0.05	68,68,68,68	0
56	MG	1A	3179	1/1	0.98	0.07	90,90,90,90	0
56	MG	1a	3006	1/1	0.98	0.04	90,90,90,90	0
56	MG	2A	3251	1/1	0.98	0.07	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3215	1/1	0.98	0.07	49,49,49,49	0
56	MG	2A	3059	1/1	0.98	0.06	93,93,93,93	0
56	MG	1A	3233	1/1	0.98	0.10	58,58,58,58	0
57	ZN	2Y	501	1/1	0.98	0.04	138,138,138,138	0
56	MG	2A	3014	1/1	0.98	0.07	72,72,72,72	0
57	ZN	2n	501	1/1	0.98	0.04	117,117,117,117	0
58	SF4	1d	501	8/8	0.98	0.04	76,91,99,101	0
56	MG	1A	3231	1/1	0.99	0.12	57,57,57,57	0
56	MG	2A	3268	1/1	0.99	0.03	82,82,82,82	0
56	MG	2A	3088	1/1	0.99	0.04	77,77,77,77	0
57	ZN	1Y	501	1/1	0.99	0.02	100,100,100,100	0
56	MG	2A	3319	1/1	0.99	0.03	78,78,78,78	0
57	ZN	16	501	1/1	0.99	0.03	87,87,87,87	0
57	ZN	1n	501	1/1	0.99	0.08	105,105,105,105	0
56	MG	1A	3544	1/1	0.99	0.04	71,71,71,71	0
56	MG	1a	3177	1/1	0.99	0.09	73,73,73,73	0
57	ZN	26	501	1/1	0.99	0.07	98,98,98,98	0
57	ZN	29	501	1/1	0.99	0.03	105,105,105,105	0
56	MG	1A	3571	1/1	0.99	0.02	98,98,98,98	0
56	MG	1A	3578	1/1	0.99	0.03	86,86,86,86	0
58	SF4	2d	501	8/8	0.99	0.03	95,106,118,119	0
57	ZN	25	501	1/1	1.00	0.04	97,97,97,97	0
57	ZN	19	501	1/1	1.00	0.07	77,77,77,77	0
57	ZN	15	501	1/1	1.00	0.03	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.