



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 12:06 AM UTC

PDB ID : 5FDU / pdb_00005fd
Title : Crystal structure of the Metalnikowin I antimicrobial peptide bound to the Thermus thermophilus 70S ribosome
Authors : Seefeldt, A.C.; Graf, M.; Perebaskine, N.; Nguyen, F.; Arenz, S.; Mardirossian, M.; Scocchi, M.; Wilson, D.N.; Innis, C.A.
Deposited on : 2015-12-16
Resolution : 2.90 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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

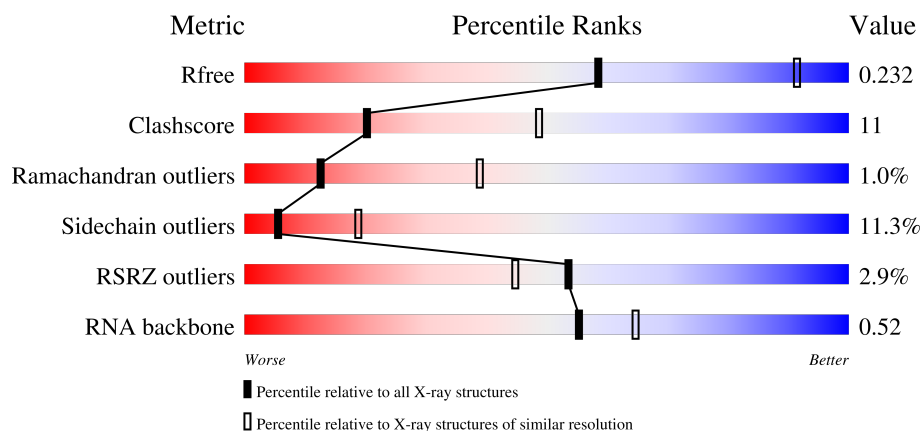
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



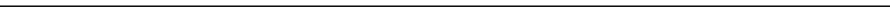
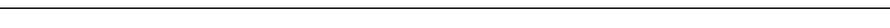
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	3% 63% 29% 6%
1	2A	2915	4% 59% 33% 6%
2	1B	120	73% 23%
2	2B	120	% 53% 42%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	1D	275	
3	2D	275	
4	1E	204	
4	2E	204	
5	1F	203	
5	2F	203	
6	1G	181	
6	2G	181	
7	1H	174	
7	2H	174	
8	1I	147	
8	2I	147	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	149	
11	2P	149	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	110	
14	2S	110	
15	1T	131	

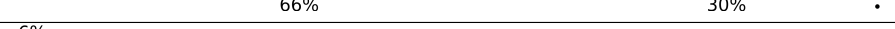
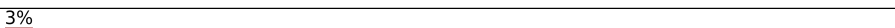
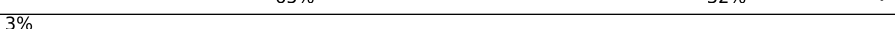
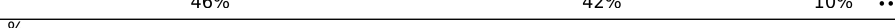
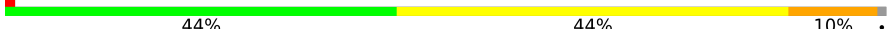
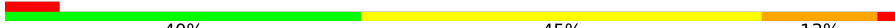
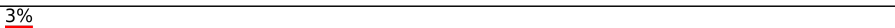
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	2T	131	
16	1U	116	
16	2U	116	
17	1V	101	
17	2V	101	
18	1W	112	
18	2W	112	
19	1X	95	
19	2X	95	
20	1Y	107	
20	2Y	107	
21	1Z	203	
21	2Z	203	
22	10	77	
22	20	77	
23	11	97	
23	21	97	
24	12	70	
24	22	70	
25	13	59	
25	23	59	
26	14	69	
26	24	69	
27	15	59	
27	25	59	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	16	53	
28	26	53	
29	17	48	
29	27	48	
30	18	64	
30	28	64	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	231	
33	2b	231	
34	1c	206	
34	2c	206	
35	1d	208	
35	2d	208	
36	1e	148	
36	2e	148	
37	1f	100	
37	2f	100	
38	1g	155	
38	2g	155	
39	1h	137	
39	2h	137	
40	1i	127	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	2i	127	
41	1j	97	
41	2j	97	
42	1k	114	
42	2k	114	
43	1l	122	
43	2l	122	
44	1m	116	
44	2m	116	
45	1n	60	
45	2n	60	
46	1o	88	
46	2o	88	
47	1p	82	
47	2p	82	
48	1q	99	
48	2q	99	
49	1r	68	
49	2r	68	
50	1s	83	
50	2s	83	
51	1t	98	
51	2t	98	
52	1u	23	
52	2u	23	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	1x	97	
53	2x	97	
54	1y	10	
54	2y	10	

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
43	OTD	1l	92	-	X	-	-
55	MG	1l	101	-	-	-	X
55	MG	1A	3165	-	-	-	X
55	MG	1A	3573	-	-	-	X
55	MG	1a	3049	-	-	-	X
55	MG	1a	3058	-	-	-	X
55	MG	1a	3063	-	-	-	X
55	MG	1a	3161	-	-	-	X
55	MG	25	103	-	-	-	X
55	MG	2A	3026	-	-	-	X
55	MG	2A	3047	-	-	-	X
55	MG	2A	3257	-	-	-	X
55	MG	2A	3624	-	-	-	X
55	MG	2A	3643	-	-	-	X
55	MG	2A	3756	-	-	-	X
55	MG	2A	3792	-	-	-	X
55	MG	2D	305	-	-	-	X
55	MG	2E	303	-	-	-	X
55	MG	2a	1606	-	-	-	X
55	MG	2a	1614	-	-	-	X
55	MG	2a	1631	-	-	-	X
55	MG	2e	3002	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 293484 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	2872	Total	C	N	O	P	0	0	0
			61862	27535	11569	19886	2872			
1	2A	2867	Total	C	N	O	P	0	0	0
			61751	27486	11547	19852	2866			

- 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
			2575	1145	476	834	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2571	1146	476	831	118			

- 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
			2131	1346	422	360	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
			1574	1004	294	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
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	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	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	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
			1121	722	208	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
			877	553	175	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
			775	498	141	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
			880	554	171	153	2			
18	2W	112	Total	C	N	O	S	0	0	0
			877	553	171	151	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
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	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
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	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
			592	368	119	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
			546	346	96	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
			536	342	98	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
			459	288	90	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	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

- 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
			1842	1175	330	332	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
			1558	979	305	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
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	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
			1133	716	214	199	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
			814	516	144	151	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
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	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
			1098	694	210	192	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
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

- 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
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	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
			834	520	156	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	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	2m	114	Total	C	N	O	S	0	0	0
			895	550	186	157	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
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	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
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	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 protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1x	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			
53	2x	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			

- Molecule 54 is a protein called Metalnikowin I.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	1y	10	Total	C	N	O	0	0	0
			87	55	17	15			
54	2y	10	Total	C	N	O	0	0	0
			87	55	17	15			

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1A	917	Total	Mg	0	0
			917	917		
55	1B	24	Total	Mg	0	0
			24	24		
55	1D	18	Total	Mg	0	0
			18	18		
55	1E	8	Total	Mg	0	0
			8	8		
55	1F	16	Total	Mg	0	0
			16	16		
55	1G	3	Total	Mg	0	0
			3	3		
55	1H	2	Total	Mg	0	0
			2	2		
55	1N	3	Total	Mg	0	0
			3	3		
55	1P	4	Total	Mg	0	0
			4	4		
55	1Q	5	Total	Mg	0	0
			5	5		
55	1R	5	Total	Mg	0	0
			5	5		
55	1S	1	Total	Mg	0	0
			1	1		
55	1T	1	Total	Mg	0	0
			1	1		
55	1U	7	Total	Mg	0	0
			7	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1V	3	Total 3	Mg 3	0	0
55	1W	3	Total 3	Mg 3	0	0
55	1X	1	Total 1	Mg 1	0	0
55	1Y	1	Total 1	Mg 1	0	0
55	10	8	Total 8	Mg 8	0	0
55	11	3	Total 3	Mg 3	0	0
55	13	2	Total 2	Mg 2	0	0
55	15	6	Total 6	Mg 6	0	0
55	17	5	Total 5	Mg 5	0	0
55	18	3	Total 3	Mg 3	0	0
55	19	2	Total 2	Mg 2	0	0
55	1a	223	Total 223	Mg 223	0	0
55	1b	1	Total 1	Mg 1	0	0
55	1d	5	Total 5	Mg 5	0	0
55	1e	2	Total 2	Mg 2	0	0
55	1f	1	Total 1	Mg 1	0	0
55	1g	1	Total 1	Mg 1	0	0
55	1h	2	Total 2	Mg 2	0	0
55	1k	1	Total 1	Mg 1	0	0
55	1l	1	Total 1	Mg 1	0	0
55	1m	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

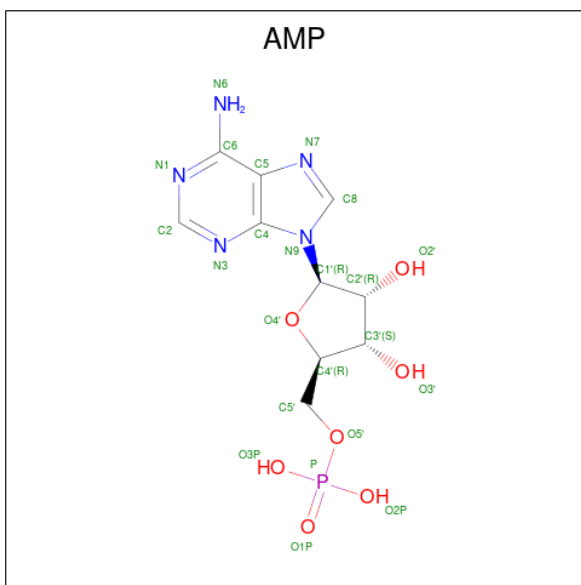
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1n	1	Total 1	Mg 1	0	0
55	1o	1	Total 1	Mg 1	0	0
55	1t	1	Total 1	Mg 1	0	0
55	2A	821	Total 821	Mg 821	0	0
55	2B	18	Total 18	Mg 18	0	0
55	2D	11	Total 11	Mg 11	0	0
55	2E	7	Total 7	Mg 7	0	0
55	2F	10	Total 10	Mg 10	0	0
55	2G	3	Total 3	Mg 3	0	0
55	2H	1	Total 1	Mg 1	0	0
55	2N	1	Total 1	Mg 1	0	0
55	2P	2	Total 2	Mg 2	0	0
55	2Q	5	Total 5	Mg 5	0	0
55	2R	3	Total 3	Mg 3	0	0
55	2S	1	Total 1	Mg 1	0	0
55	2T	1	Total 1	Mg 1	0	0
55	2U	4	Total 4	Mg 4	0	0
55	2V	5	Total 5	Mg 5	0	0
55	2W	1	Total 1	Mg 1	0	0
55	2X	3	Total 3	Mg 3	0	0
55	20	6	Total 6	Mg 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	21	2	Total 2	Mg 2	0	0
55	23	1	Total 1	Mg 1	0	0
55	25	3	Total 3	Mg 3	0	0
55	27	4	Total 4	Mg 4	0	0
55	28	3	Total 3	Mg 3	0	0
55	2a	196	Total 196	Mg 196	0	0
55	2b	1	Total 1	Mg 1	0	0
55	2d	4	Total 4	Mg 4	0	0
55	2e	2	Total 2	Mg 2	0	0
55	2f	1	Total 1	Mg 1	0	0
55	2g	1	Total 1	Mg 1	0	0
55	2h	1	Total 1	Mg 1	0	0
55	2l	1	Total 1	Mg 1	0	0
55	2m	1	Total 1	Mg 1	0	0
55	2n	2	Total 2	Mg 2	0	0
55	2o	1	Total 1	Mg 1	0	0

- Molecule 56 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1B	1	Total C 1 1	0	0
56	2A	1	Total P 1 1	0	0

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

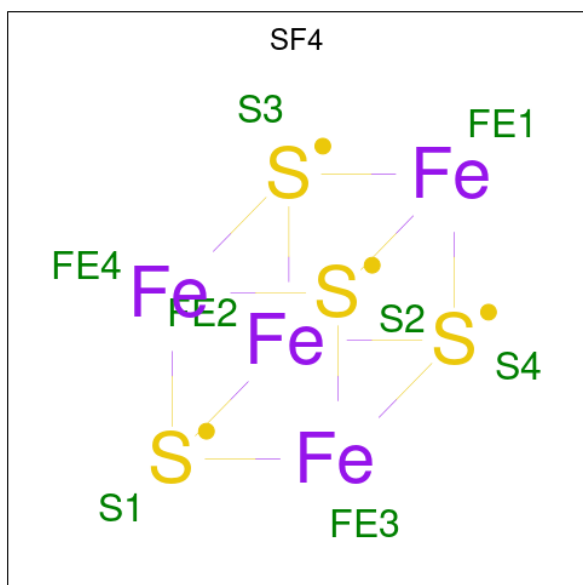
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1Y	1	Total Zn 1 1	0	0
57	14	1	Total Zn 1 1	0	0
57	15	1	Total Zn 1 1	0	0
57	16	1	Total Zn 1 1	0	0
57	19	1	Total Zn 1 1	0	0
57	1n	1	Total Zn 1 1	0	0
57	2Y	1	Total Zn 1 1	0	0
57	24	1	Total Zn 1 1	0	0
57	25	1	Total Zn 1 1	0	0
57	26	1	Total Zn 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	29	1	Total	Zn	0	0
			1	1		
57	2n	1	Total	Zn	0	0
			1	1		

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



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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	1740	Total	O	0	0
			1740	1740		
59	1B	42	Total	O	0	0
			42	42		
59	1D	14	Total	O	0	0
			14	14		
59	1E	18	Total	O	0	0
			18	18		
59	1F	11	Total	O	0	0
			11	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1G	2	Total	O	0	0
			2	2		
59	1H	3	Total	O	0	0
			3	3		
59	1N	9	Total	O	0	0
			9	9		
59	1P	13	Total	O	0	0
			13	13		
59	1Q	5	Total	O	0	0
			5	5		
59	1R	3	Total	O	0	0
			3	3		
59	1T	5	Total	O	0	0
			5	5		
59	1U	6	Total	O	0	0
			6	6		
59	1V	4	Total	O	0	0
			4	4		
59	1W	2	Total	O	0	0
			2	2		
59	1X	1	Total	O	0	0
			1	1		
59	1Y	5	Total	O	0	0
			5	5		
59	10	4	Total	O	0	0
			4	4		
59	11	2	Total	O	0	0
			2	2		
59	13	1	Total	O	0	0
			1	1		
59	15	2	Total	O	0	0
			2	2		
59	16	3	Total	O	0	0
			3	3		
59	17	1	Total	O	0	0
			1	1		
59	18	7	Total	O	0	0
			7	7		
59	19	2	Total	O	0	0
			2	2		
59	1a	393	Total	O	0	0
			393	393		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1d	10	Total 10	O 10	0	0
59	1e	3	Total 3	O 3	0	0
59	1f	1	Total 1	O 1	0	0
59	1h	1	Total 1	O 1	0	0
59	1j	1	Total 1	O 1	0	0
59	1l	3	Total 3	O 3	0	0
59	1m	2	Total 2	O 2	0	0
59	1n	1	Total 1	O 1	0	0
59	1o	1	Total 1	O 1	0	0
59	1t	2	Total 2	O 2	0	0
59	2A	1666	Total 1666	O 1666	0	0
59	2B	35	Total 35	O 35	0	0
59	2D	12	Total 12	O 12	0	0
59	2E	17	Total 17	O 17	0	0
59	2F	11	Total 11	O 11	0	0
59	2G	2	Total 2	O 2	0	0
59	2H	3	Total 3	O 3	0	0
59	2N	1	Total 1	O 1	0	0
59	2P	9	Total 9	O 9	0	0
59	2Q	5	Total 5	O 5	0	0
59	2R	3	Total 3	O 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2T	3	Total 3	O 3	0	0
59	2U	2	Total 2	O 2	0	0
59	2V	2	Total 2	O 2	0	0
59	2W	2	Total 2	O 2	0	0
59	2X	6	Total 6	O 6	0	0
59	2Y	3	Total 3	O 3	0	0
59	20	6	Total 6	O 6	0	0
59	21	3	Total 3	O 3	0	0
59	23	1	Total 1	O 1	0	0
59	25	2	Total 2	O 2	0	0
59	26	2	Total 2	O 2	0	0
59	27	1	Total 1	O 1	0	0
59	28	5	Total 5	O 5	0	0
59	29	1	Total 1	O 1	0	0
59	2a	384	Total 384	O 384	0	0
59	2c	1	Total 1	O 1	0	0
59	2d	7	Total 7	O 7	0	0
59	2e	4	Total 4	O 4	0	0
59	2f	1	Total 1	O 1	0	0
59	2h	1	Total 1	O 1	0	0
59	2j	1	Total 1	O 1	0	0

Continued on next page...

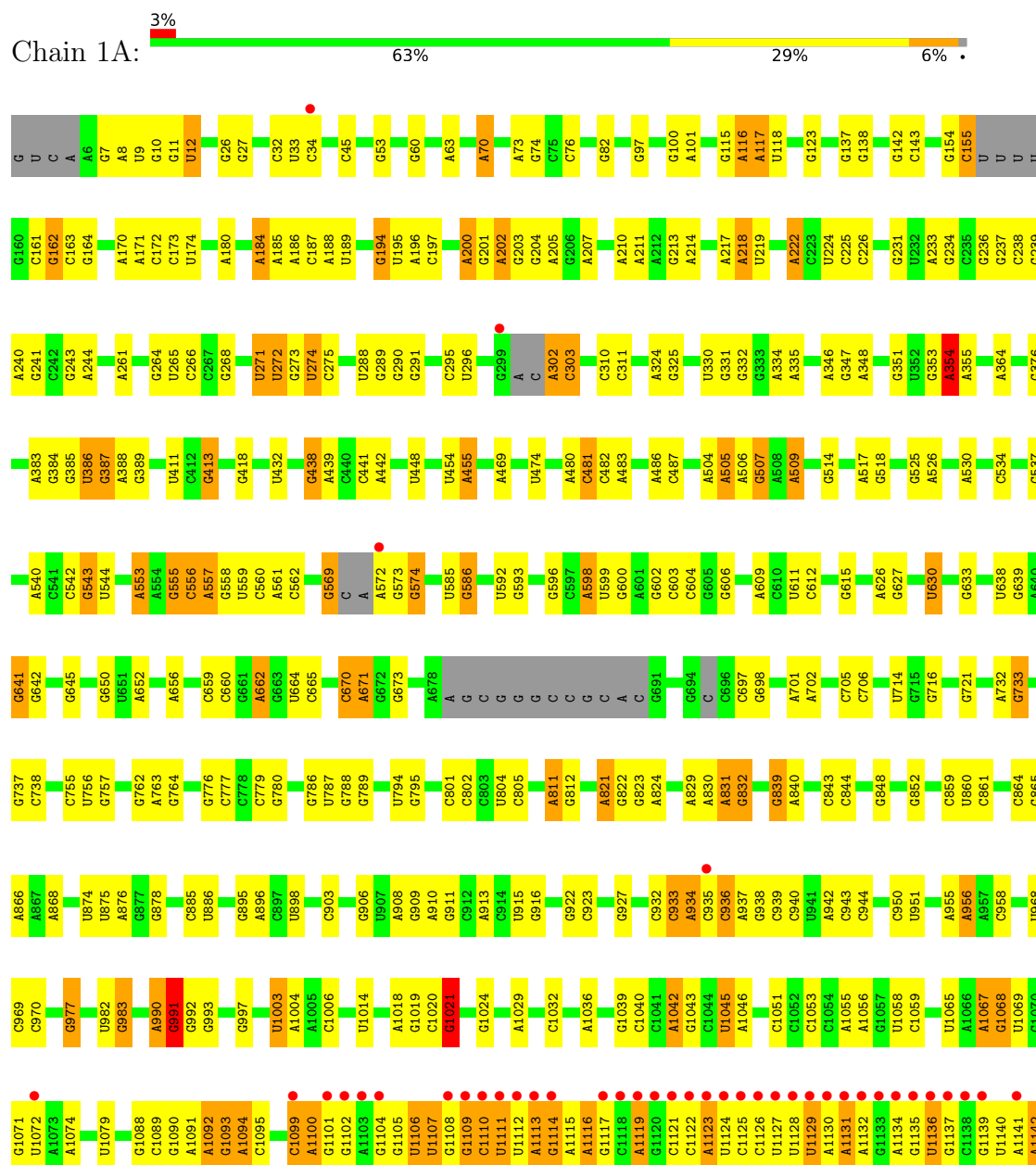
Continued from previous page...

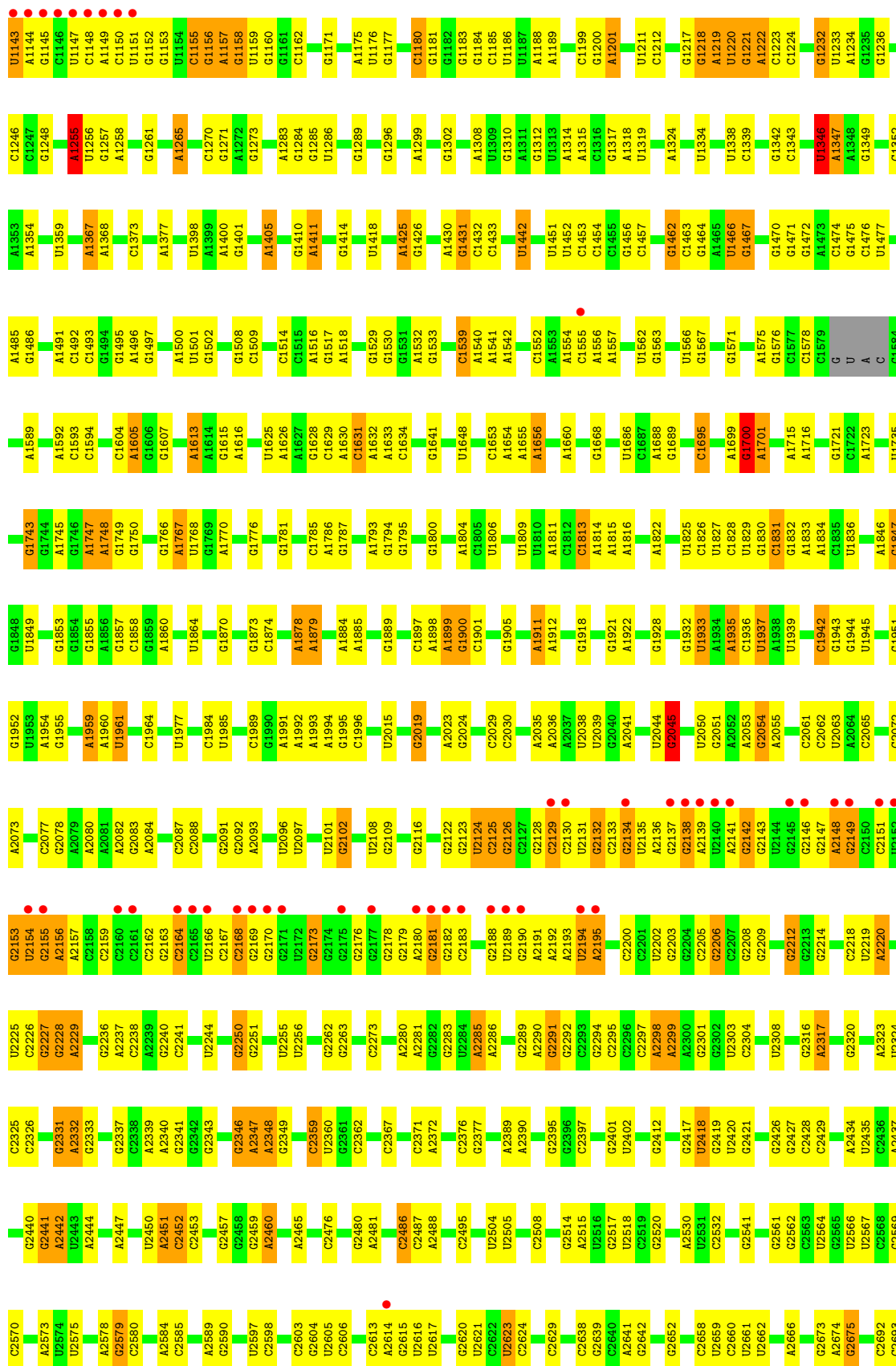
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2l	3	Total 3	O 3	0	0
59	2m	3	Total 3	O 3	0	0
59	2o	1	Total 1	O 1	0	0
59	2p	1	Total 1	O 1	0	0
59	2t	1	Total 1	O 1	0	0

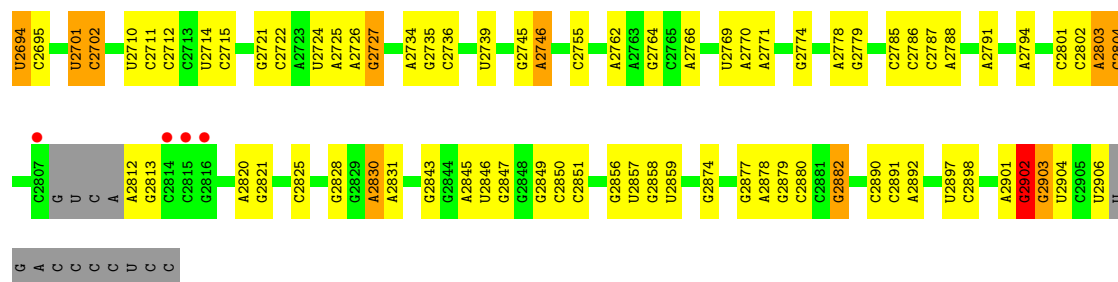
3 Residue-property plots

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.

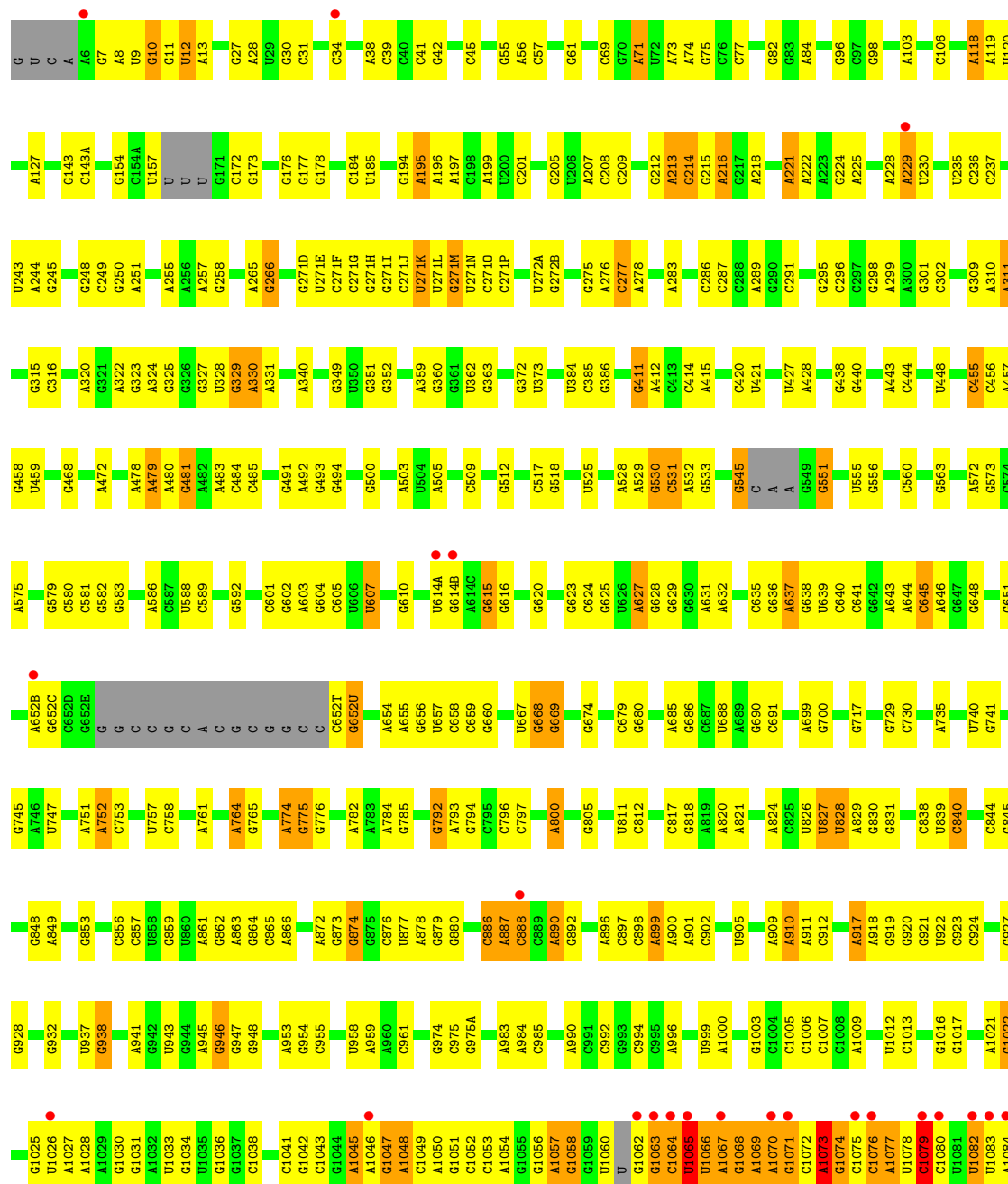
• Molecule 1: 23S ribosomal RNA



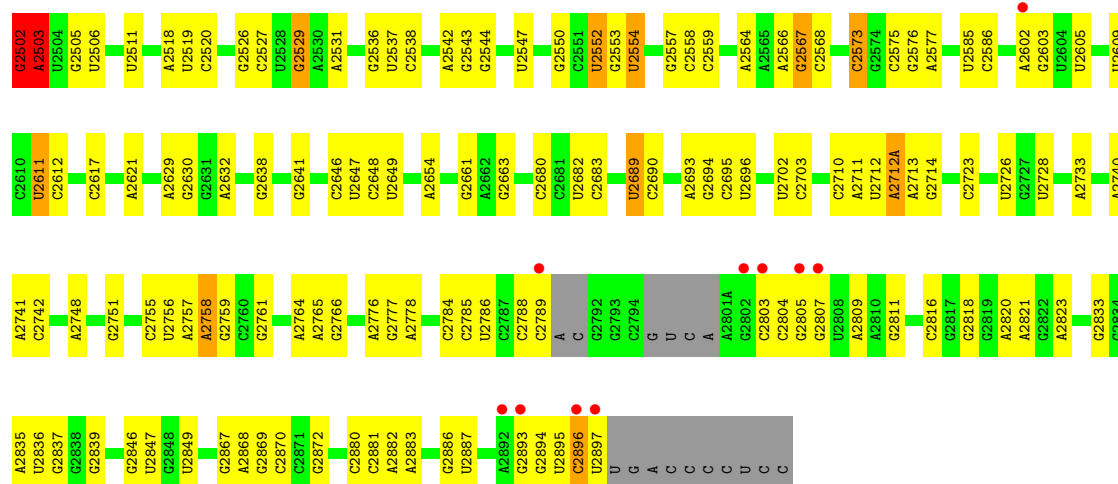




• Molecule 1: 23S ribosomal RNA



C2395	U2312	U2203	G2137	G2056	A1919	C1804	A1698	A1566	G1466	G1356	G1259	G1164	A1085
C2313	C2313	C2205	C2138	A2057	C1920	U1805	G1699	A1566	G1466	G1356	G1259	G1164	A1086
C2314	C2314	C2206	C2139	A2058	G1921	A1810	A1700	A1569	C1467	U1357	G1260	U1165	A1087
C2315	G2059	G2207	C2140	A2059	A1701	G1811	A1702	A1570	A1470	A1359	G1261	G1168	A1088
C2316	G2060	G2207	G2141	G2061	G1702	G1812	G1703	A1570	A1471	G1364	U1263	G1170	A1089
C2317	G2062	A2062	C2142	G2062	U1931	G1816	G1707	G1573	G1482	A1365	U1264	G1171	U1090
C2318	C2063	C2063	C2143	C2063	A1932	G1817	G1708	U1578	G1482	G1368	G1265	G1171	U1091
C2319	A2225	A2225	U2144	A2225	A1933	U1818	C1708	A1579	G1482	G1368	G1266	G	C1092
A2422	U2232	U2232	C2146	G2067	A1937	G1826	G1719	A1580	G1491	G1369	U1267	A	G1093
U2423	G2233	G2233	G2147	G2067	A1938	G1827	G1720	A1580	G1491	G1370	A1268	U	G1094
C2425	G2234	G2234	G2148	U2069	U1939	G1828	G1721	A1581	C1493	G1371	A1269	G	A1095
G2428	G2235	G2235	G2149	G2070	A1942	A1829	A1722	C1582	C1494	U1372	G1270	A	A1096
G2429	C2326	G2238	U2150	G2070	C1942	A1833	U1739	A1583	A1495	G1372	G1271	U1097	U1097
C2430	A2327	G2239	G2151	U2074	U1943	U1834	G1740	C1584	U1497	A1379	A1272	C1178	U1098
U2431	C2328	G2240	G2152	U2075	U1943	G1835	G1746	A1608	G1500	G1380	U1273	C1179	U1101
A2432	G2330	U2244	G2153	U2075	U1943	G1835	G1746	A1609	G1500	G1380	U1274	C1180	C1102
A2435	G2331	G2250	G2154	G2080	U1955	G1835	G1746	A1610	G1500	G1380	U1274	C1180	A1103
U2438	G2332	G2251	G2155	G2080	C1962	C1838	G1754	A1614	G1503	G1384	A1278	C1181	C1104
A2439	G2333	G2251	A2158	G2086	U1963	G1839	G1754	A1614	C1504	G1385	G1279	G1184	U1105
C2440	A2335	G2251	G2159	U2086	C1967	G1842	A1755	C1615	U1508	G1386	U1282	G1191	G1106
C2442	A2336	A2268	G2160	G2087	G1968	C1843	U1756	A1616	C1509	G1386	G1283	U1198	C1109
G2445	G2337	A2269	C2161	G2101	A1970	A1847	G1758	C1617	A1509A	G1386	U1283	U1199	A1110
A2448	C2347	A2273	G2162	U2102	A1971	A1848	G1758	G1626	A1509B	G1386	U1283	U1200	A1111
U2449	G2347	A2274	C2163	C2103	A1972	A1848	G1758	G1626	G1510	G1386	U1283	U1200	G1112
A2450	C2350	G2275	G2165	C2104	A1972	G1857	G1764	G1633	U1512	U1406	U1288	G1201	U1113
G2455	G2351	G2276	G2166	G2105	U1991	G1857	G1764	G1633	G1513	C1407	C1297	C1202	G1114
A2464	C2356	G2277	U2167	G2106	G1992	G1858	G1764	A1637	G1514	U1406	C1297	C1202	G1115
U2468	U2357	G2278	C2168	C2108	U1993	C1866	G1769	C1638	G1515	U1406	U1297	C1202	G1116
C2474	C2358	G2279	A2169	U2109	C1996	A1876	G1769	C1638	C1516	U1406	U1297	C1202	G1117
A2475	C2359	G2280	A2170	G2110	G1997	A1877	G1774	U1639	C1517	U1406	U1297	C1202	G1118
C2476	A2360	C2283	U2171	C2111	G1997	G1878	G1774	C1640	U1517	U1406	U1297	C1202	G1119
U2477	A2361	C2284	U2172	G2112	G1998	A1884	G1775	G1647	U1518	U1406	U1297	C1202	G1120
C2482	C2364	C2285	A2173	U2113	C1998	A1884	G1775	G1647	G1519	U1406	U1297	C1202	G1121
A2488	G2365	A2286	G2174	A2114	C2006	A1885	G1778	G1651	G1525	U1406	U1297	C1202	G1122
A2469	G2365	A2287	C2175	G2115	C2007	A1889	G1778	G1651	G1525	U1406	U1297	C1202	G1123
C2470	A2369	A2288	A2176	G2116	C2007	A1889	G1778	G1651	G1525	U1406	U1297	C1202	G1124
G2471	G2370	G2289	C2177	A2117	G2012	G1896	G1782	A1653	A1528A	U1406	U1297	C1202	G1125
G2472	G2371	U2291	C2178	U2118	A2013	G1897	G1782	A1654	G1529	U1406	U1297	C1202	G1126
U2473	G2372	C2292	C2179	G2120	A2014	U1898	G1784	C1657	C1530	U1406	U1297	C1202	G1127
C2474	A2376	C2293	U2180	G2121	A2019	G1899	A1785	C1658	C1532	U1406	U1297	C1202	G1128
A2475	A2377	U2296	G2181	U2122	A2020	A1900	A1786	C1658	C1532	U1406	U1297	C1202	G1129
C2476	A2378	G2297	C2182	G2123	C2021	G1903	C1790	A1665	U	U1406	U1297	C1202	G1130
U2482	C2381	G2299	C2183	G2124	U2022	C1905	A1791	A1668	C1536	U1406	U1297	C1202	G1131
A2488	G2382	G2302	G2184	A2126	G2023	G1906	U1794	A1669	C1536	U1406	U1297	C1202	G1132
G2494	G2383	G2303	C2185	G2127	A2031	U1911	C1795	G1674	U1539	U1406	U1297	C1202	G1133
C2495	G2384	G2304	U2189	C2128	G2032	U1912	C1796	G1674	U1540	U1406	U1297	C1202	G1134
C2496	A2385	G2305	U2190	G2129	A2033	A1913	C1797	C1686	G1541	U1406	U1297	C1202	G1135
A2497	C2386	A2306	G2191	U2130	C2039	G1914	G1798	G1687	A1542	U1406	U1297	C1202	G1136
C2498	U2387	G2307	G2192	U2132	C2043	U1915	C1800	U1688	C1547	U1406	U1297	C1202	G1137
C2499	U2390	G2308	C2196	G2133	C2043	A1916	G1801	G1695	C1548	U1406	U1297	C1202	G1138
C2499	U2390	G2308	C2197	G2134	C2055	U1917	A1802	G1696	C1557	U1406	U1297	C1202	G1139
C2499	U2390	G2308	A2198	C2136	C2055	A1918	A1803	G1697	A1558	U1406	U1297	C1202	G1140



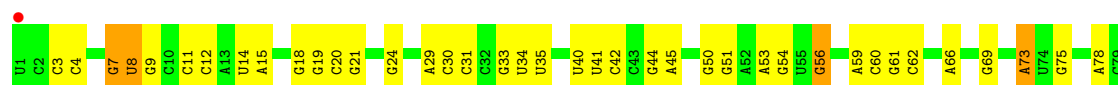
• Molecule 2: 5S ribosomal RNA

Chain 1B: 73% 23%



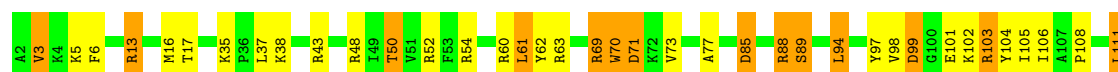
• Molecule 2: 5S ribosomal RNA

Chain 2B: 53% 42%



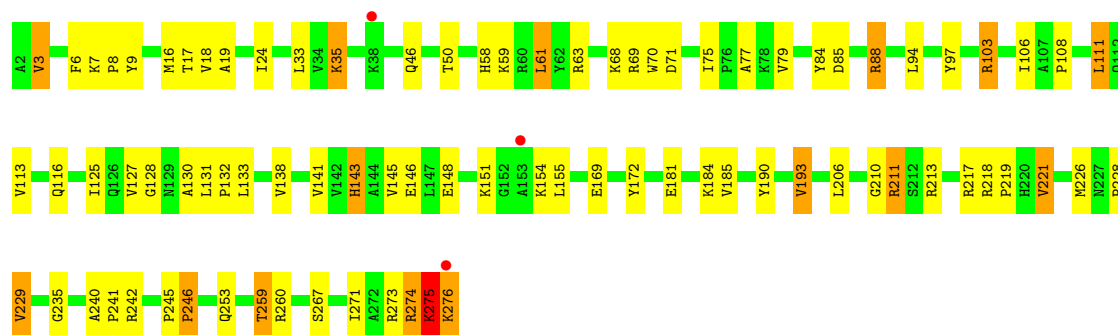
• Molecule 3: 50S ribosomal protein L2

Chain 1D: 66% 25% 8%



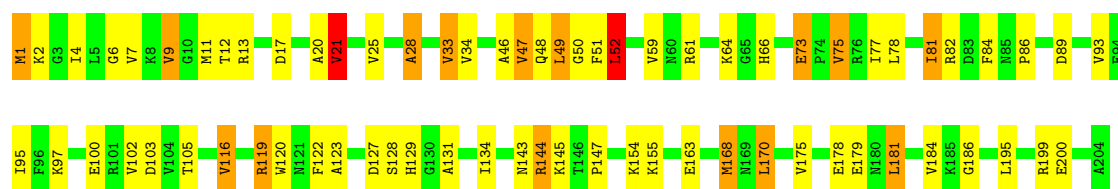
• Molecule 3: 50S ribosomal protein L2

Chain 2D: 69% 25% 5%



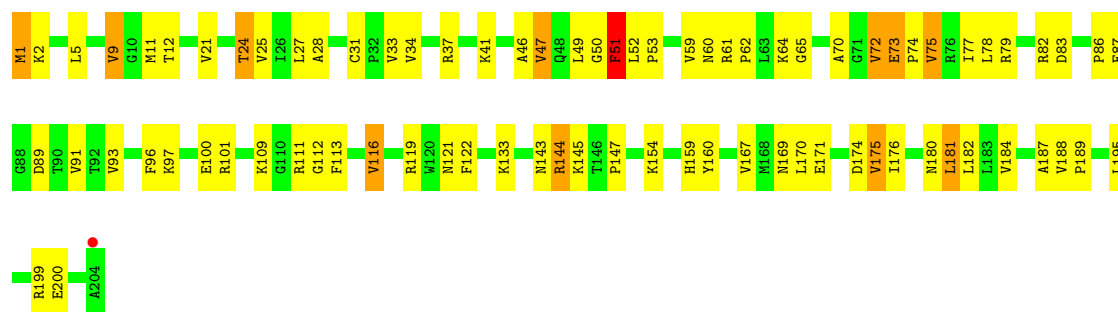
• Molecule 4: 50S ribosomal protein L3

Chain 1E: 65% 26% 7%



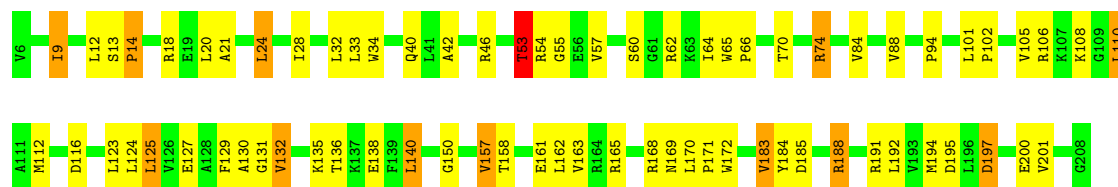
• Molecule 4: 50S ribosomal protein L3

Chain 2E: 60% 34% 5%



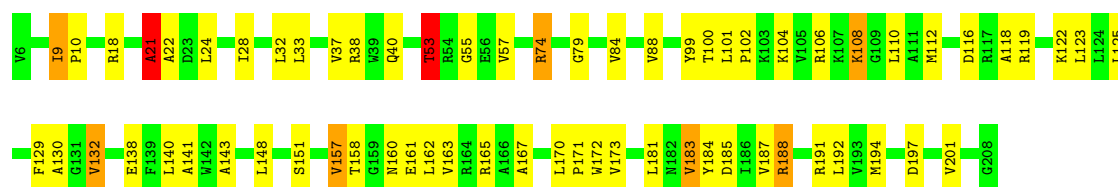
• Molecule 5: 50S ribosomal protein L4

Chain 1F: 65% 29% 6%

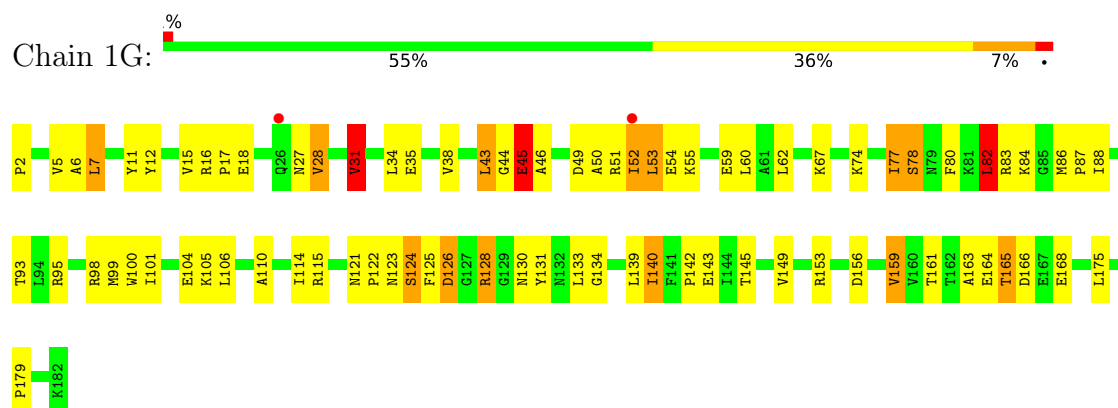


• Molecule 5: 50S ribosomal protein L4

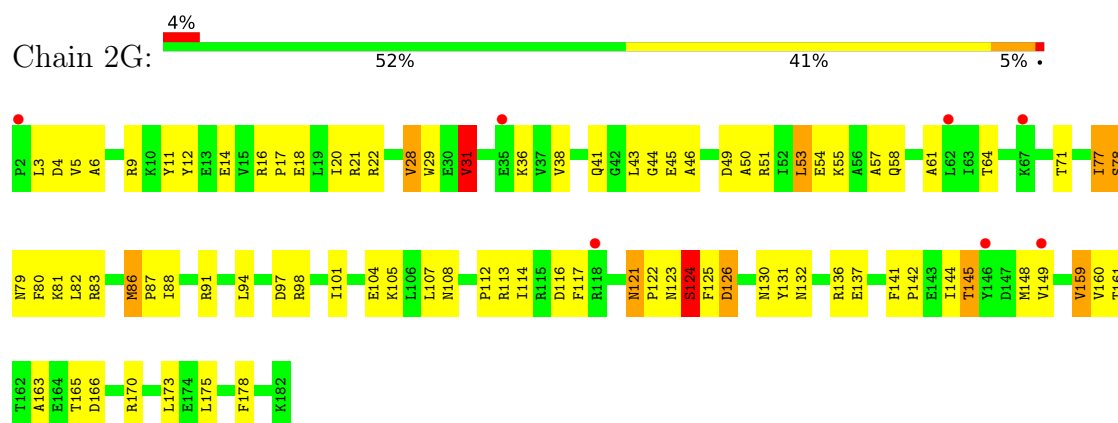
Chain 2F: 67% 28%



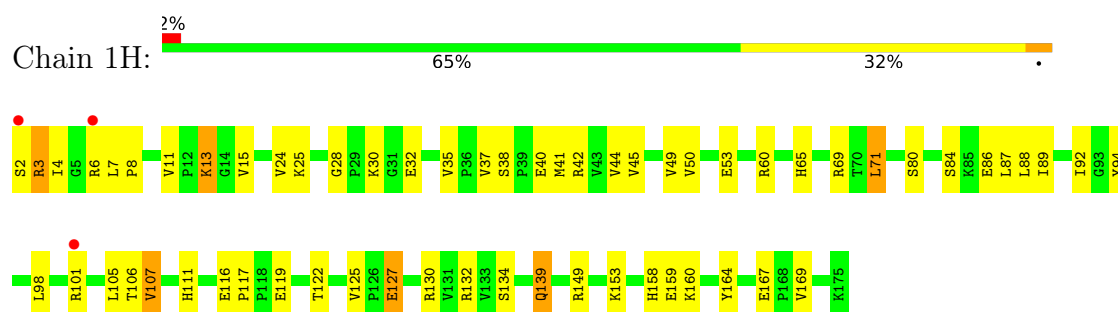
• Molecule 6: 50S ribosomal protein L5



• Molecule 6: 50S ribosomal protein L5

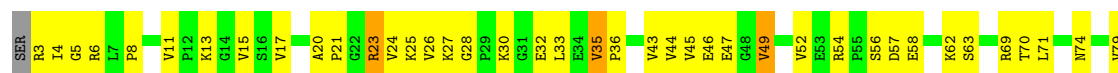


• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6

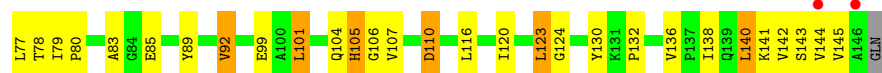




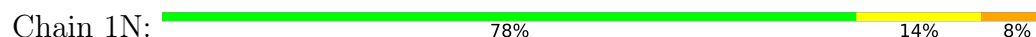
• Molecule 8: 50S ribosomal protein L9



• Molecule 8: 50S ribosomal protein L9



• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L14

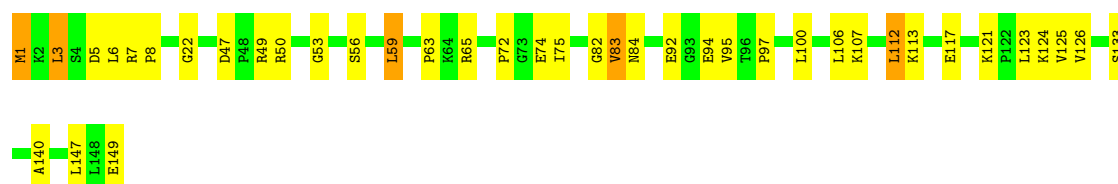
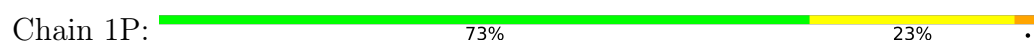




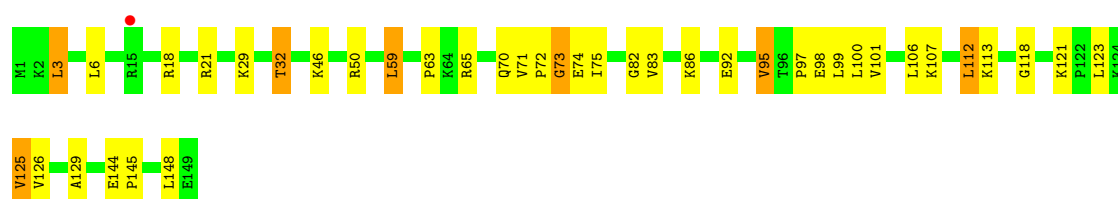
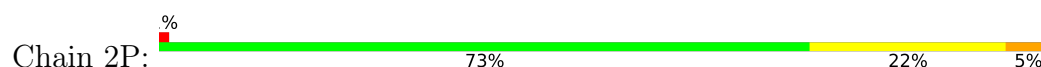
- Molecule 10: 50S ribosomal protein L14



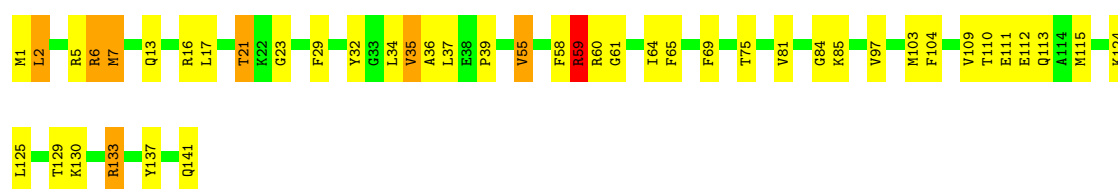
- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15

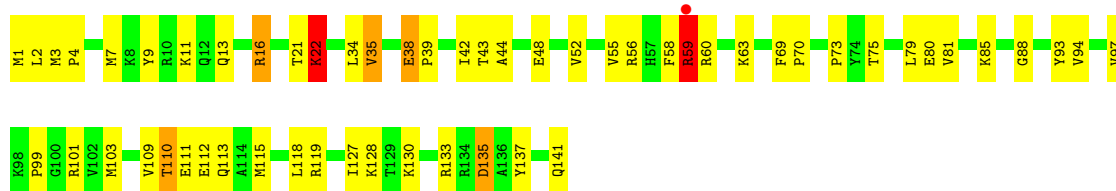


- Molecule 12: 50S ribosomal protein L16

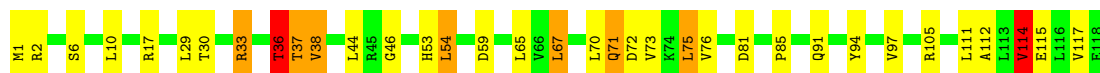


- Molecule 12: 50S ribosomal protein L16





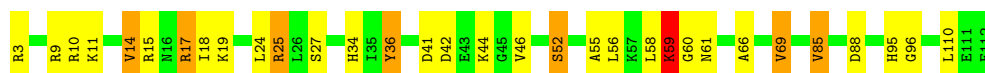
- Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17



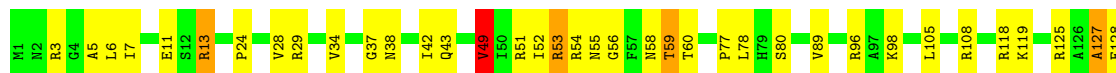
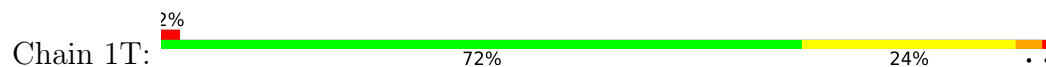
- Molecule 14: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L18

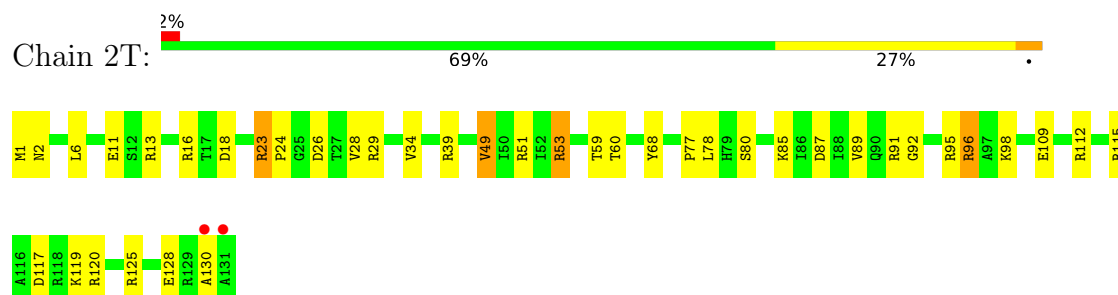


- Molecule 15: 50S ribosomal protein L19

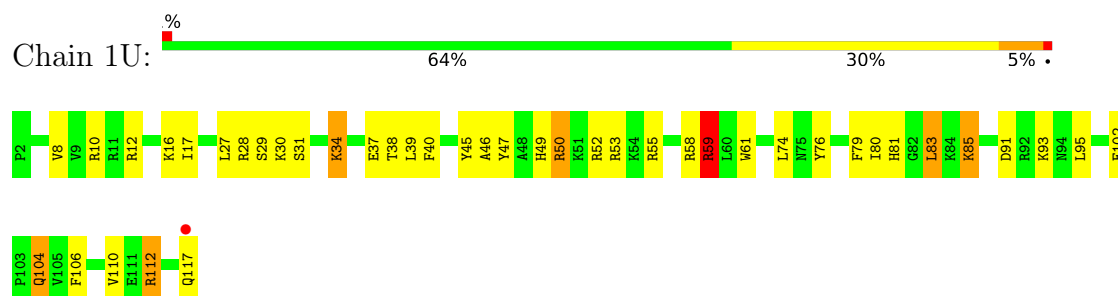




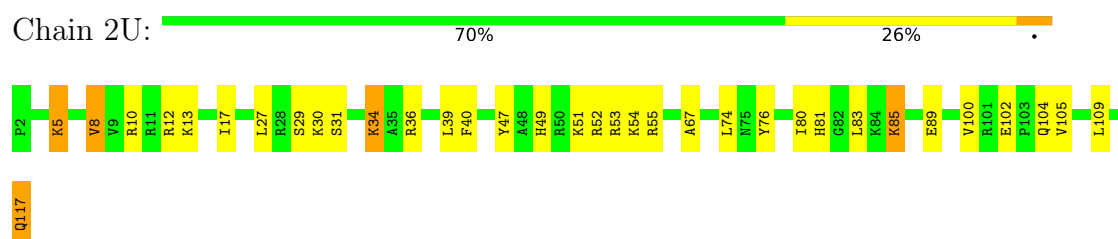
- Molecule 15: 50S ribosomal protein L19



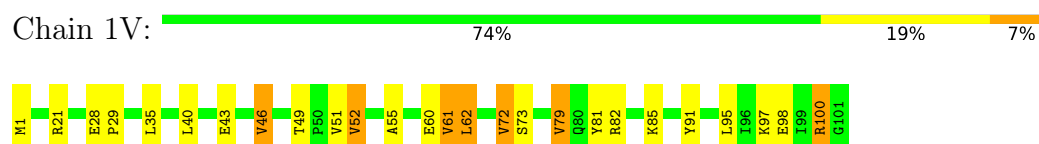
- Molecule 16: 50S ribosomal protein L20



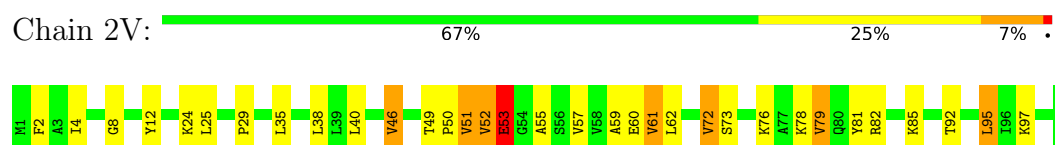
- Molecule 16: 50S ribosomal protein L20



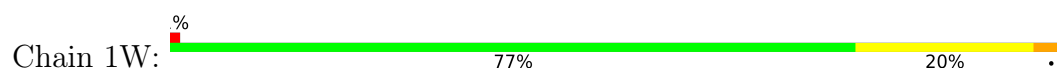
- Molecule 17: 50S ribosomal protein L21



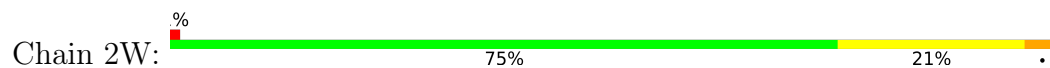
- Molecule 17: 50S ribosomal protein L21



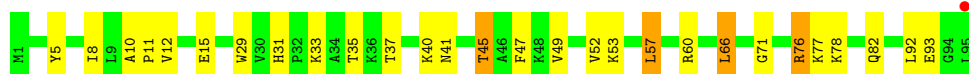
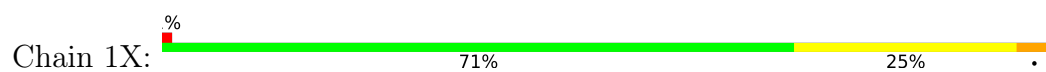
- Molecule 18: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



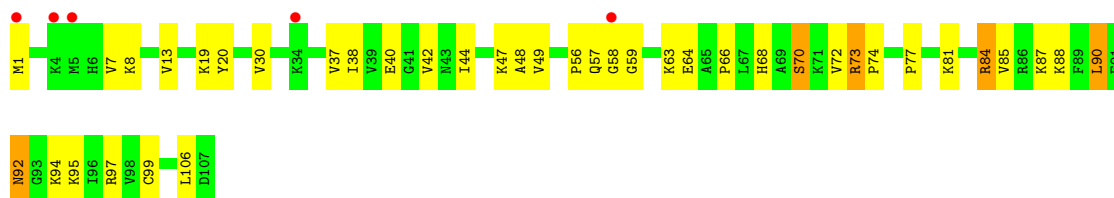
- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24

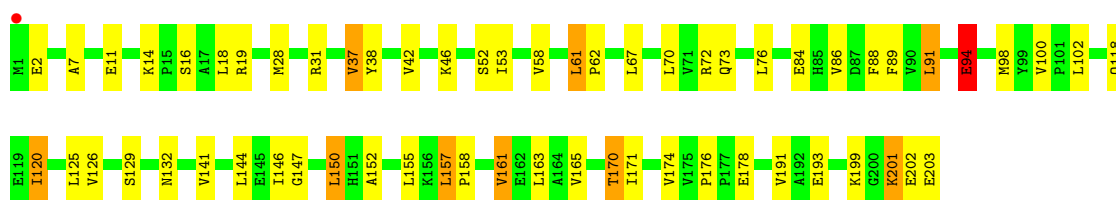


- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25





- Molecule 21: 50S ribosomal protein L25



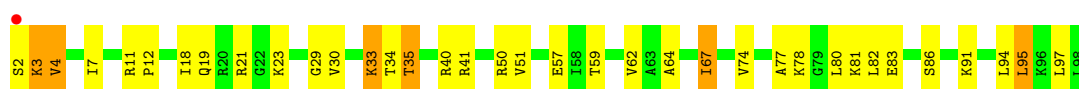
- Molecule 22: 50S ribosomal protein L27



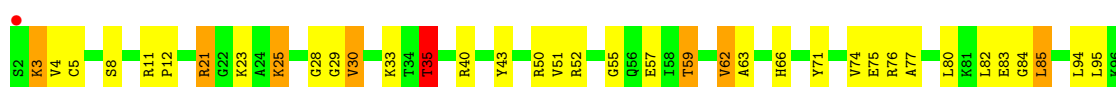
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28

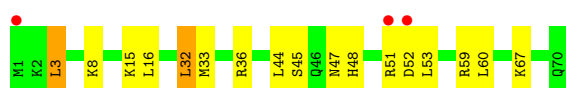
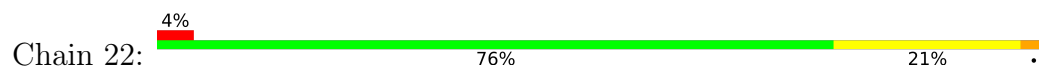




- Molecule 24: 50S ribosomal protein L29



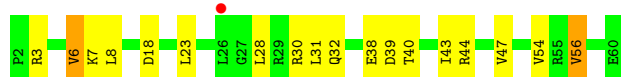
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31

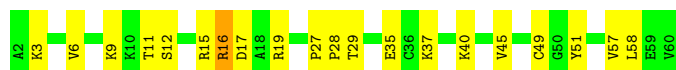


- Molecule 27: 50S ribosomal protein L32

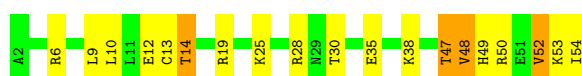




- Molecule 27: 50S ribosomal protein L32



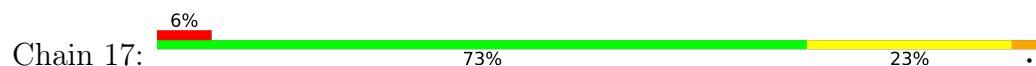
- Molecule 28: 50S ribosomal protein L33



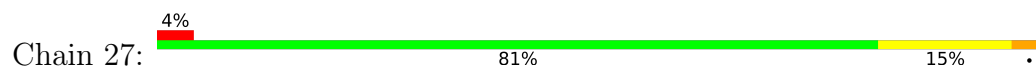
- Molecule 28: 50S ribosomal protein L33



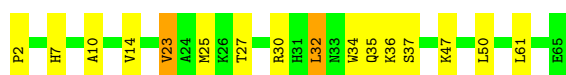
- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34

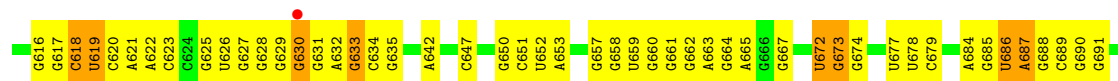


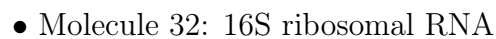
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



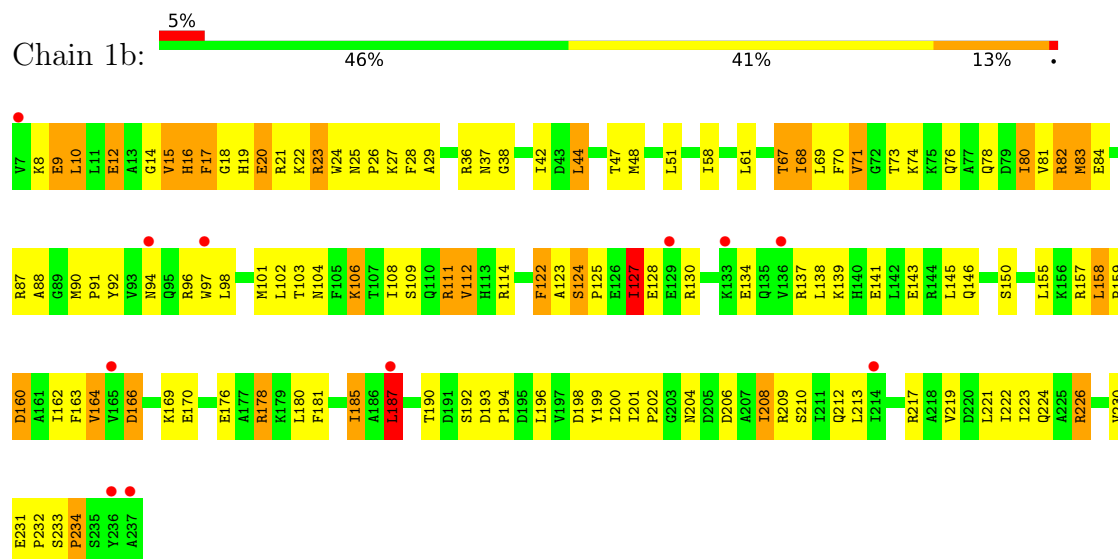




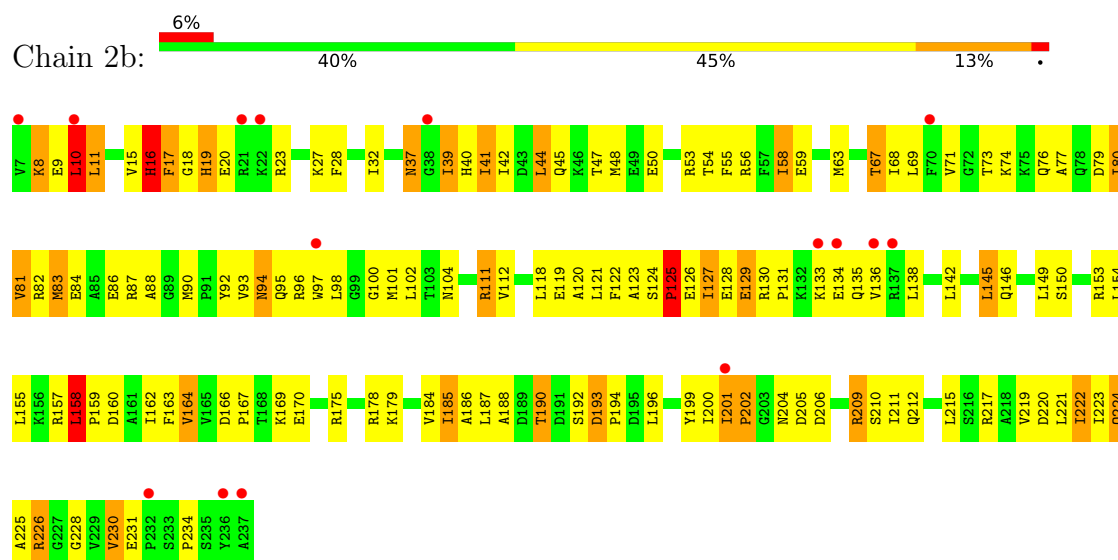
G1392	G1322	G1253	A1183	U1121	C989	G926	G818	G721	U636	G546	G473	A282
C1397	G1323	C1254	G1184	U1122	C990	G927	A819	A722	G627	A547	G474	A397
C1400	G1185	A1256	G1186	A1123	U991	G928	U820	G724	G628	G548	G475	C398
C1328	G1187	U1257	G1188	U1125	G993	G929	G826	A728	G631	U551	A477	C401
C1401	G1189	G1258	A1189	U126	A994	C930	U827	A729	G630	A553	U480	C402
C1402	G1190	C1259	G1191	G127	G985	C931	A828	G730	A632	G481	U480	G403
C1403	G1192	C1260	A1191	C1128	A996	C932	A829	G731	G633	C554	G481	U404
C1404	C1192	C1261	C1192	C1129	U997	C933	G829	G732	G634	C555	A482	U299
C1407	U1196	C1262	C1192	C1130	G998	C934	G833	A733	A642	G557	G483	G406
C1410	U1197	C1263	U1196	G1131	C999	A935	U833	A734	G485	G558	G484	G407
C1411	G1197	C1264	U1197	G1132	U1000	C936	C834	G735	U486	A559	G485	A408
C1412	G1198	A1269	G1198	G1133	A1001	A937	U835	C736	A653	U560	U487	G410
A1413	U1199	C1270	U1199	G1134	G1001A	A938	G838	A737	C656	U561	A487	A321
U1414	C1200	G1271	C1200	U1135	G1002	G939	U839	C738	G657	C489	C489	A412
U1415	U1341	G1272	A1201	C1136	A1003	C940	C840	A739	G658	C564	G490	G413
C1419	C1342	G1273	G1202	C1137	A1004	G941	U841	G741	U659	U565	G491	C328
C1426	U1351	G1274	C1203	G1138	A1005	U942	C848	C744	G660	G566	G492	G332
U1427	A1346	G1275	U1204	C1139	C1006	U943	G851	G752	G661	G567	G492	G333
C1428	U1347	G1276	U1205	C1140	G1007	G944	G852	A753	G662	C568	A496	U343
C1429	U1348	G1277	G1206	C1141	C1008	G945	G853	C754	A663	C569	U498	A344
A1434	A1349	U1278	G1207	U1142	G1009	A946	G854	G755	G664	A499	C503	C345
U1435	A1350	C1279	C1208	G1143	G1010	G947	G855	C756	U571	G500	C504	G346
U1436	A1351	A1280	C1209	G1144	G1011	A948	G857	G757	A572	C501	G505	A431
U1437	U1352	U1281	C1210	C1145	G1012	U950	C858	G758	U580	G502	A509	G350
C1353	G1353	C1282	U1211	A1146	G1013	U951	G859	A759	U581	C503	C511	G351
C1354	U1354	C1283	A1212	U1147	A1014	G952	A859	G765	A583	C504	C512	C352
G1355	G1355	A1285	A1213	U1148	A1015	U953	A860	G766	G584	C505	C513	A353
A1356	A1356	A1286	C1214	U1149	A1016	U954	A861	G767	G585	G506	C514	G354
A1357	A1357	A1287	G1215	U1150	G1017	U955	A865	G768	G586	U507	G515	G357
U1358	A1358	A1288	G1216	A1151	C1018	U956	A866	G769	G587	U508	U516	U358
C1359	C1359	C1289	C1217	A1152	C1019	A958	A867	G774	C590	U509	G517	U367
A1360	G1360	G1290	U1218	U1153	U1020	A959	A868	A777	U591	C510	C518	C372
C1362	U1362	U1292	U1219	G1154	G1023	U960	A872	G778	G592	A520	A520	A373
C1363	C1363	C1296	G1220	U1156	U1024	U961	A873	G779	G593	C526	G446	A374
G1365	U1428	A1428	G1221	A1157	G1025	U962	A874	G784	G594	U527	G447	A375
G1443	C1365	A1299	G1224	C1158	U1026	A964	C875	G785	G595	U528	A448	U376
A1447	C1366	G1300	C1225	U1159	C1027	A965	G878	A790	U598	C600	C449	G377
C1369	C1369	U1301	C1226	G1160	C1028	G966	C879	G791	C601	A532	A451	G380
G1370	G1370	C1302	A1227	C1161	C1029	A967	C880	A792	A602	A453	A453	C381
U1371	U1371	C1303	C1234	C1163	C1030	A968	G881	A793	G616	C536	C454	A382
U1372	U1372	G1304	U1235	G1164	G1030A	A969	A900	G800	G617	G537	C455	A383
C1373	C1373	G1305	A1236	C1165	G1030C	G971	A901	U801	G618	G538	C456	G384
A1374	A1374	A1306	C1237	G1166	A1030D	C972	G902	C806	U619	A539	C457	A389
C1375	C1375	U1307	A1238	A1168	G1031	C973	G903	A814	G620	G540	C458	C390
U1376	U1376	U1308	A1239	A1169	A974	U981	A918	A815	G621	G541	G460	C391
A1377	A1377	G1309	U1240	C1171	G1032	A975	A919	A816	A622	C542	A461	G392
C1378	C1378	G1310	C1243	G1172	G1033	C976	U920	C817	G623	C543	C470	A393
G1379	G1379	G1311	C1244	U1175	G1034	A977	U921	C817	G624	G544	G471	G394
C1383	C1383	U1312	A1245	A1176	A1035	A978	A913	G800	C536	C545	A472	
G1387	G1387	C1314	C1246	G1177	C1036	C979	A914	U801	G537			
C1388	C1388	A1318	U1247	C1178	C1037	C980	A918	C806	G538			
C1389	C1389	C1319	C1248	G1179	C1038	U982	A919	A712	G539			
U1390	U1390	C1320	A1250	A1180	U1040	G986	U920	G713	G540			
A1491	A1491	C1321	A1251	G1181	A1041	G987	U921	G713	G541			
A1492	A1492		A1252	G1182	C1042	G988	U922	G719	G542			



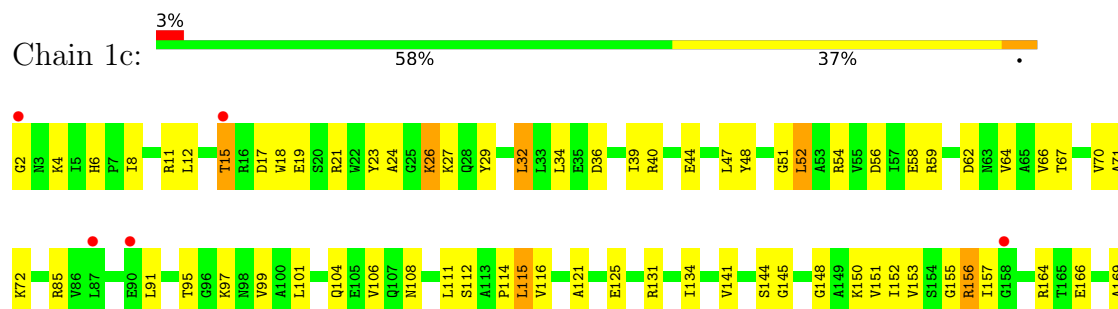
• Molecule 33: 30S ribosomal protein S2

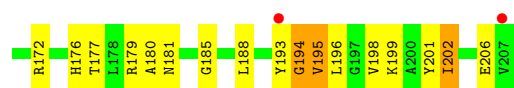


• Molecule 33: 30S ribosomal protein S2

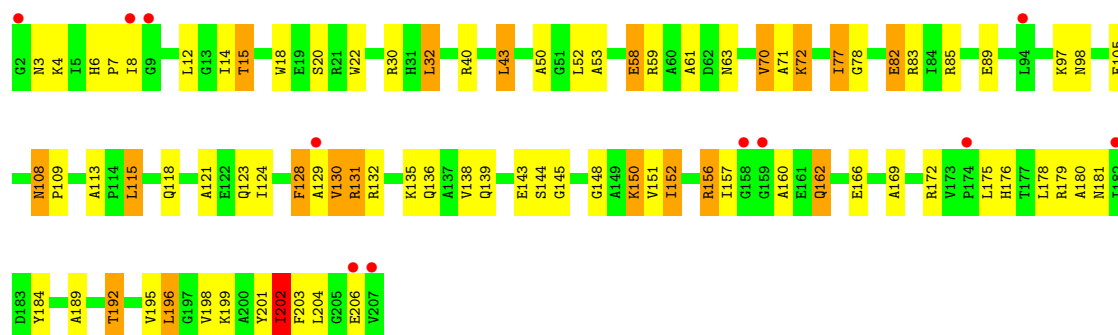


• Molecule 34: 30S ribosomal protein S3

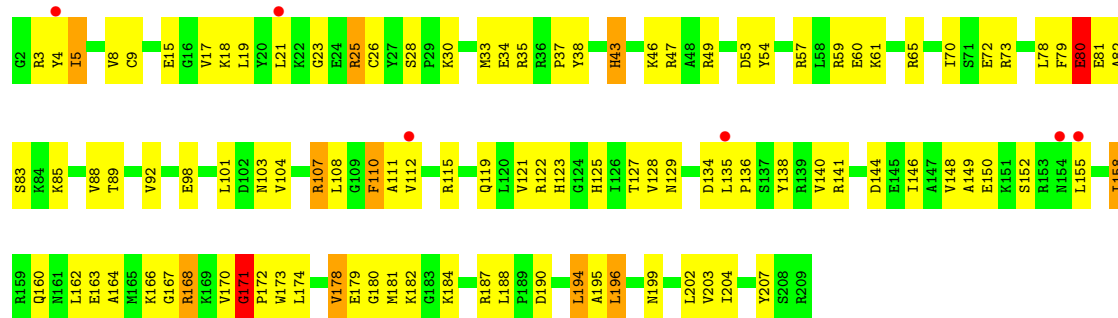




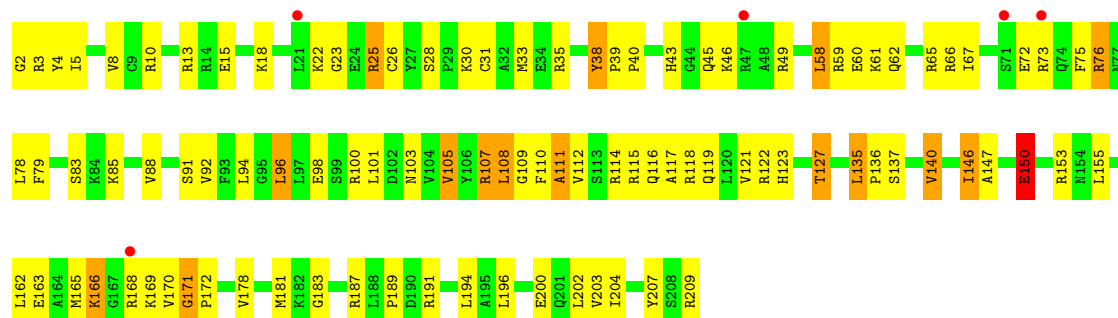
• Molecule 34: 30S ribosomal protein S3



• Molecule 35: 30S ribosomal protein S4

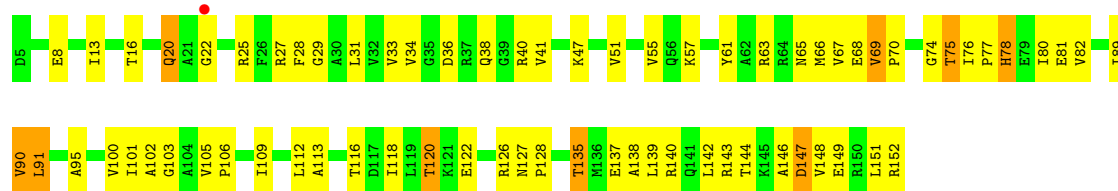


• Molecule 35: 30S ribosomal protein S4

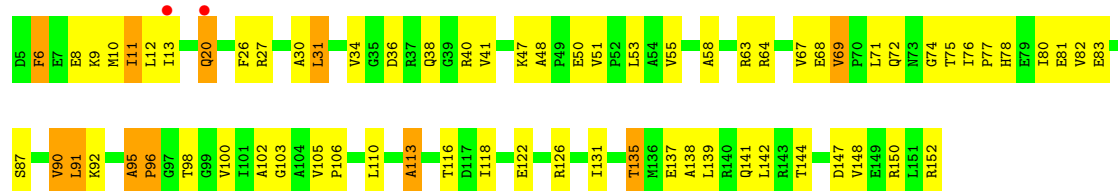


• Molecule 36: 30S ribosomal protein S5

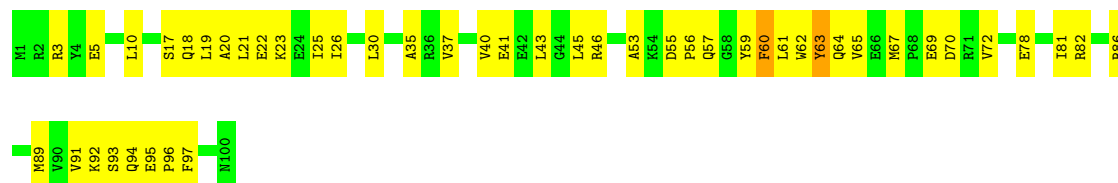




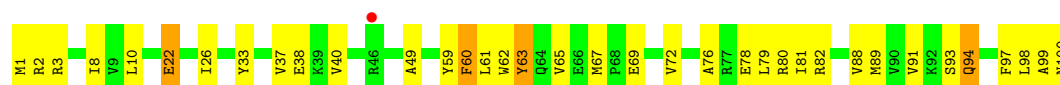
• Molecule 36: 30S ribosomal protein S5



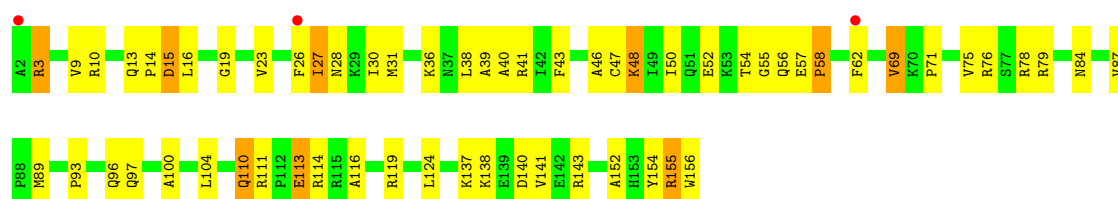
• Molecule 37: 30S ribosomal protein S6



• Molecule 37: 30S ribosomal protein S6

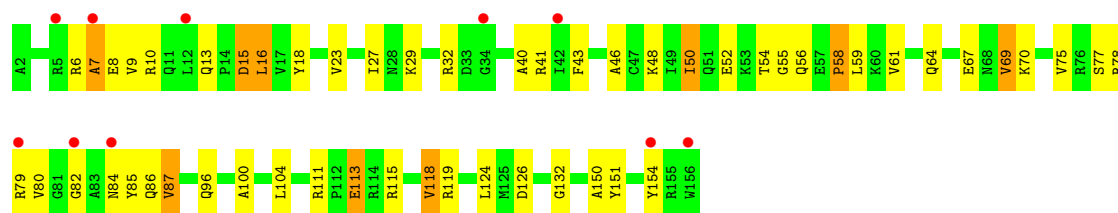


• Molecule 38: 30S ribosomal protein S7

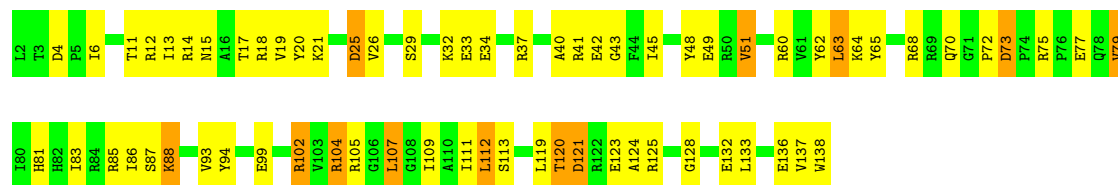


• Molecule 38: 30S ribosomal protein S7

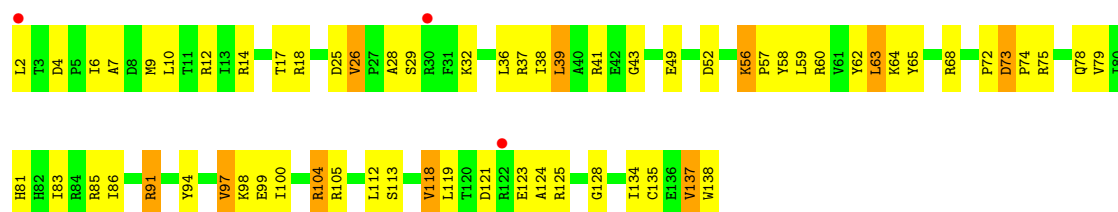




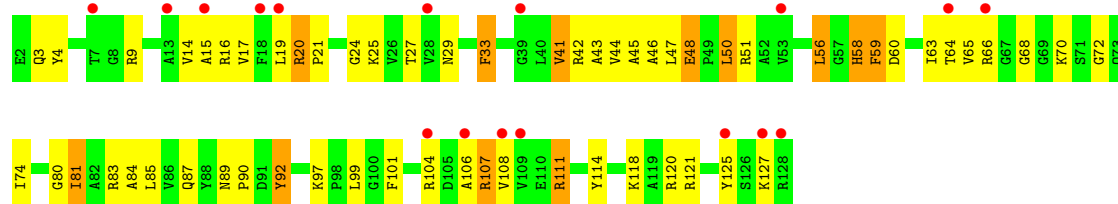
• Molecule 39: 30S ribosomal protein S8



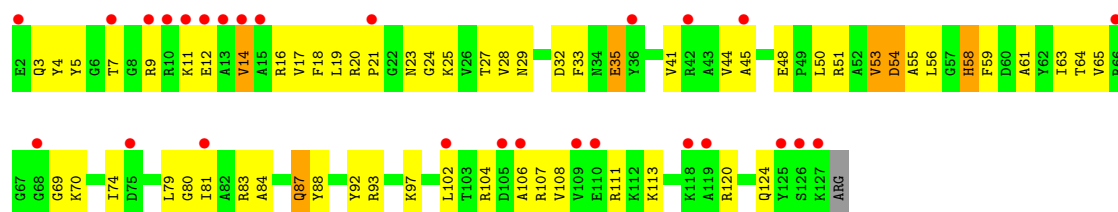
• Molecule 39: 30S ribosomal protein S8



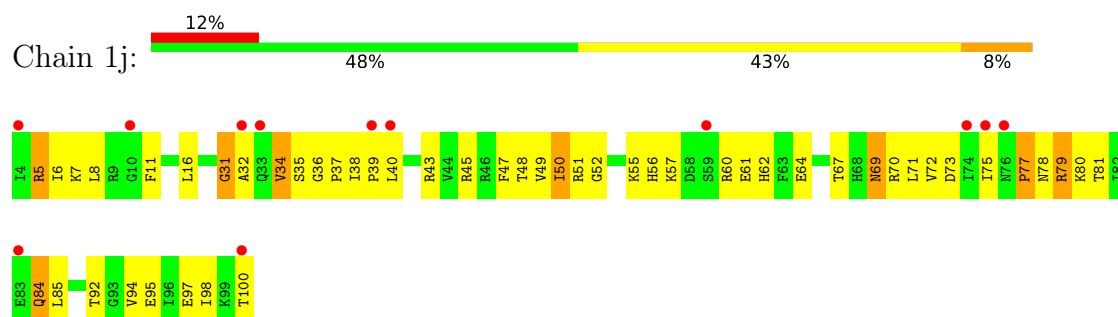
• Molecule 40: 30S ribosomal protein S9



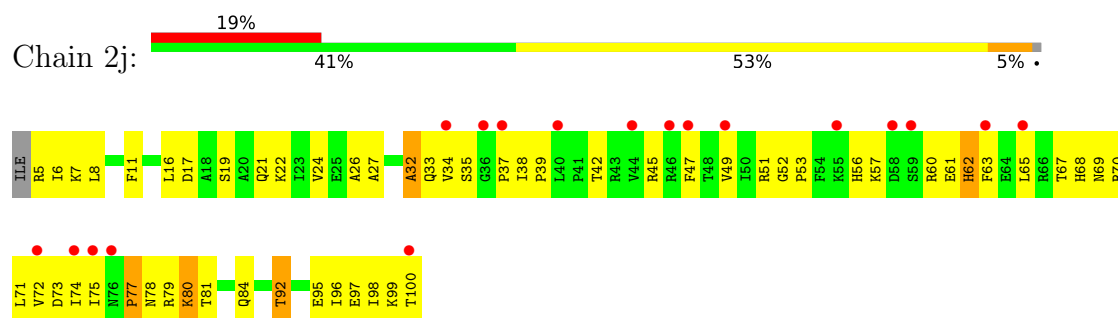
• Molecule 40: 30S ribosomal protein S9



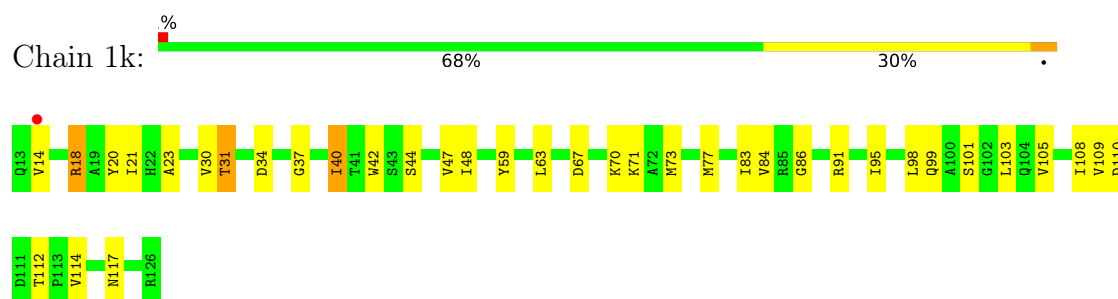
- Molecule 41: 30S ribosomal protein S10



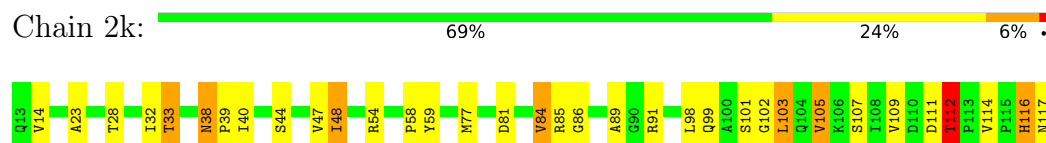
- Molecule 41: 30S ribosomal protein S10



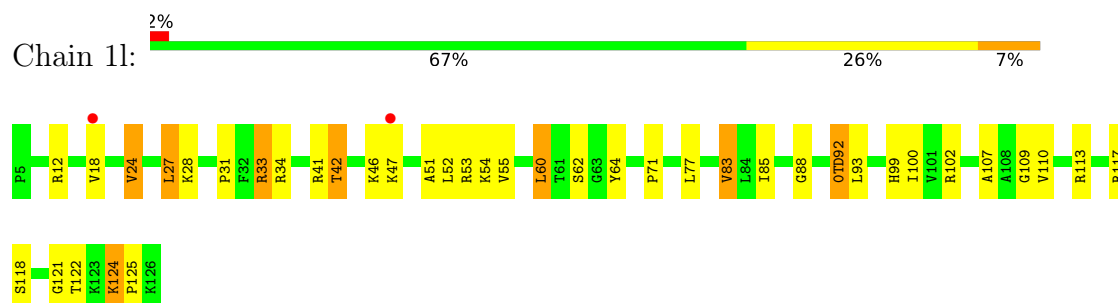
- Molecule 42: 30S ribosomal protein S11



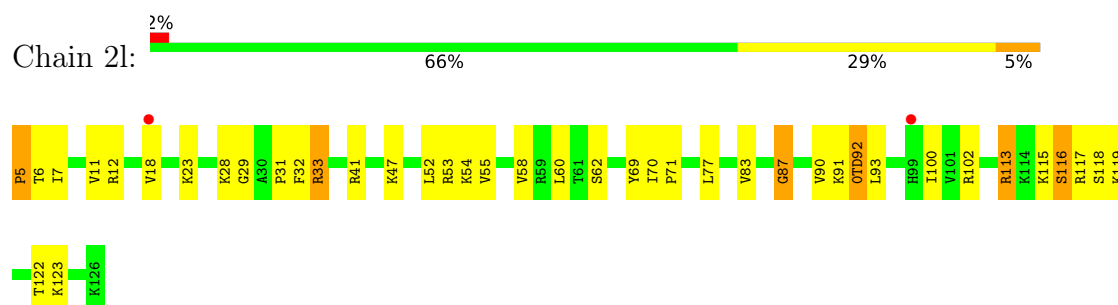
- Molecule 42: 30S ribosomal protein S11



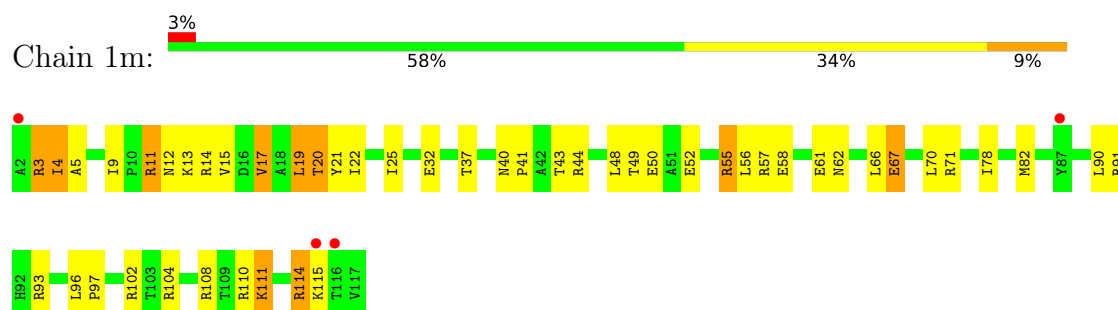
- Molecule 43: 30S ribosomal protein S12



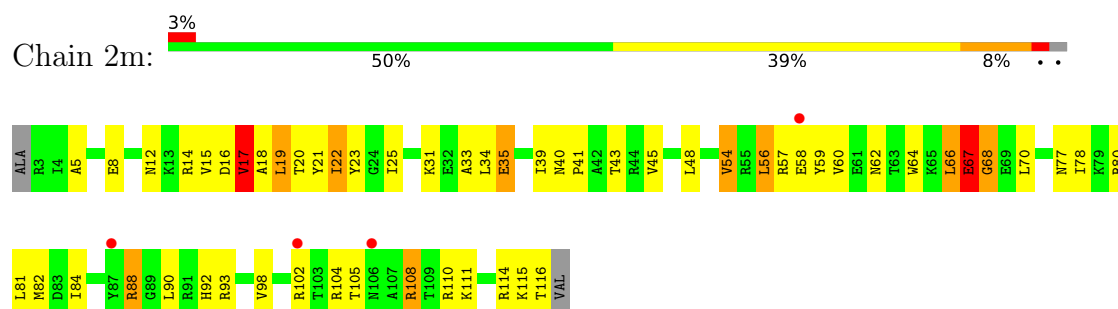
- Molecule 43: 30S ribosomal protein S12



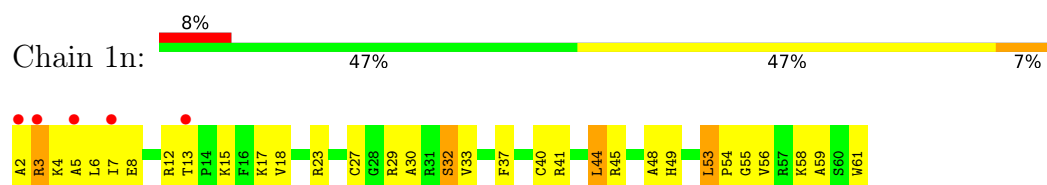
- Molecule 44: 30S ribosomal protein S13



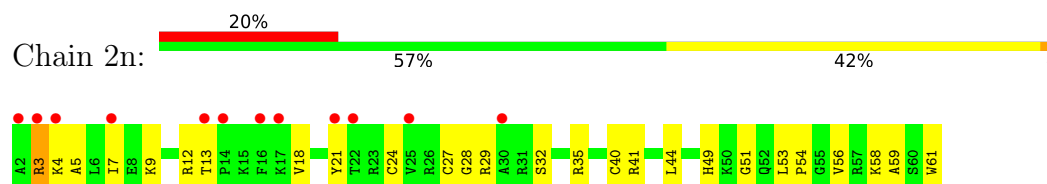
- Molecule 44: 30S ribosomal protein S13



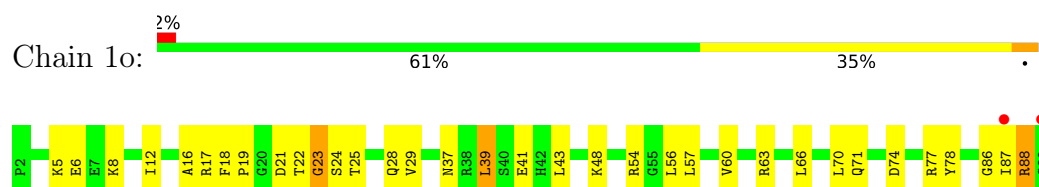
- Molecule 45: 30S ribosomal protein S14 type Z



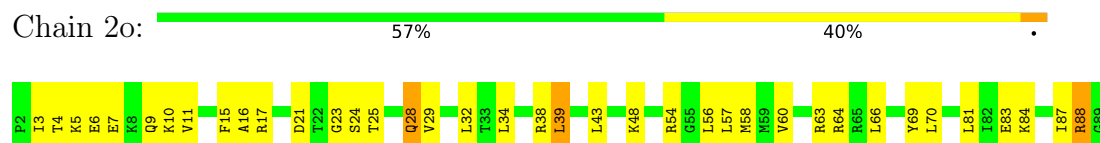
- Molecule 45: 30S ribosomal protein S14 type Z



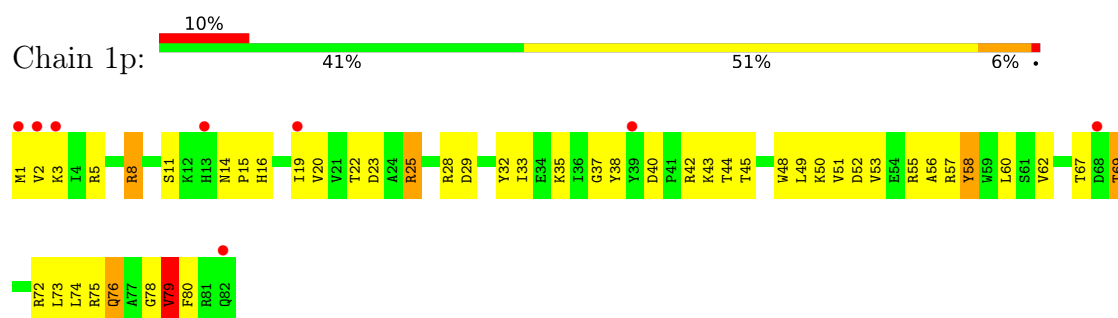
- Molecule 46: 30S ribosomal protein S15



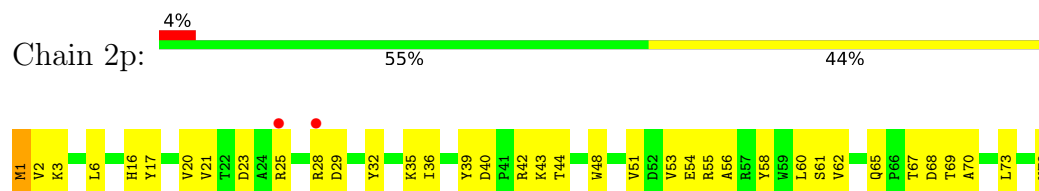
- Molecule 46: 30S ribosomal protein S15



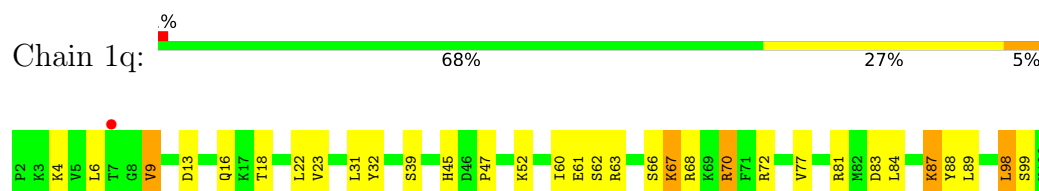
- Molecule 47: 30S ribosomal protein S16



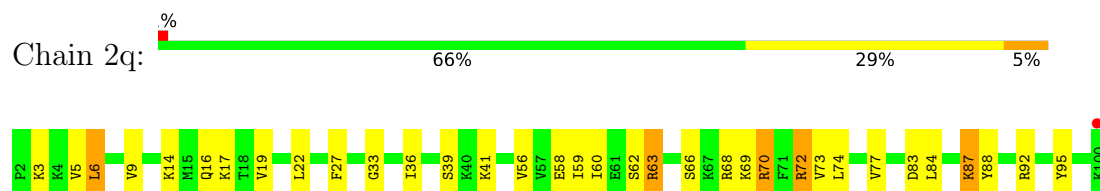
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17

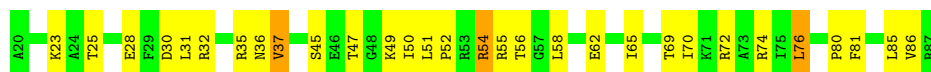


- Molecule 49: 30S ribosomal protein S18

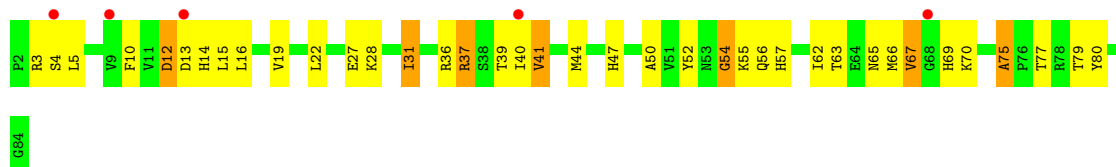




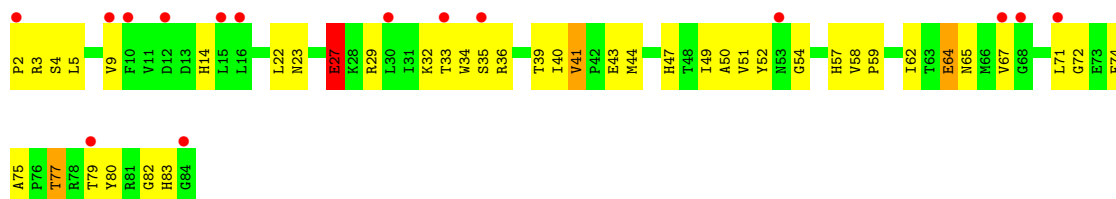
- Molecule 49: 30S ribosomal protein S18



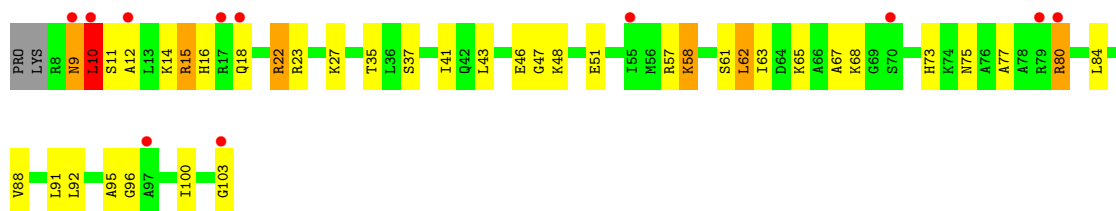
- Molecule 50: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S19

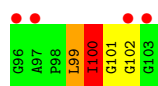


- Molecule 51: 30S ribosomal protein S20

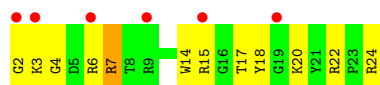


- Molecule 51: 30S ribosomal protein S20

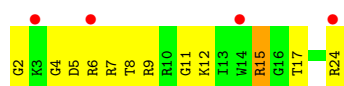




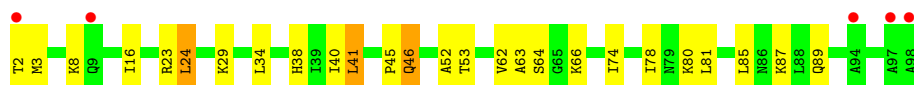
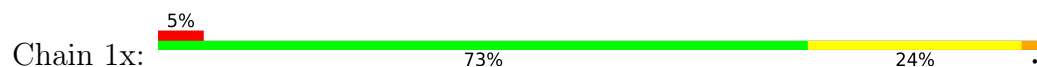
- Molecule 52: 30S ribosomal protein Thx



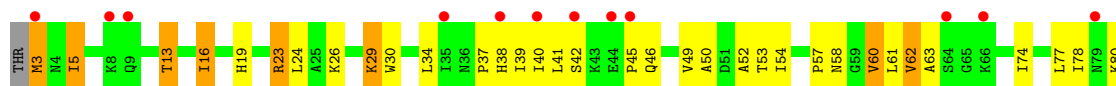
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: Ribosome-associated inhibitor A



- Molecule 53: Ribosome-associated inhibitor A



- Molecule 54: Metalnikowin I



- Molecule 54: Metalnikowin I



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.65Å 448.09Å 623.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 2.90 49.72 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.72-2.90) 99.6 (49.72-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.183 , 0.234 0.184 , 0.232	Depositor DCC
R_{free} test set	69999 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	67.9	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	293484	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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: MG, MA6, 2MG, 5MU, SF4, UR3, M2G, 7MG, ZN, OMG, 2MA, 0TD, 5MC, OMU, 4OC, PSU, AMP

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	0.85	1/69021 (0.0%)	0.94	43/107735 (0.0%)
1	2A	0.65	1/68892 (0.0%)	0.82	34/107529 (0.0%)
2	1B	0.66	0/2879	0.90	1/4490 (0.0%)
2	2B	0.53	0/2874	0.78	1/4482 (0.0%)
3	1D	1.23	6/2181 (0.3%)	1.40	27/2940 (0.9%)
3	2D	1.02	2/2186 (0.1%)	1.28	12/2944 (0.4%)
4	1E	1.29	7/1592 (0.4%)	1.35	7/2149 (0.3%)
4	2E	0.99	0/1592	1.26	5/2149 (0.2%)
5	1F	1.22	2/1619 (0.1%)	1.38	13/2193 (0.6%)
5	2F	0.90	0/1609	1.24	8/2181 (0.4%)
6	1G	0.85	0/1451	1.24	11/1961 (0.6%)
6	2G	0.82	0/1449	1.25	15/1957 (0.8%)
7	1H	1.06	1/1356 (0.1%)	1.31	10/1834 (0.5%)
7	2H	0.87	0/1350	1.29	10/1826 (0.5%)
8	1I	0.93	0/1109	1.29	11/1512 (0.7%)
8	2I	0.86	0/1091	1.20	5/1490 (0.3%)
9	1N	1.21	2/1148 (0.2%)	1.27	3/1547 (0.2%)
9	2N	0.81	1/1144 (0.1%)	1.23	9/1543 (0.6%)
10	1O	1.27	2/943 (0.2%)	1.36	7/1269 (0.6%)
10	2O	0.96	0/943	1.21	0/1269
11	1P	1.09	1/1152 (0.1%)	1.31	2/1533 (0.1%)
11	2P	0.84	0/1152	1.16	2/1533 (0.1%)
12	1Q	1.19	2/1143 (0.2%)	1.26	2/1527 (0.1%)
12	2Q	0.86	0/1143	1.13	3/1527 (0.2%)
13	1R	1.25	1/982 (0.1%)	1.30	9/1312 (0.7%)
13	2R	0.96	0/982	1.18	4/1312 (0.3%)
14	1S	0.94	0/887	1.24	2/1180 (0.2%)
14	2S	0.74	0/880	1.14	3/1172 (0.3%)
15	1T	1.14	2/1105 (0.2%)	1.29	5/1477 (0.3%)
15	2T	0.90	0/1097	1.25	6/1468 (0.4%)
16	1U	1.34	1/977 (0.1%)	1.28	4/1301 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.92	1/977 (0.1%)	1.14	0/1301
17	1V	1.13	0/786	1.28	0/1053
17	2V	0.81	0/782	1.12	1/1049 (0.1%)
18	1W	1.36	1/891 (0.1%)	1.33	2/1198 (0.2%)
18	2W	1.09	1/888 (0.1%)	1.17	3/1194 (0.3%)
19	1X	1.21	1/764 (0.1%)	1.33	3/1025 (0.3%)
19	2X	0.92	0/764	1.18	3/1025 (0.3%)
20	1Y	1.16	2/823 (0.2%)	1.40	4/1099 (0.4%)
20	2Y	0.95	0/823	1.28	2/1100 (0.2%)
21	1Z	0.97	2/1620 (0.1%)	1.28	10/2200 (0.5%)
21	2Z	0.82	0/1590	1.25	12/2162 (0.6%)
22	10	1.12	1/616 (0.2%)	1.20	0/821
22	20	0.82	1/616 (0.2%)	1.21	7/821 (0.9%)
23	11	1.23	3/761 (0.4%)	1.35	6/1013 (0.6%)
23	21	1.01	0/766	1.21	2/1018 (0.2%)
24	12	1.09	1/590 (0.2%)	1.20	0/781
24	22	0.83	0/594	1.20	1/785 (0.1%)
25	13	1.17	0/474	1.37	2/635 (0.3%)
25	23	0.80	0/469	1.11	0/630
26	14	1.02	2/559 (0.4%)	1.33	4/754 (0.5%)
26	24	1.08	1/549 (0.2%)	1.34	5/741 (0.7%)
27	15	1.31	3/473 (0.6%)	1.47	6/639 (0.9%)
27	25	0.99	1/469 (0.2%)	1.19	3/635 (0.5%)
28	16	1.14	0/460	1.21	1/613 (0.2%)
28	26	0.90	0/456	1.12	1/608 (0.2%)
29	17	1.31	0/426	1.30	1/561 (0.2%)
29	27	1.05	0/426	1.20	2/561 (0.4%)
30	18	1.26	0/525	1.27	1/691 (0.1%)
30	28	0.91	0/525	1.17	4/691 (0.6%)
31	19	1.11	0/310	1.33	0/407
31	29	0.71	0/310	1.09	0/407
32	1a	0.59	0/35795	0.80	16/55864 (0.0%)
32	2a	0.56	1/35890 (0.0%)	0.78	20/56012 (0.0%)
33	1b	0.85	0/1876	1.31	16/2533 (0.6%)
33	2b	0.88	1/1860 (0.1%)	1.28	17/2518 (0.7%)
34	1c	0.83	0/1582	1.20	9/2137 (0.4%)
34	2c	0.93	0/1566	1.26	11/2119 (0.5%)
35	1d	0.85	0/1695	1.21	15/2274 (0.7%)
35	2d	0.87	2/1698 (0.1%)	1.26	10/2277 (0.4%)
36	1e	0.81	0/1149	1.21	5/1548 (0.3%)
36	2e	0.84	0/1149	1.30	13/1548 (0.8%)
37	1f	0.83	0/827	1.17	3/1120 (0.3%)
37	2f	0.85	1/829 (0.1%)	1.18	4/1123 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.75	0/1254	1.15	4/1683 (0.2%)
38	2g	0.78	0/1248	1.20	6/1676 (0.4%)
39	1h	0.81	0/1118	1.20	5/1506 (0.3%)
39	2h	0.76	0/1108	1.26	7/1494 (0.5%)
40	1i	0.84	0/1005	1.16	6/1351 (0.4%)
40	2i	0.93	0/985	1.19	1/1329 (0.1%)
41	1j	1.01	0/732	1.28	8/993 (0.8%)
41	2j	1.03	0/723	1.25	6/984 (0.6%)
42	1k	0.86	0/849	1.20	4/1150 (0.3%)
42	2k	0.84	1/848 (0.1%)	1.27	11/1149 (1.0%)
43	1l	0.86	0/937	1.25	5/1260 (0.4%)
43	2l	0.83	0/937	1.24	7/1260 (0.6%)
44	1m	0.76	0/924	1.16	3/1242 (0.2%)
44	2m	0.86	1/905 (0.1%)	1.22	5/1217 (0.4%)
45	1n	0.77	0/501	1.23	2/664 (0.3%)
45	2n	0.73	0/501	1.06	0/664
46	1o	0.86	0/739	1.24	5/985 (0.5%)
46	2o	0.77	0/739	1.06	0/985
47	1p	0.81	0/697	1.16	1/939 (0.1%)
47	2p	0.84	0/693	1.19	0/935
48	1q	0.85	0/836	1.19	3/1117 (0.3%)
48	2q	0.78	0/836	1.11	2/1117 (0.2%)
49	1r	0.83	0/560	1.14	0/746
49	2r	0.82	0/560	1.06	0/746
50	1s	0.77	0/663	1.20	5/895 (0.6%)
50	2s	0.90	0/660	1.20	6/893 (0.7%)
51	1t	0.79	0/734	1.31	5/969 (0.5%)
51	2t	0.84	0/736	1.22	3/976 (0.3%)
52	1u	0.69	0/203	1.00	0/266
52	2u	0.73	0/203	1.24	0/266
53	1x	0.87	0/776	1.15	3/1048 (0.3%)
53	2x	0.86	0/761	1.17	1/1030 (0.1%)
54	1y	1.11	0/90	1.20	0/122
54	2y	0.93	0/90	1.17	0/122
All	All	0.79	60/310078 (0.0%)	0.98	613/463412 (0.1%)

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
19	1X	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
19	2X	0	1
33	1b	0	1
All	All	0	3

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1E	123	ALA	CA-CB	-8.68	1.39	1.53
13	1R	38	VAL	CA-CB	-8.61	1.49	1.54
9	1N	85	ILE	CA-CB	-7.42	1.48	1.54
3	2D	240	ALA	CA-CB	-6.91	1.43	1.54
3	1D	199	ALA	CA-CB	-6.87	1.41	1.53

The worst 5 of 613 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1208	C	O5'-P-OP1	-13.15	68.56	108.00
32	2a	1208	C	OP1-P-OP2	-12.36	82.53	119.60
32	1a	1520	G	O5'-P-OP2	12.06	144.18	108.00
32	1a	1520	G	OP1-P-OP2	-11.88	83.94	119.60
32	1a	1520	G	O5'-P-OP1	-11.48	73.56	108.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	1X	93	GLU	Peptide
33	1b	124	SER	Peptide
19	2X	93	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61862	0	31140	668	0
1	2A	61751	0	31143	770	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1B	2575	0	1304	29	0
2	2B	2571	0	1308	40	0
3	1D	2131	0	2207	61	0
3	2D	2136	0	2218	62	0
4	1E	1559	0	1618	47	0
4	2E	1559	0	1618	54	0
5	1F	1584	0	1625	40	0
5	2F	1574	0	1608	41	0
6	1G	1426	0	1445	63	0
6	2G	1424	0	1441	65	0
7	1H	1330	0	1407	30	0
7	2H	1324	0	1402	36	0
8	1I	1094	0	1127	44	0
8	2I	1076	0	1094	53	0
9	1N	1121	0	1195	22	0
9	2N	1117	0	1184	25	0
10	1O	933	0	996	21	0
10	2O	933	0	996	22	0
11	1P	1135	0	1212	34	0
11	2P	1135	0	1212	30	0
12	1Q	1122	0	1179	31	0
12	2Q	1122	0	1179	43	0
13	1R	968	0	1033	16	0
13	2R	968	0	1033	22	0
14	1S	877	0	938	30	0
14	2S	870	0	923	38	0
15	1T	1091	0	1151	25	0
15	2T	1083	0	1136	32	0
16	1U	959	0	1019	29	0
16	2U	959	0	1019	32	0
17	1V	775	0	841	15	0
17	2V	771	0	830	20	0
18	1W	880	0	929	12	0
18	2W	877	0	927	17	0
19	1X	750	0	814	27	0
19	2X	750	0	814	24	0
20	1Y	810	0	892	24	0
20	2Y	810	0	887	24	0
21	1Z	1587	0	1598	31	0
21	2Z	1557	0	1564	47	0
22	10	608	0	622	24	0
22	20	608	0	622	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	11	754	0	823	25	0
23	21	759	0	837	31	0
24	12	588	0	643	13	0
24	22	592	0	654	10	0
25	13	469	0	518	10	0
25	23	464	0	514	11	0
26	14	546	0	522	21	0
26	24	536	0	514	36	0
27	15	459	0	476	18	0
27	25	455	0	465	16	0
28	16	453	0	473	10	0
28	26	449	0	469	11	0
29	17	418	0	467	15	0
29	27	418	0	467	9	0
30	18	517	0	582	11	0
30	28	517	0	582	17	0
31	19	307	0	335	11	0
31	29	307	0	335	9	0
32	1a	32246	0	16296	659	0
32	2a	32331	0	16339	724	0
33	1b	1842	0	1862	101	0
33	2b	1825	0	1828	100	0
34	1c	1558	0	1557	60	0
34	2c	1542	0	1517	59	0
35	1d	1665	0	1687	86	0
35	2d	1668	0	1703	82	0
36	1e	1133	0	1191	49	0
36	2e	1133	0	1191	49	0
37	1f	814	0	808	36	0
37	2f	816	0	808	32	0
38	1g	1235	0	1249	41	0
38	2g	1229	0	1238	33	0
39	1h	1098	0	1143	55	0
39	2h	1088	0	1126	50	0
40	1i	986	0	990	47	0
40	2i	966	0	953	59	0
41	1j	719	0	672	48	0
41	2j	710	0	661	39	0
42	1k	834	0	838	27	0
42	2k	833	0	836	21	0
43	1l	932	0	981	27	0
43	2l	932	0	981	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	1m	914	0	954	32	0
44	2m	895	0	920	46	0
45	1n	492	0	529	28	0
45	2n	492	0	529	21	0
46	1o	728	0	760	22	0
46	2o	728	0	760	25	0
47	1p	681	0	697	43	0
47	2p	677	0	686	33	0
48	1q	823	0	891	25	0
48	2q	823	0	891	26	0
49	1r	555	0	618	21	0
49	2r	555	0	618	26	0
50	1s	648	0	658	30	0
50	2s	645	0	635	33	0
51	1t	732	0	809	31	0
51	2t	733	0	795	28	0
52	1u	199	0	208	8	0
52	2u	199	0	208	8	0
53	1x	764	0	786	20	0
53	2x	749	0	757	31	0
54	1y	87	0	88	1	0
54	2y	87	0	88	0	0
55	10	8	0	0	0	0
55	11	3	0	0	0	0
55	13	2	0	0	0	0
55	15	6	0	0	0	0
55	17	5	0	0	0	0
55	18	3	0	0	0	0
55	19	2	0	0	0	0
55	1A	917	0	0	0	0
55	1B	24	0	0	0	0
55	1D	18	0	0	0	0
55	1E	8	0	0	0	0
55	1F	16	0	0	0	0
55	1G	3	0	0	0	0
55	1H	2	0	0	0	0
55	1N	3	0	0	0	0
55	1P	4	0	0	0	0
55	1Q	5	0	0	0	0
55	1R	5	0	0	0	0
55	1S	1	0	0	0	0
55	1T	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	1U	7	0	0	0	0
55	1V	3	0	0	0	0
55	1W	3	0	0	0	0
55	1X	1	0	0	0	0
55	1Y	1	0	0	0	0
55	1a	223	0	0	0	0
55	1b	1	0	0	0	0
55	1d	5	0	0	0	0
55	1e	2	0	0	0	0
55	1f	1	0	0	0	0
55	1g	1	0	0	0	0
55	1h	2	0	0	0	0
55	1k	1	0	0	0	0
55	1l	1	0	0	0	0
55	1m	1	0	0	0	0
55	1n	1	0	0	0	0
55	1o	1	0	0	0	0
55	1t	1	0	0	0	0
55	20	6	0	0	0	0
55	21	2	0	0	0	0
55	23	1	0	0	0	0
55	25	3	0	0	0	0
55	27	4	0	0	0	0
55	28	3	0	0	0	0
55	2A	821	0	0	0	0
55	2B	18	0	0	0	0
55	2D	11	0	0	0	0
55	2E	7	0	0	0	0
55	2F	10	0	0	0	0
55	2G	3	0	0	0	0
55	2H	1	0	0	0	0
55	2N	1	0	0	0	0
55	2P	2	0	0	0	0
55	2Q	5	0	0	0	0
55	2R	3	0	0	0	0
55	2S	1	0	0	0	0
55	2T	1	0	0	0	0
55	2U	4	0	0	0	0
55	2V	5	0	0	0	0
55	2W	1	0	0	0	0
55	2X	3	0	0	0	0
55	2a	196	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	2b	1	0	0	0	0
55	2d	4	0	0	0	0
55	2e	2	0	0	0	0
55	2f	1	0	0	0	0
55	2g	1	0	0	0	0
55	2h	1	0	0	0	0
55	2l	1	0	0	0	0
55	2m	1	0	0	0	0
55	2n	2	0	0	0	0
55	2o	1	0	0	0	0
56	1B	1	0	0	6	0
56	2A	1	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	0	0
58	2d	8	0	0	0	0
59	10	4	0	0	0	0
59	11	2	0	0	0	0
59	13	1	0	0	0	0
59	15	2	0	0	0	0
59	16	3	0	0	0	0
59	17	1	0	0	0	0
59	18	7	0	0	0	0
59	19	2	0	0	0	0
59	1A	1740	0	0	5	0
59	1B	42	0	0	0	0
59	1D	14	0	0	0	0
59	1E	18	0	0	0	0
59	1F	11	0	0	0	0
59	1G	2	0	0	0	0
59	1H	3	0	0	0	0
59	1N	9	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1P	13	0	0	0	0
59	1Q	5	0	0	0	0
59	1R	3	0	0	0	0
59	1T	5	0	0	0	0
59	1U	6	0	0	1	0
59	1V	4	0	0	0	0
59	1W	2	0	0	0	0
59	1X	1	0	0	0	0
59	1Y	5	0	0	1	0
59	1a	393	0	0	1	0
59	1d	10	0	0	1	0
59	1e	3	0	0	0	0
59	1f	1	0	0	0	0
59	1h	1	0	0	0	0
59	1j	1	0	0	0	0
59	1l	3	0	0	0	0
59	1m	2	0	0	1	0
59	1n	1	0	0	0	0
59	1o	1	0	0	0	0
59	1t	2	0	0	0	0
59	20	6	0	0	0	0
59	21	3	0	0	0	0
59	23	1	0	0	0	0
59	25	2	0	0	0	0
59	26	2	0	0	0	0
59	27	1	0	0	0	0
59	28	5	0	0	0	0
59	29	1	0	0	0	0
59	2A	1666	0	0	8	0
59	2B	35	0	0	1	0
59	2D	12	0	0	0	0
59	2E	17	0	0	1	0
59	2F	11	0	0	0	0
59	2G	2	0	0	0	0
59	2H	3	0	0	2	0
59	2N	1	0	0	0	0
59	2P	9	0	0	0	0
59	2Q	5	0	0	0	0
59	2R	3	0	0	0	0
59	2T	3	0	0	0	0
59	2U	2	0	0	1	0
59	2V	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	2W	2	0	0	0	0
59	2X	6	0	0	0	0
59	2Y	3	0	0	0	0
59	2a	384	0	0	1	0
59	2c	1	0	0	0	0
59	2d	7	0	0	0	0
59	2e	4	0	0	0	0
59	2f	1	0	0	0	0
59	2h	1	0	0	0	0
59	2j	1	0	0	0	0
59	2l	3	0	0	0	0
59	2m	3	0	0	1	0
59	2o	1	0	0	0	0
59	2p	1	0	0	0	0
59	2t	1	0	0	0	0
All	All	293484	0	194466	5387	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 11.

The worst 5 of 5387 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)
1:2A:2552:OMU:C5	1:2A:2552:OMU:C4	1.75	1.57
1:1A:1405:A:N6	1:1A:1418:U:H3	1.21	1.38
1:1A:9:U:N3	1:1A:2641:A:H2	1.35	1.19
1:1A:2331:G:H22	14:1S:3:ARG:HD3	1.05	1.12
1:1A:1405:A:N1	1:1A:1418:U:O4	1.84	1.10

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/275 (99%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/275 (99%)	256 (94%)	17 (6%)	0	100	100
4	1E	202/204 (99%)	192 (95%)	9 (4%)	1 (0%)	24	54
4	2E	202/204 (99%)	191 (95%)	10 (5%)	1 (0%)	24	54
5	1F	201/203 (99%)	193 (96%)	7 (4%)	1 (0%)	24	54
5	2F	201/203 (99%)	192 (96%)	7 (4%)	2 (1%)	12	39
6	1G	179/181 (99%)	163 (91%)	12 (7%)	4 (2%)	5	20
6	2G	179/181 (99%)	163 (91%)	13 (7%)	3 (2%)	7	26
7	1H	172/174 (99%)	163 (95%)	9 (5%)	0	100	100
7	2H	171/174 (98%)	164 (96%)	7 (4%)	0	100	100
8	1I	145/147 (99%)	127 (88%)	15 (10%)	3 (2%)	5	21
8	2I	144/147 (98%)	125 (87%)	16 (11%)	3 (2%)	5	21
9	1N	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
9	2N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
10	1O	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	16	44
10	2O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	44
11	1P	147/149 (99%)	139 (95%)	8 (5%)	0	100	100
11	2P	147/149 (99%)	137 (93%)	9 (6%)	1 (1%)	18	48
12	1Q	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	18	48
12	2Q	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	18	48
13	1R	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
13	2R	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
14	1S	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	14	41
14	2S	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	14	41
15	1T	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
15	2T	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
16	1U	114/116 (98%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/116 (98%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	39
17	2V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	12	39
18	1W	110/112 (98%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/112 (98%)	109 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/95 (98%)	88 (95%)	5 (5%)	0	100	100
20	1Y	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
20	2Y	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
21	1Z	201/203 (99%)	187 (93%)	14 (7%)	0	100	100
21	2Z	199/203 (98%)	189 (95%)	10 (5%)	0	100	100
22	10	75/77 (97%)	70 (93%)	5 (7%)	0	100	100
22	20	75/77 (97%)	70 (93%)	5 (7%)	0	100	100
23	11	95/97 (98%)	94 (99%)	0	1 (1%)	11	36
23	21	95/97 (98%)	93 (98%)	1 (1%)	1 (1%)	11	36
24	12	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
24	22	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
25	13	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
25	23	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
26	14	67/69 (97%)	52 (78%)	11 (16%)	4 (6%)	1	4
26	24	67/69 (97%)	52 (78%)	10 (15%)	5 (8%)	1	2
27	15	57/59 (97%)	57 (100%)	0	0	100	100
27	25	57/59 (97%)	57 (100%)	0	0	100	100
28	16	51/53 (96%)	50 (98%)	1 (2%)	0	100	100
28	26	51/53 (96%)	50 (98%)	1 (2%)	0	100	100
29	17	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
29	27	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
30	18	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
30	28	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/231 (99%)	190 (83%)	27 (12%)	12 (5%)	1	5
33	2b	229/231 (99%)	192 (84%)	27 (12%)	10 (4%)	2	8
34	1c	204/206 (99%)	171 (84%)	31 (15%)	2 (1%)	12	39
34	2c	204/206 (99%)	176 (86%)	25 (12%)	3 (2%)	8	28
35	1d	206/208 (99%)	183 (89%)	19 (9%)	4 (2%)	6	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/208 (99%)	186 (90%)	17 (8%)	3 (2%)	8	28
36	1e	146/148 (99%)	126 (86%)	19 (13%)	1 (1%)	18	48
36	2e	146/148 (99%)	129 (88%)	16 (11%)	1 (1%)	18	48
37	1f	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
37	2f	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
38	1g	153/155 (99%)	143 (94%)	9 (6%)	1 (1%)	18	48
38	2g	153/155 (99%)	142 (93%)	8 (5%)	3 (2%)	6	22
39	1h	135/137 (98%)	123 (91%)	12 (9%)	0	100	100
39	2h	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
40	1i	125/127 (98%)	107 (86%)	15 (12%)	3 (2%)	4	18
40	2i	124/127 (98%)	105 (85%)	15 (12%)	4 (3%)	3	13
41	1j	95/97 (98%)	79 (83%)	13 (14%)	3 (3%)	3	13
41	2j	94/97 (97%)	79 (84%)	12 (13%)	3 (3%)	3	13
42	1k	112/114 (98%)	100 (89%)	11 (10%)	1 (1%)	14	41
42	2k	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
43	1l	119/122 (98%)	112 (94%)	7 (6%)	0	100	100
43	2l	119/122 (98%)	113 (95%)	6 (5%)	0	100	100
44	1m	114/116 (98%)	104 (91%)	5 (4%)	5 (4%)	2	8
44	2m	112/116 (97%)	103 (92%)	7 (6%)	2 (2%)	6	25
45	1n	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
45	2n	58/60 (97%)	52 (90%)	6 (10%)	0	100	100
46	1o	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	10	34
46	2o	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	10	34
47	1p	80/82 (98%)	67 (84%)	12 (15%)	1 (1%)	9	32
47	2p	80/82 (98%)	65 (81%)	15 (19%)	0	100	100
48	1q	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
48	2q	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
49	1r	66/68 (97%)	61 (92%)	4 (6%)	1 (2%)	8	28
49	2r	66/68 (97%)	62 (94%)	3 (4%)	1 (2%)	8	28
50	1s	81/83 (98%)	73 (90%)	6 (7%)	2 (2%)	4	17
50	2s	81/83 (98%)	74 (91%)	7 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1t	94/98 (96%)	87 (93%)	6 (6%)	1 (1%)	11	36
51	2t	96/98 (98%)	85 (88%)	8 (8%)	3 (3%)	3	14
52	1u	21/23 (91%)	19 (90%)	0	2 (10%)	0	1
52	2u	21/23 (91%)	17 (81%)	3 (14%)	1 (5%)	2	7
53	1x	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
53	2x	94/97 (97%)	90 (96%)	4 (4%)	0	100	100
54	1y	8/10 (80%)	8 (100%)	0	0	100	100
54	2y	8/10 (80%)	8 (100%)	0	0	100	100
All	All	11645/11862 (98%)	10762 (92%)	770 (7%)	113 (1%)	12	39

5 of 113 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1E	52	LEU
6	1G	49	ASP
6	1G	51	ARG
6	1G	78	SER
8	1I	73	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	214/217 (99%)	187 (87%)	27 (13%)	4	14
3	2D	215/217 (99%)	193 (90%)	22 (10%)	7	23
4	1E	164/165 (99%)	145 (88%)	19 (12%)	5	18
4	2E	164/165 (99%)	143 (87%)	21 (13%)	4	14
5	1F	160/161 (99%)	132 (82%)	28 (18%)	2	6
5	2F	158/161 (98%)	139 (88%)	19 (12%)	5	16
6	1G	144/155 (93%)	128 (89%)	16 (11%)	6	20
6	2G	142/155 (92%)	131 (92%)	11 (8%)	12	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	1H	144/145 (99%)	128 (89%)	16 (11%)	6	20
7	2H	143/145 (99%)	119 (83%)	24 (17%)	2	7
8	1I	111/123 (90%)	94 (85%)	17 (15%)	3	9
8	2I	108/123 (88%)	91 (84%)	17 (16%)	2	9
9	1N	119/119 (100%)	104 (87%)	15 (13%)	4	14
9	2N	118/119 (99%)	103 (87%)	15 (13%)	4	14
10	1O	100/100 (100%)	87 (87%)	13 (13%)	4	13
10	2O	100/100 (100%)	91 (91%)	9 (9%)	9	28
11	1P	115/116 (99%)	103 (90%)	12 (10%)	7	23
11	2P	115/116 (99%)	105 (91%)	10 (9%)	9	30
12	1Q	111/111 (100%)	100 (90%)	11 (10%)	7	24
12	2Q	111/111 (100%)	97 (87%)	14 (13%)	4	14
13	1R	101/101 (100%)	85 (84%)	16 (16%)	2	8
13	2R	101/101 (100%)	85 (84%)	16 (16%)	2	8
14	1S	87/87 (100%)	77 (88%)	10 (12%)	5	18
14	2S	85/87 (98%)	75 (88%)	10 (12%)	5	17
15	1T	115/115 (100%)	107 (93%)	8 (7%)	14	40
15	2T	113/115 (98%)	105 (93%)	8 (7%)	13	40
16	1U	93/93 (100%)	81 (87%)	12 (13%)	4	13
16	2U	93/93 (100%)	85 (91%)	8 (9%)	10	30
17	1V	81/82 (99%)	68 (84%)	13 (16%)	2	8
17	2V	80/82 (98%)	68 (85%)	12 (15%)	3	10
18	1W	89/91 (98%)	80 (90%)	9 (10%)	7	24
18	2W	88/91 (97%)	80 (91%)	8 (9%)	9	28
19	1X	77/77 (100%)	70 (91%)	7 (9%)	9	28
19	2X	77/77 (100%)	75 (97%)	2 (3%)	40	73
20	1Y	86/88 (98%)	75 (87%)	11 (13%)	4	14
20	2Y	86/88 (98%)	74 (86%)	12 (14%)	3	11
21	1Z	169/176 (96%)	143 (85%)	26 (15%)	2	9
21	2Z	165/176 (94%)	143 (87%)	22 (13%)	4	12
22	10	61/62 (98%)	54 (88%)	7 (12%)	5	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	20	61/62 (98%)	57 (93%)	4 (7%)	15	43
23	11	79/82 (96%)	71 (90%)	8 (10%)	7	24
23	21	81/82 (99%)	72 (89%)	9 (11%)	6	20
24	12	65/66 (98%)	61 (94%)	4 (6%)	16	46
24	22	66/66 (100%)	60 (91%)	6 (9%)	9	28
25	13	51/51 (100%)	46 (90%)	5 (10%)	7	25
25	23	50/51 (98%)	45 (90%)	5 (10%)	7	24
26	14	58/62 (94%)	48 (83%)	10 (17%)	2	7
26	24	54/62 (87%)	46 (85%)	8 (15%)	3	10
27	15	51/51 (100%)	45 (88%)	6 (12%)	5	17
27	25	50/51 (98%)	46 (92%)	4 (8%)	11	34
28	16	51/51 (100%)	45 (88%)	6 (12%)	5	17
28	26	50/51 (98%)	46 (92%)	4 (8%)	11	34
29	17	41/41 (100%)	37 (90%)	4 (10%)	7	25
29	27	41/41 (100%)	38 (93%)	3 (7%)	13	38
30	18	54/54 (100%)	50 (93%)	4 (7%)	13	38
30	28	54/54 (100%)	48 (89%)	6 (11%)	6	20
31	19	34/34 (100%)	32 (94%)	2 (6%)	18	48
31	29	34/34 (100%)	32 (94%)	2 (6%)	18	48
33	1b	191/199 (96%)	163 (85%)	28 (15%)	3	10
33	2b	187/199 (94%)	155 (83%)	32 (17%)	2	7
34	1c	144/160 (90%)	134 (93%)	10 (7%)	14	41
34	2c	140/160 (88%)	122 (87%)	18 (13%)	4	13
35	1d	171/180 (95%)	149 (87%)	22 (13%)	4	13
35	2d	172/180 (96%)	155 (90%)	17 (10%)	7	24
36	1e	114/114 (100%)	100 (88%)	14 (12%)	4	15
36	2e	114/114 (100%)	100 (88%)	14 (12%)	4	15
37	1f	85/90 (94%)	78 (92%)	7 (8%)	10	32
37	2f	85/90 (94%)	80 (94%)	5 (6%)	18	48
38	1g	120/126 (95%)	110 (92%)	10 (8%)	10	32
38	2g	119/126 (94%)	109 (92%)	10 (8%)	10	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	1h	116/118 (98%)	103 (89%)	13 (11%)	6	19
39	2h	114/118 (97%)	103 (90%)	11 (10%)	8	26
40	1i	91/98 (93%)	80 (88%)	11 (12%)	5	16
40	2i	88/98 (90%)	79 (90%)	9 (10%)	7	23
41	1j	68/87 (78%)	63 (93%)	5 (7%)	13	38
41	2j	68/87 (78%)	62 (91%)	6 (9%)	9	29
42	1k	83/86 (96%)	78 (94%)	5 (6%)	17	47
42	2k	83/86 (96%)	73 (88%)	10 (12%)	5	16
43	1l	96/102 (94%)	88 (92%)	8 (8%)	10	32
43	2l	96/102 (94%)	88 (92%)	8 (8%)	10	32
44	1m	90/94 (96%)	79 (88%)	11 (12%)	5	16
44	2m	87/94 (93%)	74 (85%)	13 (15%)	3	10
45	1n	49/49 (100%)	41 (84%)	8 (16%)	2	8
45	2n	49/49 (100%)	44 (90%)	5 (10%)	7	23
46	1o	78/79 (99%)	73 (94%)	5 (6%)	16	44
46	2o	78/79 (99%)	71 (91%)	7 (9%)	9	28
47	1p	69/71 (97%)	56 (81%)	13 (19%)	1	5
47	2p	68/71 (96%)	61 (90%)	7 (10%)	7	23
48	1q	94/94 (100%)	85 (90%)	9 (10%)	8	26
48	2q	94/94 (100%)	86 (92%)	8 (8%)	10	31
49	1r	59/59 (100%)	53 (90%)	6 (10%)	7	23
49	2r	59/59 (100%)	51 (86%)	8 (14%)	3	12
50	1s	68/72 (94%)	62 (91%)	6 (9%)	9	29
50	2s	67/72 (93%)	58 (87%)	9 (13%)	4	12
51	1t	71/76 (93%)	65 (92%)	6 (8%)	10	31
51	2t	70/76 (92%)	63 (90%)	7 (10%)	7	24
52	1u	18/18 (100%)	17 (94%)	1 (6%)	19	50
52	2u	18/18 (100%)	16 (89%)	2 (11%)	6	20
53	1x	82/83 (99%)	77 (94%)	5 (6%)	17	46
53	2x	79/83 (95%)	67 (85%)	12 (15%)	3	9
54	1y	10/10 (100%)	10 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	2y	10/10 (100%)	10 (100%)	0	100	100
All	All	9540/9882 (96%)	8466 (89%)	1074 (11%)	5	19

5 of 1074 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	2e	41	VAL
39	2h	26	VAL
36	2e	31	LEU
49	2r	65	ILE
35	1d	107	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 146 such sidechains are listed below:

Mol	Chain	Res	Type
35	2d	116	GLN
50	2s	69	HIS
36	2e	72	GLN
41	2j	69	ASN
36	1e	65	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2866/2915 (98%)	414 (14%)	58 (2%)
1	2A	2857/2915 (98%)	426 (14%)	51 (1%)
2	1B	119/120 (99%)	6 (5%)	0
2	2B	118/120 (98%)	8 (6%)	0
32	1a	1497/1521 (98%)	255 (17%)	0
32	2a	1501/1521 (98%)	252 (16%)	0
All	All	8958/9112 (98%)	1361 (15%)	109 (1%)

5 of 1361 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	60	G

5 of 109 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2902	G
1	2A	764	A
1	2A	2288	A
1	2A	196	A
1	2A	310	A

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

48 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
1	PSU	2A	2605	1	18,21,22	1.55	1 (5%)	21,30,33	1.77	2 (9%)
32	5MC	2a	1404	32	19,22,23	0.96	1 (5%)	26,32,35	1.48	5 (19%)
32	7MG	2a	527	32	23,26,27	2.26	7 (30%)	27,39,42	2.01	7 (25%)
1	OMG	2A	2251	1,55	23,26,27	1.61	4 (17%)	32,38,41	2.41	14 (43%)
43	0TD	2l	92	43	8,9,10	2.74	2 (25%)	6,11,13	3.32	4 (66%)
32	PSU	1a	516	32,55	18,21,22	1.56	4 (22%)	21,30,33	2.36	6 (28%)
1	PSU	1A	2617	1	18,21,22	1.44	4 (22%)	21,30,33	1.61	5 (23%)
32	M2G	2a	966	32	24,27,28	2.11	5 (20%)	33,40,43	1.66	8 (24%)
1	5MC	2A	1962	1,55	19,22,23	1.45	2 (10%)	26,32,35	1.52	4 (15%)
32	MA6	2a	1518	32	23,26,27	1.11	2 (8%)	33,38,41	4.04	12 (36%)
32	MA6	2a	1519	32	23,26,27	1.12	2 (8%)	33,38,41	4.45	15 (45%)
32	PSU	2a	516	32	18,21,22	1.81	3 (16%)	21,30,33	2.39	5 (23%)
1	PSU	2A	1911	1	18,21,22	1.54	3 (16%)	21,30,33	1.56	5 (23%)
32	4OC	1a	1402	32	20,23,24	2.27	7 (35%)	25,32,35	1.03	2 (8%)
1	PSU	1A	1933	1	18,21,22	1.19	3 (16%)	21,30,33	1.66	7 (33%)
1	5MC	1A	1984	1,55	19,22,23	1.42	2 (10%)	26,32,35	1.58	5 (19%)
32	5MC	2a	1400	32	19,22,23	0.87	0	26,32,35	1.39	4 (15%)
1	5MC	1A	1964	1	19,22,23	1.56	3 (15%)	26,32,35	1.37	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1A	1939	1,55	18,21,22	1.23	1 (5%)	21,30,33	1.90	6 (28%)
1	5MU	2A	1939	1,55	19,22,23	1.02	1 (5%)	27,32,35	1.52	4 (14%)
32	5MC	2a	967	32	19,22,23	1.55	3 (15%)	26,32,35	1.71	7 (26%)
32	M2G	1a	966	32	24,27,28	1.96	4 (16%)	33,40,43	1.69	8 (24%)
1	4OC	2A	1920	1	19,22,24	2.37	6 (31%)	25,31,35	1.18	3 (12%)
1	5MC	2A	1942	1	19,22,23	1.75	1 (5%)	26,32,35	1.16	3 (11%)
32	5MC	1a	1407	32	19,22,23	1.04	2 (10%)	26,32,35	1.47	5 (19%)
1	4OC	1A	1942	1,55	19,22,24	2.11	5 (26%)	25,31,35	1.31	5 (20%)
1	OMG	1A	2263	1,55	23,26,27	1.73	6 (26%)	32,38,41	2.08	13 (40%)
1	PSU	2A	1917	1	18,21,22	1.13	1 (5%)	21,30,33	1.70	5 (23%)
32	2MG	2a	1207	32	23,26,27	2.27	6 (26%)	33,38,41	2.08	10 (30%)
1	OMU	2A	2552	1,55	19,22,23	6.77	10 (52%)	25,31,34	2.44	7 (28%)
32	MA6	1a	1519	32	23,26,27	1.27	3 (13%)	33,38,41	4.25	14 (42%)
32	5MC	2a	1407	32	19,22,23	1.64	2 (10%)	26,32,35	1.28	3 (11%)
32	UR3	2a	1498	32	19,22,23	1.73	3 (15%)	26,32,35	2.22	8 (30%)
43	0TD	1l	92	43	8,9,10	4.86	3 (37%)	6,11,13	4.40	4 (66%)
32	5MC	1a	967	32	19,22,23	0.95	2 (10%)	26,32,35	1.31	4 (15%)
32	5MC	1a	1400	32	19,22,23	0.93	1 (5%)	26,32,35	1.65	6 (23%)
1	2MA	2A	2503	1,55	22,25,26	2.49	9 (40%)	32,37,40	2.81	10 (31%)
32	UR3	1a	1498	32	19,22,23	1.78	4 (21%)	26,32,35	1.55	3 (11%)
32	MA6	1a	1518	32	23,26,27	1.15	3 (13%)	33,38,41	4.17	13 (39%)
32	5MC	1a	1404	32	19,22,23	1.45	2 (10%)	26,32,35	1.53	4 (15%)
1	2MA	1A	2515	1,55	22,25,26	2.52	8 (36%)	32,37,40	3.09	14 (43%)
1	5MU	2A	1915	1	19,22,23	1.85	2 (10%)	27,32,35	1.70	6 (22%)
1	5MU	1A	1937	1	19,22,23	1.56	3 (15%)	27,32,35	1.87	7 (25%)
1	5MU	1A	1961	1,55	19,22,23	1.02	2 (10%)	27,32,35	1.52	6 (22%)
32	7MG	1a	527	32,55	23,26,27	1.93	7 (30%)	27,39,42	1.81	8 (29%)
32	2MG	1a	1207	32,55	23,26,27	2.10	4 (17%)	33,38,41	2.82	18 (54%)
32	4OC	2a	1402	32	20,23,24	2.63	7 (35%)	25,32,35	1.42	4 (16%)
1	OMU	1A	2564	1,55	19,22,23	6.42	10 (52%)	25,31,34	2.78	9 (36%)

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
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	1/7/25/26	0/2/2/2
32	7MG	2a	527	32	-	2/7/37/38	0/3/3/3
1	OMG	2A	2251	1,55	-	0/9/27/28	0/3/3/3
43	0TD	2l	92	43	-	3/7/12/14	-
32	PSU	1a	516	32,55	-	1/7/25/26	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	5MC	2A	1962	1,55	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	MA6	2a	1519	32	-	6/11/29/30	0/3/3/3
32	PSU	2a	516	32	-	1/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1984	1,55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1964	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1939	1,55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,55	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	4OC	2A	1920	1	-	2/9/27/30	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	4OC	1A	1942	1,55	-	1/9/27/30	0/2/2/2
1	OMG	1A	2263	1,55	-	1/9/27/28	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	OMU	2A	2552	1,55	-	0/9/27/28	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	1/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	6/7/12/14	-
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,55	-	3/7/25/26	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	2MA	1A	2515	1,55	-	1/7/25/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	2A	1915	1	-	3/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	4/7/25/26	0/2/2/2
1	5MU	1A	1961	1,55	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32,55	-	1/7/37/38	0/3/3/3
32	2MG	1a	1207	32,55	-	2/9/27/28	0/3/3/3
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
1	OMU	1A	2564	1,55	-	0/9/27/28	0/2/2/2

The worst 5 of 176 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	OMU	C4-N3	-16.29	1.10	1.38
1	1A	2564	OMU	C4-N3	-15.21	1.12	1.38
1	2A	2552	OMU	C5-C4	14.41	1.75	1.43
1	1A	2564	OMU	C5-C4	14.15	1.74	1.43
43	1l	92	0TD	CB-CA	-12.31	1.50	1.54

The worst 5 of 330 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1519	MA6	N1-C6-N6	-17.35	95.72	116.86
32	1a	1518	MA6	N1-C6-N6	-16.19	97.13	116.86
32	1a	1519	MA6	N1-C6-N6	-15.33	98.18	116.86
32	2a	1518	MA6	N1-C6-N6	-15.28	98.25	116.86
32	2a	1519	MA6	C5-C6-N6	12.01	144.34	125.33

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1937	5MU	O4'-C1'-N1-C2
1	1A	1937	5MU	O4'-C1'-N1-C6
1	1A	1937	5MU	O4'-C4'-C5'-O5'
1	1A	2263	OMG	C1'-C2'-O2'-CM2
32	1a	1402	4OC	O4'-C4'-C5'-O5'

There are no ring outliers.

26 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	2251	OMG	1	0
43	2l	92	0TD	2	0
32	1a	516	PSU	1	0
32	2a	966	M2G	1	0
32	2a	1518	MA6	1	0
32	2a	516	PSU	2	0
32	1a	1402	4OC	2	0
1	1A	1933	PSU	1	0
32	2a	1400	5MC	1	0
32	1a	966	M2G	2	0
1	2A	1920	4OC	1	0
1	2A	1942	5MC	1	0
32	1a	1407	5MC	1	0
1	1A	1942	4OC	1	0
1	2A	1917	PSU	1	0
32	2a	1207	2MG	3	0
1	2A	2552	OMU	2	0
32	1a	1519	MA6	3	0
32	2a	1498	UR3	1	0
43	1l	92	0TD	2	0
1	2A	2503	2MA	1	0
32	1a	1518	MA6	2	0
1	2A	1915	5MU	1	0
1	1A	1961	5MU	2	0
32	1a	1207	2MG	3	0
32	2a	1402	4OC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2435 ligands modelled in this entry, 2431 are monoatomic and 2 are modelled with single atom - 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	2d	501	35	0,12,12	-	-	-		
58	SF4	1d	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	2d	501	35	-	-	0/6/5/5
58	SF4	1d	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2A	2801(A):A	O3'	2802:G	P	3.50

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	2861/2915 (98%)	-0.79	92 (3%) 50 41	16, 34, 100, 113	0
1	2A	2856/2915 (97%)	-0.44	115 (4%) 42 34	31, 56, 101, 114	0
2	1B	120/120 (100%)	-0.78	0 100 100	27, 51, 64, 93	0
2	2B	120/120 (100%)	-0.10	1 (0%) 82 77	60, 79, 88, 96	0
3	1D	275/275 (100%)	-0.61	1 (0%) 88 85	17, 34, 49, 74	0
3	2D	275/275 (100%)	-0.26	3 (1%) 78 71	27, 49, 64, 83	0
4	1E	204/204 (100%)	-0.61	0 100 100	16, 37, 58, 73	0
4	2E	204/204 (100%)	-0.11	1 (0%) 87 83	31, 57, 73, 83	0
5	1F	203/203 (100%)	-0.47	0 100 100	16, 38, 68, 92	0
5	2F	203/203 (100%)	-0.05	0 100 100	33, 66, 82, 91	0
6	1G	181/181 (100%)	0.00	2 (1%) 78 71	47, 66, 83, 95	0
6	2G	181/181 (100%)	0.64	7 (3%) 43 35	76, 85, 92, 98	0
7	1H	174/174 (100%)	-0.30	3 (1%) 69 61	36, 51, 65, 70	0
7	2H	173/174 (99%)	0.66	3 (1%) 69 61	66, 85, 94, 98	0
8	1I	147/147 (100%)	0.12	2 (1%) 73 65	40, 71, 82, 87	0
8	2I	146/147 (99%)	0.41	3 (2%) 63 54	53, 80, 91, 97	0
9	1N	140/140 (100%)	-0.58	0 100 100	19, 33, 57, 73	0
9	2N	140/140 (100%)	-0.07	0 100 100	46, 64, 76, 88	0
10	1O	122/122 (100%)	-0.59	0 100 100	26, 38, 55, 65	0
10	2O	122/122 (100%)	-0.26	0 100 100	41, 54, 68, 76	0
11	1P	149/149 (100%)	-0.51	0 100 100	17, 43, 64, 79	0
11	2P	149/149 (100%)	-0.01	1 (0%) 84 79	38, 66, 83, 91	0
12	1Q	141/141 (100%)	-0.46	0 100 100	25, 38, 53, 68	0
12	2Q	141/141 (100%)	0.02	1 (0%) 84 79	46, 63, 76, 81	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%)	-0.64	0 100 100	21, 32, 51, 61	0
13	2R	118/118 (100%)	-0.22	0 100 100	39, 53, 63, 76	0
14	1S	110/110 (100%)	-0.36	0 100 100	37, 51, 66, 69	0
14	2S	110/110 (100%)	0.57	5 (4%) 38 30	63, 75, 84, 86	0
15	1T	131/131 (100%)	-0.37	2 (1%) 72 64	32, 43, 70, 84	0
15	2T	131/131 (100%)	-0.09	2 (1%) 72 64	48, 59, 79, 86	0
16	1U	116/116 (100%)	-0.80	1 (0%) 81 75	19, 27, 42, 62	0
16	2U	116/116 (100%)	-0.01	0 100 100	41, 61, 77, 86	0
17	1V	101/101 (100%)	-0.79	0 100 100	17, 36, 54, 69	0
17	2V	101/101 (100%)	-0.08	0 100 100	39, 72, 81, 89	0
18	1W	112/112 (100%)	-0.72	1 (0%) 81 75	19, 27, 50, 92	0
18	2W	112/112 (100%)	-0.15	1 (0%) 81 75	38, 48, 67, 87	0
19	1X	95/95 (100%)	-0.43	1 (1%) 78 71	22, 35, 62, 71	0
19	2X	95/95 (100%)	0.14	1 (1%) 78 71	45, 61, 74, 78	0
20	1Y	107/107 (100%)	-0.18	1 (0%) 81 75	32, 47, 68, 78	0
20	2Y	107/107 (100%)	0.53	5 (4%) 36 28	55, 72, 84, 94	0
21	1Z	203/203 (100%)	-0.11	1 (0%) 87 83	40, 58, 77, 88	0
21	2Z	201/203 (99%)	0.37	3 (1%) 72 64	64, 79, 88, 95	0
22	10	77/77 (100%)	-0.51	0 100 100	26, 35, 58, 65	0
22	20	77/77 (100%)	0.35	4 (5%) 33 26	53, 62, 74, 78	0
23	11	97/97 (100%)	-0.34	1 (1%) 79 73	25, 39, 67, 80	0
23	21	97/97 (100%)	-0.11	1 (1%) 79 73	40, 57, 79, 88	0
24	12	70/70 (100%)	-0.22	1 (1%) 73 65	33, 47, 62, 82	0
24	22	70/70 (100%)	0.38	3 (4%) 40 31	61, 71, 81, 83	0
25	13	59/59 (100%)	-0.60	0 100 100	21, 32, 58, 77	0
25	23	59/59 (100%)	-0.02	1 (1%) 69 61	48, 62, 77, 82	0
26	14	69/69 (100%)	0.47	9 (13%) 7 6	63, 82, 96, 98	0
26	24	69/69 (100%)	1.10	12 (17%) 4 3	80, 92, 99, 100	0
27	15	59/59 (100%)	-0.73	0 100 100	15, 32, 48, 62	0
27	25	59/59 (100%)	-0.35	0 100 100	35, 52, 70, 76	0
28	16	53/53 (100%)	-0.62	0 100 100	32, 40, 55, 62	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/53 (100%)	-0.12	1 (1%) 66 58	52, 62, 69, 76	0
29	17	48/48 (100%)	-0.54	3 (6%) 26 20	18, 24, 58, 65	0
29	27	48/48 (100%)	-0.10	2 (4%) 40 32	32, 40, 66, 79	0
30	18	64/64 (100%)	-0.71	0 100 100	23, 30, 39, 48	0
30	28	64/64 (100%)	-0.02	2 (3%) 51 42	41, 54, 64, 72	0
31	19	37/37 (100%)	-0.37	1 (2%) 56 47	30, 40, 59, 71	0
31	29	37/37 (100%)	0.59	1 (2%) 56 47	61, 68, 79, 82	0
32	1a	1488/1521 (97%)	-0.10	29 (1%) 66 58	31, 74, 100, 114	0
32	2a	1492/1521 (98%)	-0.09	18 (1%) 76 69	41, 76, 100, 112	0
33	1b	231/231 (100%)	0.59	11 (4%) 35 28	67, 82, 92, 101	0
33	2b	231/231 (100%)	0.70	15 (6%) 25 20	68, 85, 94, 98	0
34	1c	206/206 (100%)	0.59	7 (3%) 48 39	70, 83, 92, 97	0
34	2c	206/206 (100%)	0.80	11 (5%) 32 25	77, 86, 93, 99	0
35	1d	208/208 (100%)	0.60	6 (2%) 53 45	59, 76, 87, 91	0
35	2d	208/208 (100%)	0.56	5 (2%) 59 50	61, 73, 84, 88	0
36	1e	148/148 (100%)	0.05	1 (0%) 84 79	48, 69, 79, 96	0
36	2e	148/148 (100%)	0.21	2 (1%) 73 65	58, 71, 81, 89	0
37	1f	100/100 (100%)	0.21	0 100 100	53, 73, 80, 84	0
37	2f	100/100 (100%)	0.06	1 (1%) 79 73	57, 70, 82, 87	0
38	1g	155/155 (100%)	0.32	3 (1%) 66 58	67, 77, 86, 90	0
38	2g	155/155 (100%)	0.49	10 (6%) 25 20	73, 81, 89, 95	0
39	1h	137/137 (100%)	0.17	0 100 100	55, 69, 77, 89	0
39	2h	137/137 (100%)	0.23	3 (2%) 62 53	60, 72, 80, 87	0
40	1i	127/127 (100%)	1.09	17 (13%) 7 5	68, 86, 93, 97	0
40	2i	126/127 (99%)	1.29	27 (21%) 2 2	74, 88, 94, 97	0
41	1j	97/97 (100%)	1.19	12 (12%) 8 7	70, 87, 95, 98	0
41	2j	96/97 (98%)	1.30	18 (18%) 3 3	75, 89, 95, 97	0
42	1k	114/114 (100%)	-0.01	1 (0%) 81 75	40, 65, 81, 87	0
42	2k	114/114 (100%)	0.10	0 100 100	54, 71, 85, 91	0
43	1l	121/122 (99%)	0.13	2 (1%) 69 61	47, 63, 75, 78	0
43	2l	121/122 (99%)	0.27	2 (1%) 69 61	54, 66, 75, 80	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/116 (100%)	0.40	4 (3%) 48 39	71, 81, 88, 91	0
44	2m	114/116 (98%)	0.78	4 (3%) 47 38	76, 88, 93, 95	0
45	1n	60/60 (100%)	0.91	5 (8%) 17 14	71, 80, 88, 89	0
45	2n	60/60 (100%)	1.28	12 (20%) 3 2	76, 88, 92, 95	0
46	1o	88/88 (100%)	0.12	2 (2%) 61 52	46, 68, 80, 84	0
46	2o	88/88 (100%)	0.06	0 100 100	55, 71, 83, 86	0
47	1p	82/82 (100%)	0.89	8 (9%) 13 11	64, 77, 86, 90	0
47	2p	82/82 (100%)	0.51	3 (3%) 45 37	58, 70, 79, 86	0
48	1q	99/99 (100%)	0.33	1 (1%) 79 73	53, 68, 80, 84	0
48	2q	99/99 (100%)	0.11	1 (1%) 79 73	57, 70, 79, 83	0
49	1r	68/68 (100%)	0.10	0 100 100	55, 67, 80, 86	0
49	2r	68/68 (100%)	-0.01	0 100 100	61, 71, 82, 86	0
50	1s	83/83 (100%)	0.93	5 (6%) 27 21	76, 84, 91, 94	0
50	2s	83/83 (100%)	1.27	15 (18%) 3 3	84, 90, 97, 99	0
51	1t	96/98 (97%)	0.74	11 (11%) 9 8	64, 75, 86, 92	0
51	2t	98/98 (100%)	0.45	6 (6%) 27 21	56, 69, 83, 85	0
52	1u	23/23 (100%)	1.22	6 (26%) 1 1	72, 77, 83, 85	0
52	2u	23/23 (100%)	1.50	4 (17%) 4 3	79, 86, 89, 90	0
53	1x	97/97 (100%)	0.26	5 (5%) 33 26	52, 67, 81, 86	0
53	2x	96/97 (98%)	0.98	14 (14%) 6 4	72, 82, 93, 96	0
54	1y	10/10 (100%)	-0.37	0 100 100	30, 33, 40, 40	0
54	2y	10/10 (100%)	0.38	0 100 100	43, 47, 58, 58	0
All	All	20786/20974 (99%)	-0.11	608 (2%) 53 45	15, 64, 93, 114	0

The worst 5 of 608 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1133	G	13.9
1	1A	1137	G	10.1
1	1A	1118	C	9.3
1	1A	1135	G	9.0
1	1A	1132	A	8.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	5MU	1A	1937	21/22	0.84	0.11	79,86,100,113	0
32	2MG	2a	1207	24/25	0.86	0.10	81,90,95,99	0
32	PSU	2a	516	20/21	0.88	0.10	72,83,88,90	0
1	5MU	2A	1915	21/22	0.89	0.08	79,87,92,108	0
32	PSU	1a	516	20/21	0.91	0.09	66,74,77,77	0
1	PSU	1A	1939	20/21	0.91	0.10	62,78,87,88	0
32	7MG	2a	527	24/25	0.92	0.12	69,74,77,79	0
1	PSU	2A	1917	20/21	0.92	0.07	72,79,85,102	0
32	5MC	2a	967	21/22	0.93	0.10	67,73,82,90	0
1	PSU	1A	1933	20/21	0.93	0.08	57,70,74,76	0
43	0TD	2l	92	10/11	0.93	0.10	71,73,77,92	0
32	M2G	2a	966	25/26	0.94	0.11	67,71,86,94	0
43	0TD	1l	92	10/11	0.94	0.11	63,65,74,80	0
1	PSU	2A	1911	20/21	0.94	0.07	65,73,80,81	0
32	2MG	1a	1207	24/25	0.94	0.07	76,81,85,85	0
32	M2G	1a	966	25/26	0.95	0.09	52,62,74,77	0
32	4OC	2a	1402	22/23	0.95	0.08	52,60,65,67	0
32	7MG	1a	527	24/25	0.95	0.09	50,63,66,71	0
1	5MC	2A	1962	21/22	0.96	0.08	34,44,51,60	0
32	5MC	1a	1407	21/22	0.96	0.08	44,53,58,61	0
32	5MC	1a	967	21/22	0.96	0.08	57,65,75,83	0
1	4OC	1A	1942	21/23	0.96	0.08	47,59,64,65	0
32	5MC	1a	1400	21/22	0.96	0.09	54,59,64,67	0
32	5MC	1a	1404	21/22	0.96	0.08	44,48,55,59	0
32	5MC	2a	1400	21/22	0.96	0.10	65,74,78,83	0
1	4OC	2A	1920	21/23	0.96	0.08	54,65,70,72	0
32	5MC	2a	1404	21/22	0.96	0.07	49,53,60,64	0
32	5MC	2a	1407	21/22	0.96	0.08	50,59,63,65	0
32	UR3	2a	1498	21/22	0.96	0.07	47,56,64,66	0
1	5MC	2A	1942	21/22	0.96	0.07	46,53,57,61	0
1	2MA	2A	2503	23/24	0.97	0.09	30,35,40,48	0
32	UR3	1a	1498	21/22	0.97	0.08	41,50,56,59	0
32	MA6	1a	1518	24/25	0.97	0.08	38,49,52,57	0
32	4OC	1a	1402	22/23	0.97	0.07	45,52,58,61	0
1	PSU	2A	2605	20/21	0.98	0.07	33,35,41,41	0
1	2MA	1A	2515	23/24	0.98	0.06	16,20,24,25	0
1	OMU	1A	2564	21/22	0.98	0.05	21,26,29,32	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	PSU	1A	2617	20/21	0.98	0.06	20,24,30,33	0
1	5MU	1A	1961	21/22	0.98	0.06	20,26,29,33	0
1	5MC	1A	1964	21/22	0.98	0.05	25,36,39,42	0
1	5MU	2A	1939	21/22	0.98	0.06	30,36,42,44	0
1	5MC	1A	1984	21/22	0.98	0.06	30,32,36,41	0
1	OMG	1A	2263	24/25	0.98	0.05	16,22,25,27	0
1	OMG	2A	2251	24/25	0.98	0.06	35,39,44,46	0
32	MA6	1a	1519	24/25	0.98	0.08	41,50,55,58	0
32	MA6	2a	1518	24/25	0.98	0.07	50,59,65,66	0
32	MA6	2a	1519	24/25	0.98	0.08	52,58,64,69	0
1	OMU	2A	2552	21/22	0.98	0.05	30,36,40,42	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
55	MG	2a	1718	1/1	0.03	0.27	88,88,88,88	0
55	MG	1a	3154	1/1	0.26	0.30	100,100,100,100	0
55	MG	2A	3768	1/1	0.29	0.15	95,95,95,95	0
55	MG	1a	3146	1/1	0.32	0.20	80,80,80,80	0
55	MG	2A	3553	1/1	0.32	0.38	89,89,89,89	0
55	MG	2A	3533	1/1	0.34	0.21	99,99,99,99	0
55	MG	2A	3802	1/1	0.36	0.33	97,97,97,97	0
55	MG	1A	3516	1/1	0.37	0.32	35,35,35,35	0
55	MG	2A	3471	1/1	0.41	0.21	79,79,79,79	0
55	MG	1a	3143	1/1	0.42	0.24	87,87,87,87	0
55	MG	2B	3011	1/1	0.44	0.17	90,90,90,90	0
55	MG	2a	1747	1/1	0.45	0.30	94,94,94,94	0
55	MG	1a	3058	1/1	0.46	0.49	82,82,82,82	0
55	MG	2A	3511	1/1	0.47	0.19	90,90,90,90	0
55	MG	2n	502	1/1	0.48	0.26	82,82,82,82	0
55	MG	2A	3792	1/1	0.51	0.60	79,79,79,79	0
55	MG	1A	3608	1/1	0.51	0.20	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2e	3002	1/1	0.52	0.43	83,83,83,83	0
55	MG	2A	3252	1/1	0.55	0.28	69,69,69,69	0
55	MG	1a	3009	1/1	0.55	0.32	69,69,69,69	0
55	MG	2A	3171	1/1	0.55	0.29	74,74,74,74	0
55	MG	2G	3002	1/1	0.55	0.10	90,90,90,90	0
55	MG	2A	3585	1/1	0.56	0.15	68,68,68,68	0
55	MG	2A	3510	1/1	0.56	0.15	103,103,103,103	0
55	MG	1a	3077	1/1	0.56	0.31	81,81,81,81	0
55	MG	2a	1710	1/1	0.56	0.27	86,86,86,86	0
55	MG	2A	3634	1/1	0.57	0.17	83,83,83,83	0
55	MG	2a	1641	1/1	0.57	0.27	77,77,77,77	0
55	MG	2a	1719	1/1	0.57	0.32	75,75,75,75	0
55	MG	1a	3161	1/1	0.58	0.62	77,77,77,77	0
55	MG	1a	3169	1/1	0.58	0.25	95,95,95,95	0
55	MG	2A	3101	1/1	0.58	0.24	74,74,74,74	0
55	MG	1a	3048	1/1	0.58	0.22	66,66,66,66	0
55	MG	2A	3582	1/1	0.59	0.25	64,64,64,64	0
55	MG	2a	1770	1/1	0.60	0.14	75,75,75,75	0
55	MG	2A	3606	1/1	0.60	0.21	68,68,68,68	0
55	MG	1A	3778	1/1	0.60	0.21	83,83,83,83	0
55	MG	2A	3647	1/1	0.61	0.10	88,88,88,88	0
55	MG	1a	3064	1/1	0.61	0.26	78,78,78,78	0
55	MG	2G	3001	1/1	0.61	0.11	90,90,90,90	0
55	MG	2A	3563	1/1	0.61	0.32	77,77,77,77	0
55	MG	2A	3256	1/1	0.62	0.24	84,84,84,84	0
55	MG	2a	1670	1/1	0.62	0.13	84,84,84,84	0
55	MG	1A	3702	1/1	0.62	0.40	55,55,55,55	0
55	MG	1a	3074	1/1	0.63	0.28	65,65,65,65	0
55	MG	2a	1708	1/1	0.63	0.17	83,83,83,83	0
55	MG	2a	1632	1/1	0.63	0.34	75,75,75,75	0
55	MG	2a	1772	1/1	0.63	0.15	92,92,92,92	0
55	MG	2a	1717	1/1	0.63	0.22	73,73,73,73	0
55	MG	2A	3642	1/1	0.63	0.16	82,82,82,82	0
55	MG	2A	3693	1/1	0.64	0.18	95,95,95,95	0
55	MG	2A	3712	1/1	0.64	0.15	63,63,63,63	0
55	MG	2a	1686	1/1	0.64	0.14	108,108,108,108	0
55	MG	1a	3170	1/1	0.64	0.13	82,82,82,82	0
55	MG	2a	1736	1/1	0.64	0.21	78,78,78,78	0
55	MG	2a	1636	1/1	0.65	0.30	83,83,83,83	0
55	MG	1a	3215	1/1	0.65	0.27	86,86,86,86	0
55	MG	1a	3134	1/1	0.65	0.24	78,78,78,78	0
55	MG	2a	1614	1/1	0.66	0.51	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
55	MG	1A	3578	1/1	0.66	0.17	86,86,86,86	0
55	MG	2A	3090	1/1	0.66	0.32	76,76,76,76	0
55	MG	2a	1727	1/1	0.66	0.21	91,91,91,91	0
55	MG	2A	3290	1/1	0.66	0.28	64,64,64,64	0
55	MG	2a	1649	1/1	0.66	0.21	83,83,83,83	0
55	MG	2A	3194	1/1	0.66	0.27	84,84,84,84	0
55	MG	2B	3018	1/1	0.66	0.19	92,92,92,92	0
55	MG	2A	3472	1/1	0.66	0.20	88,88,88,88	0
55	MG	2A	3215	1/1	0.66	0.29	80,80,80,80	0
55	MG	2H	201	1/1	0.67	0.22	108,108,108,108	0
55	MG	2A	3455	1/1	0.67	0.39	59,59,59,59	0
55	MG	2A	3303	1/1	0.67	0.16	88,88,88,88	0
55	MG	2B	3015	1/1	0.67	0.22	85,85,85,85	0
55	MG	1A	3456	1/1	0.68	0.20	59,59,59,59	0
55	MG	1a	3189	1/1	0.68	0.11	84,84,84,84	0
55	MG	1A	3790	1/1	0.68	0.22	84,84,84,84	0
55	MG	2A	3328	1/1	0.68	0.33	72,72,72,72	0
55	MG	2A	3027	1/1	0.68	0.29	70,70,70,70	0
55	MG	2A	3456	1/1	0.68	0.35	70,70,70,70	0
55	MG	1B	3024	1/1	0.68	0.14	62,62,62,62	0
55	MG	2A	3105	1/1	0.69	0.24	82,82,82,82	0
55	MG	1a	3175	1/1	0.69	0.34	85,85,85,85	0
55	MG	2A	3789	1/1	0.69	0.19	62,62,62,62	0
55	MG	2A	3575	1/1	0.69	0.18	48,48,48,48	0
55	MG	1a	3016	1/1	0.69	0.23	80,80,80,80	0
55	MG	2a	1704	1/1	0.69	0.17	68,68,68,68	0
55	MG	2B	3002	1/1	0.69	0.28	78,78,78,78	0
55	MG	2a	1620	1/1	0.69	0.21	77,77,77,77	0
55	MG	1a	3034	1/1	0.69	0.21	84,84,84,84	0
55	MG	2A	3040	1/1	0.70	0.21	63,63,63,63	0
55	MG	2a	1711	1/1	0.70	0.39	80,80,80,80	0
55	MG	2A	3162	1/1	0.70	0.13	82,82,82,82	0
55	MG	2a	1642	1/1	0.70	0.25	68,68,68,68	0
55	MG	2a	1647	1/1	0.70	0.26	81,81,81,81	0
55	MG	2A	3653	1/1	0.70	0.23	77,77,77,77	0
55	MG	1a	3078	1/1	0.70	0.40	78,78,78,78	0
55	MG	2a	1739	1/1	0.70	0.19	86,86,86,86	0
55	MG	2a	1674	1/1	0.70	0.13	89,89,89,89	0
55	MG	2a	1682	1/1	0.70	0.20	88,88,88,88	0
55	MG	2B	3006	1/1	0.70	0.26	80,80,80,80	0
55	MG	1A	3165	1/1	0.70	0.49	80,80,80,80	0
55	MG	2A	3210	1/1	0.70	0.16	95,95,95,95	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1F	314	1/1	0.71	0.13	53,53,53,53	0
55	MG	1a	3123	1/1	0.71	0.13	86,86,86,86	0
55	MG	1a	3005	1/1	0.71	0.10	81,81,81,81	0
55	MG	2A	3759	1/1	0.71	0.15	88,88,88,88	0
55	MG	2A	3631	1/1	0.71	0.20	86,86,86,86	0
55	MG	2A	3026	1/1	0.71	0.46	73,73,73,73	0
55	MG	2A	3196	1/1	0.71	0.21	77,77,77,77	0
55	MG	2G	3003	1/1	0.71	0.18	81,81,81,81	0
55	MG	2h	8001	1/1	0.71	0.12	77,77,77,77	0
55	MG	2A	3292	1/1	0.71	0.28	77,77,77,77	0
55	MG	2a	1769	1/1	0.72	0.28	76,76,76,76	0
55	MG	1a	3092	1/1	0.72	0.18	85,85,85,85	0
55	MG	2a	1602	1/1	0.72	0.26	55,55,55,55	0
55	MG	1A	3267	1/1	0.72	0.23	79,79,79,79	0
55	MG	2A	3752	1/1	0.72	0.19	77,77,77,77	0
55	MG	1a	3084	1/1	0.72	0.26	64,64,64,64	0
55	MG	1A	3058	1/1	0.73	0.28	65,65,65,65	0
55	MG	2B	3014	1/1	0.73	0.14	76,76,76,76	0
55	MG	2A	3072	1/1	0.73	0.23	57,57,57,57	0
55	MG	1a	3117	1/1	0.73	0.22	61,61,61,61	0
55	MG	2A	3610	1/1	0.73	0.13	81,81,81,81	0
55	MG	1A	3026	1/1	0.73	0.21	63,63,63,63	0
55	MG	2A	3546	1/1	0.73	0.15	87,87,87,87	0
55	MG	1A	3859	1/1	0.73	0.13	87,87,87,87	0
55	MG	28	101	1/1	0.73	0.22	64,64,64,64	0
55	MG	2A	3798	1/1	0.73	0.36	93,93,93,93	0
55	MG	2b	3001	1/1	0.73	0.22	85,85,85,85	0
55	MG	2A	3643	1/1	0.73	0.41	60,60,60,60	0
55	MG	2A	3125	1/1	0.73	0.38	58,58,58,58	0
55	MG	1A	3209	1/1	0.73	0.13	72,72,72,72	0
55	MG	1A	3725	1/1	0.74	0.32	44,44,44,44	0
55	MG	1a	3145	1/1	0.74	0.23	77,77,77,77	0
55	MG	2A	3386	1/1	0.74	0.15	102,102,102,102	0
55	MG	1A	3731	1/1	0.74	0.12	72,72,72,72	0
55	MG	1A	3760	1/1	0.74	0.12	65,65,65,65	0
55	MG	2E	303	1/1	0.74	0.44	71,71,71,71	0
55	MG	2A	3756	1/1	0.74	0.50	95,95,95,95	0
55	MG	2A	3047	1/1	0.74	0.53	63,63,63,63	0
55	MG	1A	3183	1/1	0.74	0.23	46,46,46,46	0
55	MG	1A	3610	1/1	0.74	0.15	70,70,70,70	0
55	MG	1A	3611	1/1	0.74	0.19	65,65,65,65	0
55	MG	2A	3641	1/1	0.74	0.26	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
55	MG	1B	3013	1/1	0.74	0.14	58,58,58,58	0
55	MG	1A	3592	1/1	0.74	0.18	70,70,70,70	0
55	MG	1A	3901	1/1	0.75	0.18	42,42,42,42	0
55	MG	1A	3246	1/1	0.75	0.17	78,78,78,78	0
55	MG	1a	3200	1/1	0.75	0.20	93,93,93,93	0
55	MG	2A	3624	1/1	0.75	0.64	62,62,62,62	0
55	MG	20	106	1/1	0.75	0.19	78,78,78,78	0
55	MG	1B	3015	1/1	0.75	0.15	66,66,66,66	0
55	MG	1A	3840	1/1	0.75	0.17	61,61,61,61	0
55	MG	2a	1610	1/1	0.75	0.08	74,74,74,74	0
55	MG	2A	3794	1/1	0.75	0.17	75,75,75,75	0
55	MG	1A	3371	1/1	0.75	0.20	63,63,63,63	0
55	MG	2A	3131	1/1	0.75	0.34	65,65,65,65	0
55	MG	2A	3141	1/1	0.75	0.23	51,51,51,51	0
55	MG	2A	3030	1/1	0.75	0.37	69,69,69,69	0
55	MG	1a	3083	1/1	0.75	0.22	67,67,67,67	0
55	MG	2A	3678	1/1	0.75	0.11	92,92,92,92	0
55	MG	2A	3180	1/1	0.75	0.33	63,63,63,63	0
55	MG	2A	3707	1/1	0.75	0.21	75,75,75,75	0
55	MG	2D	305	1/1	0.75	0.46	59,59,59,59	0
55	MG	2A	3446	1/1	0.75	0.26	62,62,62,62	0
55	MG	1A	3630	1/1	0.76	0.13	55,55,55,55	0
55	MG	2A	3554	1/1	0.76	0.17	58,58,58,58	0
55	MG	2A	3038	1/1	0.76	0.17	49,49,49,49	0
55	MG	2A	3331	1/1	0.76	0.15	61,61,61,61	0
55	MG	2a	1677	1/1	0.76	0.22	71,71,71,71	0
55	MG	2A	3727	1/1	0.76	0.16	65,65,65,65	0
55	MG	1a	3041	1/1	0.76	0.21	72,72,72,72	0
55	MG	2a	1699	1/1	0.76	0.11	74,74,74,74	0
55	MG	2A	3437	1/1	0.76	0.19	78,78,78,78	0
55	MG	1A	3262	1/1	0.76	0.20	84,84,84,84	0
55	MG	2A	3195	1/1	0.76	0.22	55,55,55,55	0
55	MG	2X	102	1/1	0.76	0.19	82,82,82,82	0
55	MG	1a	3113	1/1	0.76	0.26	66,66,66,66	0
55	MG	1A	3703	1/1	0.76	0.33	30,30,30,30	0
55	MG	28	102	1/1	0.76	0.25	59,59,59,59	0
55	MG	2a	1726	1/1	0.76	0.16	78,78,78,78	0
55	MG	1a	3062	1/1	0.76	0.22	79,79,79,79	0
55	MG	2a	1606	1/1	0.76	0.47	69,69,69,69	0
55	MG	2A	3796	1/1	0.76	0.29	67,67,67,67	0
55	MG	2A	3476	1/1	0.76	0.27	78,78,78,78	0
55	MG	1P	203	1/1	0.76	0.07	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
55	MG	2a	1625	1/1	0.76	0.31	70,70,70,70	0
55	MG	2a	1629	1/1	0.76	0.19	90,90,90,90	0
55	MG	2a	1790	1/1	0.76	0.25	80,80,80,80	0
55	MG	1A	3348	1/1	0.76	0.21	71,71,71,71	0
55	MG	1A	3618	1/1	0.76	0.20	72,72,72,72	0
55	MG	2B	3007	1/1	0.76	0.26	81,81,81,81	0
55	MG	1A	3623	1/1	0.76	0.19	56,56,56,56	0
55	MG	2a	1635	1/1	0.77	0.24	77,77,77,77	0
55	MG	2A	3777	1/1	0.77	0.15	83,83,83,83	0
55	MG	2A	3064	1/1	0.77	0.26	72,72,72,72	0
55	MG	1A	3602	1/1	0.77	0.22	76,76,76,76	0
55	MG	1A	3446	1/1	0.77	0.15	49,49,49,49	0
55	MG	2A	3502	1/1	0.77	0.22	70,70,70,70	0
55	MG	2a	1656	1/1	0.77	0.38	72,72,72,72	0
55	MG	2A	3593	1/1	0.77	0.26	68,68,68,68	0
55	MG	2A	3414	1/1	0.77	0.24	72,72,72,72	0
55	MG	27	103	1/1	0.77	0.17	70,70,70,70	0
55	MG	2A	3809	1/1	0.77	0.20	75,75,75,75	0
55	MG	1A	3101	1/1	0.78	0.34	63,63,63,63	0
55	MG	2A	3612	1/1	0.78	0.16	38,38,38,38	0
55	MG	1a	3059	1/1	0.78	0.16	80,80,80,80	0
55	MG	2A	3629	1/1	0.78	0.16	74,74,74,74	0
55	MG	2A	3044	1/1	0.78	0.17	79,79,79,79	0
55	MG	2E	307	1/1	0.78	0.17	73,73,73,73	0
55	MG	1a	3138	1/1	0.78	0.18	58,58,58,58	0
55	MG	1a	3061	1/1	0.78	0.14	74,74,74,74	0
55	MG	1a	3144	1/1	0.78	0.33	75,75,75,75	0
55	MG	2a	1646	1/1	0.78	0.32	56,56,56,56	0
55	MG	1A	3829	1/1	0.78	0.17	60,60,60,60	0
55	MG	2A	3011	1/1	0.78	0.38	58,58,58,58	0
55	MG	2A	3024	1/1	0.78	0.21	58,58,58,58	0
55	MG	1l	101	1/1	0.78	0.49	54,54,54,54	0
55	MG	2A	3812	1/1	0.78	0.16	60,60,60,60	0
55	MG	1a	3049	1/1	0.78	0.44	69,69,69,69	0
55	MG	1a	3076	1/1	0.78	0.25	74,74,74,74	0
55	MG	2A	3599	1/1	0.78	0.18	75,75,75,75	0
55	MG	2a	1690	1/1	0.78	0.22	83,83,83,83	0
55	MG	2A	3497	1/1	0.78	0.16	89,89,89,89	0
55	MG	1A	3573	1/1	0.79	0.44	37,37,37,37	0
55	MG	1a	3063	1/1	0.79	0.44	64,64,64,64	0
55	MG	2A	3685	1/1	0.79	0.17	54,54,54,54	0
55	MG	1A	3258	1/1	0.79	0.26	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3579	1/1	0.79	0.23	64,64,64,64	0
55	MG	2A	3535	1/1	0.79	0.22	86,86,86,86	0
55	MG	1A	3671	1/1	0.79	0.26	46,46,46,46	0
55	MG	1A	3011	1/1	0.79	0.25	41,41,41,41	0
55	MG	1A	3886	1/1	0.79	0.19	61,61,61,61	0
55	MG	1A	3190	1/1	0.79	0.20	72,72,72,72	0
55	MG	25	103	1/1	0.79	0.48	62,62,62,62	0
55	MG	2A	3320	1/1	0.79	0.17	79,79,79,79	0
55	MG	1a	3044	1/1	0.79	0.24	66,66,66,66	0
55	MG	1a	3184	1/1	0.79	0.14	73,73,73,73	0
55	MG	2A	3113	1/1	0.79	0.24	66,66,66,66	0
55	MG	1A	3247	1/1	0.79	0.15	86,86,86,86	0
55	MG	2A	3420	1/1	0.79	0.12	60,60,60,60	0
55	MG	1A	3552	1/1	0.79	0.28	45,45,45,45	0
55	MG	2A	3441	1/1	0.79	0.17	90,90,90,90	0
55	MG	1a	3054	1/1	0.79	0.21	82,82,82,82	0
55	MG	2A	3008	1/1	0.79	0.34	69,69,69,69	0
55	MG	2a	1631	1/1	0.79	0.52	85,85,85,85	0
55	MG	1a	3119	1/1	0.79	0.21	81,81,81,81	0
55	MG	1A	3742	1/1	0.79	0.32	71,71,71,71	0
55	MG	2A	3181	1/1	0.79	0.24	79,79,79,79	0
55	MG	1D	316	1/1	0.79	0.17	73,73,73,73	0
55	MG	2d	505	1/1	0.79	0.18	101,101,101,101	0
55	MG	2A	3478	1/1	0.79	0.25	94,94,94,94	0
55	MG	1A	3554	1/1	0.79	0.33	69,69,69,69	0
55	MG	2B	3016	1/1	0.79	0.14	90,90,90,90	0
55	MG	2A	3457	1/1	0.80	0.29	90,90,90,90	0
55	MG	1a	3149	1/1	0.80	0.11	104,104,104,104	0
55	MG	1A	3574	1/1	0.80	0.29	64,64,64,64	0
55	MG	2A	3646	1/1	0.80	0.10	53,53,53,53	0
55	MG	1A	3359	1/1	0.80	0.13	64,64,64,64	0
55	MG	1a	3116	1/1	0.80	0.34	76,76,76,76	0
55	MG	1a	3027	1/1	0.80	0.39	70,70,70,70	0
55	MG	1A	3853	1/1	0.80	0.11	25,25,25,25	0
55	MG	2A	3250	1/1	0.80	0.08	31,31,31,31	0
55	MG	1a	3039	1/1	0.80	0.27	62,62,62,62	0
55	MG	1a	3132	1/1	0.80	0.16	91,91,91,91	0
55	MG	2A	3257	1/1	0.80	0.42	68,68,68,68	0
55	MG	2A	3538	1/1	0.80	0.26	62,62,62,62	0
55	MG	2A	3258	1/1	0.80	0.14	59,59,59,59	0
55	MG	1A	3124	1/1	0.80	0.21	63,63,63,63	0
55	MG	2A	3762	1/1	0.80	0.32	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
55	MG	2A	3096	1/1	0.80	0.18	46,46,46,46	0
55	MG	1a	3208	1/1	0.80	0.20	75,75,75,75	0
55	MG	1a	3210	1/1	0.80	0.15	78,78,78,78	0
55	MG	2A	3107	1/1	0.80	0.23	57,57,57,57	0
55	MG	2a	1737	1/1	0.80	0.23	69,69,69,69	0
55	MG	2a	1738	1/1	0.80	0.46	85,85,85,85	0
55	MG	2A	3108	1/1	0.80	0.38	84,84,84,84	0
55	MG	1N	8002	1/1	0.80	0.12	64,64,64,64	0
55	MG	1t	3001	1/1	0.80	0.33	76,76,76,76	0
55	MG	1A	3233	1/1	0.80	0.39	63,63,63,63	0
55	MG	2A	3426	1/1	0.80	0.29	70,70,70,70	0
55	MG	1A	3787	1/1	0.80	0.16	59,59,59,59	0
55	MG	2a	1795	1/1	0.80	0.20	57,57,57,57	0
55	MG	2A	3819	1/1	0.80	0.13	90,90,90,90	0
55	MG	2A	3019	1/1	0.80	0.14	45,45,45,45	0
55	MG	1a	3004	1/1	0.80	0.36	69,69,69,69	0
55	MG	2A	3172	1/1	0.80	0.15	69,69,69,69	0
55	MG	1A	3244	1/1	0.80	0.20	72,72,72,72	0
55	MG	1F	302	1/1	0.81	0.19	35,35,35,35	0
55	MG	1A	3878	1/1	0.81	0.22	46,46,46,46	0
55	MG	2U	201	1/1	0.81	0.20	64,64,64,64	0
55	MG	2A	3771	1/1	0.81	0.15	68,68,68,68	0
55	MG	1A	3631	1/1	0.81	0.14	59,59,59,59	0
55	MG	1A	3898	1/1	0.81	0.20	63,63,63,63	0
55	MG	1Q	204	1/1	0.81	0.16	52,52,52,52	0
55	MG	1A	3658	1/1	0.81	0.26	38,38,38,38	0
55	MG	2A	3486	1/1	0.81	0.64	57,57,57,57	0
55	MG	1B	3006	1/1	0.81	0.26	59,59,59,59	0
55	MG	1a	3152	1/1	0.81	0.29	91,91,91,91	0
55	MG	2A	3507	1/1	0.81	0.20	69,69,69,69	0
55	MG	1a	3097	1/1	0.81	0.19	61,61,61,61	0
55	MG	2A	3149	1/1	0.81	0.14	63,63,63,63	0
55	MG	2a	1730	1/1	0.81	0.12	92,92,92,92	0
55	MG	2a	1734	1/1	0.81	0.23	57,57,57,57	0
55	MG	1A	3398	1/1	0.81	0.18	37,37,37,37	0
55	MG	2A	3163	1/1	0.81	0.41	78,78,78,78	0
55	MG	2A	3672	1/1	0.81	0.15	59,59,59,59	0
55	MG	1a	3163	1/1	0.81	0.25	74,74,74,74	0
55	MG	2a	1634	1/1	0.81	0.27	81,81,81,81	0
55	MG	1a	3165	1/1	0.81	0.33	75,75,75,75	0
55	MG	1A	3471	1/1	0.81	0.18	65,65,65,65	0
55	MG	2A	3700	1/1	0.81	0.21	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
55	MG	1a	3010	1/1	0.81	0.27	78,78,78,78	0
55	MG	2a	1791	1/1	0.81	0.16	71,71,71,71	0
55	MG	1A	3501	1/1	0.81	0.15	64,64,64,64	0
55	MG	2D	307	1/1	0.81	0.36	64,64,64,64	0
55	MG	1a	3122	1/1	0.81	0.27	71,71,71,71	0
55	MG	1A	3781	1/1	0.81	0.36	28,28,28,28	0
55	MG	2A	3449	1/1	0.81	0.14	84,84,84,84	0
55	MG	1a	3028	1/1	0.81	0.25	55,55,55,55	0
55	MG	2n	503	1/1	0.81	0.24	85,85,85,85	0
55	MG	2A	3475	1/1	0.82	0.11	76,76,76,76	0
55	MG	1a	3128	1/1	0.82	0.19	71,71,71,71	0
55	MG	2A	3477	1/1	0.82	0.13	68,68,68,68	0
55	MG	1A	3503	1/1	0.82	0.20	77,77,77,77	0
55	MG	2U	203	1/1	0.82	0.19	71,71,71,71	0
55	MG	2V	202	1/1	0.82	0.36	55,55,55,55	0
55	MG	2V	204	1/1	0.82	0.17	77,77,77,77	0
55	MG	1A	3236	1/1	0.82	0.23	79,79,79,79	0
55	MG	10	101	1/1	0.82	0.14	52,52,52,52	0
55	MG	2A	3633	1/1	0.82	0.22	82,82,82,82	0
55	MG	2A	3793	1/1	0.82	0.15	67,67,67,67	0
55	MG	2A	3342	1/1	0.82	0.32	76,76,76,76	0
55	MG	1A	3533	1/1	0.82	0.27	60,60,60,60	0
55	MG	2A	3509	1/1	0.82	0.75	53,53,53,53	0
55	MG	2A	3412	1/1	0.82	0.19	70,70,70,70	0
55	MG	1A	3862	1/1	0.82	0.19	59,59,59,59	0
55	MG	2A	3209	1/1	0.82	0.17	81,81,81,81	0
55	MG	1A	3400	1/1	0.82	0.34	63,63,63,63	0
55	MG	2A	3660	1/1	0.82	0.12	71,71,71,71	0
55	MG	2B	3005	1/1	0.82	0.23	69,69,69,69	0
55	MG	2A	3671	1/1	0.82	0.28	73,73,73,73	0
55	MG	2A	3115	1/1	0.82	0.30	66,66,66,66	0
55	MG	1A	3500	1/1	0.82	0.26	65,65,65,65	0
55	MG	1A	3726	1/1	0.82	0.22	29,29,29,29	0
55	MG	1A	3021	1/1	0.82	0.07	42,42,42,42	0
55	MG	1a	3056	1/1	0.82	0.18	69,69,69,69	0
55	MG	1a	3218	1/1	0.82	0.12	72,72,72,72	0
55	MG	2D	304	1/1	0.82	0.12	55,55,55,55	0
55	MG	1a	3124	1/1	0.82	0.21	77,77,77,77	0
55	MG	2A	3459	1/1	0.82	0.17	71,71,71,71	0
55	MG	2A	3083	1/1	0.82	0.34	57,57,57,57	0
55	MG	2A	3753	1/1	0.82	0.07	71,71,71,71	0
55	MG	2A	3297	1/1	0.82	0.12	78,78,78,78	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	AMP	1B	3025	1/23	0.82	0.23	57,57,57,57	0
55	MG	1A	3076	1/1	0.83	0.20	63,63,63,63	0
55	MG	2a	1633	1/1	0.83	0.23	79,79,79,79	0
55	MG	1A	3838	1/1	0.83	0.21	45,45,45,45	0
55	MG	2A	3814	1/1	0.83	0.27	68,68,68,68	0
55	MG	2A	3815	1/1	0.83	0.27	67,67,67,67	0
55	MG	2A	3192	1/1	0.83	0.23	64,64,64,64	0
55	MG	2A	3041	1/1	0.83	0.21	73,73,73,73	0
55	MG	2B	3004	1/1	0.83	0.20	76,76,76,76	0
55	MG	1A	3313	1/1	0.83	0.19	55,55,55,55	0
55	MG	1a	3186	1/1	0.83	0.26	69,69,69,69	0
55	MG	2a	1652	1/1	0.83	0.32	90,90,90,90	0
55	MG	1A	3465	1/1	0.83	0.17	54,54,54,54	0
55	MG	2A	3068	1/1	0.83	0.11	56,56,56,56	0
55	MG	1A	3314	1/1	0.83	0.16	52,52,52,52	0
55	MG	2A	3222	1/1	0.83	0.38	62,62,62,62	0
55	MG	1A	3055	1/1	0.83	0.21	53,53,53,53	0
55	MG	1a	3081	1/1	0.83	0.21	69,69,69,69	0
55	MG	1a	3213	1/1	0.83	0.09	64,64,64,64	0
55	MG	1A	3877	1/1	0.83	0.13	63,63,63,63	0
55	MG	2A	3489	1/1	0.83	0.14	81,81,81,81	0
55	MG	1A	3034	1/1	0.83	0.14	57,57,57,57	0
55	MG	1h	3001	1/1	0.83	0.34	63,63,63,63	0
55	MG	2A	3506	1/1	0.83	0.30	47,47,47,47	0
55	MG	2a	1713	1/1	0.83	0.13	69,69,69,69	0
55	MG	1h	3002	1/1	0.83	0.12	76,76,76,76	0
55	MG	1A	3195	1/1	0.83	0.17	46,46,46,46	0
55	MG	1A	3890	1/1	0.83	0.18	73,73,73,73	0
55	MG	2P	202	1/1	0.83	0.22	73,73,73,73	0
55	MG	2A	3121	1/1	0.83	0.15	81,81,81,81	0
55	MG	2A	3519	1/1	0.83	0.10	73,73,73,73	0
55	MG	2A	3009	1/1	0.83	0.27	59,59,59,59	0
55	MG	18	3302	1/1	0.83	0.33	40,40,40,40	0
55	MG	2X	101	1/1	0.83	0.15	61,61,61,61	0
55	MG	2A	3537	1/1	0.83	0.19	61,61,61,61	0
55	MG	20	104	1/1	0.83	0.09	81,81,81,81	0
55	MG	2A	3134	1/1	0.83	0.42	70,70,70,70	0
55	MG	2A	3013	1/1	0.83	0.31	60,60,60,60	0
55	MG	2A	3387	1/1	0.83	0.12	68,68,68,68	0
55	MG	2A	3398	1/1	0.83	0.15	81,81,81,81	0
55	MG	2A	3410	1/1	0.83	0.22	83,83,83,83	0
55	MG	1A	3664	1/1	0.83	0.14	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
55	MG	1A	3131	1/1	0.83	0.10	62,62,62,62	0
55	MG	1A	3157	1/1	0.83	0.19	57,57,57,57	0
55	MG	2A	3592	1/1	0.83	0.08	89,89,89,89	0
55	MG	1a	3121	1/1	0.83	0.31	62,62,62,62	0
55	MG	2a	1623	1/1	0.83	0.16	78,78,78,78	0
55	MG	2A	3598	1/1	0.83	0.21	62,62,62,62	0
55	MG	1A	3794	1/1	0.83	0.14	59,59,59,59	0
55	MG	2A	3605	1/1	0.83	0.26	63,63,63,63	0
55	MG	2A	3542	1/1	0.84	0.19	88,88,88,88	0
55	MG	1A	3792	1/1	0.84	0.13	55,55,55,55	0
55	MG	1a	3029	1/1	0.84	0.21	55,55,55,55	0
55	MG	1a	3031	1/1	0.84	0.17	61,61,61,61	0
55	MG	2A	3561	1/1	0.84	0.09	59,59,59,59	0
55	MG	1A	3161	1/1	0.84	0.31	55,55,55,55	0
55	MG	2A	3719	1/1	0.84	0.11	70,70,70,70	0
55	MG	2A	3720	1/1	0.84	0.21	58,58,58,58	0
55	MG	2A	3721	1/1	0.84	0.13	42,42,42,42	0
55	MG	1a	3166	1/1	0.84	0.22	80,80,80,80	0
55	MG	2A	3740	1/1	0.84	0.14	68,68,68,68	0
55	MG	2A	3117	1/1	0.84	0.18	58,58,58,58	0
55	MG	2a	1692	1/1	0.84	0.14	85,85,85,85	0
55	MG	1A	3214	1/1	0.84	0.16	40,40,40,40	0
55	MG	2A	3589	1/1	0.84	0.22	82,82,82,82	0
55	MG	1A	3208	1/1	0.84	0.17	37,37,37,37	0
55	MG	2A	3129	1/1	0.84	0.28	75,75,75,75	0
55	MG	1A	3912	1/1	0.84	0.12	43,43,43,43	0
55	MG	1a	3182	1/1	0.84	0.30	71,71,71,71	0
55	MG	2A	3299	1/1	0.84	0.14	75,75,75,75	0
55	MG	1A	3753	1/1	0.84	0.13	67,67,67,67	0
55	MG	1A	3841	1/1	0.84	0.17	64,64,64,64	0
55	MG	1A	3506	1/1	0.84	0.16	71,71,71,71	0
55	MG	1a	3139	1/1	0.84	0.26	69,69,69,69	0
55	MG	27	104	1/1	0.84	0.19	67,67,67,67	0
55	MG	1A	3507	1/1	0.84	0.23	48,48,48,48	0
55	MG	2A	3345	1/1	0.84	0.12	81,81,81,81	0
55	MG	1A	3614	1/1	0.84	0.18	70,70,70,70	0
55	MG	1a	3104	1/1	0.84	0.17	82,82,82,82	0
55	MG	1A	3486	1/1	0.84	0.17	63,63,63,63	0
55	MG	2a	1742	1/1	0.84	0.16	113,113,113,113	0
55	MG	2A	3813	1/1	0.84	0.19	57,57,57,57	0
55	MG	2a	1759	1/1	0.84	0.18	72,72,72,72	0
55	MG	2a	1618	1/1	0.84	0.19	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
55	MG	1a	3115	1/1	0.84	0.26	66,66,66,66	0
55	MG	2a	1622	1/1	0.84	0.31	50,50,50,50	0
55	MG	1b	3001	1/1	0.84	0.15	81,81,81,81	0
55	MG	2A	3816	1/1	0.84	0.18	51,51,51,51	0
55	MG	1a	3150	1/1	0.84	0.11	99,99,99,99	0
55	MG	2A	3521	1/1	0.84	0.16	68,68,68,68	0
55	MG	1A	3517	1/1	0.84	0.27	68,68,68,68	0
55	MG	2A	3657	1/1	0.84	0.12	66,66,66,66	0
55	MG	2A	3421	1/1	0.84	0.18	58,58,58,58	0
55	MG	2l	201	1/1	0.84	0.14	79,79,79,79	0
55	MG	2A	3668	1/1	0.84	0.15	66,66,66,66	0
55	MG	2A	3423	1/1	0.84	0.21	79,79,79,79	0
55	MG	1n	502	1/1	0.84	0.15	63,63,63,63	0
55	MG	1a	3068	1/1	0.85	0.16	73,73,73,73	0
55	MG	1A	3895	1/1	0.85	0.35	65,65,65,65	0
55	MG	2a	1609	1/1	0.85	0.37	77,77,77,77	0
55	MG	2A	3729	1/1	0.85	0.16	70,70,70,70	0
55	MG	2A	3732	1/1	0.85	0.32	61,61,61,61	0
55	MG	1a	3006	1/1	0.85	0.14	74,74,74,74	0
55	MG	1a	3008	1/1	0.85	0.30	60,60,60,60	0
55	MG	1A	3186	1/1	0.85	0.34	72,72,72,72	0
55	MG	1A	3038	1/1	0.85	0.46	66,66,66,66	0
55	MG	2A	3050	1/1	0.85	0.15	64,64,64,64	0
55	MG	1a	3013	1/1	0.85	0.18	72,72,72,72	0
55	MG	1A	3568	1/1	0.85	0.14	63,63,63,63	0
55	MG	1a	3087	1/1	0.85	0.11	57,57,57,57	0
55	MG	2A	3078	1/1	0.85	0.19	51,51,51,51	0
55	MG	1a	3023	1/1	0.85	0.30	53,53,53,53	0
55	MG	1B	3003	1/1	0.85	0.17	64,64,64,64	0
55	MG	1A	3816	1/1	0.85	0.03	19,19,19,19	0
55	MG	2A	3543	1/1	0.85	0.18	82,82,82,82	0
55	MG	2A	3327	1/1	0.85	0.20	67,67,67,67	0
55	MG	2a	1644	1/1	0.85	0.17	67,67,67,67	0
55	MG	2a	1645	1/1	0.85	0.27	63,63,63,63	0
55	MG	2A	3099	1/1	0.85	0.12	52,52,52,52	0
55	MG	2A	3800	1/1	0.85	0.14	112,112,112,112	0
55	MG	2A	3329	1/1	0.85	0.12	88,88,88,88	0
55	MG	1a	3109	1/1	0.85	0.20	53,53,53,53	0
55	MG	2A	3340	1/1	0.85	0.13	52,52,52,52	0
55	MG	1a	3112	1/1	0.85	0.23	86,86,86,86	0
55	MG	2A	3344	1/1	0.85	0.10	55,55,55,55	0
55	MG	1A	3053	1/1	0.85	0.13	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3831	1/1	0.85	0.15	51,51,51,51	0
55	MG	2A	3111	1/1	0.85	0.30	52,52,52,52	0
55	MG	2A	3112	1/1	0.85	0.40	77,77,77,77	0
55	MG	2A	3594	1/1	0.85	0.18	56,56,56,56	0
55	MG	2A	3406	1/1	0.85	0.41	62,62,62,62	0
55	MG	2A	3408	1/1	0.85	0.16	67,67,67,67	0
55	MG	1A	3730	1/1	0.85	0.12	65,65,65,65	0
55	MG	1A	3839	1/1	0.85	0.10	59,59,59,59	0
55	MG	1A	3136	1/1	0.85	0.14	68,68,68,68	0
55	MG	2A	3417	1/1	0.85	0.61	58,58,58,58	0
55	MG	2a	1715	1/1	0.85	0.15	82,82,82,82	0
55	MG	1a	3043	1/1	0.85	0.29	68,68,68,68	0
55	MG	1A	3173	1/1	0.85	0.22	63,63,63,63	0
55	MG	2D	302	1/1	0.85	0.21	58,58,58,58	0
55	MG	2a	1722	1/1	0.85	0.12	82,82,82,82	0
55	MG	1a	3221	1/1	0.85	0.19	71,71,71,71	0
55	MG	1G	3002	1/1	0.85	0.14	62,62,62,62	0
55	MG	2A	3432	1/1	0.85	0.14	74,74,74,74	0
55	MG	1d	504	1/1	0.85	0.20	75,75,75,75	0
55	MG	1A	3210	1/1	0.85	0.23	45,45,45,45	0
55	MG	1a	3127	1/1	0.85	0.17	53,53,53,53	0
55	MG	2A	3151	1/1	0.85	0.55	62,62,62,62	0
55	MG	2A	3453	1/1	0.85	0.18	81,81,81,81	0
55	MG	1A	3758	1/1	0.85	0.28	53,53,53,53	0
55	MG	2N	201	1/1	0.85	0.14	82,82,82,82	0
55	MG	2a	1758	1/1	0.85	0.23	70,70,70,70	0
55	MG	2A	3655	1/1	0.85	0.16	60,60,60,60	0
55	MG	1A	3147	1/1	0.85	0.10	40,40,40,40	0
55	MG	2A	3007	1/1	0.85	0.21	61,61,61,61	0
55	MG	1a	3057	1/1	0.85	0.33	81,81,81,81	0
55	MG	2a	1782	1/1	0.85	0.18	70,70,70,70	0
55	MG	2a	1787	1/1	0.85	0.19	80,80,80,80	0
55	MG	2A	3468	1/1	0.85	0.17	80,80,80,80	0
55	MG	1A	3771	1/1	0.85	0.11	71,71,71,71	0
55	MG	10	105	1/1	0.85	0.15	57,57,57,57	0
55	MG	2A	3184	1/1	0.85	0.16	73,73,73,73	0
55	MG	1a	3141	1/1	0.85	0.17	75,75,75,75	0
55	MG	1A	3596	1/1	0.85	0.18	58,58,58,58	0
55	MG	27	102	1/1	0.85	0.21	49,49,49,49	0
55	MG	11	103	1/1	0.85	0.14	50,50,50,50	0
55	MG	2A	3480	1/1	0.85	0.10	81,81,81,81	0
55	MG	1A	3538	1/1	0.85	0.28	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
55	MG	1A	3604	1/1	0.85	0.14	52,52,52,52	0
55	MG	1a	3126	1/1	0.86	0.19	74,74,74,74	0
55	MG	2A	3487	1/1	0.86	0.15	68,68,68,68	0
55	MG	1P	201	1/1	0.86	0.39	30,30,30,30	0
55	MG	1A	3148	1/1	0.86	0.11	58,58,58,58	0
55	MG	2A	3167	1/1	0.86	0.14	56,56,56,56	0
55	MG	2A	3352	1/1	0.86	0.15	59,59,59,59	0
55	MG	2A	3379	1/1	0.86	0.09	61,61,61,61	0
55	MG	1A	3253	1/1	0.86	0.16	53,53,53,53	0
55	MG	1R	204	1/1	0.86	0.18	53,53,53,53	0
55	MG	1A	3013	1/1	0.86	0.18	51,51,51,51	0
55	MG	2A	3673	1/1	0.86	0.19	65,65,65,65	0
55	MG	2a	1673	1/1	0.86	0.18	63,63,63,63	0
55	MG	1A	3514	1/1	0.86	0.13	35,35,35,35	0
55	MG	1A	3216	1/1	0.86	0.17	52,52,52,52	0
55	MG	2A	3689	1/1	0.86	0.11	67,67,67,67	0
55	MG	2A	3690	1/1	0.86	0.20	84,84,84,84	0
55	MG	1A	3428	1/1	0.86	0.18	68,68,68,68	0
55	MG	1A	3014	1/1	0.86	0.27	41,41,41,41	0
55	MG	2a	1698	1/1	0.86	0.38	58,58,58,58	0
55	MG	2A	3086	1/1	0.86	0.28	56,56,56,56	0
55	MG	1a	3001	1/1	0.86	0.15	76,76,76,76	0
55	MG	2A	3540	1/1	0.86	0.16	64,64,64,64	0
55	MG	2A	3095	1/1	0.86	0.28	64,64,64,64	0
55	MG	2S	201	1/1	0.86	0.32	67,67,67,67	0
55	MG	1e	3001	1/1	0.86	0.27	55,55,55,55	0
55	MG	1a	3096	1/1	0.86	0.09	78,78,78,78	0
55	MG	2V	201	1/1	0.86	0.54	55,55,55,55	0
55	MG	2A	3425	1/1	0.86	0.18	71,71,71,71	0
55	MG	1a	3002	1/1	0.86	0.16	82,82,82,82	0
55	MG	2V	205	1/1	0.86	0.13	73,73,73,73	0
55	MG	1a	3003	1/1	0.86	0.19	65,65,65,65	0
55	MG	2A	3748	1/1	0.86	0.14	68,68,68,68	0
55	MG	2A	3435	1/1	0.86	0.12	76,76,76,76	0
55	MG	2A	3564	1/1	0.86	0.37	57,57,57,57	0
55	MG	2A	3251	1/1	0.86	0.16	79,79,79,79	0
55	MG	2A	3439	1/1	0.86	0.21	64,64,64,64	0
55	MG	1a	3053	1/1	0.86	0.26	82,82,82,82	0
55	MG	2A	3002	1/1	0.86	0.21	63,63,63,63	0
55	MG	1A	3269	1/1	0.86	0.11	62,62,62,62	0
55	MG	1a	3055	1/1	0.86	0.22	47,47,47,47	0
55	MG	2a	1756	1/1	0.86	0.11	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3260	1/1	0.86	0.15	66,66,66,66	0
55	MG	2a	1603	1/1	0.86	0.18	69,69,69,69	0
55	MG	1A	3287	1/1	0.86	0.11	45,45,45,45	0
55	MG	1A	3146	1/1	0.86	0.20	54,54,54,54	0
55	MG	2A	3604	1/1	0.86	0.15	65,65,65,65	0
55	MG	2a	1773	1/1	0.86	0.09	89,89,89,89	0
55	MG	1A	3475	1/1	0.86	0.62	32,32,32,32	0
55	MG	2A	3464	1/1	0.86	0.19	90,90,90,90	0
55	MG	2A	3607	1/1	0.86	0.12	80,80,80,80	0
55	MG	1A	3172	1/1	0.86	0.18	50,50,50,50	0
55	MG	2A	3022	1/1	0.86	0.23	68,68,68,68	0
55	MG	1A	3499	1/1	0.86	0.19	59,59,59,59	0
55	MG	2a	1628	1/1	0.86	0.23	54,54,54,54	0
55	MG	2e	3001	1/1	0.86	0.32	67,67,67,67	0
55	MG	2A	3323	1/1	0.86	0.13	66,66,66,66	0
55	MG	1a	3173	1/1	0.86	0.19	71,71,71,71	0
55	MG	1A	3317	1/1	0.86	0.13	73,73,73,73	0
55	MG	1A	3039	1/1	0.86	0.36	55,55,55,55	0
55	MG	1a	3019	1/1	0.86	0.15	54,54,54,54	0
55	MG	2A	3483	1/1	0.86	0.40	55,55,55,55	0
56	AMP	2A	3821	1/23	0.86	0.12	79,79,79,79	0
55	MG	2A	3146	1/1	0.87	0.17	53,53,53,53	0
55	MG	2A	3782	1/1	0.87	0.17	82,82,82,82	0
55	MG	1B	3005	1/1	0.87	0.13	54,54,54,54	0
55	MG	1A	3640	1/1	0.87	0.21	34,34,34,34	0
55	MG	1A	3464	1/1	0.87	0.59	35,35,35,35	0
55	MG	2A	3588	1/1	0.87	0.15	67,67,67,67	0
55	MG	1A	3660	1/1	0.87	0.16	56,56,56,56	0
55	MG	2A	3018	1/1	0.87	0.52	52,52,52,52	0
55	MG	1B	3023	1/1	0.87	0.14	63,63,63,63	0
55	MG	2A	3431	1/1	0.87	0.31	77,77,77,77	0
55	MG	2A	3805	1/1	0.87	0.11	74,74,74,74	0
55	MG	1A	3800	1/1	0.87	0.10	64,64,64,64	0
55	MG	1a	3022	1/1	0.87	0.44	66,66,66,66	0
55	MG	2A	3600	1/1	0.87	0.29	54,54,54,54	0
55	MG	1D	307	1/1	0.87	0.42	44,44,44,44	0
55	MG	1A	3577	1/1	0.87	0.34	40,40,40,40	0
55	MG	1A	3191	1/1	0.87	0.14	66,66,66,66	0
55	MG	1A	3691	1/1	0.87	0.09	26,26,26,26	0
55	MG	2a	1653	1/1	0.87	0.48	85,85,85,85	0
55	MG	1a	3030	1/1	0.87	0.33	61,61,61,61	0
55	MG	1F	316	1/1	0.87	0.13	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3377	1/1	0.87	0.18	70,70,70,70	0
55	MG	2A	3627	1/1	0.87	0.17	66,66,66,66	0
55	MG	2A	3628	1/1	0.87	0.20	63,63,63,63	0
55	MG	2B	3008	1/1	0.87	0.08	83,83,83,83	0
55	MG	1a	3037	1/1	0.87	0.22	68,68,68,68	0
55	MG	1A	3515	1/1	0.87	0.17	54,54,54,54	0
55	MG	2A	3054	1/1	0.87	0.19	51,51,51,51	0
55	MG	2A	3463	1/1	0.87	0.28	76,76,76,76	0
55	MG	2A	3248	1/1	0.87	0.09	81,81,81,81	0
55	MG	2A	3059	1/1	0.87	0.33	64,64,64,64	0
55	MG	1a	3180	1/1	0.87	0.12	102,102,102,102	0
55	MG	1A	3472	1/1	0.87	0.19	58,58,58,58	0
55	MG	1A	3254	1/1	0.87	0.29	50,50,50,50	0
55	MG	2D	308	1/1	0.87	0.25	55,55,55,55	0
55	MG	2A	3650	1/1	0.87	0.18	55,55,55,55	0
55	MG	1a	3185	1/1	0.87	0.26	68,68,68,68	0
55	MG	1A	3519	1/1	0.87	0.11	46,46,46,46	0
55	MG	1A	3484	1/1	0.87	0.12	47,47,47,47	0
55	MG	2A	3264	1/1	0.87	0.17	65,65,65,65	0
55	MG	1A	3103	1/1	0.87	0.21	35,35,35,35	0
55	MG	1A	3551	1/1	0.87	0.17	60,60,60,60	0
55	MG	2A	3295	1/1	0.87	0.15	71,71,71,71	0
55	MG	2a	1733	1/1	0.87	0.10	67,67,67,67	0
55	MG	2Q	8004	1/1	0.87	0.28	66,66,66,66	0
55	MG	2R	202	1/1	0.87	0.22	74,74,74,74	0
55	MG	1A	3402	1/1	0.87	0.15	43,43,43,43	0
55	MG	2A	3677	1/1	0.87	0.12	56,56,56,56	0
55	MG	1A	3230	1/1	0.87	0.14	50,50,50,50	0
55	MG	1a	3125	1/1	0.87	0.18	74,74,74,74	0
55	MG	2A	3103	1/1	0.87	0.10	65,65,65,65	0
55	MG	2a	1755	1/1	0.87	0.40	81,81,81,81	0
55	MG	15	102	1/1	0.87	0.54	43,43,43,43	0
55	MG	2A	3508	1/1	0.87	0.37	57,57,57,57	0
55	MG	1A	3889	1/1	0.87	0.23	46,46,46,46	0
55	MG	1a	3222	1/1	0.87	0.22	62,62,62,62	0
55	MG	1A	3764	1/1	0.87	0.15	67,67,67,67	0
55	MG	1d	502	1/1	0.87	0.15	80,80,80,80	0
55	MG	1a	3130	1/1	0.87	0.20	62,62,62,62	0
55	MG	1A	3563	1/1	0.87	0.18	59,59,59,59	0
55	MG	1f	8001	1/1	0.87	0.14	60,60,60,60	0
55	MG	2A	3118	1/1	0.87	0.24	52,52,52,52	0
55	MG	1A	3775	1/1	0.87	0.17	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
55	MG	2a	1792	1/1	0.87	0.13	52,52,52,52	0
55	MG	1a	3135	1/1	0.87	0.26	77,77,77,77	0
55	MG	2A	3128	1/1	0.87	0.25	61,61,61,61	0
55	MG	2d	504	1/1	0.87	0.15	90,90,90,90	0
55	MG	1a	3136	1/1	0.87	0.24	79,79,79,79	0
55	MG	1A	3204	1/1	0.87	0.64	39,39,39,39	0
55	MG	1A	3248	1/1	0.87	0.32	51,51,51,51	0
55	MG	2A	3758	1/1	0.87	0.17	77,77,77,77	0
55	MG	2A	3140	1/1	0.87	0.23	61,61,61,61	0
55	MG	2a	1617	1/1	0.87	0.35	65,65,65,65	0
55	MG	2A	3559	1/1	0.87	0.21	64,64,64,64	0
55	MG	1A	3638	1/1	0.87	0.33	31,31,31,31	0
55	MG	2A	3145	1/1	0.87	0.08	79,79,79,79	0
55	MG	2A	3085	1/1	0.88	0.24	62,62,62,62	0
55	MG	2A	3223	1/1	0.88	0.16	68,68,68,68	0
55	MG	1A	3098	1/1	0.88	0.13	38,38,38,38	0
55	MG	1A	3581	1/1	0.88	0.24	35,35,35,35	0
55	MG	2a	1637	1/1	0.88	0.49	71,71,71,71	0
55	MG	1A	3701	1/1	0.88	0.18	40,40,40,40	0
55	MG	2B	3001	1/1	0.88	0.13	64,64,64,64	0
55	MG	2a	1643	1/1	0.88	0.44	73,73,73,73	0
55	MG	1a	3047	1/1	0.88	0.16	68,68,68,68	0
55	MG	1A	3033	1/1	0.88	0.20	45,45,45,45	0
55	MG	1A	3470	1/1	0.88	0.10	28,28,28,28	0
55	MG	1A	3722	1/1	0.88	0.19	62,62,62,62	0
55	MG	2A	3104	1/1	0.88	0.09	56,56,56,56	0
55	MG	1W	3003	1/1	0.88	0.24	41,41,41,41	0
55	MG	1A	3855	1/1	0.88	0.13	48,48,48,48	0
55	MG	2B	3013	1/1	0.88	0.11	84,84,84,84	0
55	MG	1A	3723	1/1	0.88	0.08	47,47,47,47	0
55	MG	1A	3724	1/1	0.88	0.12	71,71,71,71	0
55	MG	1A	3863	1/1	0.88	0.17	58,58,58,58	0
55	MG	1A	3597	1/1	0.88	0.35	38,38,38,38	0
55	MG	2A	3481	1/1	0.88	0.16	67,67,67,67	0
55	MG	1A	3598	1/1	0.88	0.13	83,83,83,83	0
55	MG	1A	3320	1/1	0.88	0.19	62,62,62,62	0
55	MG	2A	3322	1/1	0.88	0.14	62,62,62,62	0
55	MG	1A	3887	1/1	0.88	0.15	44,44,44,44	0
55	MG	1A	3083	1/1	0.88	0.13	57,57,57,57	0
55	MG	1a	3066	1/1	0.88	0.27	68,68,68,68	0
55	MG	2a	1707	1/1	0.88	0.11	92,92,92,92	0
55	MG	1A	3605	1/1	0.88	0.21	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1a	3070	1/1	0.88	0.17	62,62,62,62	0
55	MG	2A	3337	1/1	0.88	0.11	79,79,79,79	0
55	MG	1A	3163	1/1	0.88	0.13	65,65,65,65	0
55	MG	1A	3537	1/1	0.88	0.15	38,38,38,38	0
55	MG	1A	3478	1/1	0.88	0.15	44,44,44,44	0
55	MG	1A	3223	1/1	0.88	0.09	42,42,42,42	0
55	MG	2A	3348	1/1	0.88	0.09	76,76,76,76	0
55	MG	2A	3531	1/1	0.88	0.14	83,83,83,83	0
55	MG	2A	3144	1/1	0.88	0.19	73,73,73,73	0
55	MG	1a	3157	1/1	0.88	0.08	82,82,82,82	0
55	MG	2A	3381	1/1	0.88	0.09	77,77,77,77	0
55	MG	1a	3159	1/1	0.88	0.13	65,65,65,65	0
55	MG	1A	3116	1/1	0.88	0.17	74,74,74,74	0
55	MG	2A	3394	1/1	0.88	0.10	65,65,65,65	0
55	MG	2W	3001	1/1	0.88	0.19	60,60,60,60	0
55	MG	1A	3622	1/1	0.88	0.16	76,76,76,76	0
55	MG	2A	3152	1/1	0.88	0.11	59,59,59,59	0
55	MG	1A	3492	1/1	0.88	0.20	50,50,50,50	0
55	MG	1A	3168	1/1	0.88	0.12	53,53,53,53	0
55	MG	2I	101	1/1	0.88	0.17	61,61,61,61	0
55	MG	1A	3202	1/1	0.88	0.23	63,63,63,63	0
55	MG	1B	3020	1/1	0.88	0.15	73,73,73,73	0
55	MG	2A	3416	1/1	0.88	0.21	56,56,56,56	0
55	MG	1B	3022	1/1	0.88	0.25	63,63,63,63	0
55	MG	2A	3569	1/1	0.88	0.31	48,48,48,48	0
55	MG	2A	3574	1/1	0.88	0.09	98,98,98,98	0
55	MG	1A	3272	1/1	0.88	0.24	56,56,56,56	0
55	MG	2a	1781	1/1	0.88	0.11	76,76,76,76	0
55	MG	2A	3579	1/1	0.88	0.25	75,75,75,75	0
55	MG	2A	3775	1/1	0.88	0.09	57,57,57,57	0
55	MG	2A	3580	1/1	0.88	0.13	73,73,73,73	0
55	MG	2A	3048	1/1	0.88	0.12	56,56,56,56	0
55	MG	1A	3169	1/1	0.88	0.32	62,62,62,62	0
55	MG	2a	1616	1/1	0.88	0.21	68,68,68,68	0
55	MG	2A	3187	1/1	0.88	0.15	73,73,73,73	0
55	MG	1A	3576	1/1	0.88	0.27	47,47,47,47	0
55	MG	2a	1619	1/1	0.88	0.30	72,72,72,72	0
55	MG	2A	3427	1/1	0.88	0.12	61,61,61,61	0
55	MG	1A	3308	1/1	0.88	0.12	42,42,42,42	0
55	MG	1A	3118	1/1	0.88	0.29	63,63,63,63	0
55	MG	1A	3820	1/1	0.88	0.42	41,41,41,41	0
55	MG	2A	3197	1/1	0.88	0.23	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1a	3038	1/1	0.88	0.55	79,79,79,79	0
55	MG	1a	3197	1/1	0.88	0.14	82,82,82,82	0
55	MG	1A	3668	1/1	0.88	0.08	85,85,85,85	0
55	MG	2A	3403	1/1	0.89	0.08	79,79,79,79	0
55	MG	1a	3174	1/1	0.89	0.13	70,70,70,70	0
55	MG	1A	3087	1/1	0.89	0.34	33,33,33,33	0
55	MG	2A	3045	1/1	0.89	0.22	46,46,46,46	0
55	MG	2A	3179	1/1	0.89	0.47	48,48,48,48	0
55	MG	1a	3178	1/1	0.89	0.10	75,75,75,75	0
55	MG	1A	3848	1/1	0.89	0.35	68,68,68,68	0
55	MG	1A	3539	1/1	0.89	0.17	62,62,62,62	0
55	MG	2A	3418	1/1	0.89	0.10	55,55,55,55	0
55	MG	1A	3255	1/1	0.89	0.16	34,34,34,34	0
55	MG	1A	3856	1/1	0.89	0.12	46,46,46,46	0
55	MG	1a	3042	1/1	0.89	0.20	53,53,53,53	0
55	MG	1A	3734	1/1	0.89	0.22	45,45,45,45	0
55	MG	2A	3591	1/1	0.89	0.19	53,53,53,53	0
55	MG	1A	3741	1/1	0.89	0.08	56,56,56,56	0
55	MG	2A	3075	1/1	0.89	0.13	53,53,53,53	0
55	MG	2A	3428	1/1	0.89	0.20	71,71,71,71	0
55	MG	1a	3199	1/1	0.89	0.13	68,68,68,68	0
55	MG	2A	3080	1/1	0.89	0.11	69,69,69,69	0
55	MG	1A	3648	1/1	0.89	0.07	90,90,90,90	0
55	MG	1A	3865	1/1	0.89	0.13	75,75,75,75	0
55	MG	1A	3866	1/1	0.89	0.14	61,61,61,61	0
55	MG	2A	3225	1/1	0.89	0.12	51,51,51,51	0
55	MG	2A	3246	1/1	0.89	0.07	92,92,92,92	0
55	MG	2a	1660	1/1	0.89	0.17	79,79,79,79	0
55	MG	2a	1664	1/1	0.89	0.21	69,69,69,69	0
55	MG	2a	1667	1/1	0.89	0.15	64,64,64,64	0
55	MG	2A	3089	1/1	0.89	0.13	56,56,56,56	0
55	MG	1a	3050	1/1	0.89	0.14	45,45,45,45	0
55	MG	2A	3454	1/1	0.89	0.15	81,81,81,81	0
55	MG	10	104	1/1	0.89	0.11	50,50,50,50	0
55	MG	2a	1678	1/1	0.89	0.29	65,65,65,65	0
55	MG	1A	3654	1/1	0.89	0.10	41,41,41,41	0
55	MG	2a	1683	1/1	0.89	0.27	67,67,67,67	0
55	MG	1A	3656	1/1	0.89	0.20	79,79,79,79	0
55	MG	2A	3100	1/1	0.89	0.10	58,58,58,58	0
55	MG	2A	3462	1/1	0.89	0.19	62,62,62,62	0
55	MG	2a	1694	1/1	0.89	0.35	78,78,78,78	0
55	MG	1A	3008	1/1	0.89	0.13	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1a	3223	1/1	0.89	0.19	54,54,54,54	0
55	MG	2a	1700	1/1	0.89	0.17	76,76,76,76	0
55	MG	2a	1703	1/1	0.89	0.10	61,61,61,61	0
55	MG	1A	3762	1/1	0.89	0.26	48,48,48,48	0
55	MG	2A	3267	1/1	0.89	0.20	61,61,61,61	0
55	MG	1A	3041	1/1	0.89	0.20	62,62,62,62	0
55	MG	1A	3353	1/1	0.89	0.18	67,67,67,67	0
55	MG	1A	3567	1/1	0.89	0.18	30,30,30,30	0
55	MG	2F	302	1/1	0.89	0.18	55,55,55,55	0
55	MG	1A	3243	1/1	0.89	0.36	44,44,44,44	0
55	MG	1A	3675	1/1	0.89	0.31	47,47,47,47	0
55	MG	1A	3684	1/1	0.89	0.11	49,49,49,49	0
55	MG	2A	3309	1/1	0.89	0.16	65,65,65,65	0
55	MG	2a	1720	1/1	0.89	0.12	73,73,73,73	0
55	MG	2A	3310	1/1	0.89	0.17	57,57,57,57	0
55	MG	1a	3065	1/1	0.89	0.31	65,65,65,65	0
55	MG	2Q	8002	1/1	0.89	0.09	62,62,62,62	0
55	MG	1A	3689	1/1	0.89	0.14	68,68,68,68	0
55	MG	1A	3361	1/1	0.89	0.13	75,75,75,75	0
55	MG	2A	3674	1/1	0.89	0.07	66,66,66,66	0
55	MG	2A	3676	1/1	0.89	0.17	73,73,73,73	0
55	MG	1A	3695	1/1	0.89	0.23	60,60,60,60	0
55	MG	1A	3187	1/1	0.89	0.08	52,52,52,52	0
55	MG	1A	3057	1/1	0.89	0.12	54,54,54,54	0
55	MG	2A	3330	1/1	0.89	0.12	57,57,57,57	0
55	MG	1B	3019	1/1	0.89	0.26	60,60,60,60	0
55	MG	2a	1752	1/1	0.89	0.10	86,86,86,86	0
55	MG	1a	3017	1/1	0.89	0.10	65,65,65,65	0
55	MG	1A	3817	1/1	0.89	0.27	72,72,72,72	0
55	MG	2a	1757	1/1	0.89	0.21	71,71,71,71	0
55	MG	1a	3082	1/1	0.89	0.19	62,62,62,62	0
55	MG	1A	3134	1/1	0.89	0.25	65,65,65,65	0
55	MG	2a	1761	1/1	0.89	0.18	67,67,67,67	0
55	MG	2A	3023	1/1	0.89	0.25	47,47,47,47	0
55	MG	2A	3523	1/1	0.89	0.10	61,61,61,61	0
55	MG	25	101	1/1	0.89	0.20	58,58,58,58	0
55	MG	25	102	1/1	0.89	0.08	62,62,62,62	0
55	MG	2a	1779	1/1	0.89	0.14	75,75,75,75	0
55	MG	2A	3530	1/1	0.89	0.35	52,52,52,52	0
55	MG	1A	3707	1/1	0.89	0.20	72,72,72,72	0
55	MG	1A	3160	1/1	0.89	0.49	40,40,40,40	0
55	MG	2A	3534	1/1	0.89	0.21	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
55	MG	1A	3201	1/1	0.89	0.16	41,41,41,41	0
55	MG	2A	3380	1/1	0.89	0.14	81,81,81,81	0
55	MG	2A	3750	1/1	0.89	0.12	63,63,63,63	0
55	MG	1A	3624	1/1	0.89	0.41	68,68,68,68	0
55	MG	2A	3031	1/1	0.89	0.34	59,59,59,59	0
55	MG	2a	1607	1/1	0.89	0.15	52,52,52,52	0
55	MG	1D	318	1/1	0.89	0.09	50,50,50,50	0
55	MG	1A	3406	1/1	0.89	0.09	46,46,46,46	0
55	MG	2f	8001	1/1	0.89	0.13	56,56,56,56	0
55	MG	2A	3396	1/1	0.89	0.10	71,71,71,71	0
55	MG	2a	1615	1/1	0.89	0.14	47,47,47,47	0
55	MG	2A	3164	1/1	0.89	0.10	56,56,56,56	0
55	MG	2A	3765	1/1	0.89	0.22	59,59,59,59	0
55	MG	2A	3400	1/1	0.89	0.11	43,43,43,43	0
55	MG	2A	3555	1/1	0.89	0.29	52,52,52,52	0
55	MG	15	107	1/1	0.90	0.10	52,52,52,52	0
55	MG	18	3301	1/1	0.90	0.39	70,70,70,70	0
55	MG	2a	1621	1/1	0.90	0.33	58,58,58,58	0
55	MG	1B	3002	1/1	0.90	0.31	69,69,69,69	0
55	MG	2A	3147	1/1	0.90	0.15	78,78,78,78	0
55	MG	1A	3488	1/1	0.90	0.24	43,43,43,43	0
55	MG	1a	3151	1/1	0.90	0.10	76,76,76,76	0
55	MG	1A	3736	1/1	0.90	0.19	55,55,55,55	0
55	MG	2A	3157	1/1	0.90	0.15	62,62,62,62	0
55	MG	2A	3786	1/1	0.90	0.07	49,49,49,49	0
55	MG	1A	3318	1/1	0.90	0.16	61,61,61,61	0
55	MG	1A	3676	1/1	0.90	0.20	70,70,70,70	0
55	MG	1a	3069	1/1	0.90	0.30	62,62,62,62	0
55	MG	1a	3160	1/1	0.90	0.19	84,84,84,84	0
55	MG	1A	3680	1/1	0.90	0.09	59,59,59,59	0
55	MG	2a	1640	1/1	0.90	0.43	61,61,61,61	0
55	MG	2A	3039	1/1	0.90	0.35	60,60,60,60	0
55	MG	2A	3174	1/1	0.90	0.09	58,58,58,58	0
55	MG	2A	3413	1/1	0.90	0.09	70,70,70,70	0
55	MG	2A	3175	1/1	0.90	0.28	69,69,69,69	0
55	MG	2A	3806	1/1	0.90	0.15	73,73,73,73	0
55	MG	2A	3808	1/1	0.90	0.25	44,44,44,44	0
55	MG	1A	3529	1/1	0.90	0.21	58,58,58,58	0
55	MG	2a	1648	1/1	0.90	0.09	63,63,63,63	0
55	MG	1A	3532	1/1	0.90	0.13	69,69,69,69	0
55	MG	1A	3117	1/1	0.90	0.10	44,44,44,44	0
55	MG	2A	3182	1/1	0.90	0.31	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
55	MG	2a	1655	1/1	0.90	0.09	84,84,84,84	0
55	MG	1A	3854	1/1	0.90	0.12	72,72,72,72	0
55	MG	2a	1658	1/1	0.90	0.08	74,74,74,74	0
55	MG	2A	3590	1/1	0.90	0.32	65,65,65,65	0
55	MG	1A	3346	1/1	0.90	0.13	52,52,52,52	0
55	MG	2A	3190	1/1	0.90	0.17	68,68,68,68	0
55	MG	1A	3189	1/1	0.90	0.14	43,43,43,43	0
55	MG	1A	3774	1/1	0.90	0.19	45,45,45,45	0
55	MG	1A	3099	1/1	0.90	0.10	62,62,62,62	0
55	MG	2A	3430	1/1	0.90	0.16	74,74,74,74	0
55	MG	1a	3085	1/1	0.90	0.26	64,64,64,64	0
55	MG	1a	3021	1/1	0.90	0.10	63,63,63,63	0
55	MG	2B	3009	1/1	0.90	0.09	71,71,71,71	0
55	MG	1E	306	1/1	0.90	0.10	52,52,52,52	0
55	MG	2B	3012	1/1	0.90	0.09	87,87,87,87	0
55	MG	2A	3436	1/1	0.90	0.08	72,72,72,72	0
55	MG	1a	3183	1/1	0.90	0.16	84,84,84,84	0
55	MG	2A	3074	1/1	0.90	0.17	48,48,48,48	0
55	MG	2A	3221	1/1	0.90	0.32	52,52,52,52	0
55	MG	2A	3622	1/1	0.90	0.16	49,49,49,49	0
55	MG	2A	3623	1/1	0.90	0.10	66,66,66,66	0
55	MG	1A	3593	1/1	0.90	0.10	34,34,34,34	0
55	MG	2a	1705	1/1	0.90	0.08	69,69,69,69	0
55	MG	2a	1706	1/1	0.90	0.18	63,63,63,63	0
55	MG	1a	3026	1/1	0.90	0.30	58,58,58,58	0
55	MG	2A	3451	1/1	0.90	0.33	67,67,67,67	0
55	MG	1F	304	1/1	0.90	0.28	39,39,39,39	0
55	MG	2A	3235	1/1	0.90	0.09	69,69,69,69	0
55	MG	2E	304	1/1	0.90	0.32	46,46,46,46	0
55	MG	2a	1714	1/1	0.90	0.26	71,71,71,71	0
55	MG	2A	3245	1/1	0.90	0.20	78,78,78,78	0
55	MG	1a	3188	1/1	0.90	0.17	64,64,64,64	0
55	MG	2F	310	1/1	0.90	0.07	75,75,75,75	0
55	MG	1A	3474	1/1	0.90	0.14	69,69,69,69	0
55	MG	1a	3111	1/1	0.90	0.12	56,56,56,56	0
55	MG	2A	3088	1/1	0.90	0.12	81,81,81,81	0
55	MG	2a	1724	1/1	0.90	0.12	93,93,93,93	0
55	MG	2A	3644	1/1	0.90	0.17	63,63,63,63	0
55	MG	1F	315	1/1	0.90	0.29	43,43,43,43	0
55	MG	1A	3783	1/1	0.90	0.09	55,55,55,55	0
55	MG	2A	3094	1/1	0.90	0.47	59,59,59,59	0
55	MG	1G	3001	1/1	0.90	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
55	MG	2R	201	1/1	0.90	0.24	56,56,56,56	0
55	MG	1A	3869	1/1	0.90	0.10	39,39,39,39	0
55	MG	1a	3036	1/1	0.90	0.17	49,49,49,49	0
55	MG	1H	8001	1/1	0.90	0.15	76,76,76,76	0
55	MG	1A	3710	1/1	0.90	0.09	42,42,42,42	0
55	MG	2U	204	1/1	0.90	0.17	55,55,55,55	0
55	MG	1A	3408	1/1	0.90	0.13	43,43,43,43	0
55	MG	1A	3509	1/1	0.90	0.12	38,38,38,38	0
55	MG	1A	3112	1/1	0.90	0.19	42,42,42,42	0
55	MG	1R	201	1/1	0.90	0.33	46,46,46,46	0
55	MG	2A	3485	1/1	0.90	0.48	73,73,73,73	0
55	MG	1A	3194	1/1	0.90	0.22	34,34,34,34	0
55	MG	2A	3109	1/1	0.90	0.18	64,64,64,64	0
55	MG	2A	3488	1/1	0.90	0.21	58,58,58,58	0
55	MG	1T	201	1/1	0.90	0.14	54,54,54,54	0
55	MG	2A	3494	1/1	0.90	0.11	77,77,77,77	0
55	MG	1V	201	1/1	0.90	0.19	25,25,25,25	0
55	MG	2A	3697	1/1	0.90	0.10	57,57,57,57	0
55	MG	2A	3321	1/1	0.90	0.08	34,34,34,34	0
55	MG	1W	3002	1/1	0.90	0.20	49,49,49,49	0
55	MG	1A	3807	1/1	0.90	0.09	48,48,48,48	0
55	MG	2A	3717	1/1	0.90	0.13	92,92,92,92	0
55	MG	2A	3325	1/1	0.90	0.13	51,51,51,51	0
55	MG	1a	3052	1/1	0.90	0.32	51,51,51,51	0
55	MG	2a	1793	1/1	0.90	0.17	61,61,61,61	0
55	MG	1m	201	1/1	0.90	0.10	72,72,72,72	0
55	MG	2a	1796	1/1	0.90	0.14	60,60,60,60	0
55	MG	1A	3010	1/1	0.90	0.24	37,37,37,37	0
55	MG	2A	3512	1/1	0.90	0.11	61,61,61,61	0
55	MG	10	103	1/1	0.90	0.18	65,65,65,65	0
55	MG	2a	1608	1/1	0.90	0.18	51,51,51,51	0
55	MG	1A	3569	1/1	0.90	0.14	43,43,43,43	0
55	MG	2A	3005	1/1	0.90	0.18	44,44,44,44	0
55	MG	2a	1613	1/1	0.90	0.33	61,61,61,61	0
55	MG	1A	3899	1/1	0.90	0.25	51,51,51,51	0
55	MG	1A	3570	1/1	0.90	0.12	48,48,48,48	0
55	MG	2A	3135	1/1	0.90	0.33	71,71,71,71	0
55	MG	1A	3907	1/1	0.90	0.15	46,46,46,46	0
55	MG	1A	3828	1/1	0.90	0.11	61,61,61,61	0
55	MG	2A	3769	1/1	0.91	0.10	75,75,75,75	0
55	MG	2A	3010	1/1	0.91	0.18	63,63,63,63	0
55	MG	2a	1630	1/1	0.91	0.17	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3338	1/1	0.91	0.51	70,70,70,70	0
55	MG	2A	3137	1/1	0.91	0.24	60,60,60,60	0
55	MG	1A	3095	1/1	0.91	0.18	61,61,61,61	0
55	MG	1A	3682	1/1	0.91	0.15	61,61,61,61	0
55	MG	1A	3188	1/1	0.91	0.22	34,34,34,34	0
55	MG	10	108	1/1	0.91	0.36	43,43,43,43	0
55	MG	2A	3351	1/1	0.91	0.11	68,68,68,68	0
55	MG	2A	3550	1/1	0.91	0.12	48,48,48,48	0
55	MG	1A	3905	1/1	0.91	0.35	45,45,45,45	0
55	MG	2A	3797	1/1	0.91	0.12	75,75,75,75	0
55	MG	2A	3377	1/1	0.91	0.07	94,94,94,94	0
55	MG	1A	3113	1/1	0.91	0.22	41,41,41,41	0
55	MG	1A	3690	1/1	0.91	0.14	67,67,67,67	0
55	MG	1B	3001	1/1	0.91	0.20	55,55,55,55	0
55	MG	1A	3468	1/1	0.91	0.11	49,49,49,49	0
55	MG	2A	3154	1/1	0.91	0.37	61,61,61,61	0
55	MG	2A	3567	1/1	0.91	0.31	51,51,51,51	0
55	MG	2a	1651	1/1	0.91	0.11	69,69,69,69	0
55	MG	2A	3388	1/1	0.91	0.15	60,60,60,60	0
55	MG	1A	3115	1/1	0.91	0.15	54,54,54,54	0
55	MG	1A	3808	1/1	0.91	0.20	38,38,38,38	0
55	MG	2A	3032	1/1	0.91	0.45	66,66,66,66	0
55	MG	1A	3078	1/1	0.91	0.33	39,39,39,39	0
55	MG	2a	1659	1/1	0.91	0.13	71,71,71,71	0
55	MG	1B	3007	1/1	0.91	0.11	51,51,51,51	0
55	MG	1a	3073	1/1	0.91	0.23	74,74,74,74	0
55	MG	2A	3586	1/1	0.91	0.13	101,101,101,101	0
55	MG	1B	3009	1/1	0.91	0.09	60,60,60,60	0
55	MG	1A	3079	1/1	0.91	0.11	40,40,40,40	0
55	MG	1A	3232	1/1	0.91	0.74	35,35,35,35	0
55	MG	2A	3046	1/1	0.91	0.12	51,51,51,51	0
55	MG	1A	3007	1/1	0.91	0.07	38,38,38,38	0
55	MG	1A	3476	1/1	0.91	0.09	45,45,45,45	0
55	MG	2A	3049	1/1	0.91	0.16	38,38,38,38	0
55	MG	1A	3714	1/1	0.91	0.16	68,68,68,68	0
55	MG	1A	3834	1/1	0.91	0.07	61,61,61,61	0
55	MG	2A	3055	1/1	0.91	0.12	49,49,49,49	0
55	MG	2A	3057	1/1	0.91	0.45	49,49,49,49	0
55	MG	2A	3193	1/1	0.91	0.28	76,76,76,76	0
55	MG	1A	3368	1/1	0.91	0.09	29,29,29,29	0
55	MG	2A	3063	1/1	0.91	0.66	49,49,49,49	0
55	MG	2a	1701	1/1	0.91	0.15	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
55	MG	1a	3181	1/1	0.91	0.08	74,74,74,74	0
55	MG	2A	3065	1/1	0.91	0.25	56,56,56,56	0
55	MG	2A	3200	1/1	0.91	0.49	65,65,65,65	0
55	MG	2A	3203	1/1	0.91	0.35	63,63,63,63	0
55	MG	1D	305	1/1	0.91	0.22	42,42,42,42	0
55	MG	1A	3196	1/1	0.91	0.13	36,36,36,36	0
55	MG	2a	1709	1/1	0.91	0.16	82,82,82,82	0
55	MG	2A	3212	1/1	0.91	0.09	60,60,60,60	0
55	MG	1a	3088	1/1	0.91	0.18	63,63,63,63	0
55	MG	2A	3440	1/1	0.91	0.15	74,74,74,74	0
55	MG	1A	3286	1/1	0.91	0.12	64,64,64,64	0
55	MG	2A	3442	1/1	0.91	0.17	81,81,81,81	0
55	MG	2A	3640	1/1	0.91	0.14	78,78,78,78	0
55	MG	2A	3076	1/1	0.91	0.26	55,55,55,55	0
55	MG	1A	3381	1/1	0.91	0.12	62,62,62,62	0
55	MG	2A	3224	1/1	0.91	0.09	69,69,69,69	0
55	MG	1A	3395	1/1	0.91	0.10	44,44,44,44	0
55	MG	2A	3228	1/1	0.91	0.13	51,51,51,51	0
55	MG	2A	3229	1/1	0.91	0.15	82,82,82,82	0
55	MG	1A	3635	1/1	0.91	0.12	39,39,39,39	0
55	MG	2A	3652	1/1	0.91	0.18	53,53,53,53	0
55	MG	2a	1731	1/1	0.91	0.11	90,90,90,90	0
55	MG	2A	3242	1/1	0.91	0.17	40,40,40,40	0
55	MG	2A	3243	1/1	0.91	0.11	72,72,72,72	0
55	MG	1a	3193	1/1	0.91	0.18	74,74,74,74	0
55	MG	1a	3194	1/1	0.91	0.08	83,83,83,83	0
55	MG	1A	3497	1/1	0.91	0.16	66,66,66,66	0
55	MG	1A	3156	1/1	0.91	0.29	54,54,54,54	0
55	MG	2a	1740	1/1	0.91	0.09	70,70,70,70	0
55	MG	2A	3470	1/1	0.91	0.11	63,63,63,63	0
55	MG	2a	1745	1/1	0.91	0.20	67,67,67,67	0
55	MG	1A	3642	1/1	0.91	0.24	36,36,36,36	0
55	MG	2a	1751	1/1	0.91	0.10	107,107,107,107	0
55	MG	1A	3646	1/1	0.91	0.10	31,31,31,31	0
55	MG	2a	1753	1/1	0.91	0.27	69,69,69,69	0
55	MG	2A	3255	1/1	0.91	0.12	62,62,62,62	0
55	MG	1A	3289	1/1	0.91	0.08	53,53,53,53	0
55	MG	1a	3033	1/1	0.91	0.12	50,50,50,50	0
55	MG	1A	3307	1/1	0.91	0.12	63,63,63,63	0
55	MG	23	101	1/1	0.91	0.23	64,64,64,64	0
55	MG	1A	3404	1/1	0.91	0.10	60,60,60,60	0
55	MG	2a	1768	1/1	0.91	0.08	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
55	MG	2A	3261	1/1	0.91	0.11	88,88,88,88	0
55	MG	1N	8001	1/1	0.91	0.19	51,51,51,51	0
55	MG	1A	3177	1/1	0.91	0.20	52,52,52,52	0
55	MG	1A	3077	1/1	0.91	0.27	47,47,47,47	0
55	MG	1a	3040	1/1	0.91	0.24	75,75,75,75	0
55	MG	2A	3708	1/1	0.91	0.15	66,66,66,66	0
55	MG	1A	3130	1/1	0.91	0.08	33,33,33,33	0
55	MG	1A	3666	1/1	0.91	0.14	45,45,45,45	0
55	MG	1A	3881	1/1	0.91	0.12	43,43,43,43	0
55	MG	2A	3301	1/1	0.91	0.09	49,49,49,49	0
55	MG	1A	3773	1/1	0.91	0.06	44,44,44,44	0
55	MG	1a	3129	1/1	0.91	0.10	66,66,66,66	0
55	MG	1a	3046	1/1	0.91	0.21	54,54,54,54	0
55	MG	2A	3315	1/1	0.91	0.11	67,67,67,67	0
55	MG	2A	3114	1/1	0.91	0.20	62,62,62,62	0
55	MG	2d	503	1/1	0.91	0.10	79,79,79,79	0
55	MG	2A	3742	1/1	0.91	0.26	70,70,70,70	0
55	MG	1A	3589	1/1	0.91	0.10	36,36,36,36	0
55	MG	1U	203	1/1	0.91	0.19	42,42,42,42	0
55	MG	1A	3444	1/1	0.91	0.15	75,75,75,75	0
55	MG	2A	3515	1/1	0.91	0.15	52,52,52,52	0
55	MG	1V	203	1/1	0.91	0.13	60,60,60,60	0
55	MG	1A	3315	1/1	0.91	0.18	45,45,45,45	0
55	MG	2A	3006	1/1	0.91	0.09	36,36,36,36	0
55	MG	1A	3892	1/1	0.91	0.14	62,62,62,62	0
55	MG	2o	3001	1/1	0.91	0.16	60,60,60,60	0
55	MG	1A	3452	1/1	0.91	0.22	76,76,76,76	0
55	MG	10	102	1/1	0.91	0.13	52,52,52,52	0
55	MG	1A	3073	1/1	0.92	0.26	43,43,43,43	0
55	MG	1A	3743	1/1	0.92	0.07	45,45,45,45	0
55	MG	2A	3130	1/1	0.92	0.12	58,58,58,58	0
55	MG	2A	3445	1/1	0.92	0.09	48,48,48,48	0
55	MG	2A	3810	1/1	0.92	0.23	51,51,51,51	0
55	MG	1A	3220	1/1	0.92	0.31	77,77,77,77	0
55	MG	2A	3448	1/1	0.92	0.09	51,51,51,51	0
55	MG	2A	3132	1/1	0.92	0.15	63,63,63,63	0
55	MG	1a	3100	1/1	0.92	0.29	60,60,60,60	0
55	MG	2A	3262	1/1	0.92	0.14	74,74,74,74	0
55	MG	2A	3818	1/1	0.92	0.15	57,57,57,57	0
55	MG	2A	3036	1/1	0.92	0.17	48,48,48,48	0
55	MG	1A	3755	1/1	0.92	0.09	69,69,69,69	0
55	MG	1A	3560	1/1	0.92	0.07	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
55	MG	2a	1654	1/1	0.92	0.38	70,70,70,70	0
55	MG	2B	3003	1/1	0.92	0.07	73,73,73,73	0
55	MG	1A	3759	1/1	0.92	0.26	61,61,61,61	0
55	MG	2A	3142	1/1	0.92	0.34	60,60,60,60	0
55	MG	1A	3845	1/1	0.92	0.09	43,43,43,43	0
55	MG	1A	3457	1/1	0.92	0.06	24,24,24,24	0
55	MG	1a	3114	1/1	0.92	0.08	74,74,74,74	0
55	MG	2a	1665	1/1	0.92	0.10	74,74,74,74	0
55	MG	2a	1666	1/1	0.92	0.14	79,79,79,79	0
55	MG	1A	3459	1/1	0.92	0.22	50,50,50,50	0
55	MG	2A	3148	1/1	0.92	0.10	57,57,57,57	0
55	MG	1A	3763	1/1	0.92	0.12	22,22,22,22	0
55	MG	2A	3150	1/1	0.92	0.16	49,49,49,49	0
55	MG	2A	3639	1/1	0.92	0.10	76,76,76,76	0
55	MG	1A	3378	1/1	0.92	0.06	20,20,20,20	0
55	MG	1A	3316	1/1	0.92	0.12	58,58,58,58	0
55	MG	1A	3388	1/1	0.92	0.13	48,48,48,48	0
55	MG	2D	301	1/1	0.92	0.47	47,47,47,47	0
55	MG	1A	3861	1/1	0.92	0.08	82,82,82,82	0
55	MG	2D	303	1/1	0.92	0.16	50,50,50,50	0
55	MG	2A	3324	1/1	0.92	0.18	61,61,61,61	0
55	MG	2A	3158	1/1	0.92	0.16	72,72,72,72	0
55	MG	2D	306	1/1	0.92	0.17	57,57,57,57	0
55	MG	2A	3159	1/1	0.92	0.17	58,58,58,58	0
55	MG	2A	3649	1/1	0.92	0.17	49,49,49,49	0
55	MG	2A	3161	1/1	0.92	0.30	54,54,54,54	0
55	MG	1a	3051	1/1	0.92	0.21	57,57,57,57	0
55	MG	15	105	1/1	0.92	0.17	43,43,43,43	0
55	MG	2A	3654	1/1	0.92	0.09	34,34,34,34	0
55	MG	2F	309	1/1	0.92	0.17	60,60,60,60	0
55	MG	1A	3093	1/1	0.92	0.12	43,43,43,43	0
55	MG	2A	3165	1/1	0.92	0.30	58,58,58,58	0
55	MG	1A	3004	1/1	0.92	0.06	41,41,41,41	0
55	MG	1D	304	1/1	0.92	0.23	37,37,37,37	0
55	MG	2A	3501	1/1	0.92	0.16	76,76,76,76	0
55	MG	1A	3575	1/1	0.92	0.19	23,23,23,23	0
55	MG	1A	3193	1/1	0.92	0.14	42,42,42,42	0
55	MG	2A	3069	1/1	0.92	0.40	52,52,52,52	0
55	MG	2A	3675	1/1	0.92	0.06	70,70,70,70	0
55	MG	2Q	8005	1/1	0.92	0.12	62,62,62,62	0
55	MG	2A	3177	1/1	0.92	0.09	62,62,62,62	0
55	MG	2a	1721	1/1	0.92	0.06	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1D	308	1/1	0.92	0.08	58,58,58,58	0
55	MG	1a	3131	1/1	0.92	0.09	76,76,76,76	0
55	MG	2A	3370	1/1	0.92	0.15	76,76,76,76	0
55	MG	2A	3688	1/1	0.92	0.09	66,66,66,66	0
55	MG	1A	3111	1/1	0.92	0.10	42,42,42,42	0
55	MG	2A	3513	1/1	0.92	0.30	47,47,47,47	0
55	MG	1A	3870	1/1	0.92	0.18	54,54,54,54	0
55	MG	2A	3518	1/1	0.92	0.07	71,71,71,71	0
55	MG	2A	3183	1/1	0.92	0.10	75,75,75,75	0
55	MG	1A	3874	1/1	0.92	0.09	59,59,59,59	0
55	MG	2A	3186	1/1	0.92	0.22	61,61,61,61	0
55	MG	2A	3527	1/1	0.92	0.19	73,73,73,73	0
55	MG	1d	503	1/1	0.92	0.18	63,63,63,63	0
55	MG	1A	3293	1/1	0.92	0.12	75,75,75,75	0
55	MG	1F	303	1/1	0.92	0.26	43,43,43,43	0
55	MG	1e	3002	1/1	0.92	0.18	58,58,58,58	0
55	MG	2A	3087	1/1	0.92	0.19	62,62,62,62	0
55	MG	1A	3349	1/1	0.92	0.09	25,25,25,25	0
55	MG	2A	3401	1/1	0.92	0.15	66,66,66,66	0
55	MG	2a	1754	1/1	0.92	0.17	85,85,85,85	0
55	MG	1a	3140	1/1	0.92	0.12	84,84,84,84	0
55	MG	1a	3012	1/1	0.92	0.14	68,68,68,68	0
55	MG	2A	3407	1/1	0.92	0.36	74,74,74,74	0
55	MG	1A	3525	1/1	0.92	0.14	57,57,57,57	0
55	MG	1A	3885	1/1	0.92	0.11	37,37,37,37	0
55	MG	1o	3001	1/1	0.92	0.17	52,52,52,52	0
55	MG	2a	1765	1/1	0.92	0.17	71,71,71,71	0
55	MG	2a	1766	1/1	0.92	0.08	91,91,91,91	0
55	MG	1A	3306	1/1	0.92	0.08	14,14,14,14	0
55	MG	1a	3071	1/1	0.92	0.26	53,53,53,53	0
55	MG	2A	3556	1/1	0.92	0.31	57,57,57,57	0
55	MG	1A	3479	1/1	0.92	0.10	39,39,39,39	0
55	MG	2A	3763	1/1	0.92	0.07	41,41,41,41	0
55	MG	1A	3084	1/1	0.92	0.14	47,47,47,47	0
55	MG	1a	3075	1/1	0.92	0.16	48,48,48,48	0
55	MG	1A	3242	1/1	0.92	0.23	29,29,29,29	0
55	MG	2a	1784	1/1	0.92	0.10	80,80,80,80	0
55	MG	1A	3891	1/1	0.92	0.20	64,64,64,64	0
55	MG	2A	3773	1/1	0.92	0.10	85,85,85,85	0
55	MG	1A	3815	1/1	0.92	0.14	51,51,51,51	0
55	MG	2A	3776	1/1	0.92	0.09	43,43,43,43	0
55	MG	1a	3080	1/1	0.92	0.12	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3778	1/1	0.92	0.09	50,50,50,50	0
55	MG	2A	3110	1/1	0.92	0.15	53,53,53,53	0
55	MG	1A	3445	1/1	0.92	0.13	65,65,65,65	0
55	MG	2A	3788	1/1	0.92	0.07	88,88,88,88	0
55	MG	2A	3014	1/1	0.92	0.21	66,66,66,66	0
55	MG	2a	1626	1/1	0.92	0.18	60,60,60,60	0
55	MG	2a	1627	1/1	0.92	0.17	84,84,84,84	0
55	MG	1A	3144	1/1	0.92	0.18	64,64,64,64	0
55	MG	2A	3583	1/1	0.92	0.17	72,72,72,72	0
55	MG	1A	3600	1/1	0.92	0.08	67,67,67,67	0
55	MG	2A	3021	1/1	0.92	0.12	43,43,43,43	0
55	MG	1A	3900	1/1	0.92	0.20	58,58,58,58	0
55	MG	1A	3549	1/1	0.92	0.22	31,31,31,31	0
55	MG	1A	3494	1/1	0.92	0.20	59,59,59,59	0
55	MG	1U	202	1/1	0.92	0.13	43,43,43,43	0
55	MG	2A	3803	1/1	0.92	0.44	69,69,69,69	0
55	MG	2A	3784	1/1	0.93	0.09	94,94,94,94	0
55	MG	1A	3440	1/1	0.93	0.13	47,47,47,47	0
55	MG	1A	3512	1/1	0.93	0.23	46,46,46,46	0
55	MG	2A	3189	1/1	0.93	0.10	43,43,43,43	0
55	MG	1A	3835	1/1	0.93	0.07	48,48,48,48	0
55	MG	1A	3135	1/1	0.93	0.07	37,37,37,37	0
55	MG	2a	1638	1/1	0.93	0.09	73,73,73,73	0
55	MG	2A	3572	1/1	0.93	0.13	55,55,55,55	0
55	MG	2A	3411	1/1	0.93	0.13	63,63,63,63	0
55	MG	1A	3072	1/1	0.93	0.07	43,43,43,43	0
55	MG	2A	3576	1/1	0.93	0.22	52,52,52,52	0
55	MG	1D	302	1/1	0.93	0.69	35,35,35,35	0
55	MG	1A	3139	1/1	0.93	0.27	59,59,59,59	0
55	MG	1A	3049	1/1	0.93	0.22	45,45,45,45	0
55	MG	2A	3804	1/1	0.93	0.12	35,35,35,35	0
55	MG	1a	3107	1/1	0.93	0.13	67,67,67,67	0
55	MG	2A	3584	1/1	0.93	0.12	62,62,62,62	0
55	MG	2a	1650	1/1	0.93	0.44	55,55,55,55	0
55	MG	2A	3199	1/1	0.93	0.23	65,65,65,65	0
55	MG	1a	3211	1/1	0.93	0.22	59,59,59,59	0
55	MG	1a	3108	1/1	0.93	0.06	81,81,81,81	0
55	MG	1A	3051	1/1	0.93	0.38	30,30,30,30	0
55	MG	2A	3424	1/1	0.93	0.15	50,50,50,50	0
55	MG	1A	3524	1/1	0.93	0.11	52,52,52,52	0
55	MG	1D	314	1/1	0.93	0.13	34,34,34,34	0
55	MG	1a	3024	1/1	0.93	0.13	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3092	1/1	0.93	0.35	49,49,49,49	0
55	MG	2a	1662	1/1	0.93	0.09	74,74,74,74	0
55	MG	2a	1663	1/1	0.93	0.21	63,63,63,63	0
55	MG	1A	3035	1/1	0.93	0.08	37,37,37,37	0
55	MG	1A	3528	1/1	0.93	0.13	57,57,57,57	0
55	MG	1A	3107	1/1	0.93	0.28	36,36,36,36	0
55	MG	2A	3602	1/1	0.93	0.06	73,73,73,73	0
55	MG	2A	3434	1/1	0.93	0.18	65,65,65,65	0
55	MG	1A	3031	1/1	0.93	0.10	22,22,22,22	0
55	MG	1A	3046	1/1	0.93	0.22	38,38,38,38	0
55	MG	1A	3860	1/1	0.93	0.10	53,53,53,53	0
55	MG	2A	3232	1/1	0.93	0.10	67,67,67,67	0
55	MG	1a	3032	1/1	0.93	0.12	45,45,45,45	0
55	MG	2A	3618	1/1	0.93	0.18	55,55,55,55	0
55	MG	2A	3619	1/1	0.93	0.08	50,50,50,50	0
55	MG	2a	1689	1/1	0.93	0.13	58,58,58,58	0
55	MG	1F	305	1/1	0.93	0.17	29,29,29,29	0
55	MG	1F	306	1/1	0.93	0.13	39,39,39,39	0
55	MG	2A	3106	1/1	0.93	0.14	60,60,60,60	0
55	MG	1A	3467	1/1	0.93	0.14	32,32,32,32	0
55	MG	1l	201	1/1	0.93	0.07	74,74,74,74	0
55	MG	1A	3082	1/1	0.93	0.46	37,37,37,37	0
55	MG	1A	3351	1/1	0.93	0.23	54,54,54,54	0
55	MG	1A	3541	1/1	0.93	0.33	34,34,34,34	0
55	MG	1A	3547	1/1	0.93	0.26	35,35,35,35	0
55	MG	2A	3001	1/1	0.93	0.14	55,55,55,55	0
55	MG	1A	3868	1/1	0.93	0.08	29,29,29,29	0
55	MG	1H	8002	1/1	0.93	0.08	46,46,46,46	0
55	MG	1A	3048	1/1	0.93	0.33	33,33,33,33	0
55	MG	1A	3637	1/1	0.93	0.12	38,38,38,38	0
55	MG	1A	3060	1/1	0.93	0.07	36,36,36,36	0
55	MG	1A	3875	1/1	0.93	0.10	44,44,44,44	0
55	MG	2a	1712	1/1	0.93	0.24	69,69,69,69	0
55	MG	1A	3260	1/1	0.93	0.19	36,36,36,36	0
55	MG	2F	307	1/1	0.93	0.22	60,60,60,60	0
55	MG	2A	3268	1/1	0.93	0.13	69,69,69,69	0
55	MG	2a	1716	1/1	0.93	0.22	73,73,73,73	0
55	MG	2A	3281	1/1	0.93	0.07	61,61,61,61	0
55	MG	2A	3285	1/1	0.93	0.08	47,47,47,47	0
55	MG	1A	3062	1/1	0.93	0.13	37,37,37,37	0
55	MG	1A	3088	1/1	0.93	0.46	30,30,30,30	0
55	MG	2A	3294	1/1	0.93	0.09	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3374	1/1	0.93	0.13	62,62,62,62	0
55	MG	2a	1723	1/1	0.93	0.11	110,110,110,110	0
55	MG	2A	3659	1/1	0.93	0.13	73,73,73,73	0
55	MG	2A	3015	1/1	0.93	0.32	50,50,50,50	0
55	MG	1A	3649	1/1	0.93	0.08	33,33,33,33	0
55	MG	2a	1728	1/1	0.93	0.07	86,86,86,86	0
55	MG	2a	1729	1/1	0.93	0.12	60,60,60,60	0
55	MG	2A	3482	1/1	0.93	0.23	54,54,54,54	0
55	MG	1A	3066	1/1	0.93	0.26	45,45,45,45	0
55	MG	1A	3094	1/1	0.93	0.34	30,30,30,30	0
55	MG	2R	203	1/1	0.93	0.14	39,39,39,39	0
55	MG	2A	3304	1/1	0.93	0.06	48,48,48,48	0
55	MG	2A	3305	1/1	0.93	0.08	84,84,84,84	0
55	MG	2A	3307	1/1	0.93	0.09	54,54,54,54	0
55	MG	1A	3485	1/1	0.93	0.24	47,47,47,47	0
55	MG	1a	3148	1/1	0.93	0.08	82,82,82,82	0
55	MG	1W	3001	1/1	0.93	0.23	38,38,38,38	0
55	MG	1A	3070	1/1	0.93	0.31	32,32,32,32	0
55	MG	1A	3572	1/1	0.93	0.10	41,41,41,41	0
55	MG	2A	3028	1/1	0.93	0.29	64,64,64,64	0
55	MG	2A	3029	1/1	0.93	0.14	61,61,61,61	0
55	MG	2A	3694	1/1	0.93	0.06	65,65,65,65	0
55	MG	20	101	1/1	0.93	0.24	64,64,64,64	0
55	MG	20	103	1/1	0.93	0.07	59,59,59,59	0
55	MG	1A	3665	1/1	0.93	0.23	51,51,51,51	0
55	MG	1A	3175	1/1	0.93	0.23	56,56,56,56	0
55	MG	1A	3667	1/1	0.93	0.16	46,46,46,46	0
55	MG	1A	3132	1/1	0.93	0.10	35,35,35,35	0
55	MG	1A	3181	1/1	0.93	0.10	51,51,51,51	0
55	MG	1A	3299	1/1	0.93	0.17	28,28,28,28	0
55	MG	2A	3156	1/1	0.93	0.23	39,39,39,39	0
55	MG	1A	3226	1/1	0.93	0.27	31,31,31,31	0
55	MG	1A	3910	1/1	0.93	0.23	35,35,35,35	0
55	MG	2A	3520	1/1	0.93	0.14	65,65,65,65	0
55	MG	13	102	1/1	0.93	0.17	44,44,44,44	0
55	MG	1A	3677	1/1	0.93	0.10	56,56,56,56	0
55	MG	2a	1778	1/1	0.93	0.07	79,79,79,79	0
55	MG	2A	3526	1/1	0.93	0.15	73,73,73,73	0
55	MG	15	104	1/1	0.93	0.22	26,26,26,26	0
55	MG	2A	3743	1/1	0.93	0.14	59,59,59,59	0
55	MG	1A	3403	1/1	0.93	0.13	53,53,53,53	0
55	MG	1A	3182	1/1	0.93	0.39	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	17	101	1/1	0.93	0.18	35,35,35,35	0
55	MG	1A	3683	1/1	0.93	0.14	51,51,51,51	0
55	MG	2A	3168	1/1	0.93	0.22	53,53,53,53	0
55	MG	2A	3051	1/1	0.93	0.20	61,61,61,61	0
55	MG	1A	3097	1/1	0.93	0.28	48,48,48,48	0
55	MG	1A	3687	1/1	0.93	0.14	56,56,56,56	0
55	MG	2A	3541	1/1	0.93	0.11	78,78,78,78	0
55	MG	2A	3764	1/1	0.93	0.07	72,72,72,72	0
55	MG	2A	3056	1/1	0.93	0.07	59,59,59,59	0
55	MG	1A	3582	1/1	0.93	0.14	69,69,69,69	0
55	MG	2A	3178	1/1	0.93	0.39	38,38,38,38	0
55	MG	1A	3824	1/1	0.93	0.13	47,47,47,47	0
55	MG	2A	3772	1/1	0.93	0.08	63,63,63,63	0
55	MG	2g	3001	1/1	0.93	0.27	72,72,72,72	0
55	MG	2A	3062	1/1	0.93	0.36	47,47,47,47	0
55	MG	2A	3774	1/1	0.93	0.13	79,79,79,79	0
55	MG	1A	3309	1/1	0.93	0.07	32,32,32,32	0
55	MG	1B	3014	1/1	0.93	0.08	41,41,41,41	0
55	MG	1A	3312	1/1	0.93	0.10	64,64,64,64	0
55	MG	2A	3557	1/1	0.93	0.10	67,67,67,67	0
55	MG	2A	3066	1/1	0.93	0.21	58,58,58,58	0
55	MG	1A	3609	1/1	0.94	0.07	62,62,62,62	0
55	MG	1A	3510	1/1	0.94	0.08	70,70,70,70	0
55	MG	1A	3159	1/1	0.94	0.14	30,30,30,30	0
55	MG	2A	3191	1/1	0.94	0.18	61,61,61,61	0
55	MG	2A	3664	1/1	0.94	0.07	75,75,75,75	0
55	MG	2A	3035	1/1	0.94	0.20	32,32,32,32	0
55	MG	1A	3110	1/1	0.94	0.25	38,38,38,38	0
55	MG	1a	3011	1/1	0.94	0.16	32,32,32,32	0
55	MG	1A	3914	1/1	0.94	0.17	62,62,62,62	0
55	MG	1A	3047	1/1	0.94	0.13	24,24,24,24	0
55	MG	1a	3014	1/1	0.94	0.18	81,81,81,81	0
55	MG	2A	3043	1/1	0.94	0.08	72,72,72,72	0
55	MG	1a	3015	1/1	0.94	0.11	74,74,74,74	0
55	MG	1a	3133	1/1	0.94	0.06	74,74,74,74	0
55	MG	2a	1611	1/1	0.94	0.11	58,58,58,58	0
55	MG	2a	1612	1/1	0.94	0.07	51,51,51,51	0
55	MG	2A	3681	1/1	0.94	0.08	71,71,71,71	0
55	MG	2A	3204	1/1	0.94	0.08	54,54,54,54	0
55	MG	1A	3056	1/1	0.94	0.16	28,28,28,28	0
55	MG	1A	3164	1/1	0.94	0.17	59,59,59,59	0
55	MG	1a	3018	1/1	0.94	0.06	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3691	1/1	0.94	0.07	70,70,70,70	0
55	MG	1A	3518	1/1	0.94	0.17	77,77,77,77	0
55	MG	2A	3465	1/1	0.94	0.10	71,71,71,71	0
55	MG	2A	3467	1/1	0.94	0.11	57,57,57,57	0
55	MG	1A	3767	1/1	0.94	0.07	51,51,51,51	0
55	MG	2A	3705	1/1	0.94	0.14	75,75,75,75	0
55	MG	2A	3706	1/1	0.94	0.08	90,90,90,90	0
55	MG	1A	3411	1/1	0.94	0.12	52,52,52,52	0
55	MG	2A	3053	1/1	0.94	0.10	57,57,57,57	0
55	MG	1A	3521	1/1	0.94	0.07	45,45,45,45	0
55	MG	2A	3474	1/1	0.94	0.08	70,70,70,70	0
55	MG	1A	3427	1/1	0.94	0.08	42,42,42,42	0
55	MG	1a	3025	1/1	0.94	0.06	55,55,55,55	0
55	MG	1A	3133	1/1	0.94	0.37	35,35,35,35	0
55	MG	2A	3058	1/1	0.94	0.34	53,53,53,53	0
55	MG	2A	3479	1/1	0.94	0.10	40,40,40,40	0
55	MG	2A	3233	1/1	0.94	0.10	73,73,73,73	0
55	MG	2A	3234	1/1	0.94	0.10	45,45,45,45	0
55	MG	1A	3433	1/1	0.94	0.30	51,51,51,51	0
55	MG	1B	3018	1/1	0.94	0.08	37,37,37,37	0
55	MG	2a	1639	1/1	0.94	0.38	50,50,50,50	0
55	MG	1A	3436	1/1	0.94	0.08	49,49,49,49	0
55	MG	1A	3437	1/1	0.94	0.06	34,34,34,34	0
55	MG	1A	3439	1/1	0.94	0.07	54,54,54,54	0
55	MG	2A	3247	1/1	0.94	0.09	35,35,35,35	0
55	MG	2A	3754	1/1	0.94	0.14	101,101,101,101	0
55	MG	1A	3534	1/1	0.94	0.09	52,52,52,52	0
55	MG	1A	3535	1/1	0.94	0.07	38,38,38,38	0
55	MG	1a	3156	1/1	0.94	0.10	69,69,69,69	0
55	MG	2A	3760	1/1	0.94	0.09	40,40,40,40	0
55	MG	1A	3653	1/1	0.94	0.09	62,62,62,62	0
55	MG	1a	3035	1/1	0.94	0.45	64,64,64,64	0
55	MG	1A	3795	1/1	0.94	0.21	46,46,46,46	0
55	MG	1A	3536	1/1	0.94	0.08	44,44,44,44	0
55	MG	1A	3001	1/1	0.94	0.05	32,32,32,32	0
55	MG	1a	3164	1/1	0.94	0.10	61,61,61,61	0
55	MG	1A	3005	1/1	0.94	0.14	22,22,22,22	0
55	MG	1D	309	1/1	0.94	0.20	41,41,41,41	0
55	MG	1a	3168	1/1	0.94	0.09	79,79,79,79	0
55	MG	1A	3086	1/1	0.94	0.16	50,50,50,50	0
55	MG	2A	3514	1/1	0.94	0.22	53,53,53,53	0
55	MG	1A	3002	1/1	0.94	0.08	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3273	1/1	0.94	0.08	60,60,60,60	0
55	MG	1A	3143	1/1	0.94	0.15	45,45,45,45	0
55	MG	1E	303	1/1	0.94	0.09	39,39,39,39	0
55	MG	1a	3045	1/1	0.94	0.25	57,57,57,57	0
55	MG	2A	3785	1/1	0.94	0.07	60,60,60,60	0
55	MG	1A	3321	1/1	0.94	0.09	55,55,55,55	0
55	MG	1a	3179	1/1	0.94	0.07	78,78,78,78	0
55	MG	1F	301	1/1	0.94	0.19	28,28,28,28	0
55	MG	2a	1676	1/1	0.94	0.09	55,55,55,55	0
55	MG	2A	3791	1/1	0.94	0.09	45,45,45,45	0
55	MG	2A	3529	1/1	0.94	0.07	75,75,75,75	0
55	MG	2A	3098	1/1	0.94	0.18	53,53,53,53	0
55	MG	1A	3322	1/1	0.94	0.13	48,48,48,48	0
55	MG	1A	3827	1/1	0.94	0.10	64,64,64,64	0
55	MG	2a	1687	1/1	0.94	0.18	55,55,55,55	0
55	MG	1A	3345	1/1	0.94	0.12	45,45,45,45	0
55	MG	1A	3669	1/1	0.94	0.18	56,56,56,56	0
55	MG	1A	3012	1/1	0.94	0.10	22,22,22,22	0
55	MG	1F	310	1/1	0.94	0.13	27,27,27,27	0
55	MG	1A	3672	1/1	0.94	0.07	49,49,49,49	0
55	MG	1A	3259	1/1	0.94	0.11	52,52,52,52	0
55	MG	1A	3179	1/1	0.94	0.23	38,38,38,38	0
55	MG	1A	3350	1/1	0.94	0.09	46,46,46,46	0
55	MG	1A	3678	1/1	0.94	0.13	37,37,37,37	0
55	MG	1A	3211	1/1	0.94	0.39	31,31,31,31	0
55	MG	2A	3551	1/1	0.94	0.06	71,71,71,71	0
55	MG	1a	3060	1/1	0.94	0.14	69,69,69,69	0
55	MG	1A	3843	1/1	0.94	0.06	49,49,49,49	0
55	MG	1A	3264	1/1	0.94	0.07	37,37,37,37	0
55	MG	1A	3355	1/1	0.94	0.08	53,53,53,53	0
55	MG	2A	3116	1/1	0.94	0.19	43,43,43,43	0
55	MG	2A	3817	1/1	0.94	0.09	65,65,65,65	0
55	MG	1N	8003	1/1	0.94	0.14	69,69,69,69	0
55	MG	1A	3571	1/1	0.94	0.13	54,54,54,54	0
55	MG	2A	3820	1/1	0.94	0.12	69,69,69,69	0
55	MG	2A	3822	1/1	0.94	0.23	53,53,53,53	0
55	MG	2A	3120	1/1	0.94	0.30	56,56,56,56	0
55	MG	1a	3216	1/1	0.94	0.08	100,100,100,100	0
55	MG	1A	3685	1/1	0.94	0.17	52,52,52,52	0
55	MG	2A	3568	1/1	0.94	0.18	68,68,68,68	0
55	MG	1Q	201	1/1	0.94	0.25	44,44,44,44	0
55	MG	2A	3570	1/1	0.94	0.07	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3180	1/1	0.94	0.20	48,48,48,48	0
55	MG	1A	3121	1/1	0.94	0.08	43,43,43,43	0
55	MG	1A	3365	1/1	0.94	0.13	40,40,40,40	0
55	MG	2a	1725	1/1	0.94	0.08	86,86,86,86	0
55	MG	1a	3072	1/1	0.94	0.07	65,65,65,65	0
55	MG	2A	3578	1/1	0.94	0.07	61,61,61,61	0
55	MG	1S	201	1/1	0.94	0.23	55,55,55,55	0
55	MG	1A	3366	1/1	0.94	0.15	26,26,26,26	0
55	MG	2A	3356	1/1	0.94	0.10	43,43,43,43	0
55	MG	2A	3359	1/1	0.94	0.09	51,51,51,51	0
55	MG	2A	3369	1/1	0.94	0.09	58,58,58,58	0
55	MG	1d	506	1/1	0.94	0.07	91,91,91,91	0
55	MG	2A	3374	1/1	0.94	0.11	62,62,62,62	0
55	MG	1A	3217	1/1	0.94	0.14	45,45,45,45	0
55	MG	1A	3481	1/1	0.94	0.06	23,23,23,23	0
55	MG	1A	3276	1/1	0.94	0.14	3,3,3,3	0
55	MG	1g	3001	1/1	0.94	0.34	66,66,66,66	0
55	MG	2A	3383	1/1	0.94	0.10	57,57,57,57	0
55	MG	1A	3279	1/1	0.94	0.09	56,56,56,56	0
55	MG	2D	310	1/1	0.94	0.13	55,55,55,55	0
55	MG	2E	301	1/1	0.94	0.14	43,43,43,43	0
55	MG	1A	3705	1/1	0.94	0.12	48,48,48,48	0
55	MG	1k	3001	1/1	0.94	0.16	48,48,48,48	0
55	MG	1A	3376	1/1	0.94	0.07	72,72,72,72	0
55	MG	2F	301	1/1	0.94	0.35	47,47,47,47	0
55	MG	1A	3709	1/1	0.94	0.09	49,49,49,49	0
55	MG	2F	303	1/1	0.94	0.12	62,62,62,62	0
55	MG	2F	304	1/1	0.94	0.15	49,49,49,49	0
55	MG	2F	306	1/1	0.94	0.25	43,43,43,43	0
55	MG	1A	3123	1/1	0.94	0.32	27,27,27,27	0
55	MG	1A	3712	1/1	0.94	0.09	52,52,52,52	0
55	MG	1A	3583	1/1	0.94	0.11	37,37,37,37	0
55	MG	1A	3586	1/1	0.94	0.07	59,59,59,59	0
55	MG	1A	3221	1/1	0.94	0.21	56,56,56,56	0
55	MG	2A	3004	1/1	0.94	0.10	56,56,56,56	0
55	MG	2A	3611	1/1	0.94	0.12	83,83,83,83	0
55	MG	1A	3064	1/1	0.94	0.19	29,29,29,29	0
55	MG	1a	3095	1/1	0.94	0.15	62,62,62,62	0
55	MG	2A	3160	1/1	0.94	0.14	46,46,46,46	0
55	MG	1A	3882	1/1	0.94	0.14	62,62,62,62	0
55	MG	1A	3386	1/1	0.94	0.16	61,61,61,61	0
55	MG	1A	3387	1/1	0.94	0.11	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3415	1/1	0.94	0.07	80,80,80,80	0
55	MG	1A	3727	1/1	0.94	0.14	40,40,40,40	0
55	MG	15	103	1/1	0.94	0.15	34,34,34,34	0
55	MG	2A	3630	1/1	0.94	0.21	58,58,58,58	0
55	MG	2A	3012	1/1	0.94	0.11	38,38,38,38	0
55	MG	1A	3149	1/1	0.94	0.23	43,43,43,43	0
55	MG	1A	3389	1/1	0.94	0.11	48,48,48,48	0
55	MG	1A	3733	1/1	0.94	0.26	27,27,27,27	0
55	MG	2V	203	1/1	0.94	0.06	59,59,59,59	0
55	MG	1A	3502	1/1	0.94	0.11	62,62,62,62	0
55	MG	17	102	1/1	0.94	0.22	36,36,36,36	0
55	MG	17	104	1/1	0.94	0.12	61,61,61,61	0
55	MG	1A	3894	1/1	0.94	0.26	38,38,38,38	0
55	MG	1A	3125	1/1	0.94	0.18	45,45,45,45	0
55	MG	1A	3737	1/1	0.94	0.07	14,14,14,14	0
55	MG	2A	3025	1/1	0.94	0.14	38,38,38,38	0
55	MG	1A	3396	1/1	0.94	0.43	66,66,66,66	0
55	MG	2m	201	1/1	0.94	0.08	79,79,79,79	0
55	MG	1A	3301	1/1	0.94	0.10	41,41,41,41	0
55	MG	1A	3129	1/1	0.94	0.10	36,36,36,36	0
55	MG	21	102	1/1	0.94	0.07	60,60,60,60	0
55	MG	2A	3185	1/1	0.94	0.38	62,62,62,62	0
55	MG	1A	3903	1/1	0.94	0.15	59,59,59,59	0
55	MG	2A	3686	1/1	0.95	0.06	95,95,95,95	0
55	MG	2A	3079	1/1	0.95	0.12	50,50,50,50	0
55	MG	1F	308	1/1	0.95	0.20	32,32,32,32	0
55	MG	2A	3081	1/1	0.95	0.15	46,46,46,46	0
55	MG	1A	3218	1/1	0.95	0.22	35,35,35,35	0
55	MG	2A	3244	1/1	0.95	0.31	53,53,53,53	0
55	MG	1F	312	1/1	0.95	0.19	44,44,44,44	0
55	MG	1A	3686	1/1	0.95	0.09	35,35,35,35	0
55	MG	1A	3119	1/1	0.95	0.17	33,33,33,33	0
55	MG	2A	3703	1/1	0.95	0.10	93,93,93,93	0
55	MG	2A	3704	1/1	0.95	0.12	62,62,62,62	0
55	MG	1A	3120	1/1	0.95	0.28	34,34,34,34	0
55	MG	1A	3438	1/1	0.95	0.08	57,57,57,57	0
55	MG	1A	3588	1/1	0.95	0.18	62,62,62,62	0
55	MG	2A	3091	1/1	0.95	0.13	54,54,54,54	0
55	MG	2A	3253	1/1	0.95	0.07	56,56,56,56	0
55	MG	2A	3484	1/1	0.95	0.23	46,46,46,46	0
55	MG	1A	3278	1/1	0.95	0.25	37,37,37,37	0
55	MG	2A	3093	1/1	0.95	0.17	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3699	1/1	0.95	0.07	38,38,38,38	0
55	MG	1A	3080	1/1	0.95	0.43	36,36,36,36	0
55	MG	1A	3441	1/1	0.95	0.09	40,40,40,40	0
55	MG	2A	3493	1/1	0.95	0.11	51,51,51,51	0
55	MG	2A	3738	1/1	0.95	0.10	86,86,86,86	0
55	MG	2A	3739	1/1	0.95	0.07	69,69,69,69	0
55	MG	1A	3857	1/1	0.95	0.14	71,71,71,71	0
55	MG	1A	3442	1/1	0.95	0.07	49,49,49,49	0
55	MG	2A	3500	1/1	0.95	0.17	41,41,41,41	0
55	MG	1A	3137	1/1	0.95	0.59	46,46,46,46	0
55	MG	2A	3265	1/1	0.95	0.09	59,59,59,59	0
55	MG	2A	3751	1/1	0.95	0.10	67,67,67,67	0
55	MG	2A	3266	1/1	0.95	0.09	65,65,65,65	0
55	MG	1A	3228	1/1	0.95	0.18	28,28,28,28	0
55	MG	1Q	202	1/1	0.95	0.06	39,39,39,39	0
55	MG	1A	3599	1/1	0.95	0.06	50,50,50,50	0
55	MG	2A	3757	1/1	0.95	0.12	53,53,53,53	0
55	MG	2A	3280	1/1	0.95	0.08	51,51,51,51	0
55	MG	1A	3138	1/1	0.95	0.18	52,52,52,52	0
55	MG	1a	3067	1/1	0.95	0.21	65,65,65,65	0
55	MG	2A	3289	1/1	0.95	0.13	46,46,46,46	0
55	MG	1A	3864	1/1	0.95	0.12	49,49,49,49	0
55	MG	1R	205	1/1	0.95	0.07	34,34,34,34	0
55	MG	1A	3711	1/1	0.95	0.16	39,39,39,39	0
55	MG	1A	3292	1/1	0.95	0.11	52,52,52,52	0
55	MG	1A	3867	1/1	0.95	0.29	37,37,37,37	0
55	MG	1A	3713	1/1	0.95	0.08	98,98,98,98	0
55	MG	1U	207	1/1	0.95	0.09	47,47,47,47	0
55	MG	1A	3522	1/1	0.95	0.09	26,26,26,26	0
55	MG	1A	3718	1/1	0.95	0.16	67,67,67,67	0
55	MG	1A	3873	1/1	0.95	0.07	49,49,49,49	0
55	MG	1A	3721	1/1	0.95	0.09	50,50,50,50	0
55	MG	1A	3523	1/1	0.95	0.11	56,56,56,56	0
55	MG	1A	3607	1/1	0.95	0.06	60,60,60,60	0
55	MG	1A	3020	1/1	0.95	0.28	39,39,39,39	0
55	MG	2A	3783	1/1	0.95	0.13	78,78,78,78	0
55	MG	2A	3318	1/1	0.95	0.20	67,67,67,67	0
55	MG	2A	3122	1/1	0.95	0.15	46,46,46,46	0
55	MG	1A	3880	1/1	0.95	0.07	66,66,66,66	0
55	MG	2a	1661	1/1	0.95	0.20	63,63,63,63	0
55	MG	2A	3126	1/1	0.95	0.09	55,55,55,55	0
55	MG	2A	3127	1/1	0.95	0.25	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
55	MG	1A	3075	1/1	0.95	0.40	41,41,41,41	0
55	MG	1A	3372	1/1	0.95	0.10	29,29,29,29	0
55	MG	10	107	1/1	0.95	0.05	57,57,57,57	0
55	MG	1A	3883	1/1	0.95	0.06	58,58,58,58	0
55	MG	1a	3089	1/1	0.95	0.12	52,52,52,52	0
55	MG	2a	1671	1/1	0.95	0.06	80,80,80,80	0
55	MG	2A	3552	1/1	0.95	0.14	52,52,52,52	0
55	MG	1A	3461	1/1	0.95	0.10	63,63,63,63	0
55	MG	2a	1675	1/1	0.95	0.16	51,51,51,51	0
55	MG	2A	3799	1/1	0.95	0.17	83,83,83,83	0
55	MG	11	102	1/1	0.95	0.08	56,56,56,56	0
55	MG	2A	3801	1/1	0.95	0.12	21,21,21,21	0
55	MG	2A	3136	1/1	0.95	0.24	55,55,55,55	0
55	MG	1A	3531	1/1	0.95	0.10	46,46,46,46	0
55	MG	2a	1684	1/1	0.95	0.06	76,76,76,76	0
55	MG	2A	3138	1/1	0.95	0.32	48,48,48,48	0
55	MG	2A	3139	1/1	0.95	0.11	53,53,53,53	0
55	MG	2A	3560	1/1	0.95	0.09	53,53,53,53	0
55	MG	1A	3167	1/1	0.95	0.08	52,52,52,52	0
55	MG	2a	1691	1/1	0.95	0.14	56,56,56,56	0
55	MG	1A	3028	1/1	0.95	0.27	37,37,37,37	0
55	MG	2A	3346	1/1	0.95	0.06	77,77,77,77	0
55	MG	2a	1695	1/1	0.95	0.17	58,58,58,58	0
55	MG	2A	3811	1/1	0.95	0.08	67,67,67,67	0
55	MG	1A	3019	1/1	0.95	0.29	39,39,39,39	0
55	MG	1A	3170	1/1	0.95	0.31	34,34,34,34	0
55	MG	1A	3627	1/1	0.95	0.24	44,44,44,44	0
55	MG	1A	3740	1/1	0.95	0.08	26,26,26,26	0
55	MG	1A	3380	1/1	0.95	0.08	52,52,52,52	0
55	MG	2A	3573	1/1	0.95	0.09	71,71,71,71	0
55	MG	2A	3366	1/1	0.95	0.08	92,92,92,92	0
55	MG	1A	3071	1/1	0.95	0.17	42,42,42,42	0
55	MG	17	103	1/1	0.95	0.40	43,43,43,43	0
55	MG	1A	3632	1/1	0.95	0.07	49,49,49,49	0
55	MG	1A	3746	1/1	0.95	0.12	31,31,31,31	0
55	MG	1A	3634	1/1	0.95	0.10	38,38,38,38	0
55	MG	2A	3581	1/1	0.95	0.09	72,72,72,72	0
55	MG	19	103	1/1	0.95	0.09	61,61,61,61	0
55	MG	1A	3385	1/1	0.95	0.12	57,57,57,57	0
55	MG	1A	3904	1/1	0.95	0.16	17,17,17,17	0
55	MG	1A	3756	1/1	0.95	0.12	40,40,40,40	0
55	MG	1A	3311	1/1	0.95	0.05	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3587	1/1	0.95	0.05	68,68,68,68	0
55	MG	1A	3100	1/1	0.95	0.17	25,25,25,25	0
55	MG	1A	3911	1/1	0.95	0.10	39,39,39,39	0
55	MG	1A	3639	1/1	0.95	0.07	47,47,47,47	0
55	MG	1A	3913	1/1	0.95	0.37	63,63,63,63	0
55	MG	1A	3761	1/1	0.95	0.11	64,64,64,64	0
55	MG	1A	3544	1/1	0.95	0.18	34,34,34,34	0
55	MG	1A	3546	1/1	0.95	0.27	25,25,25,25	0
55	MG	1A	3643	1/1	0.95	0.06	34,34,34,34	0
55	MG	2A	3170	1/1	0.95	0.07	73,73,73,73	0
55	MG	1A	3044	1/1	0.95	0.14	33,33,33,33	0
55	MG	1A	3548	1/1	0.95	0.08	39,39,39,39	0
55	MG	2A	3173	1/1	0.95	0.28	42,42,42,42	0
55	MG	1A	3206	1/1	0.95	0.17	32,32,32,32	0
55	MG	2A	3034	1/1	0.95	0.13	54,54,54,54	0
55	MG	2A	3176	1/1	0.95	0.19	51,51,51,51	0
55	MG	2A	3608	1/1	0.95	0.09	62,62,62,62	0
55	MG	1B	3008	1/1	0.95	0.09	57,57,57,57	0
55	MG	1A	3652	1/1	0.95	0.12	34,34,34,34	0
55	MG	1a	3137	1/1	0.95	0.21	68,68,68,68	0
55	MG	2A	3615	1/1	0.95	0.11	56,56,56,56	0
55	MG	1A	3394	1/1	0.95	0.13	50,50,50,50	0
55	MG	2a	1744	1/1	0.95	0.09	76,76,76,76	0
55	MG	1a	3020	1/1	0.95	0.10	58,58,58,58	0
55	MG	2A	3621	1/1	0.95	0.15	54,54,54,54	0
55	MG	1A	3176	1/1	0.95	0.09	52,52,52,52	0
55	MG	2A	3422	1/1	0.95	0.09	52,52,52,52	0
55	MG	2A	3042	1/1	0.95	0.12	27,27,27,27	0
55	MG	2A	3626	1/1	0.95	0.11	60,60,60,60	0
55	MG	1A	3150	1/1	0.95	0.10	39,39,39,39	0
55	MG	1A	3657	1/1	0.95	0.11	50,50,50,50	0
55	MG	1A	3555	1/1	0.95	0.12	61,61,61,61	0
55	MG	1A	3659	1/1	0.95	0.12	57,57,57,57	0
55	MG	1A	3256	1/1	0.95	0.07	41,41,41,41	0
55	MG	1a	3147	1/1	0.95	0.06	85,85,85,85	0
55	MG	2P	201	1/1	0.95	0.27	51,51,51,51	0
55	MG	1A	3178	1/1	0.95	0.18	39,39,39,39	0
55	MG	2A	3638	1/1	0.95	0.11	86,86,86,86	0
55	MG	1A	3564	1/1	0.95	0.09	43,43,43,43	0
55	MG	1A	3487	1/1	0.95	0.25	57,57,57,57	0
55	MG	1A	3319	1/1	0.95	0.06	34,34,34,34	0
55	MG	1A	3490	1/1	0.95	0.15	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2a	1774	1/1	0.95	0.07	91,91,91,91	0
55	MG	1A	3491	1/1	0.95	0.09	55,55,55,55	0
55	MG	1A	3670	1/1	0.95	0.24	53,53,53,53	0
55	MG	1A	3151	1/1	0.95	0.16	46,46,46,46	0
55	MG	2U	202	1/1	0.95	0.28	46,46,46,46	0
55	MG	1A	3213	1/1	0.95	0.60	32,32,32,32	0
55	MG	1A	3823	1/1	0.95	0.09	28,28,28,28	0
55	MG	2A	3060	1/1	0.95	0.27	52,52,52,52	0
55	MG	2A	3207	1/1	0.95	0.09	70,70,70,70	0
55	MG	2A	3447	1/1	0.95	0.08	73,73,73,73	0
55	MG	1A	3496	1/1	0.95	0.06	51,51,51,51	0
55	MG	1A	3153	1/1	0.95	0.09	49,49,49,49	0
55	MG	1A	3324	1/1	0.95	0.13	40,40,40,40	0
55	MG	1E	308	1/1	0.95	0.19	49,49,49,49	0
55	MG	2A	3216	1/1	0.95	0.11	41,41,41,41	0
55	MG	2A	3219	1/1	0.95	0.20	22,22,22,22	0
55	MG	20	102	1/1	0.95	0.12	75,75,75,75	0
55	MG	1A	3154	1/1	0.95	0.28	28,28,28,28	0
55	MG	1A	3266	1/1	0.95	0.14	70,70,70,70	0
55	MG	1A	3090	1/1	0.95	0.14	37,37,37,37	0
55	MG	2A	3460	1/1	0.95	0.09	55,55,55,55	0
55	MG	2A	3461	1/1	0.95	0.07	34,34,34,34	0
55	MG	1A	3432	1/1	0.95	0.07	49,49,49,49	0
55	MG	2A	3073	1/1	0.95	0.22	48,48,48,48	0
55	MG	1a	3172	1/1	0.95	0.09	77,77,77,77	0
55	MG	1A	3837	1/1	0.95	0.10	84,84,84,84	0
55	MG	27	101	1/1	0.95	0.20	55,55,55,55	0
55	MG	1A	3580	1/1	0.95	0.12	61,61,61,61	0
55	MG	1F	307	1/1	0.95	0.31	29,29,29,29	0
55	MG	2A	3692	1/1	0.96	0.06	54,54,54,54	0
55	MG	2A	3119	1/1	0.96	0.15	49,49,49,49	0
55	MG	2a	1601	1/1	0.96	0.20	79,79,79,79	0
55	MG	2A	3269	1/1	0.96	0.05	45,45,45,45	0
55	MG	2A	3270	1/1	0.96	0.07	58,58,58,58	0
55	MG	2a	1604	1/1	0.96	0.05	53,53,53,53	0
55	MG	2a	1605	1/1	0.96	0.31	56,56,56,56	0
55	MG	1a	3098	1/1	0.96	0.11	61,61,61,61	0
55	MG	1A	3796	1/1	0.96	0.08	43,43,43,43	0
55	MG	1A	3067	1/1	0.96	0.33	37,37,37,37	0
55	MG	2A	3123	1/1	0.96	0.08	43,43,43,43	0
55	MG	1a	3105	1/1	0.96	0.16	58,58,58,58	0
55	MG	1A	3102	1/1	0.96	0.15	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3212	1/1	0.96	0.12	43,43,43,43	0
55	MG	1A	3809	1/1	0.96	0.07	13,13,13,13	0
55	MG	1A	3068	1/1	0.96	0.18	27,27,27,27	0
55	MG	1A	3595	1/1	0.96	0.09	67,67,67,67	0
55	MG	1A	3520	1/1	0.96	0.07	56,56,56,56	0
55	MG	1A	3069	1/1	0.96	0.06	38,38,38,38	0
55	MG	2A	3726	1/1	0.96	0.05	41,41,41,41	0
55	MG	2A	3504	1/1	0.96	0.05	55,55,55,55	0
55	MG	2A	3505	1/1	0.96	0.13	44,44,44,44	0
55	MG	2A	3133	1/1	0.96	0.12	60,60,60,60	0
55	MG	2A	3735	1/1	0.96	0.11	49,49,49,49	0
55	MG	1A	3108	1/1	0.96	0.13	24,24,24,24	0
55	MG	2a	1624	1/1	0.96	0.13	53,53,53,53	0
55	MG	1A	3109	1/1	0.96	0.04	30,30,30,30	0
55	MG	2A	3306	1/1	0.96	0.10	39,39,39,39	0
55	MG	1B	3016	1/1	0.96	0.05	51,51,51,51	0
55	MG	2A	3308	1/1	0.96	0.14	52,52,52,52	0
55	MG	2A	3746	1/1	0.96	0.11	69,69,69,69	0
55	MG	2A	3747	1/1	0.96	0.08	75,75,75,75	0
55	MG	1A	3363	1/1	0.96	0.06	26,26,26,26	0
55	MG	1A	3454	1/1	0.96	0.06	56,56,56,56	0
55	MG	2A	3313	1/1	0.96	0.05	40,40,40,40	0
55	MG	1A	3526	1/1	0.96	0.14	64,64,64,64	0
55	MG	2A	3317	1/1	0.96	0.12	55,55,55,55	0
55	MG	1A	3698	1/1	0.96	0.07	48,48,48,48	0
55	MG	2A	3755	1/1	0.96	0.06	63,63,63,63	0
55	MG	2A	3319	1/1	0.96	0.04	78,78,78,78	0
55	MG	2A	3017	1/1	0.96	0.11	54,54,54,54	0
55	MG	1A	3833	1/1	0.96	0.10	69,69,69,69	0
55	MG	1A	3527	1/1	0.96	0.07	35,35,35,35	0
55	MG	2A	3020	1/1	0.96	0.05	42,42,42,42	0
55	MG	2A	3528	1/1	0.96	0.09	34,34,34,34	0
55	MG	1A	3606	1/1	0.96	0.10	56,56,56,56	0
55	MG	1A	3836	1/1	0.96	0.10	54,54,54,54	0
55	MG	1A	3045	1/1	0.96	0.11	12,12,12,12	0
55	MG	1A	3219	1/1	0.96	0.11	49,49,49,49	0
55	MG	1A	3036	1/1	0.96	0.09	28,28,28,28	0
55	MG	1A	3023	1/1	0.96	0.12	21,21,21,21	0
55	MG	1D	310	1/1	0.96	0.15	42,42,42,42	0
55	MG	2A	3335	1/1	0.96	0.06	71,71,71,71	0
55	MG	2A	3336	1/1	0.96	0.05	56,56,56,56	0
55	MG	1D	311	1/1	0.96	0.12	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3155	1/1	0.96	0.45	50,50,50,50	0
55	MG	1D	313	1/1	0.96	0.16	51,51,51,51	0
55	MG	2A	3545	1/1	0.96	0.06	97,97,97,97	0
55	MG	2A	3779	1/1	0.96	0.06	72,72,72,72	0
55	MG	1A	3708	1/1	0.96	0.09	53,53,53,53	0
55	MG	2A	3547	1/1	0.96	0.11	41,41,41,41	0
55	MG	2A	3343	1/1	0.96	0.05	73,73,73,73	0
55	MG	1D	315	1/1	0.96	0.11	68,68,68,68	0
55	MG	1A	3281	1/1	0.96	0.07	54,54,54,54	0
55	MG	2A	3033	1/1	0.96	0.15	59,59,59,59	0
55	MG	1D	317	1/1	0.96	0.08	57,57,57,57	0
55	MG	2A	3790	1/1	0.96	0.06	71,71,71,71	0
55	MG	2A	3350	1/1	0.96	0.06	49,49,49,49	0
55	MG	1A	3844	1/1	0.96	0.07	27,27,27,27	0
55	MG	1E	302	1/1	0.96	0.39	39,39,39,39	0
55	MG	1A	3373	1/1	0.96	0.08	58,58,58,58	0
55	MG	1a	3142	1/1	0.96	0.04	85,85,85,85	0
55	MG	2A	3361	1/1	0.96	0.08	64,64,64,64	0
55	MG	2A	3362	1/1	0.96	0.11	61,61,61,61	0
55	MG	1E	304	1/1	0.96	0.09	46,46,46,46	0
55	MG	2A	3367	1/1	0.96	0.07	37,37,37,37	0
55	MG	2a	1681	1/1	0.96	0.06	84,84,84,84	0
55	MG	1A	3846	1/1	0.96	0.16	53,53,53,53	0
55	MG	1E	307	1/1	0.96	0.09	33,33,33,33	0
55	MG	2A	3373	1/1	0.96	0.06	48,48,48,48	0
55	MG	1A	3847	1/1	0.96	0.08	58,58,58,58	0
55	MG	2A	3375	1/1	0.96	0.26	49,49,49,49	0
55	MG	1A	3162	1/1	0.96	0.33	37,37,37,37	0
55	MG	1A	3850	1/1	0.96	0.09	21,21,21,21	0
55	MG	1A	3619	1/1	0.96	0.12	44,44,44,44	0
55	MG	2A	3577	1/1	0.96	0.12	56,56,56,56	0
55	MG	1A	3224	1/1	0.96	0.04	73,73,73,73	0
55	MG	2A	3382	1/1	0.96	0.13	65,65,65,65	0
55	MG	2a	1697	1/1	0.96	0.06	80,80,80,80	0
55	MG	1A	3017	1/1	0.96	0.14	31,31,31,31	0
55	MG	1A	3291	1/1	0.96	0.07	30,30,30,30	0
55	MG	1A	3625	1/1	0.96	0.22	35,35,35,35	0
55	MG	1A	3626	1/1	0.96	0.08	44,44,44,44	0
55	MG	2A	3389	1/1	0.96	0.06	46,46,46,46	0
55	MG	1F	309	1/1	0.96	0.10	28,28,28,28	0
55	MG	1A	3227	1/1	0.96	0.21	34,34,34,34	0
55	MG	2A	3397	1/1	0.96	0.07	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
55	MG	1A	3629	1/1	0.96	0.11	42,42,42,42	0
55	MG	1A	3092	1/1	0.96	0.18	37,37,37,37	0
55	MG	1A	3543	1/1	0.96	0.20	63,63,63,63	0
55	MG	1A	3384	1/1	0.96	0.23	58,58,58,58	0
55	MG	1A	3633	1/1	0.96	0.14	79,79,79,79	0
55	MG	1A	3229	1/1	0.96	0.32	62,62,62,62	0
55	MG	2A	3188	1/1	0.96	0.07	45,45,45,45	0
55	MG	2A	3596	1/1	0.96	0.07	65,65,65,65	0
55	MG	2A	3597	1/1	0.96	0.05	51,51,51,51	0
55	MG	2A	3409	1/1	0.96	0.11	48,48,48,48	0
55	MG	1A	3074	1/1	0.96	0.36	29,29,29,29	0
55	MG	1A	3192	1/1	0.96	0.09	42,42,42,42	0
55	MG	1A	3166	1/1	0.96	0.22	46,46,46,46	0
55	MG	1A	3550	1/1	0.96	0.07	44,44,44,44	0
55	MG	1A	3482	1/1	0.96	0.17	43,43,43,43	0
55	MG	1A	3641	1/1	0.96	0.24	35,35,35,35	0
55	MG	1A	3234	1/1	0.96	0.07	48,48,48,48	0
55	MG	2A	3071	1/1	0.96	0.27	62,62,62,62	0
55	MG	1A	3040	1/1	0.96	0.16	37,37,37,37	0
55	MG	1A	3645	1/1	0.96	0.15	54,54,54,54	0
55	MG	1A	3310	1/1	0.96	0.14	41,41,41,41	0
55	MG	2A	3201	1/1	0.96	0.17	48,48,48,48	0
55	MG	1A	3237	1/1	0.96	0.07	53,53,53,53	0
55	MG	1A	3238	1/1	0.96	0.28	38,38,38,38	0
55	MG	1A	3239	1/1	0.96	0.05	35,35,35,35	0
55	MG	2a	1732	1/1	0.96	0.05	74,74,74,74	0
55	MG	2A	3208	1/1	0.96	0.11	60,60,60,60	0
55	MG	1A	3142	1/1	0.96	0.48	32,32,32,32	0
55	MG	1A	3061	1/1	0.96	0.31	47,47,47,47	0
55	MG	1U	201	1/1	0.96	0.18	34,34,34,34	0
55	MG	2A	3082	1/1	0.96	0.10	56,56,56,56	0
55	MG	1A	3199	1/1	0.96	0.18	34,34,34,34	0
55	MG	2A	3084	1/1	0.96	0.07	45,45,45,45	0
55	MG	1A	3200	1/1	0.96	0.31	37,37,37,37	0
55	MG	1a	3192	1/1	0.96	0.07	49,49,49,49	0
55	MG	2F	305	1/1	0.96	0.22	46,46,46,46	0
55	MG	2A	3632	1/1	0.96	0.12	97,97,97,97	0
55	MG	2a	1750	1/1	0.96	0.06	83,83,83,83	0
55	MG	1U	204	1/1	0.96	0.36	29,29,29,29	0
55	MG	2F	308	1/1	0.96	0.30	59,59,59,59	0
55	MG	2A	3438	1/1	0.96	0.07	81,81,81,81	0
55	MG	2A	3636	1/1	0.96	0.05	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
55	MG	1U	205	1/1	0.96	0.22	29,29,29,29	0
55	MG	1a	3196	1/1	0.96	0.07	77,77,77,77	0
55	MG	1A	3015	1/1	0.96	0.29	23,23,23,23	0
55	MG	1A	3410	1/1	0.96	0.13	42,42,42,42	0
55	MG	2A	3230	1/1	0.96	0.18	51,51,51,51	0
55	MG	1V	202	1/1	0.96	0.12	25,25,25,25	0
55	MG	2a	1762	1/1	0.96	0.10	74,74,74,74	0
55	MG	2a	1764	1/1	0.96	0.06	59,59,59,59	0
55	MG	1a	3201	1/1	0.96	0.09	92,92,92,92	0
55	MG	1A	3063	1/1	0.96	0.09	49,49,49,49	0
55	MG	2Q	8003	1/1	0.96	0.13	57,57,57,57	0
55	MG	1A	3768	1/1	0.96	0.09	46,46,46,46	0
55	MG	2A	3450	1/1	0.96	0.07	40,40,40,40	0
55	MG	2A	3237	1/1	0.96	0.10	67,67,67,67	0
55	MG	1A	3769	1/1	0.96	0.06	61,61,61,61	0
55	MG	1A	3896	1/1	0.96	0.29	37,37,37,37	0
55	MG	2a	1776	1/1	0.96	0.07	80,80,80,80	0
55	MG	2a	1777	1/1	0.96	0.06	77,77,77,77	0
55	MG	1A	3417	1/1	0.96	0.06	22,22,22,22	0
55	MG	1A	3424	1/1	0.96	0.06	62,62,62,62	0
55	MG	1A	3249	1/1	0.96	0.18	21,21,21,21	0
55	MG	2A	3658	1/1	0.96	0.19	76,76,76,76	0
55	MG	2A	3102	1/1	0.96	0.06	56,56,56,56	0
55	MG	1a	3079	1/1	0.96	0.13	55,55,55,55	0
55	MG	2A	3661	1/1	0.96	0.06	85,85,85,85	0
55	MG	2A	3249	1/1	0.96	0.08	43,43,43,43	0
55	MG	1A	3251	1/1	0.96	0.32	34,34,34,34	0
55	MG	2A	3670	1/1	0.96	0.08	84,84,84,84	0
55	MG	1A	3902	1/1	0.96	0.07	56,56,56,56	0
55	MG	1A	3052	1/1	0.96	0.23	36,36,36,36	0
55	MG	1A	3779	1/1	0.96	0.06	24,24,24,24	0
55	MG	2A	3254	1/1	0.96	0.18	54,54,54,54	0
55	MG	1A	3205	1/1	0.96	0.20	44,44,44,44	0
55	MG	1A	3435	1/1	0.96	0.05	69,69,69,69	0
55	MG	1a	3086	1/1	0.96	0.18	68,68,68,68	0
55	MG	1A	3511	1/1	0.96	0.06	26,26,26,26	0
55	MG	2A	3679	1/1	0.96	0.06	52,52,52,52	0
55	MG	2A	3680	1/1	0.96	0.07	66,66,66,66	0
55	MG	1A	3174	1/1	0.96	0.08	44,44,44,44	0
55	MG	2A	3684	1/1	0.96	0.08	57,57,57,57	0
55	MG	1A	3122	1/1	0.96	0.26	30,30,30,30	0
55	MG	1A	3585	1/1	0.96	0.13	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
55	MG	1a	3094	1/1	0.96	0.06	46,46,46,46	0
55	MG	1A	3030	1/1	0.96	0.09	30,30,30,30	0
55	MG	1A	3915	1/1	0.96	0.12	60,60,60,60	0
55	MG	1A	3917	1/1	0.96	0.20	36,36,36,36	0
55	MG	1A	3469	1/1	0.97	0.11	39,39,39,39	0
55	MG	2A	3169	1/1	0.97	0.17	50,50,50,50	0
55	MG	2A	3722	1/1	0.97	0.04	67,67,67,67	0
55	MG	2A	3724	1/1	0.97	0.05	45,45,45,45	0
55	MG	1A	3621	1/1	0.97	0.10	40,40,40,40	0
55	MG	2A	3522	1/1	0.97	0.13	82,82,82,82	0
55	MG	1A	3032	1/1	0.97	0.22	45,45,45,45	0
55	MG	2A	3731	1/1	0.97	0.09	70,70,70,70	0
55	MG	1A	3252	1/1	0.97	0.25	36,36,36,36	0
55	MG	1A	3009	1/1	0.97	0.11	28,28,28,28	0
55	MG	1A	3849	1/1	0.97	0.16	89,89,89,89	0
55	MG	1A	3716	1/1	0.97	0.07	46,46,46,46	0
55	MG	1a	3153	1/1	0.97	0.07	57,57,57,57	0
55	MG	1A	3473	1/1	0.97	0.09	63,63,63,63	0
55	MG	2A	3532	1/1	0.97	0.05	84,84,84,84	0
55	MG	2A	3744	1/1	0.97	0.15	64,64,64,64	0
55	MG	1a	3155	1/1	0.97	0.04	78,78,78,78	0
55	MG	2A	3353	1/1	0.97	0.06	72,72,72,72	0
55	MG	2A	3052	1/1	0.97	0.21	42,42,42,42	0
55	MG	2A	3749	1/1	0.97	0.05	85,85,85,85	0
55	MG	2A	3536	1/1	0.97	0.07	64,64,64,64	0
55	MG	2A	3357	1/1	0.97	0.09	50,50,50,50	0
55	MG	1A	3542	1/1	0.97	0.06	77,77,77,77	0
55	MG	2A	3360	1/1	0.97	0.05	64,64,64,64	0
55	MG	1A	3042	1/1	0.97	0.14	25,25,25,25	0
55	MG	1A	3392	1/1	0.97	0.13	35,35,35,35	0
55	MG	2A	3363	1/1	0.97	0.07	50,50,50,50	0
55	MG	2A	3544	1/1	0.97	0.05	90,90,90,90	0
55	MG	2A	3365	1/1	0.97	0.10	39,39,39,39	0
55	MG	1A	3545	1/1	0.97	0.31	36,36,36,36	0
55	MG	1A	3858	1/1	0.97	0.09	56,56,56,56	0
55	MG	1A	3393	1/1	0.97	0.05	53,53,53,53	0
55	MG	1A	3081	1/1	0.97	0.24	33,33,33,33	0
55	MG	1A	3054	1/1	0.97	0.12	49,49,49,49	0
55	MG	2A	3061	1/1	0.97	0.17	62,62,62,62	0
55	MG	2A	3766	1/1	0.97	0.11	81,81,81,81	0
55	MG	1F	313	1/1	0.97	0.07	32,32,32,32	0
55	MG	2A	3376	1/1	0.97	0.05	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3770	1/1	0.97	0.04	79,79,79,79	0
55	MG	1a	3167	1/1	0.97	0.06	86,86,86,86	0
55	MG	1A	3728	1/1	0.97	0.08	54,54,54,54	0
55	MG	1A	3729	1/1	0.97	0.06	47,47,47,47	0
55	MG	1A	3257	1/1	0.97	0.11	40,40,40,40	0
55	MG	2A	3067	1/1	0.97	0.08	62,62,62,62	0
55	MG	2A	3562	1/1	0.97	0.13	74,74,74,74	0
55	MG	1A	3043	1/1	0.97	0.14	10,10,10,10	0
55	MG	1A	3636	1/1	0.97	0.06	38,38,38,38	0
55	MG	1A	3483	1/1	0.97	0.17	38,38,38,38	0
55	MG	1A	3145	1/1	0.97	0.18	29,29,29,29	0
55	MG	1a	3176	1/1	0.97	0.07	92,92,92,92	0
55	MG	2A	3391	1/1	0.97	0.04	43,43,43,43	0
55	MG	2A	3571	1/1	0.97	0.05	41,41,41,41	0
55	MG	2a	1657	1/1	0.97	0.10	65,65,65,65	0
55	MG	2A	3392	1/1	0.97	0.13	31,31,31,31	0
55	MG	2A	3787	1/1	0.97	0.08	61,61,61,61	0
55	MG	2A	3393	1/1	0.97	0.07	52,52,52,52	0
55	MG	1A	3553	1/1	0.97	0.10	37,37,37,37	0
55	MG	2A	3395	1/1	0.97	0.05	35,35,35,35	0
55	MG	2A	3202	1/1	0.97	0.07	56,56,56,56	0
55	MG	1A	3027	1/1	0.97	0.14	31,31,31,31	0
55	MG	1A	3261	1/1	0.97	0.16	28,28,28,28	0
55	MG	1A	3171	1/1	0.97	0.18	44,44,44,44	0
55	MG	2A	3795	1/1	0.97	0.07	72,72,72,72	0
55	MG	1P	202	1/1	0.97	0.28	28,28,28,28	0
55	MG	1A	3561	1/1	0.97	0.08	47,47,47,47	0
55	MG	2a	1672	1/1	0.97	0.07	57,57,57,57	0
55	MG	1A	3745	1/1	0.97	0.10	54,54,54,54	0
55	MG	2A	3211	1/1	0.97	0.07	45,45,45,45	0
55	MG	1A	3003	1/1	0.97	0.07	20,20,20,20	0
55	MG	1Q	203	1/1	0.97	0.12	38,38,38,38	0
55	MG	1A	3747	1/1	0.97	0.05	45,45,45,45	0
55	MG	1Q	205	1/1	0.97	0.06	43,43,43,43	0
55	MG	2a	1679	1/1	0.97	0.05	63,63,63,63	0
55	MG	1A	3748	1/1	0.97	0.05	50,50,50,50	0
55	MG	1R	203	1/1	0.97	0.09	19,19,19,19	0
55	MG	1A	3750	1/1	0.97	0.06	52,52,52,52	0
55	MG	2A	3807	1/1	0.97	0.11	48,48,48,48	0
55	MG	1A	3323	1/1	0.97	0.11	46,46,46,46	0
55	MG	1A	3884	1/1	0.97	0.05	18,18,18,18	0
55	MG	1A	3409	1/1	0.97	0.05	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3265	1/1	0.97	0.10	44,44,44,44	0
55	MG	2A	3595	1/1	0.97	0.05	52,52,52,52	0
55	MG	1A	3757	1/1	0.97	0.06	37,37,37,37	0
55	MG	1a	3207	1/1	0.97	0.10	76,76,76,76	0
55	MG	1A	3650	1/1	0.97	0.13	49,49,49,49	0
55	MG	2a	1696	1/1	0.97	0.05	77,77,77,77	0
55	MG	1A	3651	1/1	0.97	0.14	40,40,40,40	0
55	MG	1A	3331	1/1	0.97	0.06	22,22,22,22	0
55	MG	2A	3601	1/1	0.97	0.05	58,58,58,58	0
55	MG	2A	3236	1/1	0.97	0.09	80,80,80,80	0
55	MG	1a	3212	1/1	0.97	0.05	51,51,51,51	0
55	MG	2A	3239	1/1	0.97	0.05	38,38,38,38	0
55	MG	2A	3241	1/1	0.97	0.06	49,49,49,49	0
55	MG	1A	3495	1/1	0.97	0.09	49,49,49,49	0
55	MG	1A	3893	1/1	0.97	0.06	103,103,103,103	0
55	MG	2A	3609	1/1	0.97	0.06	38,38,38,38	0
55	MG	1A	3198	1/1	0.97	0.34	28,28,28,28	0
55	MG	2A	3433	1/1	0.97	0.04	66,66,66,66	0
55	MG	1a	3217	1/1	0.97	0.12	87,87,87,87	0
55	MG	1A	3655	1/1	0.97	0.18	41,41,41,41	0
55	MG	2A	3617	1/1	0.97	0.05	33,33,33,33	0
55	MG	1A	3419	1/1	0.97	0.07	37,37,37,37	0
55	MG	1A	3765	1/1	0.97	0.06	39,39,39,39	0
55	MG	2A	3620	1/1	0.97	0.06	45,45,45,45	0
55	MG	1A	3498	1/1	0.97	0.06	70,70,70,70	0
55	MG	1A	3423	1/1	0.97	0.04	20,20,20,20	0
55	MG	1A	3105	1/1	0.97	0.07	46,46,46,46	0
55	MG	1A	3029	1/1	0.97	0.06	38,38,38,38	0
55	MG	2A	3625	1/1	0.97	0.08	74,74,74,74	0
55	MG	1A	3661	1/1	0.97	0.05	33,33,33,33	0
55	MG	1A	3231	1/1	0.97	0.61	31,31,31,31	0
55	MG	10	106	1/1	0.97	0.09	58,58,58,58	0
55	MG	1A	3273	1/1	0.97	0.07	19,19,19,19	0
55	MG	1A	3776	1/1	0.97	0.04	43,43,43,43	0
55	MG	1A	3908	1/1	0.97	0.20	33,33,33,33	0
55	MG	1A	3126	1/1	0.97	0.14	34,34,34,34	0
55	MG	1A	3128	1/1	0.97	0.08	31,31,31,31	0
55	MG	2D	311	1/1	0.97	0.09	53,53,53,53	0
55	MG	1A	3203	1/1	0.97	0.14	35,35,35,35	0
55	MG	2A	3635	1/1	0.97	0.05	92,92,92,92	0
55	MG	2A	3263	1/1	0.97	0.06	46,46,46,46	0
55	MG	2E	306	1/1	0.97	0.07	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3637	1/1	0.97	0.06	61,61,61,61	0
55	MG	1A	3235	1/1	0.97	0.18	38,38,38,38	0
55	MG	1A	3282	1/1	0.97	0.05	26,26,26,26	0
55	MG	1a	3099	1/1	0.97	0.12	61,61,61,61	0
55	MG	2A	3458	1/1	0.97	0.08	78,78,78,78	0
55	MG	1A	3789	1/1	0.97	0.05	31,31,31,31	0
55	MG	2a	1741	1/1	0.97	0.05	75,75,75,75	0
55	MG	2A	3124	1/1	0.97	0.16	47,47,47,47	0
55	MG	1a	3103	1/1	0.97	0.07	72,72,72,72	0
55	MG	1A	3285	1/1	0.97	0.29	47,47,47,47	0
55	MG	2a	1746	1/1	0.97	0.08	69,69,69,69	0
55	MG	1A	3513	1/1	0.97	0.07	27,27,27,27	0
55	MG	2a	1748	1/1	0.97	0.05	79,79,79,79	0
55	MG	2a	1749	1/1	0.97	0.04	80,80,80,80	0
55	MG	1A	3059	1/1	0.97	0.13	35,35,35,35	0
55	MG	1A	3089	1/1	0.97	0.07	37,37,37,37	0
55	MG	2A	3651	1/1	0.97	0.12	56,56,56,56	0
55	MG	1A	3590	1/1	0.97	0.11	48,48,48,48	0
55	MG	2A	3287	1/1	0.97	0.06	39,39,39,39	0
55	MG	1A	3037	1/1	0.97	0.09	56,56,56,56	0
55	MG	1A	3802	1/1	0.97	0.06	39,39,39,39	0
55	MG	1A	3804	1/1	0.97	0.16	87,87,87,87	0
55	MG	2A	3473	1/1	0.97	0.06	61,61,61,61	0
55	MG	2A	3293	1/1	0.97	0.05	40,40,40,40	0
55	MG	2a	1760	1/1	0.97	0.04	90,90,90,90	0
55	MG	18	3303	1/1	0.97	0.06	52,52,52,52	0
55	MG	1A	3806	1/1	0.97	0.12	65,65,65,65	0
55	MG	1A	3679	1/1	0.97	0.05	44,44,44,44	0
55	MG	2A	3666	1/1	0.97	0.07	70,70,70,70	0
55	MG	2A	3298	1/1	0.97	0.05	56,56,56,56	0
55	MG	1A	3370	1/1	0.97	0.06	41,41,41,41	0
55	MG	1A	3290	1/1	0.97	0.09	49,49,49,49	0
55	MG	1A	3091	1/1	0.97	0.15	16,16,16,16	0
55	MG	2A	3016	1/1	0.97	0.43	46,46,46,46	0
55	MG	1B	3017	1/1	0.97	0.06	39,39,39,39	0
55	MG	1A	3449	1/1	0.97	0.06	21,21,21,21	0
55	MG	2A	3143	1/1	0.97	0.11	53,53,53,53	0
55	MG	1a	3007	1/1	0.97	0.04	74,74,74,74	0
55	MG	1A	3451	1/1	0.97	0.06	43,43,43,43	0
55	MG	1A	3241	1/1	0.97	0.10	30,30,30,30	0
55	MG	2A	3312	1/1	0.97	0.08	53,53,53,53	0
55	MG	1A	3822	1/1	0.97	0.17	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3682	1/1	0.97	0.07	67,67,67,67	0
55	MG	1A	3022	1/1	0.97	0.14	31,31,31,31	0
55	MG	2a	1789	1/1	0.97	0.10	86,86,86,86	0
55	MG	2A	3496	1/1	0.97	0.05	43,43,43,43	0
55	MG	1A	3601	1/1	0.97	0.15	37,37,37,37	0
55	MG	1A	3455	1/1	0.97	0.09	49,49,49,49	0
55	MG	20	105	1/1	0.97	0.08	81,81,81,81	0
55	MG	1A	3603	1/1	0.97	0.10	49,49,49,49	0
55	MG	1A	3006	1/1	0.97	0.06	21,21,21,21	0
55	MG	2A	3503	1/1	0.97	0.11	53,53,53,53	0
55	MG	1D	306	1/1	0.97	0.14	35,35,35,35	0
55	MG	1A	3696	1/1	0.97	0.08	29,29,29,29	0
55	MG	1A	3114	1/1	0.97	0.12	37,37,37,37	0
55	MG	1A	3458	1/1	0.97	0.09	46,46,46,46	0
55	MG	1A	3303	1/1	0.97	0.06	13,13,13,13	0
55	MG	1A	3184	1/1	0.97	0.17	37,37,37,37	0
55	MG	1A	3185	1/1	0.97	0.31	32,32,32,32	0
55	MG	1A	3382	1/1	0.97	0.15	52,52,52,52	0
55	MG	1A	3706	1/1	0.97	0.10	54,54,54,54	0
55	MG	1A	3466	1/1	0.97	0.05	46,46,46,46	0
55	MG	28	103	1/1	0.97	0.08	77,77,77,77	0
55	MG	1A	3050	1/1	0.97	0.23	29,29,29,29	0
55	MG	1A	3842	1/1	0.97	0.06	84,84,84,84	0
55	MG	2A	3517	1/1	0.97	0.11	64,64,64,64	0
55	MG	1A	3215	1/1	0.97	0.23	38,38,38,38	0
55	MG	2A	3278	1/1	0.98	0.04	56,56,56,56	0
55	MG	17	105	1/1	0.98	0.06	52,52,52,52	0
55	MG	1A	3770	1/1	0.98	0.08	34,34,34,34	0
55	MG	1A	3127	1/1	0.98	0.14	14,14,14,14	0
55	MG	1A	3694	1/1	0.98	0.04	35,35,35,35	0
55	MG	1A	3065	1/1	0.98	0.08	32,32,32,32	0
55	MG	1A	3104	1/1	0.98	0.38	37,37,37,37	0
55	MG	1A	3327	1/1	0.98	0.04	18,18,18,18	0
55	MG	1A	3450	1/1	0.98	0.06	19,19,19,19	0
55	MG	2A	3443	1/1	0.98	0.11	63,63,63,63	0
55	MG	2A	3444	1/1	0.98	0.05	31,31,31,31	0
55	MG	1A	3700	1/1	0.98	0.04	24,24,24,24	0
55	MG	1E	305	1/1	0.98	0.05	26,26,26,26	0
55	MG	2A	3166	1/1	0.98	0.25	44,44,44,44	0
55	MG	1A	3876	1/1	0.98	0.06	64,64,64,64	0
55	MG	1A	3508	1/1	0.98	0.09	51,51,51,51	0
55	MG	1A	3329	1/1	0.98	0.04	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3302	1/1	0.98	0.06	44,44,44,44	0
55	MG	1A	3879	1/1	0.98	0.04	41,41,41,41	0
55	MG	2A	3603	1/1	0.98	0.04	61,61,61,61	0
55	MG	1A	3784	1/1	0.98	0.04	42,42,42,42	0
55	MG	2A	3070	1/1	0.98	0.09	35,35,35,35	0
55	MG	1A	3222	1/1	0.98	0.37	36,36,36,36	0
55	MG	1A	3704	1/1	0.98	0.12	42,42,42,42	0
55	MG	1a	3106	1/1	0.98	0.04	60,60,60,60	0
55	MG	1A	3334	1/1	0.98	0.04	20,20,20,20	0
55	MG	1A	3336	1/1	0.98	0.05	21,21,21,21	0
55	MG	1A	3343	1/1	0.98	0.04	26,26,26,26	0
55	MG	2A	3077	1/1	0.98	0.08	56,56,56,56	0
55	MG	2A	3314	1/1	0.98	0.14	60,60,60,60	0
55	MG	1a	3110	1/1	0.98	0.04	52,52,52,52	0
55	MG	2A	3316	1/1	0.98	0.07	43,43,43,43	0
55	MG	2A	3466	1/1	0.98	0.09	37,37,37,37	0
55	MG	1a	3219	1/1	0.98	0.09	63,63,63,63	0
55	MG	1A	3240	1/1	0.98	0.08	58,58,58,58	0
55	MG	2A	3469	1/1	0.98	0.04	68,68,68,68	0
55	MG	1A	3207	1/1	0.98	0.07	45,45,45,45	0
55	MG	1A	3397	1/1	0.98	0.03	64,64,64,64	0
55	MG	1F	311	1/1	0.98	0.19	25,25,25,25	0
55	MG	1A	3801	1/1	0.98	0.06	56,56,56,56	0
55	MG	1A	3460	1/1	0.98	0.11	20,20,20,20	0
55	MG	1A	3018	1/1	0.98	0.30	23,23,23,23	0
55	MG	1A	3805	1/1	0.98	0.07	65,65,65,65	0
55	MG	1a	3120	1/1	0.98	0.05	65,65,65,65	0
55	MG	1A	3263	1/1	0.98	0.06	17,17,17,17	0
55	MG	1A	3401	1/1	0.98	0.05	62,62,62,62	0
55	MG	1A	3715	1/1	0.98	0.04	85,85,85,85	0
55	MG	1G	3003	1/1	0.98	0.11	47,47,47,47	0
55	MG	2A	3334	1/1	0.98	0.11	45,45,45,45	0
55	MG	1A	3897	1/1	0.98	0.11	11,11,11,11	0
55	MG	1A	3300	1/1	0.98	0.05	44,44,44,44	0
55	MG	1A	3225	1/1	0.98	0.06	34,34,34,34	0
55	MG	2A	3198	1/1	0.98	0.10	27,27,27,27	0
55	MG	2A	3339	1/1	0.98	0.04	71,71,71,71	0
55	MG	1A	3719	1/1	0.98	0.06	45,45,45,45	0
55	MG	2A	3341	1/1	0.98	0.05	34,34,34,34	0
55	MG	2A	3490	1/1	0.98	0.10	33,33,33,33	0
55	MG	2A	3491	1/1	0.98	0.05	51,51,51,51	0
55	MG	2a	1688	1/1	0.98	0.04	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3645	1/1	0.98	0.06	62,62,62,62	0
55	MG	2B	3010	1/1	0.98	0.06	72,72,72,72	0
55	MG	2A	3097	1/1	0.98	0.14	35,35,35,35	0
55	MG	1A	3302	1/1	0.98	0.05	42,42,42,42	0
55	MG	2a	1693	1/1	0.98	0.10	54,54,54,54	0
55	MG	2A	3495	1/1	0.98	0.07	59,59,59,59	0
55	MG	1A	3584	1/1	0.98	0.10	37,37,37,37	0
55	MG	1A	3140	1/1	0.98	0.05	37,37,37,37	0
55	MG	2A	3498	1/1	0.98	0.03	39,39,39,39	0
55	MG	2B	3017	1/1	0.98	0.11	84,84,84,84	0
55	MG	2A	3499	1/1	0.98	0.04	65,65,65,65	0
55	MG	1A	3407	1/1	0.98	0.06	48,48,48,48	0
55	MG	2A	3205	1/1	0.98	0.21	52,52,52,52	0
55	MG	2a	1702	1/1	0.98	0.05	67,67,67,67	0
55	MG	2A	3206	1/1	0.98	0.04	39,39,39,39	0
55	MG	1A	3304	1/1	0.98	0.05	45,45,45,45	0
55	MG	2A	3003	1/1	0.98	0.04	31,31,31,31	0
55	MG	1A	3825	1/1	0.98	0.10	68,68,68,68	0
55	MG	2A	3355	1/1	0.98	0.05	76,76,76,76	0
55	MG	2A	3662	1/1	0.98	0.04	68,68,68,68	0
55	MG	2D	309	1/1	0.98	0.06	30,30,30,30	0
55	MG	2A	3663	1/1	0.98	0.09	50,50,50,50	0
55	MG	1A	3245	1/1	0.98	0.08	46,46,46,46	0
55	MG	2A	3665	1/1	0.98	0.07	59,59,59,59	0
55	MG	2E	302	1/1	0.98	0.04	35,35,35,35	0
55	MG	1A	3909	1/1	0.98	0.09	32,32,32,32	0
55	MG	1A	3152	1/1	0.98	0.07	53,53,53,53	0
55	MG	2A	3213	1/1	0.98	0.07	33,33,33,33	0
55	MG	2A	3214	1/1	0.98	0.07	37,37,37,37	0
55	MG	1A	3591	1/1	0.98	0.04	30,30,30,30	0
55	MG	1R	202	1/1	0.98	0.06	46,46,46,46	0
55	MG	2A	3217	1/1	0.98	0.06	32,32,32,32	0
55	MG	2A	3218	1/1	0.98	0.05	52,52,52,52	0
55	MG	2A	3516	1/1	0.98	0.08	45,45,45,45	0
55	MG	1A	3268	1/1	0.98	0.08	35,35,35,35	0
55	MG	1A	3832	1/1	0.98	0.10	55,55,55,55	0
55	MG	1A	3141	1/1	0.98	0.12	37,37,37,37	0
55	MG	1A	3367	1/1	0.98	0.04	30,30,30,30	0
55	MG	1A	3477	1/1	0.98	0.11	20,20,20,20	0
55	MG	1A	3420	1/1	0.98	0.06	27,27,27,27	0
55	MG	2A	3683	1/1	0.98	0.05	60,60,60,60	0
55	MG	2A	3227	1/1	0.98	0.07	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
55	MG	2A	3524	1/1	0.98	0.09	67,67,67,67	0
55	MG	2A	3525	1/1	0.98	0.03	50,50,50,50	0
55	MG	1A	3271	1/1	0.98	0.05	22,22,22,22	0
55	MG	1A	3663	1/1	0.98	0.03	26,26,26,26	0
55	MG	1B	3004	1/1	0.98	0.04	44,44,44,44	0
55	MG	1A	3738	1/1	0.98	0.08	14,14,14,14	0
55	MG	1U	206	1/1	0.98	0.11	28,28,28,28	0
55	MG	1A	3480	1/1	0.98	0.15	34,34,34,34	0
55	MG	2A	3385	1/1	0.98	0.05	32,32,32,32	0
55	MG	2A	3695	1/1	0.98	0.05	97,97,97,97	0
55	MG	1A	3106	1/1	0.98	0.09	42,42,42,42	0
55	MG	2a	1743	1/1	0.98	0.05	55,55,55,55	0
55	MG	2A	3699	1/1	0.98	0.04	38,38,38,38	0
55	MG	2T	201	1/1	0.98	0.06	47,47,47,47	0
55	MG	1A	3425	1/1	0.98	0.08	20,20,20,20	0
55	MG	2A	3702	1/1	0.98	0.08	34,34,34,34	0
55	MG	1A	3155	1/1	0.98	0.34	27,27,27,27	0
55	MG	1A	3540	1/1	0.98	0.11	19,19,19,19	0
55	MG	2A	3240	1/1	0.98	0.04	34,34,34,34	0
55	MG	1A	3274	1/1	0.98	0.06	27,27,27,27	0
55	MG	2A	3539	1/1	0.98	0.09	74,74,74,74	0
55	MG	1A	3429	1/1	0.98	0.04	26,26,26,26	0
55	MG	1a	3158	1/1	0.98	0.04	88,88,88,88	0
55	MG	2A	3713	1/1	0.98	0.06	79,79,79,79	0
55	MG	2A	3716	1/1	0.98	0.15	92,92,92,92	0
55	MG	1A	3431	1/1	0.98	0.04	40,40,40,40	0
55	MG	2X	103	1/1	0.98	0.07	58,58,58,58	0
55	MG	1A	3250	1/1	0.98	0.10	11,11,11,11	0
55	MG	1A	3674	1/1	0.98	0.04	26,26,26,26	0
55	MG	1a	3162	1/1	0.98	0.04	77,77,77,77	0
55	MG	2A	3399	1/1	0.98	0.06	45,45,45,45	0
55	MG	2A	3723	1/1	0.98	0.05	73,73,73,73	0
55	MG	1A	3277	1/1	0.98	0.05	30,30,30,30	0
55	MG	2A	3725	1/1	0.98	0.08	64,64,64,64	0
55	MG	2a	1767	1/1	0.98	0.16	79,79,79,79	0
55	MG	1A	3852	1/1	0.98	0.16	24,24,24,24	0
55	MG	2A	3402	1/1	0.98	0.05	37,37,37,37	0
55	MG	1B	3021	1/1	0.98	0.10	66,66,66,66	0
55	MG	1A	3434	1/1	0.98	0.06	16,16,16,16	0
55	MG	2A	3037	1/1	0.98	0.08	24,24,24,24	0
55	MG	1A	3375	1/1	0.98	0.15	51,51,51,51	0
55	MG	2A	3736	1/1	0.98	0.10	95,95,95,95	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3024	1/1	0.98	0.18	30,30,30,30	0
55	MG	1A	3612	1/1	0.98	0.10	78,78,78,78	0
55	MG	2A	3558	1/1	0.98	0.08	59,59,59,59	0
55	MG	1D	303	1/1	0.98	0.21	52,52,52,52	0
55	MG	1a	3171	1/1	0.98	0.10	50,50,50,50	0
55	MG	13	101	1/1	0.98	0.19	32,32,32,32	0
55	MG	2a	1785	1/1	0.98	0.06	68,68,68,68	0
55	MG	2a	1786	1/1	0.98	0.07	90,90,90,90	0
55	MG	2A	3745	1/1	0.98	0.07	70,70,70,70	0
55	MG	2a	1788	1/1	0.98	0.04	86,86,86,86	0
55	MG	2A	3259	1/1	0.98	0.04	34,34,34,34	0
55	MG	1A	3613	1/1	0.98	0.05	82,82,82,82	0
55	MG	15	101	1/1	0.98	0.06	42,42,42,42	0
55	MG	2A	3565	1/1	0.98	0.05	56,56,56,56	0
55	MG	2A	3566	1/1	0.98	0.14	64,64,64,64	0
55	MG	2a	1794	1/1	0.98	0.05	70,70,70,70	0
55	MG	1A	3025	1/1	0.98	0.39	33,33,33,33	0
55	MG	1A	3280	1/1	0.98	0.06	29,29,29,29	0
55	MG	2A	3419	1/1	0.98	0.04	33,33,33,33	0
55	MG	2d	502	1/1	0.98	0.08	74,74,74,74	0
55	MG	1A	3379	1/1	0.98	0.06	43,43,43,43	0
55	MG	1A	3620	1/1	0.98	0.07	50,50,50,50	0
55	MG	1A	3158	1/1	0.98	0.04	37,37,37,37	0
55	MG	1A	3085	1/1	0.98	0.19	34,34,34,34	0
55	MG	1A	3096	1/1	0.98	0.50	34,34,34,34	0
55	MG	2A	3153	1/1	0.98	0.06	52,52,52,52	0
55	MG	1D	312	1/1	0.98	0.12	15,15,15,15	0
55	MG	2A	3271	1/1	0.98	0.05	36,36,36,36	0
55	MG	2A	3272	1/1	0.98	0.04	41,41,41,41	0
55	MG	2A	3429	1/1	0.98	0.05	64,64,64,64	0
55	MG	1A	3443	1/1	0.98	0.04	22,22,22,22	0
55	MG	2A	3275	1/1	0.98	0.04	47,47,47,47	0
55	MG	2A	3767	1/1	0.98	0.04	65,65,65,65	0
55	MG	2A	3276	1/1	0.98	0.04	48,48,48,48	0
55	MG	2A	3277	1/1	0.98	0.07	36,36,36,36	0
57	ZN	14	501	1/1	0.98	0.04	109,109,109,109	0
57	ZN	1n	501	1/1	0.98	0.04	88,88,88,88	0
57	ZN	2n	501	1/1	0.98	0.04	108,108,108,108	0
58	SF4	2d	501	8/8	0.98	0.04	65,69,77,88	0
55	MG	1B	3012	1/1	0.99	0.03	44,44,44,44	0
55	MG	1A	3735	1/1	0.99	0.17	27,27,27,27	0
55	MG	1A	3505	1/1	0.99	0.04	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3613	1/1	0.99	0.03	55,55,55,55	0
55	MG	2A	3614	1/1	0.99	0.05	58,58,58,58	0
55	MG	1A	3352	1/1	0.99	0.03	22,22,22,22	0
55	MG	2A	3616	1/1	0.99	0.08	53,53,53,53	0
55	MG	1A	3462	1/1	0.99	0.04	40,40,40,40	0
55	MG	1a	3187	1/1	0.99	0.06	89,89,89,89	0
55	MG	1A	3421	1/1	0.99	0.04	28,28,28,28	0
55	MG	1A	3422	1/1	0.99	0.03	30,30,30,30	0
55	MG	1a	3190	1/1	0.99	0.03	79,79,79,79	0
55	MG	1a	3191	1/1	0.99	0.05	47,47,47,47	0
55	MG	1A	3326	1/1	0.99	0.04	24,24,24,24	0
55	MG	1A	3556	1/1	0.99	0.03	14,14,14,14	0
55	MG	2A	3326	1/1	0.99	0.03	35,35,35,35	0
55	MG	1A	3557	1/1	0.99	0.04	24,24,24,24	0
55	MG	1a	3195	1/1	0.99	0.09	62,62,62,62	0
55	MG	1A	3558	1/1	0.99	0.03	27,27,27,27	0
55	MG	1A	3559	1/1	0.99	0.05	26,26,26,26	0
55	MG	1a	3198	1/1	0.99	0.04	47,47,47,47	0
55	MG	2A	3332	1/1	0.99	0.04	46,46,46,46	0
55	MG	1A	3383	1/1	0.99	0.03	20,20,20,20	0
55	MG	1D	301	1/1	0.99	0.10	32,32,32,32	0
55	MG	1a	3090	1/1	0.99	0.03	40,40,40,40	0
55	MG	1a	3203	1/1	0.99	0.03	67,67,67,67	0
55	MG	1a	3204	1/1	0.99	0.05	72,72,72,72	0
55	MG	1a	3205	1/1	0.99	0.04	77,77,77,77	0
55	MG	1a	3206	1/1	0.99	0.03	68,68,68,68	0
55	MG	1a	3091	1/1	0.99	0.04	37,37,37,37	0
55	MG	2a	1668	1/1	0.99	0.04	51,51,51,51	0
55	MG	2a	1669	1/1	0.99	0.06	46,46,46,46	0
55	MG	1A	3615	1/1	0.99	0.07	19,19,19,19	0
55	MG	1a	3209	1/1	0.99	0.04	52,52,52,52	0
55	MG	1a	3093	1/1	0.99	0.04	73,73,73,73	0
55	MG	2A	3492	1/1	0.99	0.03	52,52,52,52	0
55	MG	1A	3751	1/1	0.99	0.07	39,39,39,39	0
55	MG	1A	3616	1/1	0.99	0.08	48,48,48,48	0
55	MG	2A	3347	1/1	0.99	0.04	80,80,80,80	0
55	MG	1A	3617	1/1	0.99	0.06	38,38,38,38	0
55	MG	2A	3648	1/1	0.99	0.03	34,34,34,34	0
55	MG	2A	3349	1/1	0.99	0.07	77,77,77,77	0
55	MG	2a	1680	1/1	0.99	0.05	55,55,55,55	0
55	MG	1a	3214	1/1	0.99	0.03	71,71,71,71	0
55	MG	1A	3354	1/1	0.99	0.03	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3681	1/1	0.99	0.04	38,38,38,38	0
55	MG	1A	3562	1/1	0.99	0.08	20,20,20,20	0
55	MG	2a	1685	1/1	0.99	0.09	56,56,56,56	0
55	MG	2A	3354	1/1	0.99	0.04	26,26,26,26	0
55	MG	1A	3275	1/1	0.99	0.04	27,27,27,27	0
55	MG	2A	3656	1/1	0.99	0.03	42,42,42,42	0
55	MG	1a	3101	1/1	0.99	0.04	39,39,39,39	0
55	MG	1a	3220	1/1	0.99	0.03	65,65,65,65	0
55	MG	2A	3358	1/1	0.99	0.03	45,45,45,45	0
55	MG	1a	3102	1/1	0.99	0.03	48,48,48,48	0
55	MG	19	101	1/1	0.99	0.19	41,41,41,41	0
55	MG	2A	3220	1/1	0.99	0.04	66,66,66,66	0
55	MG	1A	3357	1/1	0.99	0.06	20,20,20,20	0
55	MG	1A	3565	1/1	0.99	0.03	20,20,20,20	0
55	MG	2A	3364	1/1	0.99	0.03	60,60,60,60	0
55	MG	1A	3566	1/1	0.99	0.04	23,23,23,23	0
55	MG	2A	3667	1/1	0.99	0.04	57,57,57,57	0
55	MG	1A	3358	1/1	0.99	0.05	19,19,19,19	0
55	MG	1A	3688	1/1	0.99	0.05	26,26,26,26	0
55	MG	2A	3368	1/1	0.99	0.04	42,42,42,42	0
55	MG	2A	3226	1/1	0.99	0.05	44,44,44,44	0
55	MG	1d	505	1/1	0.99	0.03	74,74,74,74	0
55	MG	2A	3371	1/1	0.99	0.05	36,36,36,36	0
55	MG	2A	3372	1/1	0.99	0.03	38,38,38,38	0
55	MG	1A	3430	1/1	0.99	0.03	16,16,16,16	0
55	MG	1A	3766	1/1	0.99	0.13	39,39,39,39	0
55	MG	1A	3197	1/1	0.99	0.06	25,25,25,25	0
55	MG	1A	3360	1/1	0.99	0.02	21,21,21,21	0
55	MG	1E	301	1/1	0.99	0.04	15,15,15,15	0
55	MG	2A	3378	1/1	0.99	0.03	51,51,51,51	0
55	MG	2E	305	1/1	0.99	0.03	34,34,34,34	0
55	MG	1A	3692	1/1	0.99	0.04	43,43,43,43	0
55	MG	1A	3693	1/1	0.99	0.05	42,42,42,42	0
55	MG	1A	3628	1/1	0.99	0.07	50,50,50,50	0
55	MG	1A	3772	1/1	0.99	0.03	37,37,37,37	0
55	MG	2A	3238	1/1	0.99	0.03	38,38,38,38	0
55	MG	2A	3687	1/1	0.99	0.03	49,49,49,49	0
55	MG	2A	3384	1/1	0.99	0.04	68,68,68,68	0
55	MG	1a	3118	1/1	0.99	0.03	70,70,70,70	0
55	MG	1A	3305	1/1	0.99	0.03	16,16,16,16	0
55	MG	1A	3362	1/1	0.99	0.03	20,20,20,20	0
55	MG	1A	3697	1/1	0.99	0.04	19,19,19,19	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3294	1/1	0.99	0.04	33,33,33,33	0
55	MG	1A	3872	1/1	0.99	0.04	29,29,29,29	0
55	MG	1A	3777	1/1	0.99	0.04	41,41,41,41	0
55	MG	2A	3696	1/1	0.99	0.04	62,62,62,62	0
55	MG	1A	3364	1/1	0.99	0.16	36,36,36,36	0
55	MG	2A	3698	1/1	0.99	0.06	42,42,42,42	0
55	MG	1A	3335	1/1	0.99	0.06	19,19,19,19	0
55	MG	1A	3295	1/1	0.99	0.03	13,13,13,13	0
55	MG	2Q	8001	1/1	0.99	0.08	79,79,79,79	0
55	MG	1A	3337	1/1	0.99	0.04	39,39,39,39	0
55	MG	2a	1735	1/1	0.99	0.03	81,81,81,81	0
55	MG	1A	3399	1/1	0.99	0.05	15,15,15,15	0
55	MG	1A	3786	1/1	0.99	0.03	23,23,23,23	0
55	MG	1A	3338	1/1	0.99	0.05	20,20,20,20	0
55	MG	1A	3788	1/1	0.99	0.04	48,48,48,48	0
55	MG	2A	3548	1/1	0.99	0.03	65,65,65,65	0
55	MG	2A	3549	1/1	0.99	0.07	74,74,74,74	0
55	MG	2A	3711	1/1	0.99	0.03	70,70,70,70	0
55	MG	1A	3369	1/1	0.99	0.03	14,14,14,14	0
55	MG	1A	3340	1/1	0.99	0.03	22,22,22,22	0
55	MG	2A	3714	1/1	0.99	0.03	49,49,49,49	0
55	MG	2A	3715	1/1	0.99	0.06	66,66,66,66	0
55	MG	1A	3791	1/1	0.99	0.10	33,33,33,33	0
55	MG	2A	3404	1/1	0.99	0.03	63,63,63,63	0
55	MG	2A	3718	1/1	0.99	0.07	83,83,83,83	0
55	MG	1A	3530	1/1	0.99	0.03	44,44,44,44	0
55	MG	1A	3793	1/1	0.99	0.09	52,52,52,52	0
55	MG	1A	3341	1/1	0.99	0.05	20,20,20,20	0
55	MG	1A	3888	1/1	0.99	0.10	47,47,47,47	0
55	MG	1A	3342	1/1	0.99	0.03	21,21,21,21	0
55	MG	1A	3405	1/1	0.99	0.04	42,42,42,42	0
55	MG	1A	3798	1/1	0.99	0.04	48,48,48,48	0
55	MG	1A	3644	1/1	0.99	0.03	18,18,18,18	0
55	MG	1A	3489	1/1	0.99	0.03	33,33,33,33	0
55	MG	2A	3728	1/1	0.99	0.04	34,34,34,34	0
55	MG	1A	3587	1/1	0.99	0.06	50,50,50,50	0
55	MG	2A	3730	1/1	0.99	0.06	56,56,56,56	0
55	MG	1A	3803	1/1	0.99	0.07	39,39,39,39	0
55	MG	2a	1763	1/1	0.99	0.05	55,55,55,55	0
55	MG	1A	3647	1/1	0.99	0.03	39,39,39,39	0
55	MG	2A	3733	1/1	0.99	0.07	60,60,60,60	0
55	MG	1A	3447	1/1	0.99	0.02	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1P	204	1/1	0.99	0.04	35,35,35,35	0
55	MG	2A	3737	1/1	0.99	0.08	80,80,80,80	0
55	MG	1A	3296	1/1	0.99	0.04	20,20,20,20	0
55	MG	1A	3717	1/1	0.99	0.03	35,35,35,35	0
55	MG	2a	1771	1/1	0.99	0.02	55,55,55,55	0
55	MG	1A	3344	1/1	0.99	0.04	25,25,25,25	0
55	MG	2A	3741	1/1	0.99	0.03	70,70,70,70	0
55	MG	2A	3274	1/1	0.99	0.03	61,61,61,61	0
55	MG	2a	1775	1/1	0.99	0.05	63,63,63,63	0
55	MG	1A	3493	1/1	0.99	0.03	30,30,30,30	0
55	MG	1A	3810	1/1	0.99	0.02	27,27,27,27	0
55	MG	1A	3811	1/1	0.99	0.07	56,56,56,56	0
55	MG	1A	3812	1/1	0.99	0.04	28,28,28,28	0
55	MG	2a	1780	1/1	0.99	0.03	68,68,68,68	0
55	MG	2A	3279	1/1	0.99	0.04	45,45,45,45	0
55	MG	1A	3813	1/1	0.99	0.04	25,25,25,25	0
55	MG	2a	1783	1/1	0.99	0.07	53,53,53,53	0
55	MG	1A	3814	1/1	0.99	0.03	18,18,18,18	0
55	MG	2A	3282	1/1	0.99	0.04	34,34,34,34	0
55	MG	2A	3284	1/1	0.99	0.03	37,37,37,37	0
55	MG	1A	3298	1/1	0.99	0.04	27,27,27,27	0
55	MG	2A	3286	1/1	0.99	0.03	42,42,42,42	0
55	MG	1A	3270	1/1	0.99	0.07	18,18,18,18	0
55	MG	1A	3594	1/1	0.99	0.06	24,24,24,24	0
55	MG	1A	3818	1/1	0.99	0.11	24,24,24,24	0
55	MG	2A	3291	1/1	0.99	0.04	34,34,34,34	0
55	MG	1A	3819	1/1	0.99	0.09	58,58,58,58	0
55	MG	1A	3453	1/1	0.99	0.05	19,19,19,19	0
55	MG	1A	3821	1/1	0.99	0.13	54,54,54,54	0
55	MG	2A	3761	1/1	0.99	0.04	38,38,38,38	0
55	MG	1A	3016	1/1	0.99	0.33	19,19,19,19	0
55	MG	2A	3296	1/1	0.99	0.04	42,42,42,42	0
55	MG	1A	3916	1/1	0.99	0.21	29,29,29,29	0
55	MG	1A	3283	1/1	0.99	0.03	25,25,25,25	0
55	MG	1A	3412	1/1	0.99	0.04	12,12,12,12	0
55	MG	2A	3300	1/1	0.99	0.03	36,36,36,36	0
55	MG	1A	3414	1/1	0.99	0.03	19,19,19,19	0
55	MG	1A	3826	1/1	0.99	0.11	59,59,59,59	0
55	MG	1A	3416	1/1	0.99	0.02	26,26,26,26	0
55	MG	1A	3284	1/1	0.99	0.06	43,43,43,43	0
55	MG	2A	3452	1/1	0.99	0.06	51,51,51,51	0
55	MG	1A	3662	1/1	0.99	0.10	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1Y	502	1/1	0.99	0.10	74,74,74,74	0
55	MG	1A	3830	1/1	0.99	0.04	47,47,47,47	0
55	MG	1a	3177	1/1	0.99	0.04	74,74,74,74	0
55	MG	1A	3325	1/1	0.99	0.05	28,28,28,28	0
55	MG	1A	3504	1/1	0.99	0.04	19,19,19,19	0
55	MG	2A	3311	1/1	0.99	0.04	42,42,42,42	0
57	ZN	16	101	1/1	0.99	0.03	44,44,44,44	0
55	MG	2A	3780	1/1	0.99	0.05	40,40,40,40	0
57	ZN	2Y	501	1/1	0.99	0.03	95,95,95,95	0
57	ZN	24	501	1/1	0.99	0.08	129,129,129,129	0
57	ZN	26	101	1/1	0.99	0.04	64,64,64,64	0
57	ZN	29	501	1/1	0.99	0.03	75,75,75,75	0
55	MG	1B	3010	1/1	0.99	0.03	59,59,59,59	0
58	SF4	1d	501	8/8	0.99	0.05	65,70,75,78	0
55	MG	1B	3011	1/1	0.99	0.04	48,48,48,48	0
55	MG	1A	3782	1/1	1.00	0.03	33,33,33,33	0
55	MG	1A	3330	1/1	1.00	0.03	37,37,37,37	0
55	MG	1A	3732	1/1	1.00	0.02	21,21,21,21	0
55	MG	1A	3785	1/1	1.00	0.02	25,25,25,25	0
55	MG	1A	3297	1/1	1.00	0.02	15,15,15,15	0
55	MG	2A	3390	1/1	1.00	0.01	49,49,49,49	0
55	MG	1A	3332	1/1	1.00	0.02	28,28,28,28	0
55	MG	1A	3426	1/1	1.00	0.02	18,18,18,18	0
55	MG	1A	3390	1/1	1.00	0.02	23,23,23,23	0
55	MG	1A	3413	1/1	1.00	0.02	43,43,43,43	0
55	MG	1a	3202	1/1	1.00	0.04	47,47,47,47	0
55	MG	1A	3851	1/1	1.00	0.04	21,21,21,21	0
55	MG	1A	3391	1/1	1.00	0.01	18,18,18,18	0
55	MG	1A	3739	1/1	1.00	0.05	22,22,22,22	0
55	MG	1A	3415	1/1	1.00	0.04	20,20,20,20	0
55	MG	2A	3283	1/1	1.00	0.04	37,37,37,37	0
55	MG	2A	3734	1/1	1.00	0.06	67,67,67,67	0
55	MG	2A	3781	1/1	1.00	0.02	51,51,51,51	0
55	MG	1A	3720	1/1	1.00	0.10	65,65,65,65	0
55	MG	1A	3339	1/1	1.00	0.04	18,18,18,18	0
55	MG	1X	8001	1/1	1.00	0.03	31,31,31,31	0
55	MG	1A	3463	1/1	1.00	0.02	28,28,28,28	0
55	MG	2A	3405	1/1	1.00	0.02	43,43,43,43	0
55	MG	2A	3288	1/1	1.00	0.03	30,30,30,30	0
55	MG	1A	3797	1/1	1.00	0.04	28,28,28,28	0
55	MG	1A	3744	1/1	1.00	0.03	55,55,55,55	0
55	MG	1A	3799	1/1	1.00	0.02	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3347	1/1	1.00	0.02	18,18,18,18	0
55	MG	1A	3448	1/1	1.00	0.01	23,23,23,23	0
55	MG	1A	3418	1/1	1.00	0.03	26,26,26,26	0
55	MG	2A	3701	1/1	1.00	0.01	60,60,60,60	0
55	MG	2A	3333	1/1	1.00	0.02	42,42,42,42	0
55	MG	1A	3356	1/1	1.00	0.02	25,25,25,25	0
55	MG	1A	3749	1/1	1.00	0.04	36,36,36,36	0
55	MG	1A	3333	1/1	1.00	0.03	17,17,17,17	0
55	MG	1A	3673	1/1	1.00	0.03	35,35,35,35	0
55	MG	1A	3752	1/1	1.00	0.04	22,22,22,22	0
57	ZN	1Y	501	1/1	1.00	0.04	61,61,61,61	0
55	MG	1A	3328	1/1	1.00	0.02	22,22,22,22	0
57	ZN	15	106	1/1	1.00	0.04	47,47,47,47	0
55	MG	2A	3709	1/1	1.00	0.01	45,45,45,45	0
57	ZN	19	102	1/1	1.00	0.01	43,43,43,43	0
55	MG	2A	3710	1/1	1.00	0.02	60,60,60,60	0
55	MG	1A	3754	1/1	1.00	0.10	39,39,39,39	0
55	MG	1A	3871	1/1	1.00	0.03	21,21,21,21	0
57	ZN	25	104	1/1	1.00	0.02	54,54,54,54	0
55	MG	1A	3780	1/1	1.00	0.07	58,58,58,58	0
55	MG	2A	3669	1/1	1.00	0.02	40,40,40,40	0
55	MG	1A	3288	1/1	1.00	0.04	26,26,26,26	0
55	MG	2A	3231	1/1	1.00	0.07	48,48,48,48	0
55	MG	1A	3906	1/1	1.00	0.04	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.