



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 5, 2026 – 05:35 AM UTC

PDB ID : 10PX / pdb_000010px
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with benzoxaborole derivative of azithromycin (AZI-BB2), mRNA, aminoacylated A-site Phe-tRNA_{phe}, aminoacylated P-site fMet-tRNA_{met}, and deacylated E-site tRNA_{phe} at 2.45Å resolution
Authors : Chen, C.-W.; Volynkina, I.A.; Bortyazh, M.O.; Tereshchenkov, A.G.; Karakchieva, A.O.; Lukianov, D.A.; Komarova, E.S.; Tupikin, A.E.; Skvortsov, D.A.; Tevyashova, A.N.; Tikhomirov, A.S.; Tashlitsky, V.N.; Kabilov, M.R.; Shchekotikhin, A.E.; Dontsova, O.A.; Sergiev, P.V.; Polikanov, Y.S.
Deposited on : 2026-02-01
Resolution : 2.45 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
Buster-report	: wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	: 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	: 9.0.010 (Gargrove)

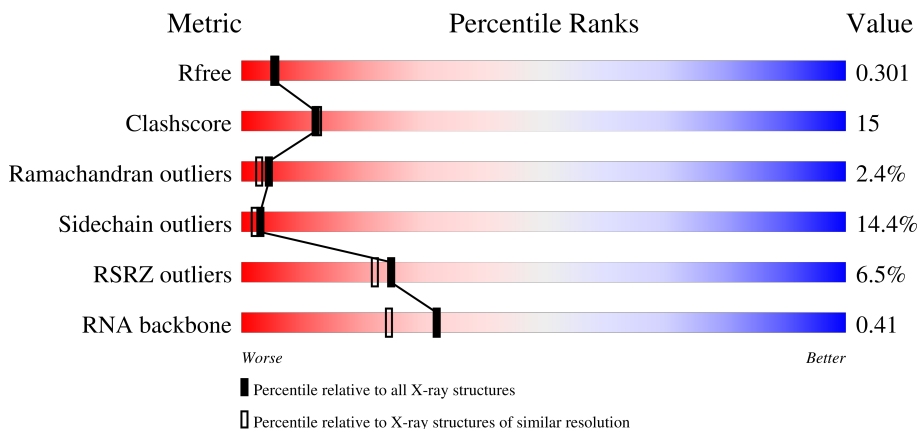
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)
RNA backbone	3983	1023 (2.72-2.20)

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	

Continued on next page...

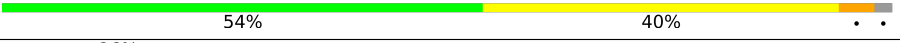



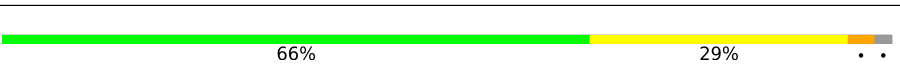

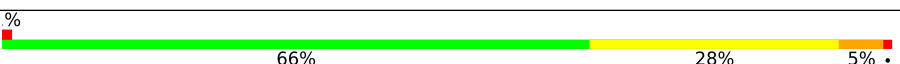

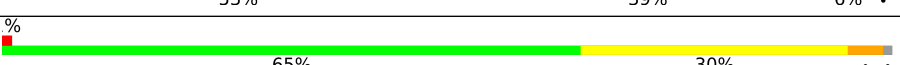
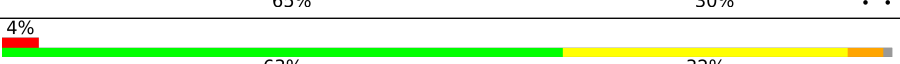
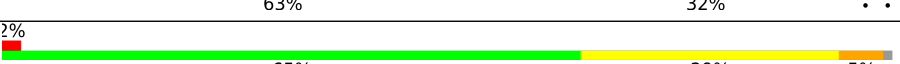
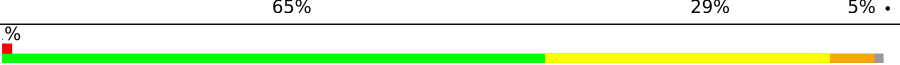



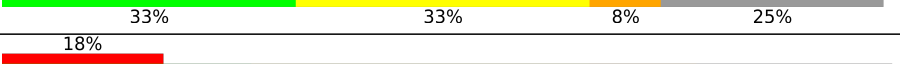
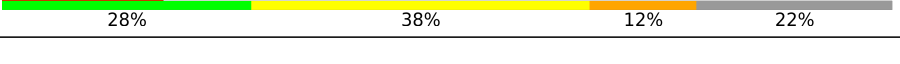
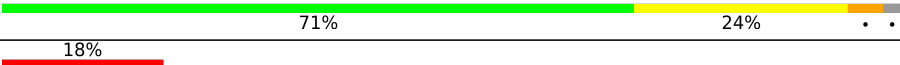

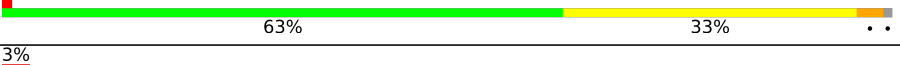
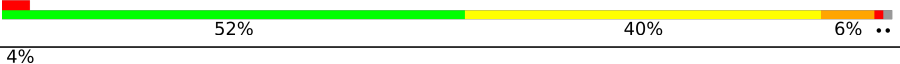


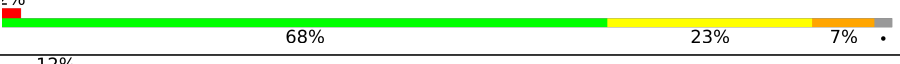
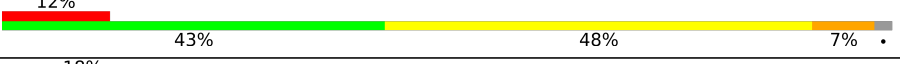
Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	2A	2915	
2	1B	121	
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	1S	112	
14	2S	112	
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
26	24	71	
27	15	60	
27	25	60	
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	




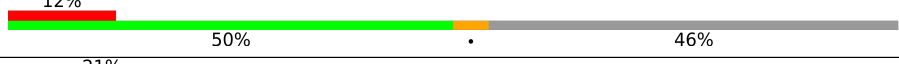
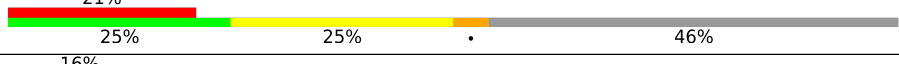
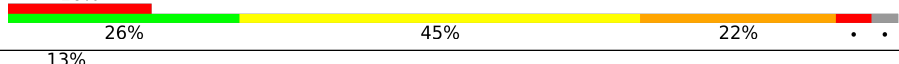
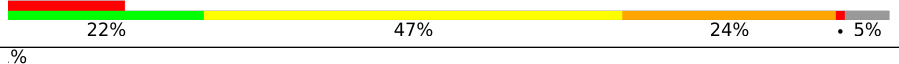

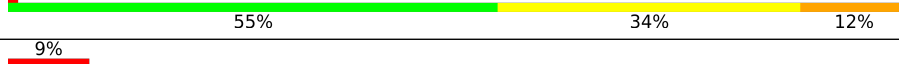
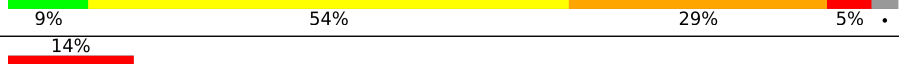
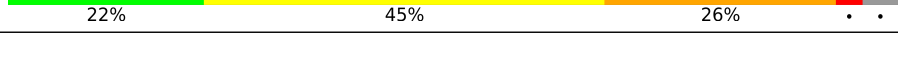
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
39	1h	138	
39	2h	138	
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
51	2t	106	
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1y	76	
56	2y	76	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	29	101	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 300377 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called MET-PHE-mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
53	2v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 54 is a RNA chain called A-site Aminoacylated Phe-tRNA^{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1603	722	287	518	74	2			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1555	699	280	502	72	2			

- Molecule 55 is a RNA chain called P-site Aminoacylated fMet-tRNA^{met}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1656	740	299	538	77	2			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1656	740	299	538	77	2			

- Molecule 56 is a RNA chain called E-site Deacylated tRNA^{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
56	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
56	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1099	Total	Mg	0	0
			1099	1099		
57	1B	36	Total	Mg	0	0
			36	36		
57	1D	13	Total	Mg	0	0
			13	13		
57	1E	14	Total	Mg	0	0
			14	14		
57	1F	12	Total	Mg	0	0
			12	12		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1G	5	Total 5	Mg 5	0	0
57	1H	1	Total 1	Mg 1	0	0
57	1I	1	Total 1	Mg 1	0	0
57	1N	6	Total 6	Mg 6	0	0
57	1O	5	Total 5	Mg 5	0	0
57	1P	3	Total 3	Mg 3	0	0
57	1Q	7	Total 7	Mg 7	0	0
57	1R	4	Total 4	Mg 4	0	0
57	1S	3	Total 3	Mg 3	0	0
57	1T	4	Total 4	Mg 4	0	0
57	1U	10	Total 10	Mg 10	0	0
57	1V	10	Total 10	Mg 10	0	0
57	1W	8	Total 8	Mg 8	0	0
57	1X	7	Total 7	Mg 7	0	0
57	1Y	3	Total 3	Mg 3	0	0
57	1Z	4	Total 4	Mg 4	0	0
57	10	8	Total 8	Mg 8	0	0
57	11	5	Total 5	Mg 5	0	0
57	12	2	Total 2	Mg 2	0	0
57	13	5	Total 5	Mg 5	0	0
57	14	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	15	9	Total 9	Mg 9	0	0
57	16	2	Total 2	Mg 2	0	0
57	17	7	Total 7	Mg 7	0	0
57	18	5	Total 5	Mg 5	0	0
57	1a	213	Total 213	Mg 213	0	0
57	1b	1	Total 1	Mg 1	0	0
57	1d	1	Total 1	Mg 1	0	0
57	1e	2	Total 2	Mg 2	0	0
57	1f	2	Total 2	Mg 2	0	0
57	1k	1	Total 1	Mg 1	0	0
57	1l	2	Total 2	Mg 2	0	0
57	1m	2	Total 2	Mg 2	0	0
57	1n	3	Total 3	Mg 3	0	0
57	1t	1	Total 1	Mg 1	0	0
57	1v	2	Total 2	Mg 2	0	0
57	1w	8	Total 8	Mg 8	0	0
57	1x	14	Total 14	Mg 14	0	0
57	1y	1	Total 1	Mg 1	0	0
57	2A	883	Total 883	Mg 883	0	0
57	2B	20	Total 20	Mg 20	0	0
57	2D	8	Total 8	Mg 8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2E	7	Total 7	Mg 7	0	0
57	2F	6	Total 6	Mg 6	0	0
57	2G	1	Total 1	Mg 1	0	0
57	2N	1	Total 1	Mg 1	0	0
57	2O	1	Total 1	Mg 1	0	0
57	2P	3	Total 3	Mg 3	0	0
57	2Q	3	Total 3	Mg 3	0	0
57	2R	3	Total 3	Mg 3	0	0
57	2T	3	Total 3	Mg 3	0	0
57	2U	1	Total 1	Mg 1	0	0
57	2V	2	Total 2	Mg 2	0	0
57	2W	3	Total 3	Mg 3	0	0
57	2X	2	Total 2	Mg 2	0	0
57	2Z	1	Total 1	Mg 1	0	0
57	20	2	Total 2	Mg 2	0	0
57	21	1	Total 1	Mg 1	0	0
57	23	1	Total 1	Mg 1	0	0
57	25	5	Total 5	Mg 5	0	0
57	27	2	Total 2	Mg 2	0	0
57	28	4	Total 4	Mg 4	0	0
57	29	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2a	234	Total 234	Mg 234	0	0
57	2d	2	Total 2	Mg 2	0	0
57	2e	1	Total 1	Mg 1	0	0
57	2f	1	Total 1	Mg 1	0	0
57	2g	1	Total 1	Mg 1	0	0
57	2i	1	Total 1	Mg 1	0	0
57	2j	2	Total 2	Mg 2	0	0
57	2k	1	Total 1	Mg 1	0	0
57	2l	4	Total 4	Mg 4	0	0
57	2m	1	Total 1	Mg 1	0	0
57	2p	1	Total 1	Mg 1	0	0
57	2q	2	Total 2	Mg 2	0	0
57	2r	2	Total 2	Mg 2	0	0
57	2t	1	Total 1	Mg 1	0	0
57	2v	3	Total 3	Mg 3	0	0
57	2w	9	Total 9	Mg 9	0	0
57	2x	6	Total 6	Mg 6	0	0
57	2y	6	Total 6	Mg 6	0	0

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

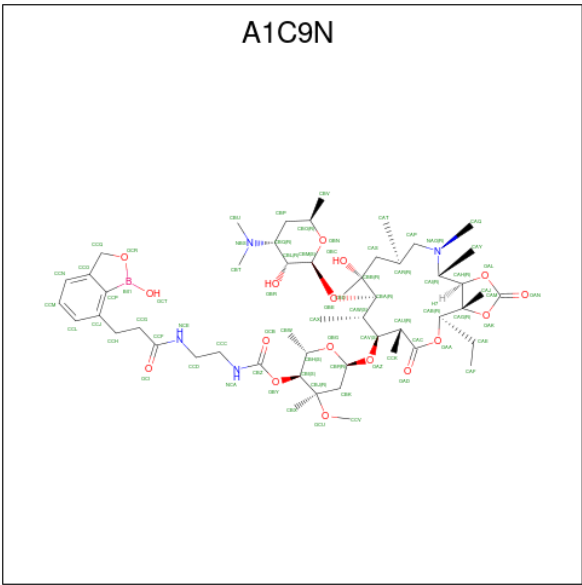
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1	Total 1	K 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2A	1	Total	K	0	0
			1	1		

- Molecule 59 is AZI-BB2 (CCD ID: A1C9N) (formula: C₅₂H₈₅BN₄O₁₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
59	1A	1	Total	B	C	N	O	0	0
			74	1	52	4	17		
59	2A	1	Total	B	C	N	O	0	0
			74	1	52	4	17		

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

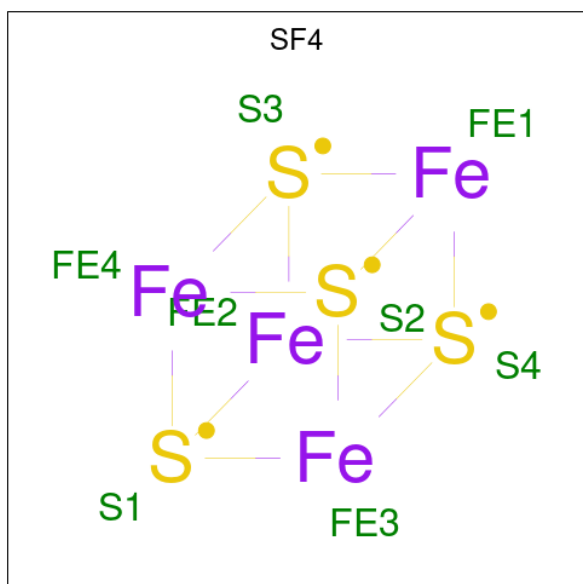
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1Y	1	Total	Zn	0	0
			1	1		
60	14	1	Total	Zn	0	0
			1	1		
60	15	1	Total	Zn	0	0
			1	1		
60	16	1	Total	Zn	0	0
			1	1		
60	19	1	Total	Zn	0	0
			1	1		
60	1n	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2Y	1	Total	Zn	0	0
			1	1		
60	24	1	Total	Zn	0	0
			1	1		
60	25	1	Total	Zn	0	0
			1	1		
60	26	1	Total	Zn	0	0
			1	1		
60	29	1	Total	Zn	0	0
			1	1		
60	2n	1	Total	Zn	0	0
			1	1		

- Molecule 61 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	1d	1	Total	Fe	S	0	0
			8	4	4		
61	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	1997	Total	O	0	0
			1997	1997		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1B	63	Total 63	O 63	0	0
62	1D	30	Total 30	O 30	0	0
62	1E	31	Total 31	O 31	0	0
62	1F	16	Total 16	O 16	0	0
62	1G	5	Total 5	O 5	0	0
62	1H	2	Total 2	O 2	0	0
62	1I	1	Total 1	O 1	0	0
62	1N	8	Total 8	O 8	0	0
62	1O	5	Total 5	O 5	0	0
62	1P	24	Total 24	O 24	0	0
62	1Q	8	Total 8	O 8	0	0
62	1R	11	Total 11	O 11	0	0
62	1S	5	Total 5	O 5	0	0
62	1T	9	Total 9	O 9	0	0
62	1U	9	Total 9	O 9	0	0
62	1V	9	Total 9	O 9	0	0
62	1W	8	Total 8	O 8	0	0
62	1X	5	Total 5	O 5	0	0
62	1Y	4	Total 4	O 4	0	0
62	1Z	1	Total 1	O 1	0	0
62	10	10	Total 10	O 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	11	14	Total 14	O 14	0	0
62	12	2	Total 2	O 2	0	0
62	13	3	Total 3	O 3	0	0
62	15	6	Total 6	O 6	0	0
62	16	4	Total 4	O 4	0	0
62	17	9	Total 9	O 9	0	0
62	18	10	Total 10	O 10	0	0
62	1a	379	Total 379	O 379	0	0
62	1b	1	Total 1	O 1	0	0
62	1e	1	Total 1	O 1	0	0
62	1f	1	Total 1	O 1	0	0
62	1i	1	Total 1	O 1	0	0
62	1l	7	Total 7	O 7	0	0
62	1p	1	Total 1	O 1	0	0
62	1q	2	Total 2	O 2	0	0
62	1u	1	Total 1	O 1	0	0
62	1v	5	Total 5	O 5	0	0
62	1w	13	Total 13	O 13	0	0
62	1x	15	Total 15	O 15	0	0
62	1y	2	Total 2	O 2	0	0
62	2A	1156	Total 1156	O 1156	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2B	24	Total 24	O 24	0	0
62	2D	22	Total 22	O 22	0	0
62	2E	14	Total 14	O 14	0	0
62	2F	12	Total 12	O 12	0	0
62	2I	3	Total 3	O 3	0	0
62	2N	1	Total 1	O 1	0	0
62	2O	3	Total 3	O 3	0	0
62	2P	12	Total 12	O 12	0	0
62	2Q	1	Total 1	O 1	0	0
62	2R	6	Total 6	O 6	0	0
62	2T	5	Total 5	O 5	0	0
62	2U	3	Total 3	O 3	0	0
62	2V	1	Total 1	O 1	0	0
62	2W	1	Total 1	O 1	0	0
62	2X	3	Total 3	O 3	0	0
62	2Z	1	Total 1	O 1	0	0
62	20	3	Total 3	O 3	0	0
62	21	12	Total 12	O 12	0	0
62	23	2	Total 2	O 2	0	0
62	25	2	Total 2	O 2	0	0
62	27	4	Total 4	O 4	0	0

Continued on next page...

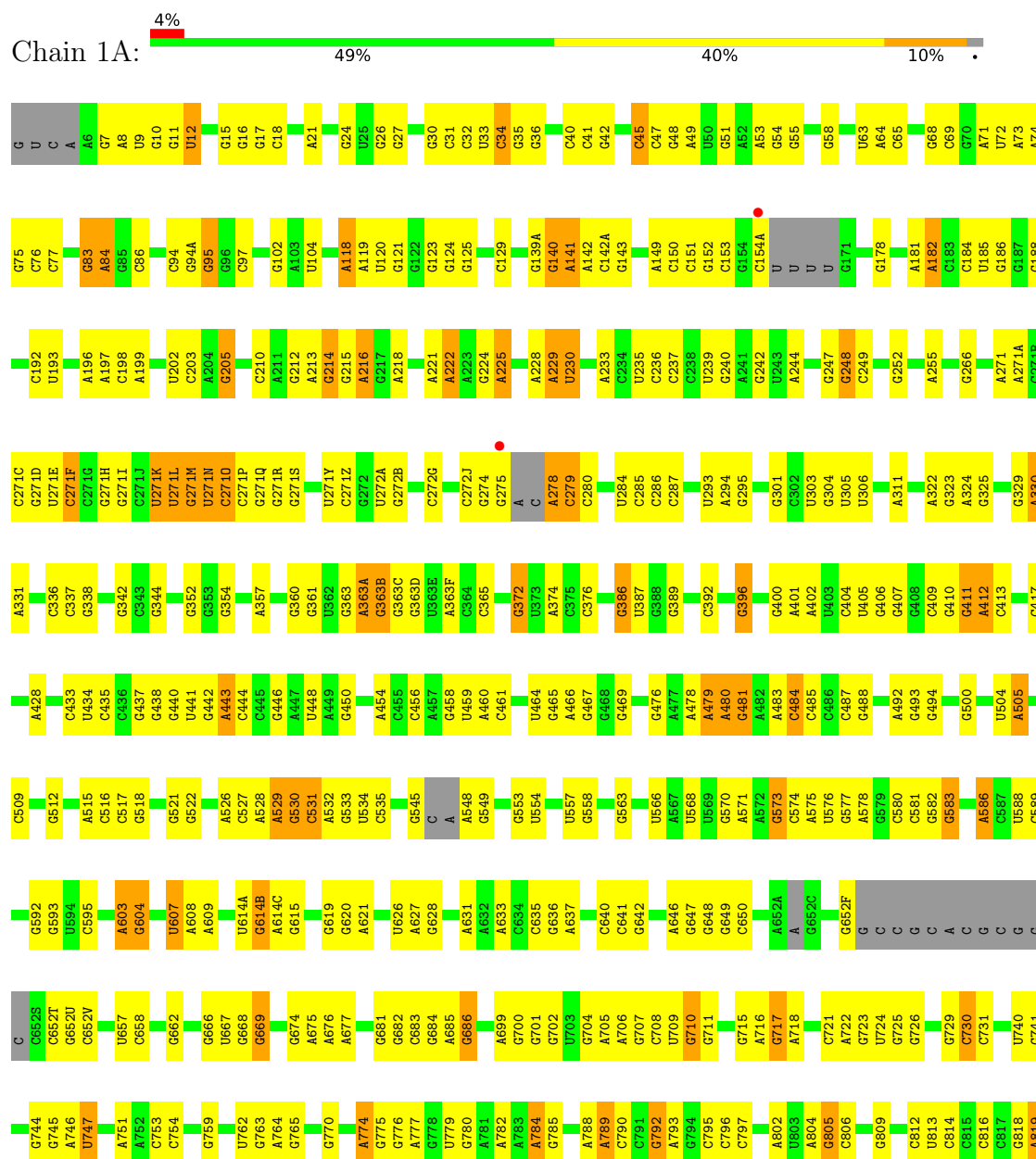
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	28	3	Total 3	O 3	0	0
62	29	1	Total 1	O 1	0	0
62	2a	267	Total 267	O 267	0	0
62	2c	1	Total 1	O 1	0	0
62	2d	1	Total 1	O 1	0	0
62	2f	1	Total 1	O 1	0	0
62	2j	3	Total 3	O 3	0	0
62	2l	6	Total 6	O 6	0	0
62	2o	1	Total 1	O 1	0	0
62	2p	2	Total 2	O 2	0	0
62	2t	2	Total 2	O 2	0	0
62	2v	2	Total 2	O 2	0	0
62	2w	3	Total 3	O 3	0	0
62	2x	6	Total 6	O 6	0	0
62	2y	8	Total 8	O 8	0	0

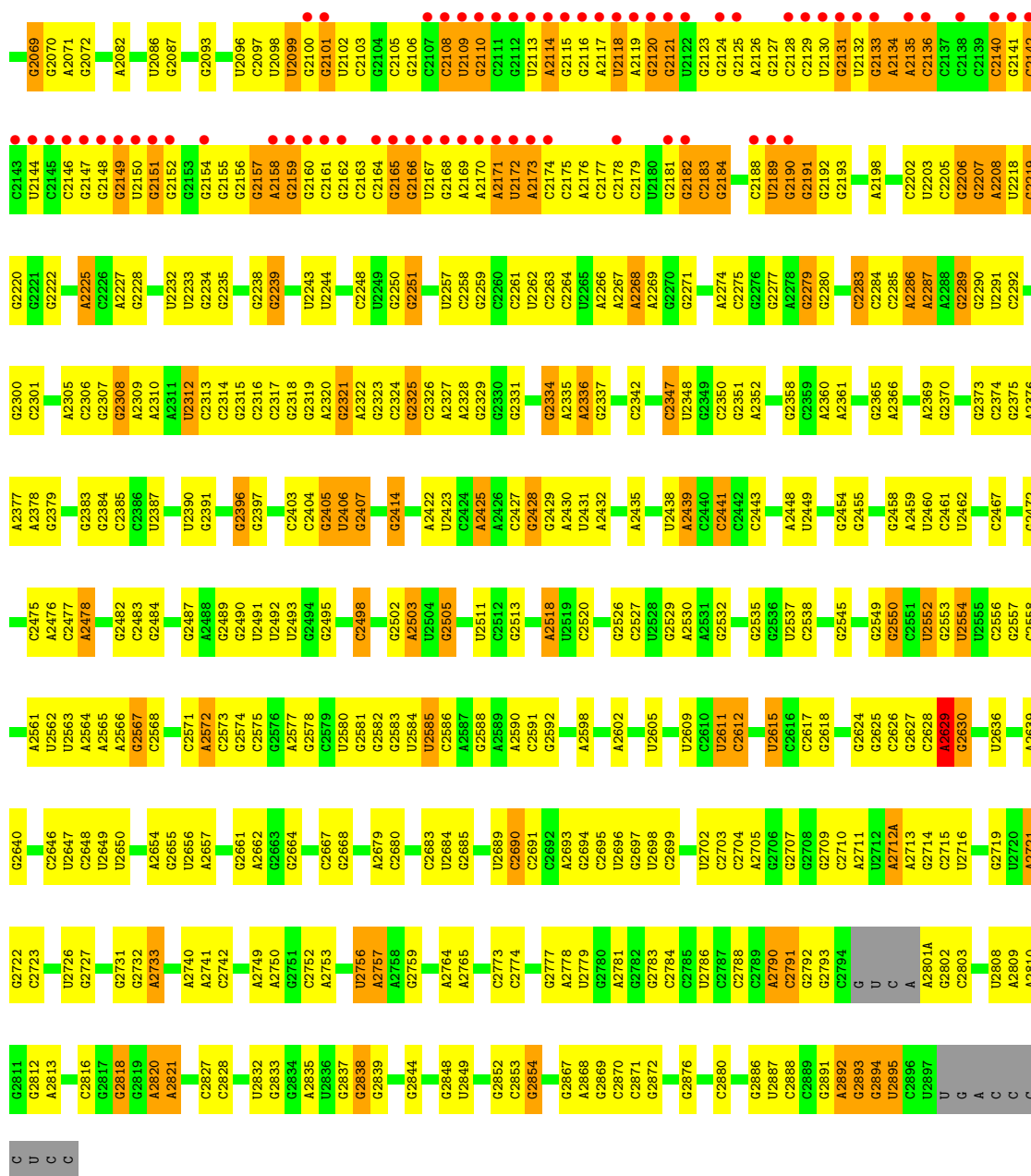
3 Residue-property plots

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

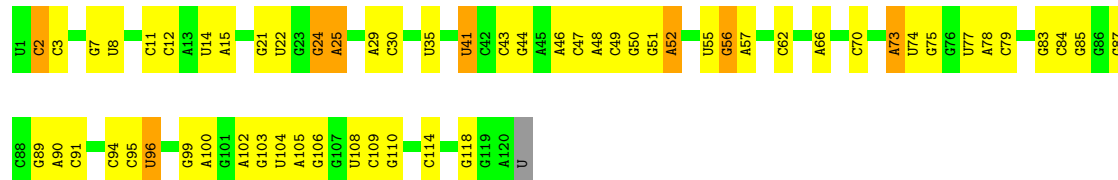


A1971	A1889	C1782	A1669	G1568	A1477	G1388	A1213	A1128	U1066	C993	A900	A820
A1972	A1890	A1783	C1670	A1569	G1482	G1389	C1224	A1129	A1067	C994	A901	A821
G1985	G1891	A1784	U1673	A1570	G1484	U1312	G1225	U1130	A1068	C995	A902	A824
A1986	C1892	A1785	G1674	A1571	G1485	U1313	G1226	U1131	A1069	A996	C902	A824
G1999	G1899	A1786	C1675	A1572	G1486	C1314	U1229	U1132	A1070	C997	C904	C825
A1900	A1900	G1676	U1676	U1578	G1487	U1315	G1230	U1133	A1071	C998	U907	U826
U1991	U1991	A1676	G1677	A1579	G1488	C1399	G1230	G1135	C1072	U999	U907	U827
G1903	G1903	C1790	U1680	A1580	G1489	G1400	G1230	G1136	A1073	A1000	U828	U828
C1904	C1904	A1791	U1681	G1581	A1490	G1401	G1236	G1137	G1074	G1003	A910	A829
G1905	G1905	U1794	G1682	A1583	C1493	C1403	G1236	U1138	C1075	C912	A910	A830
G1906	G1906	C1795	G1683	A1584	A1494	C1404	G1237	G1139	C1076	C912	C912	A831
C1908	C1908	U1796	C1684	A1586	A1495	U1405	A1237	C1140	A1077	U913	U913	U839
U1911	U1911	G1797	C1685	A1587	A1496	U1406	G1238	U1141	U1078	C1005	C914	U839
A1912	A1912	U1798	C1686	A1588	U1497	U1407	G1239	U1142	C1079	C1006	C915	C840
A1913	A1913	G1799	G1687	C1589	U1497	U1408	U1240	U1143	C1080	C1007	C915	C840
C1914	C1914	U1800	G1688	U1590	C1502	C1409	U1240	A1142A	U1081	G1011	U922	A841
U1915	U1915	G1801	U1688	G1593	G1503	C1410	G1244	A1143	U1082	G1012	C923	A842
A1916	A1916	A1802	U1689	G1594	C1504	G1411	G1244	G1144	U1083	U1012	C923	A842
U1917	U1917	C1804	U1690	G1595	G1604	A1412	G1248	U1148	U1084	A1020	G931	C846
A1918	A1918	U1805	G1696	C1599	A1508	C1413	U1249	A1149	A1085	A1021	G932	U847
A1919	A1919	C1806	U1700	C1599	C1509	G1416	G1250	C1150	G1087	U1022	G942	C848
C1920	C1920	C1806	A1701	A1603	A1509A	C1417	G1251	C1151	A1088	U1023	G942	A849
G1929	G1929	A1810	U1719	C1607	A1509B	G1418	G1252	C1153	G1089	G1024	A945	C856
C1930	C1930	G1811	G1720	A1608	C1511	U1420	A1254	A1156	U1090	U1025	G946	U858
G1931	G1931	A1812	G1721	C1609	C1512	G1421	G1256	C1161	C1092	U1026	G947	C859
C1934	C1934	G1813	G1722	A1610	C1513	G1422	U1255	C1162	G1093	A1027	U960	U860
G1935	G1935	U1814	U1738	A1616	G1514	G1426	U1256	G1163	U1094	A1028	C950	A861
A1936	A1936	A1815	G1740	C1614	G1515	A1427	C1261	G1164	A1095	U1033	C951	A862
C1937	C1937	G1816	G1741	C1615	U1518	C1428	G1264	U1165	A1096	G1036	C954	C865
A1938	A1938	U1817	A1741	A1616	G1519	G1429	A1265	C1166	U1097	G1037	C955	C865
U1939	U1939	C1818	G1742	C1617	G1520	C1430	G1266	U1167	A1098	C1038	C956	A866
A1940	A1940	U1819	U1745A	A1618	G1523	C1431	U1267	G1170	G1099	G1039	A957	U871
C1941	C1941	G1823	G1746	C1622	U1527	U1432	A1268	G1171	U1101	C1040	U958	U871
C1942	C1942	C1827	U1749	G1628	A1528	A1434	G1270	G1173	C1102	G1041	A959	G875
G1945	G1945	A1829	G1750	C1628	A1528A	G1435	G1271	A1174	C1104	G1043	A960	C876
U1946	U1946	C1837	C1754	A1634	G1532	A1439	A1272	U1175	U1105	C1043	C961	U877
C1947	C1947	U1837	G1755	G1635	U	G1441	U1273	G1176	U1106	A1045	C962	A878
U1951	U1951	A1847	G1756	C1635	A	G1442	U1279	A1177	G1107	A1046	U963	C879
U1955	U1955	G1850	U1759	A1641	C	A1445	G1279	C1178	U1108	G1047	C964	G881
C1956	C1956	U1851	A1760	G1642	G1537	C1445A	G1280	C1180	C1109	A1048	U969	G882
G1957	G1957	C1852	C1761	G1647	G1538	C1446	G1283	G1187	G1112	G1051	C970	G883
C1958	C1958	U1852	G1762	C1648	G1539	U1372	G1283	U1188	G1113	C1052	C971	C884
G1959	G1959	G1860	G1763	G1649	U1540	G1447	A1286	U1189	U1114	C1053	C972	C885
C2055	C2055	G1861	G1764	G1650	G1541	C1374	A1287	G1190	G1115	A1054	A973	C886
G2056	G2056	C1866	U1773	G1651	U1453	C1375	U1292	G1191	C1116	G1055	G974	A887
A2059	A2059	C1866	A1774	A1652	G1455	C1376	C1293	G1192	G1117	G1056	C975	C888
C2060	C2060	A1876	C1774	G1655	G1466	A1379	G1293	G1193	C1118	A1057	G975A	C889
G2061	G2061	G1877	U1775	C1656	C1467	G1380	C1297	G1193	G1059	U	C976	A890
C1967	C1967	C1879	U1778	C1663	C1468	A1384	U1300	C1200	C1119	G1060	A981	C893
G1968	G1968	C1886	U1779	C1664	A1557	A1385	U1301	C1201	G1120	G1062	A983	U895
A1969	A1969	C1886	A1780	A1664	A1558	G1386	A1302	C1209	G1124	G1063	G989	A896
C2066	C2066	C1886	C1781	C1664	A1567	C1387	G1303	C1209	G1125	U1065	C992	C898
												A899

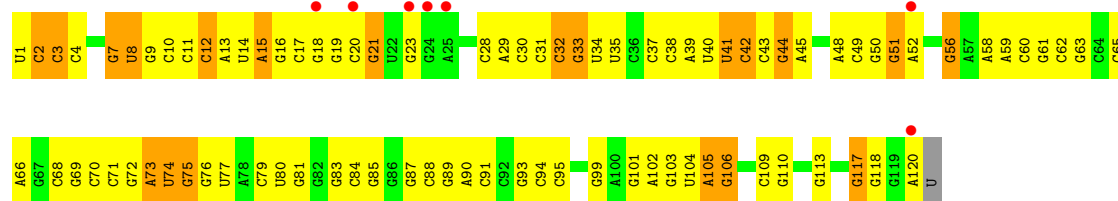




G1344	G1422	G1501	G1589	G1666	G1767	G1845	U1939	A2033	G2115	G2175	U2262	A2328	G2400
C1345	G1423	C1502	U1590	G1667	C1767	G1846	U1940	U2034	G2116	A2176	C2263	G2329	G2401
A1354	G1424	U1503	G1591	A1668	A1773	A1847	C1941	G2035	A2117	C2177	C2264	G2330	C2402
G1356	G1425	C1507	G1592	A1669	U1777	A1848	C1942	G2036	U2118	C2178	A2268	U2332	C2403
G1357	G1426	A1506	G1594	G1670	U1778	G1849	G1945	G2037	A2219	G2181	A2269	U2333	
G1358	A1427	A1508	G1595	U1671	U1779	U1851	U1946	C2040	G2120	C2182	A2273	G2334	U2406
A1359	C1428	A1509	A1596	G1674	A1780	C1852	G1954	U2041	G2121	C2183	A2274	A2335	G2407
A1360	G1429	A1509A	U1602	G1683	C1781	G1857	G1955	A2042	U2122	A2184	A2275	A2336	U2408
	U1431	A1510	G1603	C1684	C1782	G1858	U1956	C2044	G2123	C2185	G2276	G2337	G2409
	A1434		A1603	U1689	A1786	A1859	C1962		G2125	A2186	G2277	G2341	G2410
			U1517		A1787	G1860	U1963	G2049	A2126	C2187	C2188	C2342	A2411
			U1518		C1788	G1861	U1967	C2050	G2127	C2189	U2189	C2343	A2412
			U1519		A1789			A2051	C2128	G2190	G2191	U2344	G2413
			C1530		C1790	G1865	G1968	G2052	G2129	C2192	C2193	A2345	
			A1609		A1791	G1866	G1969	G2055	U2130	G2194	G2195	A2346	A2418
			C1532			A1876	A1970	G2056	G2131	C2196	C2197	A2347	U2419
			G1533		U1794	A1877	A1971		G2132	C2198	C2199	U2348	G2420
			U		C1795	G1878	A1981	A2062	G2133	C2199	A2286	G2349	G2421
			A		U1796		A1972	A2063	A2134	A2195	A2287	A2350	A2422
			C1536		U1797	G1883	G1973	G2061	A2135	C2196	A2288	G2351	U2423
			G1541		C1798			G2062	C2137	U2197	G2289	A2352	A2424
			A1542		U1798	G1884		A2064	C2138	A2198	G2290	A2353	A2425
			C1547		U1799	A1889	A1981	A2065	G2139	A2199	G2291	G2354	A2426
			U1550		C1800	G1890	G1985	C2064	C2140	C2202	A2286	G2355	C2427
			C1552		G1801			C2065	C2141	U2203	A2287	C2356	G2428
			G1557		A1802	C1893	C1990	C2066	G2142	U2204	A2288	G2357	G2429
			A1558		A1803	C1894	U1991		C2143	C2205	A2289	A2358	A2430
			G1559		C1804	G1895	G1992	G2069	U2144	G2206	A2290	A2359	U2431
			C1560		U1805	G1896	U1993	G2070	U2145	G2207	G2291	A2360	A2432
			G1561		U1808		C1994	A2071	C2146	A2208	G2292	G2361	A2433
			A1562		A1809	A1900	U1995		G2147	U2218	A2293	G2362	A2434
			A1563		A1810	A1901	C1996	G2079	G2148	G2219	G2299	A2366	A2435
			C1564		A1811	G1902	G1997		C2149	C2220	G2300	A2366	
			A1565		A1812	G1903	G1998	A2082	U2150	C2221	G2303	A2369	A2439
			C1566		G1813	G1904	C1999	G2083	G2151	A2224	A2304	G2370	G2440
			A1567		G1814	G1905	G2000	C2084	G2152	A2225	A2305	G2371	G2441
			U1570		A1815	G1906	A2001		G2153	C2226	C2306	G2372	C2442
			A1571		G1816			G2093	G2154	A2227	G2307	G2373	G2443
			C1572		C1744		C2006		G2155	G2228	G2308	G2374	G2444
			G1477		U1817	U1911	G2010	U2096	G2156	C2229	A2309	G2375	G2445
			G1478		U1818	A1912	G2011	C2097	U2157	G2237	A2310	A2376	A2448
			U1481		A1819	C1914	U2012	U2098	A2158	G2238	A2311	A2377	A2449
			U1489		U1820	U1915	G2012	U2099	G2159	G2239	U2312	A2378	A2450
			A1490		G1822	A1916	G2018	G2100	G2160	C2240	C2313	G2379	A2451
			A1580		G1823	U1917	A2019	G2101	C2161	A2241	G2314	C2380	
			C1581		G1824			G2102	G2162	G2242	G2315	G2383	G2454
			A1582		A1825		U2022	C2103	C2163	U2243	G2316	G2384	G2455
			C1583				G2023	G2104	G2164	U2244	G2317	C2385	G2456
			U1584		A1829		G2024	G2105	G2165	U2245	G2318	C2386	G2457
			A1586		U1833		G2025	G2106	G2166	U2246	G2319	A2387	G2458
			U1587		U1834		C2026	C2107	G2167		A2320	G2388	A2459
			C1588		G1761		G2027	C2108	G2168		G2321	A2389	U2460
			U1497		A1762		G2028	G2109	A2169		G2251	G2390	G2461
			A1498		G1763		G2029	G2110	G2170		G2252	U2391	U2462
			C1499		G1764		A2030	G2111	A2171		G2324	G2392	G2463
					C1765		A1936	G2112	U2172		G2325	A2392	G2464
					U1766		A1938	U2113	C2173		G2326	A2392	G2465
								A2114	C2174		A2327	C2395	G2466

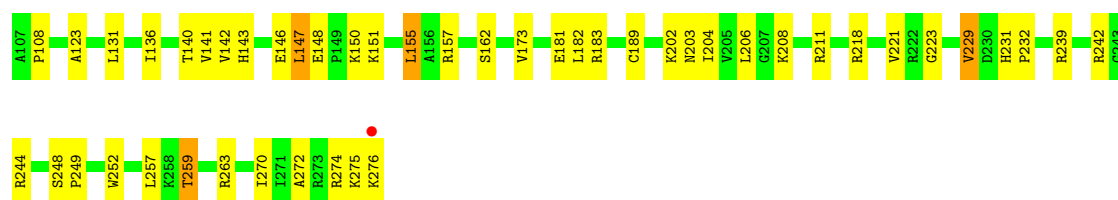


- Molecule 2: 5S Ribosomal RNA

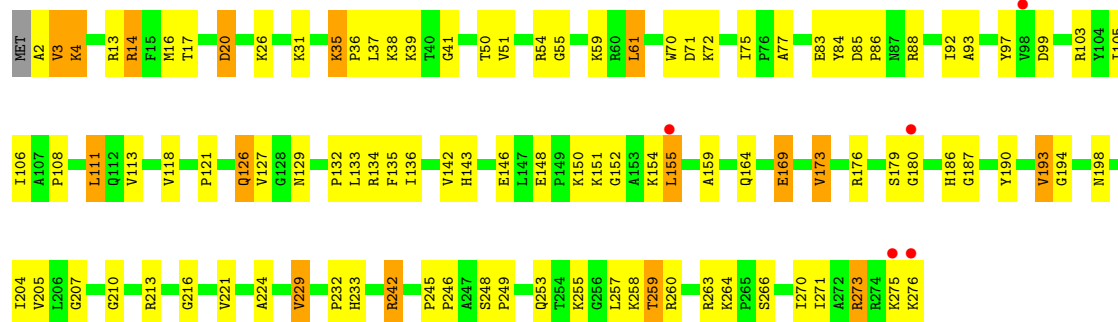


- Molecule 3: 50S ribosomal protein L2





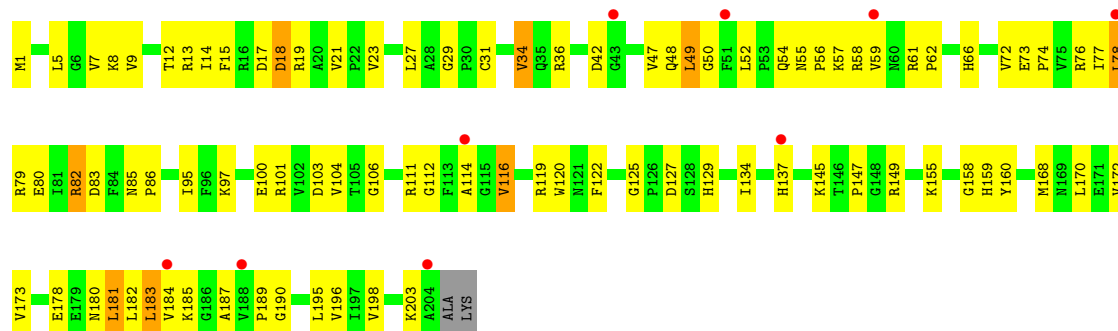
• Molecule 3: 50S ribosomal protein L2



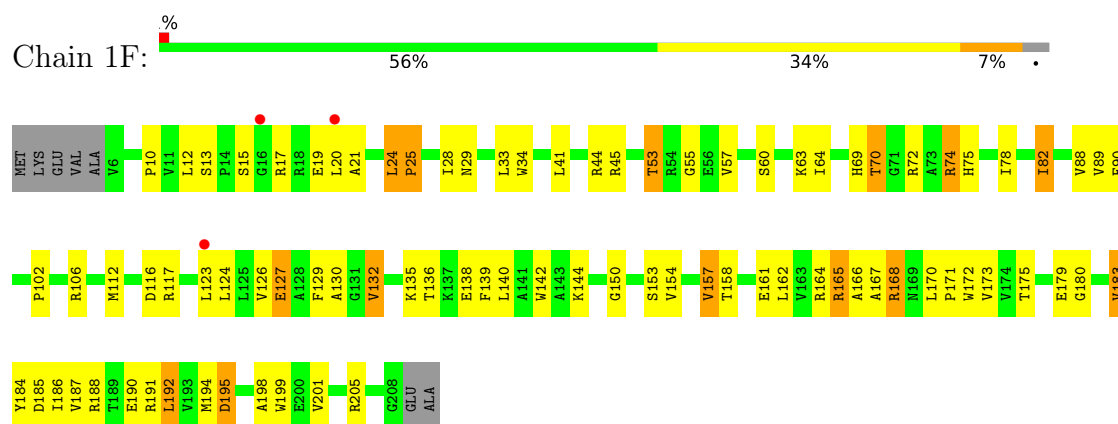
• Molecule 4: 50S ribosomal protein L3



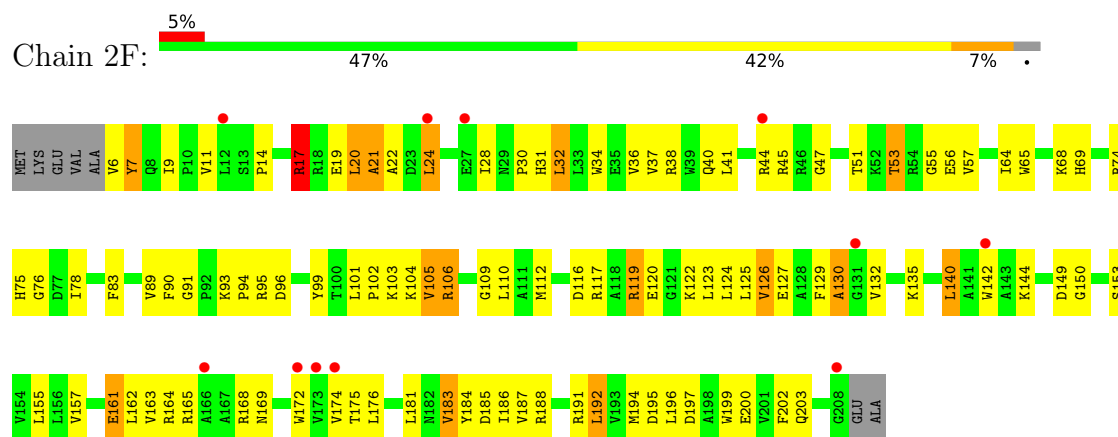
• Molecule 4: 50S ribosomal protein L3



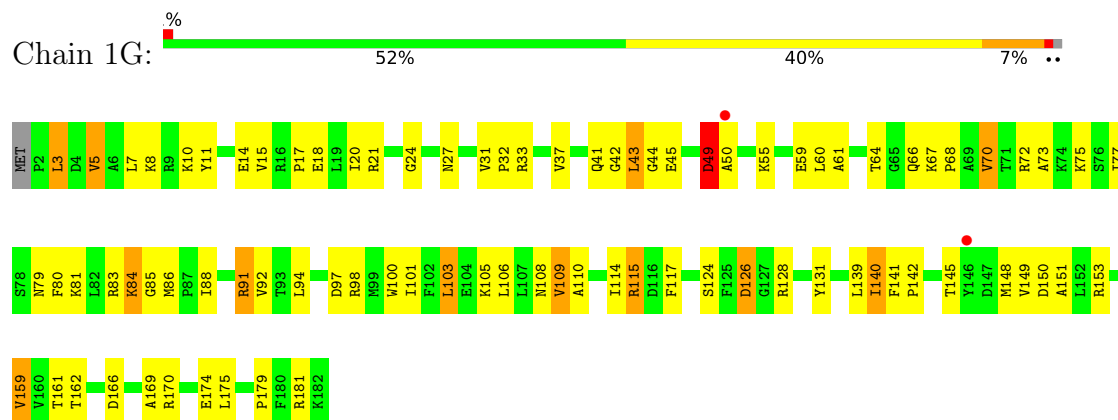
• Molecule 5: 50S ribosomal protein L4



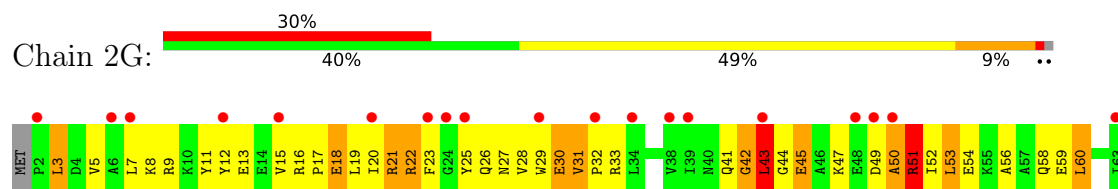
• Molecule 5: 50S ribosomal protein L4

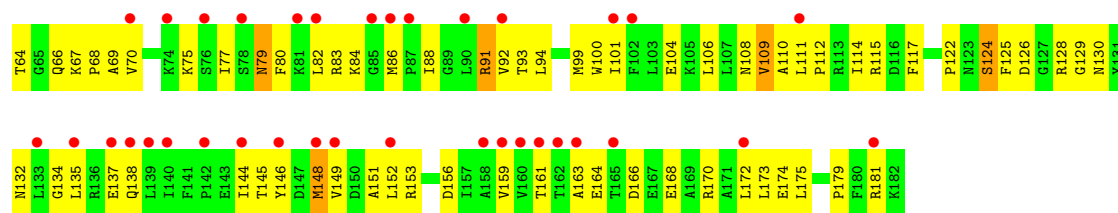


• Molecule 6: 50S ribosomal protein L5

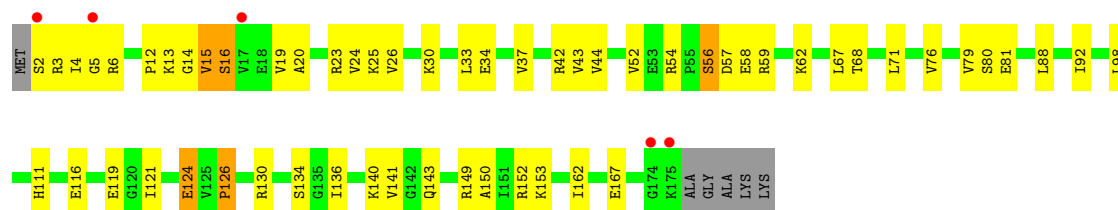


• Molecule 6: 50S ribosomal protein L5

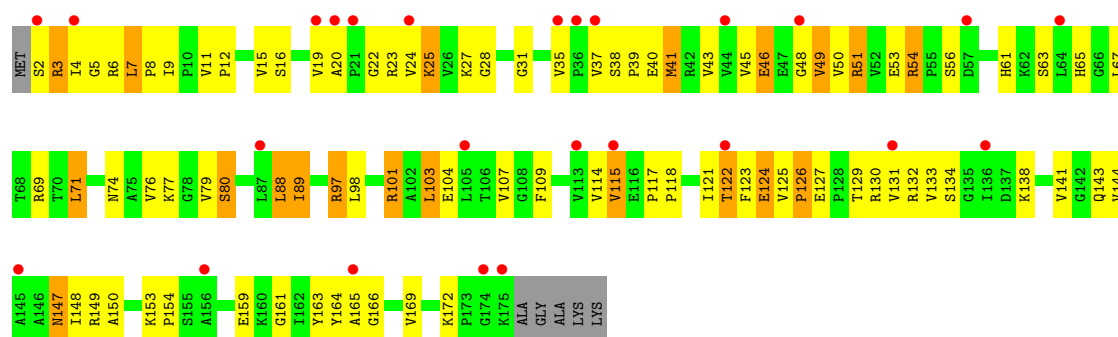




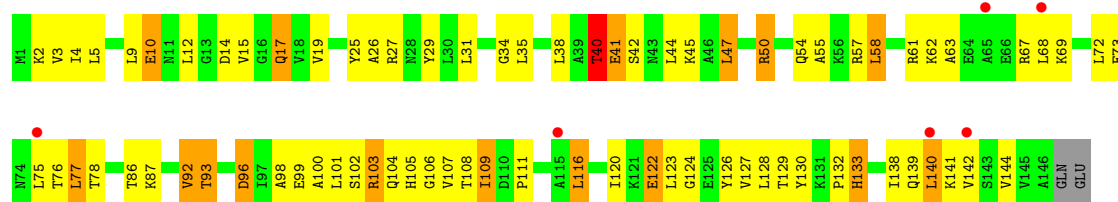
• Molecule 7: 50S ribosomal protein L6



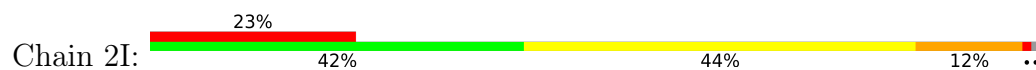
• Molecule 7: 50S ribosomal protein L6

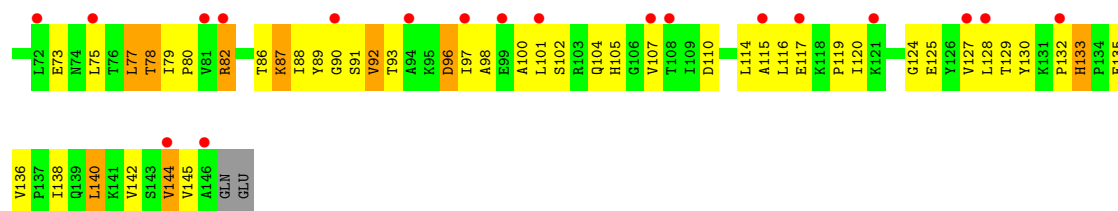


• Molecule 8: 50S ribosomal protein L9

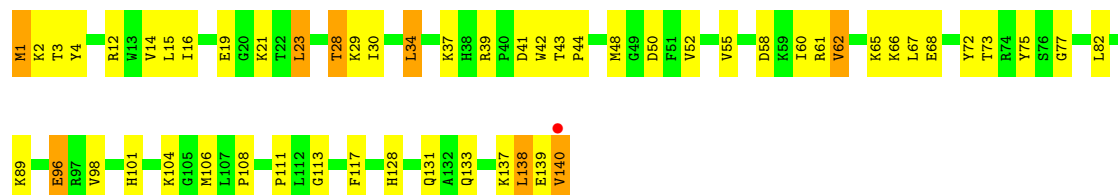


• Molecule 8: 50S ribosomal protein L9

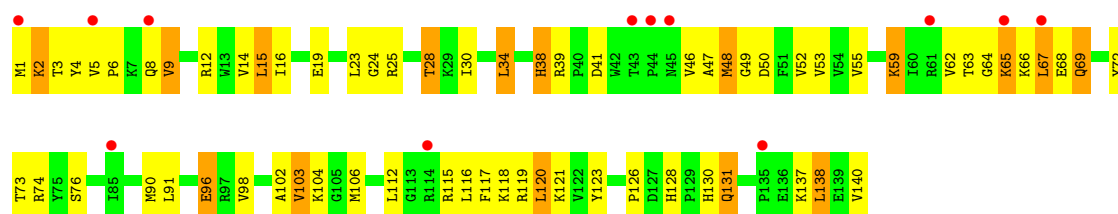




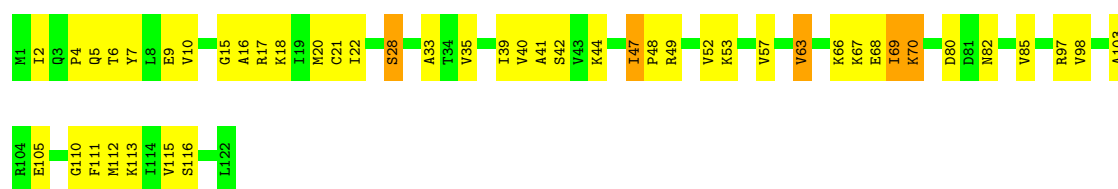
• Molecule 9: 50S ribosomal protein L13



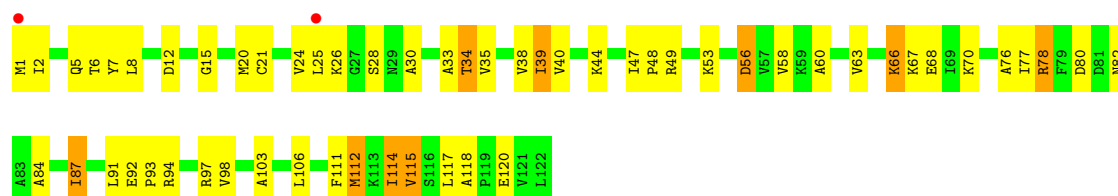
• Molecule 9: 50S ribosomal protein L13



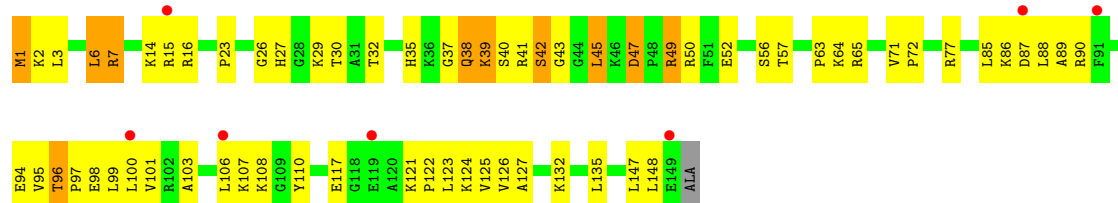
• Molecule 10: 50S ribosomal protein L14



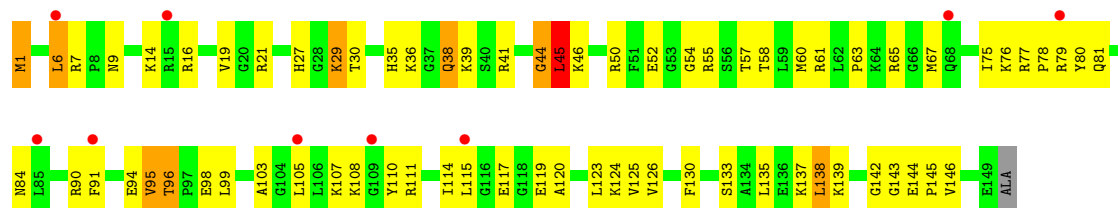
• Molecule 10: 50S ribosomal protein L14



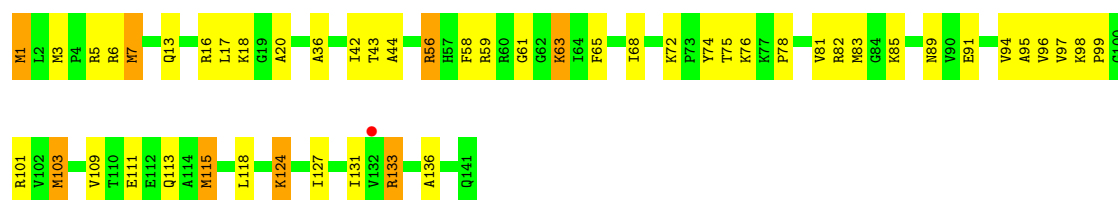
• Molecule 11: 50S ribosomal protein L15



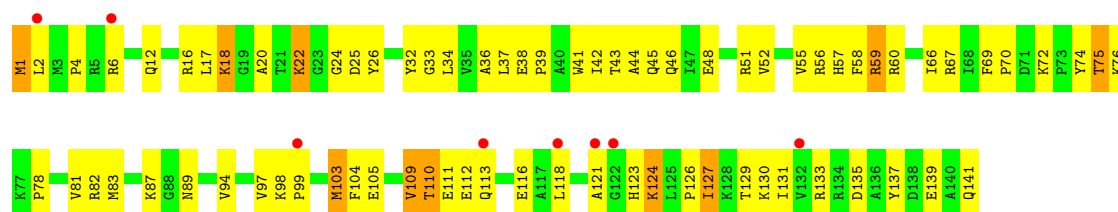
• Molecule 11: 50S ribosomal protein L15



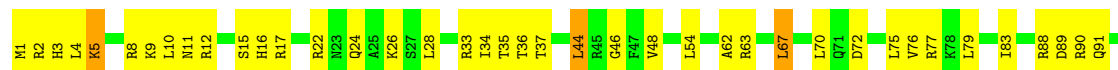
• Molecule 12: 50S ribosomal protein L16



• Molecule 12: 50S ribosomal protein L16

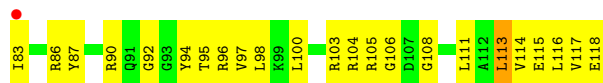


• Molecule 13: 50S ribosomal protein L17

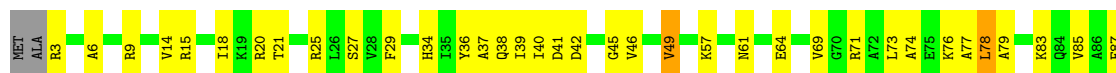




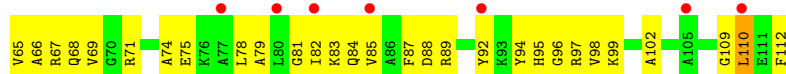
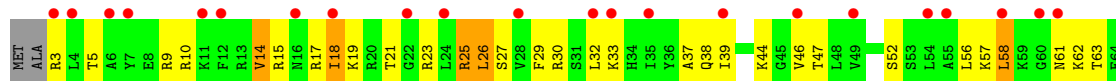
- Molecule 13: 50S ribosomal protein L17



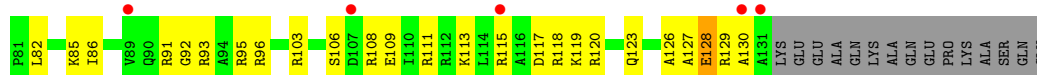
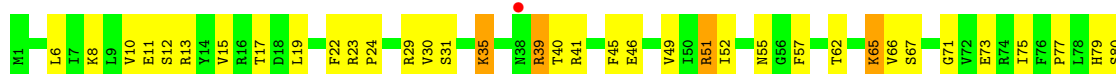
- Molecule 14: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L18

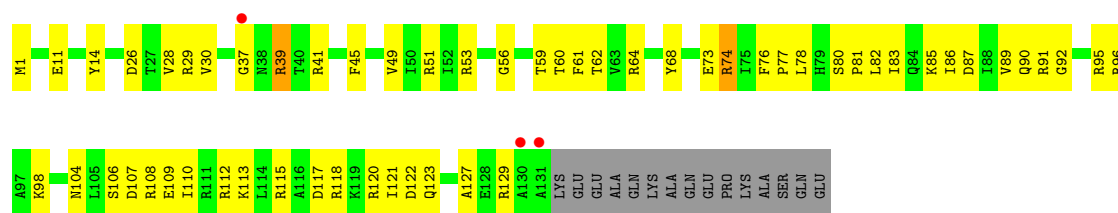


- Molecule 15: 50S ribosomal protein L19



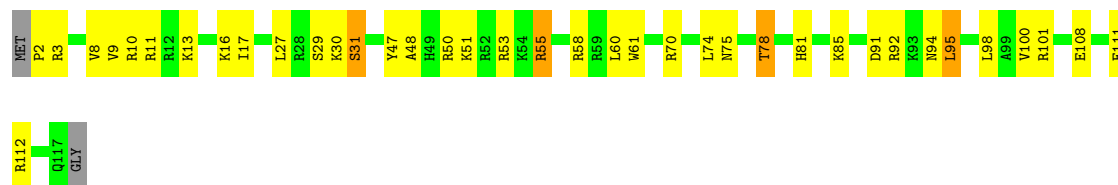
- Molecule 15: 50S ribosomal protein L19





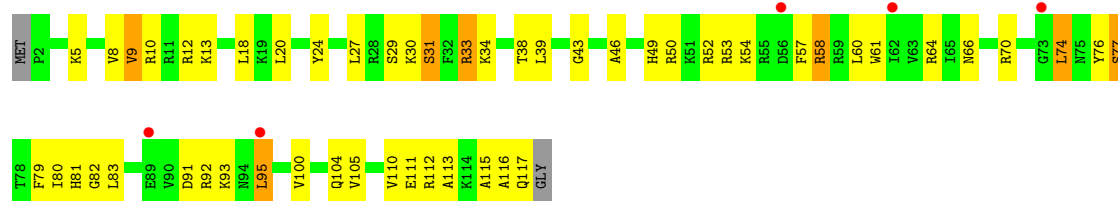
• Molecule 16: 50S ribosomal protein L20

Chain 1U: 66% 29% . .



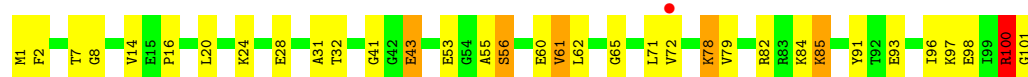
• Molecule 16: 50S ribosomal protein L20

Chain 2U: 4% 53% 39% 6% .



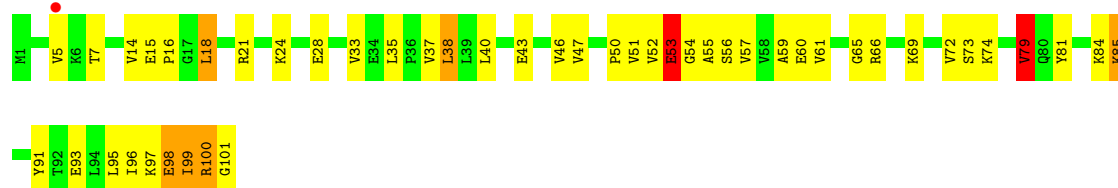
• Molecule 17: 50S ribosomal protein L21

Chain 1V: % 66% 28% 5% .



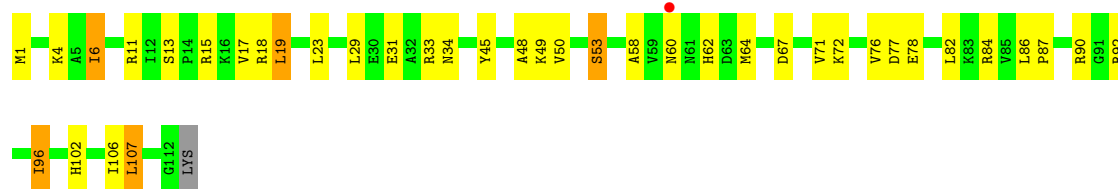
• Molecule 17: 50S ribosomal protein L21

Chain 2V: % 53% 39% 6% .

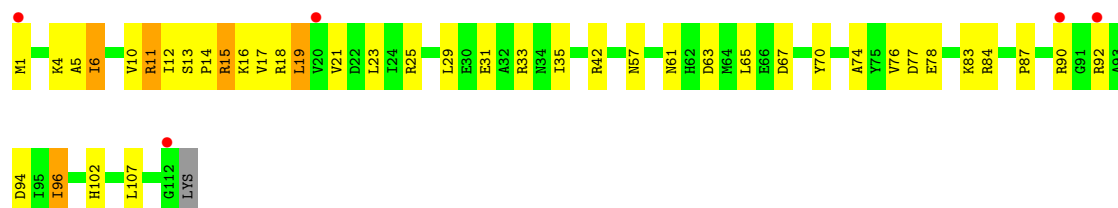


• Molecule 18: 50S ribosomal protein L22

Chain 1W: % 65% 30% . .



- Molecule 18: 50S ribosomal protein L22



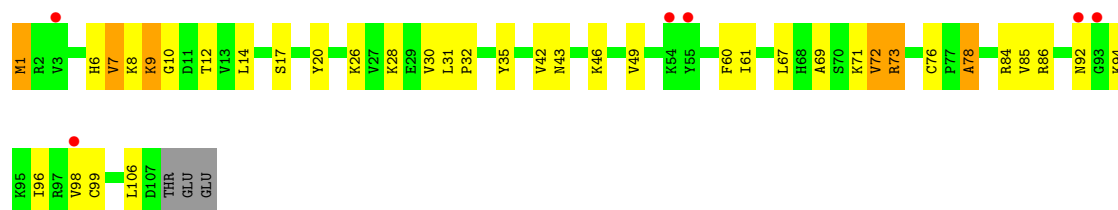
- Molecule 19: 50S ribosomal protein L23



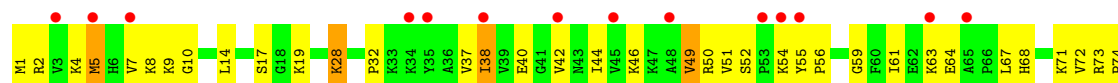
- Molecule 19: 50S ribosomal protein L23

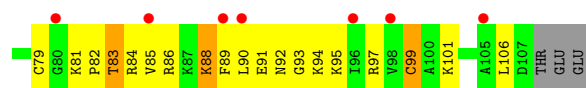


- Molecule 20: 50S ribosomal protein L24

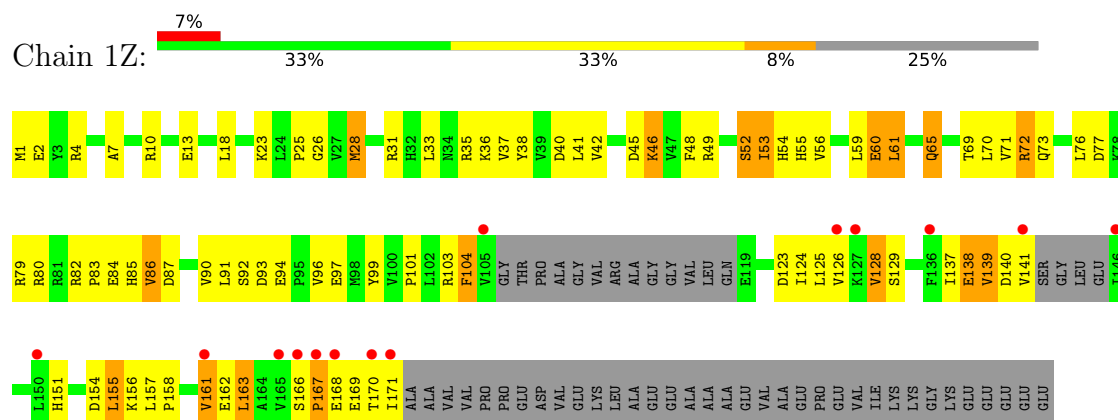


- Molecule 20: 50S ribosomal protein L24

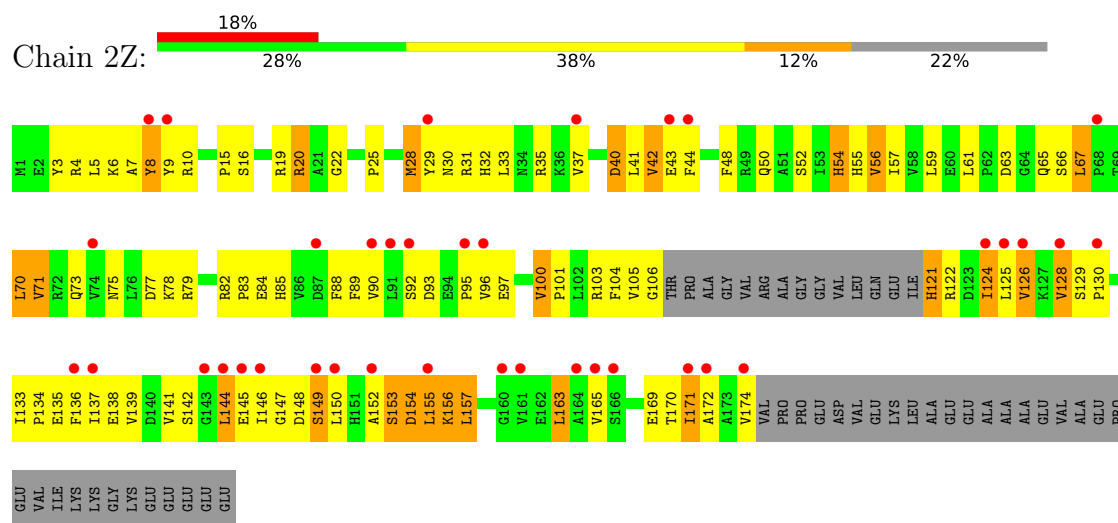




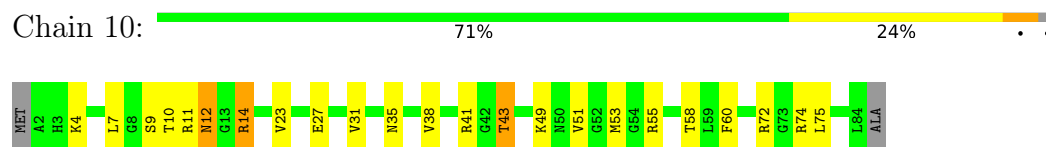
• Molecule 21: 50S ribosomal protein L25



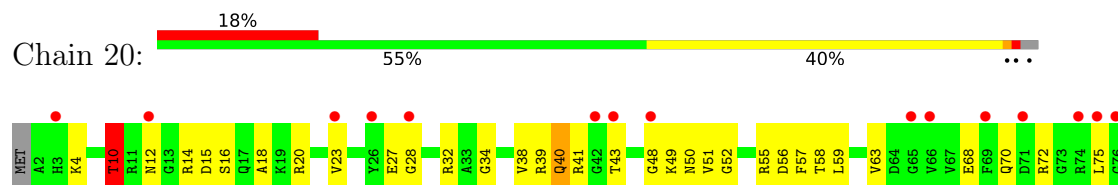
• Molecule 21: 50S ribosomal protein L25

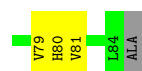


• Molecule 22: 50S ribosomal protein L27



• Molecule 22: 50S ribosomal protein L27

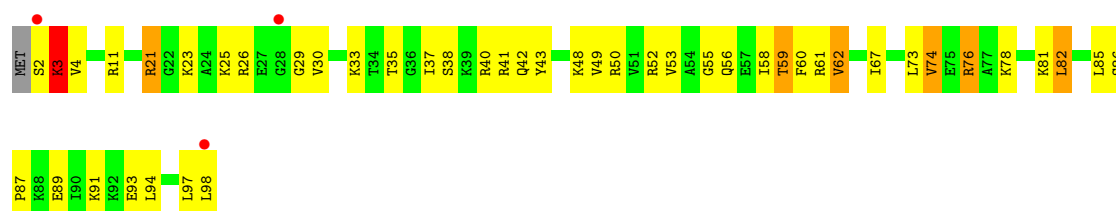




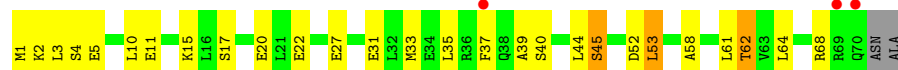
- Molecule 23: 50S ribosomal protein L28



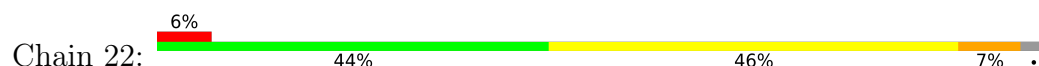
- Molecule 23: 50S ribosomal protein L28



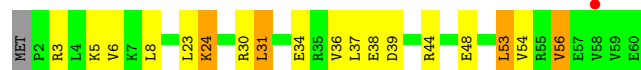
- Molecule 24: 50S ribosomal protein L29



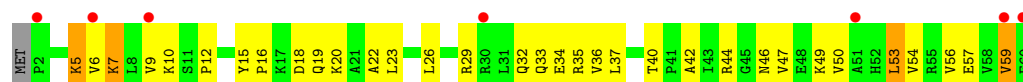
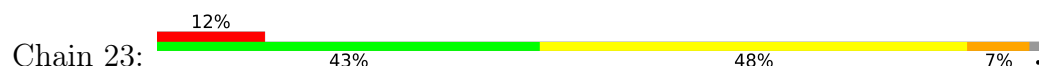
- Molecule 24: 50S ribosomal protein L29



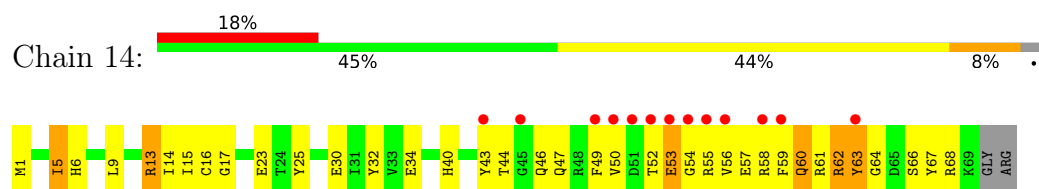
- Molecule 25: 50S ribosomal protein L30



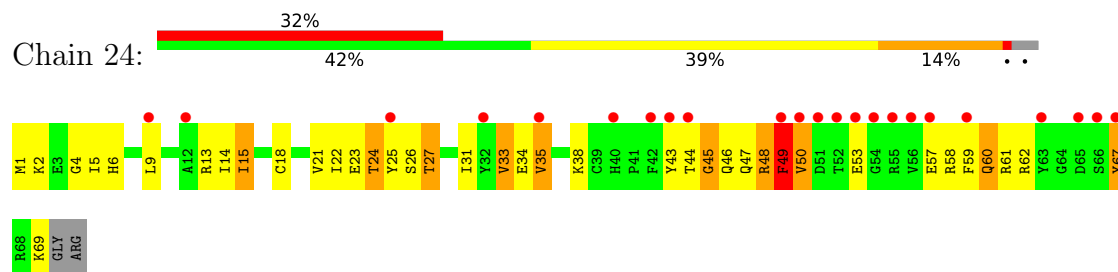
- Molecule 25: 50S ribosomal protein L30



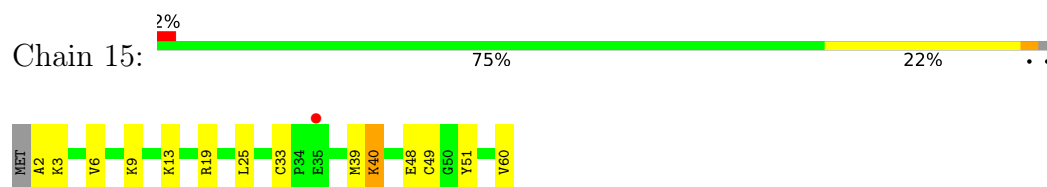
- Molecule 26: 50S ribosomal protein L31



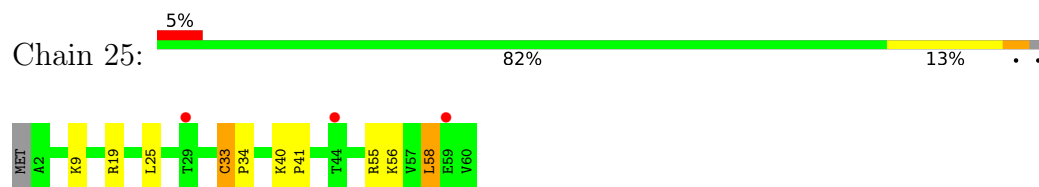
- Molecule 26: 50S ribosomal protein L31



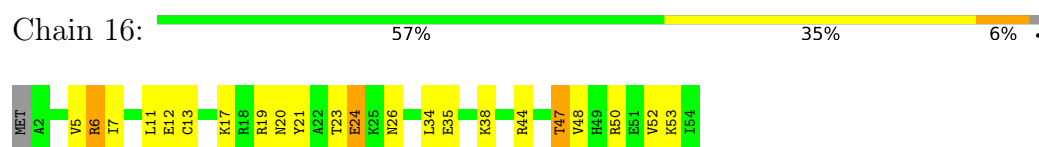
- Molecule 27: 50S ribosomal protein L32



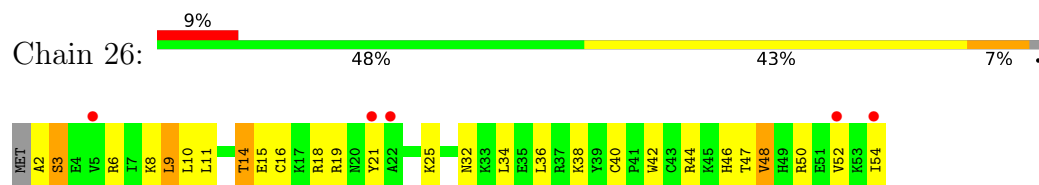
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33

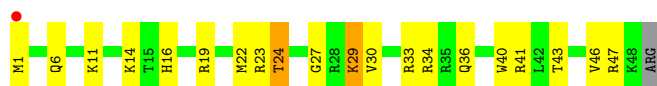


- Molecule 28: 50S ribosomal protein L33

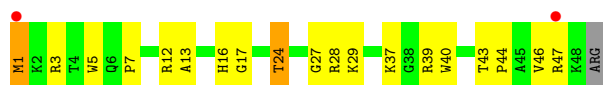


- Molecule 29: 50S ribosomal protein L34





- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



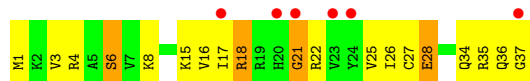
- Molecule 30: 50S ribosomal protein L35



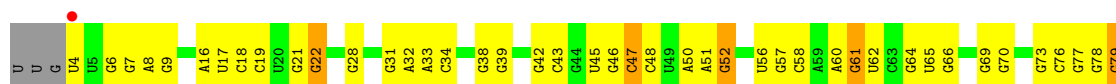
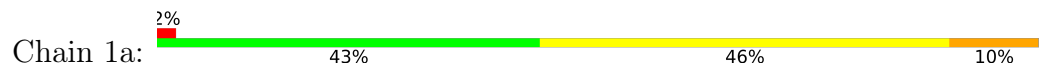
- Molecule 31: 50S ribosomal protein L36

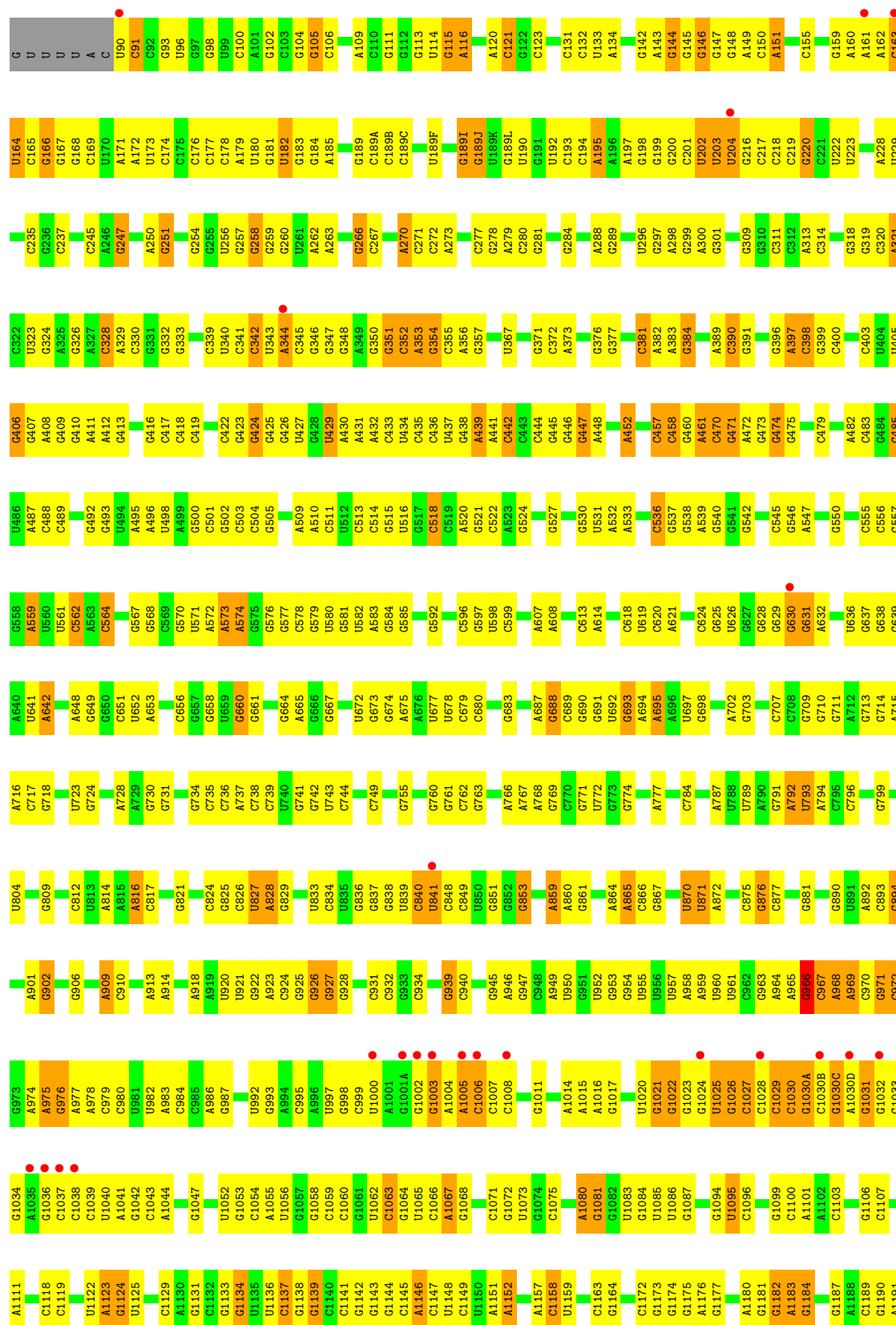


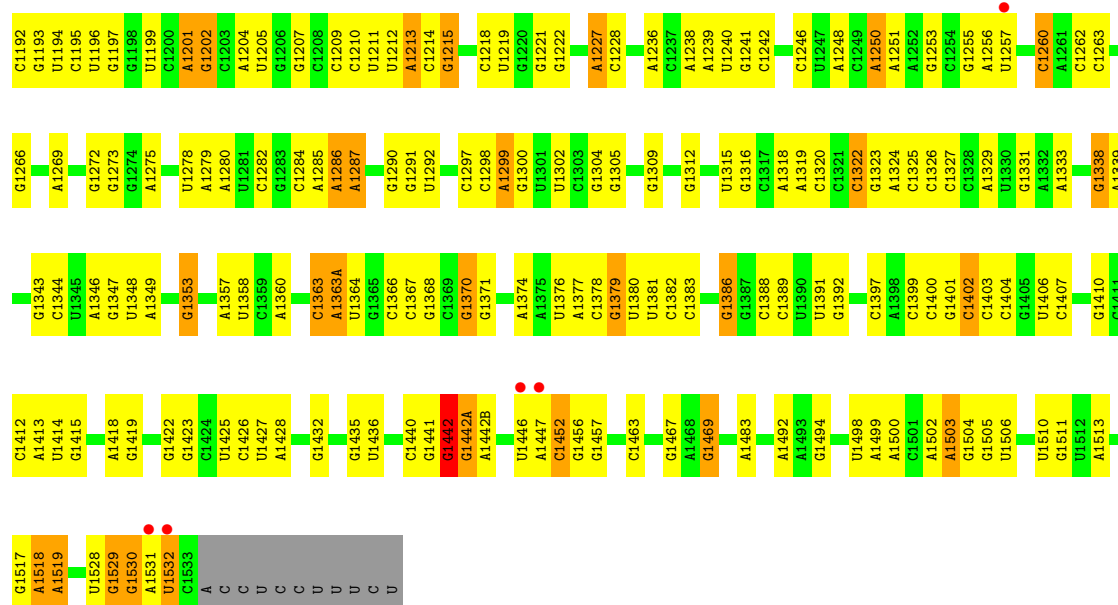
- Molecule 31: 50S ribosomal protein L36



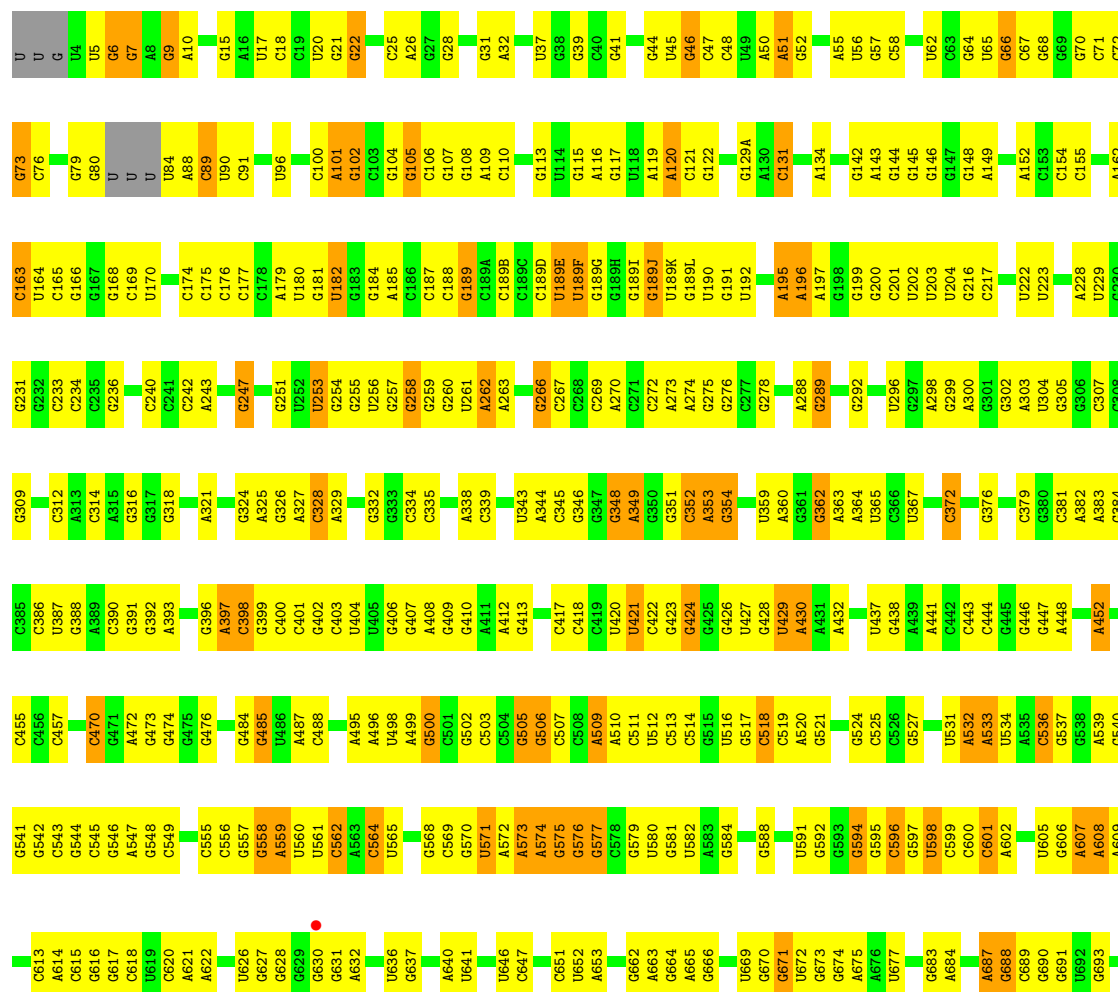
- Molecule 32: 16S Ribosomal RNA

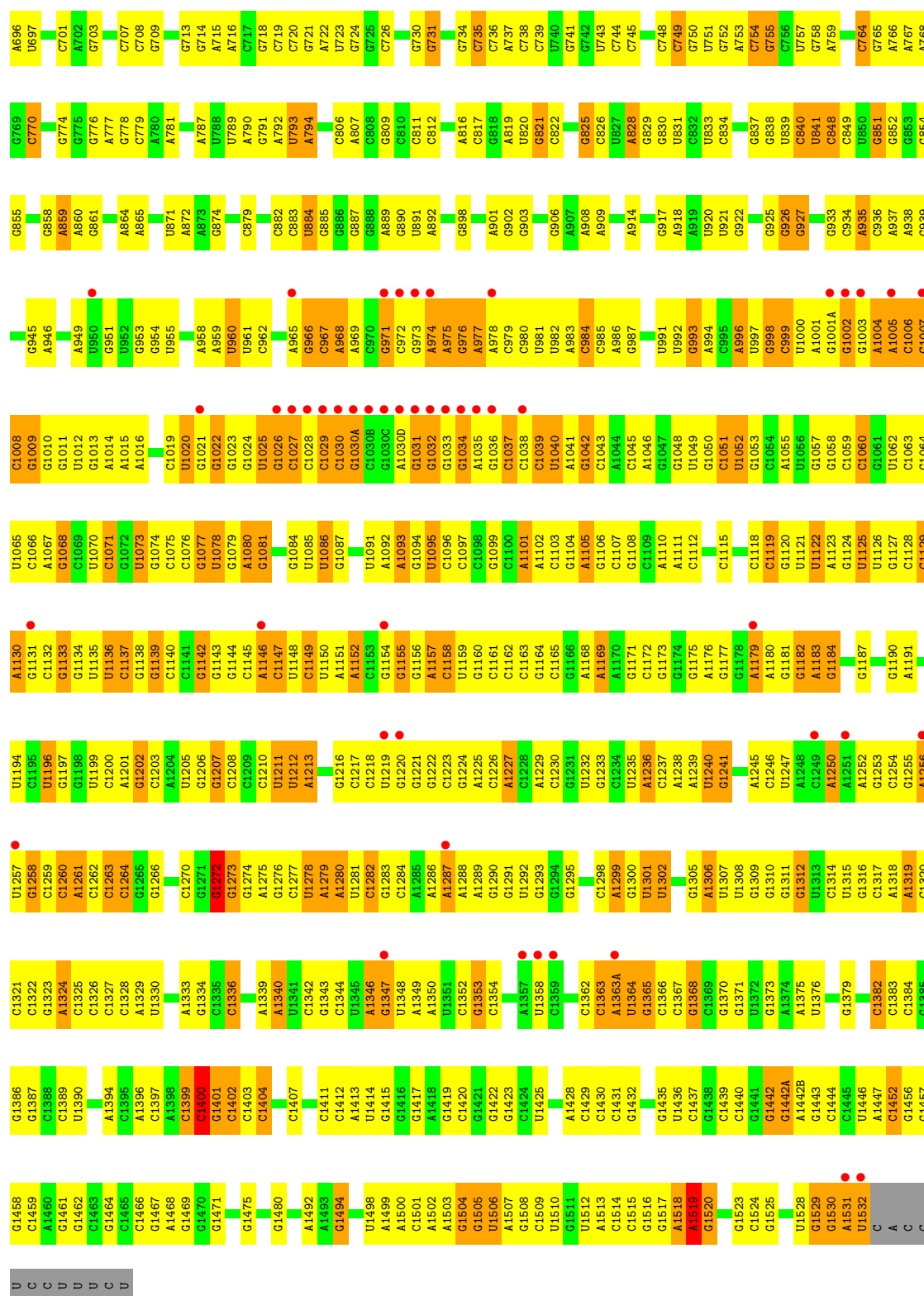


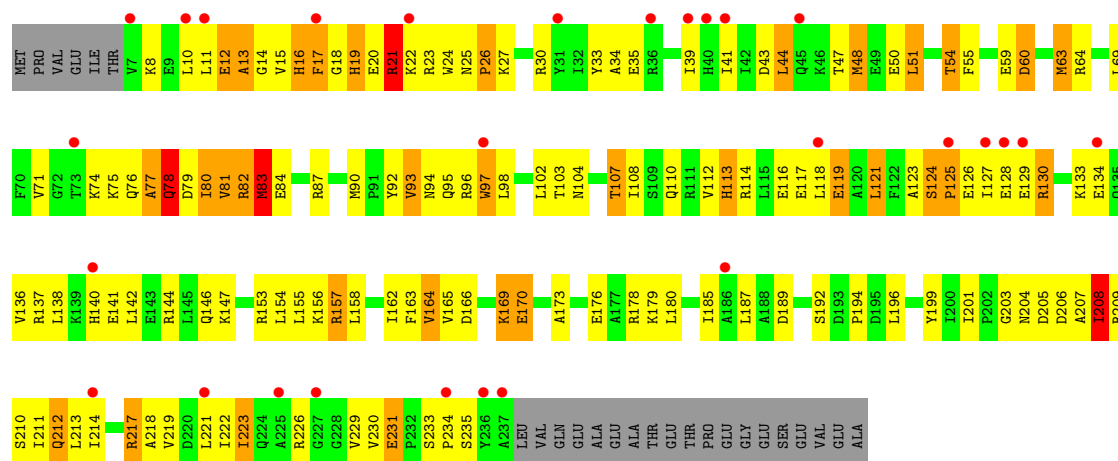




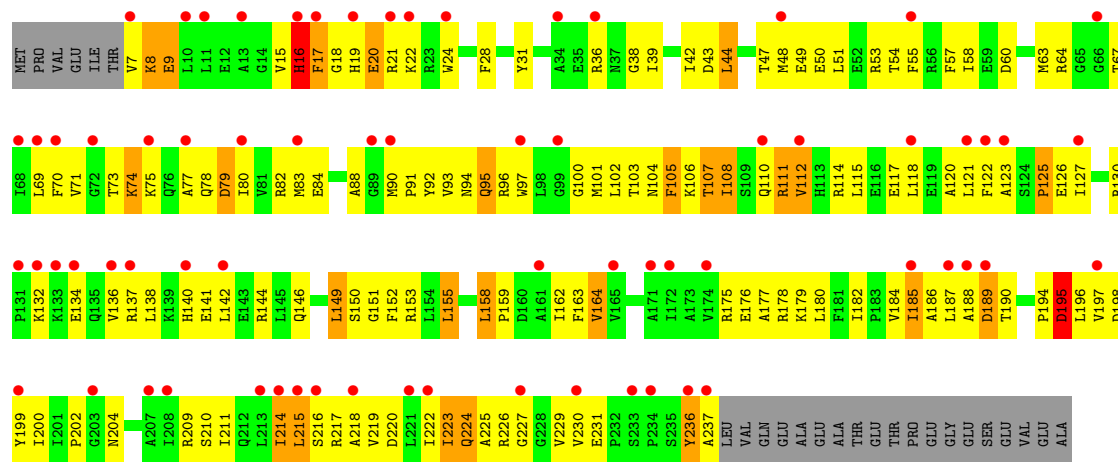
• Molecule 32: 16S Ribosomal RNA



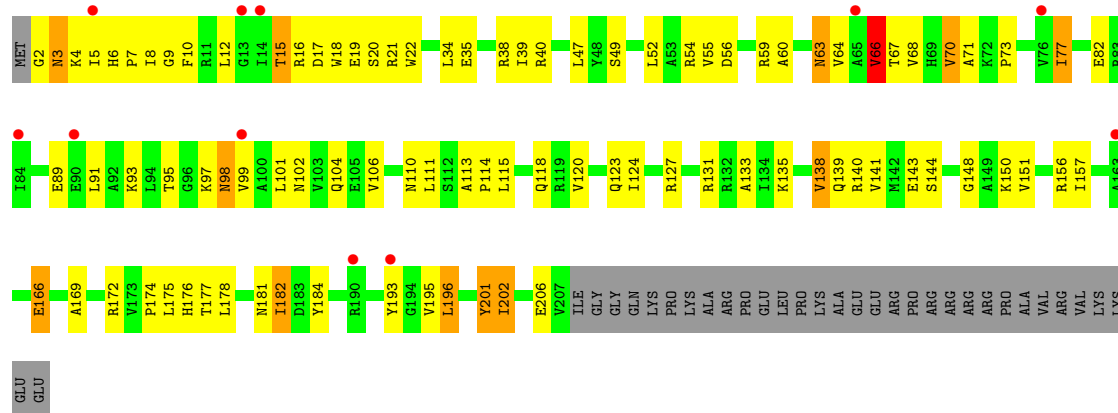




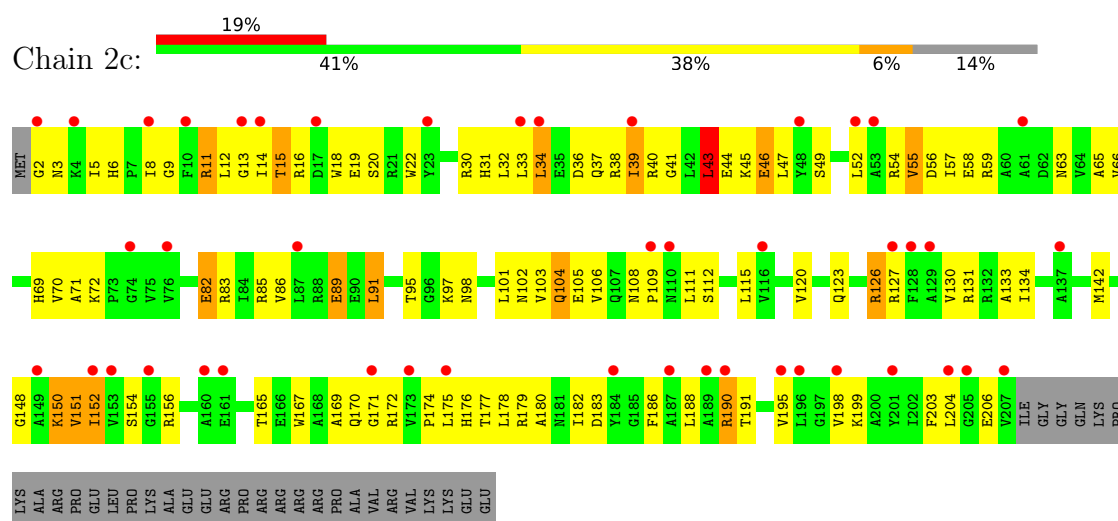
• Molecule 33: 30S ribosomal protein S2



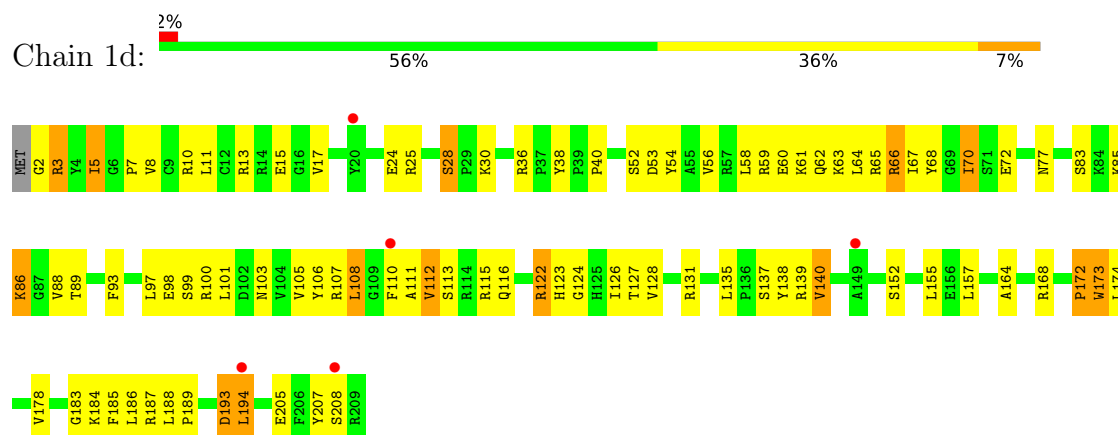
• Molecule 34: 30S ribosomal protein S3



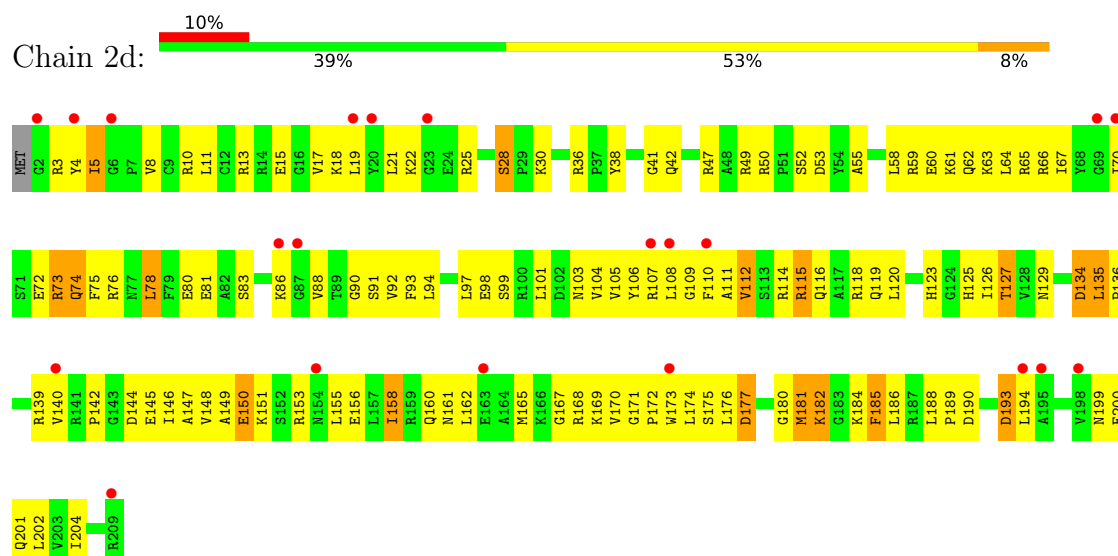
• Molecule 34: 30S ribosomal protein S3



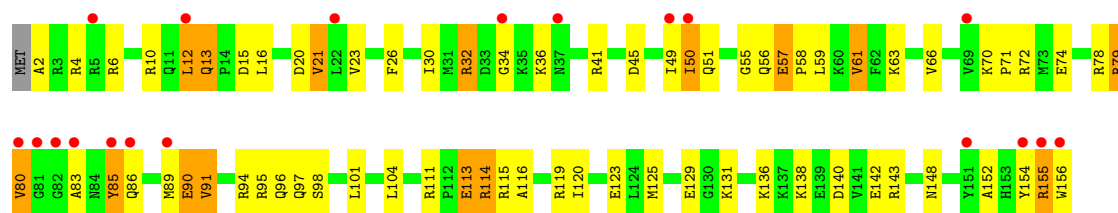
• Molecule 35: 30S ribosomal protein S4



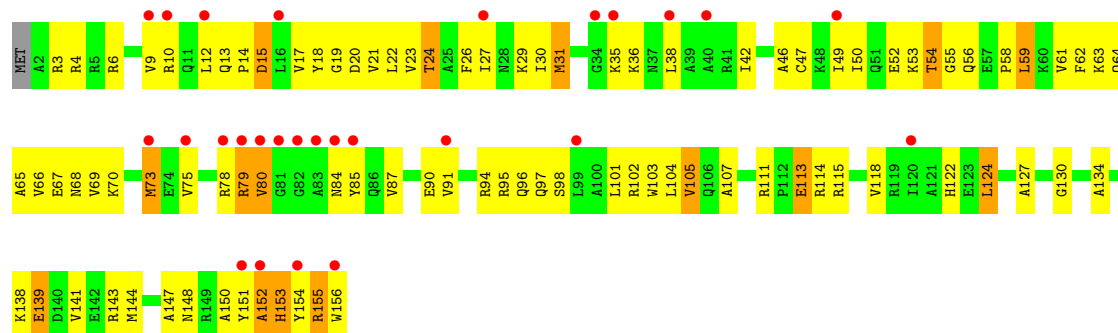
• Molecule 35: 30S ribosomal protein S4



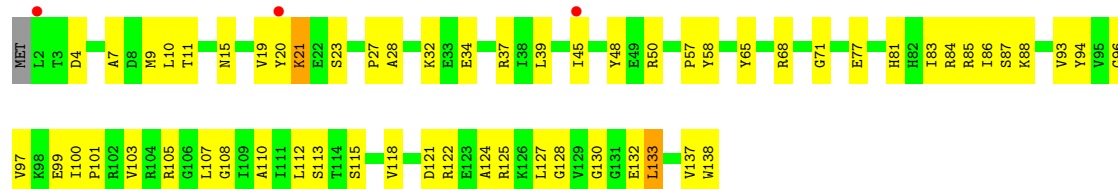
• Molecule 36: 30S ribosomal protein S5



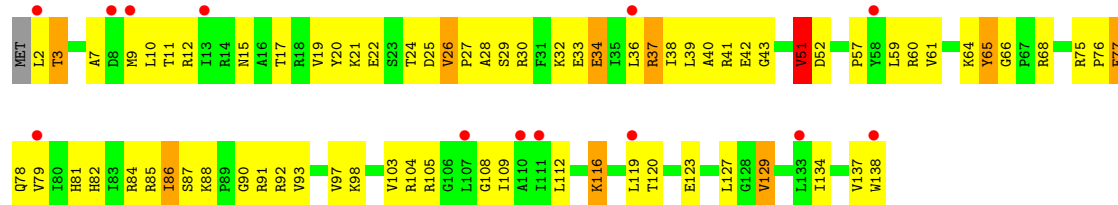
• Molecule 38: 30S ribosomal protein S7



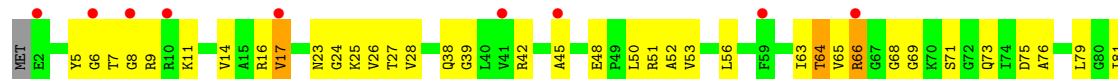
• Molecule 39: 30S ribosomal protein S8



• Molecule 39: 30S ribosomal protein S8

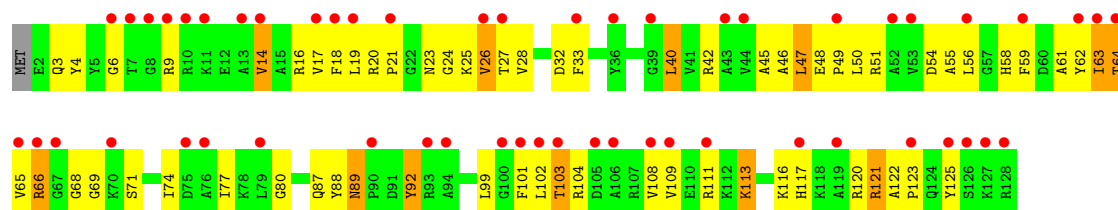
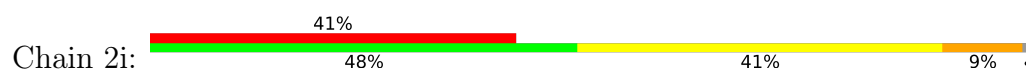


• Molecule 40: 30S ribosomal protein S9

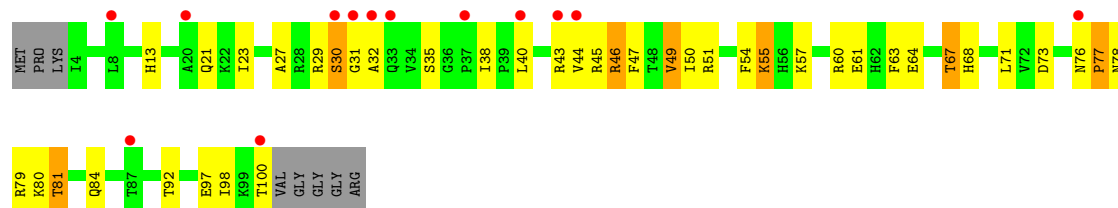




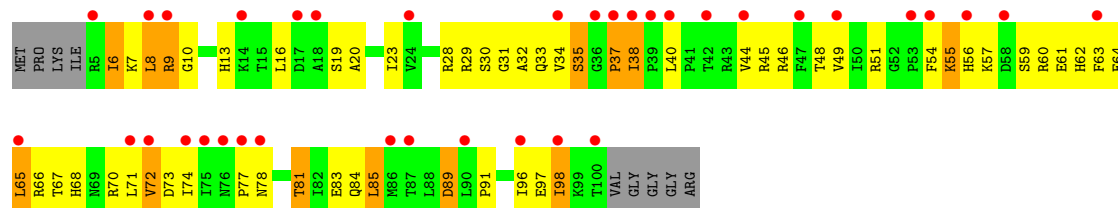
• Molecule 40: 30S ribosomal protein S9



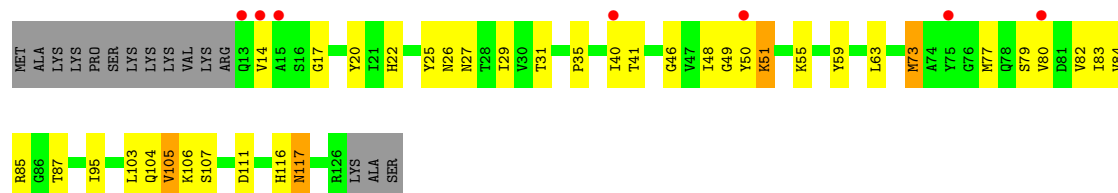
• Molecule 41: 30S ribosomal protein S10



• Molecule 41: 30S ribosomal protein S10



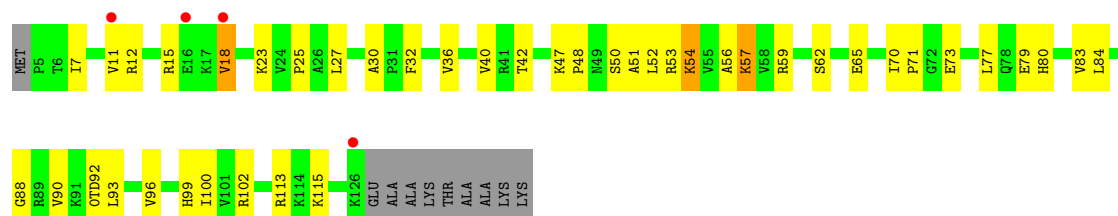
• Molecule 42: 30S ribosomal protein S11



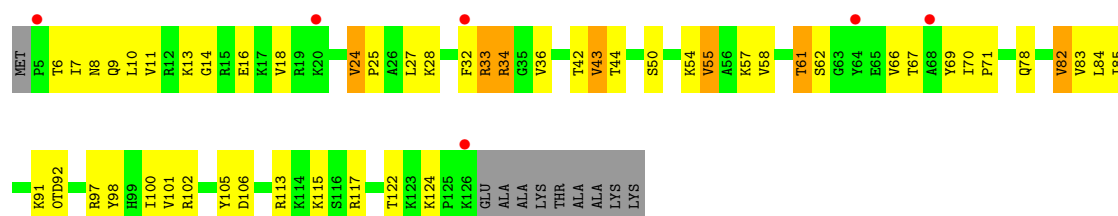
• Molecule 42: 30S ribosomal protein S11



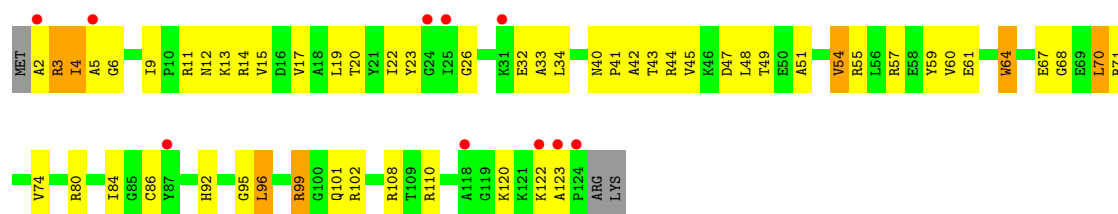
- Molecule 43: 30S ribosomal protein S12



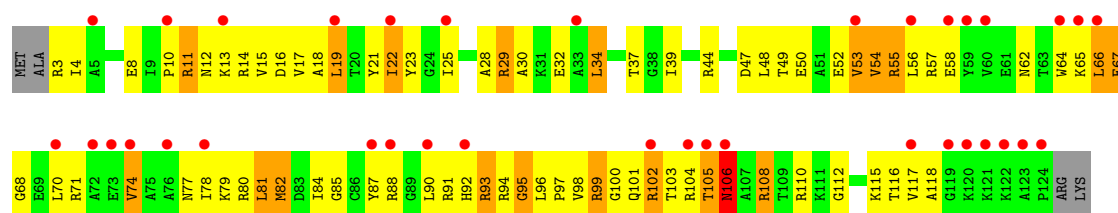
- Molecule 43: 30S ribosomal protein S12



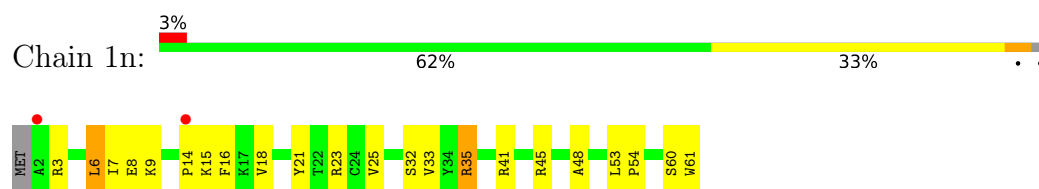
- Molecule 44: 30S ribosomal protein S13



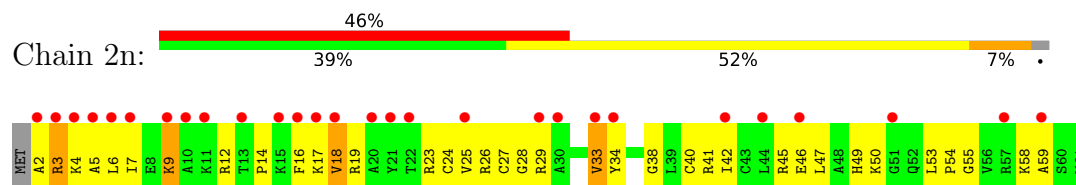
- Molecule 44: 30S ribosomal protein S13



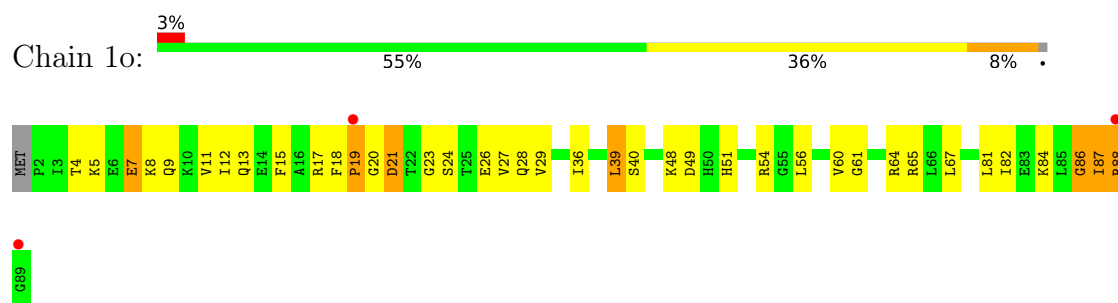
- Molecule 45: 30S ribosomal protein S14 type Z



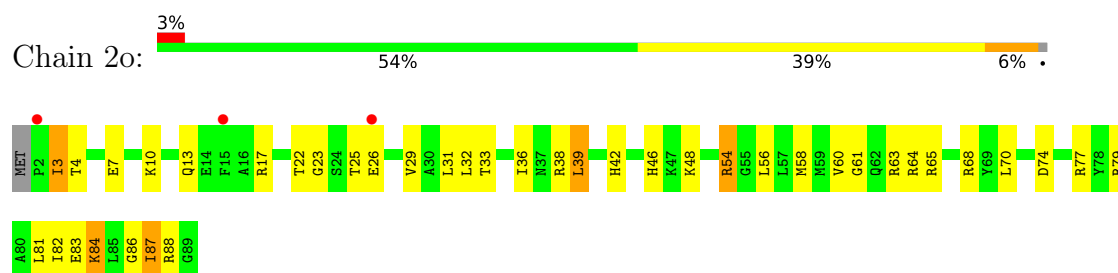
- Molecule 45: 30S ribosomal protein S14 type Z



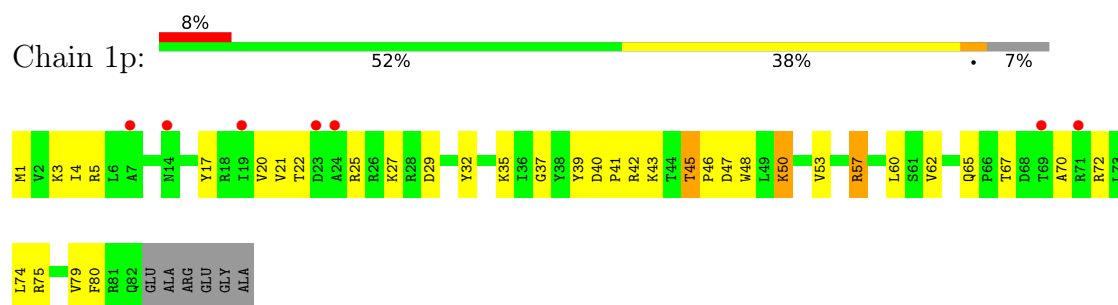
- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16

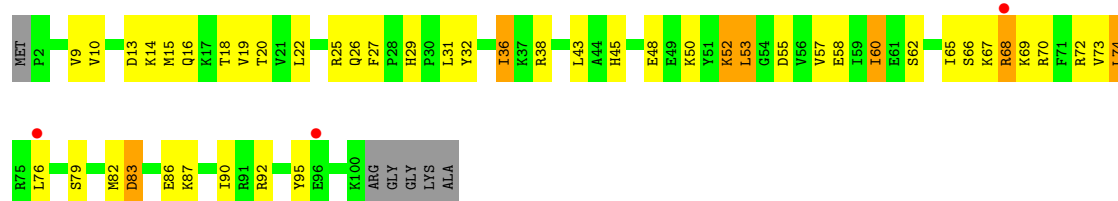


- Molecule 47: 30S ribosomal protein S16





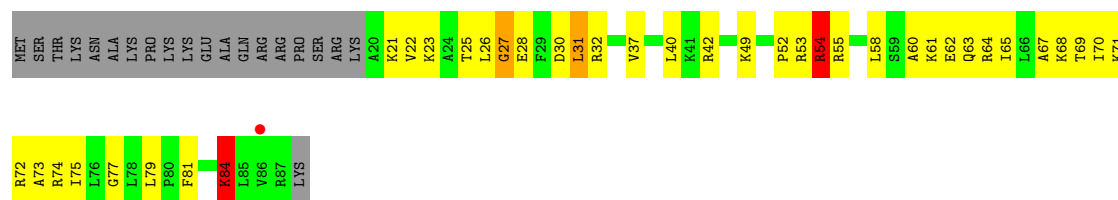
- Molecule 48: 30S ribosomal protein S17



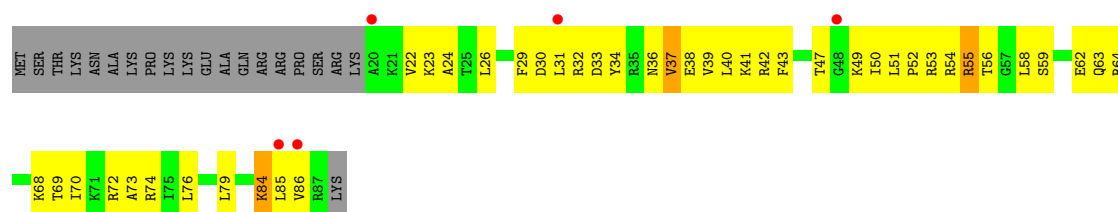
- Molecule 48: 30S ribosomal protein S17



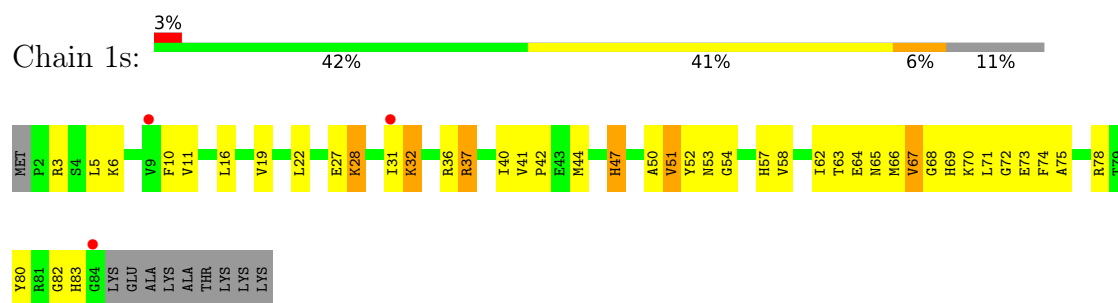
- Molecule 49: 30S ribosomal protein S18



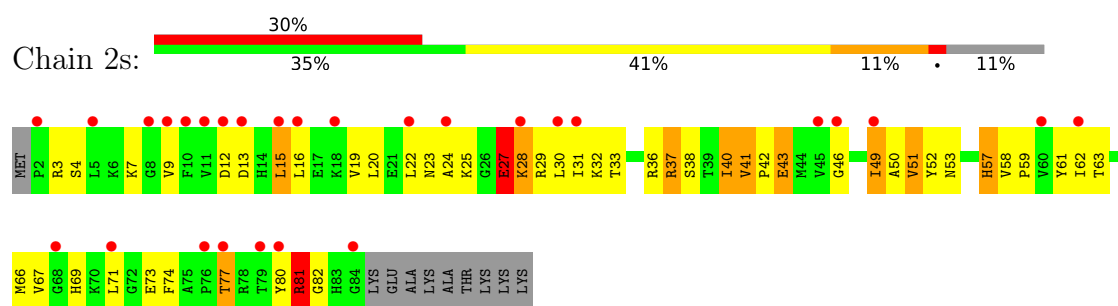
- Molecule 49: 30S ribosomal protein S18



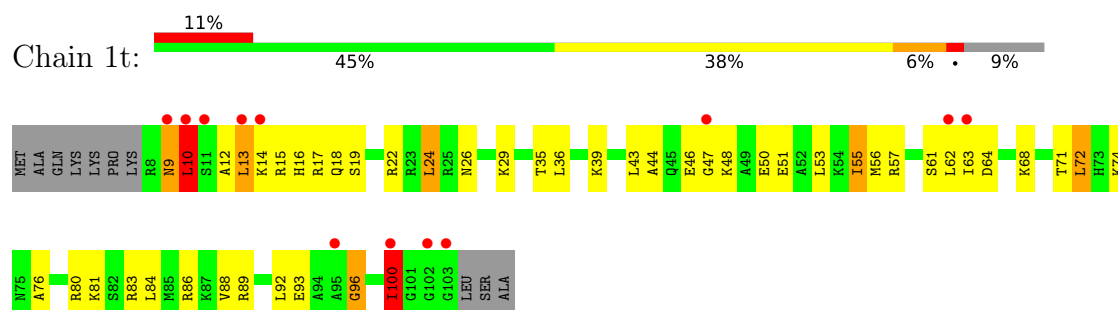
- Molecule 50: 30S ribosomal protein S19



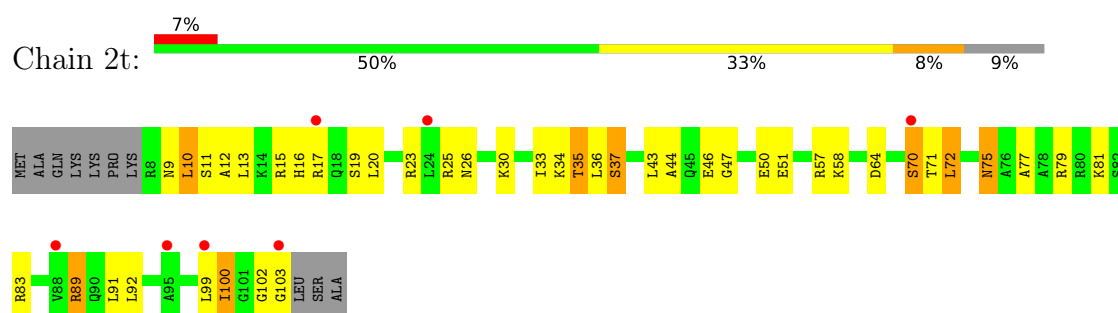
- Molecule 50: 30S ribosomal protein S19



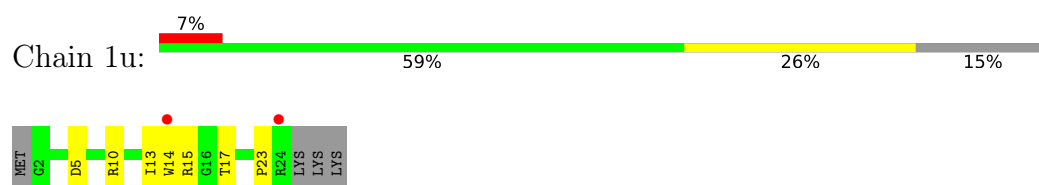
- Molecule 51: 30S ribosomal protein S20



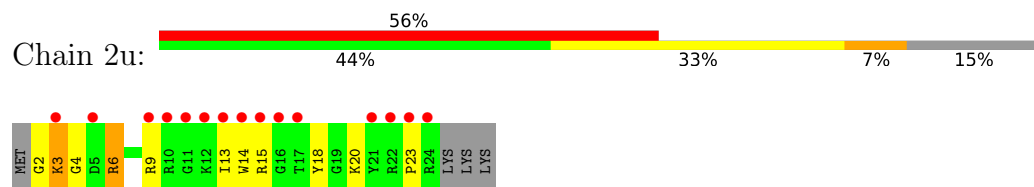
- Molecule 51: 30S ribosomal protein S20



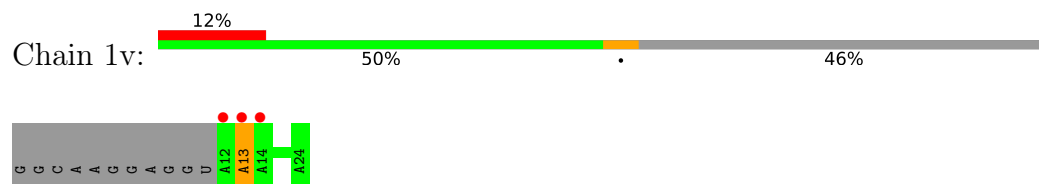
- Molecule 52: 30S ribosomal protein Thx



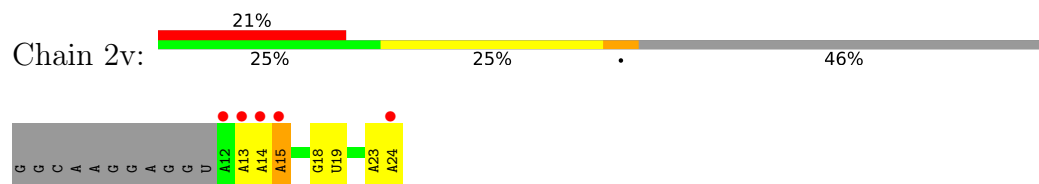
- Molecule 52: 30S ribosomal protein Thx



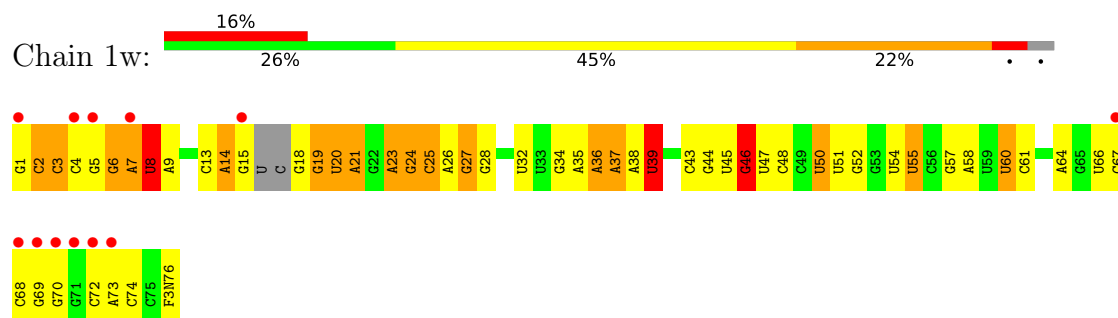
- Molecule 53: MET-PHE-mRNA



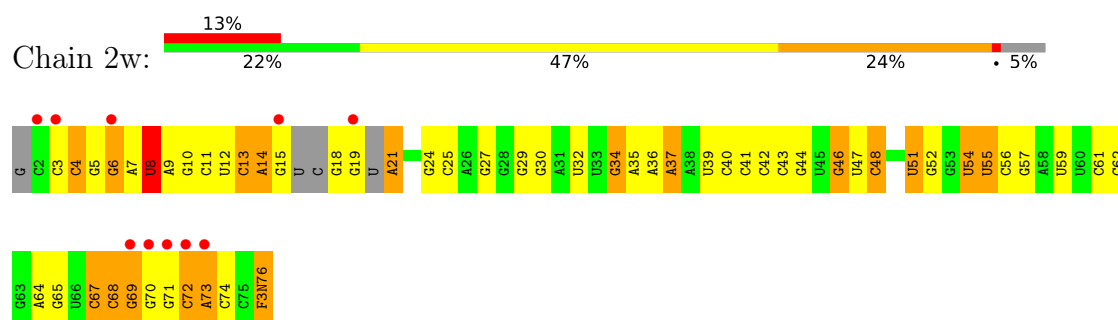
- Molecule 53: MET-PHE-mRNA



- Molecule 54: A-site Aminoacylated Phe-tRNAphe

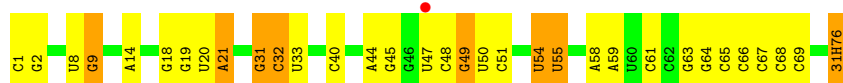


- Molecule 54: A-site Aminoacylated Phe-tRNAphe

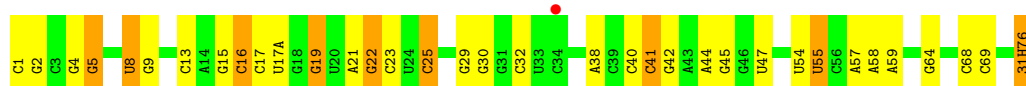


- Molecule 55: P-site Aminoacylated fMet-tRNAmet

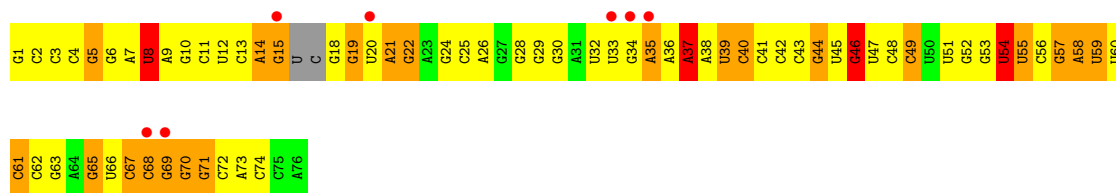
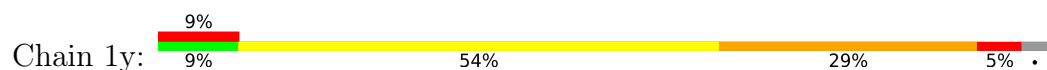




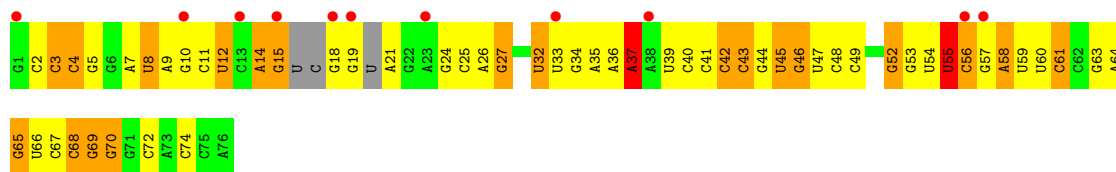
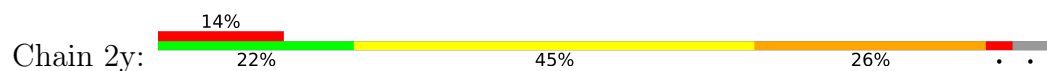
- Molecule 55: P-site Aminoacylated fMet-tRNA^{Met}



- Molecule 56: E-site Deacylated tRNA^{phe}



- Molecule 56: E-site Deacylated tRNA^{phe}



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.22Å 446.66Å 615.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.11 – 2.45 121.11 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (121.11-2.45) 99.9 (121.11-2.45)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.245 , 0.300 0.247 , 0.301	Depositor DCC
R_{free} test set	103653 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	300377	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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: OMC, A1C9N, M2G, MG, K, ZN, MIA, 0TD, F3N, 4SU, OMU, 2MA, OMG, SF4, 5MC, G7M, UR3, 5MU, 2MG, PSU, MA6, 31H, 4OC

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	0.54	0/69011	0.74	5/107720 (0.0%)
1	2A	0.41	0/67295	0.63	2/105042 (0.0%)
2	1B	0.46	0/2882	0.68	0/4494
2	2B	0.37	0/2879	0.58	0/4487
3	1D	0.57	0/2186	0.79	3/2944 (0.1%)
3	2D	0.43	0/2186	0.67	0/2944
4	1E	0.49	0/1592	0.76	0/2149
4	2E	0.43	0/1592	0.64	0/2149
5	1F	0.51	0/1619	0.72	0/2193
5	2F	0.38	0/1615	0.65	0/2188
6	1G	0.41	0/1448	0.67	0/1957
6	2G	0.38	0/1453	0.63	0/1963
7	1H	0.43	0/1356	0.65	0/1834
7	2H	0.34	0/1356	0.53	0/1834
8	1I	0.39	0/1112	0.62	0/1514
8	2I	0.37	0/1079	0.66	0/1475
9	1N	0.49	0/1144	0.71	0/1543
9	2N	0.37	0/1144	0.66	0/1543
10	1O	0.50	0/943	0.70	0/1269
10	2O	0.41	0/943	0.71	0/1269
11	1P	0.50	0/1152	0.78	0/1533
11	2P	0.39	0/1152	0.72	0/1533
12	1Q	0.52	0/1143	0.74	0/1527
12	2Q	0.40	0/1143	0.67	0/1527
13	1R	0.55	0/982	0.81	0/1312
13	2R	0.43	0/982	0.66	0/1312
14	1S	0.43	0/883	0.69	0/1176
14	2S	0.38	0/880	0.62	0/1172
15	1T	0.46	0/1105	0.67	0/1477
15	2T	0.39	0/1097	0.64	0/1468
16	1U	0.53	0/977	0.72	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.39	0/977	0.58	0/1301
17	1V	0.51	0/782	0.67	0/1049
17	2V	0.36	0/782	0.62	0/1049
18	1W	0.54	0/897	0.73	0/1205
18	2W	0.43	0/897	0.63	0/1205
19	1X	0.53	0/764	0.80	0/1025
19	2X	0.39	0/764	0.65	0/1025
20	1Y	0.45	0/819	0.67	0/1095
20	2Y	0.40	0/819	0.64	0/1095
21	1Z	0.41	0/1267	0.65	0/1717
21	2Z	0.41	0/1299	0.66	0/1763
22	10	0.53	0/662	0.85	2/881 (0.2%)
22	20	0.40	0/662	0.65	0/881
23	11	0.51	0/762	0.72	0/1014
23	21	0.40	0/762	0.64	0/1014
24	12	0.46	0/590	0.64	0/781
24	22	0.41	0/590	0.57	0/781
25	13	0.50	0/474	0.71	0/635
25	23	0.35	0/469	0.62	0/630
26	14	0.46	0/565	0.79	0/761
26	24	0.42	0/545	0.64	0/737
27	15	0.58	0/469	0.78	0/635
27	25	0.45	0/469	0.74	0/635
28	16	0.51	0/460	0.73	0/613
28	26	0.40	0/456	0.66	0/608
29	17	0.61	0/426	0.83	0/561
29	27	0.49	0/426	0.69	0/561
30	18	0.50	0/525	0.69	0/691
30	28	0.39	0/525	0.59	0/691
31	19	0.57	0/310	0.83	0/407
31	29	0.38	0/310	0.60	0/407
32	1a	0.40	0/35795	0.61	4/55864 (0.0%)
32	2a	0.37	0/35886	0.59	4/56005 (0.0%)
33	1b	0.40	0/1881	0.71	0/2542
33	2b	0.41	0/1860	0.67	0/2518
34	1c	0.38	0/1572	0.63	1/2126 (0.0%)
34	2c	0.38	0/1566	0.60	0/2119
35	1d	0.37	0/1685	0.63	0/2262
35	2d	0.39	0/1704	0.65	0/2284
36	1e	0.40	0/1145	0.63	0/1543
36	2e	0.37	0/1149	0.67	0/1548
37	1f	0.44	0/823	0.62	0/1115
37	2f	0.38	0/829	0.56	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.38	0/1250	0.59	0/1679
38	2g	0.38	0/1254	0.55	0/1683
39	1h	0.36	0/1108	0.60	0/1494
39	2h	0.35	0/1108	0.56	0/1494
40	1i	0.38	0/1002	0.70	0/1346
40	2i	0.39	0/997	0.63	0/1343
41	1j	0.36	0/722	0.59	0/982
41	2j	0.41	0/727	0.66	0/988
42	1k	0.37	0/844	0.65	0/1145
42	2k	0.34	0/848	0.53	0/1149
43	1l	0.42	0/937	0.65	0/1260
43	2l	0.36	0/937	0.61	0/1260
44	1m	0.39	0/969	0.62	0/1302
44	2m	0.41	0/961	0.66	0/1291
45	1n	0.36	0/501	0.68	0/664
45	2n	0.31	0/501	0.59	0/664
46	1o	0.41	0/739	0.63	0/985
46	2o	0.34	0/739	0.56	0/985
47	1p	0.35	0/697	0.61	0/939
47	2p	0.41	0/693	0.62	0/935
48	1q	0.39	0/836	0.59	0/1117
48	2q	0.36	0/836	0.61	0/1117
49	1r	0.44	0/560	0.64	0/746
49	2r	0.36	0/560	0.61	0/746
50	1s	0.37	0/667	0.65	0/900
50	2s	0.41	0/661	0.69	0/893
51	1t	0.37	0/730	0.66	0/965
51	2t	0.37	0/729	0.68	0/965
52	1u	0.36	0/203	0.61	0/266
52	2u	0.49	0/203	0.68	0/266
53	1v	0.45	0/310	0.56	0/480
53	2v	0.40	0/310	0.52	0/480
54	1w	0.46	1/1581 (0.1%)	0.62	0/2458
54	2w	0.47	2/1531 (0.1%)	0.61	0/2379
55	1x	0.47	0/1723	0.66	0/2684
55	2x	0.41	1/1723 (0.1%)	0.60	0/2684
56	1y	0.50	2/1606 (0.1%)	0.62	0/2497
56	2y	0.54	2/1583 (0.1%)	0.61	0/2459
All	All	0.44	8/316636 (0.0%)	0.66	21/474041 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	2F	0	1
6	1G	0	1
22	10	0	1
25	13	0	1
26	14	0	1
33	1b	0	2
All	All	0	7

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	46	G7M	O3'-P	6.24	1.62	1.56
54	2w	8	4SU	O3'-P	6.11	1.62	1.56
54	2w	46	G7M	O3'-P	5.87	1.62	1.56
55	2x	8	4SU	O3'-P	5.84	1.62	1.56
56	2y	8	4SU	O3'-P	5.78	1.62	1.56

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1992	G	C2'-C3'-O3'	7.48	120.72	109.50
1	1A	1992	G	C2'-C3'-O3'	7.39	120.58	109.50
32	1a	266	G	C2'-C3'-O3'	6.41	119.11	109.50
1	1A	2629	A	P-O3'-C3'	6.18	129.47	120.20
3	1D	98	VAL	N-CA-C	-6.18	104.92	112.76

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	10	12	ASN	Peptide
25	13	53	LEU	Peptide
26	14	67	TYR	Peptide
6	1G	50	ALA	Peptide
33	1b	125	PRO	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31189	1084	0
1	2A	60322	0	30421	1282	0
2	1B	2577	0	1305	54	0
2	2B	2575	0	1303	74	0
3	1D	2136	0	2218	58	0
3	2D	2136	0	2218	86	0
4	1E	1559	0	1618	64	0
4	2E	1559	0	1618	63	0
5	1F	1584	0	1625	58	0
5	2F	1580	0	1619	79	0
6	1G	1423	0	1436	63	0
6	2G	1428	0	1438	93	0
7	1H	1330	0	1407	30	0
7	2H	1330	0	1407	62	0
8	1I	1097	0	1140	49	0
8	2I	1064	0	1082	57	1
9	1N	1117	0	1184	34	0
9	2N	1117	0	1184	50	0
10	1O	933	0	996	30	0
10	2O	933	0	996	43	0
11	1P	1135	0	1212	71	0
11	2P	1135	0	1212	62	0
12	1Q	1122	0	1179	41	0
12	2Q	1122	0	1179	60	0
13	1R	968	0	1033	41	0
13	2R	968	0	1033	44	0
14	1S	873	0	927	29	0
14	2S	870	0	923	54	0
15	1T	1091	0	1151	33	0
15	2T	1083	0	1136	44	0
16	1U	959	0	1019	30	0
16	2U	959	0	1019	41	0
17	1V	771	0	830	21	0
17	2V	771	0	830	34	0
18	1W	886	0	940	24	0
18	2W	886	0	940	28	0
19	1X	750	0	814	31	0
19	2X	750	0	814	28	0
20	1Y	806	0	881	23	0
20	2Y	806	0	881	40	0
21	1Z	1240	0	1240	68	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	2Z	1271	0	1273	82	0
22	10	653	0	674	23	0
22	20	653	0	674	30	0
23	11	755	0	826	27	0
23	21	755	0	826	37	0
24	12	588	0	643	20	0
24	22	588	0	643	32	0
25	13	469	0	518	10	0
25	23	464	0	514	20	0
26	14	552	0	533	24	0
26	24	532	0	503	50	0
27	15	455	0	465	13	0
27	25	455	0	464	8	0
28	16	453	0	473	15	0
28	26	449	0	469	20	0
29	17	418	0	467	20	0
29	27	418	0	467	21	0
30	18	517	0	582	19	0
30	28	517	0	582	23	0
31	19	307	0	335	13	0
31	29	307	0	335	13	0
32	1a	32246	0	16294	640	1
32	2a	32327	0	16338	822	0
33	1b	1846	0	1867	105	0
33	2b	1825	0	1828	105	0
34	1c	1548	0	1535	73	0
34	2c	1542	0	1517	82	0
35	1d	1655	0	1672	67	0
35	2d	1674	0	1714	90	0
36	1e	1129	0	1185	64	0
36	2e	1133	0	1191	60	0
37	1f	810	0	804	49	0
37	2f	816	0	808	37	0
38	1g	1231	0	1238	55	0
38	2g	1235	0	1249	84	0
39	1h	1088	0	1126	36	0
39	2h	1088	0	1126	55	0
40	1i	983	0	986	38	0
40	2i	978	0	965	53	0
41	1j	709	0	650	28	0
41	2j	714	0	672	47	0
42	1k	829	0	825	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	2k	833	0	836	43	0
43	1l	932	0	981	31	0
43	2l	932	0	979	30	0
44	1m	958	0	1002	49	0
44	2m	950	0	988	78	0
45	1n	492	0	529	17	0
45	2n	492	0	529	46	0
46	1o	728	0	760	22	0
46	2o	728	0	760	29	0
47	1p	681	0	697	26	0
47	2p	677	0	686	37	0
48	1q	823	0	891	43	0
48	2q	823	0	891	38	0
49	1r	555	0	618	28	0
49	2r	555	0	618	38	0
50	1s	652	0	662	34	0
50	2s	646	0	644	53	0
51	1t	728	0	798	42	0
51	2t	727	0	796	33	0
52	1u	199	0	208	5	0
52	2u	199	0	208	8	0
53	1v	277	0	140	2	0
53	2v	277	0	140	6	0
54	1w	1603	0	828	53	0
54	2w	1555	0	797	38	0
55	1x	1656	0	848	20	0
55	2x	1656	0	849	23	0
56	1y	1585	0	803	62	0
56	2y	1565	0	794	56	0
57	10	8	0	0	0	0
57	11	5	0	0	0	0
57	12	2	0	0	0	0
57	13	5	0	0	0	0
57	14	1	0	0	0	0
57	15	9	0	0	0	0
57	16	2	0	0	0	0
57	17	7	0	0	0	0
57	18	5	0	0	0	0
57	1A	1099	0	0	0	0
57	1B	36	0	0	0	0
57	1D	13	0	0	0	0
57	1E	14	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1F	12	0	0	0	0
57	1G	5	0	0	0	0
57	1H	1	0	0	0	0
57	1I	1	0	0	0	0
57	1N	6	0	0	0	0
57	1O	5	0	0	0	0
57	1P	3	0	0	0	0
57	1Q	7	0	0	0	0
57	1R	4	0	0	0	0
57	1S	3	0	0	0	0
57	1T	4	0	0	0	0
57	1U	10	0	0	0	0
57	1V	10	0	0	0	0
57	1W	8	0	0	0	0
57	1X	7	0	0	0	0
57	1Y	3	0	0	0	0
57	1Z	4	0	0	0	0
57	1a	213	0	0	0	0
57	1b	1	0	0	0	0
57	1d	1	0	0	0	0
57	1e	2	0	0	0	0
57	1f	2	0	0	0	0
57	1k	1	0	0	0	0
57	1l	2	0	0	0	0
57	1m	2	0	0	0	0
57	1n	3	0	0	0	0
57	1t	1	0	0	0	0
57	1v	2	0	0	0	0
57	1w	8	0	0	0	0
57	1x	14	0	0	0	0
57	1y	1	0	0	0	0
57	20	2	0	0	0	0
57	21	1	0	0	0	0
57	23	1	0	0	0	0
57	25	5	0	0	0	0
57	27	2	0	0	0	0
57	28	4	0	0	0	0
57	29	1	0	0	0	0
57	2A	883	0	0	0	0
57	2B	20	0	0	0	0
57	2D	8	0	0	0	0
57	2E	7	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2F	6	0	0	0	0
57	2G	1	0	0	0	0
57	2N	1	0	0	0	0
57	2O	1	0	0	0	0
57	2P	3	0	0	0	0
57	2Q	3	0	0	0	0
57	2R	3	0	0	0	0
57	2T	3	0	0	0	0
57	2U	1	0	0	0	0
57	2V	2	0	0	0	0
57	2W	3	0	0	0	0
57	2X	2	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	234	0	0	0	0
57	2d	2	0	0	0	0
57	2e	1	0	0	0	0
57	2f	1	0	0	0	0
57	2g	1	0	0	0	0
57	2i	1	0	0	0	0
57	2j	2	0	0	0	0
57	2k	1	0	0	0	0
57	2l	4	0	0	0	0
57	2m	1	0	0	0	0
57	2p	1	0	0	0	0
57	2q	2	0	0	0	0
57	2r	2	0	0	0	0
57	2t	1	0	0	0	0
57	2v	3	0	0	0	0
57	2w	9	0	0	0	0
57	2x	6	0	0	0	0
57	2y	6	0	0	0	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	1A	74	0	0	1	0
59	2A	74	0	0	0	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	0	0
61	2d	8	0	0	0	0
62	10	10	0	0	1	0
62	11	14	0	0	0	0
62	12	2	0	0	0	0
62	13	3	0	0	1	0
62	15	6	0	0	1	0
62	16	4	0	0	0	0
62	17	9	0	0	3	0
62	18	10	0	0	0	0
62	1A	1997	0	0	151	0
62	1B	63	0	0	3	0
62	1D	30	0	0	1	0
62	1E	31	0	0	4	0
62	1F	16	0	0	1	0
62	1G	5	0	0	1	0
62	1H	2	0	0	1	0
62	1I	1	0	0	0	0
62	1N	8	0	0	1	0
62	1O	5	0	0	0	0
62	1P	24	0	0	6	0
62	1Q	8	0	0	0	0
62	1R	11	0	0	0	0
62	1S	5	0	0	0	0
62	1T	9	0	0	0	0
62	1U	9	0	0	0	0
62	1V	9	0	0	0	0
62	1W	8	0	0	1	0
62	1X	5	0	0	0	0
62	1Y	4	0	0	0	0
62	1Z	1	0	0	0	0
62	1a	379	0	0	30	0
62	1b	1	0	0	0	0
62	1e	1	0	0	0	0
62	1f	1	0	0	0	0
62	1i	1	0	0	0	0
62	1l	7	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	1p	1	0	0	0	0
62	1q	2	0	0	0	0
62	1u	1	0	0	1	0
62	1v	5	0	0	0	0
62	1w	13	0	0	1	0
62	1x	15	0	0	1	0
62	1y	2	0	0	0	0
62	20	3	0	0	0	0
62	21	12	0	0	1	0
62	23	2	0	0	0	0
62	25	2	0	0	0	0
62	27	4	0	0	0	0
62	28	3	0	0	1	0
62	29	1	0	0	0	0
62	2A	1156	0	0	135	0
62	2B	24	0	0	4	0
62	2D	22	0	0	3	0
62	2E	14	0	0	6	0
62	2F	12	0	0	0	0
62	2I	3	0	0	0	0
62	2N	1	0	0	0	0
62	2O	3	0	0	0	0
62	2P	12	0	0	3	0
62	2Q	1	0	0	0	0
62	2R	6	0	0	0	0
62	2T	5	0	0	0	0
62	2U	3	0	0	1	0
62	2V	1	0	0	0	0
62	2W	1	0	0	0	0
62	2X	3	0	0	2	0
62	2Z	1	0	0	0	0
62	2a	267	0	0	22	0
62	2c	1	0	0	0	0
62	2d	1	0	0	0	0
62	2f	1	0	0	0	0
62	2j	3	0	0	1	0
62	2l	6	0	0	1	0
62	2o	1	0	0	0	0
62	2p	2	0	0	0	0
62	2t	2	0	0	0	0
62	2v	2	0	0	0	0
62	2w	3	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	2x	6	0	0	0	0
62	2y	8	0	0	0	0
All	All	300377	0	196733	7374	1

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 15.

The worst 5 of 7374 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.15	1.37
1:1A:1082:U:N3	1:1A:1086:A:N6	1.94	1.13
54:1w:27:G:H1	54:1w:43:C:N4	1.50	1.08
54:1w:3:C:H42	54:1w:70:G:H1	1.05	1.02
32:2a:664:G:H22	32:2a:741:G:H1	1.07	1.01

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:357:G:O2'	8:2I:89:TYR:O[2_655]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	253 (93%)	20 (7%)	0	100	100
3	2D	273/276 (99%)	243 (89%)	27 (10%)	3 (1%)	11	12
4	1E	202/206 (98%)	181 (90%)	19 (9%)	2 (1%)	12	14
4	2E	202/206 (98%)	178 (88%)	18 (9%)	6 (3%)	3	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	1F	201/210 (96%)	192 (96%)	7 (4%)	2 (1%)	12	14
5	2F	201/210 (96%)	184 (92%)	13 (6%)	4 (2%)	6	4
6	1G	179/182 (98%)	151 (84%)	24 (13%)	4 (2%)	5	3
6	2G	179/182 (98%)	148 (83%)	25 (14%)	6 (3%)	3	1
7	1H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	21	27
7	2H	172/180 (96%)	147 (86%)	23 (13%)	2 (1%)	10	11
8	1I	144/148 (97%)	112 (78%)	28 (19%)	4 (3%)	4	2
8	2I	144/148 (97%)	110 (76%)	27 (19%)	7 (5%)	1	0
9	1N	138/140 (99%)	125 (91%)	10 (7%)	3 (2%)	5	3
9	2N	138/140 (99%)	123 (89%)	12 (9%)	3 (2%)	5	3
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	16	20
11	1P	147/150 (98%)	123 (84%)	18 (12%)	6 (4%)	2	1
11	2P	147/150 (98%)	121 (82%)	20 (14%)	6 (4%)	2	1
12	1Q	139/141 (99%)	125 (90%)	12 (9%)	2 (1%)	9	8
12	2Q	139/141 (99%)	120 (86%)	17 (12%)	2 (1%)	9	8
13	1R	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
13	2R	116/118 (98%)	107 (92%)	8 (7%)	1 (1%)	14	17
14	1S	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	14	17
14	2S	108/112 (96%)	90 (83%)	12 (11%)	6 (6%)	1	0
15	1T	129/146 (88%)	117 (91%)	10 (8%)	2 (2%)	7	7
15	2T	129/146 (88%)	116 (90%)	12 (9%)	1 (1%)	16	20
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
16	2U	114/118 (97%)	105 (92%)	8 (7%)	1 (1%)	14	17
17	1V	99/101 (98%)	90 (91%)	6 (6%)	3 (3%)	3	2
17	2V	99/101 (98%)	91 (92%)	5 (5%)	3 (3%)	3	2
18	1W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
18	2W	110/113 (97%)	103 (94%)	6 (6%)	1 (1%)	14	17
19	1X	93/96 (97%)	86 (92%)	5 (5%)	2 (2%)	5	3
19	2X	93/96 (97%)	82 (88%)	10 (11%)	1 (1%)	11	12
20	1Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	12	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	2Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	12	14
21	1Z	148/206 (72%)	125 (84%)	18 (12%)	5 (3%)	3	1
21	2Z	156/206 (76%)	122 (78%)	27 (17%)	7 (4%)	2	0
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	72 (89%)	7 (9%)	2 (2%)	4	3
23	11	95/98 (97%)	86 (90%)	8 (8%)	1 (1%)	11	12
23	21	95/98 (97%)	86 (90%)	8 (8%)	1 (1%)	11	12
24	12	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
24	22	68/72 (94%)	60 (88%)	8 (12%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	49 (86%)	6 (10%)	2 (4%)	3	1
26	14	67/71 (94%)	48 (72%)	15 (22%)	4 (6%)	1	0
26	24	67/71 (94%)	48 (72%)	12 (18%)	7 (10%)	0	0
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
27	25	57/60 (95%)	49 (86%)	8 (14%)	0	100	100
28	16	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
28	26	51/54 (94%)	45 (88%)	5 (10%)	1 (2%)	6	4
29	17	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
29	27	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
30	18	62/65 (95%)	60 (97%)	1 (2%)	1 (2%)	7	7
30	28	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
31	19	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
31	29	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	3	2
33	1b	229/256 (90%)	174 (76%)	36 (16%)	19 (8%)	0	0
33	2b	229/256 (90%)	166 (72%)	45 (20%)	18 (8%)	1	0
34	1c	204/239 (85%)	180 (88%)	23 (11%)	1 (0%)	24	32
34	2c	204/239 (85%)	167 (82%)	31 (15%)	6 (3%)	3	2
35	1d	206/209 (99%)	178 (86%)	24 (12%)	4 (2%)	6	5
35	2d	206/209 (99%)	174 (84%)	25 (12%)	7 (3%)	3	1
36	1e	146/162 (90%)	132 (90%)	12 (8%)	2 (1%)	9	8
36	2e	146/162 (90%)	114 (78%)	24 (16%)	8 (6%)	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
37	2f	98/101 (97%)	87 (89%)	9 (9%)	2 (2%)	6	4
38	1g	153/156 (98%)	128 (84%)	21 (14%)	4 (3%)	4	2
38	2g	153/156 (98%)	127 (83%)	17 (11%)	9 (6%)	1	0
39	1h	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
39	2h	135/138 (98%)	109 (81%)	24 (18%)	2 (2%)	8	7
40	1i	125/128 (98%)	100 (80%)	24 (19%)	1 (1%)	16	20
40	2i	125/128 (98%)	100 (80%)	23 (18%)	2 (2%)	7	7
41	1j	95/105 (90%)	77 (81%)	14 (15%)	4 (4%)	2	0
41	2j	94/105 (90%)	78 (83%)	7 (7%)	9 (10%)	0	0
42	1k	112/129 (87%)	99 (88%)	9 (8%)	4 (4%)	2	1
42	2k	112/129 (87%)	93 (83%)	12 (11%)	7 (6%)	1	0
43	1l	119/132 (90%)	104 (87%)	15 (13%)	0	100	100
43	2l	119/132 (90%)	111 (93%)	6 (5%)	2 (2%)	7	6
44	1m	121/126 (96%)	106 (88%)	15 (12%)	0	100	100
44	2m	120/126 (95%)	90 (75%)	26 (22%)	4 (3%)	3	1
45	1n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	6
46	1o	86/89 (97%)	74 (86%)	7 (8%)	5 (6%)	1	0
46	2o	86/89 (97%)	77 (90%)	8 (9%)	1 (1%)	10	11
47	1p	80/88 (91%)	68 (85%)	12 (15%)	0	100	100
47	2p	80/88 (91%)	67 (84%)	12 (15%)	1 (1%)	9	9
48	1q	97/105 (92%)	84 (87%)	12 (12%)	1 (1%)	12	14
48	2q	97/105 (92%)	79 (81%)	14 (14%)	4 (4%)	2	1
49	1r	66/88 (75%)	55 (83%)	7 (11%)	4 (6%)	1	0
49	2r	66/88 (75%)	58 (88%)	7 (11%)	1 (2%)	8	7
50	1s	81/93 (87%)	68 (84%)	10 (12%)	3 (4%)	2	1
50	2s	81/93 (87%)	62 (76%)	14 (17%)	5 (6%)	1	0
51	1t	94/106 (89%)	79 (84%)	9 (10%)	6 (6%)	1	0
51	2t	94/106 (89%)	73 (78%)	16 (17%)	5 (5%)	1	0
52	1u	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	2u	21/27 (78%)	16 (76%)	3 (14%)	2 (10%)	0	0
All	All	11370/12128 (94%)	9876 (87%)	1219 (11%)	275 (2%)	4	3

5 of 275 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	1I	107	VAL
11	1P	38	GLN
11	1P	39	LYS
20	1Y	78	ALA
21	1Z	53	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	196 (91%)	19 (9%)	9	10
3	2D	215/218 (99%)	194 (90%)	21 (10%)	7	7
4	1E	164/166 (99%)	142 (87%)	22 (13%)	4	3
4	2E	164/166 (99%)	146 (89%)	18 (11%)	6	5
5	1F	160/166 (96%)	134 (84%)	26 (16%)	2	1
5	2F	159/166 (96%)	137 (86%)	22 (14%)	3	3
6	1G	143/156 (92%)	124 (87%)	19 (13%)	4	3
6	2G	143/156 (92%)	117 (82%)	26 (18%)	2	1
7	1H	144/148 (97%)	126 (88%)	18 (12%)	4	4
7	2H	144/148 (97%)	115 (80%)	29 (20%)	1	0
8	1I	113/124 (91%)	84 (74%)	29 (26%)	0	0
8	2I	105/124 (85%)	74 (70%)	31 (30%)	0	0
9	1N	118/119 (99%)	103 (87%)	15 (13%)	4	4
9	2N	118/119 (99%)	92 (78%)	26 (22%)	1	0
10	1O	100/100 (100%)	88 (88%)	12 (12%)	5	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	2O	100/100 (100%)	87 (87%)	13 (13%)	4	3
11	1P	115/116 (99%)	105 (91%)	10 (9%)	9	11
11	2P	115/116 (99%)	103 (90%)	12 (10%)	7	6
12	1Q	111/111 (100%)	100 (90%)	11 (10%)	7	7
12	2Q	111/111 (100%)	96 (86%)	15 (14%)	4	3
13	1R	101/101 (100%)	91 (90%)	10 (10%)	7	7
13	2R	101/101 (100%)	90 (89%)	11 (11%)	6	5
14	1S	86/88 (98%)	72 (84%)	14 (16%)	2	1
14	2S	85/88 (97%)	74 (87%)	11 (13%)	4	3
15	1T	115/127 (91%)	100 (87%)	15 (13%)	4	3
15	2T	113/127 (89%)	102 (90%)	11 (10%)	8	8
16	1U	93/94 (99%)	84 (90%)	9 (10%)	8	8
16	2U	93/94 (99%)	81 (87%)	12 (13%)	4	3
17	1V	80/82 (98%)	69 (86%)	11 (14%)	3	3
17	2V	80/82 (98%)	65 (81%)	15 (19%)	1	0
18	1W	90/92 (98%)	77 (86%)	13 (14%)	3	2
18	2W	90/92 (98%)	79 (88%)	11 (12%)	5	4
19	1X	77/78 (99%)	71 (92%)	6 (8%)	11	14
19	2X	77/78 (99%)	71 (92%)	6 (8%)	11	14
20	1Y	85/91 (93%)	72 (85%)	13 (15%)	3	2
20	2Y	85/91 (93%)	69 (81%)	16 (19%)	1	0
21	1Z	135/179 (75%)	111 (82%)	24 (18%)	2	1
21	2Z	137/179 (76%)	105 (77%)	32 (23%)	1	0
22	10	65/67 (97%)	61 (94%)	4 (6%)	16	23
22	20	65/67 (97%)	61 (94%)	4 (6%)	16	23
23	11	80/83 (96%)	74 (92%)	6 (8%)	12	16
23	21	80/83 (96%)	64 (80%)	16 (20%)	1	0
24	12	65/67 (97%)	59 (91%)	6 (9%)	8	9
24	22	65/67 (97%)	58 (89%)	7 (11%)	6	6
25	13	51/52 (98%)	44 (86%)	7 (14%)	3	3
25	23	50/52 (96%)	43 (86%)	7 (14%)	3	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	14	59/63 (94%)	48 (81%)	11 (19%)	1	1
26	24	53/63 (84%)	42 (79%)	11 (21%)	1	0
27	15	50/52 (96%)	48 (96%)	2 (4%)	28	41
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	26
28	16	51/52 (98%)	43 (84%)	8 (16%)	2	1
28	26	50/52 (96%)	44 (88%)	6 (12%)	5	4
29	17	41/42 (98%)	34 (83%)	7 (17%)	2	1
29	27	41/42 (98%)	38 (93%)	3 (7%)	13	17
30	18	54/55 (98%)	48 (89%)	6 (11%)	6	5
30	28	54/55 (98%)	48 (89%)	6 (11%)	6	5
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	52
31	29	34/34 (100%)	28 (82%)	6 (18%)	2	1
33	1b	192/220 (87%)	156 (81%)	36 (19%)	1	0
33	2b	187/220 (85%)	152 (81%)	35 (19%)	1	0
34	1c	142/188 (76%)	123 (87%)	19 (13%)	4	3
34	2c	140/188 (74%)	115 (82%)	25 (18%)	2	1
35	1d	169/181 (93%)	143 (85%)	26 (15%)	2	2
35	2d	173/181 (96%)	139 (80%)	34 (20%)	1	0
36	1e	113/123 (92%)	95 (84%)	18 (16%)	2	1
36	2e	114/123 (93%)	92 (81%)	22 (19%)	1	0
37	1f	84/90 (93%)	72 (86%)	12 (14%)	3	2
37	2f	85/90 (94%)	66 (78%)	19 (22%)	1	0
38	1g	119/127 (94%)	98 (82%)	21 (18%)	2	1
38	2g	120/127 (94%)	100 (83%)	20 (17%)	2	1
39	1h	114/119 (96%)	102 (90%)	12 (10%)	6	6
39	2h	114/119 (96%)	99 (87%)	15 (13%)	4	3
40	1i	90/99 (91%)	78 (87%)	12 (13%)	4	3
40	2i	89/99 (90%)	73 (82%)	16 (18%)	2	1
41	1j	66/92 (72%)	56 (85%)	10 (15%)	3	2
41	2j	69/92 (75%)	54 (78%)	15 (22%)	1	0
42	1k	82/99 (83%)	72 (88%)	10 (12%)	5	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	2k	83/99 (84%)	62 (75%)	21 (25%)	0	0
43	1l	96/108 (89%)	89 (93%)	7 (7%)	13	17
43	2l	96/108 (89%)	81 (84%)	15 (16%)	2	1
44	1m	93/101 (92%)	80 (86%)	13 (14%)	3	3
44	2m	92/101 (91%)	68 (74%)	24 (26%)	0	0
45	1n	49/50 (98%)	41 (84%)	8 (16%)	2	1
45	2n	49/50 (98%)	45 (92%)	4 (8%)	10	13
46	1o	78/80 (98%)	68 (87%)	10 (13%)	4	3
46	2o	78/80 (98%)	69 (88%)	9 (12%)	5	5
47	1p	69/74 (93%)	59 (86%)	10 (14%)	3	2
47	2p	68/74 (92%)	59 (87%)	9 (13%)	4	3
48	1q	94/97 (97%)	85 (90%)	9 (10%)	8	8
48	2q	94/97 (97%)	82 (87%)	12 (13%)	4	3
49	1r	59/77 (77%)	53 (90%)	6 (10%)	7	6
49	2r	59/77 (77%)	54 (92%)	5 (8%)	10	11
50	1s	69/80 (86%)	60 (87%)	9 (13%)	4	3
50	2s	67/80 (84%)	56 (84%)	11 (16%)	2	1
51	1t	70/82 (85%)	60 (86%)	10 (14%)	3	2
51	2t	70/82 (85%)	60 (86%)	10 (14%)	3	2
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	27
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	27
All	All	9303/10064 (92%)	7961 (86%)	1342 (14%)	3	2

5 of 1342 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	2Z	54	HIS
37	2f	70	ASP
22	20	40	GLN
21	2Z	42	VAL
33	2b	142	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 165 such sidechains are listed below:

Mol	Chain	Res	Type
23	21	56	GLN
40	2i	3	GLN
25	23	32	GLN
34	2c	181	ASN
42	2k	104	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	532 (18%)	36 (1%)
1	2A	2791/2915 (95%)	550 (19%)	26 (0%)
2	1B	119/121 (98%)	14 (11%)	0
2	2B	118/121 (97%)	35 (29%)	0
32	1a	1497/1521 (98%)	293 (19%)	0
32	2a	1501/1521 (98%)	359 (23%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	71/76 (93%)	25 (35%)	0
54	2w	69/76 (90%)	27 (39%)	0
55	1x	75/77 (97%)	12 (16%)	0
55	2x	75/77 (97%)	13 (17%)	0
56	1y	72/76 (94%)	35 (48%)	0
56	2y	70/76 (92%)	28 (40%)	0
All	All	9346/9620 (97%)	1927 (20%)	62 (0%)

5 of 1927 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	21	A
1	1A	32	C
1	1A	33	U

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2183	C
1	2A	1653	G
1	1A	2756	U
1	2A	1530	C
1	2A	2126	A

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

88 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$
56	4SU	2y	8	56	18,21,22	1.74	4 (22%)	25,30,33	2.62	6 (24%)
55	5MU	2x	54	55	19,22,23	1.48	5 (26%)	27,32,35	2.44	8 (29%)
32	4OC	2a	1402	32	20,23,24	0.76	1 (5%)	25,32,35	1.39	5 (20%)
54	5MU	1w	54	54	19,22,23	1.31	4 (21%)	27,32,35	2.29	6 (22%)
55	31H	2x	76	57,58,55	31,34,35	1.34	4 (12%)	35,47,50	2.02	11 (31%)
56	PSU	2y	39	56	18,21,22	1.35	2 (11%)	21,30,33	2.09	4 (19%)
32	UR3	2a	1498	32	19,22,23	1.28	1 (5%)	26,32,35	1.82	5 (19%)
32	5MC	2a	1407	32	19,22,23	1.85	3 (15%)	26,32,35	1.20	3 (11%)
32	5MC	2a	1400	32	19,22,23	1.42	2 (10%)	26,32,35	1.05	1 (3%)
1	5MC	1A	1942	57,1	19,22,23	1.69	3 (15%)	26,32,35	1.40	3 (11%)
54	PSU	1w	39	54	18,21,22	1.18	2 (11%)	21,30,33	2.67	6 (28%)
1	PSU	2A	1911	1	18,21,22	1.40	2 (11%)	21,30,33	2.52	5 (23%)
56	PSU	2y	32	56	18,21,22	1.40	3 (16%)	21,30,33	1.99	4 (19%)
1	5MU	2A	1915	57,1	19,22,23	1.47	6 (31%)	27,32,35	2.20	8 (29%)
1	2MA	1A	2503	57,1	22,25,26	1.28	4 (18%)	32,37,40	2.66	11 (34%)
54	MIA	2w	37	54	24,27,32	2.10	4 (16%)	32,39,47	2.45	11 (34%)
43	0TD	2l	92	43	8,9,10	5.25	2 (25%)	6,11,13	4.63	1 (16%)
55	5MC	1x	32	55	19,22,23	1.37	3 (15%)	26,32,35	1.38	2 (7%)
32	UR3	1a	1498	32	19,22,23	1.27	2 (10%)	26,32,35	2.27	6 (23%)
32	M2G	2a	966	32	24,27,28	1.36	4 (16%)	33,40,43	1.85	6 (18%)
32	4OC	1a	1402	32	20,23,24	0.84	1 (5%)	25,32,35	1.06	1 (4%)
1	PSU	1A	1911	1	18,21,22	1.54	3 (16%)	21,30,33	2.28	4 (19%)
32	MA6	2a	1519	32	23,26,27	0.43	0	33,38,41	2.15	10 (30%)
1	5MU	1A	1939	1	19,22,23	1.53	5 (26%)	27,32,35	2.75	8 (29%)
1	PSU	2A	2605	1	18,21,22	1.44	3 (16%)	21,30,33	2.00	4 (19%)
1	OMU	2A	2552	57,1	19,22,23	1.11	3 (15%)	25,31,34	1.83	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	MA6	2a	1518	32	23,26,27	0.39	0	33,38,41	2.06	9 (27%)
1	PSU	2A	1917	1	18,21,22	1.50	3 (16%)	21,30,33	2.26	5 (23%)
56	4SU	1y	8	56	18,21,22	1.62	3 (16%)	25,30,33	2.30	5 (20%)
32	PSU	2a	516	32	18,21,22	1.38	2 (11%)	21,30,33	2.06	6 (28%)
55	5MU	1x	54	57,55	19,22,23	1.36	3 (15%)	27,32,35	1.75	6 (22%)
55	PSU	2x	55	55	18,21,22	1.36	2 (11%)	21,30,33	1.91	4 (19%)
32	5MC	1a	967	32	19,22,23	1.83	3 (15%)	26,32,35	1.27	3 (11%)
1	PSU	1A	2605	57,1	18,21,22	1.44	3 (16%)	21,30,33	2.06	4 (19%)
54	F3N	2w	76	54,1	33,36,37	1.46	5 (15%)	41,51,54	1.83	9 (21%)
1	OMC	2A	1920	1	19,22,23	0.73	0	25,31,34	0.97	1 (4%)
56	PSU	1y	32	56	18,21,22	1.42	2 (11%)	21,30,33	2.03	4 (19%)
32	5MC	2a	1404	32	19,22,23	1.81	3 (15%)	26,32,35	1.20	4 (15%)
1	5MC	2A	1942	1	19,22,23	1.77	2 (10%)	26,32,35	1.46	4 (15%)
1	5MU	2A	1939	57,1	19,22,23	1.64	5 (26%)	27,32,35	2.78	8 (29%)
56	PSU	1y	55	56	18,21,22	1.35	2 (11%)	21,30,33	1.99	4 (19%)
1	OMG	2A	2251	57,1,55	23,26,27	1.26	4 (17%)	32,38,41	1.97	7 (21%)
54	PSU	2w	39	54	18,21,22	1.40	2 (11%)	21,30,33	1.69	4 (19%)
32	G7M	1a	527	32	23,26,27	1.66	3 (13%)	34,39,42	1.74	4 (11%)
55	5MC	2x	32	55	19,22,23	1.36	2 (10%)	26,32,35	1.38	4 (15%)
1	5MC	1A	1962	57,1	19,22,23	1.81	3 (15%)	26,32,35	1.52	6 (23%)
1	5MC	2A	1962	57,1	19,22,23	1.74	3 (15%)	26,32,35	1.33	3 (11%)
54	4SU	1w	8	54	18,21,22	1.90	4 (22%)	25,30,33	2.66	7 (28%)
32	MA6	1a	1518	32	23,26,27	0.43	0	33,38,41	1.94	9 (27%)
54	F3N	1w	76	54,1	33,36,37	1.69	4 (12%)	41,51,54	1.62	8 (19%)
54	G7M	2w	46	54	23,26,27	1.56	4 (17%)	34,39,42	1.88	5 (14%)
32	G7M	2a	527	32	23,26,27	1.41	5 (21%)	34,39,42	1.61	4 (11%)
43	0TD	1l	92	43	8,9,10	3.95	1 (12%)	6,11,13	9.18	3 (50%)
54	5MU	2w	54	54	19,22,23	1.50	6 (31%)	27,32,35	1.89	7 (25%)
1	2MA	2A	2503	57,1	22,25,26	1.54	6 (27%)	32,37,40	2.34	7 (21%)
55	4SU	1x	8	55	18,21,22	2.34	6 (33%)	25,30,33	1.97	6 (24%)
55	PSU	1x	55	55	18,21,22	1.41	2 (11%)	21,30,33	2.00	3 (14%)
32	PSU	1a	516	32,57	18,21,22	1.38	2 (11%)	21,30,33	2.07	5 (23%)
56	PSU	1y	39	56	18,21,22	1.46	3 (16%)	21,30,33	2.06	3 (14%)
32	MA6	1a	1519	32	23,26,27	0.45	0	33,38,41	1.95	8 (24%)
32	2MG	2a	1207	32,57	23,26,27	1.28	3 (13%)	33,38,41	2.09	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PSU	2w	55	54	18,21,22	1.42	3 (16%)	21,30,33	2.07	6 (28%)
56	MIA	1y	37	56	21,24,32	1.68	3 (14%)	30,35,47	2.16	6 (20%)
32	5MC	1a	1404	32	19,22,23	1.60	3 (15%)	26,32,35	1.48	3 (11%)
1	PSU	1A	1917	1	18,21,22	1.33	2 (11%)	21,30,33	2.15	6 (28%)
54	4SU	2w	8	54	18,21,22	1.82	5 (27%)	25,30,33	2.51	5 (20%)
1	OMU	1A	2552	57,1	19,22,23	1.30	4 (21%)	25,31,34	1.94	6 (24%)
56	PSU	2y	55	56	18,21,22	1.36	1 (5%)	21,30,33	2.01	5 (23%)
32	5MC	1a	1407	32	19,22,23	1.91	3 (15%)	26,32,35	1.21	4 (15%)
32	2MG	1a	1207	32	23,26,27	1.33	3 (13%)	33,38,41	2.42	10 (30%)
56	MIA	2y	37	56	21,24,32	1.72	3 (14%)	30,35,47	1.87	9 (30%)
56	5MU	1y	54	56	19,22,23	1.57	4 (21%)	27,32,35	1.97	6 (22%)
54	PSU	1w	32	57,54	18,21,22	1.27	1 (5%)	21,30,33	1.61	4 (19%)
32	5MC	2a	967	32	19,22,23	1.67	3 (15%)	26,32,35	1.10	3 (11%)
54	PSU	1w	55	54	18,21,22	1.55	3 (16%)	21,30,33	2.39	5 (23%)
54	PSU	2w	32	54	18,21,22	1.44	2 (11%)	21,30,33	1.82	4 (19%)
56	G7M	2y	46	56	23,26,27	1.66	5 (21%)	34,39,42	1.92	4 (11%)
1	5MU	1A	1915	1	19,22,23	1.41	4 (21%)	27,32,35	2.42	6 (22%)
54	MIA	1w	37	54	28,31,32	2.28	6 (21%)	38,44,47	2.72	10 (26%)
32	5MC	1a	1400	32	19,22,23	1.39	2 (10%)	26,32,35	1.37	3 (11%)
56	G7M	1y	46	56	23,26,27	1.71	6 (26%)	34,39,42	2.20	9 (26%)
56	5MU	2y	54	56	19,22,23	1.49	4 (21%)	27,32,35	1.57	5 (18%)
1	OMG	1A	2251	57,1,55	23,26,27	1.28	3 (13%)	32,38,41	2.10	6 (18%)
55	31H	1x	76	57,55	31,34,35	1.19	3 (9%)	35,47,50	2.41	14 (40%)
54	G7M	1w	46	54	23,26,27	1.57	3 (13%)	34,39,42	1.79	4 (11%)
32	M2G	1a	966	32	24,27,28	1.32	4 (16%)	33,40,43	2.03	7 (21%)
55	4SU	2x	8	55	18,21,22	2.22	6 (33%)	25,30,33	1.52	6 (24%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	1.18	2 (8%)

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
56	4SU	2y	8	56	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
55	31H	2x	76	57,58,55	-	5/22/40/41	0/3/3/3
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
1	5MC	1A	1942	57,1	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	2/7/25/26	0/2/2/2
56	PSU	2y	32	56	-	2/7/25/26	0/2/2/2
1	5MU	2A	1915	57,1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	57,1	-	1/7/25/26	0/3/3/3
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
43	0TD	2l	92	43	-	3/7/12/14	-
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	57,1	-	0/9/27/28	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
56	4SU	1y	8	56	-	3/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	2/7/25/26	0/2/2/2
55	5MU	1x	54	57,55	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	57,1	-	0/7/25/26	0/2/2/2
54	F3N	2w	76	54,1	-	1/19/37/38	0/4/4/4
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	57,1	-	0/7/25/26	0/2/2/2
56	PSU	1y	55	56	-	2/7/25/26	0/2/2/2
1	OMG	2A	2251	57,1,55	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32	-	2/7/25/26	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	57,1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	57,1	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
54	F3N	1w	76	54,1	-	0/19/37/38	0/4/4/4
54	G7M	2w	46	54	-	0/7/25/26	0/3/3/3
32	G7M	2a	527	32	-	3/7/25/26	0/3/3/3
43	0TD	1l	92	43	-	3/7/12/14	-
54	5MU	2w	54	54	-	1/7/25/26	0/2/2/2
1	2MA	2A	2503	57,1	-	1/7/25/26	0/3/3/3
55	4SU	1x	8	55	-	1/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,57	-	0/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
32	2MG	2a	1207	32,57	-	2/9/27/28	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
56	MIA	1y	37	56	-	2/7/25/34	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	57,1	-	0/9/27/28	0/2/2/2
56	PSU	2y	55	56	-	3/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
56	MIA	2y	37	56	-	3/7/25/34	0/3/3/3
56	5MU	1y	54	56	-	2/7/25/26	0/2/2/2
54	PSU	1w	32	57,54	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	2/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
56	G7M	2y	46	56	-	4/7/25/26	0/3/3/3
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	2/15/33/34	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
56	G7M	1y	46	56	-	2/7/25/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	5MU	2y	54	56	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	57,1,55	-	0/9/27/28	0/3/3/3
55	31H	1x	76	57,55	-	4/22/40/41	0/3/3/3
54	G7M	1w	46	54	-	0/7/25/26	0/3/3/3
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2

The worst 5 of 266 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-11.57	1.70	1.82
43	1l	92	0TD	CB-SB	-10.64	1.71	1.82
43	2l	92	0TD	CB-CA	8.77	1.57	1.54
32	1a	1407	5MC	C5-C4	7.52	1.49	1.44
32	1a	967	5MC	C5-C4	7.04	1.49	1.44

The worst 5 of 490 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	21.91	141.76	102.36
43	2l	92	0TD	CSB-SB-CB	-11.05	82.51	102.36
54	1w	37	MIA	C12-C13-C14	-9.37	110.19	127.01
54	2w	37	MIA	C5-C4-N3	-8.33	118.40	127.18
54	1w	39	PSU	N1-C2-N3	8.04	123.66	115.17

There are no chirality outliers.

5 of 71 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	1w	37	MIA	C12-C13-C14-C16
56	1y	46	G7M	C4'-C5'-O5'-P
32	2a	1207	2MG	N1-C2-N2-CM2
32	2a	1207	2MG	N3-C2-N2-CM2
32	2a	1519	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

47 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	2y	8	4SU	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1402	4OC	2	0
55	2x	76	31H	3	0
32	2a	1400	5MC	4	0
1	1A	1942	5MC	1	0
54	1w	39	PSU	2	0
1	2A	1915	5MU	1	0
1	1A	2503	2MA	1	0
54	2w	37	MIA	2	0
55	1x	32	5MC	1	0
32	2a	966	M2G	2	0
32	1a	1402	4OC	2	0
32	2a	1519	MA6	3	0
1	2A	2552	OMU	1	0
32	2a	1518	MA6	1	0
56	1y	8	4SU	2	0
55	1x	54	5MU	1	0
55	2x	55	PSU	2	0
32	1a	967	5MC	2	0
54	2w	76	F3N	2	0
56	1y	55	PSU	1	0
1	2A	2251	OMG	1	0
54	1w	8	4SU	1	0
32	1a	1518	MA6	2	0
54	2w	54	5MU	3	0
1	2A	2503	2MA	1	0
55	1x	55	PSU	1	0
56	1y	39	PSU	1	0
32	1a	1519	MA6	2	0
32	2a	1207	2MG	2	0
54	2w	55	PSU	1	0
56	1y	37	MIA	3	0
54	2w	8	4SU	2	0
1	1A	2552	OMU	2	0
56	2y	55	PSU	5	0
56	2y	37	MIA	1	0
56	1y	54	5MU	2	0
32	2a	967	5MC	4	0
54	1w	55	PSU	1	0
1	1A	1915	5MU	1	0
54	1w	37	MIA	1	0
56	1y	46	G7M	1	0
1	1A	2251	OMG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	1x	76	31H	1	0
54	1w	46	G7M	1	0
32	1a	966	M2G	2	0
55	2x	8	4SU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2812 ligands modelled in this entry, 2808 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	A1C9N	2A	3885	-	77,79,79	1.97	11 (14%)	107,118,118	2.17	28 (26%)
61	SF4	2d	303	35	0,12,12	-	-	-	-	-
59	A1C9N	1A	4101	-	77,79,79	3.00	12 (15%)	107,118,118	2.38	29 (27%)
61	SF4	1d	302	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
59	A1C9N	2A	3885	-	-	14/82/141/141	1/6/6/6
61	SF4	2d	303	35	-	-	0/6/5/5
59	A1C9N	1A	4101	-	-	14/82/141/141	1/6/6/6
61	SF4	1d	302	35	-	-	0/6/5/5

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1A	4101	A1C9N	B01-OCR	19.21	1.63	1.39
59	1A	4101	A1C9N	B01-OCT	12.44	1.54	1.35
59	2A	3885	A1C9N	B01-OCT	-8.76	1.22	1.35
59	2A	3885	A1C9N	CCQ-CCO	-6.37	1.41	1.50
59	1A	4101	A1C9N	CAU-CAC	-5.50	1.39	1.51

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	1A	4101	A1C9N	B01-OCR-CCQ	-16.14	97.70	110.48
59	2A	3885	A1C9N	B01-OCR-CCQ	-12.64	100.47	110.48
59	1A	4101	A1C9N	OBY-CBZ-NCA	5.88	120.59	111.01
59	2A	3885	A1C9N	OBY-CBZ-NCA	5.40	119.81	111.01
59	2A	3885	A1C9N	CAE-CAB-CAG	-5.36	107.83	115.23

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1A	4101	A1C9N	CBI-CBJ-OCU-CCV
59	1A	4101	A1C9N	CBK-CBJ-OCU-CCV
59	1A	4101	A1C9N	CBX-CBJ-OCU-CCV
59	1A	4101	A1C9N	CBP-CBQ-NBS-CBU
59	2A	3885	A1C9N	CBI-CBJ-OCU-CCV

All (2) ring outliers are listed below:

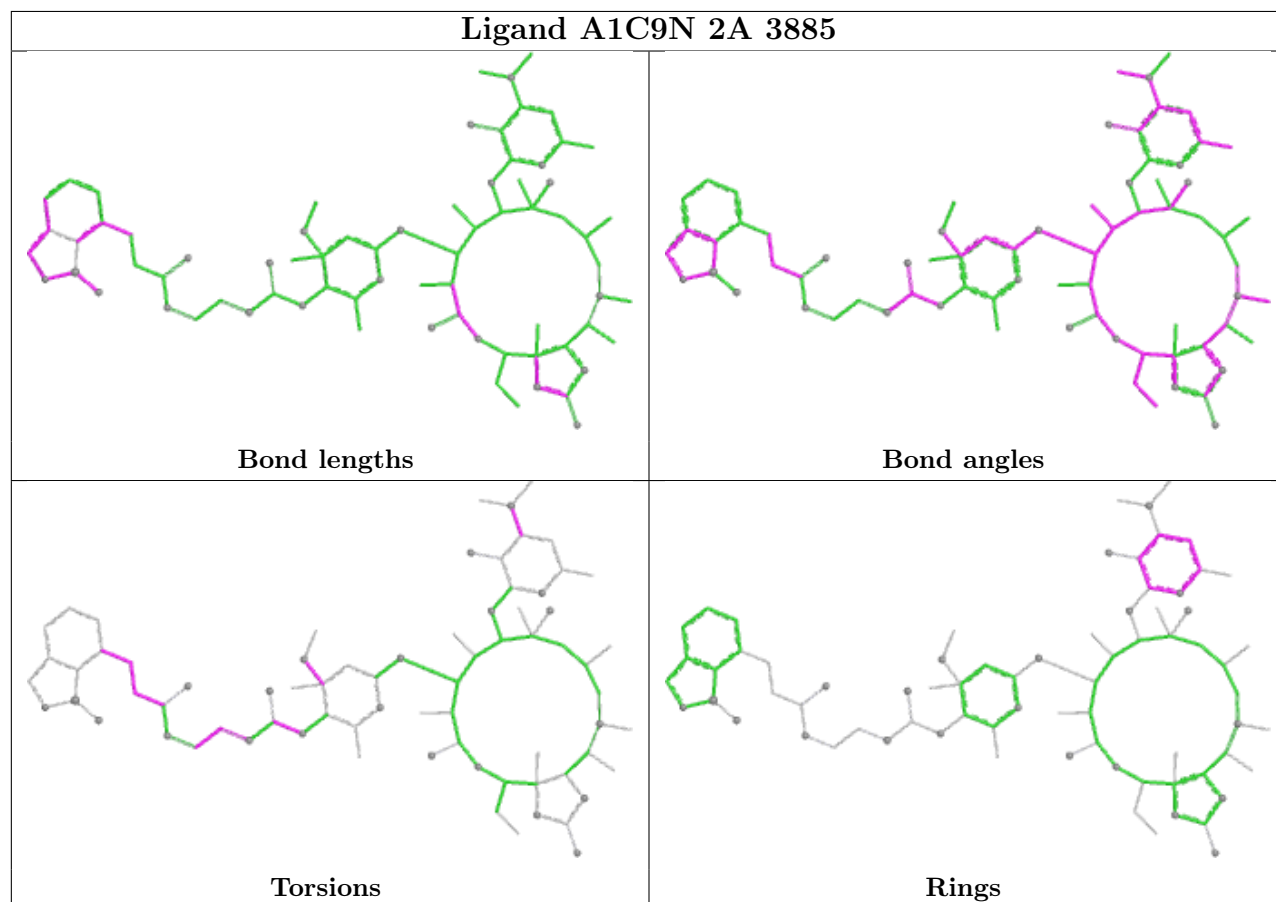
Mol	Chain	Res	Type	Atoms
59	2A	3885	A1C9N	CBL-CBM-CBO-CBP-CBQ-OBN
59	1A	4101	A1C9N	CBL-CBM-CBO-CBP-CBQ-OBN

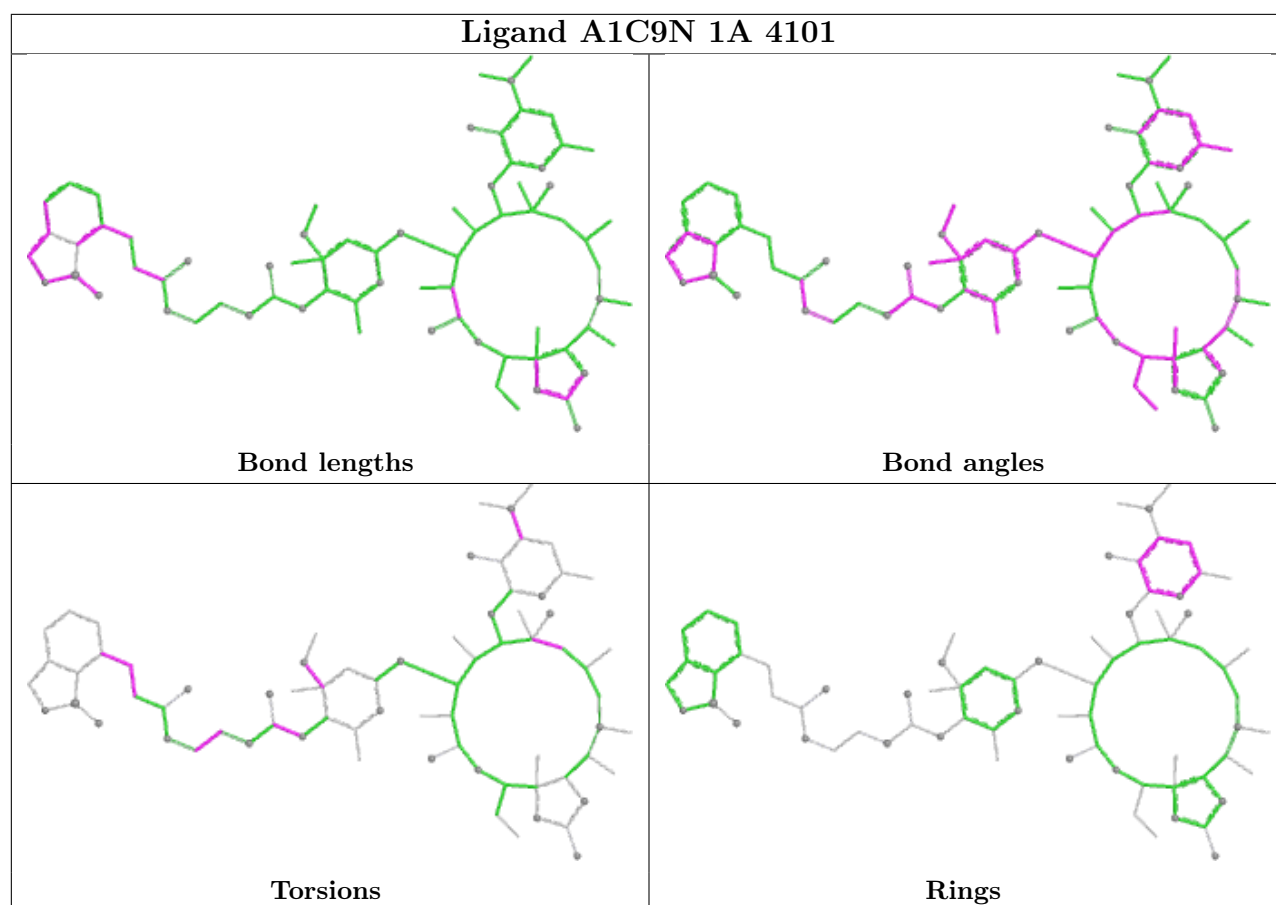
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	1A	4101	A1C9N	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	-0.40	115 (4%) 42 41	14, 32, 79, 89	0
1	2A	2789/2915 (95%)	0.14	99 (3%) 47 47	28, 51, 76, 89	0
2	1B	120/121 (99%)	-0.41	0 100 100	25, 41, 53, 76	0
2	2B	120/121 (99%)	0.82	7 (5%) 29 26	52, 65, 73, 75	0
3	1D	275/276 (99%)	-0.00	1 (0%) 88 89	16, 32, 46, 60	0
3	2D	275/276 (99%)	0.46	5 (1%) 67 69	24, 45, 54, 69	0
4	1E	204/206 (99%)	0.19	1 (0%) 87 88	15, 38, 52, 60	0
4	2E	204/206 (99%)	0.66	9 (4%) 39 38	29, 51, 61, 66	0
5	1F	203/210 (96%)	0.21	3 (1%) 72 74	14, 41, 61, 71	0
5	2F	203/210 (96%)	0.90	11 (5%) 31 29	28, 58, 66, 71	0
6	1G	181/182 (99%)	0.67	2 (1%) 78 79	34, 50, 62, 75	0
6	2G	181/182 (99%)	1.66	54 (29%) 1 1	56, 65, 71, 75	0
7	1H	174/180 (96%)	0.60	5 (2%) 53 55	32, 49, 57, 60	0
7	2H	174/180 (96%)	1.32	25 (14%) 6 4	57, 68, 74, 78	0
8	1I	146/148 (98%)	0.82	6 (4%) 41 41	37, 59, 68, 71	0
8	2I	146/148 (98%)	1.47	34 (23%) 2 1	51, 64, 71, 75	0
9	1N	140/140 (100%)	0.12	1 (0%) 84 86	24, 36, 52, 65	0
9	2N	140/140 (100%)	1.06	12 (8%) 16 14	37, 56, 64, 68	0
10	1O	122/122 (100%)	0.10	0 100 100	24, 36, 50, 56	0
10	2O	122/122 (100%)	0.53	2 (1%) 70 73	33, 49, 58, 64	0
11	1P	149/150 (99%)	0.45	7 (4%) 36 35	15, 43, 61, 67	0
11	2P	149/150 (99%)	0.91	9 (6%) 27 24	35, 56, 69, 76	0
12	1Q	141/141 (100%)	0.10	1 (0%) 84 86	22, 35, 47, 58	0
12	2Q	141/141 (100%)	1.02	8 (5%) 29 26	37, 56, 63, 69	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%)	0.01	0 100 100	19, 31, 42, 48	0
13	2R	118/118 (100%)	0.56	1 (0%) 82 83	32, 44, 56, 64	0
14	1S	110/112 (98%)	0.30	0 100 100	31, 42, 52, 55	0
14	2S	110/112 (98%)	1.49	29 (26%) 1 1	51, 60, 67, 70	0
15	1T	131/146 (89%)	0.44	6 (4%) 37 36	25, 42, 62, 72	0
15	2T	131/146 (89%)	0.65	3 (2%) 61 63	41, 51, 63, 72	0
16	1U	116/118 (98%)	-0.07	0 100 100	20, 30, 42, 48	0
16	2U	116/118 (98%)	0.81	5 (4%) 40 39	38, 56, 64, 72	0
17	1V	101/101 (100%)	-0.01	1 (0%) 79 80	17, 37, 51, 55	0
17	2V	101/101 (100%)	0.87	1 (0%) 79 80	40, 61, 66, 69	0
18	1W	112/113 (99%)	0.12	1 (0%) 81 82	21, 31, 46, 63	0
18	2W	112/113 (99%)	0.77	5 (4%) 38 37	35, 45, 59, 81	0
19	1X	95/96 (98%)	-0.01	2 (2%) 63 65	19, 32, 53, 69	0
19	2X	95/96 (98%)	0.68	1 (1%) 78 79	39, 51, 61, 67	0
20	1Y	107/110 (97%)	0.52	6 (5%) 30 27	32, 43, 58, 67	0
20	2Y	107/110 (97%)	1.39	21 (19%) 3 2	52, 61, 67, 72	0
21	1Z	154/206 (74%)	0.90	14 (9%) 15 12	34, 54, 67, 75	0
21	2Z	160/206 (77%)	1.51	37 (23%) 2 1	54, 66, 73, 76	0
22	10	83/85 (97%)	0.03	0 100 100	21, 31, 41, 56	0
22	20	83/85 (97%)	1.33	15 (18%) 3 3	38, 53, 60, 62	0
23	11	97/98 (98%)	0.30	1 (1%) 79 80	21, 40, 59, 64	0
23	21	97/98 (98%)	0.68	3 (3%) 51 52	35, 49, 61, 67	0
24	12	70/72 (97%)	0.30	3 (4%) 40 39	28, 43, 52, 68	0
24	22	70/72 (97%)	0.97	4 (5%) 29 26	50, 57, 64, 70	0
25	13	59/60 (98%)	0.09	1 (1%) 69 71	20, 33, 50, 57	0
25	23	59/60 (98%)	1.23	7 (11%) 9 7	46, 57, 69, 72	0
26	14	69/71 (97%)	1.14	13 (18%) 3 2	39, 59, 74, 79	0
26	24	69/71 (97%)	1.77	23 (33%) 1 1	61, 70, 77, 79	0
27	15	59/60 (98%)	-0.03	1 (1%) 69 71	17, 30, 43, 48	0
27	25	59/60 (98%)	0.61	3 (5%) 33 31	28, 45, 57, 62	0
28	16	53/54 (98%)	0.12	0 100 100	26, 36, 46, 52	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.94	5 (9%) 14 11	43, 53, 60, 64	0
29	17	48/49 (97%)	-0.19	1 (2%) 63 65	15, 24, 39, 49	0
29	27	48/49 (97%)	0.36	2 (4%) 40 40	26, 39, 50, 63	0
30	18	64/65 (98%)	-0.01	1 (1%) 70 73	22, 29, 37, 40	0
30	28	64/65 (98%)	0.78	6 (9%) 14 11	37, 48, 54, 57	0
31	19	37/37 (100%)	0.20	1 (2%) 56 57	29, 36, 49, 55	0
31	29	37/37 (100%)	1.40	6 (16%) 4 3	54, 59, 66, 70	0
32	1a	1488/1521 (97%)	0.13	29 (1%) 66 67	29, 53, 76, 88	0
32	2a	1491/1521 (98%)	0.53	48 (3%) 50 51	39, 62, 78, 90	0
33	1b	231/256 (90%)	1.11	28 (12%) 8 7	49, 62, 72, 78	0
33	2b	231/256 (90%)	1.59	69 (29%) 1 1	59, 70, 75, 78	0
34	1c	206/239 (86%)	0.81	11 (5%) 32 30	45, 56, 67, 74	0
34	2c	206/239 (86%)	1.50	45 (21%) 2 2	55, 67, 73, 77	0
35	1d	208/209 (99%)	0.72	5 (2%) 59 62	44, 54, 61, 66	0
35	2d	208/209 (99%)	1.13	21 (10%) 12 10	43, 55, 63, 72	0
36	1e	148/162 (91%)	0.63	5 (3%) 48 48	40, 52, 61, 72	0
36	2e	148/162 (91%)	1.09	12 (8%) 18 16	52, 62, 67, 74	0
37	1f	100/101 (99%)	0.50	1 (1%) 79 80	37, 49, 60, 67	0
37	2f	100/101 (99%)	0.74	3 (3%) 52 53	49, 58, 65, 70	0
38	1g	155/156 (99%)	1.04	19 (12%) 8 7	46, 56, 67, 73	0
38	2g	155/156 (99%)	1.22	27 (17%) 4 3	58, 66, 73, 81	0
39	1h	137/138 (99%)	0.69	3 (2%) 62 64	46, 54, 61, 65	0
39	2h	137/138 (99%)	1.17	13 (9%) 14 11	55, 63, 69, 71	0
40	1i	127/128 (99%)	1.13	12 (9%) 14 11	40, 58, 68, 72	0
40	2i	127/128 (99%)	1.96	53 (41%) 0 0	58, 68, 72, 75	0
41	1j	97/105 (92%)	1.18	13 (13%) 7 6	43, 61, 70, 74	0
41	2j	96/105 (91%)	1.82	36 (37%) 1 0	57, 68, 73, 77	0
42	1k	114/129 (88%)	0.78	7 (6%) 27 24	35, 53, 62, 66	0
42	2k	114/129 (88%)	1.03	9 (7%) 18 16	47, 61, 68, 70	0
43	1l	121/132 (91%)	0.40	4 (3%) 49 50	36, 44, 53, 63	0
43	2l	121/132 (91%)	0.84	6 (4%) 34 32	43, 54, 61, 67	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	1.01	10 (8%) 18 16	41, 56, 64, 69	0
44	2m	122/126 (96%)	1.77	36 (29%) 1 1	60, 67, 72, 74	0
45	1n	60/61 (98%)	0.77	2 (3%) 49 50	43, 51, 60, 60	0
45	2n	60/61 (98%)	2.09	28 (46%) 0 0	61, 66, 71, 73	0
46	1o	88/89 (98%)	0.81	3 (3%) 48 48	38, 51, 61, 63	0
46	2o	88/89 (98%)	0.98	3 (3%) 48 48	50, 58, 65, 70	0
47	1p	82/88 (93%)	1.17	7 (8%) 16 14	47, 56, 61, 64	0
47	2p	82/88 (93%)	0.92	7 (8%) 16 14	46, 54, 60, 65	0
48	1q	99/105 (94%)	0.99	3 (3%) 52 53	41, 54, 62, 67	0
48	2q	99/105 (94%)	1.04	9 (9%) 15 12	52, 60, 66, 70	0
49	1r	68/88 (77%)	0.49	1 (1%) 72 74	43, 51, 60, 65	0
49	2r	68/88 (77%)	0.88	5 (7%) 20 18	53, 61, 66, 70	0
50	1s	83/93 (89%)	0.81	3 (3%) 46 46	46, 56, 64, 69	0
50	2s	83/93 (89%)	1.71	28 (33%) 1 1	60, 68, 73, 77	0
51	1t	96/106 (90%)	1.08	12 (12%) 8 6	51, 57, 66, 71	0
51	2t	96/106 (90%)	0.98	7 (7%) 21 18	48, 56, 67, 69	0
52	1u	23/27 (85%)	1.26	2 (8%) 16 14	51, 54, 58, 62	0
52	2u	23/27 (85%)	2.55	15 (65%) 0 0	61, 68, 72, 73	0
53	1v	13/24 (54%)	0.57	3 (23%) 2 1	37, 43, 77, 83	0
53	2v	13/24 (54%)	1.47	5 (38%) 1 0	53, 62, 80, 84	0
54	1w	66/76 (86%)	0.97	12 (18%) 3 3	23, 69, 79, 83	0
54	2w	64/76 (84%)	1.16	10 (15%) 5 3	40, 77, 82, 87	0
55	1x	72/77 (93%)	0.22	1 (1%) 73 75	19, 52, 67, 77	0
55	2x	72/77 (93%)	0.58	1 (1%) 73 75	34, 63, 71, 78	0
56	1y	67/76 (88%)	1.28	7 (10%) 11 9	48, 80, 84, 86	0
56	2y	66/76 (86%)	1.53	11 (16%) 4 3	59, 82, 85, 87	0
All	All	20873/21748 (95%)	0.49	1356 (6%) 25 22	14, 53, 73, 90	0

The worst 5 of 1356 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	7.4
1	2A	882	G	6.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2146	C	6.3
1	2A	883	G	6.1
44	2m	124	PRO	5.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	G7M	2y	46	24/25	0.49	0.16	67,84,89,96	0
56	PSU	2y	55	20/21	0.59	0.16	75,82,88,102	0
56	G7M	1y	46	24/25	0.60	0.15	76,84,88,94	0
56	4SU	2y	8	20/21	0.65	0.14	73,83,93,99	0
56	5MU	2y	54	21/22	0.67	0.14	66,79,92,103	0
54	G7M	2w	46	24/25	0.68	0.14	69,76,88,94	0
56	MIA	2y	37	22/30	0.69	0.16	68,75,94,99	0
56	4SU	1y	8	20/21	0.70	0.13	79,84,92,103	0
56	MIA	1y	37	22/30	0.71	0.15	63,72,80,94	0
56	PSU	1y	32	20/21	0.71	0.16	70,76,94,100	0
56	5MU	1y	54	21/22	0.73	0.13	66,78,83,96	0
56	PSU	2y	39	20/21	0.74	0.18	72,79,86,94	0
56	PSU	1y	55	20/21	0.75	0.13	71,78,93,93	0
54	G7M	1w	46	24/25	0.75	0.14	57,67,87,98	0
56	PSU	2y	32	20/21	0.77	0.15	62,78,87,90	0
56	PSU	1y	39	20/21	0.81	0.14	68,74,78,79	0
54	4SU	2w	8	20/21	0.82	0.12	68,73,87,88	0
32	2MG	2a	1207	24/25	0.86	0.13	61,66,74,75	0
55	4SU	2x	8	20/21	0.87	0.11	58,62,73,75	0
55	5MU	2x	54	21/22	0.88	0.12	58,67,72,77	0
54	5MU	2w	54	21/22	0.88	0.10	57,66,69,72	0
54	PSU	2w	55	20/21	0.88	0.10	63,69,75,77	0
54	PSU	2w	32	20/21	0.88	0.13	59,64,73,73	0
55	PSU	2x	55	20/21	0.89	0.12	58,63,73,79	0
54	PSU	2w	39	20/21	0.89	0.12	56,65,68,70	0
55	5MC	2x	32	21/22	0.89	0.16	52,57,65,66	0
32	PSU	2a	516	20/21	0.89	0.12	54,60,64,66	0
43	0TD	2l	92	10/11	0.90	0.14	46,53,58,65	0
1	PSU	2A	1917	20/21	0.90	0.11	42,52,59,63	0
54	PSU	1w	55	20/21	0.91	0.10	55,61,67,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	4SU	1x	8	20/21	0.91	0.12	47,55,62,63	0
54	PSU	1w	32	20/21	0.91	0.12	47,51,58,61	0
1	OMC	2A	1920	21/22	0.92	0.10	46,52,56,57	0
32	5MC	2a	1407	21/22	0.92	0.12	46,52,55,61	0
55	5MU	1x	54	21/22	0.92	0.11	46,54,59,61	0
32	G7M	2a	527	24/25	0.92	0.11	48,56,62,67	0
32	5MC	2a	967	21/22	0.92	0.14	54,61,64,70	0
32	M2G	2a	966	25/26	0.93	0.14	56,62,69,72	0
1	5MU	1A	1915	21/22	0.93	0.11	38,42,50,58	0
55	PSU	1x	55	20/21	0.93	0.09	45,51,59,63	0
32	5MC	2a	1400	21/22	0.93	0.14	46,57,64,70	0
32	5MC	2a	1404	21/22	0.93	0.12	41,53,57,60	0
1	5MC	2A	1942	21/22	0.93	0.11	42,53,59,64	0
54	4SU	1w	8	20/21	0.93	0.11	56,67,72,74	0
1	PSU	2A	1911	20/21	0.93	0.11	44,56,64,66	0
54	5MU	1w	54	21/22	0.94	0.09	45,50,58,66	0
1	5MU	2A	1915	21/22	0.94	0.09	47,56,60,62	0
32	4OC	2a	1402	22/23	0.94	0.11	48,56,58,62	0
32	2MG	1a	1207	24/25	0.94	0.10	43,51,55,65	0
54	MIA	2w	37	25/30	0.94	0.10	50,60,63,65	0
32	MA6	2a	1518	24/25	0.95	0.10	48,54,60,65	0
32	MA6	2a	1519	24/25	0.95	0.12	42,53,57,60	0
1	OMU	2A	2552	21/22	0.95	0.09	34,40,43,47	0
1	OMC	1A	1920	21/22	0.95	0.08	29,37,39,41	0
32	PSU	1a	516	20/21	0.95	0.09	32,47,51,51	0
1	PSU	1A	1911	20/21	0.95	0.08	36,40,47,51	0
43	0TD	1l	92	10/11	0.95	0.09	36,42,45,47	0
54	PSU	1w	39	20/21	0.96	0.08	39,48,51,52	0
32	5MC	1a	1400	21/22	0.96	0.10	28,38,45,49	0
32	4OC	1a	1402	22/23	0.96	0.09	32,38,41,46	0
32	5MC	1a	1404	21/22	0.96	0.08	28,32,37,40	0
32	MA6	1a	1518	24/25	0.96	0.10	32,38,42,42	0
55	5MC	1x	32	21/22	0.96	0.08	35,39,44,49	0
32	MA6	1a	1519	24/25	0.96	0.09	30,37,41,42	0
32	M2G	1a	966	25/26	0.96	0.08	34,41,47,48	0
55	31H	2x	76	32/33	0.96	0.09	26,34,39,49	0
32	UR3	2a	1498	21/22	0.96	0.11	42,51,56,57	0
32	5MC	1a	967	21/22	0.96	0.09	31,41,48,50	0
1	5MC	2A	1962	21/22	0.96	0.10	28,42,48,53	0
1	OMG	2A	2251	24/25	0.96	0.09	29,34,40,42	0
1	5MC	1A	1942	21/22	0.96	0.08	33,38,41,51	0
1	PSU	2A	2605	20/21	0.96	0.08	25,36,39,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MIA	1w	37	29/30	0.96	0.09	38,46,53,54	0
32	G7M	1a	527	24/25	0.97	0.07	30,35,44,47	0
1	2MA	2A	2503	23/24	0.97	0.07	25,31,39,39	0
32	5MC	1a	1407	21/22	0.97	0.07	26,31,34,40	0
54	F3N	2w	76	33/34	0.97	0.09	27,33,37,42	0
1	OMG	1A	2251	24/25	0.97	0.07	16,21,28,30	0
1	PSU	1A	1917	20/21	0.97	0.08	26,36,45,46	0
55	31H	1x	76	32/33	0.97	0.08	16,21,26,30	10
54	F3N	1w	76	33/34	0.97	0.07	15,19,23,28	0
1	5MC	1A	1962	21/22	0.98	0.07	22,26,38,41	0
1	5MU	1A	1939	21/22	0.98	0.07	20,24,26,27	0
1	5MU	2A	1939	21/22	0.98	0.06	24,33,39,43	0
1	2MA	1A	2503	23/24	0.98	0.06	11,18,23,23	0
1	OMU	1A	2552	21/22	0.98	0.07	20,25,30,33	0
32	UR3	1a	1498	21/22	0.98	0.06	22,32,35,39	0
1	PSU	1A	2605	20/21	0.98	0.07	17,22,27,29	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3246	1/1	0.48	0.32	74,74,74,74	0
57	MG	2a	1818	1/1	0.48	0.20	78,78,78,78	0
57	MG	2a	1788	1/1	0.55	0.25	69,69,69,69	0
57	MG	2A	3506	1/1	0.56	0.33	82,82,82,82	0
57	MG	2A	3562	1/1	0.56	0.20	64,64,64,64	0
57	MG	1A	4008	1/1	0.60	0.13	77,77,77,77	0
57	MG	2A	3884	1/1	0.62	0.24	75,75,75,75	0
57	MG	2a	1618	1/1	0.62	0.24	70,70,70,70	0
57	MG	2A	3730	1/1	0.63	0.18	74,74,74,74	0
57	MG	1A	3292	1/1	0.64	0.32	59,59,59,59	0
57	MG	1A	3467	1/1	0.66	0.27	71,71,71,71	0
57	MG	1a	1613	1/1	0.67	0.23	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1A	3948	1/1	0.67	0.13	57,57,57,57	0
57	MG	1A	3516	1/1	0.67	0.28	66,66,66,66	0
57	MG	2a	1624	1/1	0.68	0.34	76,76,76,76	0
57	MG	2a	1711	1/1	0.68	0.34	73,73,73,73	0
57	MG	2A	3289	1/1	0.68	0.19	73,73,73,73	0
57	MG	2A	3004	1/1	0.68	0.27	66,66,66,66	0
57	MG	2a	1822	1/1	0.68	0.20	60,60,60,60	0
57	MG	2A	3607	1/1	0.69	0.18	59,59,59,59	0
57	MG	1A	3978	1/1	0.69	0.22	79,79,79,79	0
57	MG	2A	3761	1/1	0.69	0.25	60,60,60,60	0
57	MG	2a	1629	1/1	0.69	0.21	60,60,60,60	0
57	MG	1B	233	1/1	0.70	0.19	71,71,71,71	0
57	MG	2A	3670	1/1	0.70	0.18	66,66,66,66	0
57	MG	2A	3059	1/1	0.71	0.29	69,69,69,69	0
57	MG	2A	3103	1/1	0.71	0.27	62,62,62,62	0
57	MG	2A	3554	1/1	0.71	0.25	53,53,53,53	0
57	MG	2A	3807	1/1	0.71	0.18	68,68,68,68	0
57	MG	2A	3196	1/1	0.71	0.22	71,71,71,71	0
57	MG	1w	102	1/1	0.71	0.13	73,73,73,73	0
57	MG	2B	202	1/1	0.72	0.23	76,76,76,76	0
57	MG	10	106	1/1	0.72	0.17	46,46,46,46	0
57	MG	1A	4073	1/1	0.72	0.17	57,57,57,57	0
57	MG	2A	3596	1/1	0.72	0.21	76,76,76,76	0
57	MG	2B	212	1/1	0.73	0.32	81,81,81,81	0
57	MG	1A	3884	1/1	0.73	0.15	64,64,64,64	0
57	MG	2A	3501	1/1	0.73	0.14	71,71,71,71	0
57	MG	1A	3887	1/1	0.73	0.21	42,42,42,42	0
57	MG	1A	3858	1/1	0.73	0.16	64,64,64,64	0
57	MG	1A	4094	1/1	0.73	0.18	77,77,77,77	0
57	MG	1x	101	1/1	0.73	0.24	65,65,65,65	0
57	MG	2a	1821	1/1	0.73	0.19	53,53,53,53	0
57	MG	2A	3599	1/1	0.73	0.14	59,59,59,59	0
57	MG	2y	106	1/1	0.73	0.17	73,73,73,73	0
57	MG	1A	3269	1/1	0.74	0.22	65,65,65,65	0
57	MG	1A	3944	1/1	0.74	0.18	40,40,40,40	0
57	MG	29	101	1/1	0.74	0.52	71,71,71,71	0
57	MG	2A	3868	1/1	0.74	0.19	69,69,69,69	0
57	MG	1A	3612	1/1	0.74	0.14	57,57,57,57	0
57	MG	2w	103	1/1	0.74	0.18	62,62,62,62	0
57	MG	2B	201	1/1	0.74	0.22	62,62,62,62	0
57	MG	2A	3344	1/1	0.75	0.16	72,72,72,72	0
57	MG	2a	1771	1/1	0.75	0.15	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3955	1/1	0.75	0.17	59,59,59,59	0
57	MG	2a	1798	1/1	0.75	0.17	54,54,54,54	0
57	MG	1A	3838	1/1	0.75	0.22	65,65,65,65	0
57	MG	2A	3243	1/1	0.75	0.19	68,68,68,68	0
57	MG	1a	1676	1/1	0.75	0.31	73,73,73,73	0
57	MG	1a	1743	1/1	0.75	0.20	61,61,61,61	0
57	MG	2A	3322	1/1	0.75	0.23	74,74,74,74	0
57	MG	1A	3675	1/1	0.76	0.11	48,48,48,48	0
57	MG	2A	3192	1/1	0.76	0.18	69,69,69,69	0
57	MG	2A	3414	1/1	0.76	0.13	72,72,72,72	0
57	MG	2A	3262	1/1	0.76	0.34	61,61,61,61	0
57	MG	2A	3606	1/1	0.76	0.12	65,65,65,65	0
57	MG	2j	202	1/1	0.76	0.14	62,62,62,62	0
57	MG	1A	3874	1/1	0.76	0.18	26,26,26,26	0
57	MG	2w	105	1/1	0.76	0.19	77,77,77,77	0
57	MG	2A	3539	1/1	0.76	0.19	54,54,54,54	0
57	MG	1A	3544	1/1	0.77	0.20	67,67,67,67	0
57	MG	1A	4017	1/1	0.77	0.11	38,38,38,38	0
57	MG	2A	3614	1/1	0.77	0.14	55,55,55,55	0
57	MG	1A	4025	1/1	0.77	0.12	59,59,59,59	0
57	MG	2a	1641	1/1	0.77	0.20	64,64,64,64	0
57	MG	2A	3106	1/1	0.77	0.20	73,73,73,73	0
57	MG	1A	3651	1/1	0.77	0.10	35,35,35,35	0
57	MG	2T	203	1/1	0.77	0.21	64,64,64,64	0
57	MG	2A	3348	1/1	0.78	0.16	62,62,62,62	0
57	MG	2a	1644	1/1	0.78	0.33	69,69,69,69	0
57	MG	2A	3370	1/1	0.78	0.28	73,73,73,73	0
57	MG	1A	3805	1/1	0.78	0.14	53,53,53,53	0
57	MG	1w	105	1/1	0.78	0.13	73,73,73,73	0
57	MG	2A	3283	1/1	0.78	0.24	63,63,63,63	0
57	MG	1A	3986	1/1	0.78	0.29	77,77,77,77	0
57	MG	1A	3551	1/1	0.78	0.13	61,61,61,61	0
57	MG	2A	3747	1/1	0.78	0.18	57,57,57,57	0
57	MG	2a	1610	1/1	0.78	0.18	69,69,69,69	0
57	MG	2p	101	1/1	0.78	0.17	53,53,53,53	0
57	MG	1A	3695	1/1	0.78	0.10	30,30,30,30	0
57	MG	2A	3768	1/1	0.78	0.13	56,56,56,56	0
57	MG	2A	3779	1/1	0.78	0.23	60,60,60,60	0
57	MG	2A	3461	1/1	0.79	0.22	64,64,64,64	0
57	MG	1A	4057	1/1	0.79	0.13	47,47,47,47	0
57	MG	2a	1695	1/1	0.79	0.25	66,66,66,66	0
57	MG	1A	4021	1/1	0.79	0.14	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3102	1/1	0.79	0.29	66,66,66,66	0
57	MG	2A	3687	1/1	0.79	0.15	62,62,62,62	0
57	MG	2B	211	1/1	0.79	0.20	64,64,64,64	0
57	MG	2A	3713	1/1	0.79	0.12	58,58,58,58	0
57	MG	1A	3646	1/1	0.79	0.14	54,54,54,54	0
57	MG	1A	4097	1/1	0.79	0.17	65,65,65,65	0
57	MG	2A	3750	1/1	0.79	0.15	64,64,64,64	0
57	MG	2A	3568	1/1	0.79	0.17	50,50,50,50	0
57	MG	2A	3110	1/1	0.79	0.13	65,65,65,65	0
57	MG	2A	3446	1/1	0.79	0.20	54,54,54,54	0
57	MG	2x	104	1/1	0.79	0.20	60,60,60,60	0
57	MG	2a	1630	1/1	0.79	0.33	67,67,67,67	0
57	MG	2a	1620	1/1	0.80	0.19	61,61,61,61	0
57	MG	1A	3428	1/1	0.80	0.20	66,66,66,66	0
57	MG	1A	3965	1/1	0.80	0.09	18,18,18,18	0
57	MG	1a	1804	1/1	0.80	0.12	39,39,39,39	0
57	MG	2A	3410	1/1	0.80	0.17	71,71,71,71	0
57	MG	2A	3412	1/1	0.80	0.12	61,61,61,61	0
57	MG	2A	3809	1/1	0.80	0.16	61,61,61,61	0
57	MG	2A	3820	1/1	0.80	0.14	58,58,58,58	0
57	MG	2a	1743	1/1	0.80	0.27	68,68,68,68	0
57	MG	1A	4048	1/1	0.80	0.11	24,24,24,24	0
57	MG	1A	4009	1/1	0.80	0.15	57,57,57,57	0
57	MG	2A	3663	1/1	0.80	0.16	76,76,76,76	0
57	MG	2A	3272	1/1	0.80	0.13	76,76,76,76	0
57	MG	1A	3418	1/1	0.80	0.21	65,65,65,65	0
57	MG	2A	3689	1/1	0.80	0.14	65,65,65,65	0
57	MG	2B	216	1/1	0.80	0.15	69,69,69,69	0
57	MG	2B	220	1/1	0.80	0.25	58,58,58,58	0
57	MG	2v	101	1/1	0.80	0.17	74,74,74,74	0
57	MG	2A	3115	1/1	0.80	0.24	55,55,55,55	0
57	MG	2A	3718	1/1	0.80	0.15	59,59,59,59	0
57	MG	2A	3116	1/1	0.80	0.22	57,57,57,57	0
57	MG	2A	3326	1/1	0.80	0.21	59,59,59,59	0
57	MG	1v	101	1/1	0.81	0.16	59,59,59,59	0
57	MG	1a	1623	1/1	0.81	0.27	58,58,58,58	0
57	MG	2A	3349	1/1	0.81	0.18	68,68,68,68	0
57	MG	2a	1748	1/1	0.81	0.14	73,73,73,73	0
57	MG	2A	3255	1/1	0.81	0.09	69,69,69,69	0
57	MG	2A	3748	1/1	0.81	0.17	59,59,59,59	0
57	MG	2G	201	1/1	0.81	0.25	56,56,56,56	0
57	MG	2a	1803	1/1	0.81	0.26	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3380	1/1	0.81	0.23	72,72,72,72	0
57	MG	1a	1642	1/1	0.81	0.16	64,64,64,64	0
57	MG	1U	210	1/1	0.81	0.22	43,43,43,43	0
57	MG	1A	3725	1/1	0.81	0.15	49,49,49,49	0
57	MG	2A	3430	1/1	0.81	0.32	60,60,60,60	0
57	MG	2A	3187	1/1	0.81	0.14	68,68,68,68	0
57	MG	2A	3304	1/1	0.81	0.14	74,74,74,74	0
57	MG	2w	104	1/1	0.81	0.14	81,81,81,81	0
57	MG	1A	3956	1/1	0.81	0.13	66,66,66,66	0
57	MG	1a	1810	1/1	0.81	0.18	63,63,63,63	0
57	MG	2A	3695	1/1	0.81	0.17	57,57,57,57	0
57	MG	2A	3275	1/1	0.82	0.22	64,64,64,64	0
57	MG	2A	3276	1/1	0.82	0.19	74,74,74,74	0
57	MG	1a	1789	1/1	0.82	0.22	69,69,69,69	0
57	MG	1A	3964	1/1	0.82	0.08	46,46,46,46	0
57	MG	2A	3301	1/1	0.82	0.20	58,58,58,58	0
57	MG	1A	3722	1/1	0.82	0.11	52,52,52,52	0
57	MG	1e	201	1/1	0.82	0.11	65,65,65,65	0
57	MG	2a	1726	1/1	0.82	0.16	58,58,58,58	0
57	MG	2A	3111	1/1	0.82	0.19	60,60,60,60	0
57	MG	2a	1744	1/1	0.82	0.14	78,78,78,78	0
57	MG	1m	3002	1/1	0.82	0.20	57,57,57,57	0
57	MG	2A	3879	1/1	0.82	0.19	57,57,57,57	0
57	MG	1B	209	1/1	0.82	0.12	60,60,60,60	0
57	MG	1A	3233	1/1	0.82	0.15	59,59,59,59	0
57	MG	2A	3354	1/1	0.82	0.16	70,70,70,70	0
57	MG	1H	201	1/1	0.82	0.12	63,63,63,63	0
57	MG	1a	1697	1/1	0.82	0.28	59,59,59,59	0
57	MG	2A	3213	1/1	0.82	0.14	56,56,56,56	0
57	MG	1A	4091	1/1	0.82	0.09	71,71,71,71	0
57	MG	2E	306	1/1	0.82	0.20	49,49,49,49	0
57	MG	2A	3705	1/1	0.82	0.23	60,60,60,60	0
57	MG	2A	3709	1/1	0.82	0.09	71,71,71,71	0
57	MG	2A	3008	1/1	0.82	0.21	59,59,59,59	0
57	MG	2A	3031	1/1	0.82	0.22	67,67,67,67	0
57	MG	1a	1753	1/1	0.82	0.18	58,58,58,58	0
57	MG	2A	3101	1/1	0.82	0.20	66,66,66,66	0
57	MG	1A	4029	1/1	0.83	0.11	52,52,52,52	0
57	MG	10	107	1/1	0.83	0.16	60,60,60,60	0
57	MG	1A	3664	1/1	0.83	0.09	27,27,27,27	0
57	MG	1A	3775	1/1	0.83	0.07	12,12,12,12	0
57	MG	1A	4071	1/1	0.83	0.09	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3980	1/1	0.83	0.10	58,58,58,58	0
57	MG	2A	3488	1/1	0.83	0.16	61,61,61,61	0
57	MG	2A	3090	1/1	0.83	0.16	50,50,50,50	0
57	MG	2a	1656	1/1	0.83	0.23	72,72,72,72	0
57	MG	1A	3623	1/1	0.83	0.12	57,57,57,57	0
57	MG	1A	3996	1/1	0.83	0.11	54,54,54,54	0
57	MG	2A	3292	1/1	0.83	0.14	77,77,77,77	0
57	MG	1a	1749	1/1	0.83	0.16	54,54,54,54	0
57	MG	1A	3312	1/1	0.83	0.11	52,52,52,52	0
57	MG	2A	3587	1/1	0.83	0.17	55,55,55,55	0
57	MG	2A	3854	1/1	0.83	0.28	63,63,63,63	0
57	MG	1a	1768	1/1	0.83	0.08	48,48,48,48	0
57	MG	1A	3952	1/1	0.83	0.12	57,57,57,57	0
57	MG	1B	228	1/1	0.83	0.10	68,68,68,68	0
57	MG	2a	1809	1/1	0.83	0.16	64,64,64,64	0
57	MG	1B	229	1/1	0.83	0.20	60,60,60,60	0
57	MG	1A	3713	1/1	0.83	0.13	50,50,50,50	0
57	MG	2A	3654	1/1	0.83	0.18	60,60,60,60	0
57	MG	2A	3658	1/1	0.83	0.18	54,54,54,54	0
57	MG	1A	3866	1/1	0.83	0.21	32,32,32,32	0
57	MG	2A	3363	1/1	0.83	0.17	61,61,61,61	0
57	MG	2w	101	1/1	0.83	0.23	59,59,59,59	0
57	MG	2A	3366	1/1	0.83	0.13	50,50,50,50	0
57	MG	1A	3250	1/1	0.83	0.18	60,60,60,60	0
57	MG	1Z	3702	1/1	0.83	0.11	63,63,63,63	0
57	MG	2A	3701	1/1	0.83	0.12	63,63,63,63	0
57	MG	2a	1601	1/1	0.83	0.17	59,59,59,59	0
57	MG	2A	3558	1/1	0.84	0.12	48,48,48,48	0
57	MG	2A	3759	1/1	0.84	0.17	54,54,54,54	0
57	MG	2A	3068	1/1	0.84	0.16	62,62,62,62	0
57	MG	2A	3072	1/1	0.84	0.12	57,57,57,57	0
57	MG	2A	3219	1/1	0.84	0.14	60,60,60,60	0
57	MG	1S	203	1/1	0.84	0.13	61,61,61,61	0
57	MG	2a	1665	1/1	0.84	0.13	57,57,57,57	0
57	MG	1A	3511	1/1	0.84	0.14	65,65,65,65	0
57	MG	1A	3730	1/1	0.84	0.17	64,64,64,64	0
57	MG	10	102	1/1	0.84	0.36	63,63,63,63	0
57	MG	2A	3611	1/1	0.84	0.17	51,51,51,51	0
57	MG	2A	3266	1/1	0.84	0.18	52,52,52,52	0
57	MG	2A	3882	1/1	0.84	0.16	65,65,65,65	0
57	MG	2A	3372	1/1	0.84	0.11	67,67,67,67	0
57	MG	2A	3376	1/1	0.84	0.12	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3738	1/1	0.84	0.12	52,52,52,52	0
57	MG	2A	3387	1/1	0.84	0.13	60,60,60,60	0
57	MG	1A	3060	1/1	0.84	0.13	58,58,58,58	0
57	MG	1x	102	1/1	0.84	0.15	62,62,62,62	0
57	MG	2B	217	1/1	0.84	0.14	54,54,54,54	0
57	MG	1a	1785	1/1	0.84	0.15	53,53,53,53	0
57	MG	2a	1829	1/1	0.84	0.12	57,57,57,57	0
57	MG	1A	3979	1/1	0.84	0.09	30,30,30,30	0
57	MG	2l	203	1/1	0.84	0.14	62,62,62,62	0
57	MG	2A	3291	1/1	0.84	0.20	67,67,67,67	0
57	MG	2A	3171	1/1	0.84	0.17	62,62,62,62	0
57	MG	2V	202	1/1	0.84	0.15	59,59,59,59	0
57	MG	2A	3295	1/1	0.84	0.31	65,65,65,65	0
57	MG	2A	3176	1/1	0.84	0.11	49,49,49,49	0
57	MG	1A	3679	1/1	0.84	0.09	19,19,19,19	0
57	MG	2A	3316	1/1	0.84	0.26	58,58,58,58	0
57	MG	2y	104	1/1	0.84	0.09	71,71,71,71	0
57	MG	1A	4024	1/1	0.84	0.20	50,50,50,50	0
57	MG	1l	104	1/1	0.85	0.11	50,50,50,50	0
57	MG	2A	3320	1/1	0.85	0.15	55,55,55,55	0
57	MG	2E	301	1/1	0.85	0.11	58,58,58,58	0
57	MG	2A	3122	1/1	0.85	0.14	58,58,58,58	0
57	MG	1w	103	1/1	0.85	0.09	55,55,55,55	0
57	MG	1A	3487	1/1	0.85	0.13	62,62,62,62	0
57	MG	2A	3178	1/1	0.85	0.17	61,61,61,61	0
57	MG	27	101	1/1	0.85	0.26	58,58,58,58	0
57	MG	2A	3184	1/1	0.85	0.21	56,56,56,56	0
57	MG	1w	106	1/1	0.85	0.10	42,42,42,42	0
57	MG	2A	3684	1/1	0.85	0.10	62,62,62,62	0
57	MG	1A	3596	1/1	0.85	0.16	60,60,60,60	0
57	MG	1A	3492	1/1	0.85	0.18	50,50,50,50	0
57	MG	2A	3206	1/1	0.85	0.18	62,62,62,62	0
57	MG	2A	3211	1/1	0.85	0.10	64,64,64,64	0
57	MG	1x	112	1/1	0.85	0.11	54,54,54,54	0
57	MG	2A	3707	1/1	0.85	0.12	57,57,57,57	0
57	MG	1a	1649	1/1	0.85	0.12	57,57,57,57	0
57	MG	2A	3382	1/1	0.85	0.16	47,47,47,47	0
57	MG	1A	3752	1/1	0.85	0.23	57,57,57,57	0
57	MG	2A	3399	1/1	0.85	0.14	64,64,64,64	0
57	MG	2A	3406	1/1	0.85	0.16	65,65,65,65	0
57	MG	2a	1714	1/1	0.85	0.17	62,62,62,62	0
57	MG	1A	3204	1/1	0.85	0.14	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4001	1/1	0.85	0.08	24,24,24,24	0
57	MG	1A	3947	1/1	0.85	0.10	23,23,23,23	0
57	MG	1A	3122	1/1	0.85	0.13	35,35,35,35	0
57	MG	2a	1756	1/1	0.85	0.15	64,64,64,64	0
57	MG	2A	3075	1/1	0.85	0.13	63,63,63,63	0
57	MG	2A	3776	1/1	0.85	0.11	65,65,65,65	0
57	MG	1A	3718	1/1	0.85	0.09	58,58,58,58	0
57	MG	2A	3094	1/1	0.85	0.18	38,38,38,38	0
57	MG	1A	3844	1/1	0.85	0.12	42,42,42,42	0
57	MG	2a	1812	1/1	0.85	0.13	70,70,70,70	0
57	MG	2A	3285	1/1	0.85	0.13	53,53,53,53	0
57	MG	2A	3839	1/1	0.85	0.09	28,28,28,28	0
57	MG	2A	3847	1/1	0.85	0.19	70,70,70,70	0
57	MG	1A	3352	1/1	0.85	0.12	45,45,45,45	0
57	MG	2a	1833	1/1	0.85	0.14	62,62,62,62	0
57	MG	1A	3958	1/1	0.85	0.13	54,54,54,54	0
57	MG	1A	3864	1/1	0.85	0.22	31,31,31,31	0
57	MG	2A	3294	1/1	0.85	0.11	55,55,55,55	0
57	MG	2A	3564	1/1	0.85	0.13	47,47,47,47	0
57	MG	1A	4047	1/1	0.85	0.14	31,31,31,31	0
57	MG	2A	3583	1/1	0.85	0.14	44,44,44,44	0
57	MG	2B	209	1/1	0.85	0.23	56,56,56,56	0
57	MG	1A	3865	1/1	0.85	0.12	50,50,50,50	0
57	MG	1A	3966	1/1	0.85	0.18	48,48,48,48	0
57	MG	2B	215	1/1	0.85	0.10	47,47,47,47	0
57	MG	2A	3310	1/1	0.85	0.25	64,64,64,64	0
57	MG	2a	1639	1/1	0.86	0.15	65,65,65,65	0
57	MG	1O	205	1/1	0.86	0.18	56,56,56,56	0
57	MG	1a	1731	1/1	0.86	0.10	39,39,39,39	0
57	MG	2A	3273	1/1	0.86	0.14	65,65,65,65	0
57	MG	2A	3851	1/1	0.86	0.12	59,59,59,59	0
57	MG	2A	3853	1/1	0.86	0.11	32,32,32,32	0
57	MG	2a	1706	1/1	0.86	0.11	53,53,53,53	0
57	MG	1A	3193	1/1	0.86	0.11	47,47,47,47	0
57	MG	1A	3962	1/1	0.86	0.10	42,42,42,42	0
57	MG	2a	1717	1/1	0.86	0.17	70,70,70,70	0
57	MG	2a	1720	1/1	0.86	0.22	66,66,66,66	0
57	MG	1x	111	1/1	0.86	0.13	55,55,55,55	0
57	MG	2a	1731	1/1	0.86	0.16	64,64,64,64	0
57	MG	1A	3721	1/1	0.86	0.15	43,43,43,43	0
57	MG	2A	3409	1/1	0.86	0.16	64,64,64,64	0
57	MG	2A	3682	1/1	0.86	0.13	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3003	1/1	0.86	0.13	47,47,47,47	0
57	MG	2A	3175	1/1	0.86	0.18	57,57,57,57	0
57	MG	1a	1760	1/1	0.86	0.11	60,60,60,60	0
57	MG	1A	3510	1/1	0.86	0.10	55,55,55,55	0
57	MG	2B	213	1/1	0.86	0.21	58,58,58,58	0
57	MG	2a	1804	1/1	0.86	0.17	64,64,64,64	0
57	MG	1A	3843	1/1	0.86	0.14	56,56,56,56	0
57	MG	1A	4095	1/1	0.86	0.10	37,37,37,37	0
57	MG	2A	3189	1/1	0.86	0.19	68,68,68,68	0
57	MG	1a	1798	1/1	0.86	0.15	81,81,81,81	0
57	MG	2A	3502	1/1	0.86	0.09	61,61,61,61	0
57	MG	2a	1823	1/1	0.86	0.19	59,59,59,59	0
57	MG	2a	1826	1/1	0.86	0.14	62,62,62,62	0
57	MG	2A	3195	1/1	0.86	0.24	53,53,53,53	0
57	MG	1A	3469	1/1	0.86	0.12	55,55,55,55	0
57	MG	2A	3204	1/1	0.86	0.13	45,45,45,45	0
57	MG	2A	3555	1/1	0.86	0.11	42,42,42,42	0
57	MG	15	109	1/1	0.86	0.11	45,45,45,45	0
57	MG	1A	3712	1/1	0.86	0.13	34,34,34,34	0
57	MG	2A	3091	1/1	0.86	0.14	66,66,66,66	0
57	MG	1A	3737	1/1	0.86	0.15	65,65,65,65	0
57	MG	2A	3097	1/1	0.86	0.15	58,58,58,58	0
57	MG	1A	4036	1/1	0.86	0.11	45,45,45,45	0
57	MG	2A	3791	1/1	0.86	0.10	49,49,49,49	0
57	MG	1A	3210	1/1	0.86	0.12	64,64,64,64	0
57	MG	1A	3716	1/1	0.86	0.15	45,45,45,45	0
57	MG	2A	3440	1/1	0.87	0.19	53,53,53,53	0
57	MG	1a	1755	1/1	0.87	0.09	47,47,47,47	0
57	MG	2A	3449	1/1	0.87	0.17	49,49,49,49	0
57	MG	2A	3735	1/1	0.87	0.14	51,51,51,51	0
57	MG	2A	3740	1/1	0.87	0.11	50,50,50,50	0
57	MG	1A	3382	1/1	0.87	0.09	61,61,61,61	0
57	MG	2a	1638	1/1	0.87	0.30	54,54,54,54	0
57	MG	2A	3299	1/1	0.87	0.16	56,56,56,56	0
57	MG	1A	3038	1/1	0.87	0.14	56,56,56,56	0
57	MG	1a	1774	1/1	0.87	0.11	70,70,70,70	0
57	MG	2a	1649	1/1	0.87	0.24	61,61,61,61	0
57	MG	2a	1653	1/1	0.87	0.22	57,57,57,57	0
57	MG	1A	3989	1/1	0.87	0.09	30,30,30,30	0
57	MG	2A	3762	1/1	0.87	0.17	37,37,37,37	0
57	MG	2A	3514	1/1	0.87	0.13	56,56,56,56	0
57	MG	2a	1701	1/1	0.87	0.14	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3198	1/1	0.87	0.23	55,55,55,55	0
57	MG	2a	1708	1/1	0.87	0.16	54,54,54,54	0
57	MG	2A	3083	1/1	0.87	0.10	37,37,37,37	0
57	MG	1A	3535	1/1	0.87	0.25	53,53,53,53	0
57	MG	2A	3323	1/1	0.87	0.19	52,52,52,52	0
57	MG	1A	3341	1/1	0.87	0.14	53,53,53,53	0
57	MG	2A	3814	1/1	0.87	0.12	49,49,49,49	0
57	MG	2a	1727	1/1	0.87	0.18	66,66,66,66	0
57	MG	1A	3860	1/1	0.87	0.09	21,21,21,21	0
57	MG	2A	3838	1/1	0.87	0.12	68,68,68,68	0
57	MG	2A	3565	1/1	0.87	0.18	42,42,42,42	0
57	MG	1A	3545	1/1	0.87	0.19	50,50,50,50	0
57	MG	2A	3222	1/1	0.87	0.16	57,57,57,57	0
57	MG	2a	1766	1/1	0.87	0.14	54,54,54,54	0
57	MG	2A	3224	1/1	0.87	0.10	50,50,50,50	0
57	MG	2A	3357	1/1	0.87	0.12	62,62,62,62	0
57	MG	17	105	1/1	0.87	0.30	48,48,48,48	0
57	MG	1A	3493	1/1	0.87	0.11	51,51,51,51	0
57	MG	2A	3367	1/1	0.87	0.25	62,62,62,62	0
57	MG	1A	3561	1/1	0.87	0.14	55,55,55,55	0
57	MG	2A	3612	1/1	0.87	0.13	63,63,63,63	0
57	MG	1a	1628	1/1	0.87	0.25	60,60,60,60	0
57	MG	2B	207	1/1	0.87	0.11	62,62,62,62	0
57	MG	2A	3623	1/1	0.87	0.13	42,42,42,42	0
57	MG	1a	1634	1/1	0.87	0.09	46,46,46,46	0
57	MG	1B	214	1/1	0.87	0.10	44,44,44,44	0
57	MG	1B	225	1/1	0.87	0.11	49,49,49,49	0
57	MG	2A	3274	1/1	0.87	0.12	61,61,61,61	0
57	MG	2a	1834	1/1	0.87	0.21	63,63,63,63	0
57	MG	2e	201	1/1	0.87	0.10	59,59,59,59	0
57	MG	2A	3677	1/1	0.87	0.18	56,56,56,56	0
57	MG	2l	202	1/1	0.87	0.14	53,53,53,53	0
57	MG	2A	3391	1/1	0.87	0.15	63,63,63,63	0
57	MG	2A	3397	1/1	0.87	0.14	58,58,58,58	0
57	MG	1A	3562	1/1	0.87	0.12	52,52,52,52	0
57	MG	1A	3710	1/1	0.87	0.11	21,21,21,21	0
57	MG	1A	3972	1/1	0.87	0.12	62,62,62,62	0
57	MG	1a	1739	1/1	0.87	0.16	64,64,64,64	0
57	MG	1A	3591	1/1	0.87	0.29	45,45,45,45	0
57	MG	2w	109	1/1	0.87	0.20	65,65,65,65	0
57	MG	1A	4038	1/1	0.87	0.08	26,26,26,26	0
57	MG	1A	3265	1/1	0.87	0.10	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3710	1/1	0.87	0.11	60,60,60,60	0
57	MG	2A	3359	1/1	0.88	0.10	50,50,50,50	0
57	MG	2A	3778	1/1	0.88	0.10	56,56,56,56	0
57	MG	1A	3649	1/1	0.88	0.12	47,47,47,47	0
57	MG	2A	3098	1/1	0.88	0.17	61,61,61,61	0
57	MG	2A	3799	1/1	0.88	0.16	58,58,58,58	0
57	MG	1A	3470	1/1	0.88	0.10	41,41,41,41	0
57	MG	1A	3405	1/1	0.88	0.16	50,50,50,50	0
57	MG	2A	3811	1/1	0.88	0.08	43,43,43,43	0
57	MG	1A	3277	1/1	0.88	0.07	48,48,48,48	0
57	MG	1A	3821	1/1	0.88	0.12	49,49,49,49	0
57	MG	18	102	1/1	0.88	0.15	50,50,50,50	0
57	MG	1B	203	1/1	0.88	0.19	55,55,55,55	0
57	MG	1A	3064	1/1	0.88	0.11	50,50,50,50	0
57	MG	1A	3891	1/1	0.88	0.12	35,35,35,35	0
57	MG	2a	1719	1/1	0.88	0.15	65,65,65,65	0
57	MG	1B	217	1/1	0.88	0.09	40,40,40,40	0
57	MG	2a	1721	1/1	0.88	0.18	54,54,54,54	0
57	MG	2A	3137	1/1	0.88	0.11	47,47,47,47	0
57	MG	2A	3401	1/1	0.88	0.19	65,65,65,65	0
57	MG	1B	223	1/1	0.88	0.13	59,59,59,59	0
57	MG	2a	1741	1/1	0.88	0.10	44,44,44,44	0
57	MG	1a	1643	1/1	0.88	0.18	53,53,53,53	0
57	MG	2A	3679	1/1	0.88	0.18	51,51,51,51	0
57	MG	1A	3897	1/1	0.88	0.07	23,23,23,23	0
57	MG	1a	1658	1/1	0.88	0.20	45,45,45,45	0
57	MG	2a	1758	1/1	0.88	0.08	49,49,49,49	0
57	MG	2a	1761	1/1	0.88	0.09	54,54,54,54	0
57	MG	2B	203	1/1	0.88	0.18	61,61,61,61	0
57	MG	1a	1663	1/1	0.88	0.18	61,61,61,61	0
57	MG	2a	1785	1/1	0.88	0.16	54,54,54,54	0
57	MG	2B	208	1/1	0.88	0.11	51,51,51,51	0
57	MG	1A	3196	1/1	0.88	0.25	33,33,33,33	0
57	MG	2B	210	1/1	0.88	0.16	67,67,67,67	0
57	MG	1A	3727	1/1	0.88	0.16	49,49,49,49	0
57	MG	2A	3698	1/1	0.88	0.08	34,34,34,34	0
57	MG	1a	1711	1/1	0.88	0.17	56,56,56,56	0
57	MG	1a	1724	1/1	0.88	0.14	62,62,62,62	0
57	MG	2A	3311	1/1	0.88	0.24	63,63,63,63	0
57	MG	2A	3464	1/1	0.88	0.20	49,49,49,49	0
57	MG	1A	4039	1/1	0.88	0.08	38,38,38,38	0
57	MG	2D	307	1/1	0.88	0.21	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1D	312	1/1	0.88	0.16	39,39,39,39	0
57	MG	1A	4040	1/1	0.88	0.11	28,28,28,28	0
57	MG	2A	3729	1/1	0.88	0.08	39,39,39,39	0
57	MG	1A	3855	1/1	0.88	0.23	56,56,56,56	0
57	MG	1A	3644	1/1	0.88	0.09	19,19,19,19	0
57	MG	2A	3736	1/1	0.88	0.12	69,69,69,69	0
57	MG	2A	3522	1/1	0.88	0.17	50,50,50,50	0
57	MG	2A	3338	1/1	0.88	0.19	55,55,55,55	0
57	MG	2a	1609	1/1	0.88	0.15	62,62,62,62	0
57	MG	1A	3395	1/1	0.88	0.13	56,56,56,56	0
57	MG	1Y	202	1/1	0.88	0.09	53,53,53,53	0
57	MG	1A	4068	1/1	0.88	0.10	38,38,38,38	0
57	MG	2a	1623	1/1	0.88	0.26	58,58,58,58	0
57	MG	1A	4000	1/1	0.88	0.12	41,41,41,41	0
57	MG	2A	3355	1/1	0.88	0.09	37,37,37,37	0
57	MG	2A	3767	1/1	0.88	0.11	56,56,56,56	0
57	MG	2A	3228	1/1	0.88	0.15	53,53,53,53	0
57	MG	1A	3434	1/1	0.89	0.17	51,51,51,51	0
57	MG	2A	3622	1/1	0.89	0.12	40,40,40,40	0
57	MG	1a	1772	1/1	0.89	0.09	47,47,47,47	0
57	MG	2A	3639	1/1	0.89	0.08	44,44,44,44	0
57	MG	1Z	3700	1/1	0.89	0.11	50,50,50,50	0
57	MG	2A	3656	1/1	0.89	0.26	61,61,61,61	0
57	MG	2R	202	1/1	0.89	0.18	45,45,45,45	0
57	MG	2R	203	1/1	0.89	0.12	43,43,43,43	0
57	MG	1A	3436	1/1	0.89	0.10	53,53,53,53	0
57	MG	2A	3351	1/1	0.89	0.08	73,73,73,73	0
57	MG	23	101	1/1	0.89	0.13	58,58,58,58	0
57	MG	1A	3236	1/1	0.89	0.13	52,52,52,52	0
57	MG	2A	3675	1/1	0.89	0.18	52,52,52,52	0
57	MG	1A	3653	1/1	0.89	0.10	59,59,59,59	0
57	MG	2A	3356	1/1	0.89	0.21	40,40,40,40	0
57	MG	1A	4060	1/1	0.89	0.10	45,45,45,45	0
57	MG	1a	1809	1/1	0.89	0.14	61,61,61,61	0
57	MG	2A	3360	1/1	0.89	0.11	60,60,60,60	0
57	MG	2A	3191	1/1	0.89	0.07	50,50,50,50	0
57	MG	1A	3468	1/1	0.89	0.12	54,54,54,54	0
57	MG	2A	3194	1/1	0.89	0.15	58,58,58,58	0
57	MG	1A	3173	1/1	0.89	0.09	34,34,34,34	0
57	MG	1A	3026	1/1	0.89	0.09	49,49,49,49	0
57	MG	1A	4081	1/1	0.89	0.09	29,29,29,29	0
57	MG	2a	1640	1/1	0.89	0.23	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3377	1/1	0.89	0.13	67,67,67,67	0
57	MG	1A	3990	1/1	0.89	0.10	33,33,33,33	0
57	MG	2a	1648	1/1	0.89	0.10	50,50,50,50	0
57	MG	1A	3795	1/1	0.89	0.11	67,67,67,67	0
57	MG	1A	3917	1/1	0.89	0.24	38,38,38,38	0
57	MG	2a	1655	1/1	0.89	0.14	63,63,63,63	0
57	MG	2A	3723	1/1	0.89	0.08	42,42,42,42	0
57	MG	2A	3724	1/1	0.89	0.10	56,56,56,56	0
57	MG	2a	1675	1/1	0.89	0.28	54,54,54,54	0
57	MG	2a	1679	1/1	0.89	0.14	56,56,56,56	0
57	MG	1A	3933	1/1	0.89	0.08	31,31,31,31	0
57	MG	2a	1699	1/1	0.89	0.11	65,65,65,65	0
57	MG	2a	1700	1/1	0.89	0.18	56,56,56,56	0
57	MG	2A	3217	1/1	0.89	0.11	51,51,51,51	0
57	MG	1A	3479	1/1	0.89	0.17	38,38,38,38	0
57	MG	1B	208	1/1	0.89	0.09	58,58,58,58	0
57	MG	2a	1710	1/1	0.89	0.11	55,55,55,55	0
57	MG	1A	3814	1/1	0.89	0.41	50,50,50,50	0
57	MG	1a	1651	1/1	0.89	0.16	50,50,50,50	0
57	MG	2A	3241	1/1	0.89	0.23	52,52,52,52	0
57	MG	2A	3749	1/1	0.89	0.09	66,66,66,66	0
57	MG	1A	4016	1/1	0.89	0.08	33,33,33,33	0
57	MG	2A	3752	1/1	0.89	0.14	44,44,44,44	0
57	MG	1a	1659	1/1	0.89	0.11	48,48,48,48	0
57	MG	2A	3417	1/1	0.89	0.10	64,64,64,64	0
57	MG	2A	3418	1/1	0.89	0.18	66,66,66,66	0
57	MG	2A	3764	1/1	0.89	0.09	48,48,48,48	0
57	MG	2A	3428	1/1	0.89	0.14	39,39,39,39	0
57	MG	2A	3253	1/1	0.89	0.22	63,63,63,63	0
57	MG	2A	3005	1/1	0.89	0.11	52,52,52,52	0
57	MG	1A	3323	1/1	0.89	0.11	50,50,50,50	0
57	MG	2A	3028	1/1	0.89	0.31	43,43,43,43	0
57	MG	2a	1760	1/1	0.89	0.10	68,68,68,68	0
57	MG	1A	3408	1/1	0.89	0.10	54,54,54,54	0
57	MG	2A	3035	1/1	0.89	0.11	53,53,53,53	0
57	MG	2A	3053	1/1	0.89	0.18	55,55,55,55	0
57	MG	1a	1677	1/1	0.89	0.13	53,53,53,53	0
57	MG	1a	1679	1/1	0.89	0.20	45,45,45,45	0
57	MG	2A	3279	1/1	0.89	0.11	53,53,53,53	0
57	MG	2a	1799	1/1	0.89	0.09	55,55,55,55	0
57	MG	1a	1681	1/1	0.89	0.11	58,58,58,58	0
57	MG	2A	3823	1/1	0.89	0.09	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1806	1/1	0.89	0.09	58,58,58,58	0
57	MG	2A	3826	1/1	0.89	0.10	49,49,49,49	0
57	MG	2A	3515	1/1	0.89	0.15	54,54,54,54	0
57	MG	2A	3520	1/1	0.89	0.13	38,38,38,38	0
57	MG	2a	1819	1/1	0.89	0.10	52,52,52,52	0
57	MG	1A	3604	1/1	0.89	0.13	44,44,44,44	0
57	MG	2A	3536	1/1	0.89	0.09	40,40,40,40	0
57	MG	1a	1702	1/1	0.89	0.17	55,55,55,55	0
57	MG	2A	3550	1/1	0.89	0.10	44,44,44,44	0
57	MG	1a	1708	1/1	0.89	0.12	50,50,50,50	0
57	MG	2a	1831	1/1	0.89	0.11	61,61,61,61	0
57	MG	1A	3413	1/1	0.89	0.10	47,47,47,47	0
57	MG	1a	1718	1/1	0.89	0.20	45,45,45,45	0
57	MG	2d	302	1/1	0.89	0.09	65,65,65,65	0
57	MG	1a	1720	1/1	0.89	0.11	64,64,64,64	0
57	MG	1A	4028	1/1	0.89	0.10	61,61,61,61	0
57	MG	1A	3613	1/1	0.89	0.09	26,26,26,26	0
57	MG	1a	1738	1/1	0.89	0.07	36,36,36,36	0
57	MG	2l	204	1/1	0.89	0.08	55,55,55,55	0
57	MG	2B	204	1/1	0.89	0.13	65,65,65,65	0
57	MG	1A	4033	1/1	0.89	0.11	44,44,44,44	0
57	MG	1A	4035	1/1	0.89	0.08	41,41,41,41	0
57	MG	2w	102	1/1	0.89	0.20	73,73,73,73	0
57	MG	2A	3588	1/1	0.89	0.11	60,60,60,60	0
57	MG	1A	3340	1/1	0.89	0.20	46,46,46,46	0
57	MG	1Q	205	1/1	0.89	0.09	36,36,36,36	0
57	MG	1A	3859	1/1	0.89	0.09	55,55,55,55	0
57	MG	2x	102	1/1	0.89	0.17	57,57,57,57	0
57	MG	1A	3235	1/1	0.89	0.09	31,31,31,31	0
57	MG	2y	101	1/1	0.89	0.13	71,71,71,71	0
57	MG	1a	1761	1/1	0.89	0.11	47,47,47,47	0
57	MG	2y	105	1/1	0.89	0.23	65,65,65,65	0
57	MG	2A	3337	1/1	0.89	0.13	52,52,52,52	0
57	MG	1A	3481	1/1	0.90	0.09	43,43,43,43	0
57	MG	1a	1725	1/1	0.90	0.10	39,39,39,39	0
57	MG	2A	3231	1/1	0.90	0.21	42,42,42,42	0
57	MG	2a	1616	1/1	0.90	0.16	51,51,51,51	0
57	MG	1A	3848	1/1	0.90	0.08	47,47,47,47	0
57	MG	2A	3057	1/1	0.90	0.12	47,47,47,47	0
57	MG	1A	3853	1/1	0.90	0.08	40,40,40,40	0
57	MG	2A	3715	1/1	0.90	0.10	61,61,61,61	0
57	MG	2a	1625	1/1	0.90	0.29	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3717	1/1	0.90	0.09	55,55,55,55	0
57	MG	2A	3250	1/1	0.90	0.12	51,51,51,51	0
57	MG	2a	1635	1/1	0.90	0.19	51,51,51,51	0
57	MG	2A	3411	1/1	0.90	0.20	60,60,60,60	0
57	MG	2A	3067	1/1	0.90	0.08	40,40,40,40	0
57	MG	2A	3254	1/1	0.90	0.10	52,52,52,52	0
57	MG	1A	3317	1/1	0.90	0.17	43,43,43,43	0
57	MG	2A	3256	1/1	0.90	0.15	58,58,58,58	0
57	MG	2A	3426	1/1	0.90	0.15	47,47,47,47	0
57	MG	1a	1741	1/1	0.90	0.07	42,42,42,42	0
57	MG	2A	3745	1/1	0.90	0.12	47,47,47,47	0
57	MG	2A	3074	1/1	0.90	0.14	55,55,55,55	0
57	MG	2A	3436	1/1	0.90	0.28	55,55,55,55	0
57	MG	1A	3281	1/1	0.90	0.11	47,47,47,47	0
57	MG	2a	1670	1/1	0.90	0.15	69,69,69,69	0
57	MG	2A	3080	1/1	0.90	0.09	53,53,53,53	0
57	MG	1a	1745	1/1	0.90	0.12	54,54,54,54	0
57	MG	2a	1684	1/1	0.90	0.19	50,50,50,50	0
57	MG	2a	1688	1/1	0.90	0.09	63,63,63,63	0
57	MG	2A	3086	1/1	0.90	0.17	43,43,43,43	0
57	MG	2a	1698	1/1	0.90	0.14	49,49,49,49	0
57	MG	2A	3462	1/1	0.90	0.14	42,42,42,42	0
57	MG	1A	3655	1/1	0.90	0.10	30,30,30,30	0
57	MG	2A	3486	1/1	0.90	0.18	49,49,49,49	0
57	MG	2A	3277	1/1	0.90	0.12	56,56,56,56	0
57	MG	2A	3497	1/1	0.90	0.10	59,59,59,59	0
57	MG	2A	3278	1/1	0.90	0.17	45,45,45,45	0
57	MG	1A	3389	1/1	0.90	0.10	52,52,52,52	0
57	MG	13	105	1/1	0.90	0.12	46,46,46,46	0
57	MG	1a	1758	1/1	0.90	0.15	43,43,43,43	0
57	MG	2A	3792	1/1	0.90	0.10	35,35,35,35	0
57	MG	1A	3731	1/1	0.90	0.08	40,40,40,40	0
57	MG	2A	3802	1/1	0.90	0.09	56,56,56,56	0
57	MG	1A	3667	1/1	0.90	0.12	53,53,53,53	0
57	MG	1A	4088	1/1	0.90	0.16	50,50,50,50	0
57	MG	2A	3810	1/1	0.90	0.11	63,63,63,63	0
57	MG	1a	1769	1/1	0.90	0.08	69,69,69,69	0
57	MG	18	103	1/1	0.90	0.20	50,50,50,50	0
57	MG	2A	3815	1/1	0.90	0.10	50,50,50,50	0
57	MG	2a	1745	1/1	0.90	0.09	45,45,45,45	0
57	MG	1A	3668	1/1	0.90	0.07	31,31,31,31	0
57	MG	1a	1780	1/1	0.90	0.11	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3873	1/1	0.90	0.10	42,42,42,42	0
57	MG	2A	3837	1/1	0.90	0.12	74,74,74,74	0
57	MG	2A	3305	1/1	0.90	0.13	53,53,53,53	0
57	MG	1A	3744	1/1	0.90	0.10	45,45,45,45	0
57	MG	2A	3118	1/1	0.90	0.13	50,50,50,50	0
57	MG	2a	1775	1/1	0.90	0.13	62,62,62,62	0
57	MG	1A	3335	1/1	0.90	0.17	36,36,36,36	0
57	MG	2A	3318	1/1	0.90	0.08	44,44,44,44	0
57	MG	2a	1789	1/1	0.90	0.09	53,53,53,53	0
57	MG	1a	1637	1/1	0.90	0.26	66,66,66,66	0
57	MG	2A	3153	1/1	0.90	0.24	55,55,55,55	0
57	MG	2A	3869	1/1	0.90	0.09	50,50,50,50	0
57	MG	2A	3870	1/1	0.90	0.12	46,46,46,46	0
57	MG	2A	3162	1/1	0.90	0.14	53,53,53,53	0
57	MG	2A	3590	1/1	0.90	0.08	44,44,44,44	0
57	MG	1A	4098	1/1	0.90	0.12	54,54,54,54	0
57	MG	1A	3761	1/1	0.90	0.13	34,34,34,34	0
57	MG	1a	1812	1/1	0.90	0.14	60,60,60,60	0
57	MG	1A	3888	1/1	0.90	0.09	13,13,13,13	0
57	MG	2A	3610	1/1	0.90	0.13	53,53,53,53	0
57	MG	2B	205	1/1	0.90	0.13	45,45,45,45	0
57	MG	1A	3769	1/1	0.90	0.10	37,37,37,37	0
57	MG	1t	201	1/1	0.90	0.19	56,56,56,56	0
57	MG	1A	4012	1/1	0.90	0.07	27,27,27,27	0
57	MG	2A	3619	1/1	0.90	0.10	65,65,65,65	0
57	MG	1A	3895	1/1	0.90	0.11	18,18,18,18	0
57	MG	1A	3770	1/1	0.90	0.08	22,22,22,22	0
57	MG	1a	1670	1/1	0.90	0.16	49,49,49,49	0
57	MG	2B	214	1/1	0.90	0.18	55,55,55,55	0
57	MG	1A	3337	1/1	0.90	0.24	47,47,47,47	0
57	MG	1A	3338	1/1	0.90	0.08	39,39,39,39	0
57	MG	1A	3532	1/1	0.90	0.09	45,45,45,45	0
57	MG	2A	3202	1/1	0.90	0.11	46,46,46,46	0
57	MG	2q	202	1/1	0.90	0.16	61,61,61,61	0
57	MG	1A	3946	1/1	0.90	0.08	21,21,21,21	0
57	MG	2v	103	1/1	0.90	0.23	56,56,56,56	0
57	MG	1A	3272	1/1	0.90	0.11	36,36,36,36	0
57	MG	2A	3209	1/1	0.90	0.11	44,44,44,44	0
57	MG	2F	306	1/1	0.90	0.16	53,53,53,53	0
57	MG	2A	3371	1/1	0.90	0.18	61,61,61,61	0
57	MG	1A	3476	1/1	0.90	0.13	39,39,39,39	0
57	MG	1A	3822	1/1	0.90	0.23	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3830	1/1	0.90	0.11	40,40,40,40	0
57	MG	1A	3100	1/1	0.90	0.12	60,60,60,60	0
57	MG	2A	3220	1/1	0.90	0.14	56,56,56,56	0
57	MG	25	103	1/1	0.90	0.22	47,47,47,47	0
57	MG	2A	3696	1/1	0.90	0.11	54,54,54,54	0
57	MG	1A	3647	1/1	0.90	0.09	52,52,52,52	0
59	A1C9N	2A	3885	74/74	0.90	0.15	27,48,58,59	0
57	MG	1A	3232	1/1	0.91	0.14	48,48,48,48	0
57	MG	1A	3366	1/1	0.91	0.11	28,28,28,28	0
57	MG	1E	314	1/1	0.91	0.06	34,34,34,34	0
57	MG	2D	303	1/1	0.91	0.21	57,57,57,57	0
57	MG	1A	4007	1/1	0.91	0.07	40,40,40,40	0
57	MG	1A	3615	1/1	0.91	0.09	30,30,30,30	0
57	MG	2E	302	1/1	0.91	0.09	41,41,41,41	0
57	MG	2A	3334	1/1	0.91	0.16	56,56,56,56	0
57	MG	2F	302	1/1	0.91	0.08	39,39,39,39	0
57	MG	1A	3170	1/1	0.91	0.12	56,56,56,56	0
57	MG	2A	3139	1/1	0.91	0.10	44,44,44,44	0
57	MG	2A	3340	1/1	0.91	0.09	43,43,43,43	0
57	MG	2A	3146	1/1	0.91	0.14	55,55,55,55	0
57	MG	2T	202	1/1	0.91	0.15	59,59,59,59	0
57	MG	2A	3345	1/1	0.91	0.11	64,64,64,64	0
57	MG	1R	202	1/1	0.91	0.18	56,56,56,56	0
57	MG	2Z	301	1/1	0.91	0.13	57,57,57,57	0
57	MG	2I	101	1/1	0.91	0.17	33,33,33,33	0
57	MG	2A	3632	1/1	0.91	0.14	61,61,61,61	0
57	MG	1a	1767	1/1	0.91	0.09	54,54,54,54	0
57	MG	2A	3644	1/1	0.91	0.08	40,40,40,40	0
57	MG	28	102	1/1	0.91	0.12	41,41,41,41	0
57	MG	2A	3653	1/1	0.91	0.08	41,41,41,41	0
57	MG	2A	3350	1/1	0.91	0.11	61,61,61,61	0
57	MG	2a	1603	1/1	0.91	0.11	57,57,57,57	0
57	MG	2a	1606	1/1	0.91	0.14	52,52,52,52	0
57	MG	2a	1607	1/1	0.91	0.26	54,54,54,54	0
57	MG	1A	3875	1/1	0.91	0.10	27,27,27,27	0
57	MG	2A	3353	1/1	0.91	0.10	45,45,45,45	0
57	MG	1A	4015	1/1	0.91	0.09	28,28,28,28	0
57	MG	2A	3668	1/1	0.91	0.14	54,54,54,54	0
57	MG	1A	3878	1/1	0.91	0.24	27,27,27,27	0
57	MG	1A	3733	1/1	0.91	0.09	37,37,37,37	0
57	MG	1A	3885	1/1	0.91	0.08	29,29,29,29	0
57	MG	2A	3358	1/1	0.91	0.23	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1626	1/1	0.91	0.10	46,46,46,46	0
57	MG	1a	1783	1/1	0.91	0.11	52,52,52,52	0
57	MG	1A	3641	1/1	0.91	0.14	53,53,53,53	0
57	MG	2a	1632	1/1	0.91	0.07	73,73,73,73	0
57	MG	2A	3685	1/1	0.91	0.10	51,51,51,51	0
57	MG	2A	3362	1/1	0.91	0.10	49,49,49,49	0
57	MG	1A	3098	1/1	0.91	0.08	50,50,50,50	0
57	MG	1a	1791	1/1	0.91	0.08	41,41,41,41	0
57	MG	1a	1792	1/1	0.91	0.08	68,68,68,68	0
57	MG	2a	1642	1/1	0.91	0.31	69,69,69,69	0
57	MG	1A	3186	1/1	0.91	0.06	28,28,28,28	0
57	MG	2A	3700	1/1	0.91	0.19	46,46,46,46	0
57	MG	1A	3751	1/1	0.91	0.08	46,46,46,46	0
57	MG	1A	3896	1/1	0.91	0.07	12,12,12,12	0
57	MG	1A	3047	1/1	0.91	0.06	12,12,12,12	0
57	MG	1A	3910	1/1	0.91	0.17	18,18,18,18	0
57	MG	2a	1659	1/1	0.91	0.14	63,63,63,63	0
57	MG	2A	3378	1/1	0.91	0.15	56,56,56,56	0
57	MG	2a	1666	1/1	0.91	0.08	49,49,49,49	0
57	MG	2A	3711	1/1	0.91	0.07	39,39,39,39	0
57	MG	2a	1673	1/1	0.91	0.13	58,58,58,58	0
57	MG	1A	3914	1/1	0.91	0.08	32,32,32,32	0
57	MG	2a	1678	1/1	0.91	0.31	66,66,66,66	0
57	MG	1l	201	1/1	0.91	0.10	55,55,55,55	0
57	MG	1A	3407	1/1	0.91	0.15	53,53,53,53	0
57	MG	18	105	1/1	0.91	0.20	54,54,54,54	0
57	MG	1a	1608	1/1	0.91	0.15	48,48,48,48	0
57	MG	1A	3923	1/1	0.91	0.13	50,50,50,50	0
57	MG	2A	3400	1/1	0.91	0.20	55,55,55,55	0
57	MG	1A	3929	1/1	0.91	0.10	41,41,41,41	0
57	MG	2A	3731	1/1	0.91	0.10	34,34,34,34	0
57	MG	1A	3494	1/1	0.91	0.10	43,43,43,43	0
57	MG	1A	4050	1/1	0.91	0.07	41,41,41,41	0
57	MG	1a	1636	1/1	0.91	0.17	50,50,50,50	0
57	MG	1A	4055	1/1	0.91	0.17	62,62,62,62	0
57	MG	1a	1640	1/1	0.91	0.15	46,46,46,46	0
57	MG	2a	1715	1/1	0.91	0.19	56,56,56,56	0
57	MG	2A	3413	1/1	0.91	0.09	58,58,58,58	0
57	MG	1A	3322	1/1	0.91	0.08	34,34,34,34	0
57	MG	1A	4058	1/1	0.91	0.09	54,54,54,54	0
57	MG	1A	3409	1/1	0.91	0.10	39,39,39,39	0
57	MG	2A	3753	1/1	0.91	0.11	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3784	1/1	0.91	0.09	32,32,32,32	0
57	MG	2A	3760	1/1	0.91	0.11	32,32,32,32	0
57	MG	2a	1733	1/1	0.91	0.14	48,48,48,48	0
57	MG	1A	3785	1/1	0.91	0.10	41,41,41,41	0
57	MG	2A	3017	1/1	0.91	0.10	45,45,45,45	0
57	MG	2A	3763	1/1	0.91	0.11	39,39,39,39	0
57	MG	1A	3659	1/1	0.91	0.09	33,33,33,33	0
57	MG	2A	3765	1/1	0.91	0.10	49,49,49,49	0
57	MG	2a	1753	1/1	0.91	0.08	55,55,55,55	0
57	MG	2A	3438	1/1	0.91	0.26	56,56,56,56	0
57	MG	2a	1757	1/1	0.91	0.07	72,72,72,72	0
57	MG	2A	3257	1/1	0.91	0.16	55,55,55,55	0
57	MG	2a	1759	1/1	0.91	0.11	63,63,63,63	0
57	MG	2A	3441	1/1	0.91	0.11	53,53,53,53	0
57	MG	2A	3777	1/1	0.91	0.09	52,52,52,52	0
57	MG	2A	3261	1/1	0.91	0.10	47,47,47,47	0
57	MG	2A	3447	1/1	0.91	0.21	54,54,54,54	0
57	MG	2a	1773	1/1	0.91	0.08	64,64,64,64	0
57	MG	1a	1660	1/1	0.91	0.11	59,59,59,59	0
57	MG	2a	1777	1/1	0.91	0.18	47,47,47,47	0
57	MG	2a	1778	1/1	0.91	0.14	48,48,48,48	0
57	MG	2A	3450	1/1	0.91	0.19	56,56,56,56	0
57	MG	2a	1787	1/1	0.91	0.09	65,65,65,65	0
57	MG	2A	3795	1/1	0.91	0.20	58,58,58,58	0
57	MG	2A	3452	1/1	0.91	0.08	46,46,46,46	0
57	MG	2A	3457	1/1	0.91	0.15	46,46,46,46	0
57	MG	1A	3258	1/1	0.91	0.12	54,54,54,54	0
57	MG	2A	3271	1/1	0.91	0.31	61,61,61,61	0
57	MG	1a	1665	1/1	0.91	0.13	54,54,54,54	0
57	MG	2A	3465	1/1	0.91	0.10	39,39,39,39	0
57	MG	2A	3470	1/1	0.91	0.17	62,62,62,62	0
57	MG	1A	3327	1/1	0.91	0.12	49,49,49,49	0
57	MG	1A	3330	1/1	0.91	0.08	39,39,39,39	0
57	MG	1A	4093	1/1	0.91	0.16	59,59,59,59	0
57	MG	1A	3264	1/1	0.91	0.17	59,59,59,59	0
57	MG	2A	3827	1/1	0.91	0.09	41,41,41,41	0
57	MG	1A	3073	1/1	0.91	0.22	66,66,66,66	0
57	MG	2A	3503	1/1	0.91	0.07	18,18,18,18	0
57	MG	2A	3505	1/1	0.91	0.12	38,38,38,38	0
57	MG	2a	1830	1/1	0.91	0.17	50,50,50,50	0
57	MG	1a	1689	1/1	0.91	0.13	69,69,69,69	0
57	MG	2A	3508	1/1	0.91	0.10	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3512	1/1	0.91	0.07	47,47,47,47	0
57	MG	2d	301	1/1	0.91	0.20	54,54,54,54	0
57	MG	2A	3513	1/1	0.91	0.10	64,64,64,64	0
57	MG	2A	3856	1/1	0.91	0.09	40,40,40,40	0
57	MG	2A	3864	1/1	0.91	0.10	51,51,51,51	0
57	MG	1A	3686	1/1	0.91	0.12	46,46,46,46	0
57	MG	2A	3281	1/1	0.91	0.11	54,54,54,54	0
57	MG	2A	3517	1/1	0.91	0.18	55,55,55,55	0
57	MG	2A	3518	1/1	0.91	0.10	56,56,56,56	0
57	MG	2A	3078	1/1	0.91	0.09	39,39,39,39	0
57	MG	1A	3450	1/1	0.91	0.07	47,47,47,47	0
57	MG	1a	1707	1/1	0.91	0.10	61,61,61,61	0
57	MG	2A	3290	1/1	0.91	0.12	65,65,65,65	0
57	MG	1A	3457	1/1	0.91	0.25	34,34,34,34	0
57	MG	1A	3466	1/1	0.91	0.14	49,49,49,49	0
57	MG	1A	3570	1/1	0.91	0.13	54,54,54,54	0
57	MG	1B	210	1/1	0.91	0.10	45,45,45,45	0
57	MG	2w	107	1/1	0.91	0.12	55,55,55,55	0
57	MG	1A	3131	1/1	0.91	0.19	47,47,47,47	0
57	MG	1A	3271	1/1	0.91	0.07	25,25,25,25	0
57	MG	2x	103	1/1	0.91	0.13	64,64,64,64	0
57	MG	1A	3598	1/1	0.91	0.31	60,60,60,60	0
57	MG	1B	224	1/1	0.91	0.09	45,45,45,45	0
57	MG	2A	3577	1/1	0.91	0.07	33,33,33,33	0
57	MG	1A	3158	1/1	0.91	0.12	32,32,32,32	0
57	MG	1A	3723	1/1	0.91	0.07	36,36,36,36	0
57	MG	1A	3997	1/1	0.91	0.11	54,54,54,54	0
57	MG	1A	3460	1/1	0.92	0.06	34,34,34,34	0
57	MG	1A	3572	1/1	0.92	0.08	42,42,42,42	0
57	MG	1A	3870	1/1	0.92	0.12	34,34,34,34	0
57	MG	1a	1799	1/1	0.92	0.10	52,52,52,52	0
57	MG	1A	3872	1/1	0.92	0.23	40,40,40,40	0
57	MG	1A	3359	1/1	0.92	0.15	46,46,46,46	0
57	MG	1A	3057	1/1	0.92	0.11	48,48,48,48	0
57	MG	2A	3527	1/1	0.92	0.11	45,45,45,45	0
57	MG	2A	3529	1/1	0.92	0.14	45,45,45,45	0
57	MG	1A	3058	1/1	0.92	0.09	29,29,29,29	0
57	MG	1a	1813	1/1	0.92	0.07	56,56,56,56	0
57	MG	2A	3547	1/1	0.92	0.10	49,49,49,49	0
57	MG	1b	301	1/1	0.92	0.17	56,56,56,56	0
57	MG	1A	3385	1/1	0.92	0.10	47,47,47,47	0
57	MG	2A	3269	1/1	0.92	0.15	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3605	1/1	0.92	0.11	47,47,47,47	0
57	MG	2E	304	1/1	0.92	0.11	35,35,35,35	0
57	MG	15	103	1/1	0.92	0.19	29,29,29,29	0
57	MG	2F	301	1/1	0.92	0.31	40,40,40,40	0
57	MG	1n	102	1/1	0.92	0.14	38,38,38,38	0
57	MG	15	106	1/1	0.92	0.19	35,35,35,35	0
57	MG	1A	4026	1/1	0.92	0.08	37,37,37,37	0
57	MG	2P	202	1/1	0.92	0.17	47,47,47,47	0
57	MG	2P	203	1/1	0.92	0.07	52,52,52,52	0
57	MG	2A	3575	1/1	0.92	0.07	29,29,29,29	0
57	MG	1A	3729	1/1	0.92	0.09	37,37,37,37	0
57	MG	2A	3581	1/1	0.92	0.16	64,64,64,64	0
57	MG	2A	3582	1/1	0.92	0.10	33,33,33,33	0
57	MG	1A	3326	1/1	0.92	0.11	25,25,25,25	0
57	MG	1A	3391	1/1	0.92	0.24	39,39,39,39	0
57	MG	20	101	1/1	0.92	0.10	48,48,48,48	0
57	MG	1A	3392	1/1	0.92	0.11	53,53,53,53	0
57	MG	2A	3589	1/1	0.92	0.12	27,27,27,27	0
57	MG	1a	1604	1/1	0.92	0.16	53,53,53,53	0
57	MG	1a	1606	1/1	0.92	0.12	57,57,57,57	0
57	MG	28	101	1/1	0.92	0.10	54,54,54,54	0
57	MG	1x	108	1/1	0.92	0.23	58,58,58,58	0
57	MG	2A	3287	1/1	0.92	0.14	60,60,60,60	0
57	MG	1A	3892	1/1	0.92	0.07	29,29,29,29	0
57	MG	2A	3609	1/1	0.92	0.17	51,51,51,51	0
57	MG	1A	3197	1/1	0.92	0.19	39,39,39,39	0
57	MG	1y	101	1/1	0.92	0.08	58,58,58,58	0
57	MG	2a	1608	1/1	0.92	0.20	58,58,58,58	0
57	MG	1a	1614	1/1	0.92	0.07	57,57,57,57	0
57	MG	2A	3293	1/1	0.92	0.14	54,54,54,54	0
57	MG	2a	1611	1/1	0.92	0.14	45,45,45,45	0
57	MG	1a	1615	1/1	0.92	0.14	54,54,54,54	0
57	MG	2A	3621	1/1	0.92	0.07	25,25,25,25	0
57	MG	1A	3484	1/1	0.92	0.14	45,45,45,45	0
57	MG	2A	3297	1/1	0.92	0.18	53,53,53,53	0
57	MG	2A	3625	1/1	0.92	0.07	47,47,47,47	0
57	MG	1A	3328	1/1	0.92	0.13	39,39,39,39	0
57	MG	2A	3300	1/1	0.92	0.11	54,54,54,54	0
57	MG	1A	4042	1/1	0.92	0.08	25,25,25,25	0
57	MG	2A	3652	1/1	0.92	0.07	43,43,43,43	0
57	MG	2A	3303	1/1	0.92	0.10	63,63,63,63	0
57	MG	1a	1635	1/1	0.92	0.11	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1636	1/1	0.92	0.22	52,52,52,52	0
57	MG	2A	3029	1/1	0.92	0.15	61,61,61,61	0
57	MG	2A	3307	1/1	0.92	0.16	49,49,49,49	0
57	MG	2A	3308	1/1	0.92	0.18	43,43,43,43	0
57	MG	2A	3667	1/1	0.92	0.17	50,50,50,50	0
57	MG	2A	3030	1/1	0.92	0.14	43,43,43,43	0
57	MG	1A	4043	1/1	0.92	0.14	40,40,40,40	0
57	MG	2A	3672	1/1	0.92	0.11	46,46,46,46	0
57	MG	2A	3674	1/1	0.92	0.09	40,40,40,40	0
57	MG	2a	1650	1/1	0.92	0.13	61,61,61,61	0
57	MG	2a	1652	1/1	0.92	0.12	42,42,42,42	0
57	MG	1A	4044	1/1	0.92	0.10	50,50,50,50	0
57	MG	2A	3043	1/1	0.92	0.25	45,45,45,45	0
57	MG	2A	3319	1/1	0.92	0.17	62,62,62,62	0
57	MG	2a	1658	1/1	0.92	0.08	48,48,48,48	0
57	MG	2A	3046	1/1	0.92	0.24	58,58,58,58	0
57	MG	2a	1663	1/1	0.92	0.16	57,57,57,57	0
57	MG	2A	3048	1/1	0.92	0.09	41,41,41,41	0
57	MG	2A	3052	1/1	0.92	0.07	42,42,42,42	0
57	MG	2A	3686	1/1	0.92	0.17	58,58,58,58	0
57	MG	1A	3906	1/1	0.92	0.08	53,53,53,53	0
57	MG	2A	3055	1/1	0.92	0.12	47,47,47,47	0
57	MG	1A	3909	1/1	0.92	0.13	24,24,24,24	0
57	MG	1A	3750	1/1	0.92	0.13	56,56,56,56	0
57	MG	1a	1645	1/1	0.92	0.10	47,47,47,47	0
57	MG	2A	3699	1/1	0.92	0.09	52,52,52,52	0
57	MG	2a	1691	1/1	0.92	0.27	56,56,56,56	0
57	MG	1a	1646	1/1	0.92	0.18	49,49,49,49	0
57	MG	1A	3248	1/1	0.92	0.18	51,51,51,51	0
57	MG	1A	3332	1/1	0.92	0.07	37,37,37,37	0
57	MG	1A	3757	1/1	0.92	0.17	43,43,43,43	0
57	MG	1A	3928	1/1	0.92	0.09	53,53,53,53	0
57	MG	2a	1702	1/1	0.92	0.14	47,47,47,47	0
57	MG	1A	3129	1/1	0.92	0.09	34,34,34,34	0
57	MG	1A	3495	1/1	0.92	0.11	39,39,39,39	0
57	MG	1A	3940	1/1	0.92	0.07	45,45,45,45	0
57	MG	1a	1668	1/1	0.92	0.12	49,49,49,49	0
57	MG	2a	1712	1/1	0.92	0.17	56,56,56,56	0
57	MG	2a	1713	1/1	0.92	0.11	48,48,48,48	0
57	MG	1a	1669	1/1	0.92	0.22	44,44,44,44	0
57	MG	1A	3410	1/1	0.92	0.07	34,34,34,34	0
57	MG	1A	3183	1/1	0.92	0.11	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3658	1/1	0.92	0.05	18,18,18,18	0
57	MG	1A	3415	1/1	0.92	0.30	59,59,59,59	0
57	MG	1A	3662	1/1	0.92	0.07	37,37,37,37	0
57	MG	1a	1683	1/1	0.92	0.20	57,57,57,57	0
57	MG	2A	3105	1/1	0.92	0.10	52,52,52,52	0
57	MG	1a	1684	1/1	0.92	0.08	43,43,43,43	0
57	MG	1A	3804	1/1	0.92	0.09	33,33,33,33	0
57	MG	2a	1737	1/1	0.92	0.13	55,55,55,55	0
57	MG	2a	1740	1/1	0.92	0.08	51,51,51,51	0
57	MG	1a	1692	1/1	0.92	0.24	43,43,43,43	0
57	MG	2A	3112	1/1	0.92	0.11	44,44,44,44	0
57	MG	2A	3374	1/1	0.92	0.16	33,33,33,33	0
57	MG	2A	3114	1/1	0.92	0.18	56,56,56,56	0
57	MG	1A	3525	1/1	0.92	0.14	55,55,55,55	0
57	MG	1A	3416	1/1	0.92	0.09	39,39,39,39	0
57	MG	2a	1754	1/1	0.92	0.13	52,52,52,52	0
57	MG	1A	3818	1/1	0.92	0.09	51,51,51,51	0
57	MG	1A	3534	1/1	0.92	0.10	33,33,33,33	0
57	MG	2A	3129	1/1	0.92	0.11	66,66,66,66	0
57	MG	1A	3670	1/1	0.92	0.15	33,33,33,33	0
57	MG	1A	3296	1/1	0.92	0.17	50,50,50,50	0
57	MG	2A	3143	1/1	0.92	0.19	41,41,41,41	0
57	MG	1a	1719	1/1	0.92	0.31	54,54,54,54	0
57	MG	2a	1770	1/1	0.92	0.10	64,64,64,64	0
57	MG	2A	3147	1/1	0.92	0.21	59,59,59,59	0
57	MG	1B	213	1/1	0.92	0.20	63,63,63,63	0
57	MG	2A	3159	1/1	0.92	0.27	51,51,51,51	0
57	MG	2A	3771	1/1	0.92	0.16	57,57,57,57	0
57	MG	2A	3775	1/1	0.92	0.15	48,48,48,48	0
57	MG	2a	1783	1/1	0.92	0.15	56,56,56,56	0
57	MG	1A	3970	1/1	0.92	0.07	24,24,24,24	0
57	MG	2A	3164	1/1	0.92	0.14	53,53,53,53	0
57	MG	1B	215	1/1	0.92	0.08	45,45,45,45	0
57	MG	1A	3540	1/1	0.92	0.15	30,30,30,30	0
57	MG	2a	1791	1/1	0.92	0.11	66,66,66,66	0
57	MG	2a	1796	1/1	0.92	0.08	43,43,43,43	0
57	MG	1a	1736	1/1	0.92	0.16	51,51,51,51	0
57	MG	2A	3177	1/1	0.92	0.10	44,44,44,44	0
57	MG	2a	1802	1/1	0.92	0.07	42,42,42,42	0
57	MG	2A	3793	1/1	0.92	0.10	58,58,58,58	0
57	MG	1a	1737	1/1	0.92	0.10	45,45,45,45	0
57	MG	1B	218	1/1	0.92	0.14	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1808	1/1	0.92	0.11	50,50,50,50	0
57	MG	2A	3801	1/1	0.92	0.09	52,52,52,52	0
57	MG	2a	1810	1/1	0.92	0.15	51,51,51,51	0
57	MG	1A	3681	1/1	0.92	0.10	16,16,16,16	0
57	MG	2a	1816	1/1	0.92	0.12	60,60,60,60	0
57	MG	2A	3804	1/1	0.92	0.09	36,36,36,36	0
57	MG	2A	3806	1/1	0.92	0.10	46,46,46,46	0
57	MG	1A	3339	1/1	0.92	0.08	40,40,40,40	0
57	MG	2A	3432	1/1	0.92	0.13	56,56,56,56	0
57	MG	1A	3298	1/1	0.92	0.08	38,38,38,38	0
57	MG	1A	3981	1/1	0.92	0.08	73,73,73,73	0
57	MG	1A	3851	1/1	0.92	0.10	43,43,43,43	0
57	MG	1a	1752	1/1	0.92	0.08	41,41,41,41	0
57	MG	1A	3987	1/1	0.92	0.09	44,44,44,44	0
57	MG	2A	3197	1/1	0.92	0.13	55,55,55,55	0
57	MG	2A	3448	1/1	0.92	0.13	38,38,38,38	0
57	MG	1D	306	1/1	0.92	0.10	36,36,36,36	0
57	MG	2A	3828	1/1	0.92	0.08	33,33,33,33	0
57	MG	2A	3835	1/1	0.92	0.10	43,43,43,43	0
57	MG	2i	201	1/1	0.92	0.17	66,66,66,66	0
57	MG	1A	3852	1/1	0.92	0.12	42,42,42,42	0
57	MG	2l	201	1/1	0.92	0.08	59,59,59,59	0
57	MG	1E	310	1/1	0.92	0.08	24,24,24,24	0
57	MG	2A	3453	1/1	0.92	0.09	44,44,44,44	0
57	MG	2A	3455	1/1	0.92	0.10	49,49,49,49	0
57	MG	1E	313	1/1	0.92	0.10	39,39,39,39	0
57	MG	2A	3208	1/1	0.92	0.08	53,53,53,53	0
57	MG	1a	1765	1/1	0.92	0.14	53,53,53,53	0
57	MG	1A	3702	1/1	0.92	0.11	28,28,28,28	0
57	MG	2A	3857	1/1	0.92	0.08	39,39,39,39	0
57	MG	1A	3706	1/1	0.92	0.10	17,17,17,17	0
57	MG	2A	3867	1/1	0.92	0.16	45,45,45,45	0
57	MG	2A	3214	1/1	0.92	0.18	45,45,45,45	0
57	MG	2A	3215	1/1	0.92	0.09	47,47,47,47	0
57	MG	1A	3708	1/1	0.92	0.15	49,49,49,49	0
57	MG	2A	3871	1/1	0.92	0.10	50,50,50,50	0
57	MG	1Q	204	1/1	0.92	0.08	58,58,58,58	0
57	MG	1A	3220	1/1	0.92	0.08	39,39,39,39	0
57	MG	1a	1775	1/1	0.92	0.11	44,44,44,44	0
57	MG	1A	3345	1/1	0.92	0.13	50,50,50,50	0
57	MG	2y	103	1/1	0.92	0.12	59,59,59,59	0
57	MG	1A	3027	1/1	0.92	0.13	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1T	203	1/1	0.92	0.13	43,43,43,43	0
57	MG	2A	3237	1/1	0.92	0.10	50,50,50,50	0
57	MG	1U	203	1/1	0.92	0.09	47,47,47,47	0
57	MG	2A	3042	1/1	0.93	0.16	39,39,39,39	0
57	MG	1A	3300	1/1	0.93	0.17	49,49,49,49	0
57	MG	2A	3044	1/1	0.93	0.13	57,57,57,57	0
57	MG	1A	3453	1/1	0.93	0.10	44,44,44,44	0
57	MG	1A	3346	1/1	0.93	0.11	33,33,33,33	0
57	MG	1A	3302	1/1	0.93	0.17	34,34,34,34	0
57	MG	1A	3357	1/1	0.93	0.14	54,54,54,54	0
57	MG	2N	201	1/1	0.93	0.06	45,45,45,45	0
57	MG	1A	3924	1/1	0.93	0.08	41,41,41,41	0
57	MG	1A	3925	1/1	0.93	0.06	39,39,39,39	0
57	MG	2A	3604	1/1	0.93	0.10	50,50,50,50	0
57	MG	2A	3058	1/1	0.93	0.17	46,46,46,46	0
57	MG	1A	4096	1/1	0.93	0.14	54,54,54,54	0
57	MG	1a	1678	1/1	0.93	0.08	41,41,41,41	0
57	MG	1A	3739	1/1	0.93	0.09	35,35,35,35	0
57	MG	2W	201	1/1	0.93	0.14	57,57,57,57	0
57	MG	2W	203	1/1	0.93	0.09	35,35,35,35	0
57	MG	2A	3069	1/1	0.93	0.12	53,53,53,53	0
57	MG	1A	3610	1/1	0.93	0.07	35,35,35,35	0
57	MG	2A	3073	1/1	0.93	0.11	43,43,43,43	0
57	MG	2A	3617	1/1	0.93	0.08	57,57,57,57	0
57	MG	25	101	1/1	0.93	0.15	49,49,49,49	0
57	MG	1A	3930	1/1	0.93	0.09	28,28,28,28	0
57	MG	1A	3358	1/1	0.93	0.08	53,53,53,53	0
57	MG	1a	1686	1/1	0.93	0.09	47,47,47,47	0
57	MG	1A	3310	1/1	0.93	0.22	39,39,39,39	0
57	MG	2A	3082	1/1	0.93	0.09	40,40,40,40	0
57	MG	2A	3627	1/1	0.93	0.13	51,51,51,51	0
57	MG	1A	3311	1/1	0.93	0.09	45,45,45,45	0
57	MG	2a	1605	1/1	0.93	0.24	56,56,56,56	0
57	MG	2A	3636	1/1	0.93	0.07	25,25,25,25	0
57	MG	2A	3638	1/1	0.93	0.09	37,37,37,37	0
57	MG	2A	3321	1/1	0.93	0.13	46,46,46,46	0
57	MG	2A	3642	1/1	0.93	0.10	39,39,39,39	0
57	MG	1A	3619	1/1	0.93	0.08	21,21,21,21	0
57	MG	2A	3650	1/1	0.93	0.13	38,38,38,38	0
57	MG	1a	1698	1/1	0.93	0.09	40,40,40,40	0
57	MG	2a	1617	1/1	0.93	0.06	41,41,41,41	0
57	MG	1a	1699	1/1	0.93	0.20	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3092	1/1	0.93	0.11	47,47,47,47	0
57	MG	2A	3655	1/1	0.93	0.07	42,42,42,42	0
57	MG	1a	1701	1/1	0.93	0.23	54,54,54,54	0
57	MG	1A	3759	1/1	0.93	0.06	31,31,31,31	0
57	MG	1A	3053	1/1	0.93	0.14	41,41,41,41	0
57	MG	1A	3949	1/1	0.93	0.15	51,51,51,51	0
57	MG	1a	1709	1/1	0.93	0.11	54,54,54,54	0
57	MG	2A	3669	1/1	0.93	0.10	55,55,55,55	0
57	MG	2a	1633	1/1	0.93	0.15	49,49,49,49	0
57	MG	1A	3764	1/1	0.93	0.11	33,33,33,33	0
57	MG	2A	3671	1/1	0.93	0.10	48,48,48,48	0
57	MG	2a	1637	1/1	0.93	0.14	50,50,50,50	0
57	MG	1a	1713	1/1	0.93	0.17	53,53,53,53	0
57	MG	1a	1715	1/1	0.93	0.18	48,48,48,48	0
57	MG	1A	3767	1/1	0.93	0.08	19,19,19,19	0
57	MG	1A	3062	1/1	0.93	0.27	51,51,51,51	0
57	MG	1A	3109	1/1	0.93	0.06	29,29,29,29	0
57	MG	1A	3390	1/1	0.93	0.25	31,31,31,31	0
57	MG	1A	3207	1/1	0.93	0.09	45,45,45,45	0
57	MG	1B	230	1/1	0.93	0.07	50,50,50,50	0
57	MG	1A	3485	1/1	0.93	0.09	43,43,43,43	0
57	MG	2a	1651	1/1	0.93	0.12	47,47,47,47	0
57	MG	1A	3325	1/1	0.93	0.11	38,38,38,38	0
57	MG	2A	3128	1/1	0.93	0.10	37,37,37,37	0
57	MG	1A	3797	1/1	0.93	0.11	51,51,51,51	0
57	MG	1E	302	1/1	0.93	0.09	45,45,45,45	0
57	MG	1A	3802	1/1	0.93	0.08	13,13,13,13	0
57	MG	1A	3115	1/1	0.93	0.16	36,36,36,36	0
57	MG	2a	1660	1/1	0.93	0.12	51,51,51,51	0
57	MG	2A	3368	1/1	0.93	0.17	45,45,45,45	0
57	MG	2a	1664	1/1	0.93	0.08	48,48,48,48	0
57	MG	1A	3399	1/1	0.93	0.11	44,44,44,44	0
57	MG	2A	3703	1/1	0.93	0.10	76,76,76,76	0
57	MG	1a	1748	1/1	0.93	0.07	51,51,51,51	0
57	MG	2a	1672	1/1	0.93	0.09	44,44,44,44	0
57	MG	1A	3401	1/1	0.93	0.08	40,40,40,40	0
57	MG	2A	3155	1/1	0.93	0.11	49,49,49,49	0
57	MG	1N	205	1/1	0.93	0.08	49,49,49,49	0
57	MG	1A	3219	1/1	0.93	0.08	42,42,42,42	0
57	MG	2a	1681	1/1	0.93	0.08	55,55,55,55	0
57	MG	1a	1754	1/1	0.93	0.10	57,57,57,57	0
57	MG	2A	3165	1/1	0.93	0.06	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3381	1/1	0.93	0.07	56,56,56,56	0
57	MG	2a	1693	1/1	0.93	0.12	46,46,46,46	0
57	MG	2a	1694	1/1	0.93	0.15	33,33,33,33	0
57	MG	2A	3170	1/1	0.93	0.14	48,48,48,48	0
57	MG	2a	1696	1/1	0.93	0.14	51,51,51,51	0
57	MG	2A	3385	1/1	0.93	0.17	56,56,56,56	0
57	MG	1A	3496	1/1	0.93	0.21	36,36,36,36	0
57	MG	2A	3388	1/1	0.93	0.12	44,44,44,44	0
57	MG	1A	3500	1/1	0.93	0.09	53,53,53,53	0
57	MG	1Q	206	1/1	0.93	0.15	40,40,40,40	0
57	MG	2a	1703	1/1	0.93	0.17	58,58,58,58	0
57	MG	1A	3118	1/1	0.93	0.12	38,38,38,38	0
57	MG	1A	3184	1/1	0.93	0.12	46,46,46,46	0
57	MG	2a	1709	1/1	0.93	0.11	61,61,61,61	0
57	MG	2A	3181	1/1	0.93	0.19	47,47,47,47	0
57	MG	2A	3744	1/1	0.93	0.06	36,36,36,36	0
57	MG	2A	3402	1/1	0.93	0.10	45,45,45,45	0
57	MG	2A	3403	1/1	0.93	0.11	41,41,41,41	0
57	MG	2A	3182	1/1	0.93	0.22	54,54,54,54	0
57	MG	2A	3408	1/1	0.93	0.08	58,58,58,58	0
57	MG	1T	202	1/1	0.93	0.08	57,57,57,57	0
57	MG	2a	1718	1/1	0.93	0.09	56,56,56,56	0
57	MG	1A	3991	1/1	0.93	0.05	23,23,23,23	0
57	MG	1A	3993	1/1	0.93	0.06	26,26,26,26	0
57	MG	2A	3757	1/1	0.93	0.08	35,35,35,35	0
57	MG	1A	3994	1/1	0.93	0.10	42,42,42,42	0
57	MG	1A	3006	1/1	0.93	0.07	27,27,27,27	0
57	MG	2a	1728	1/1	0.93	0.15	43,43,43,43	0
57	MG	1A	3673	1/1	0.93	0.10	23,23,23,23	0
57	MG	1A	3845	1/1	0.93	0.06	26,26,26,26	0
57	MG	2a	1735	1/1	0.93	0.15	42,42,42,42	0
57	MG	2a	1736	1/1	0.93	0.10	54,54,54,54	0
57	MG	1Z	3703	1/1	0.93	0.07	32,32,32,32	0
57	MG	2a	1738	1/1	0.93	0.18	50,50,50,50	0
57	MG	2A	3423	1/1	0.93	0.19	43,43,43,43	0
57	MG	1A	3523	1/1	0.93	0.08	62,62,62,62	0
57	MG	10	105	1/1	0.93	0.13	62,62,62,62	0
57	MG	1a	1790	1/1	0.93	0.06	47,47,47,47	0
57	MG	2A	3769	1/1	0.93	0.11	64,64,64,64	0
57	MG	1A	3850	1/1	0.93	0.13	46,46,46,46	0
57	MG	1A	3524	1/1	0.93	0.18	53,53,53,53	0
57	MG	1A	3334	1/1	0.93	0.10	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3189	1/1	0.93	0.08	39,39,39,39	0
57	MG	2A	3210	1/1	0.93	0.06	37,37,37,37	0
57	MG	2A	3442	1/1	0.93	0.35	60,60,60,60	0
57	MG	2A	3782	1/1	0.93	0.09	46,46,46,46	0
57	MG	2A	3443	1/1	0.93	0.15	48,48,48,48	0
57	MG	2A	3444	1/1	0.93	0.14	58,58,58,58	0
57	MG	1a	1802	1/1	0.93	0.10	52,52,52,52	0
57	MG	2a	1769	1/1	0.93	0.12	40,40,40,40	0
57	MG	1a	1803	1/1	0.93	0.08	67,67,67,67	0
57	MG	2A	3797	1/1	0.93	0.13	47,47,47,47	0
57	MG	1A	3688	1/1	0.93	0.07	32,32,32,32	0
57	MG	1A	3690	1/1	0.93	0.08	43,43,43,43	0
57	MG	1A	3694	1/1	0.93	0.08	24,24,24,24	0
57	MG	1A	3533	1/1	0.93	0.11	39,39,39,39	0
57	MG	17	107	1/1	0.93	0.11	39,39,39,39	0
57	MG	2A	3221	1/1	0.93	0.13	41,41,41,41	0
57	MG	2A	3808	1/1	0.93	0.08	48,48,48,48	0
57	MG	1A	3863	1/1	0.93	0.10	44,44,44,44	0
57	MG	2A	3223	1/1	0.93	0.21	49,49,49,49	0
57	MG	1d	301	1/1	0.93	0.16	50,50,50,50	0
57	MG	2a	1794	1/1	0.93	0.14	55,55,55,55	0
57	MG	1A	3701	1/1	0.93	0.10	26,26,26,26	0
57	MG	2A	3230	1/1	0.93	0.17	40,40,40,40	0
57	MG	2A	3816	1/1	0.93	0.11	55,55,55,55	0
57	MG	2a	1801	1/1	0.93	0.21	56,56,56,56	0
57	MG	2A	3466	1/1	0.93	0.06	44,44,44,44	0
57	MG	1A	3288	1/1	0.93	0.11	54,54,54,54	0
57	MG	2A	3471	1/1	0.93	0.08	46,46,46,46	0
57	MG	2A	3475	1/1	0.93	0.10	62,62,62,62	0
57	MG	2A	3483	1/1	0.93	0.14	53,53,53,53	0
57	MG	2A	3232	1/1	0.93	0.10	40,40,40,40	0
57	MG	2A	3233	1/1	0.93	0.24	52,52,52,52	0
57	MG	2A	3495	1/1	0.93	0.09	59,59,59,59	0
57	MG	2a	1813	1/1	0.93	0.11	54,54,54,54	0
57	MG	1A	3016	1/1	0.93	0.09	50,50,50,50	0
57	MG	2A	3842	1/1	0.93	0.08	54,54,54,54	0
57	MG	2A	3240	1/1	0.93	0.10	32,32,32,32	0
57	MG	2a	1820	1/1	0.93	0.12	56,56,56,56	0
57	MG	1A	3417	1/1	0.93	0.12	36,36,36,36	0
57	MG	2A	3852	1/1	0.93	0.08	60,60,60,60	0
57	MG	1A	3295	1/1	0.93	0.10	42,42,42,42	0
57	MG	2a	1825	1/1	0.93	0.12	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1611	1/1	0.93	0.11	51,51,51,51	0
57	MG	2A	3248	1/1	0.93	0.15	51,51,51,51	0
57	MG	1A	3421	1/1	0.93	0.10	33,33,33,33	0
57	MG	1A	3550	1/1	0.93	0.11	51,51,51,51	0
57	MG	2a	1832	1/1	0.93	0.15	41,41,41,41	0
57	MG	1A	3715	1/1	0.93	0.10	65,65,65,65	0
57	MG	1a	1621	1/1	0.93	0.15	49,49,49,49	0
57	MG	1A	3876	1/1	0.93	0.06	25,25,25,25	0
57	MG	2A	3516	1/1	0.93	0.11	33,33,33,33	0
57	MG	1A	3427	1/1	0.93	0.07	52,52,52,52	0
57	MG	2A	3872	1/1	0.93	0.15	56,56,56,56	0
57	MG	2j	201	1/1	0.93	0.07	52,52,52,52	0
57	MG	2A	3875	1/1	0.93	0.22	52,52,52,52	0
57	MG	1x	104	1/1	0.93	0.12	48,48,48,48	0
57	MG	2A	3881	1/1	0.93	0.09	51,51,51,51	0
57	MG	1a	1629	1/1	0.93	0.15	44,44,44,44	0
57	MG	1A	3560	1/1	0.93	0.10	26,26,26,26	0
57	MG	1A	3719	1/1	0.93	0.05	10,10,10,10	0
57	MG	2q	201	1/1	0.93	0.19	59,59,59,59	0
57	MG	1A	3886	1/1	0.93	0.07	31,31,31,31	0
57	MG	2r	102	1/1	0.93	0.14	61,61,61,61	0
57	MG	1A	4045	1/1	0.93	0.07	42,42,42,42	0
57	MG	1A	3720	1/1	0.93	0.14	57,57,57,57	0
57	MG	2A	3541	1/1	0.93	0.07	40,40,40,40	0
57	MG	1A	3241	1/1	0.93	0.07	30,30,30,30	0
57	MG	1A	3245	1/1	0.93	0.13	39,39,39,39	0
57	MG	1A	3565	1/1	0.93	0.12	45,45,45,45	0
57	MG	2A	3023	1/1	0.93	0.17	63,63,63,63	0
57	MG	2w	106	1/1	0.93	0.09	50,50,50,50	0
57	MG	1A	3566	1/1	0.93	0.07	40,40,40,40	0
57	MG	1A	3726	1/1	0.93	0.07	23,23,23,23	0
57	MG	2A	3563	1/1	0.93	0.11	40,40,40,40	0
57	MG	1A	3344	1/1	0.93	0.07	35,35,35,35	0
57	MG	1A	3900	1/1	0.93	0.20	58,58,58,58	0
57	MG	2A	3566	1/1	0.93	0.07	42,42,42,42	0
57	MG	2A	3284	1/1	0.93	0.16	45,45,45,45	0
57	MG	2A	3572	1/1	0.93	0.12	50,50,50,50	0
57	MG	1A	3439	1/1	0.93	0.26	49,49,49,49	0
57	MG	2A	3037	1/1	0.93	0.08	37,37,37,37	0
59	A1C9N	1A	4101	74/74	0.93	0.12	13,37,50,51	0
57	MG	2A	3579	1/1	0.93	0.09	54,54,54,54	0
57	MG	2A	3238	1/1	0.94	0.08	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3580	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3458	1/1	0.94	0.11	46,46,46,46	0
57	MG	2A	3242	1/1	0.94	0.09	50,50,50,50	0
57	MG	1A	3305	1/1	0.94	0.12	36,36,36,36	0
57	MG	2A	3525	1/1	0.94	0.07	53,53,53,53	0
57	MG	1A	4030	1/1	0.94	0.07	33,33,33,33	0
57	MG	2A	3528	1/1	0.94	0.08	48,48,48,48	0
57	MG	2A	3247	1/1	0.94	0.09	52,52,52,52	0
57	MG	1m	3001	1/1	0.94	0.08	36,36,36,36	0
57	MG	17	106	1/1	0.94	0.07	35,35,35,35	0
57	MG	2A	3251	1/1	0.94	0.10	53,53,53,53	0
57	MG	2A	3544	1/1	0.94	0.07	32,32,32,32	0
57	MG	2A	3546	1/1	0.94	0.16	41,41,41,41	0
57	MG	1n	101	1/1	0.94	0.17	40,40,40,40	0
57	MG	1A	3728	1/1	0.94	0.13	42,42,42,42	0
57	MG	2A	3552	1/1	0.94	0.07	32,32,32,32	0
57	MG	2F	304	1/1	0.94	0.17	39,39,39,39	0
57	MG	1A	3375	1/1	0.94	0.08	43,43,43,43	0
57	MG	1A	3377	1/1	0.94	0.14	39,39,39,39	0
57	MG	18	104	1/1	0.94	0.11	49,49,49,49	0
57	MG	1A	3234	1/1	0.94	0.09	40,40,40,40	0
57	MG	1A	3028	1/1	0.94	0.10	42,42,42,42	0
57	MG	2Q	201	1/1	0.94	0.15	52,52,52,52	0
57	MG	2Q	202	1/1	0.94	0.12	52,52,52,52	0
57	MG	1A	3178	1/1	0.94	0.05	23,23,23,23	0
57	MG	1w	107	1/1	0.94	0.06	56,56,56,56	0
57	MG	1a	1607	1/1	0.94	0.07	35,35,35,35	0
57	MG	1A	3893	1/1	0.94	0.09	41,41,41,41	0
57	MG	2A	3571	1/1	0.94	0.06	37,37,37,37	0
57	MG	1a	1609	1/1	0.94	0.07	44,44,44,44	0
57	MG	2W	202	1/1	0.94	0.08	40,40,40,40	0
57	MG	1x	106	1/1	0.94	0.23	51,51,51,51	0
57	MG	2X	101	1/1	0.94	0.07	60,60,60,60	0
57	MG	1A	3180	1/1	0.94	0.06	34,34,34,34	0
57	MG	1A	3112	1/1	0.94	0.13	27,27,27,27	0
57	MG	20	102	1/1	0.94	0.18	50,50,50,50	0
57	MG	1A	3740	1/1	0.94	0.08	55,55,55,55	0
57	MG	1x	114	1/1	0.94	0.10	36,36,36,36	0
57	MG	1A	3743	1/1	0.94	0.07	39,39,39,39	0
57	MG	2A	3280	1/1	0.94	0.11	37,37,37,37	0
57	MG	2A	3002	1/1	0.94	0.22	44,44,44,44	0
57	MG	27	102	1/1	0.94	0.08	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1619	1/1	0.94	0.08	37,37,37,37	0
57	MG	1A	3903	1/1	0.94	0.09	31,31,31,31	0
57	MG	1A	3618	1/1	0.94	0.05	20,20,20,20	0
57	MG	2A	3006	1/1	0.94	0.20	45,45,45,45	0
57	MG	1A	3054	1/1	0.94	0.10	24,24,24,24	0
57	MG	2a	1604	1/1	0.94	0.13	54,54,54,54	0
57	MG	2A	3605	1/1	0.94	0.08	40,40,40,40	0
57	MG	1A	3324	1/1	0.94	0.15	43,43,43,43	0
57	MG	2A	3018	1/1	0.94	0.18	48,48,48,48	0
57	MG	2A	3022	1/1	0.94	0.16	41,41,41,41	0
57	MG	1a	1631	1/1	0.94	0.14	39,39,39,39	0
57	MG	1a	1633	1/1	0.94	0.24	55,55,55,55	0
57	MG	1A	3912	1/1	0.94	0.07	36,36,36,36	0
57	MG	2a	1614	1/1	0.94	0.09	52,52,52,52	0
57	MG	1A	4059	1/1	0.94	0.09	35,35,35,35	0
57	MG	1A	3637	1/1	0.94	0.14	43,43,43,43	0
57	MG	2A	3032	1/1	0.94	0.07	47,47,47,47	0
57	MG	1A	4065	1/1	0.94	0.05	34,34,34,34	0
57	MG	2a	1621	1/1	0.94	0.10	54,54,54,54	0
57	MG	2A	3302	1/1	0.94	0.13	50,50,50,50	0
57	MG	1A	4066	1/1	0.94	0.10	51,51,51,51	0
57	MG	1A	3397	1/1	0.94	0.06	27,27,27,27	0
57	MG	1A	3920	1/1	0.94	0.05	24,24,24,24	0
57	MG	2a	1628	1/1	0.94	0.22	52,52,52,52	0
57	MG	2A	3629	1/1	0.94	0.07	45,45,45,45	0
57	MG	1A	3643	1/1	0.94	0.06	34,34,34,34	0
57	MG	2A	3633	1/1	0.94	0.17	48,48,48,48	0
57	MG	1A	4078	1/1	0.94	0.07	30,30,30,30	0
57	MG	1A	4080	1/1	0.94	0.08	44,44,44,44	0
57	MG	1a	1650	1/1	0.94	0.12	56,56,56,56	0
57	MG	1A	3185	1/1	0.94	0.10	56,56,56,56	0
57	MG	1a	1655	1/1	0.94	0.07	42,42,42,42	0
57	MG	2A	3648	1/1	0.94	0.13	44,44,44,44	0
57	MG	1a	1656	1/1	0.94	0.12	42,42,42,42	0
57	MG	1A	3488	1/1	0.94	0.10	36,36,36,36	0
57	MG	1A	3007	1/1	0.94	0.07	32,32,32,32	0
57	MG	1A	4092	1/1	0.94	0.10	44,44,44,44	0
57	MG	2a	1645	1/1	0.94	0.09	44,44,44,44	0
57	MG	2a	1647	1/1	0.94	0.11	52,52,52,52	0
57	MG	1A	3402	1/1	0.94	0.12	31,31,31,31	0
57	MG	2A	3325	1/1	0.94	0.12	52,52,52,52	0
57	MG	1A	3263	1/1	0.94	0.18	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3660	1/1	0.94	0.15	53,53,53,53	0
57	MG	2A	3332	1/1	0.94	0.10	57,57,57,57	0
57	MG	2A	3665	1/1	0.94	0.06	49,49,49,49	0
57	MG	2A	3333	1/1	0.94	0.34	54,54,54,54	0
57	MG	1A	3771	1/1	0.94	0.07	26,26,26,26	0
57	MG	2A	3336	1/1	0.94	0.13	56,56,56,56	0
57	MG	1A	3406	1/1	0.94	0.25	28,28,28,28	0
57	MG	1A	3187	1/1	0.94	0.10	28,28,28,28	0
57	MG	2A	3339	1/1	0.94	0.09	57,57,57,57	0
57	MG	2A	3673	1/1	0.94	0.07	27,27,27,27	0
57	MG	1a	1671	1/1	0.94	0.08	52,52,52,52	0
57	MG	2A	3341	1/1	0.94	0.08	48,48,48,48	0
57	MG	2a	1669	1/1	0.94	0.07	47,47,47,47	0
57	MG	1a	1674	1/1	0.94	0.06	44,44,44,44	0
57	MG	1a	1675	1/1	0.94	0.07	37,37,37,37	0
57	MG	2A	3680	1/1	0.94	0.14	41,41,41,41	0
57	MG	2A	3346	1/1	0.94	0.15	46,46,46,46	0
57	MG	1A	3081	1/1	0.94	0.20	28,28,28,28	0
57	MG	1A	3793	1/1	0.94	0.07	42,42,42,42	0
57	MG	1A	3503	1/1	0.94	0.07	52,52,52,52	0
57	MG	1A	3796	1/1	0.94	0.12	43,43,43,43	0
57	MG	1A	3088	1/1	0.94	0.07	33,33,33,33	0
57	MG	2a	1689	1/1	0.94	0.10	48,48,48,48	0
57	MG	2a	1690	1/1	0.94	0.08	49,49,49,49	0
57	MG	1B	212	1/1	0.94	0.05	44,44,44,44	0
57	MG	1A	3333	1/1	0.94	0.13	44,44,44,44	0
57	MG	2A	3697	1/1	0.94	0.09	46,46,46,46	0
57	MG	1A	3195	1/1	0.94	0.09	25,25,25,25	0
57	MG	1a	1688	1/1	0.94	0.10	46,46,46,46	0
57	MG	1A	3093	1/1	0.94	0.06	44,44,44,44	0
57	MG	1A	3961	1/1	0.94	0.10	40,40,40,40	0
57	MG	1A	3275	1/1	0.94	0.08	39,39,39,39	0
57	MG	1A	3145	1/1	0.94	0.08	36,36,36,36	0
57	MG	1A	3674	1/1	0.94	0.06	32,32,32,32	0
57	MG	2A	3107	1/1	0.94	0.13	42,42,42,42	0
57	MG	2a	1704	1/1	0.94	0.11	49,49,49,49	0
57	MG	2a	1705	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3528	1/1	0.94	0.28	52,52,52,52	0
57	MG	2a	1707	1/1	0.94	0.13	53,53,53,53	0
57	MG	1A	3149	1/1	0.94	0.17	30,30,30,30	0
57	MG	2A	3369	1/1	0.94	0.10	57,57,57,57	0
57	MG	1a	1705	1/1	0.94	0.12	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3832	1/1	0.94	0.06	31,31,31,31	0
57	MG	1A	3835	1/1	0.94	0.10	37,37,37,37	0
57	MG	2A	3373	1/1	0.94	0.07	48,48,48,48	0
57	MG	1B	231	1/1	0.94	0.19	42,42,42,42	0
57	MG	1B	232	1/1	0.94	0.07	43,43,43,43	0
57	MG	1A	3836	1/1	0.94	0.12	50,50,50,50	0
57	MG	2A	3127	1/1	0.94	0.09	53,53,53,53	0
57	MG	2A	3734	1/1	0.94	0.06	23,23,23,23	0
57	MG	2A	3379	1/1	0.94	0.20	48,48,48,48	0
57	MG	1D	303	1/1	0.94	0.10	34,34,34,34	0
57	MG	2a	1724	1/1	0.94	0.10	41,41,41,41	0
57	MG	2A	3738	1/1	0.94	0.09	60,60,60,60	0
57	MG	1a	1716	1/1	0.94	0.16	41,41,41,41	0
57	MG	2A	3743	1/1	0.94	0.07	42,42,42,42	0
57	MG	2A	3132	1/1	0.94	0.12	51,51,51,51	0
57	MG	2A	3134	1/1	0.94	0.08	47,47,47,47	0
57	MG	2A	3386	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	3419	1/1	0.94	0.07	44,44,44,44	0
57	MG	1A	3151	1/1	0.94	0.07	20,20,20,20	0
57	MG	1A	3984	1/1	0.94	0.08	54,54,54,54	0
57	MG	2A	3751	1/1	0.94	0.09	51,51,51,51	0
57	MG	2A	3393	1/1	0.94	0.10	47,47,47,47	0
57	MG	2a	1742	1/1	0.94	0.20	60,60,60,60	0
57	MG	1E	303	1/1	0.94	0.10	41,41,41,41	0
57	MG	1E	307	1/1	0.94	0.08	40,40,40,40	0
57	MG	2A	3148	1/1	0.94	0.21	49,49,49,49	0
57	MG	2A	3151	1/1	0.94	0.07	57,57,57,57	0
57	MG	2a	1752	1/1	0.94	0.07	55,55,55,55	0
57	MG	1E	308	1/1	0.94	0.10	35,35,35,35	0
57	MG	1A	3985	1/1	0.94	0.08	67,67,67,67	0
57	MG	1A	3687	1/1	0.94	0.05	15,15,15,15	0
57	MG	2A	3161	1/1	0.94	0.08	40,40,40,40	0
57	MG	1A	3290	1/1	0.94	0.11	46,46,46,46	0
57	MG	1F	311	1/1	0.94	0.07	34,34,34,34	0
57	MG	1F	312	1/1	0.94	0.10	38,38,38,38	0
57	MG	2A	3169	1/1	0.94	0.10	42,42,42,42	0
57	MG	2A	3770	1/1	0.94	0.11	48,48,48,48	0
57	MG	1G	203	1/1	0.94	0.07	60,60,60,60	0
57	MG	2A	3774	1/1	0.94	0.11	34,34,34,34	0
57	MG	1A	3153	1/1	0.94	0.10	34,34,34,34	0
57	MG	1a	1747	1/1	0.94	0.07	48,48,48,48	0
57	MG	1N	202	1/1	0.94	0.07	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3419	1/1	0.94	0.12	43,43,43,43	0
57	MG	2A	3421	1/1	0.94	0.20	41,41,41,41	0
57	MG	1N	204	1/1	0.94	0.23	43,43,43,43	0
57	MG	2A	3790	1/1	0.94	0.10	49,49,49,49	0
57	MG	1a	1751	1/1	0.94	0.07	38,38,38,38	0
57	MG	1A	3542	1/1	0.94	0.08	36,36,36,36	0
57	MG	1A	3429	1/1	0.94	0.06	27,27,27,27	0
57	MG	2a	1790	1/1	0.94	0.07	41,41,41,41	0
57	MG	1P	203	1/1	0.94	0.21	32,32,32,32	0
57	MG	2A	3796	1/1	0.94	0.07	47,47,47,47	0
57	MG	2A	3433	1/1	0.94	0.14	42,42,42,42	0
57	MG	2A	3798	1/1	0.94	0.10	59,59,59,59	0
57	MG	2A	3434	1/1	0.94	0.26	52,52,52,52	0
57	MG	2a	1800	1/1	0.94	0.15	53,53,53,53	0
57	MG	2A	3800	1/1	0.94	0.10	52,52,52,52	0
57	MG	1Q	201	1/1	0.94	0.22	32,32,32,32	0
57	MG	2A	3437	1/1	0.94	0.09	48,48,48,48	0
57	MG	2A	3803	1/1	0.94	0.11	44,44,44,44	0
57	MG	2a	1805	1/1	0.94	0.15	51,51,51,51	0
57	MG	2A	3188	1/1	0.94	0.08	46,46,46,46	0
57	MG	2a	1807	1/1	0.94	0.24	52,52,52,52	0
57	MG	2A	3439	1/1	0.94	0.24	51,51,51,51	0
57	MG	1A	3431	1/1	0.94	0.09	37,37,37,37	0
57	MG	1a	1759	1/1	0.94	0.13	47,47,47,47	0
57	MG	1A	3548	1/1	0.94	0.10	49,49,49,49	0
57	MG	1A	3995	1/1	0.94	0.47	35,35,35,35	0
57	MG	2a	1814	1/1	0.94	0.10	56,56,56,56	0
57	MG	1a	1763	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	3294	1/1	0.94	0.07	31,31,31,31	0
57	MG	1A	3435	1/1	0.94	0.12	38,38,38,38	0
57	MG	1T	201	1/1	0.94	0.15	42,42,42,42	0
57	MG	2A	3819	1/1	0.94	0.06	57,57,57,57	0
57	MG	2A	3199	1/1	0.94	0.09	42,42,42,42	0
57	MG	2A	3201	1/1	0.94	0.08	43,43,43,43	0
57	MG	2A	3451	1/1	0.94	0.07	40,40,40,40	0
57	MG	1A	3999	1/1	0.94	0.08	42,42,42,42	0
57	MG	2a	1828	1/1	0.94	0.09	49,49,49,49	0
57	MG	2A	3203	1/1	0.94	0.06	42,42,42,42	0
57	MG	2A	3830	1/1	0.94	0.06	35,35,35,35	0
57	MG	2A	3831	1/1	0.94	0.09	34,34,34,34	0
57	MG	1A	3552	1/1	0.94	0.10	31,31,31,31	0
57	MG	1A	3217	1/1	0.94	0.17	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3207	1/1	0.94	0.08	44,44,44,44	0
57	MG	1A	3042	1/1	0.94	0.14	23,23,23,23	0
57	MG	1a	1779	1/1	0.94	0.10	57,57,57,57	0
57	MG	2A	3843	1/1	0.94	0.08	39,39,39,39	0
57	MG	1W	206	1/1	0.94	0.14	41,41,41,41	0
57	MG	2A	3848	1/1	0.94	0.09	58,58,58,58	0
57	MG	1X	107	1/1	0.94	0.06	44,44,44,44	0
57	MG	2A	3467	1/1	0.94	0.17	45,45,45,45	0
57	MG	2A	3468	1/1	0.94	0.09	54,54,54,54	0
57	MG	1Y	201	1/1	0.94	0.06	40,40,40,40	0
57	MG	2A	3855	1/1	0.94	0.08	54,54,54,54	0
57	MG	2m	201	1/1	0.94	0.08	60,60,60,60	0
57	MG	1A	3448	1/1	0.94	0.10	49,49,49,49	0
57	MG	1A	3563	1/1	0.94	0.11	35,35,35,35	0
57	MG	2A	3860	1/1	0.94	0.16	46,46,46,46	0
57	MG	2r	101	1/1	0.94	0.13	54,54,54,54	0
57	MG	2A	3482	1/1	0.94	0.08	58,58,58,58	0
57	MG	2t	201	1/1	0.94	0.11	35,35,35,35	0
57	MG	1A	3159	1/1	0.94	0.06	47,47,47,47	0
57	MG	2A	3484	1/1	0.94	0.09	53,53,53,53	0
57	MG	1A	4013	1/1	0.94	0.08	27,27,27,27	0
57	MG	1A	3869	1/1	0.94	0.05	39,39,39,39	0
57	MG	2A	3490	1/1	0.94	0.13	52,52,52,52	0
57	MG	2A	3494	1/1	0.94	0.09	29,29,29,29	0
57	MG	1A	3168	1/1	0.94	0.10	24,24,24,24	0
57	MG	1A	3454	1/1	0.94	0.11	49,49,49,49	0
57	MG	2A	3880	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	3025	1/1	0.94	0.09	34,34,34,34	0
57	MG	10	108	1/1	0.94	0.07	48,48,48,48	0
57	MG	2A	3225	1/1	0.94	0.22	54,54,54,54	0
57	MG	1a	1807	1/1	0.94	0.07	36,36,36,36	0
57	MG	2x	105	1/1	0.94	0.16	39,39,39,39	0
57	MG	1a	1808	1/1	0.94	0.12	56,56,56,56	0
57	MG	2A	3507	1/1	0.94	0.08	63,63,63,63	0
57	MG	1A	3576	1/1	0.94	0.15	35,35,35,35	0
57	MG	12	101	1/1	0.94	0.07	38,38,38,38	0
57	MG	13	103	1/1	0.94	0.10	40,40,40,40	0
57	MG	2A	3236	1/1	0.94	0.07	46,46,46,46	0
57	MG	1A	3577	1/1	0.94	0.17	36,36,36,36	0
57	MG	1A	3932	1/1	0.95	0.07	44,44,44,44	0
57	MG	1a	1722	1/1	0.95	0.14	41,41,41,41	0
57	MG	1D	308	1/1	0.95	0.12	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3070	1/1	0.95	0.07	26,26,26,26	0
57	MG	2A	3186	1/1	0.95	0.09	39,39,39,39	0
57	MG	2A	3474	1/1	0.95	0.08	47,47,47,47	0
57	MG	1a	1727	1/1	0.95	0.07	55,55,55,55	0
57	MG	2A	3476	1/1	0.95	0.09	32,32,32,32	0
57	MG	2A	3874	1/1	0.95	0.12	48,48,48,48	0
57	MG	2A	3479	1/1	0.95	0.11	35,35,35,35	0
57	MG	2A	3876	1/1	0.95	0.14	44,44,44,44	0
57	MG	2A	3877	1/1	0.95	0.08	59,59,59,59	0
57	MG	2A	3480	1/1	0.95	0.14	46,46,46,46	0
57	MG	2A	3481	1/1	0.95	0.11	30,30,30,30	0
57	MG	1a	1728	1/1	0.95	0.12	44,44,44,44	0
57	MG	1A	3579	1/1	0.95	0.09	39,39,39,39	0
57	MG	1a	1733	1/1	0.95	0.07	31,31,31,31	0
57	MG	1a	1734	1/1	0.95	0.06	30,30,30,30	0
57	MG	1a	1735	1/1	0.95	0.07	43,43,43,43	0
57	MG	1A	3941	1/1	0.95	0.10	46,46,46,46	0
57	MG	2A	3492	1/1	0.95	0.19	50,50,50,50	0
57	MG	1A	3742	1/1	0.95	0.07	54,54,54,54	0
57	MG	2B	206	1/1	0.95	0.17	54,54,54,54	0
57	MG	1A	3182	1/1	0.95	0.05	28,28,28,28	0
57	MG	2A	3496	1/1	0.95	0.10	42,42,42,42	0
57	MG	1A	3583	1/1	0.95	0.04	22,22,22,22	0
57	MG	2A	3499	1/1	0.95	0.05	49,49,49,49	0
57	MG	1E	312	1/1	0.95	0.06	51,51,51,51	0
57	MG	1a	1742	1/1	0.95	0.08	35,35,35,35	0
57	MG	1A	3749	1/1	0.95	0.06	9,9,9,9	0
57	MG	1A	3584	1/1	0.95	0.06	32,32,32,32	0
57	MG	1F	305	1/1	0.95	0.04	39,39,39,39	0
57	MG	1F	310	1/1	0.95	0.19	29,29,29,29	0
57	MG	1A	3587	1/1	0.95	0.05	39,39,39,39	0
57	MG	2B	218	1/1	0.95	0.09	60,60,60,60	0
57	MG	2B	219	1/1	0.95	0.16	55,55,55,55	0
57	MG	2A	3510	1/1	0.95	0.16	52,52,52,52	0
57	MG	1A	3954	1/1	0.95	0.06	45,45,45,45	0
57	MG	2D	305	1/1	0.95	0.05	20,20,20,20	0
57	MG	1G	202	1/1	0.95	0.15	48,48,48,48	0
57	MG	1A	3462	1/1	0.95	0.07	44,44,44,44	0
57	MG	1G	204	1/1	0.95	0.07	47,47,47,47	0
57	MG	1A	3593	1/1	0.95	0.05	23,23,23,23	0
57	MG	1A	3957	1/1	0.95	0.12	47,47,47,47	0
57	MG	2E	307	1/1	0.95	0.07	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3465	1/1	0.95	0.10	41,41,41,41	0
57	MG	2A	3519	1/1	0.95	0.08	25,25,25,25	0
57	MG	2F	303	1/1	0.95	0.12	56,56,56,56	0
57	MG	1A	3959	1/1	0.95	0.13	37,37,37,37	0
57	MG	2A	3521	1/1	0.95	0.07	17,17,17,17	0
57	MG	1N	206	1/1	0.95	0.22	28,28,28,28	0
57	MG	2A	3523	1/1	0.95	0.06	39,39,39,39	0
57	MG	1a	1762	1/1	0.95	0.16	49,49,49,49	0
57	MG	1A	3597	1/1	0.95	0.24	39,39,39,39	0
57	MG	1A	3762	1/1	0.95	0.05	38,38,38,38	0
57	MG	1A	3301	1/1	0.95	0.08	34,34,34,34	0
57	MG	2A	3532	1/1	0.95	0.06	44,44,44,44	0
57	MG	1A	3120	1/1	0.95	0.14	33,33,33,33	0
57	MG	2T	201	1/1	0.95	0.09	47,47,47,47	0
57	MG	1A	3383	1/1	0.95	0.10	44,44,44,44	0
57	MG	2A	3227	1/1	0.95	0.13	41,41,41,41	0
57	MG	1A	3002	1/1	0.95	0.06	38,38,38,38	0
57	MG	2A	3545	1/1	0.95	0.07	36,36,36,36	0
57	MG	1A	3971	1/1	0.95	0.07	30,30,30,30	0
57	MG	1A	3388	1/1	0.95	0.12	15,15,15,15	0
57	MG	1a	1776	1/1	0.95	0.09	43,43,43,43	0
57	MG	1A	3772	1/1	0.95	0.07	18,18,18,18	0
57	MG	1A	3773	1/1	0.95	0.09	25,25,25,25	0
57	MG	1A	3471	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3780	1/1	0.95	0.06	52,52,52,52	0
57	MG	1U	209	1/1	0.95	0.14	40,40,40,40	0
57	MG	1A	3473	1/1	0.95	0.10	39,39,39,39	0
57	MG	1V	204	1/1	0.95	0.20	36,36,36,36	0
57	MG	25	104	1/1	0.95	0.11	45,45,45,45	0
57	MG	1V	208	1/1	0.95	0.11	44,44,44,44	0
57	MG	2A	3244	1/1	0.95	0.09	58,58,58,58	0
57	MG	1W	204	1/1	0.95	0.09	44,44,44,44	0
57	MG	1A	3306	1/1	0.95	0.13	32,32,32,32	0
57	MG	1X	101	1/1	0.95	0.12	48,48,48,48	0
57	MG	1X	102	1/1	0.95	0.13	27,27,27,27	0
57	MG	2a	1602	1/1	0.95	0.12	60,60,60,60	0
57	MG	1A	3788	1/1	0.95	0.06	43,43,43,43	0
57	MG	2A	3252	1/1	0.95	0.10	59,59,59,59	0
57	MG	1a	1806	1/1	0.95	0.08	58,58,58,58	0
57	MG	1A	3478	1/1	0.95	0.11	25,25,25,25	0
57	MG	1A	3622	1/1	0.95	0.08	23,23,23,23	0
57	MG	2A	3586	1/1	0.95	0.09	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3307	1/1	0.95	0.09	27,27,27,27	0
57	MG	1Z	3701	1/1	0.95	0.05	31,31,31,31	0
57	MG	1A	3624	1/1	0.95	0.05	20,20,20,20	0
57	MG	2a	1612	1/1	0.95	0.07	52,52,52,52	0
57	MG	2a	1613	1/1	0.95	0.13	51,51,51,51	0
57	MG	1A	3800	1/1	0.95	0.06	16,16,16,16	0
57	MG	2A	3592	1/1	0.95	0.09	48,48,48,48	0
57	MG	2A	3265	1/1	0.95	0.12	38,38,38,38	0
57	MG	2A	3598	1/1	0.95	0.07	38,38,38,38	0
57	MG	1A	3629	1/1	0.95	0.09	35,35,35,35	0
57	MG	1A	3803	1/1	0.95	0.06	35,35,35,35	0
57	MG	1A	3633	1/1	0.95	0.05	29,29,29,29	0
57	MG	1e	202	1/1	0.95	0.22	48,48,48,48	0
57	MG	1A	3238	1/1	0.95	0.18	19,19,19,19	0
57	MG	1A	3998	1/1	0.95	0.07	40,40,40,40	0
57	MG	1A	3808	1/1	0.95	0.06	22,22,22,22	0
57	MG	1A	3640	1/1	0.95	0.10	55,55,55,55	0
57	MG	1A	3815	1/1	0.95	0.08	26,26,26,26	0
57	MG	2a	1631	1/1	0.95	0.21	51,51,51,51	0
57	MG	2A	3613	1/1	0.95	0.13	52,52,52,52	0
57	MG	1n	103	1/1	0.95	0.18	44,44,44,44	0
57	MG	2a	1634	1/1	0.95	0.08	59,59,59,59	0
57	MG	1A	3074	1/1	0.95	0.08	27,27,27,27	0
57	MG	14	101	1/1	0.95	0.10	46,46,46,46	0
57	MG	2A	3620	1/1	0.95	0.05	26,26,26,26	0
57	MG	1A	3819	1/1	0.95	0.09	39,39,39,39	0
57	MG	1A	3393	1/1	0.95	0.07	52,52,52,52	0
57	MG	1w	104	1/1	0.95	0.20	64,64,64,64	0
57	MG	1A	3394	1/1	0.95	0.12	53,53,53,53	0
57	MG	2A	3626	1/1	0.95	0.14	53,53,53,53	0
57	MG	16	101	1/1	0.95	0.06	39,39,39,39	0
57	MG	17	103	1/1	0.95	0.10	29,29,29,29	0
57	MG	17	104	1/1	0.95	0.12	42,42,42,42	0
57	MG	1A	3243	1/1	0.95	0.21	27,27,27,27	0
57	MG	2A	3635	1/1	0.95	0.15	44,44,44,44	0
57	MG	1A	3313	1/1	0.95	0.06	30,30,30,30	0
57	MG	1x	105	1/1	0.95	0.12	45,45,45,45	0
57	MG	1A	3833	1/1	0.95	0.11	42,42,42,42	0
57	MG	1x	107	1/1	0.95	0.06	42,42,42,42	0
57	MG	2a	1654	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	3079	1/1	0.95	0.08	44,44,44,44	0
57	MG	2A	3646	1/1	0.95	0.09	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1657	1/1	0.95	0.12	56,56,56,56	0
57	MG	2A	3647	1/1	0.95	0.08	28,28,28,28	0
57	MG	1A	3321	1/1	0.95	0.13	25,25,25,25	0
57	MG	2A	3649	1/1	0.95	0.09	39,39,39,39	0
57	MG	1A	3837	1/1	0.95	0.12	33,33,33,33	0
57	MG	1A	3246	1/1	0.95	0.11	50,50,50,50	0
57	MG	1a	1601	1/1	0.95	0.06	42,42,42,42	0
57	MG	2A	3001	1/1	0.95	0.19	41,41,41,41	0
57	MG	2a	1667	1/1	0.95	0.18	55,55,55,55	0
57	MG	1A	3840	1/1	0.95	0.06	27,27,27,27	0
57	MG	1A	3842	1/1	0.95	0.06	39,39,39,39	0
57	MG	1A	3247	1/1	0.95	0.23	49,49,49,49	0
57	MG	2A	3659	1/1	0.95	0.14	54,54,54,54	0
57	MG	1A	3656	1/1	0.95	0.06	27,27,27,27	0
57	MG	2A	3661	1/1	0.95	0.15	40,40,40,40	0
57	MG	2A	3662	1/1	0.95	0.07	56,56,56,56	0
57	MG	2A	3309	1/1	0.95	0.07	45,45,45,45	0
57	MG	2a	1683	1/1	0.95	0.07	44,44,44,44	0
57	MG	1A	3052	1/1	0.95	0.06	40,40,40,40	0
57	MG	2a	1686	1/1	0.95	0.17	47,47,47,47	0
57	MG	2A	3666	1/1	0.95	0.07	53,53,53,53	0
57	MG	1a	1610	1/1	0.95	0.15	42,42,42,42	0
57	MG	2A	3312	1/1	0.95	0.07	64,64,64,64	0
57	MG	2A	3314	1/1	0.95	0.09	53,53,53,53	0
57	MG	2a	1692	1/1	0.95	0.16	46,46,46,46	0
57	MG	2A	3016	1/1	0.95	0.13	54,54,54,54	0
57	MG	1A	3501	1/1	0.95	0.06	36,36,36,36	0
57	MG	1a	1612	1/1	0.95	0.12	29,29,29,29	0
57	MG	1A	3661	1/1	0.95	0.06	31,31,31,31	0
57	MG	1A	3188	1/1	0.95	0.16	25,25,25,25	0
57	MG	2A	3025	1/1	0.95	0.08	39,39,39,39	0
57	MG	1A	3504	1/1	0.95	0.07	27,27,27,27	0
57	MG	1A	3506	1/1	0.95	0.11	29,29,29,29	0
57	MG	1A	3257	1/1	0.95	0.13	45,45,45,45	0
57	MG	2A	3330	1/1	0.95	0.08	49,49,49,49	0
57	MG	1A	3856	1/1	0.95	0.07	13,13,13,13	0
57	MG	1a	1624	1/1	0.95	0.09	47,47,47,47	0
57	MG	1a	1625	1/1	0.95	0.06	40,40,40,40	0
57	MG	2A	3335	1/1	0.95	0.09	43,43,43,43	0
57	MG	2A	3688	1/1	0.95	0.07	46,46,46,46	0
57	MG	1a	1626	1/1	0.95	0.19	42,42,42,42	0
57	MG	2A	3691	1/1	0.95	0.14	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3692	1/1	0.95	0.11	55,55,55,55	0
57	MG	2A	3693	1/1	0.95	0.12	42,42,42,42	0
57	MG	2A	3040	1/1	0.95	0.21	50,50,50,50	0
57	MG	2A	3041	1/1	0.95	0.10	48,48,48,48	0
57	MG	1a	1627	1/1	0.95	0.14	48,48,48,48	0
57	MG	1A	3085	1/1	0.95	0.17	35,35,35,35	0
57	MG	1A	3191	1/1	0.95	0.12	25,25,25,25	0
57	MG	2A	3045	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	4046	1/1	0.95	0.06	40,40,40,40	0
57	MG	2A	3047	1/1	0.95	0.07	56,56,56,56	0
57	MG	2a	1722	1/1	0.95	0.19	54,54,54,54	0
57	MG	2A	3704	1/1	0.95	0.05	48,48,48,48	0
57	MG	2a	1725	1/1	0.95	0.06	39,39,39,39	0
57	MG	1a	1632	1/1	0.95	0.23	50,50,50,50	0
57	MG	2A	3049	1/1	0.95	0.07	55,55,55,55	0
57	MG	2A	3708	1/1	0.95	0.06	47,47,47,47	0
57	MG	2A	3050	1/1	0.95	0.16	31,31,31,31	0
57	MG	2a	1732	1/1	0.95	0.16	36,36,36,36	0
57	MG	2A	3051	1/1	0.95	0.20	49,49,49,49	0
57	MG	2a	1734	1/1	0.95	0.18	41,41,41,41	0
57	MG	2A	3352	1/1	0.95	0.12	48,48,48,48	0
57	MG	2A	3712	1/1	0.95	0.10	61,61,61,61	0
57	MG	1A	3017	1/1	0.95	0.13	41,41,41,41	0
57	MG	1A	3862	1/1	0.95	0.08	33,33,33,33	0
57	MG	2a	1739	1/1	0.95	0.27	53,53,53,53	0
57	MG	1A	3414	1/1	0.95	0.05	26,26,26,26	0
57	MG	1A	4054	1/1	0.95	0.11	38,38,38,38	0
57	MG	2A	3722	1/1	0.95	0.06	38,38,38,38	0
57	MG	1A	3194	1/1	0.95	0.12	21,21,21,21	0
57	MG	1a	1639	1/1	0.95	0.13	47,47,47,47	0
57	MG	2A	3726	1/1	0.95	0.07	51,51,51,51	0
57	MG	2a	1747	1/1	0.95	0.07	50,50,50,50	0
57	MG	2A	3727	1/1	0.95	0.07	48,48,48,48	0
57	MG	2a	1749	1/1	0.95	0.17	72,72,72,72	0
57	MG	2A	3061	1/1	0.95	0.11	45,45,45,45	0
57	MG	1A	3526	1/1	0.95	0.05	36,36,36,36	0
57	MG	2A	3361	1/1	0.95	0.14	53,53,53,53	0
57	MG	1A	3683	1/1	0.95	0.08	52,52,52,52	0
57	MG	1A	3527	1/1	0.95	0.07	40,40,40,40	0
57	MG	2A	3364	1/1	0.95	0.07	56,56,56,56	0
57	MG	2A	3071	1/1	0.95	0.09	48,48,48,48	0
57	MG	1A	3092	1/1	0.95	0.18	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3741	1/1	0.95	0.12	50,50,50,50	0
57	MG	2A	3742	1/1	0.95	0.09	47,47,47,47	0
57	MG	1A	3157	1/1	0.95	0.50	22,22,22,22	0
57	MG	1a	1647	1/1	0.95	0.13	36,36,36,36	0
57	MG	1A	3018	1/1	0.95	0.11	22,22,22,22	0
57	MG	2a	1772	1/1	0.95	0.12	58,58,58,58	0
57	MG	1A	3693	1/1	0.95	0.07	33,33,33,33	0
57	MG	1A	3336	1/1	0.95	0.05	38,38,38,38	0
57	MG	1A	3274	1/1	0.95	0.10	29,29,29,29	0
57	MG	1A	3538	1/1	0.95	0.10	38,38,38,38	0
57	MG	2a	1782	1/1	0.95	0.21	48,48,48,48	0
57	MG	2A	3084	1/1	0.95	0.06	35,35,35,35	0
57	MG	2a	1784	1/1	0.95	0.08	56,56,56,56	0
57	MG	1A	3881	1/1	0.95	0.15	35,35,35,35	0
57	MG	2a	1786	1/1	0.95	0.09	45,45,45,45	0
57	MG	2A	3089	1/1	0.95	0.14	45,45,45,45	0
57	MG	2A	3755	1/1	0.95	0.10	50,50,50,50	0
57	MG	1A	3882	1/1	0.95	0.08	22,22,22,22	0
57	MG	1A	4086	1/1	0.95	0.07	36,36,36,36	0
57	MG	1A	4087	1/1	0.95	0.11	48,48,48,48	0
57	MG	2a	1792	1/1	0.95	0.18	55,55,55,55	0
57	MG	1a	1664	1/1	0.95	0.04	38,38,38,38	0
57	MG	2A	3384	1/1	0.95	0.10	35,35,35,35	0
57	MG	2a	1797	1/1	0.95	0.08	46,46,46,46	0
57	MG	2A	3095	1/1	0.95	0.10	35,35,35,35	0
57	MG	1A	3539	1/1	0.95	0.27	54,54,54,54	0
57	MG	1a	1666	1/1	0.95	0.13	42,42,42,42	0
57	MG	2A	3766	1/1	0.95	0.10	66,66,66,66	0
57	MG	2A	3100	1/1	0.95	0.12	36,36,36,36	0
57	MG	1A	3705	1/1	0.95	0.07	25,25,25,25	0
57	MG	2A	3392	1/1	0.95	0.09	48,48,48,48	0
57	MG	1A	3426	1/1	0.95	0.11	40,40,40,40	0
57	MG	2A	3395	1/1	0.95	0.19	52,52,52,52	0
57	MG	2A	3773	1/1	0.95	0.10	45,45,45,45	0
57	MG	2A	3396	1/1	0.95	0.14	42,42,42,42	0
57	MG	1A	3541	1/1	0.95	0.04	18,18,18,18	0
57	MG	1A	3019	1/1	0.95	0.13	32,32,32,32	0
57	MG	2a	1811	1/1	0.95	0.16	50,50,50,50	0
57	MG	1a	1673	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3276	1/1	0.95	0.21	38,38,38,38	0
57	MG	1A	3164	1/1	0.95	0.07	40,40,40,40	0
57	MG	1A	3714	1/1	0.95	0.09	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3789	1/1	0.95	0.08	42,42,42,42	0
57	MG	2A	3404	1/1	0.95	0.12	38,38,38,38	0
57	MG	1A	3547	1/1	0.95	0.05	36,36,36,36	0
57	MG	2A	3407	1/1	0.95	0.12	60,60,60,60	0
57	MG	2A	3113	1/1	0.95	0.17	48,48,48,48	0
57	MG	1A	3209	1/1	0.95	0.09	33,33,33,33	0
57	MG	1B	205	1/1	0.95	0.13	48,48,48,48	0
57	MG	1a	1680	1/1	0.95	0.16	34,34,34,34	0
57	MG	2a	1827	1/1	0.95	0.20	42,42,42,42	0
57	MG	1B	206	1/1	0.95	0.07	36,36,36,36	0
57	MG	1a	1682	1/1	0.95	0.13	43,43,43,43	0
57	MG	1A	3342	1/1	0.95	0.27	31,31,31,31	0
57	MG	2A	3415	1/1	0.95	0.09	46,46,46,46	0
57	MG	1A	3032	1/1	0.95	0.22	25,25,25,25	0
57	MG	1a	1685	1/1	0.95	0.14	50,50,50,50	0
57	MG	2A	3131	1/1	0.95	0.22	50,50,50,50	0
57	MG	1A	3901	1/1	0.95	0.07	32,32,32,32	0
57	MG	2A	3422	1/1	0.95	0.14	33,33,33,33	0
57	MG	1A	3169	1/1	0.95	0.12	31,31,31,31	0
57	MG	2A	3135	1/1	0.95	0.06	33,33,33,33	0
57	MG	2A	3136	1/1	0.95	0.17	41,41,41,41	0
57	MG	1A	3555	1/1	0.95	0.20	34,34,34,34	0
57	MG	2k	201	1/1	0.95	0.13	52,52,52,52	0
57	MG	2A	3813	1/1	0.95	0.06	54,54,54,54	0
57	MG	1a	1690	1/1	0.95	0.09	37,37,37,37	0
57	MG	1a	1691	1/1	0.95	0.19	43,43,43,43	0
57	MG	2A	3145	1/1	0.95	0.11	40,40,40,40	0
57	MG	2A	3818	1/1	0.95	0.13	59,59,59,59	0
57	MG	1A	3556	1/1	0.95	0.07	26,26,26,26	0
57	MG	1a	1696	1/1	0.95	0.20	43,43,43,43	0
57	MG	1A	3559	1/1	0.95	0.08	36,36,36,36	0
57	MG	2A	3824	1/1	0.95	0.09	42,42,42,42	0
57	MG	2A	3825	1/1	0.95	0.09	43,43,43,43	0
57	MG	2A	3149	1/1	0.95	0.18	42,42,42,42	0
57	MG	1A	3437	1/1	0.95	0.08	40,40,40,40	0
57	MG	1A	3020	1/1	0.95	0.09	40,40,40,40	0
57	MG	2A	3829	1/1	0.95	0.09	40,40,40,40	0
57	MG	2A	3154	1/1	0.95	0.10	48,48,48,48	0
57	MG	1A	3441	1/1	0.95	0.12	31,31,31,31	0
57	MG	2A	3834	1/1	0.95	0.06	43,43,43,43	0
57	MG	2A	3156	1/1	0.95	0.10	55,55,55,55	0
57	MG	1A	3350	1/1	0.95	0.18	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3160	1/1	0.95	0.06	46,46,46,46	0
57	MG	1A	3922	1/1	0.95	0.10	30,30,30,30	0
57	MG	1B	227	1/1	0.95	0.04	23,23,23,23	0
57	MG	1A	3039	1/1	0.95	0.06	22,22,22,22	0
57	MG	1A	3223	1/1	0.95	0.10	20,20,20,20	0
57	MG	1A	3024	1/1	0.95	0.16	44,44,44,44	0
57	MG	2x	106	1/1	0.95	0.10	48,48,48,48	0
57	MG	1A	3927	1/1	0.95	0.06	27,27,27,27	0
57	MG	2y	102	1/1	0.95	0.08	55,55,55,55	0
57	MG	1A	3456	1/1	0.95	0.09	37,37,37,37	0
57	MG	2A	3172	1/1	0.95	0.07	55,55,55,55	0
57	MG	2A	3174	1/1	0.95	0.09	47,47,47,47	0
57	MG	1A	3574	1/1	0.95	0.09	41,41,41,41	0
57	MG	1D	302	1/1	0.95	0.10	40,40,40,40	0
57	MG	1A	3297	1/1	0.95	0.09	41,41,41,41	0
57	MG	2A	3849	1/1	0.96	0.06	37,37,37,37	0
57	MG	2A	3850	1/1	0.96	0.07	19,19,19,19	0
57	MG	1a	1657	1/1	0.96	0.09	34,34,34,34	0
57	MG	1A	3639	1/1	0.96	0.04	10,10,10,10	0
57	MG	2A	3120	1/1	0.96	0.10	31,31,31,31	0
57	MG	1A	3480	1/1	0.96	0.08	40,40,40,40	0
57	MG	2A	3124	1/1	0.96	0.21	56,56,56,56	0
57	MG	2A	3125	1/1	0.96	0.22	44,44,44,44	0
57	MG	2A	3126	1/1	0.96	0.05	41,41,41,41	0
57	MG	1A	3289	1/1	0.96	0.07	19,19,19,19	0
57	MG	1A	3642	1/1	0.96	0.05	36,36,36,36	0
57	MG	1A	3482	1/1	0.96	0.08	37,37,37,37	0
57	MG	1A	4061	1/1	0.96	0.24	40,40,40,40	0
57	MG	2A	3460	1/1	0.96	0.17	51,51,51,51	0
57	MG	1A	4064	1/1	0.96	0.04	14,14,14,14	0
57	MG	1a	1667	1/1	0.96	0.07	40,40,40,40	0
57	MG	2A	3463	1/1	0.96	0.14	48,48,48,48	0
57	MG	1A	3483	1/1	0.96	0.06	44,44,44,44	0
57	MG	1A	3203	1/1	0.96	0.05	29,29,29,29	0
57	MG	1A	4067	1/1	0.96	0.07	46,46,46,46	0
57	MG	2A	3138	1/1	0.96	0.17	32,32,32,32	0
57	MG	2A	3878	1/1	0.96	0.08	45,45,45,45	0
57	MG	1A	3379	1/1	0.96	0.04	37,37,37,37	0
57	MG	2A	3469	1/1	0.96	0.05	32,32,32,32	0
57	MG	2A	3140	1/1	0.96	0.12	51,51,51,51	0
57	MG	1A	4069	1/1	0.96	0.10	16,16,16,16	0
57	MG	2A	3883	1/1	0.96	0.09	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3473	1/1	0.96	0.14	17,17,17,17	0
57	MG	1A	3648	1/1	0.96	0.09	24,24,24,24	0
57	MG	1A	3846	1/1	0.96	0.13	42,42,42,42	0
57	MG	1A	4074	1/1	0.96	0.07	36,36,36,36	0
57	MG	2A	3478	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	4077	1/1	0.96	0.09	42,42,42,42	0
57	MG	1A	3486	1/1	0.96	0.11	44,44,44,44	0
57	MG	1A	3381	1/1	0.96	0.10	28,28,28,28	0
57	MG	1A	3138	1/1	0.96	0.11	29,29,29,29	0
57	MG	1A	4085	1/1	0.96	0.10	27,27,27,27	0
57	MG	1A	3654	1/1	0.96	0.10	44,44,44,44	0
57	MG	2A	3485	1/1	0.96	0.10	42,42,42,42	0
57	MG	1A	3142	1/1	0.96	0.10	10,10,10,10	0
57	MG	2A	3157	1/1	0.96	0.09	31,31,31,31	0
57	MG	2A	3158	1/1	0.96	0.05	26,26,26,26	0
57	MG	1A	3854	1/1	0.96	0.08	43,43,43,43	0
57	MG	1A	3208	1/1	0.96	0.08	27,27,27,27	0
57	MG	1A	3657	1/1	0.96	0.08	30,30,30,30	0
57	MG	1a	1687	1/1	0.96	0.11	46,46,46,46	0
57	MG	1A	3857	1/1	0.96	0.11	38,38,38,38	0
57	MG	2A	3498	1/1	0.96	0.11	45,45,45,45	0
57	MG	2D	302	1/1	0.96	0.17	39,39,39,39	0
57	MG	1A	3087	1/1	0.96	0.06	37,37,37,37	0
57	MG	2D	304	1/1	0.96	0.14	35,35,35,35	0
57	MG	2A	3500	1/1	0.96	0.13	48,48,48,48	0
57	MG	2D	306	1/1	0.96	0.24	35,35,35,35	0
57	MG	2A	3166	1/1	0.96	0.17	34,34,34,34	0
57	MG	2A	3168	1/1	0.96	0.13	38,38,38,38	0
57	MG	1A	3009	1/1	0.96	0.06	26,26,26,26	0
57	MG	2E	303	1/1	0.96	0.11	45,45,45,45	0
57	MG	1A	3660	1/1	0.96	0.05	30,30,30,30	0
57	MG	2E	305	1/1	0.96	0.06	40,40,40,40	0
57	MG	1A	3211	1/1	0.96	0.08	41,41,41,41	0
57	MG	1a	1695	1/1	0.96	0.22	41,41,41,41	0
57	MG	2A	3173	1/1	0.96	0.06	52,52,52,52	0
57	MG	1A	3497	1/1	0.96	0.08	23,23,23,23	0
57	MG	1B	201	1/1	0.96	0.06	30,30,30,30	0
57	MG	1B	202	1/1	0.96	0.11	42,42,42,42	0
57	MG	1A	3663	1/1	0.96	0.07	35,35,35,35	0
57	MG	1a	1700	1/1	0.96	0.14	42,42,42,42	0
57	MG	1A	3498	1/1	0.96	0.17	36,36,36,36	0
57	MG	2O	201	1/1	0.96	0.06	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3666	1/1	0.96	0.05	15,15,15,15	0
57	MG	1a	1703	1/1	0.96	0.17	49,49,49,49	0
57	MG	2A	3185	1/1	0.96	0.12	41,41,41,41	0
57	MG	1a	1704	1/1	0.96	0.09	49,49,49,49	0
57	MG	2Q	203	1/1	0.96	0.10	48,48,48,48	0
57	MG	2R	201	1/1	0.96	0.06	32,32,32,32	0
57	MG	1B	207	1/1	0.96	0.17	37,37,37,37	0
57	MG	1A	3868	1/1	0.96	0.05	37,37,37,37	0
57	MG	1A	3499	1/1	0.96	0.10	30,30,30,30	0
57	MG	2A	3524	1/1	0.96	0.06	42,42,42,42	0
57	MG	2A	3190	1/1	0.96	0.09	46,46,46,46	0
57	MG	2V	201	1/1	0.96	0.16	51,51,51,51	0
57	MG	2A	3526	1/1	0.96	0.09	44,44,44,44	0
57	MG	1A	3216	1/1	0.96	0.06	37,37,37,37	0
57	MG	1B	211	1/1	0.96	0.10	43,43,43,43	0
57	MG	1a	1712	1/1	0.96	0.04	35,35,35,35	0
57	MG	2A	3530	1/1	0.96	0.06	43,43,43,43	0
57	MG	1A	3089	1/1	0.96	0.07	36,36,36,36	0
57	MG	2A	3534	1/1	0.96	0.04	36,36,36,36	0
57	MG	2A	3535	1/1	0.96	0.09	28,28,28,28	0
57	MG	1a	1714	1/1	0.96	0.06	29,29,29,29	0
57	MG	2A	3538	1/1	0.96	0.08	45,45,45,45	0
57	MG	1A	3672	1/1	0.96	0.04	15,15,15,15	0
57	MG	1A	3090	1/1	0.96	0.06	32,32,32,32	0
57	MG	2A	3543	1/1	0.96	0.13	42,42,42,42	0
57	MG	1a	1717	1/1	0.96	0.11	44,44,44,44	0
57	MG	2A	3200	1/1	0.96	0.23	51,51,51,51	0
57	MG	1A	3155	1/1	0.96	0.08	33,33,33,33	0
57	MG	1A	3221	1/1	0.96	0.06	27,27,27,27	0
57	MG	28	104	1/1	0.96	0.09	47,47,47,47	0
57	MG	2A	3548	1/1	0.96	0.12	36,36,36,36	0
57	MG	2A	3549	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3877	1/1	0.96	0.15	32,32,32,32	0
57	MG	1A	3396	1/1	0.96	0.17	28,28,28,28	0
57	MG	1a	1723	1/1	0.96	0.18	54,54,54,54	0
57	MG	1A	3222	1/1	0.96	0.06	26,26,26,26	0
57	MG	1A	3398	1/1	0.96	0.13	16,16,16,16	0
57	MG	2A	3559	1/1	0.96	0.05	20,20,20,20	0
57	MG	2A	3561	1/1	0.96	0.14	38,38,38,38	0
57	MG	1a	1726	1/1	0.96	0.20	57,57,57,57	0
57	MG	1A	3518	1/1	0.96	0.14	34,34,34,34	0
57	MG	1A	3522	1/1	0.96	0.08	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3309	1/1	0.96	0.10	35,35,35,35	0
57	MG	1A	3400	1/1	0.96	0.05	31,31,31,31	0
57	MG	1A	3091	1/1	0.96	0.09	21,21,21,21	0
57	MG	2a	1615	1/1	0.96	0.06	37,37,37,37	0
57	MG	2A	3216	1/1	0.96	0.11	43,43,43,43	0
57	MG	1A	3225	1/1	0.96	0.18	37,37,37,37	0
57	MG	2A	3573	1/1	0.96	0.05	37,37,37,37	0
57	MG	2a	1619	1/1	0.96	0.14	48,48,48,48	0
57	MG	1A	3404	1/1	0.96	0.10	27,27,27,27	0
57	MG	1B	235	1/1	0.96	0.06	39,39,39,39	0
57	MG	2a	1622	1/1	0.96	0.17	57,57,57,57	0
57	MG	2A	3578	1/1	0.96	0.17	38,38,38,38	0
57	MG	1A	3697	1/1	0.96	0.13	59,59,59,59	0
57	MG	2A	3580	1/1	0.96	0.07	43,43,43,43	0
57	MG	1A	3699	1/1	0.96	0.07	33,33,33,33	0
57	MG	1D	304	1/1	0.96	0.09	30,30,30,30	0
57	MG	1D	305	1/1	0.96	0.04	16,16,16,16	0
57	MG	1A	3227	1/1	0.96	0.17	39,39,39,39	0
57	MG	2A	3226	1/1	0.96	0.31	40,40,40,40	0
57	MG	1A	3228	1/1	0.96	0.10	36,36,36,36	0
57	MG	1a	1746	1/1	0.96	0.04	48,48,48,48	0
57	MG	2A	3229	1/1	0.96	0.17	45,45,45,45	0
57	MG	2A	3591	1/1	0.96	0.12	49,49,49,49	0
57	MG	1D	311	1/1	0.96	0.24	23,23,23,23	0
57	MG	1A	3703	1/1	0.96	0.05	10,10,10,10	0
57	MG	1E	301	1/1	0.96	0.05	21,21,21,21	0
57	MG	1A	3314	1/1	0.96	0.13	33,33,33,33	0
57	MG	2A	3600	1/1	0.96	0.14	43,43,43,43	0
57	MG	2A	3235	1/1	0.96	0.14	55,55,55,55	0
57	MG	1A	3902	1/1	0.96	0.11	29,29,29,29	0
57	MG	2a	1643	1/1	0.96	0.22	54,54,54,54	0
57	MG	1A	3316	1/1	0.96	0.12	33,33,33,33	0
57	MG	1A	3230	1/1	0.96	0.09	20,20,20,20	0
57	MG	1A	3907	1/1	0.96	0.07	32,32,32,32	0
57	MG	1A	3908	1/1	0.96	0.06	29,29,29,29	0
57	MG	1A	3536	1/1	0.96	0.11	36,36,36,36	0
57	MG	1A	3537	1/1	0.96	0.10	35,35,35,35	0
57	MG	1A	3911	1/1	0.96	0.11	41,41,41,41	0
57	MG	2A	3245	1/1	0.96	0.09	47,47,47,47	0
57	MG	1F	308	1/1	0.96	0.12	46,46,46,46	0
57	MG	2A	3618	1/1	0.96	0.12	45,45,45,45	0
57	MG	1A	3319	1/1	0.96	0.06	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3411	1/1	0.96	0.06	40,40,40,40	0
57	MG	2A	3249	1/1	0.96	0.07	51,51,51,51	0
57	MG	1a	1766	1/1	0.96	0.07	50,50,50,50	0
57	MG	1A	3915	1/1	0.96	0.07	34,34,34,34	0
57	MG	1G	201	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	3916	1/1	0.96	0.14	27,27,27,27	0
57	MG	1A	3065	1/1	0.96	0.08	30,30,30,30	0
57	MG	1A	3918	1/1	0.96	0.04	31,31,31,31	0
57	MG	1A	3066	1/1	0.96	0.05	19,19,19,19	0
57	MG	1I	201	1/1	0.96	0.08	49,49,49,49	0
57	MG	2a	1668	1/1	0.96	0.09	57,57,57,57	0
57	MG	2A	3260	1/1	0.96	0.08	39,39,39,39	0
57	MG	1a	1777	1/1	0.96	0.06	49,49,49,49	0
57	MG	2a	1671	1/1	0.96	0.10	45,45,45,45	0
57	MG	1a	1778	1/1	0.96	0.08	36,36,36,36	0
57	MG	1N	201	1/1	0.96	0.12	42,42,42,42	0
57	MG	2a	1674	1/1	0.96	0.05	42,42,42,42	0
57	MG	1A	3094	1/1	0.96	0.12	31,31,31,31	0
57	MG	2a	1676	1/1	0.96	0.10	51,51,51,51	0
57	MG	2A	3643	1/1	0.96	0.05	34,34,34,34	0
57	MG	1A	3004	1/1	0.96	0.06	19,19,19,19	0
57	MG	2a	1680	1/1	0.96	0.10	64,64,64,64	0
57	MG	1a	1784	1/1	0.96	0.06	35,35,35,35	0
57	MG	1A	3099	1/1	0.96	0.07	32,32,32,32	0
57	MG	1A	3546	1/1	0.96	0.11	36,36,36,36	0
57	MG	1O	201	1/1	0.96	0.08	51,51,51,51	0
57	MG	2a	1687	1/1	0.96	0.10	43,43,43,43	0
57	MG	1O	202	1/1	0.96	0.07	48,48,48,48	0
57	MG	1A	3926	1/1	0.96	0.09	34,34,34,34	0
57	MG	1a	1795	1/1	0.96	0.06	56,56,56,56	0
57	MG	1A	3033	1/1	0.96	0.04	29,29,29,29	0
57	MG	1A	3102	1/1	0.96	0.07	16,16,16,16	0
57	MG	1a	1800	1/1	0.96	0.08	56,56,56,56	0
57	MG	1Q	202	1/1	0.96	0.06	30,30,30,30	0
57	MG	1Q	203	1/1	0.96	0.10	43,43,43,43	0
57	MG	1A	3724	1/1	0.96	0.07	40,40,40,40	0
57	MG	1A	3420	1/1	0.96	0.05	29,29,29,29	0
57	MG	2A	3286	1/1	0.96	0.16	34,34,34,34	0
57	MG	1A	3931	1/1	0.96	0.04	31,31,31,31	0
57	MG	1Q	207	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3104	1/1	0.96	0.07	24,24,24,24	0
57	MG	1R	203	1/1	0.96	0.09	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1R	204	1/1	0.96	0.07	16,16,16,16	0
57	MG	1A	3425	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3936	1/1	0.96	0.07	34,34,34,34	0
57	MG	1A	3939	1/1	0.96	0.04	34,34,34,34	0
57	MG	1A	3329	1/1	0.96	0.15	44,44,44,44	0
57	MG	2A	3298	1/1	0.96	0.06	36,36,36,36	0
57	MG	1U	202	1/1	0.96	0.10	33,33,33,33	0
57	MG	1A	3045	1/1	0.96	0.07	17,17,17,17	0
57	MG	2A	3676	1/1	0.96	0.07	53,53,53,53	0
57	MG	1A	3111	1/1	0.96	0.05	31,31,31,31	0
57	MG	1A	3945	1/1	0.96	0.07	43,43,43,43	0
57	MG	1A	3075	1/1	0.96	0.08	27,27,27,27	0
57	MG	2a	1716	1/1	0.96	0.13	39,39,39,39	0
57	MG	2A	3681	1/1	0.96	0.10	44,44,44,44	0
57	MG	1V	205	1/1	0.96	0.07	24,24,24,24	0
57	MG	1A	3114	1/1	0.96	0.15	30,30,30,30	0
57	MG	2A	3306	1/1	0.96	0.06	37,37,37,37	0
57	MG	1V	210	1/1	0.96	0.05	41,41,41,41	0
57	MG	1W	202	1/1	0.96	0.12	46,46,46,46	0
57	MG	1W	203	1/1	0.96	0.05	27,27,27,27	0
57	MG	1A	3433	1/1	0.96	0.07	28,28,28,28	0
57	MG	1A	3076	1/1	0.96	0.22	35,35,35,35	0
57	MG	1W	207	1/1	0.96	0.08	28,28,28,28	0
57	MG	1A	3253	1/1	0.96	0.06	35,35,35,35	0
57	MG	2A	3694	1/1	0.96	0.13	48,48,48,48	0
57	MG	2A	3315	1/1	0.96	0.07	35,35,35,35	0
57	MG	1A	3034	1/1	0.96	0.08	32,32,32,32	0
57	MG	1X	103	1/1	0.96	0.05	25,25,25,25	0
57	MG	1A	3741	1/1	0.96	0.12	41,41,41,41	0
57	MG	1x	103	1/1	0.96	0.14	41,41,41,41	0
57	MG	1A	3119	1/1	0.96	0.05	36,36,36,36	0
57	MG	1A	3261	1/1	0.96	0.07	32,32,32,32	0
57	MG	2A	3702	1/1	0.96	0.08	33,33,33,33	0
57	MG	1Y	203	1/1	0.96	0.15	40,40,40,40	0
57	MG	1A	3440	1/1	0.96	0.14	36,36,36,36	0
57	MG	1A	3746	1/1	0.96	0.08	20,20,20,20	0
57	MG	2A	3706	1/1	0.96	0.10	42,42,42,42	0
57	MG	1A	3748	1/1	0.96	0.10	23,23,23,23	0
57	MG	1A	3080	1/1	0.96	0.14	25,25,25,25	0
57	MG	10	101	1/1	0.96	0.13	36,36,36,36	0
57	MG	1A	3446	1/1	0.96	0.06	27,27,27,27	0
57	MG	10	103	1/1	0.96	0.11	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3447	1/1	0.96	0.06	42,42,42,42	0
57	MG	1A	3048	1/1	0.96	0.15	34,34,34,34	0
57	MG	2A	3714	1/1	0.96	0.11	20,20,20,20	0
57	MG	1A	3581	1/1	0.96	0.14	39,39,39,39	0
57	MG	1A	3582	1/1	0.96	0.06	32,32,32,32	0
57	MG	11	101	1/1	0.96	0.17	32,32,32,32	0
57	MG	11	102	1/1	0.96	0.10	34,34,34,34	0
57	MG	2A	3010	1/1	0.96	0.08	45,45,45,45	0
57	MG	2A	3015	1/1	0.96	0.15	37,37,37,37	0
57	MG	2a	1763	1/1	0.96	0.08	51,51,51,51	0
57	MG	2a	1765	1/1	0.96	0.06	49,49,49,49	0
57	MG	11	103	1/1	0.96	0.07	36,36,36,36	0
57	MG	1A	3760	1/1	0.96	0.05	50,50,50,50	0
57	MG	11	105	1/1	0.96	0.06	29,29,29,29	0
57	MG	2A	3019	1/1	0.96	0.07	33,33,33,33	0
57	MG	2A	3021	1/1	0.96	0.09	24,24,24,24	0
57	MG	1A	3976	1/1	0.96	0.10	53,53,53,53	0
57	MG	12	102	1/1	0.96	0.08	26,26,26,26	0
57	MG	1A	3977	1/1	0.96	0.08	58,58,58,58	0
57	MG	1A	3449	1/1	0.96	0.10	31,31,31,31	0
57	MG	2A	3739	1/1	0.96	0.16	44,44,44,44	0
57	MG	1A	3190	1/1	0.96	0.08	32,32,32,32	0
57	MG	1A	3763	1/1	0.96	0.06	14,14,14,14	0
57	MG	1A	3585	1/1	0.96	0.07	40,40,40,40	0
57	MG	15	108	1/1	0.96	0.15	33,33,33,33	0
57	MG	2A	3034	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	3766	1/1	0.96	0.07	13,13,13,13	0
57	MG	2A	3746	1/1	0.96	0.07	40,40,40,40	0
57	MG	2A	3036	1/1	0.96	0.04	25,25,25,25	0
57	MG	1A	3124	1/1	0.96	0.15	28,28,28,28	0
57	MG	17	101	1/1	0.96	0.07	23,23,23,23	0
57	MG	1A	3083	1/1	0.96	0.09	19,19,19,19	0
57	MG	1A	3592	1/1	0.96	0.08	24,24,24,24	0
57	MG	1A	3130	1/1	0.96	0.07	66,66,66,66	0
57	MG	1A	3594	1/1	0.96	0.14	36,36,36,36	0
57	MG	2A	3754	1/1	0.96	0.12	59,59,59,59	0
57	MG	1A	3347	1/1	0.96	0.22	23,23,23,23	0
57	MG	1A	3992	1/1	0.96	0.03	26,26,26,26	0
57	MG	1A	3051	1/1	0.96	0.07	27,27,27,27	0
57	MG	1A	3777	1/1	0.96	0.04	18,18,18,18	0
57	MG	1A	3459	1/1	0.96	0.25	50,50,50,50	0
57	MG	2A	3375	1/1	0.96	0.09	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3781	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	3782	1/1	0.96	0.06	26,26,26,26	0
57	MG	1a	1605	1/1	0.96	0.11	52,52,52,52	0
57	MG	1A	3783	1/1	0.96	0.04	18,18,18,18	0
57	MG	1A	3351	1/1	0.96	0.06	32,32,32,32	0
57	MG	2A	3056	1/1	0.96	0.06	33,33,33,33	0
57	MG	1A	3135	1/1	0.96	0.13	31,31,31,31	0
57	MG	2A	3383	1/1	0.96	0.21	56,56,56,56	0
57	MG	1A	3786	1/1	0.96	0.12	46,46,46,46	0
57	MG	2a	1815	1/1	0.96	0.04	54,54,54,54	0
57	MG	1A	4003	1/1	0.96	0.09	19,19,19,19	0
57	MG	2a	1817	1/1	0.96	0.07	59,59,59,59	0
57	MG	1A	3607	1/1	0.96	0.06	24,24,24,24	0
57	MG	2A	3062	1/1	0.96	0.05	47,47,47,47	0
57	MG	2A	3063	1/1	0.96	0.17	38,38,38,38	0
57	MG	2A	3389	1/1	0.96	0.16	46,46,46,46	0
57	MG	2A	3066	1/1	0.96	0.07	42,42,42,42	0
57	MG	1A	3789	1/1	0.96	0.10	42,42,42,42	0
57	MG	2a	1824	1/1	0.96	0.15	57,57,57,57	0
57	MG	2A	3780	1/1	0.96	0.09	39,39,39,39	0
57	MG	1A	3790	1/1	0.96	0.05	19,19,19,19	0
57	MG	2A	3394	1/1	0.96	0.08	52,52,52,52	0
57	MG	1A	3608	1/1	0.96	0.07	29,29,29,29	0
57	MG	1A	3794	1/1	0.96	0.04	17,17,17,17	0
57	MG	1a	1616	1/1	0.96	0.05	46,46,46,46	0
57	MG	2A	3398	1/1	0.96	0.08	36,36,36,36	0
57	MG	1A	3463	1/1	0.96	0.12	26,26,26,26	0
57	MG	1A	3611	1/1	0.96	0.06	15,15,15,15	0
57	MG	1A	3353	1/1	0.96	0.05	28,28,28,28	0
57	MG	2A	3076	1/1	0.96	0.21	41,41,41,41	0
57	MG	2A	3077	1/1	0.96	0.05	32,32,32,32	0
57	MG	1A	3137	1/1	0.96	0.32	23,23,23,23	0
57	MG	2g	201	1/1	0.96	0.08	63,63,63,63	0
57	MG	1A	4022	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3801	1/1	0.96	0.10	20,20,20,20	0
57	MG	1A	3614	1/1	0.96	0.06	30,30,30,30	0
57	MG	1A	3198	1/1	0.96	0.04	30,30,30,30	0
57	MG	2A	3085	1/1	0.96	0.11	55,55,55,55	0
57	MG	1A	3616	1/1	0.96	0.06	40,40,40,40	0
57	MG	2A	3087	1/1	0.96	0.07	36,36,36,36	0
57	MG	2A	3088	1/1	0.96	0.09	42,42,42,42	0
57	MG	1A	3200	1/1	0.96	0.08	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3806	1/1	0.96	0.06	35,35,35,35	0
57	MG	2A	3416	1/1	0.96	0.05	47,47,47,47	0
57	MG	1A	3807	1/1	0.96	0.06	31,31,31,31	0
57	MG	1A	3202	1/1	0.96	0.06	30,30,30,30	0
57	MG	1A	3812	1/1	0.96	0.28	19,19,19,19	0
57	MG	2A	3420	1/1	0.96	0.16	48,48,48,48	0
57	MG	1A	4037	1/1	0.96	0.08	31,31,31,31	0
57	MG	1A	3368	1/1	0.96	0.05	25,25,25,25	0
57	MG	2A	3822	1/1	0.96	0.05	30,30,30,30	0
57	MG	1A	3369	1/1	0.96	0.16	34,34,34,34	0
57	MG	1A	3817	1/1	0.96	0.10	66,66,66,66	0
57	MG	1A	4041	1/1	0.96	0.06	38,38,38,38	0
57	MG	2A	3429	1/1	0.96	0.07	34,34,34,34	0
57	MG	1A	3370	1/1	0.96	0.07	36,36,36,36	0
57	MG	2A	3431	1/1	0.96	0.12	40,40,40,40	0
57	MG	2w	108	1/1	0.96	0.06	58,58,58,58	0
57	MG	1a	1644	1/1	0.96	0.08	55,55,55,55	0
57	MG	1A	3626	1/1	0.96	0.05	16,16,16,16	0
57	MG	1A	3628	1/1	0.96	0.13	34,34,34,34	0
57	MG	2A	3833	1/1	0.96	0.04	31,31,31,31	0
57	MG	2A	3435	1/1	0.96	0.05	31,31,31,31	0
57	MG	1A	3371	1/1	0.96	0.10	42,42,42,42	0
57	MG	2A	3109	1/1	0.96	0.15	31,31,31,31	0
57	MG	1a	1648	1/1	0.96	0.14	39,39,39,39	0
57	MG	1A	3824	1/1	0.96	0.05	28,28,28,28	0
57	MG	2A	3840	1/1	0.96	0.08	35,35,35,35	0
57	MG	1A	3373	1/1	0.96	0.06	42,42,42,42	0
57	MG	1A	3831	1/1	0.96	0.05	22,22,22,22	0
57	MG	1A	3635	1/1	0.96	0.04	26,26,26,26	0
57	MG	1A	3374	1/1	0.96	0.11	32,32,32,32	0
60	ZN	24	501	1/1	0.96	0.09	105,105,105,105	0
60	ZN	2n	501	1/1	0.96	0.06	81,81,81,81	0
57	MG	1v	102	1/1	0.97	0.05	41,41,41,41	0
57	MG	1w	101	1/1	0.97	0.04	40,40,40,40	0
57	MG	1A	4032	1/1	0.97	0.07	21,21,21,21	0
57	MG	1A	3841	1/1	0.97	0.04	40,40,40,40	0
57	MG	1A	3171	1/1	0.97	0.08	8,8,8,8	0
57	MG	1A	3172	1/1	0.97	0.06	38,38,38,38	0
57	MG	2D	301	1/1	0.97	0.07	25,25,25,25	0
57	MG	1A	3113	1/1	0.97	0.10	28,28,28,28	0
57	MG	1A	3176	1/1	0.97	0.22	26,26,26,26	0
57	MG	1A	3671	1/1	0.97	0.06	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3553	1/1	0.97	0.05	37,37,37,37	0
57	MG	1A	3847	1/1	0.97	0.04	26,26,26,26	0
57	MG	1A	3077	1/1	0.97	0.18	29,29,29,29	0
57	MG	2D	308	1/1	0.97	0.07	49,49,49,49	0
57	MG	1A	3849	1/1	0.97	0.06	46,46,46,46	0
57	MG	2A	3258	1/1	0.97	0.07	53,53,53,53	0
57	MG	2A	3259	1/1	0.97	0.09	38,38,38,38	0
57	MG	1A	3529	1/1	0.97	0.04	29,29,29,29	0
57	MG	1A	3021	1/1	0.97	0.04	15,15,15,15	0
57	MG	1A	3181	1/1	0.97	0.07	27,27,27,27	0
57	MG	2A	3263	1/1	0.97	0.05	35,35,35,35	0
57	MG	2A	3264	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3676	1/1	0.97	0.08	13,13,13,13	0
57	MG	1x	109	1/1	0.97	0.07	13,13,13,13	0
57	MG	2A	3267	1/1	0.97	0.09	59,59,59,59	0
57	MG	2A	3268	1/1	0.97	0.13	44,44,44,44	0
57	MG	1x	110	1/1	0.97	0.11	46,46,46,46	0
57	MG	2A	3576	1/1	0.97	0.04	40,40,40,40	0
57	MG	2A	3270	1/1	0.97	0.08	39,39,39,39	0
57	MG	1A	3677	1/1	0.97	0.04	27,27,27,27	0
57	MG	1A	3117	1/1	0.97	0.05	21,21,21,21	0
57	MG	1x	113	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	4049	1/1	0.97	0.04	26,26,26,26	0
57	MG	1a	1602	1/1	0.97	0.14	45,45,45,45	0
57	MG	1A	3022	1/1	0.97	0.04	29,29,29,29	0
57	MG	1A	4052	1/1	0.97	0.03	25,25,25,25	0
57	MG	1A	3682	1/1	0.97	0.06	24,24,24,24	0
57	MG	1A	3008	1/1	0.97	0.03	23,23,23,23	0
57	MG	1A	4056	1/1	0.97	0.06	11,11,11,11	0
57	MG	1A	3684	1/1	0.97	0.07	53,53,53,53	0
57	MG	2U	201	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3685	1/1	0.97	0.05	28,28,28,28	0
57	MG	1A	3861	1/1	0.97	0.10	24,24,24,24	0
57	MG	2A	3593	1/1	0.97	0.14	36,36,36,36	0
57	MG	2A	3594	1/1	0.97	0.06	39,39,39,39	0
57	MG	2A	3011	1/1	0.97	0.06	36,36,36,36	0
57	MG	2A	3012	1/1	0.97	0.06	30,30,30,30	0
57	MG	2X	102	1/1	0.97	0.07	46,46,46,46	0
57	MG	2A	3013	1/1	0.97	0.06	40,40,40,40	0
57	MG	2A	3288	1/1	0.97	0.12	36,36,36,36	0
57	MG	2A	3603	1/1	0.97	0.11	47,47,47,47	0
57	MG	2A	3014	1/1	0.97	0.06	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3037	1/1	0.97	0.14	20,20,20,20	0
57	MG	1A	3422	1/1	0.97	0.07	30,30,30,30	0
57	MG	25	102	1/1	0.97	0.19	41,41,41,41	0
57	MG	1A	4063	1/1	0.97	0.04	27,27,27,27	0
57	MG	2A	3608	1/1	0.97	0.08	26,26,26,26	0
57	MG	25	105	1/1	0.97	0.09	50,50,50,50	0
57	MG	1A	3424	1/1	0.97	0.13	38,38,38,38	0
57	MG	1A	3249	1/1	0.97	0.18	28,28,28,28	0
57	MG	2A	3020	1/1	0.97	0.05	47,47,47,47	0
57	MG	2A	3296	1/1	0.97	0.07	42,42,42,42	0
57	MG	28	103	1/1	0.97	0.06	44,44,44,44	0
57	MG	1a	1617	1/1	0.97	0.08	29,29,29,29	0
57	MG	1A	3121	1/1	0.97	0.13	24,24,24,24	0
57	MG	2A	3616	1/1	0.97	0.11	36,36,36,36	0
57	MG	1A	3252	1/1	0.97	0.04	43,43,43,43	0
57	MG	2A	3024	1/1	0.97	0.10	48,48,48,48	0
57	MG	1A	3543	1/1	0.97	0.09	42,42,42,42	0
57	MG	2A	3026	1/1	0.97	0.17	40,40,40,40	0
57	MG	1A	3055	1/1	0.97	0.08	25,25,25,25	0
57	MG	1A	3698	1/1	0.97	0.06	18,18,18,18	0
57	MG	1A	3254	1/1	0.97	0.04	43,43,43,43	0
57	MG	1A	3255	1/1	0.97	0.06	35,35,35,35	0
57	MG	1A	3056	1/1	0.97	0.05	20,20,20,20	0
57	MG	1A	3126	1/1	0.97	0.15	32,32,32,32	0
57	MG	1A	4079	1/1	0.97	0.05	25,25,25,25	0
57	MG	2A	3630	1/1	0.97	0.04	31,31,31,31	0
57	MG	1A	3704	1/1	0.97	0.07	36,36,36,36	0
57	MG	1A	3549	1/1	0.97	0.06	45,45,45,45	0
57	MG	1A	4082	1/1	0.97	0.04	19,19,19,19	0
57	MG	1A	3879	1/1	0.97	0.11	30,30,30,30	0
57	MG	1A	3880	1/1	0.97	0.14	35,35,35,35	0
57	MG	1A	3259	1/1	0.97	0.05	24,24,24,24	0
57	MG	2A	3640	1/1	0.97	0.06	47,47,47,47	0
57	MG	2A	3641	1/1	0.97	0.04	37,37,37,37	0
57	MG	2A	3317	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3001	1/1	0.97	0.07	33,33,33,33	0
57	MG	1A	3883	1/1	0.97	0.14	29,29,29,29	0
57	MG	1a	1641	1/1	0.97	0.05	56,56,56,56	0
57	MG	1A	3343	1/1	0.97	0.04	43,43,43,43	0
57	MG	2a	1627	1/1	0.97	0.09	39,39,39,39	0
57	MG	1A	3711	1/1	0.97	0.07	34,34,34,34	0
57	MG	1A	3554	1/1	0.97	0.14	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3324	1/1	0.97	0.07	39,39,39,39	0
57	MG	1A	3438	1/1	0.97	0.18	43,43,43,43	0
57	MG	1A	3010	1/1	0.97	0.04	26,26,26,26	0
57	MG	2A	3327	1/1	0.97	0.05	40,40,40,40	0
57	MG	1A	3192	1/1	0.97	0.19	32,32,32,32	0
57	MG	2A	3331	1/1	0.97	0.06	52,52,52,52	0
57	MG	1A	3040	1/1	0.97	0.06	25,25,25,25	0
57	MG	2A	3054	1/1	0.97	0.11	42,42,42,42	0
57	MG	1A	4100	1/1	0.97	0.13	38,38,38,38	0
57	MG	1A	3442	1/1	0.97	0.17	39,39,39,39	0
57	MG	1A	3894	1/1	0.97	0.08	25,25,25,25	0
57	MG	1a	1654	1/1	0.97	0.15	41,41,41,41	0
57	MG	2A	3664	1/1	0.97	0.14	52,52,52,52	0
57	MG	1A	3445	1/1	0.97	0.06	40,40,40,40	0
57	MG	1B	204	1/1	0.97	0.04	22,22,22,22	0
57	MG	1A	3267	1/1	0.97	0.21	27,27,27,27	0
57	MG	2a	1646	1/1	0.97	0.06	52,52,52,52	0
57	MG	1A	3348	1/1	0.97	0.08	25,25,25,25	0
57	MG	2A	3342	1/1	0.97	0.07	36,36,36,36	0
57	MG	2A	3343	1/1	0.97	0.09	41,41,41,41	0
57	MG	2A	3065	1/1	0.97	0.08	66,66,66,66	0
57	MG	1A	3898	1/1	0.97	0.04	24,24,24,24	0
57	MG	1A	3899	1/1	0.97	0.05	11,11,11,11	0
57	MG	2A	3347	1/1	0.97	0.05	41,41,41,41	0
57	MG	1a	1662	1/1	0.97	0.16	37,37,37,37	0
57	MG	1A	3349	1/1	0.97	0.12	27,27,27,27	0
57	MG	1A	3567	1/1	0.97	0.07	47,47,47,47	0
57	MG	1A	3568	1/1	0.97	0.13	21,21,21,21	0
57	MG	1A	3268	1/1	0.97	0.10	25,25,25,25	0
57	MG	1A	3905	1/1	0.97	0.04	31,31,31,31	0
57	MG	1A	3571	1/1	0.97	0.07	43,43,43,43	0
57	MG	2A	3683	1/1	0.97	0.07	40,40,40,40	0
57	MG	1A	3134	1/1	0.97	0.07	33,33,33,33	0
57	MG	1A	3451	1/1	0.97	0.09	44,44,44,44	0
57	MG	1A	3270	1/1	0.97	0.10	25,25,25,25	0
57	MG	1B	221	1/1	0.97	0.09	36,36,36,36	0
57	MG	2A	3081	1/1	0.97	0.11	52,52,52,52	0
57	MG	1A	3061	1/1	0.97	0.12	33,33,33,33	0
57	MG	2A	3690	1/1	0.97	0.08	32,32,32,32	0
57	MG	1A	3455	1/1	0.97	0.07	37,37,37,37	0
57	MG	1A	3732	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3913	1/1	0.97	0.07	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3355	1/1	0.97	0.05	42,42,42,42	0
57	MG	2A	3365	1/1	0.97	0.09	36,36,36,36	0
57	MG	1A	3734	1/1	0.97	0.09	41,41,41,41	0
57	MG	2a	1677	1/1	0.97	0.19	45,45,45,45	0
57	MG	1A	3736	1/1	0.97	0.03	9,9,9,9	0
57	MG	1A	3356	1/1	0.97	0.14	27,27,27,27	0
57	MG	1A	3041	1/1	0.97	0.10	17,17,17,17	0
57	MG	1A	3011	1/1	0.97	0.06	31,31,31,31	0
57	MG	2a	1682	1/1	0.97	0.14	51,51,51,51	0
57	MG	1A	3921	1/1	0.97	0.08	20,20,20,20	0
57	MG	2A	3093	1/1	0.97	0.14	35,35,35,35	0
57	MG	1A	3139	1/1	0.97	0.04	14,14,14,14	0
57	MG	1A	3461	1/1	0.97	0.06	26,26,26,26	0
57	MG	1A	3586	1/1	0.97	0.19	37,37,37,37	0
57	MG	1A	3360	1/1	0.97	0.08	31,31,31,31	0
57	MG	2A	3099	1/1	0.97	0.09	41,41,41,41	0
57	MG	1A	3361	1/1	0.97	0.07	36,36,36,36	0
57	MG	1D	307	1/1	0.97	0.05	26,26,26,26	0
57	MG	1A	3745	1/1	0.97	0.05	42,42,42,42	0
57	MG	1A	3464	1/1	0.97	0.15	45,45,45,45	0
57	MG	1a	1693	1/1	0.97	0.07	35,35,35,35	0
57	MG	1a	1694	1/1	0.97	0.18	37,37,37,37	0
57	MG	1A	3364	1/1	0.97	0.12	21,21,21,21	0
57	MG	2A	3108	1/1	0.97	0.10	41,41,41,41	0
57	MG	1A	3365	1/1	0.97	0.09	24,24,24,24	0
57	MG	1A	3595	1/1	0.97	0.09	27,27,27,27	0
57	MG	2A	3719	1/1	0.97	0.06	48,48,48,48	0
57	MG	2A	3721	1/1	0.97	0.05	25,25,25,25	0
57	MG	1A	3140	1/1	0.97	0.09	31,31,31,31	0
57	MG	1E	306	1/1	0.97	0.08	24,24,24,24	0
57	MG	2A	3390	1/1	0.97	0.05	52,52,52,52	0
57	MG	2A	3725	1/1	0.97	0.07	46,46,46,46	0
57	MG	1A	3367	1/1	0.97	0.10	33,33,33,33	0
57	MG	1A	3934	1/1	0.97	0.04	30,30,30,30	0
57	MG	1E	309	1/1	0.97	0.12	40,40,40,40	0
57	MG	1A	3756	1/1	0.97	0.04	38,38,38,38	0
57	MG	2A	3117	1/1	0.97	0.08	38,38,38,38	0
57	MG	2A	3732	1/1	0.97	0.05	35,35,35,35	0
57	MG	2A	3733	1/1	0.97	0.12	37,37,37,37	0
57	MG	1A	3937	1/1	0.97	0.04	51,51,51,51	0
57	MG	2A	3119	1/1	0.97	0.08	49,49,49,49	0
57	MG	1A	3141	1/1	0.97	0.09	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3121	1/1	0.97	0.07	35,35,35,35	0
57	MG	1a	1706	1/1	0.97	0.07	39,39,39,39	0
57	MG	1A	3600	1/1	0.97	0.17	45,45,45,45	0
57	MG	1A	3601	1/1	0.97	0.08	40,40,40,40	0
57	MG	1F	306	1/1	0.97	0.10	21,21,21,21	0
57	MG	2a	1723	1/1	0.97	0.10	52,52,52,52	0
57	MG	1a	1710	1/1	0.97	0.05	32,32,32,32	0
57	MG	2A	3405	1/1	0.97	0.05	43,43,43,43	0
57	MG	1A	3602	1/1	0.97	0.09	42,42,42,42	0
57	MG	1F	309	1/1	0.97	0.06	40,40,40,40	0
57	MG	2A	3130	1/1	0.97	0.07	38,38,38,38	0
57	MG	2a	1730	1/1	0.97	0.10	45,45,45,45	0
57	MG	1A	3603	1/1	0.97	0.09	29,29,29,29	0
57	MG	1A	3278	1/1	0.97	0.09	21,21,21,21	0
57	MG	2A	3133	1/1	0.97	0.05	52,52,52,52	0
57	MG	1A	3279	1/1	0.97	0.29	31,31,31,31	0
57	MG	1A	3606	1/1	0.97	0.04	18,18,18,18	0
57	MG	1A	3472	1/1	0.97	0.20	32,32,32,32	0
57	MG	1A	3951	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3043	1/1	0.97	0.07	35,35,35,35	0
57	MG	1G	205	1/1	0.97	0.05	34,34,34,34	0
57	MG	2A	3758	1/1	0.97	0.08	49,49,49,49	0
57	MG	1A	3953	1/1	0.97	0.06	56,56,56,56	0
57	MG	2A	3141	1/1	0.97	0.13	34,34,34,34	0
57	MG	2A	3142	1/1	0.97	0.14	51,51,51,51	0
57	MG	1A	3474	1/1	0.97	0.04	27,27,27,27	0
57	MG	2A	3144	1/1	0.97	0.12	29,29,29,29	0
57	MG	2a	1746	1/1	0.97	0.07	59,59,59,59	0
57	MG	1A	3285	1/1	0.97	0.04	34,34,34,34	0
57	MG	2A	3424	1/1	0.97	0.22	40,40,40,40	0
57	MG	2A	3425	1/1	0.97	0.22	48,48,48,48	0
57	MG	2a	1750	1/1	0.97	0.05	59,59,59,59	0
57	MG	2a	1751	1/1	0.97	0.06	52,52,52,52	0
57	MG	1A	3477	1/1	0.97	0.11	39,39,39,39	0
57	MG	2A	3427	1/1	0.97	0.12	48,48,48,48	0
57	MG	1N	203	1/1	0.97	0.11	43,43,43,43	0
57	MG	2a	1755	1/1	0.97	0.05	58,58,58,58	0
57	MG	1A	3286	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3144	1/1	0.97	0.06	47,47,47,47	0
57	MG	2A	3772	1/1	0.97	0.04	36,36,36,36	0
57	MG	1a	1730	1/1	0.97	0.07	37,37,37,37	0
57	MG	2A	3152	1/1	0.97	0.05	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3205	1/1	0.97	0.05	15,15,15,15	0
57	MG	1A	3378	1/1	0.97	0.04	31,31,31,31	0
57	MG	1A	3097	1/1	0.97	0.09	42,42,42,42	0
57	MG	1O	203	1/1	0.97	0.09	42,42,42,42	0
57	MG	2a	1767	1/1	0.97	0.05	53,53,53,53	0
57	MG	2a	1768	1/1	0.97	0.08	64,64,64,64	0
57	MG	1O	204	1/1	0.97	0.09	45,45,45,45	0
57	MG	1A	3963	1/1	0.97	0.05	21,21,21,21	0
57	MG	2A	3781	1/1	0.97	0.13	35,35,35,35	0
57	MG	1P	202	1/1	0.97	0.15	19,19,19,19	0
57	MG	2A	3785	1/1	0.97	0.05	47,47,47,47	0
57	MG	2A	3787	1/1	0.97	0.07	45,45,45,45	0
57	MG	2a	1776	1/1	0.97	0.07	53,53,53,53	0
57	MG	1A	3146	1/1	0.97	0.33	29,29,29,29	0
57	MG	1A	3620	1/1	0.97	0.09	7,7,7,7	0
57	MG	2a	1779	1/1	0.97	0.10	35,35,35,35	0
57	MG	2a	1781	1/1	0.97	0.09	30,30,30,30	0
57	MG	1A	3621	1/1	0.97	0.06	33,33,33,33	0
57	MG	2A	3163	1/1	0.97	0.10	40,40,40,40	0
57	MG	1A	3967	1/1	0.97	0.06	54,54,54,54	0
57	MG	2A	3794	1/1	0.97	0.06	48,48,48,48	0
57	MG	1A	3969	1/1	0.97	0.08	34,34,34,34	0
57	MG	1A	3044	1/1	0.97	0.04	16,16,16,16	0
57	MG	2A	3167	1/1	0.97	0.25	52,52,52,52	0
57	MG	1A	3067	1/1	0.97	0.11	35,35,35,35	0
57	MG	1A	3152	1/1	0.97	0.14	23,23,23,23	0
57	MG	1A	3212	1/1	0.97	0.08	37,37,37,37	0
57	MG	1a	1750	1/1	0.97	0.08	30,30,30,30	0
57	MG	2a	1793	1/1	0.97	0.19	50,50,50,50	0
57	MG	1A	3213	1/1	0.97	0.18	21,21,21,21	0
57	MG	2a	1795	1/1	0.97	0.12	47,47,47,47	0
57	MG	1A	3490	1/1	0.97	0.13	37,37,37,37	0
57	MG	2A	3456	1/1	0.97	0.13	34,34,34,34	0
57	MG	2A	3805	1/1	0.97	0.05	35,35,35,35	0
57	MG	1S	201	1/1	0.97	0.25	37,37,37,37	0
57	MG	2A	3459	1/1	0.97	0.23	45,45,45,45	0
57	MG	1S	202	1/1	0.97	0.04	37,37,37,37	0
57	MG	1A	3630	1/1	0.97	0.06	19,19,19,19	0
57	MG	1a	1757	1/1	0.97	0.05	41,41,41,41	0
57	MG	1A	3491	1/1	0.97	0.08	45,45,45,45	0
57	MG	2A	3179	1/1	0.97	0.05	37,37,37,37	0
57	MG	2A	3180	1/1	0.97	0.06	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3299	1/1	0.97	0.21	23,23,23,23	0
57	MG	1A	3983	1/1	0.97	0.05	48,48,48,48	0
57	MG	2A	3183	1/1	0.97	0.09	56,56,56,56	0
57	MG	1T	204	1/1	0.97	0.06	37,37,37,37	0
57	MG	1A	3636	1/1	0.97	0.04	22,22,22,22	0
57	MG	2A	3821	1/1	0.97	0.06	40,40,40,40	0
57	MG	1A	3799	1/1	0.97	0.04	16,16,16,16	0
57	MG	1U	206	1/1	0.97	0.31	40,40,40,40	0
57	MG	1U	207	1/1	0.97	0.11	23,23,23,23	0
57	MG	1U	208	1/1	0.97	0.23	32,32,32,32	0
57	MG	1A	3215	1/1	0.97	0.07	32,32,32,32	0
57	MG	2A	3477	1/1	0.97	0.08	46,46,46,46	0
57	MG	1A	3638	1/1	0.97	0.05	27,27,27,27	0
57	MG	1a	1770	1/1	0.97	0.04	37,37,37,37	0
57	MG	1a	1771	1/1	0.97	0.05	50,50,50,50	0
57	MG	1A	3988	1/1	0.97	0.11	18,18,18,18	0
57	MG	1A	3012	1/1	0.97	0.03	19,19,19,19	0
57	MG	1V	206	1/1	0.97	0.08	28,28,28,28	0
57	MG	1A	3101	1/1	0.97	0.10	19,19,19,19	0
57	MG	1V	209	1/1	0.97	0.05	27,27,27,27	0
57	MG	1A	3156	1/1	0.97	0.06	28,28,28,28	0
57	MG	2A	3487	1/1	0.97	0.05	17,17,17,17	0
57	MG	1W	201	1/1	0.97	0.09	32,32,32,32	0
57	MG	1A	3071	1/1	0.97	0.11	17,17,17,17	0
57	MG	1a	1781	1/1	0.97	0.06	48,48,48,48	0
57	MG	2A	3845	1/1	0.97	0.05	45,45,45,45	0
57	MG	2A	3493	1/1	0.97	0.05	45,45,45,45	0
57	MG	1A	3046	1/1	0.97	0.05	20,20,20,20	0
57	MG	2A	3205	1/1	0.97	0.23	48,48,48,48	0
57	MG	1A	3308	1/1	0.97	0.07	24,24,24,24	0
57	MG	1A	3107	1/1	0.97	0.12	22,22,22,22	0
57	MG	1a	1786	1/1	0.97	0.05	55,55,55,55	0
57	MG	1a	1787	1/1	0.97	0.06	48,48,48,48	0
57	MG	1A	3810	1/1	0.97	0.04	27,27,27,27	0
57	MG	1A	3161	1/1	0.97	0.07	26,26,26,26	0
57	MG	2A	3212	1/1	0.97	0.06	37,37,37,37	0
57	MG	1A	3162	1/1	0.97	0.05	22,22,22,22	0
57	MG	2A	3504	1/1	0.97	0.17	37,37,37,37	0
57	MG	2A	3861	1/1	0.97	0.05	40,40,40,40	0
57	MG	2A	3862	1/1	0.97	0.06	27,27,27,27	0
57	MG	2A	3863	1/1	0.97	0.05	30,30,30,30	0
57	MG	1A	3226	1/1	0.97	0.09	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1X	106	1/1	0.97	0.04	37,37,37,37	0
57	MG	1A	3816	1/1	0.97	0.06	34,34,34,34	0
57	MG	1A	3505	1/1	0.97	0.09	41,41,41,41	0
57	MG	1A	4002	1/1	0.97	0.03	6,6,6,6	0
57	MG	1A	3652	1/1	0.97	0.06	27,27,27,27	0
57	MG	1A	3029	1/1	0.97	0.15	22,22,22,22	0
57	MG	1A	3509	1/1	0.97	0.07	44,44,44,44	0
57	MG	1A	3110	1/1	0.97	0.14	25,25,25,25	0
57	MG	1A	4010	1/1	0.97	0.05	12,12,12,12	0
57	MG	1A	3031	1/1	0.97	0.11	11,11,11,11	0
57	MG	1A	3827	1/1	0.97	0.09	17,17,17,17	0
57	MG	1A	4014	1/1	0.97	0.06	31,31,31,31	0
57	MG	10	104	1/1	0.97	0.05	28,28,28,28	0
57	MG	1A	3829	1/1	0.97	0.07	30,30,30,30	0
57	MG	1A	3515	1/1	0.97	0.16	23,23,23,23	0
57	MG	1A	3231	1/1	0.97	0.07	19,19,19,19	0
57	MG	2x	101	1/1	0.97	0.09	29,29,29,29	0
57	MG	1A	4019	1/1	0.97	0.08	33,33,33,33	0
57	MG	1A	3517	1/1	0.97	0.21	30,30,30,30	0
57	MG	2A	3234	1/1	0.97	0.12	25,25,25,25	0
57	MG	1f	202	1/1	0.97	0.09	43,43,43,43	0
57	MG	1k	201	1/1	0.97	0.08	33,33,33,33	0
57	MG	1A	3318	1/1	0.97	0.08	37,37,37,37	0
57	MG	1A	4023	1/1	0.97	0.10	28,28,28,28	0
57	MG	2A	3239	1/1	0.97	0.08	43,43,43,43	0
57	MG	1A	3834	1/1	0.97	0.05	37,37,37,37	0
57	MG	1A	3520	1/1	0.97	0.05	33,33,33,33	0
57	MG	1A	3521	1/1	0.97	0.12	49,49,49,49	0
58	K	2A	3472	1/1	0.97	0.06	41,41,41,41	0
57	MG	2A	3537	1/1	0.97	0.07	26,26,26,26	0
57	MG	1A	3049	1/1	0.97	0.04	10,10,10,10	0
60	ZN	14	102	1/1	0.97	0.06	58,58,58,58	0
57	MG	1A	3320	1/1	0.97	0.06	24,24,24,24	0
57	MG	1A	3665	1/1	0.97	0.03	20,20,20,20	0
57	MG	1A	3237	1/1	0.98	0.16	24,24,24,24	0
57	MG	1A	3108	1/1	0.98	0.11	22,22,22,22	0
57	MG	1A	3578	1/1	0.98	0.14	33,33,33,33	0
57	MG	1A	3239	1/1	0.98	0.05	25,25,25,25	0
57	MG	1A	3787	1/1	0.98	0.08	13,13,13,13	0
57	MG	1A	3423	1/1	0.98	0.07	35,35,35,35	0
57	MG	2A	3737	1/1	0.98	0.05	51,51,51,51	0
57	MG	1A	3023	1/1	0.98	0.04	9,9,9,9	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1U	201	1/1	0.98	0.15	27,27,27,27	0
57	MG	2A	3489	1/1	0.98	0.14	37,37,37,37	0
57	MG	1A	3242	1/1	0.98	0.07	22,22,22,22	0
57	MG	2A	3491	1/1	0.98	0.03	31,31,31,31	0
57	MG	1A	4051	1/1	0.98	0.05	23,23,23,23	0
57	MG	2A	3060	1/1	0.98	0.05	34,34,34,34	0
57	MG	1U	204	1/1	0.98	0.12	25,25,25,25	0
57	MG	1U	205	1/1	0.98	0.16	24,24,24,24	0
57	MG	1A	3791	1/1	0.98	0.03	33,33,33,33	0
57	MG	1A	3678	1/1	0.98	0.06	14,14,14,14	0
57	MG	1A	3072	1/1	0.98	0.04	9,9,9,9	0
57	MG	1A	3244	1/1	0.98	0.05	32,32,32,32	0
57	MG	1A	3362	1/1	0.98	0.06	37,37,37,37	0
57	MG	2A	3282	1/1	0.98	0.04	33,33,33,33	0
57	MG	1V	201	1/1	0.98	0.16	22,22,22,22	0
57	MG	1V	203	1/1	0.98	0.27	35,35,35,35	0
57	MG	1A	3363	1/1	0.98	0.05	36,36,36,36	0
57	MG	2A	3756	1/1	0.98	0.04	42,42,42,42	0
57	MG	1A	3798	1/1	0.98	0.07	35,35,35,35	0
57	MG	1A	3430	1/1	0.98	0.04	29,29,29,29	0
57	MG	1V	207	1/1	0.98	0.18	23,23,23,23	0
57	MG	1A	3589	1/1	0.98	0.04	30,30,30,30	0
57	MG	1A	3590	1/1	0.98	0.22	38,38,38,38	0
57	MG	2A	3511	1/1	0.98	0.06	45,45,45,45	0
57	MG	1A	3502	1/1	0.98	0.07	51,51,51,51	0
57	MG	1a	1721	1/1	0.98	0.11	26,26,26,26	0
57	MG	1A	3160	1/1	0.98	0.06	22,22,22,22	0
57	MG	1A	3432	1/1	0.98	0.14	27,27,27,27	0
57	MG	1A	3691	1/1	0.98	0.04	29,29,29,29	0
57	MG	1A	3132	1/1	0.98	0.04	16,16,16,16	0
57	MG	2a	1661	1/1	0.98	0.15	54,54,54,54	0
57	MG	2a	1662	1/1	0.98	0.04	32,32,32,32	0
57	MG	1W	205	1/1	0.98	0.09	31,31,31,31	0
57	MG	1A	3199	1/1	0.98	0.08	32,32,32,32	0
57	MG	1A	4070	1/1	0.98	0.11	26,26,26,26	0
57	MG	1a	1729	1/1	0.98	0.06	46,46,46,46	0
57	MG	1W	208	1/1	0.98	0.05	24,24,24,24	0
57	MG	1A	3507	1/1	0.98	0.04	13,13,13,13	0
57	MG	1a	1732	1/1	0.98	0.04	28,28,28,28	0
57	MG	1A	4072	1/1	0.98	0.04	15,15,15,15	0
57	MG	1A	3696	1/1	0.98	0.02	22,22,22,22	0
57	MG	1X	104	1/1	0.98	0.18	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1X	105	1/1	0.98	0.09	24,24,24,24	0
57	MG	1A	3811	1/1	0.98	0.02	15,15,15,15	0
57	MG	1A	4076	1/1	0.98	0.04	17,17,17,17	0
57	MG	1A	3508	1/1	0.98	0.07	39,39,39,39	0
57	MG	2A	3783	1/1	0.98	0.10	34,34,34,34	0
57	MG	2A	3784	1/1	0.98	0.05	43,43,43,43	0
57	MG	2A	3533	1/1	0.98	0.03	26,26,26,26	0
57	MG	2A	3786	1/1	0.98	0.04	47,47,47,47	0
57	MG	1a	1740	1/1	0.98	0.06	31,31,31,31	0
57	MG	2A	3788	1/1	0.98	0.09	48,48,48,48	0
57	MG	1A	3813	1/1	0.98	0.05	31,31,31,31	0
57	MG	2A	3313	1/1	0.98	0.14	52,52,52,52	0
57	MG	2a	1685	1/1	0.98	0.24	45,45,45,45	0
57	MG	1A	3133	1/1	0.98	0.13	22,22,22,22	0
57	MG	1A	3201	1/1	0.98	0.07	16,16,16,16	0
57	MG	1a	1744	1/1	0.98	0.07	33,33,33,33	0
57	MG	1A	3938	1/1	0.98	0.07	36,36,36,36	0
57	MG	1A	3700	1/1	0.98	0.04	32,32,32,32	0
57	MG	1A	4083	1/1	0.98	0.09	28,28,28,28	0
57	MG	1A	3163	1/1	0.98	0.28	23,23,23,23	0
57	MG	1A	3512	1/1	0.98	0.14	19,19,19,19	0
57	MG	1A	3942	1/1	0.98	0.04	40,40,40,40	0
57	MG	1A	3943	1/1	0.98	0.03	43,43,43,43	0
57	MG	1A	4089	1/1	0.98	0.04	22,22,22,22	0
57	MG	2a	1697	1/1	0.98	0.09	33,33,33,33	0
57	MG	1A	4090	1/1	0.98	0.06	34,34,34,34	0
57	MG	2A	3551	1/1	0.98	0.08	31,31,31,31	0
57	MG	1A	3513	1/1	0.98	0.04	16,16,16,16	0
57	MG	1A	3820	1/1	0.98	0.06	24,24,24,24	0
57	MG	2A	3328	1/1	0.98	0.07	32,32,32,32	0
57	MG	1A	3082	1/1	0.98	0.07	25,25,25,25	0
57	MG	2A	3556	1/1	0.98	0.05	47,47,47,47	0
57	MG	1A	3165	1/1	0.98	0.03	28,28,28,28	0
57	MG	1A	3823	1/1	0.98	0.04	32,32,32,32	0
57	MG	1A	3372	1/1	0.98	0.15	29,29,29,29	0
57	MG	2A	3812	1/1	0.98	0.04	41,41,41,41	0
57	MG	1A	3950	1/1	0.98	0.04	38,38,38,38	0
57	MG	1A	3826	1/1	0.98	0.03	28,28,28,28	0
57	MG	2A	3123	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	4099	1/1	0.98	0.14	40,40,40,40	0
57	MG	2A	3817	1/1	0.98	0.07	36,36,36,36	0
57	MG	13	102	1/1	0.98	0.09	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3567	1/1	0.98	0.04	28,28,28,28	0
57	MG	1A	3707	1/1	0.98	0.07	10,10,10,10	0
57	MG	2A	3569	1/1	0.98	0.06	52,52,52,52	0
57	MG	2A	3570	1/1	0.98	0.07	55,55,55,55	0
57	MG	13	104	1/1	0.98	0.04	28,28,28,28	0
57	MG	1A	3828	1/1	0.98	0.11	20,20,20,20	0
57	MG	1A	3315	1/1	0.98	0.03	31,31,31,31	0
57	MG	15	101	1/1	0.98	0.18	24,24,24,24	0
57	MG	1A	3519	1/1	0.98	0.07	38,38,38,38	0
57	MG	15	105	1/1	0.98	0.13	28,28,28,28	0
57	MG	1a	1773	1/1	0.98	0.04	55,55,55,55	0
57	MG	1A	3166	1/1	0.98	0.13	29,29,29,29	0
57	MG	15	107	1/1	0.98	0.08	23,23,23,23	0
57	MG	1A	3444	1/1	0.98	0.10	21,21,21,21	0
57	MG	2a	1729	1/1	0.98	0.12	48,48,48,48	0
57	MG	1A	3206	1/1	0.98	0.05	16,16,16,16	0
57	MG	1A	3376	1/1	0.98	0.08	23,23,23,23	0
57	MG	2A	3584	1/1	0.98	0.04	29,29,29,29	0
57	MG	2A	3585	1/1	0.98	0.09	29,29,29,29	0
57	MG	16	102	1/1	0.98	0.10	24,24,24,24	0
57	MG	1A	3256	1/1	0.98	0.03	16,16,16,16	0
57	MG	2A	3841	1/1	0.98	0.06	33,33,33,33	0
57	MG	17	102	1/1	0.98	0.04	17,17,17,17	0
57	MG	1a	1782	1/1	0.98	0.04	56,56,56,56	0
57	MG	1A	3167	1/1	0.98	0.05	22,22,22,22	0
57	MG	1A	3717	1/1	0.98	0.04	51,51,51,51	0
57	MG	1A	3096	1/1	0.98	0.05	9,9,9,9	0
57	MG	1A	3380	1/1	0.98	0.04	20,20,20,20	0
57	MG	1A	3136	1/1	0.98	0.06	33,33,33,33	0
57	MG	1a	1788	1/1	0.98	0.03	38,38,38,38	0
57	MG	2A	3597	1/1	0.98	0.08	51,51,51,51	0
57	MG	18	101	1/1	0.98	0.10	37,37,37,37	0
57	MG	2A	3150	1/1	0.98	0.04	28,28,28,28	0
57	MG	1A	3452	1/1	0.98	0.07	40,40,40,40	0
57	MG	2A	3602	1/1	0.98	0.04	28,28,28,28	0
57	MG	1A	3968	1/1	0.98	0.05	27,27,27,27	0
57	MG	2A	3858	1/1	0.98	0.06	37,37,37,37	0
57	MG	2A	3859	1/1	0.98	0.09	41,41,41,41	0
57	MG	1B	216	1/1	0.98	0.04	34,34,34,34	0
57	MG	1a	1793	1/1	0.98	0.05	47,47,47,47	0
57	MG	1A	3530	1/1	0.98	0.17	25,25,25,25	0
57	MG	1a	1796	1/1	0.98	0.04	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1797	1/1	0.98	0.04	60,60,60,60	0
57	MG	2A	3865	1/1	0.98	0.04	44,44,44,44	0
57	MG	1A	3531	1/1	0.98	0.04	20,20,20,20	0
57	MG	1B	219	1/1	0.98	0.04	35,35,35,35	0
57	MG	1a	1603	1/1	0.98	0.11	42,42,42,42	0
57	MG	2a	1762	1/1	0.98	0.04	41,41,41,41	0
57	MG	1a	1801	1/1	0.98	0.04	49,49,49,49	0
57	MG	1B	220	1/1	0.98	0.05	42,42,42,42	0
57	MG	1A	3063	1/1	0.98	0.06	27,27,27,27	0
57	MG	2A	3873	1/1	0.98	0.07	37,37,37,37	0
57	MG	2A	3615	1/1	0.98	0.08	43,43,43,43	0
57	MG	1B	222	1/1	0.98	0.03	28,28,28,28	0
57	MG	1a	1805	1/1	0.98	0.07	48,48,48,48	0
57	MG	1A	3084	1/1	0.98	0.13	18,18,18,18	0
57	MG	1A	3973	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3625	1/1	0.98	0.07	25,25,25,25	0
57	MG	2a	1774	1/1	0.98	0.05	48,48,48,48	0
57	MG	1A	3015	1/1	0.98	0.09	27,27,27,27	0
57	MG	1A	3627	1/1	0.98	0.09	32,32,32,32	0
57	MG	1a	1811	1/1	0.98	0.03	31,31,31,31	0
57	MG	2A	3624	1/1	0.98	0.11	29,29,29,29	0
57	MG	1A	3387	1/1	0.98	0.10	22,22,22,22	0
57	MG	2a	1780	1/1	0.98	0.08	52,52,52,52	0
57	MG	1A	3116	1/1	0.98	0.06	18,18,18,18	0
57	MG	1A	3266	1/1	0.98	0.04	35,35,35,35	0
57	MG	2A	3628	1/1	0.98	0.07	36,36,36,36	0
57	MG	1A	3982	1/1	0.98	0.03	30,30,30,30	0
57	MG	1A	3632	1/1	0.98	0.03	28,28,28,28	0
57	MG	1A	3214	1/1	0.98	0.08	23,23,23,23	0
57	MG	1f	201	1/1	0.98	0.08	38,38,38,38	0
57	MG	2A	3634	1/1	0.98	0.05	22,22,22,22	0
57	MG	1a	1618	1/1	0.98	0.09	41,41,41,41	0
57	MG	1A	3634	1/1	0.98	0.05	11,11,11,11	0
57	MG	2A	3637	1/1	0.98	0.09	40,40,40,40	0
57	MG	1a	1620	1/1	0.98	0.05	41,41,41,41	0
57	MG	1l	202	1/1	0.98	0.07	41,41,41,41	0
57	MG	1A	3735	1/1	0.98	0.03	22,22,22,22	0
57	MG	1A	3174	1/1	0.98	0.11	19,19,19,19	0
57	MG	1A	3175	1/1	0.98	0.07	27,27,27,27	0
57	MG	1A	3035	1/1	0.98	0.09	16,16,16,16	0
57	MG	1A	3331	1/1	0.98	0.09	39,39,39,39	0
57	MG	1A	3218	1/1	0.98	0.08	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1D	309	1/1	0.98	0.06	34,34,34,34	0
57	MG	1D	310	1/1	0.98	0.05	29,29,29,29	0
57	MG	1a	1630	1/1	0.98	0.05	41,41,41,41	0
57	MG	1A	3177	1/1	0.98	0.04	18,18,18,18	0
57	MG	2A	3651	1/1	0.98	0.13	44,44,44,44	0
57	MG	2A	3193	1/1	0.98	0.16	43,43,43,43	0
57	MG	1A	3059	1/1	0.98	0.05	26,26,26,26	0
57	MG	1D	313	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3143	1/1	0.98	0.07	36,36,36,36	0
57	MG	1A	3003	1/1	0.98	0.04	20,20,20,20	0
57	MG	2A	3657	1/1	0.98	0.06	46,46,46,46	0
57	MG	1A	3103	1/1	0.98	0.05	40,40,40,40	0
57	MG	1w	108	1/1	0.98	0.06	48,48,48,48	0
57	MG	1E	304	1/1	0.98	0.07	27,27,27,27	0
57	MG	1a	1638	1/1	0.98	0.14	37,37,37,37	0
57	MG	1E	305	1/1	0.98	0.11	23,23,23,23	0
57	MG	1A	3867	1/1	0.98	0.03	28,28,28,28	0
57	MG	1A	3645	1/1	0.98	0.10	10,10,10,10	0
57	MG	1A	3747	1/1	0.98	0.07	32,32,32,32	0
57	MG	1A	3224	1/1	0.98	0.09	31,31,31,31	0
57	MG	2F	305	1/1	0.98	0.17	40,40,40,40	0
57	MG	1A	3078	1/1	0.98	0.06	22,22,22,22	0
57	MG	1E	311	1/1	0.98	0.05	24,24,24,24	0
57	MG	1A	3403	1/1	0.98	0.10	34,34,34,34	0
57	MG	1A	3147	1/1	0.98	0.04	26,26,26,26	0
57	MG	1A	4004	1/1	0.98	0.13	14,14,14,14	0
57	MG	1F	301	1/1	0.98	0.04	22,22,22,22	0
57	MG	1F	304	1/1	0.98	0.06	21,21,21,21	0
57	MG	1A	4005	1/1	0.98	0.04	25,25,25,25	0
57	MG	1a	1652	1/1	0.98	0.07	31,31,31,31	0
57	MG	1a	1653	1/1	0.98	0.06	36,36,36,36	0
57	MG	1A	4006	1/1	0.98	0.04	32,32,32,32	0
57	MG	2A	3218	1/1	0.98	0.11	42,42,42,42	0
57	MG	1F	307	1/1	0.98	0.08	25,25,25,25	0
57	MG	1A	3650	1/1	0.98	0.03	19,19,19,19	0
57	MG	1A	3753	1/1	0.98	0.05	25,25,25,25	0
57	MG	2A	3007	1/1	0.98	0.16	41,41,41,41	0
57	MG	1A	3754	1/1	0.98	0.05	33,33,33,33	0
57	MG	2f	201	1/1	0.98	0.07	41,41,41,41	0
57	MG	1A	3755	1/1	0.98	0.06	39,39,39,39	0
57	MG	1A	4011	1/1	0.98	0.03	16,16,16,16	0
57	MG	1a	1661	1/1	0.98	0.03	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3282	1/1	0.98	0.12	18,18,18,18	0
57	MG	1A	3475	1/1	0.98	0.05	21,21,21,21	0
57	MG	1A	3284	1/1	0.98	0.15	22,22,22,22	0
57	MG	1A	3557	1/1	0.98	0.31	30,30,30,30	0
57	MG	1A	3558	1/1	0.98	0.08	23,23,23,23	0
57	MG	2A	3445	1/1	0.98	0.08	45,45,45,45	0
57	MG	1A	3148	1/1	0.98	0.05	21,21,21,21	0
57	MG	1A	4018	1/1	0.98	0.04	25,25,25,25	0
57	MG	1A	3105	1/1	0.98	0.06	18,18,18,18	0
57	MG	1A	4020	1/1	0.98	0.05	45,45,45,45	0
57	MG	1A	3229	1/1	0.98	0.05	18,18,18,18	0
57	MG	1a	1672	1/1	0.98	0.04	40,40,40,40	0
57	MG	1A	3150	1/1	0.98	0.16	21,21,21,21	0
57	MG	1A	3123	1/1	0.98	0.11	25,25,25,25	0
57	MG	2v	102	1/1	0.98	0.05	45,45,45,45	0
57	MG	2A	3454	1/1	0.98	0.09	40,40,40,40	0
57	MG	1A	3889	1/1	0.98	0.06	18,18,18,18	0
57	MG	2A	3027	1/1	0.98	0.05	30,30,30,30	0
57	MG	1A	3890	1/1	0.98	0.06	32,32,32,32	0
57	MG	2A	3458	1/1	0.98	0.14	34,34,34,34	0
57	MG	1A	3768	1/1	0.98	0.04	24,24,24,24	0
57	MG	1A	4027	1/1	0.98	0.04	31,31,31,31	0
57	MG	1A	3412	1/1	0.98	0.06	46,46,46,46	0
57	MG	1A	3106	1/1	0.98	0.09	23,23,23,23	0
57	MG	2A	3033	1/1	0.98	0.03	35,35,35,35	0
57	MG	1P	201	1/1	0.98	0.05	23,23,23,23	0
57	MG	1A	3293	1/1	0.98	0.11	25,25,25,25	0
57	MG	1A	4031	1/1	0.98	0.04	48,48,48,48	0
57	MG	1A	3125	1/1	0.98	0.16	24,24,24,24	0
57	MG	2A	3716	1/1	0.98	0.06	35,35,35,35	0
57	MG	2A	3038	1/1	0.98	0.03	32,32,32,32	0
57	MG	2A	3039	1/1	0.98	0.03	27,27,27,27	0
57	MG	1A	3569	1/1	0.98	0.09	18,18,18,18	0
57	MG	2A	3720	1/1	0.98	0.06	37,37,37,37	0
57	MG	1A	3774	1/1	0.98	0.06	25,25,25,25	0
57	MG	1A	3154	1/1	0.98	0.06	25,25,25,25	0
57	MG	1A	3050	1/1	0.98	0.15	28,28,28,28	0
58	K	1A	3564	1/1	0.98	0.03	17,17,17,17	0
57	MG	1A	3778	1/1	0.98	0.04	19,19,19,19	0
57	MG	1A	3127	1/1	0.98	0.13	32,32,32,32	0
57	MG	1R	201	1/1	0.98	0.05	24,24,24,24	0
57	MG	1A	3669	1/1	0.98	0.03	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	ZN	2Y	501	1/1	0.98	0.05	87,87,87,87	0
57	MG	1A	3354	1/1	0.98	0.12	27,27,27,27	0
57	MG	1A	3904	1/1	0.98	0.04	26,26,26,26	0
57	MG	1A	3689	1/1	0.99	0.05	25,25,25,25	0
57	MG	1A	3251	1/1	0.99	0.05	34,34,34,34	0
57	MG	2A	3678	1/1	0.99	0.04	26,26,26,26	0
57	MG	1A	3588	1/1	0.99	0.09	25,25,25,25	0
57	MG	2A	3866	1/1	0.99	0.12	29,29,29,29	0
57	MG	1A	4062	1/1	0.99	0.04	33,33,33,33	0
57	MG	1A	3692	1/1	0.99	0.02	21,21,21,21	0
57	MG	1A	3386	1/1	0.99	0.10	20,20,20,20	0
57	MG	1A	3240	1/1	0.99	0.04	15,15,15,15	0
57	MG	2A	3509	1/1	0.99	0.03	55,55,55,55	0
57	MG	2A	3595	1/1	0.99	0.05	35,35,35,35	0
57	MG	1A	3283	1/1	0.99	0.05	30,30,30,30	0
57	MG	1A	3960	1/1	0.99	0.03	33,33,33,33	0
57	MG	1A	3303	1/1	0.99	0.07	21,21,21,21	0
57	MG	1a	1756	1/1	0.99	0.03	33,33,33,33	0
57	MG	1B	226	1/1	0.99	0.03	27,27,27,27	0
57	MG	2A	3601	1/1	0.99	0.03	38,38,38,38	0
57	MG	1A	3304	1/1	0.99	0.06	16,16,16,16	0
57	MG	1a	1622	1/1	0.99	0.04	39,39,39,39	0
57	MG	1A	3776	1/1	0.99	0.03	38,38,38,38	0
57	MG	1A	3086	1/1	0.99	0.11	28,28,28,28	0
57	MG	1A	3068	1/1	0.99	0.03	24,24,24,24	0
57	MG	1A	3779	1/1	0.99	0.02	33,33,33,33	0
57	MG	1a	1764	1/1	0.99	0.07	35,35,35,35	0
57	MG	1A	3095	1/1	0.99	0.02	12,12,12,12	0
57	MG	1A	4075	1/1	0.99	0.06	30,30,30,30	0
57	MG	1B	234	1/1	0.99	0.03	38,38,38,38	0
57	MG	1A	3871	1/1	0.99	0.06	10,10,10,10	0
57	MG	1B	236	1/1	0.99	0.03	22,22,22,22	0
57	MG	1D	301	1/1	0.99	0.09	17,17,17,17	0
57	MG	1A	3919	1/1	0.99	0.01	18,18,18,18	0
57	MG	1A	3825	1/1	0.99	0.03	10,10,10,10	0
57	MG	1A	3287	1/1	0.99	0.05	25,25,25,25	0
57	MG	2A	3531	1/1	0.99	0.04	32,32,32,32	0
57	MG	2A	3064	1/1	0.99	0.04	55,55,55,55	0
57	MG	1A	3631	1/1	0.99	0.05	30,30,30,30	0
57	MG	1A	3514	1/1	0.99	0.07	25,25,25,25	0
57	MG	1A	3974	1/1	0.99	0.04	44,44,44,44	0
57	MG	1A	3975	1/1	0.99	0.04	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	13	101	1/1	0.99	0.06	23,23,23,23	0
57	MG	2A	3070	1/1	0.99	0.07	26,26,26,26	0
57	MG	1A	4084	1/1	0.99	0.04	29,29,29,29	0
57	MG	2A	3540	1/1	0.99	0.03	26,26,26,26	0
57	MG	1A	3599	1/1	0.99	0.10	41,41,41,41	0
57	MG	2A	3542	1/1	0.99	0.12	33,33,33,33	0
57	MG	1A	3489	1/1	0.99	0.14	30,30,30,30	0
57	MG	2A	3631	1/1	0.99	0.04	32,32,32,32	0
57	MG	1A	3128	1/1	0.99	0.08	37,37,37,37	0
57	MG	1A	3069	1/1	0.99	0.06	9,9,9,9	0
57	MG	1A	3443	1/1	0.99	0.07	20,20,20,20	0
57	MG	15	102	1/1	0.99	0.06	23,23,23,23	0
57	MG	1A	3709	1/1	0.99	0.03	21,21,21,21	0
57	MG	2A	3079	1/1	0.99	0.10	21,21,21,21	0
57	MG	2A	3728	1/1	0.99	0.06	40,40,40,40	0
57	MG	15	104	1/1	0.99	0.20	24,24,24,24	0
57	MG	1A	4034	1/1	0.99	0.05	19,19,19,19	0
57	MG	1A	3573	1/1	0.99	0.12	21,21,21,21	0
57	MG	1A	3005	1/1	0.99	0.07	27,27,27,27	0
57	MG	2A	3009	1/1	0.99	0.08	29,29,29,29	0
57	MG	1A	3792	1/1	0.99	0.04	25,25,25,25	0
57	MG	1A	3575	1/1	0.99	0.09	30,30,30,30	0
57	MG	2A	3645	1/1	0.99	0.04	27,27,27,27	0
57	MG	2A	3557	1/1	0.99	0.05	36,36,36,36	0
57	MG	1A	3839	1/1	0.99	0.05	29,29,29,29	0
57	MG	1a	1794	1/1	0.99	0.03	36,36,36,36	0
57	MG	2A	3560	1/1	0.99	0.06	30,30,30,30	0
57	MG	2A	3832	1/1	0.99	0.03	23,23,23,23	0
57	MG	2P	201	1/1	0.99	0.07	52,52,52,52	0
57	MG	1A	3935	1/1	0.99	0.02	4,4,4,4	0
57	MG	1A	3291	1/1	0.99	0.05	37,37,37,37	0
57	MG	1A	3273	1/1	0.99	0.05	39,39,39,39	0
57	MG	2A	3836	1/1	0.99	0.05	32,32,32,32	0
57	MG	1A	3609	1/1	0.99	0.10	15,15,15,15	0
57	MG	2a	1764	1/1	0.99	0.08	54,54,54,54	0
57	MG	1A	3013	1/1	0.99	0.08	11,11,11,11	0
57	MG	1V	202	1/1	0.99	0.13	18,18,18,18	0
57	MG	1A	3260	1/1	0.99	0.03	29,29,29,29	0
57	MG	2A	3096	1/1	0.99	0.06	30,30,30,30	0
57	MG	1A	3680	1/1	0.99	0.04	15,15,15,15	0
57	MG	2A	3329	1/1	0.99	0.11	26,26,26,26	0
57	MG	2A	3844	1/1	0.99	0.03	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1F	302	1/1	0.99	0.04	28,28,28,28	0
57	MG	2A	3846	1/1	0.99	0.04	45,45,45,45	0
57	MG	1F	303	1/1	0.99	0.15	23,23,23,23	0
57	MG	1A	3014	1/1	0.99	0.09	19,19,19,19	0
57	MG	2A	3574	1/1	0.99	0.04	36,36,36,36	0
57	MG	1A	3758	1/1	0.99	0.04	16,16,16,16	0
57	MG	1A	3262	1/1	0.99	0.05	36,36,36,36	0
57	MG	1A	3030	1/1	0.99	0.07	16,16,16,16	0
57	MG	2A	3104	1/1	0.99	0.08	22,22,22,22	0
57	MG	1A	3553	1/1	0.99	0.12	22,22,22,22	0
57	MG	1A	3179	1/1	0.99	0.02	10,10,10,10	0
57	MG	1A	4053	1/1	0.99	0.02	22,22,22,22	0
57	MG	1A	3617	1/1	0.99	0.11	31,31,31,31	0
60	ZN	1Y	204	1/1	0.99	0.03	59,59,59,59	0
57	MG	1A	3280	1/1	0.99	0.16	23,23,23,23	0
60	ZN	15	110	1/1	0.99	0.05	35,35,35,35	0
60	ZN	16	103	1/1	0.99	0.03	34,34,34,34	0
60	ZN	1n	104	1/1	0.99	0.03	48,48,48,48	0
57	MG	1A	3765	1/1	0.99	0.04	28,28,28,28	0
57	MG	1A	3809	1/1	0.99	0.05	17,17,17,17	0
60	ZN	25	106	1/1	0.99	0.04	52,52,52,52	0
60	ZN	26	501	1/1	0.99	0.03	47,47,47,47	0
60	ZN	29	102	1/1	0.99	0.04	59,59,59,59	0
57	MG	1A	3384	1/1	0.99	0.04	34,34,34,34	0
61	SF4	1d	302	8/8	0.99	0.05	43,47,53,61	0
61	SF4	2d	303	8/8	0.99	0.04	42,45,50,53	0
60	ZN	19	501	1/1	1.00	0.03	34,34,34,34	0
57	MG	1A	3036	1/1	1.00	0.07	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.