



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:18 PM UTC

PDB ID : 9MTQ / pdb_00009mtq
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with mRNA, A-site GGD-mutant Release Factor 1, and P-site fMEAAA KC-peptidyl-tRNA_{cys} at 2.55Å resolution
Authors : Aleksandrova, E.V.; Syroegin, E.A.; Basu, R.S.; Vassilevski, A.A.; Gagnon, M.G.; Polikanov, Y.S.
Deposited on : 2025-01-12
Resolution : 2.55 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

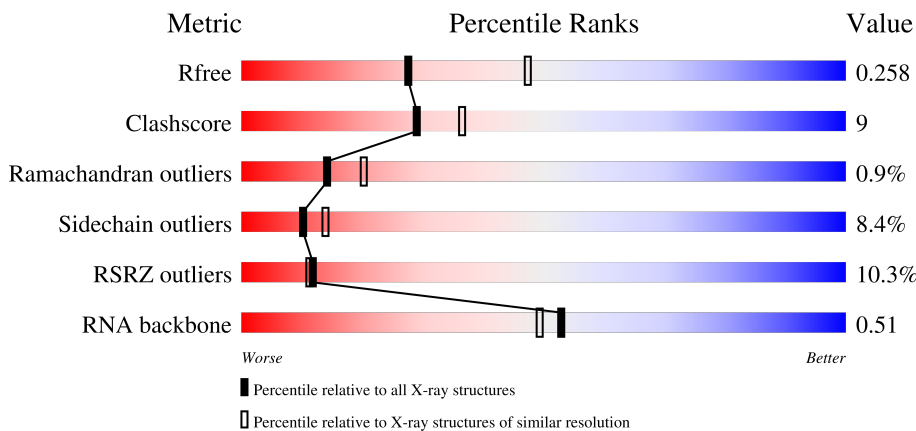
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)
RNA backbone	3983	1112 (2.80-2.28)

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	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 64%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin: 0;">5% 64% 27% 7% •</p>
1	2A	2915	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin: 0;">4% 59% 30% 6% •</p>
2	1B	121	<div style="display: flex; align-items: center;"> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 26%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin: 0;">69% 26% ••</p>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	2B	121	 2% 64% 27% 7%
3	1D	276	 % 82% 15%
3	2D	276	 % 76% 21%
4	1E	206	 2% 79% 19%
4	2E	206	 2% 82% 16%
5	1F	210	 69% 24%
5	2F	210	 2% 61% 31%
6	1G	182	 17% 63% 34%
6	2G	182	 19% 60% 32% 7%
7	1H	180	 2% 75% 21%
7	2H	180	 27% 62% 31%
8	1I	148	 10% 70% 26%
8	2I	148	 22% 61% 30% 6%
9	1N	140	 % 84% 14%
9	2N	140	 4% 74% 26%
10	1O	122	 80% 17%
10	2O	122	 78% 21%
11	1P	150	 % 79% 17%
11	2P	150	 2% 78% 20%
12	1Q	141	 4% 87% 13%
12	2Q	141	 6% 74% 24%
13	1R	118	 85% 14%
13	2R	118	 81% 18%
14	1S	112	 3% 74% 21%
14	2S	112	 12% 71% 23%



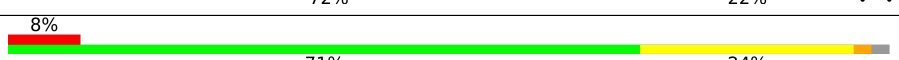
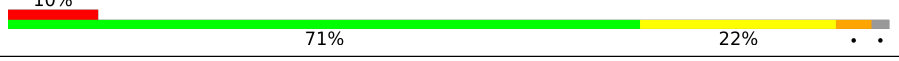
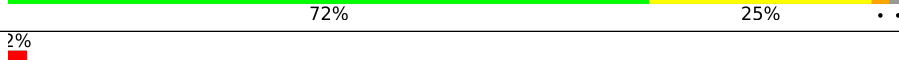
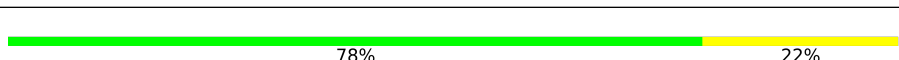
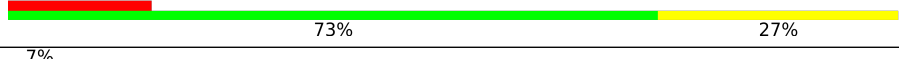




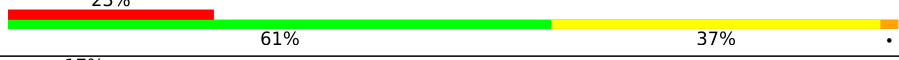
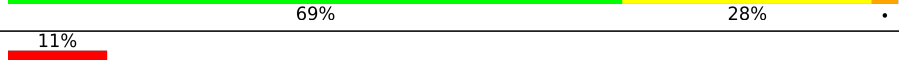

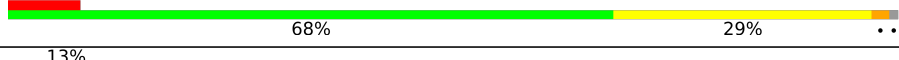
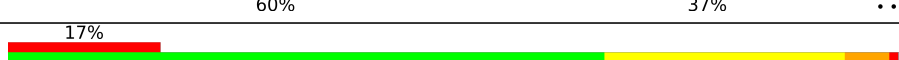





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	1T	146	% 67% 21% 10%
15	2T	146	4% 58% 30% 10%
16	1U	118	86% 12% ..
16	2U	118	% 76% 20% ..
17	1V	101	86% 13% .
17	2V	101	4% 80% 18% ..
18	1W	113	88% 9% ..
18	2W	113	3% 79% 20% .
19	1X	96	% 74% 24% ..
19	2X	96	7% 78% 20% ..
20	1Y	110	2% 73% 19% 5% .
20	2Y	110	11% 70% 23% 5% .
21	1Z	206	5% 53% 18% . 25%
21	2Z	206	14% 44% 30% . 22%
22	10	85	4% 71% 16% . 11%
22	20	85	5% 79% 11% 11%
23	11	98	3% 77% 20% ..
23	21	98	3% 78% 16% 5% .
24	12	72	3% 78% 17% . .
24	22	72	8% 64% 32% . .
25	13	60	3% 78% 17% . .
25	23	60	3% 65% 28% 5% .
26	14	71	38% 48% 37% 11% . .
26	24	71	30% 52% 37% 8% .
27	15	60	2% 83% 15% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	25	60	 3% 87% 12%
28	16	54	 80% 11% 7%
28	26	54	 2% 72% 22%
29	17	49	 8% 71% 24%
29	27	49	 10% 71% 22%
30	18	65	 72% 25%
30	28	65	 2% 78% 18%
31	19	37	 78% 22%
31	29	37	 16% 73% 27%
32	1a	1521	 7% 51% 38%
32	2a	1521	 7% 50% 39% 9%
33	1b	256	 30% 50% 32% 8% 10%
33	2b	256	 34% 51% 33% 7% 10%
34	1c	239	 28% 56% 27% 14%
34	2c	239	 35% 50% 33% 14%
35	1d	209	 23% 61% 37%
35	2d	209	 17% 69% 28%
36	1e	162	 11% 55% 31% 6% 9%
36	2e	162	 10% 48% 38% 6% 9%
37	1f	101	 8% 68% 29%
37	2f	101	 13% 60% 37%
38	1g	156	17% 67% 27% 5%
38	2g	156	26% 63% 33%
39	1h	138	12% 66% 30%
39	2h	138	9% 72% 25%


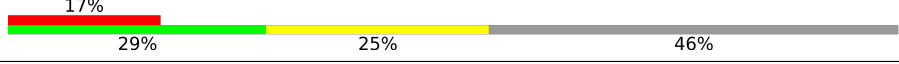
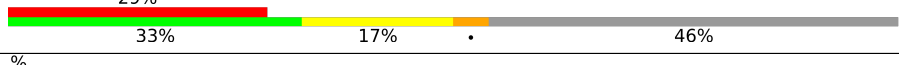
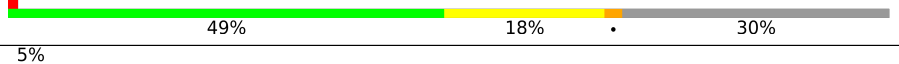

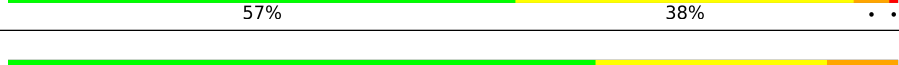
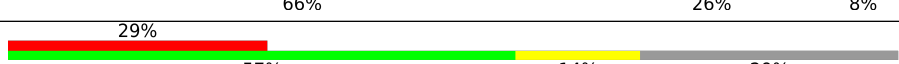
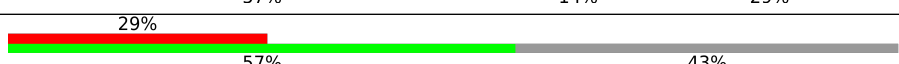

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
51	2t	106	
52	1u	27	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	354	
54	2w	354	
55	1x	74	
55	2x	74	
56	1z	7	
56	2z	7	

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	2A	3239	-	-	-	X
57	MG	2A	3259	-	-	-	X
57	MG	2A	3435	-	-	-	X
57	MG	2a	1645	-	-	-	X

2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 297259 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
			Total	C	N	O	P			
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
			Total	C	N	O	P			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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	76	Total	C	N	O	S	0	0	0
			604	373	128	102	1			
22	20	76	Total	C	N	O	S	0	0	0
			604	373	128	102	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
			Total	C	N	O	S			
42	2k	114	833	519	156	155	3	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	1m	118	919	566	190	161	2	0	0	0
44	2m	116	907	558	188	159	2	0	0	0

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

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

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

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

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

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

- 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 CYS-Stop 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 protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	249	Total	C	N	O	S	0	0	0
			1937	1197	359	372	9			
54	2w	253	Total	C	N	O	S	0	0	0
			1955	1208	360	378	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1w	230	ASP	GLN	engineered mutation	UNP P96077
2w	230	ASP	GLN	engineered mutation	UNP P96077

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA fMEAAAKC-tRNA_{cys} RNA-part.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	74	Total	C	N	O	P	S	0	0	0
			1577	704	281	517	74	1			
55	2x	74	Total	C	N	O	P	S	0	0	0
			1577	704	281	517	74	1			

- Molecule 56 is a protein called P-site Peptidyl-tRNA fMEAAAKC-tRNA_{cys} Peptide-part.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1z	5	Total	C	N	O	S	0	0	0
			30	18	6	5	1			
56	2z	4	Total	C	N	O	S	0	0	0
			25	15	5	4	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1088	Total	Mg	0	0
			1088	1088		
57	1B	36	Total	Mg	0	0
			36	36		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1D	13	Total Mg 13 13	0	0
57	1E	15	Total Mg 15 15	0	0
57	1F	15	Total Mg 15 15	0	0
57	1G	4	Total Mg 4 4	0	0
57	1I	1	Total Mg 1 1	0	0
57	1N	6	Total Mg 6 6	0	0
57	1O	4	Total Mg 4 4	0	0
57	1P	4	Total Mg 4 4	0	0
57	1Q	8	Total Mg 8 8	0	0
57	1R	5	Total Mg 5 5	0	0
57	1S	3	Total Mg 3 3	0	0
57	1T	2	Total Mg 2 2	0	0
57	1U	10	Total Mg 10 10	0	0
57	1V	6	Total Mg 6 6	0	0
57	1W	6	Total Mg 6 6	0	0
57	1X	5	Total Mg 5 5	0	0
57	1Y	4	Total Mg 4 4	0	0
57	1Z	2	Total Mg 2 2	0	0
57	10	8	Total Mg 8 8	0	0
57	11	4	Total Mg 4 4	0	0
57	12	2	Total Mg 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	13	4	Total Mg 4 4	0	0
57	15	8	Total Mg 8 8	0	0
57	16	1	Total Mg 1 1	0	0
57	17	6	Total Mg 6 6	0	0
57	18	4	Total Mg 4 4	0	0
57	19	1	Total Mg 1 1	0	0
57	1a	223	Total Mg 223 223	0	0
57	1b	1	Total Mg 1 1	0	0
57	1d	1	Total Mg 1 1	0	0
57	1e	3	Total Mg 3 3	0	0
57	1f	1	Total Mg 1 1	0	0
57	1l	2	Total Mg 2 2	0	0
57	1m	1	Total Mg 1 1	0	0
57	1n	1	Total Mg 1 1	0	0
57	1p	1	Total Mg 1 1	0	0
57	1r	1	Total Mg 1 1	0	0
57	1t	1	Total Mg 1 1	0	0
57	1v	1	Total Mg 1 1	0	0
57	1w	2	Total Mg 2 2	0	0
57	1x	13	Total Mg 13 13	0	0
57	2A	853	Total Mg 853 853	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2B	22	Total Mg 22 22	0	0
57	2D	9	Total Mg 9 9	0	0
57	2E	9	Total Mg 9 9	0	0
57	2F	9	Total Mg 9 9	0	0
57	2G	1	Total Mg 1 1	0	0
57	2N	1	Total Mg 1 1	0	0
57	2O	2	Total Mg 2 2	0	0
57	2P	1	Total Mg 1 1	0	0
57	2Q	4	Total Mg 4 4	0	0
57	2R	2	Total Mg 2 2	0	0
57	2T	3	Total Mg 3 3	0	0
57	2U	2	Total Mg 2 2	0	0
57	2V	2	Total Mg 2 2	0	0
57	2W	2	Total Mg 2 2	0	0
57	2X	2	Total Mg 2 2	0	0
57	2Z	1	Total Mg 1 1	0	0
57	20	2	Total Mg 2 2	0	0
57	21	1	Total Mg 1 1	0	0
57	23	3	Total Mg 3 3	0	0
57	25	7	Total Mg 7 7	0	0
57	26	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	27	2	Total Mg 2 2	0	0
57	28	4	Total Mg 4 4	0	0
57	29	1	Total Mg 1 1	0	0
57	2a	176	Total Mg 176 176	0	0
57	2d	2	Total Mg 2 2	0	0
57	2e	1	Total Mg 1 1	0	0
57	2f	3	Total Mg 3 3	0	0
57	2g	1	Total Mg 1 1	0	0
57	2i	1	Total Mg 1 1	0	0
57	2j	1	Total Mg 1 1	0	0
57	2k	1	Total Mg 1 1	0	0
57	2l	2	Total Mg 2 2	0	0
57	2q	3	Total Mg 3 3	0	0
57	2t	1	Total Mg 1 1	0	0
57	2v	2	Total Mg 2 2	0	0
57	2w	1	Total Mg 1 1	0	0
57	2x	10	Total Mg 10 10	0	0

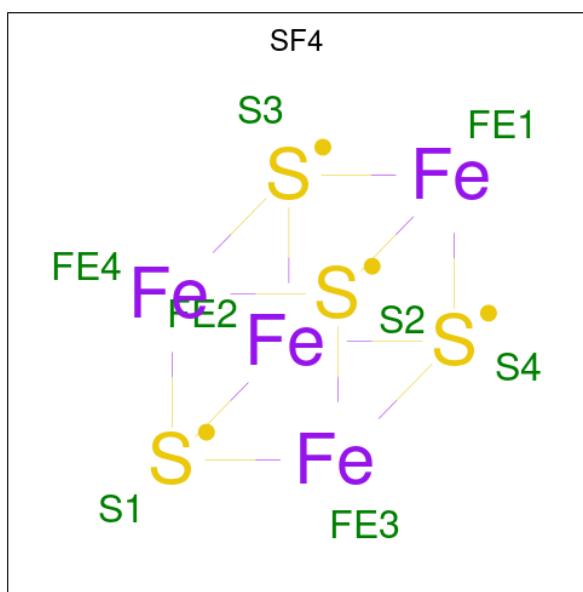
- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1Y	1	Total Zn 1 1	0	0
59	14	1	Total Zn 1 1	0	0
59	15	1	Total Zn 1 1	0	0
59	16	1	Total Zn 1 1	0	0
59	19	1	Total Zn 1 1	0	0
59	1n	1	Total Zn 1 1	0	0
59	2Y	1	Total Zn 1 1	0	0
59	24	1	Total Zn 1 1	0	0
59	25	1	Total Zn 1 1	0	0
59	26	1	Total Zn 1 1	0	0
59	29	1	Total Zn 1 1	0	0
59	2n	1	Total Zn 1 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	1d	1	Total	Fe	S	0	0
			8	4	4		
60	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2032	Total	O	0	0
			2032	2032		
61	1B	62	Total	O	0	0
			62	62		
61	1D	24	Total	O	0	0
			24	24		
61	1E	31	Total	O	0	0
			31	31		
61	1F	15	Total	O	0	0
			15	15		
61	1G	7	Total	O	0	0
			7	7		
61	1H	2	Total	O	0	0
			2	2		
61	1I	1	Total	O	0	0
			1	1		
61	1N	5	Total	O	0	0
			5	5		
61	1O	7	Total	O	0	0
			7	7		
61	1P	20	Total	O	0	0
			20	20		
61	1Q	7	Total	O	0	0
			7	7		
61	1R	15	Total	O	0	0
			15	15		
61	1S	4	Total	O	0	0
			4	4		
61	1T	9	Total	O	0	0
			9	9		
61	1U	13	Total	O	0	0
			13	13		
61	1V	9	Total	O	0	0
			9	9		
61	1W	11	Total	O	0	0
			11	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1X	4	Total 4	O 4	0	0
61	1Y	2	Total 2	O 2	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	9	Total 9	O 9	0	0
61	11	10	Total 10	O 10	0	0
61	12	3	Total 3	O 3	0	0
61	13	4	Total 4	O 4	0	0
61	15	5	Total 5	O 5	0	0
61	16	1	Total 1	O 1	0	0
61	17	6	Total 6	O 6	0	0
61	18	10	Total 10	O 10	0	0
61	1a	289	Total 289	O 289	0	0
61	1d	1	Total 1	O 1	0	0
61	1j	1	Total 1	O 1	0	0
61	1l	4	Total 4	O 4	0	0
61	1q	2	Total 2	O 2	0	0
61	1v	5	Total 5	O 5	0	0
61	1w	5	Total 5	O 5	0	0
61	1x	24	Total 24	O 24	0	0
61	2A	1200	Total 1200	O 1200	0	0
61	2B	20	Total 20	O 20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2D	23	Total 23	O 23	0	0
61	2E	12	Total 12	O 12	0	0
61	2F	15	Total 15	O 15	0	0
61	2I	2	Total 2	O 2	0	0
61	2O	3	Total 3	O 3	0	0
61	2P	14	Total 14	O 14	0	0
61	2Q	1	Total 1	O 1	0	0
61	2R	3	Total 3	O 3	0	0
61	2T	4	Total 4	O 4	0	0
61	2U	3	Total 3	O 3	0	0
61	2W	2	Total 2	O 2	0	0
61	2X	3	Total 3	O 3	0	0
61	2Z	1	Total 1	O 1	0	0
61	20	2	Total 2	O 2	0	0
61	21	7	Total 7	O 7	0	0
61	22	1	Total 1	O 1	0	0
61	23	2	Total 2	O 2	0	0
61	25	1	Total 1	O 1	0	0
61	27	3	Total 3	O 3	0	0
61	28	2	Total 2	O 2	0	0
61	29	1	Total 1	O 1	0	0

Continued on next page...

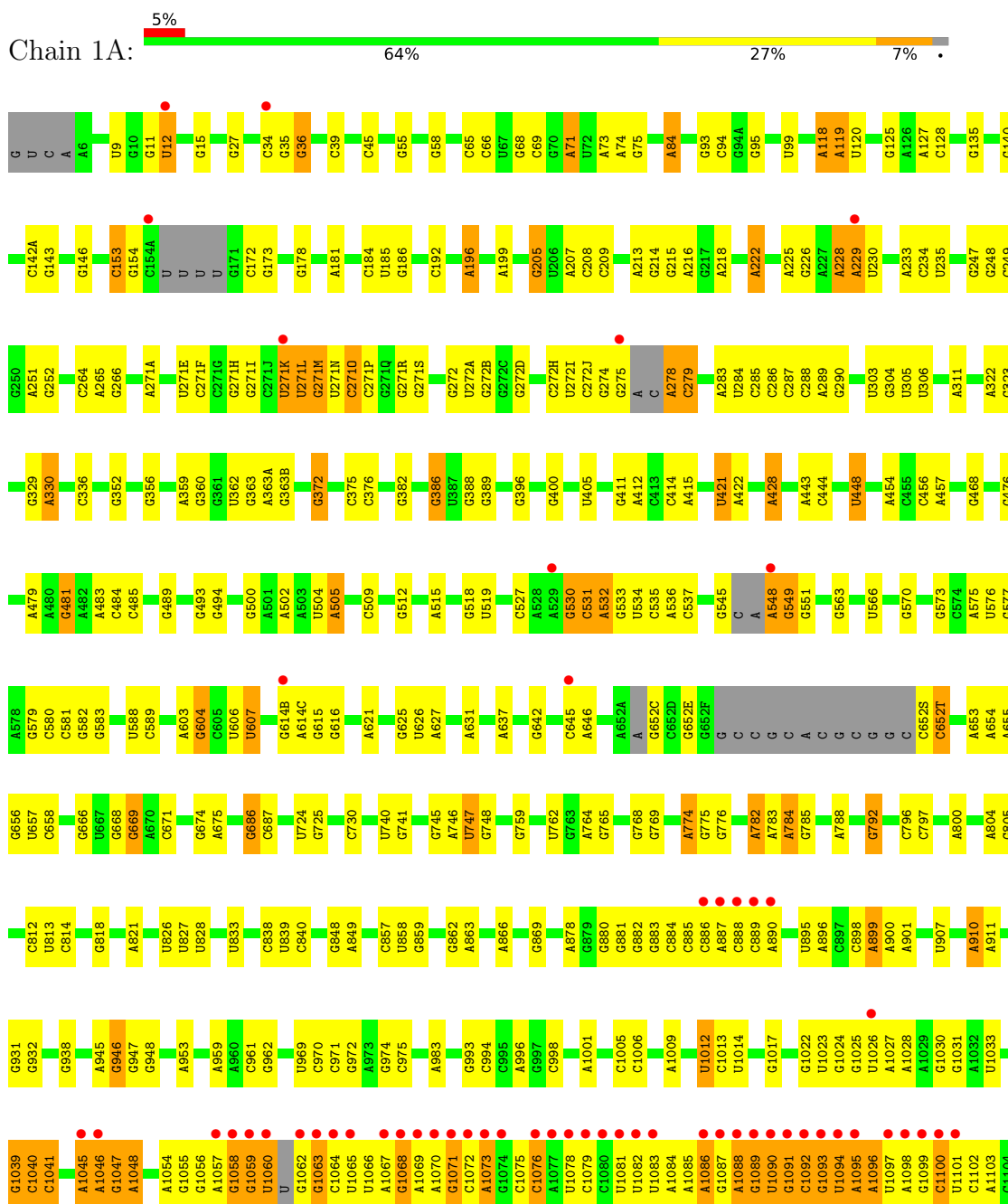
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2a	152	Total 152	O 152	0	0
61	2e	2	Total 2	O 2	0	0
61	2j	1	Total 1	O 1	0	0
61	2l	5	Total 5	O 5	0	0
61	2o	1	Total 1	O 1	0	0
61	2q	2	Total 2	O 2	0	0
61	2t	1	Total 1	O 1	0	0
61	2v	1	Total 1	O 1	0	0
61	2w	3	Total 3	O 3	0	0
61	2x	28	Total 28	O 28	0	0
61	2z	1	Total 1	O 1	0	0

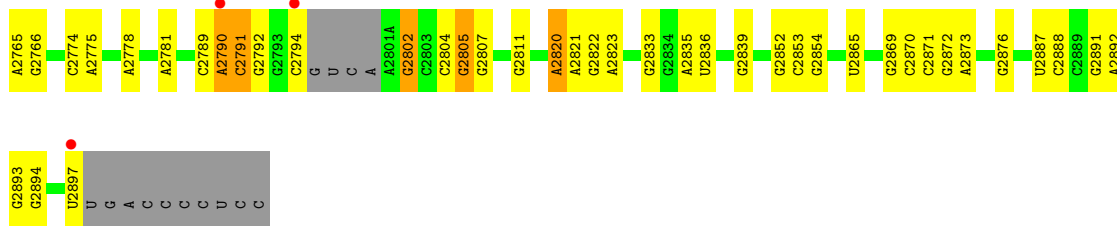
3 Residue-property plots i

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.

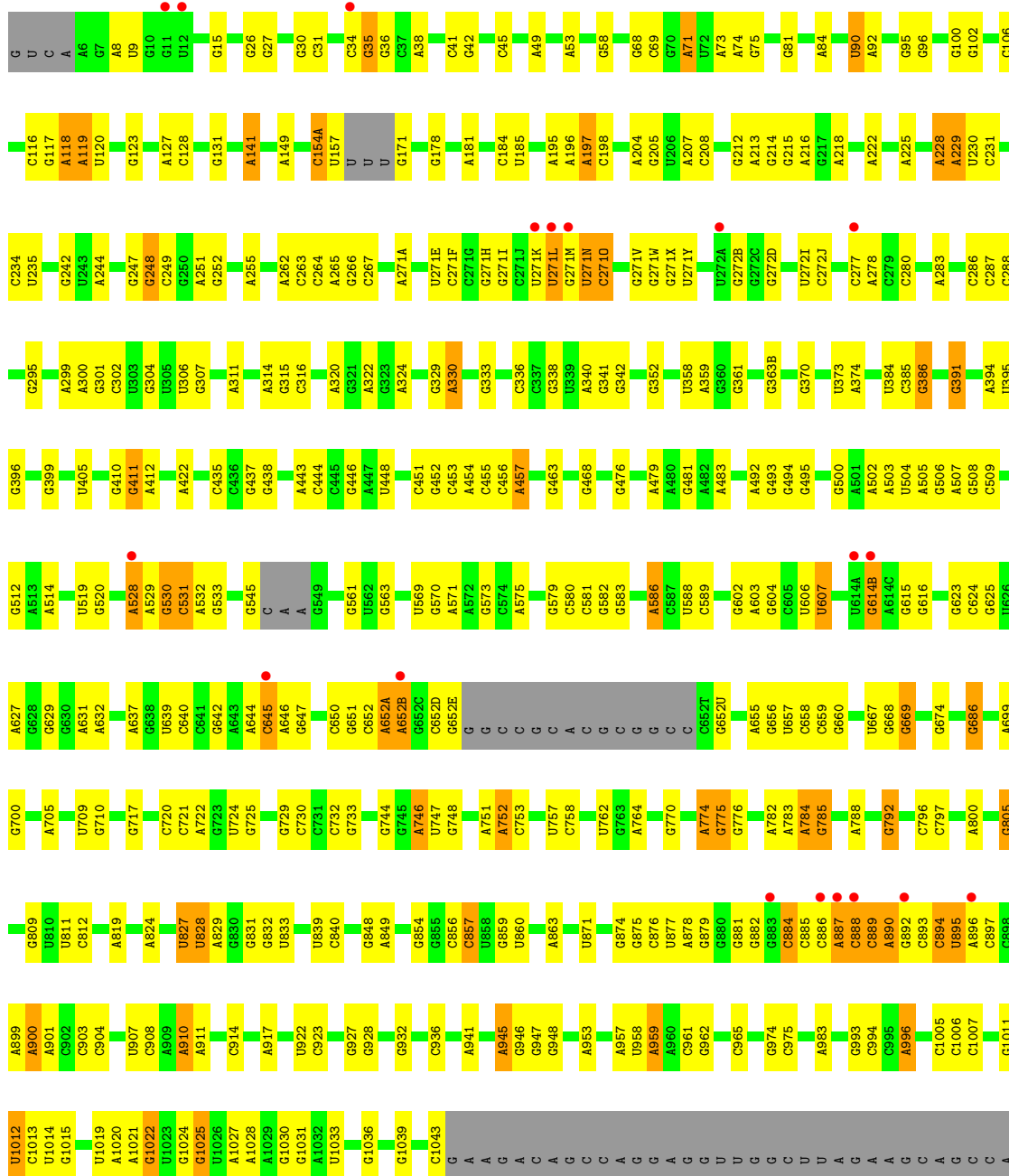
- Molecule 1: 23S Ribosomal RNA

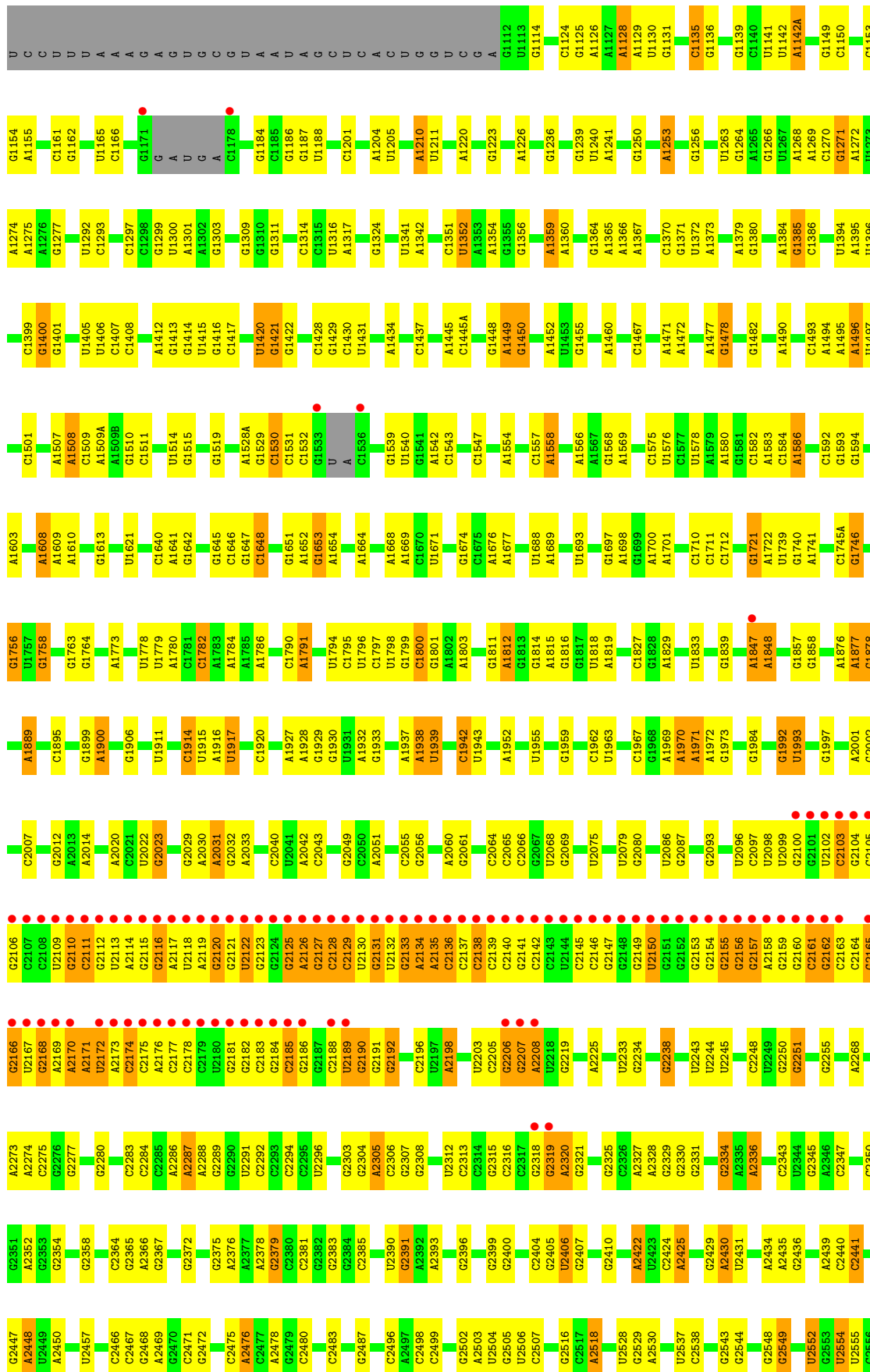


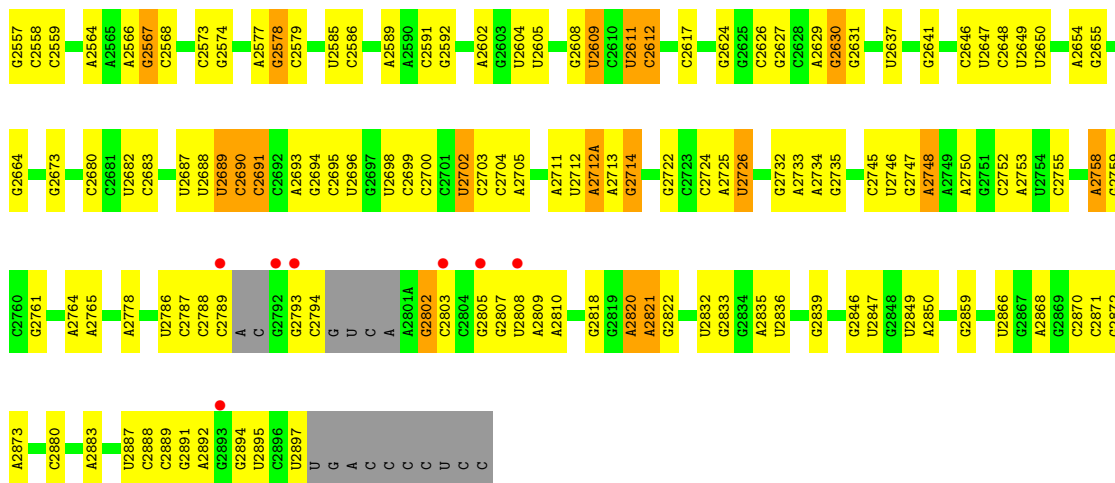
U1105	A1241	G1364	G1470	C1607	U1778	A1889	U2028	A2136	G2186	C2306	U2422	C2538	U2649
G1106	A1241	A1365	G1478	A1608	U1779	G1899	G2030	G2127	G2187	G2307	U2423	C2539	A2654
G1107	A1253	A1365	G1478	A1609	A1780	C1928	A2030	C2129	C2188	G2308	C2424	A2541	A2654
U1108	A1253	A1365	G1482	A1610	C1781	A1900	A2031	C2130	U2189	A2309	C2425	A2542	C2658
G1109	G1266	G1370	G1482	U1629	A1782	A1901	G2032	G2131	G2190	A2426	C2426	G2543	C2659
C1110	G1266	G1371	C1493	U1636	A1783	C1902	A2033	U2132	G2191	G2427	C2428	G2544	G2663
A1111	G1280	U1372	A1494	A1637	A1784	G1903	A2033	G2133	G2192	G2428	G2429	C2550	G2663
U1112	G1280	A1373	A1495	A1637	A1785	G1906	G2038	A2134	G2193	G2319	G2429	C2551	C2663
U1113	A1265	A1379	U1503	A1641	A1791	U1911	C2043	A2135	A2198	A2320	U2430	U2552	G2673
G1114	A1265	G1380	C1504	G1642	U1794	C1914	U1916	C2136	U2015	G2325	A2435	U2553	C2678
G1115	U1267	U1267	C1504	G1643	C1795	U1915	C2055	C2137	C2203	A2327	A2436	U2554	A2679
G1116	U1268	U1268	C1504	G1644	C1796	U1916	G2056	C2138	G2206	A2328	A2437	U2555	C2683
G1125	A1289	U1385	A1508	G1644	C1797	U1917	A2059	C2139	G2207	A2329	A2438	U2556	U2687
A1128	C1270	U1393	C1509	G1647	U1798	U1918	A2060	C2140	G2208	A2330	C2440	U2557	U2688
A1129	C1271	A1393	A1509A	G1648	C1799	U1919	A2061	C2141	G2209	G2330	C2441	U2558	U2689
U1135	U1273	U1396	A1509B	C1648	G1799	A1919	G2062	C2142	G2210	G2331	G2442	U2559	C2690
G1136	A1274	U1399	U1518	A1654	C1800	C1920	A2062	U2144	G2211	G2332	A2448	C2567	U2699
A1142A	U1288	C1403	G1519	A1668	A1801	G1921	G2067	C2145	G2212	G2333	G2454	C2568	A2693
A1143	U1292	C1404	G1520	A1669	A1802	G1929	U2068	G2147	U2233	A2336	C2467	C2573	G2694
G1144	C1293	U1405	G1525	A1670	A1803	G1930	G2069	G2148	G2234	A2337	G2468	C2574	U2702
C1152	C1297	U1406	G1532	U1673	U1805	U1931	U2079	G2149	G2238	A2345	A2469	U2578	C2703
C1153	C1298	C1407	G	G1674	A1810	G1932	U2079	C2150	G2239	A2346	G2470	C2579	A2705
G1154	C1299	C1407	U	G1674	G1811	G1933	U2086	C2151	U2243	A2347	C2471	C2580	U2712
A1155	U1300	A1412	A	C1683	G1812	A1938	G2087	G2152	U2244	A2348	G2472	C2581	A2713
G1161	A1301	G1413	C	C1684	G1813	U1939	G2088	C2153	U2244	A2349	C2473	C2582	G2714
G1164	A1302	U1406	G1637	U1688	G1814	U1942	G2093	G2154	G2251	A2354	A2476	C2583	G2722
U1165	G1303	C1417	A1542	U1693	G1815	C1942	U2096	G2155	G2255	A2355	C2477	C2584	C2723
U1166	G1309	U1420	C1543	U1693	G1816	U1955	U2096	G2156	G2255	A2356	A2478	C2585	U2726
U1167	G1310	G1421	C1547	G1696	U1818	C1958	G2099	G2157	G2255	A2357	C2483	C2586	G2732
G1171	G1311	U1424	C1548	G1696	G1822	C1962	G2100	G2158	G2255	A2358	C2484	C2587	A2733
G1173	U1312	G1424	C1557	A1700	C1827	U1963	G2101	G2159	G2255	A2359	A2268	C2588	A2740
A1174	U1313	G1425	A1558	A1701	G1828	U1963	G2102	G2160	G2255	A2360	A2268	C2589	A2741
U1175	C1314	G1426	A1558	A1702	G1829	U1963	C2103	G2161	G2255	A2361	A2268	C2590	G2742
G1176	C1315	A1427	A1558	G1702	A1829	C1967	C2104	C2162	G2271	A2362	A2274	C2591	C2743
A1177	U1321	G1428	A1566	G1703	U1833	C1967	G2105	G2163	U2272	A2363	A2274	C2592	G2743
G1178	A1321	U1429	A1566	G1703	U1833	C1967	G2106	G2164	U2272	A2364	A2274	C2593	G2743
C1179	G1332	C1430	A1569	G1740	A1847	U1971	C2108	G2165	G2277	A2365	A2274	C2594	G2743
C1180	G1332	C1430	A1569	G1740	A1847	U1971	U2109	G2166	G2277	A2366	A2274	C2595	G2743
G1187	U1335	U1442	U1578	C1745A	U1851	A1972	G2110	G2167	G2283	A2367	A2274	C2596	G2743
U1188	A1336	A1445	A1579	G1746	C1852	U1992	G2111	G2168	G2283	A2368	A2274	C2597	G2743
C1201	G1337	G1447	G1581	G1756	G1858	U1993	U2113	G2169	G2283	A2369	A2274	C2598	G2743
A1210	U1338	A1448	A1586	U1757	A1859	C1996	G2115	G2170	G2283	A2370	A2274	C2599	G2743
U1211	A1342	A1449	A1586	G1758	U1864	G1997	G2116	G2171	G2283	A2371	A2274	C2600	G2743
G1212	U1352	G1450	C1588	G1758	G1865	U1997	G2117	G2172	G2283	A2372	A2274	C2601	G2743
A1220	A1353	U1453	C1588	G1758	G1866	A2014	U2118	U2172	G2283	A2373	A2274	C2602	G2743
G1223	A1354	G1455	C1589	G1762	A1876	A2014	G2120	A2173	G2283	A2374	A2274	C2603	G2743
A1226	G1355	G1461	G1593	G1769	A1877	A2019	G2121	G2174	G2283	A2375	A2274	C2604	G2743
	U1359	C1467	G1594	G1773	A1883	A2020	U2122	G2175	G2283	A2376	A2274	C2605	G2743
	A1360	C1467	U1602	A1773	G2023	A2021	G2123	G2176	G2283	A2377	A2274	C2606	G2743
						A2022	G2124	G2177	G2283	A2378	A2274	C2607	G2743
						U2022	G2125	G2178	G2283	A2379	A2274	C2608	G2743
						G2023	G2125	G2179	G2283	A2380	A2274	C2609	G2743
							G2126	G2180	G2283	A2381	A2274	C2610	G2743
							G2127	G2181	G2283	A2382	A2274	C2611	G2743
							G2128	G2182	G2283	A2383	A2274	C2612	G2743
							G2129	G2183	G2283	A2384	A2274	C2613	G2743
							G2130	G2184	G2283	A2385	A2274	C2614	G2743
							G2131	G2185	G2283	A2386	A2274	C2615	G2743
							G2132	G2186	G2283	A2387	A2274	C2616	G2743
							G2133	G2187	G2283	A2388	A2274	C2617	G2743
							G2134	G2188	G2283	A2389	A2274	C2618	G2743
							G2135	G2189	G2283	A2390	A2274	C2619	G2743
							G2136	G2190	G2283	A2391	A2274	C2620	G2743
							G2137	G2191	G2283	A2392	A2274	C2621	G2743
							G2138	G2192	G2283	A2393	A2274	C2622	G2743
							G2139	G2193	G2283	A2394	A2274	C2623	G2743
							G2140	G2194	G2283	A2395	A2274	C2624	G2743
							G2141	G2195	G2283	A2396	A2274	C2625	G2743
							G2142	G2196	G2283	A2397	A2274	C2626	G2743
							G2143	G2197	G2283	A2398	A2274	C2627	G2743
							G2144	G2198	G2283	A2399	A2274	C2628	G2743
							G2145	G2199	G2283	A2400	A2274	C2629	G2743
							G2146	G2200	G2283	A2401	A2274	C2630	G2743
							G2147	G2201	G2283	A2402	A2274	C2631	G2743
							G2148	G2202	G2283	A2403	A2274	C2632	G2743
							G2149	G2203	G2283	A2404	A2274	C2633	G2743
							G2150	G2204	G2283	A2405	A2274	C2634	G2743
							G2151	G2205	G2283	A2406	A2274	C2635	G2743
							G2152	G2206	G2283	A2407	A2274	C2636	G2743
							G2153	G2207	G2283	A2408	A2274	C2637	G2743
							G2154	G2208	G2283	A2409	A2274	C2638	G2743
							G2155	G2209	G2283	A2410	A2274	C2639	G2743
							G2156	G2210	G2283	A2411	A2274	C2640	G2743
							G2157	G2211	G2283	A2412	A2274	C2641	G2743
							G2158	G2212	G2283	A2413	A2274	C2642	G2743
							G2159	G2213	G2283	A2414	A2274	C2643	G2743
							G2160	G2214	G2283	A2415	A2274	C2644	G2743
							G2161	G2215	G2283	A2416	A2274	C2645	G2743
							G2162	G2216	G2283	A2417	A2274	C2646	G2743
							G2163	G2217	G2283	A2418	A2274	C2647	G2743
							G2164	G2218	G2283	A2419	A2274	C2648	G2743
							G2165	G2219	G2283	A2420	A2274	C2649	G2743
							G2166	G2220	G2283	A2421	A2274	C2650	G2743
							G2167	G2221	G2283	A2422	A2274	C2651	G2743
							G2168	G2222	G2283	A2423	A2274	C2652	G2743
							G2169	G2223	G2283	A2424	A2274	C2653	G2743
							G2170	G2224	G2283	A2425	A2274	C2654	G2743
							G2171	G2225	G2283	A2426	A2274	C2655	G2743
							G2172	G2226	G2283	A2427	A2274	C2656	G2743
							G2173	G2227	G2283	A2428	A2274	C2657	G2743
							G2174	G2228	G2283	A2429	A2274	C2658	G2743
							G2175	G2229	G2283	A2430	A2274	C2659	G2743
							G2176	G2230	G2283	A2431	A2274	C2660	G2743
							G2177	G2231	G2283	A2432	A2274	C2661	G2743
							G2178	G2232	G2283	A2433	A2274	C2662	G2743
							G2179	G2233	G2283	A2434	A2274	C2663	G2743
							G2180	G2234	G2283	A2435	A2274	C2664	G2743
							G2181	G2235	G2283	A2436	A2274	C2665	G2743
							G2						



• Molecule 1: 23S Ribosomal RNA

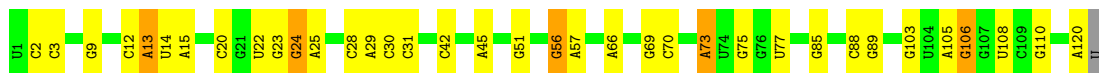






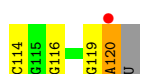
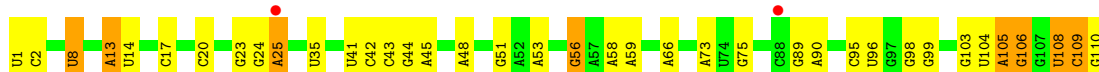
• Molecule 2: 5S Ribosomal RNA

Chain 1B:



• Molecule 2: 5S Ribosomal RNA

Chain 2B:



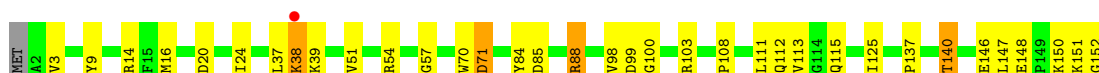
• Molecule 3: 50S ribosomal protein L2

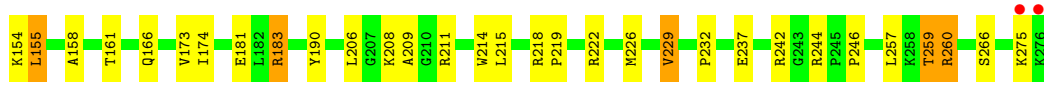
Chain 1D:



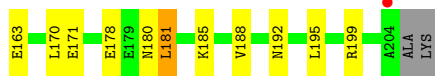
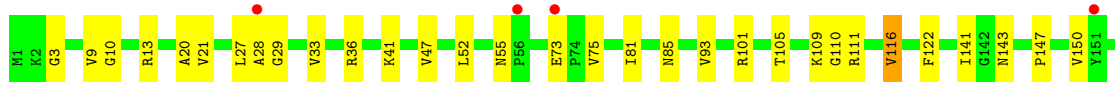
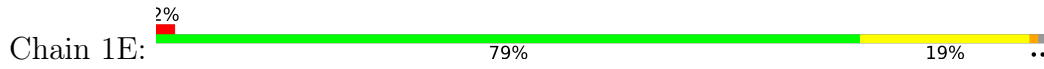
• Molecule 3: 50S ribosomal protein L2

Chain 2D:

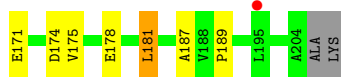
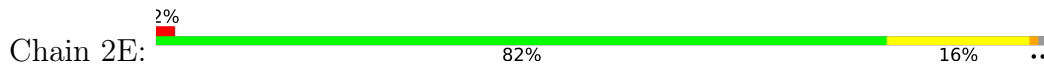




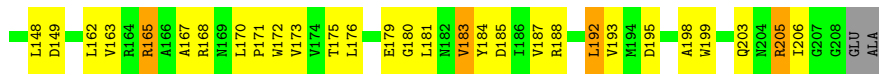
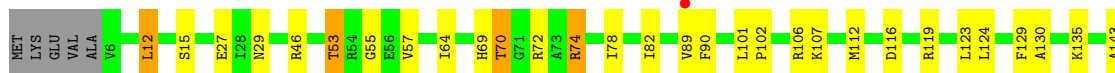
• Molecule 4: 50S ribosomal protein L3



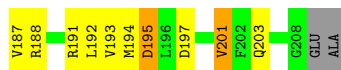
• Molecule 4: 50S ribosomal protein L3



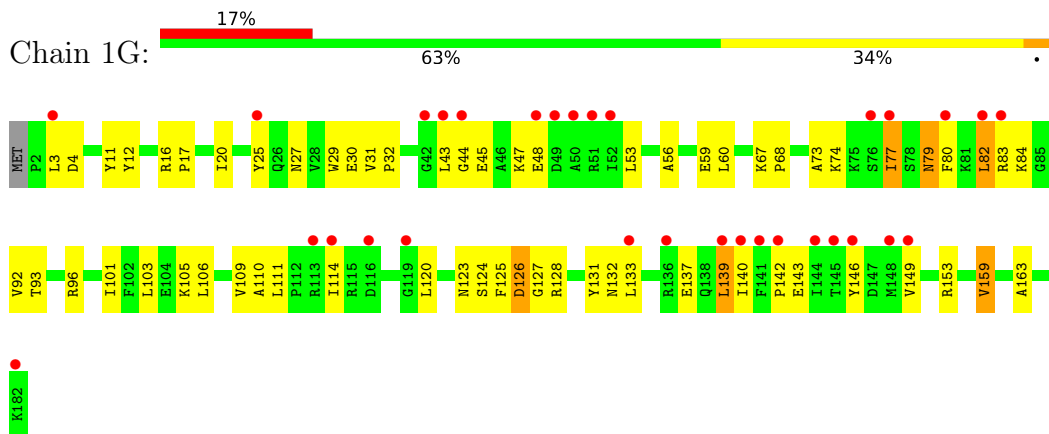
• Molecule 5: 50S ribosomal protein L4



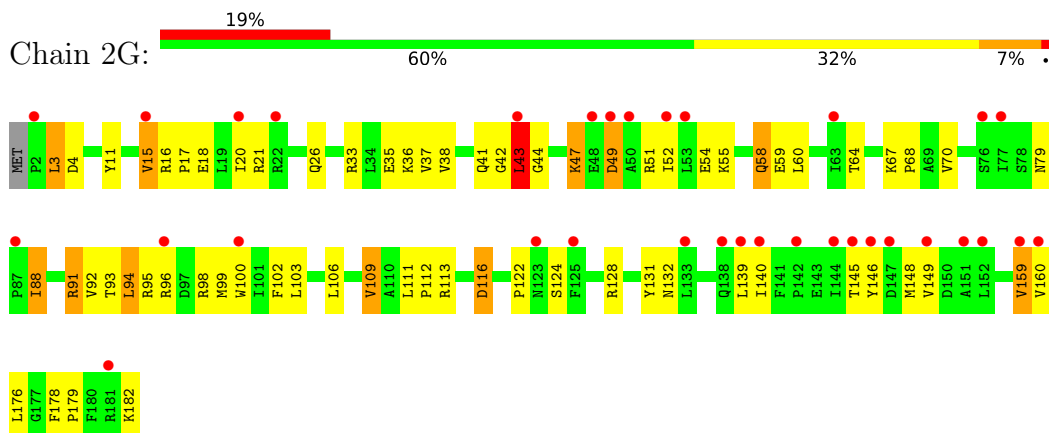
• Molecule 5: 50S ribosomal protein L4



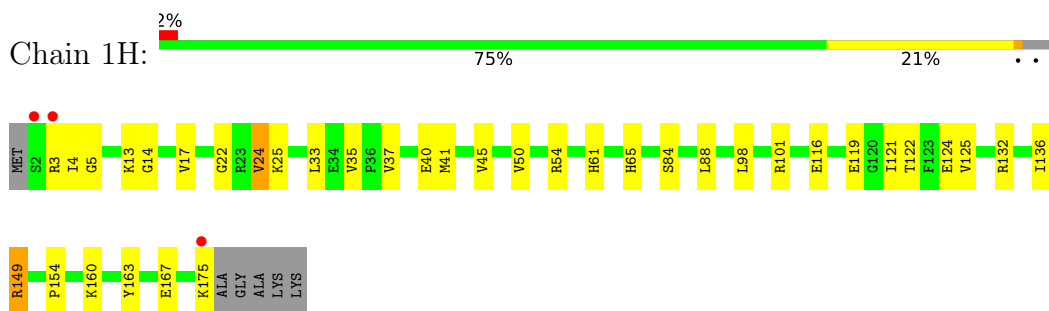
- Molecule 6: 50S ribosomal protein L5



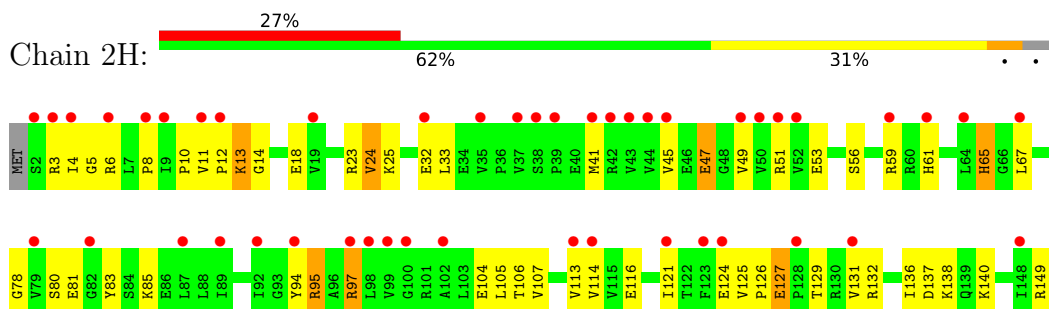
- Molecule 6: 50S ribosomal protein L5

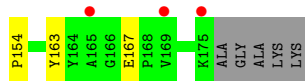


- Molecule 7: 50S ribosomal protein L6

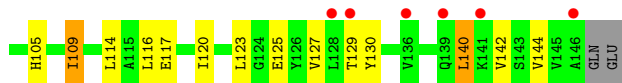


- Molecule 7: 50S ribosomal protein L6

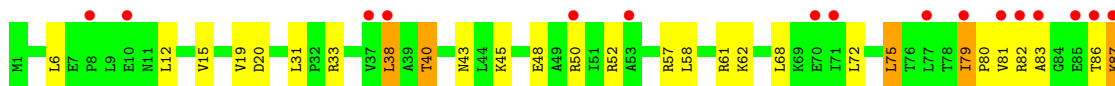




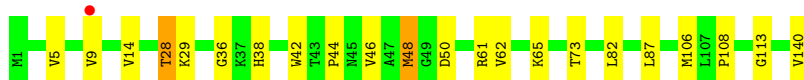
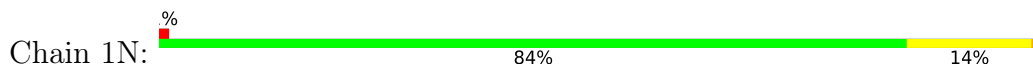
• Molecule 8: 50S ribosomal protein L9



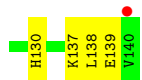
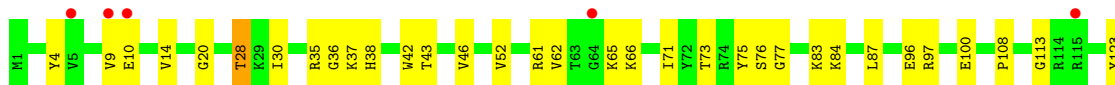
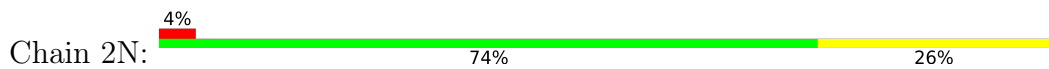
• Molecule 8: 50S ribosomal protein L9



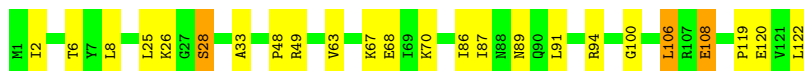
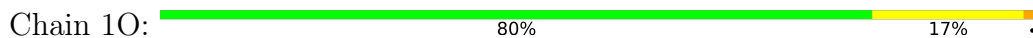
• Molecule 9: 50S ribosomal protein L13




• Molecule 9: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L14




- Molecule 10: 50S ribosomal protein L14

Chain 2O:  78% 21%




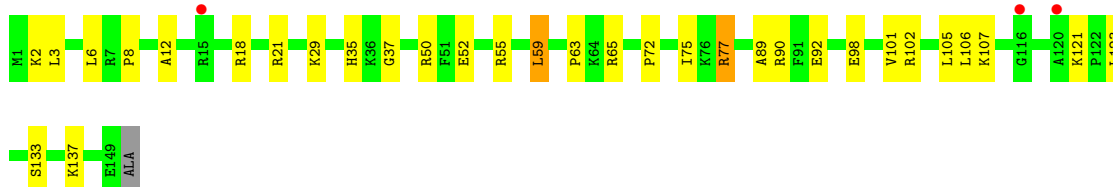
- Molecule 11: 50S ribosomal protein L15

Chain 1P:  79% 17%




- Molecule 11: 50S ribosomal protein L15

Chain 2P:  78% 20%




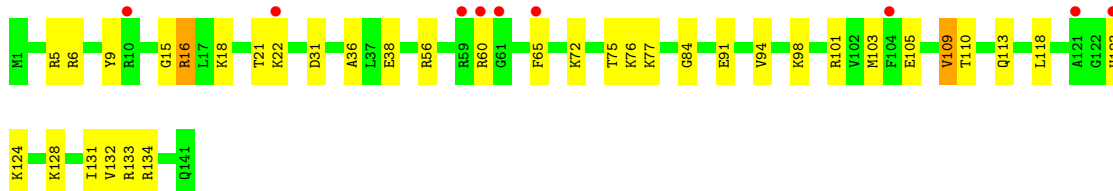
- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  87% 13%




- Molecule 12: 50S ribosomal protein L16

Chain 2Q:  74% 24%




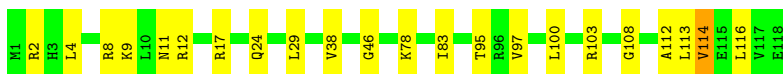
- Molecule 13: 50S ribosomal protein L17

Chain 1R:  85% 14%




- Molecule 13: 50S ribosomal protein L17

Chain 2R:  81% 18%



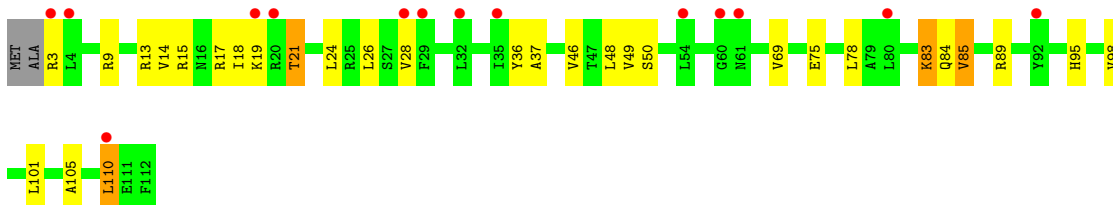
- Molecule 14: 50S ribosomal protein L18

Chain 1S:  3% 74% 21%



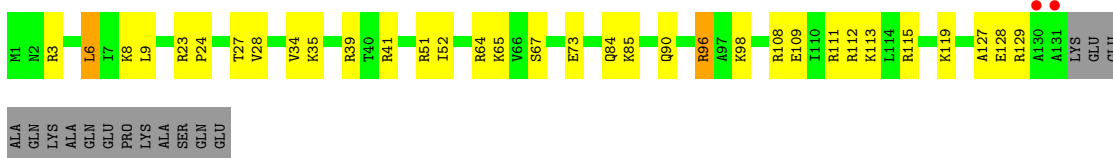
- Molecule 14: 50S ribosomal protein L18

Chain 2S:  12% 71% 23%



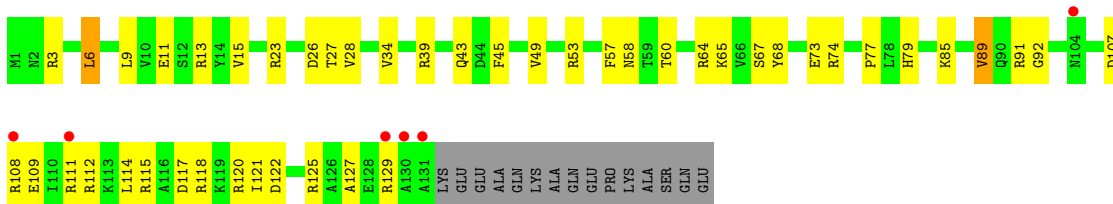
- Molecule 15: 50S ribosomal protein L19

Chain 1T:  67% 21% 10%




- Molecule 15: 50S ribosomal protein L19

Chain 2T:  4% 58% 30% 10%

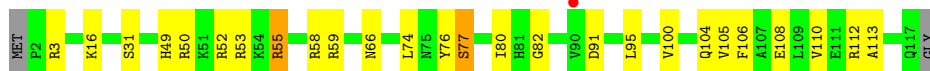
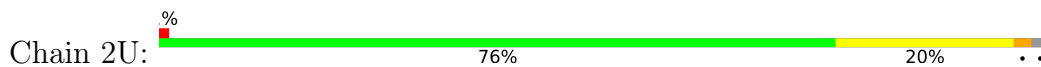


- Molecule 16: 50S ribosomal protein L20

Chain 1U:  86% 12%



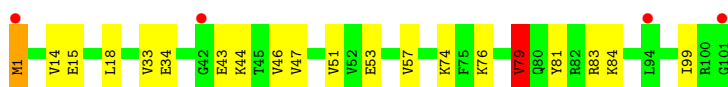
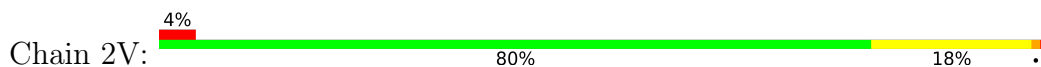
- Molecule 16: 50S ribosomal protein L20



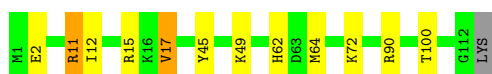
- Molecule 17: 50S ribosomal protein L21



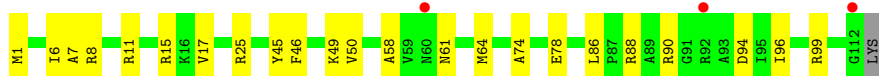
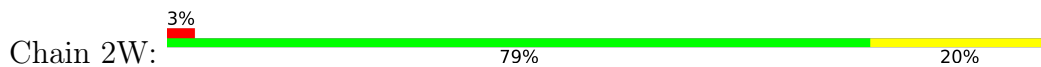
- Molecule 17: 50S ribosomal protein L21



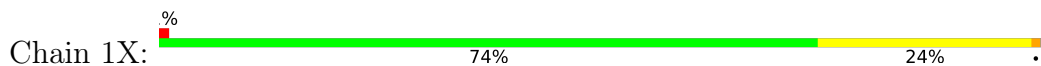
- Molecule 18: 50S ribosomal protein L22



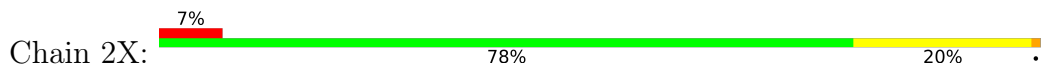
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23

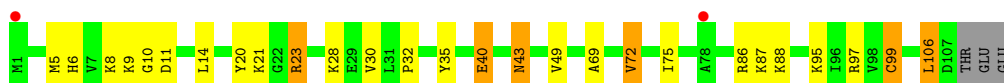
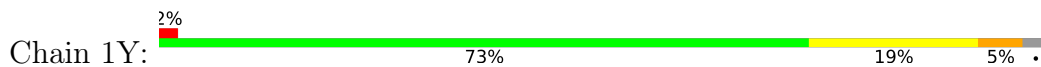


- Molecule 19: 50S ribosomal protein L23





- Molecule 20: 50S ribosomal protein L24

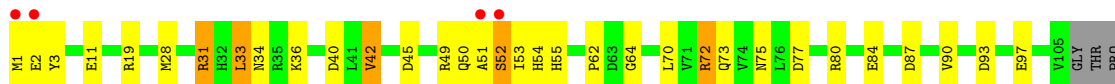


- Molecule 20: 50S ribosomal protein L24



THR
GLU
GLU

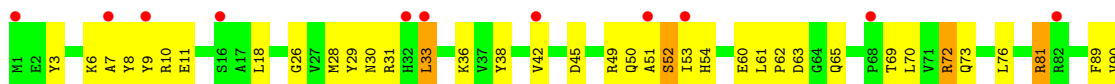
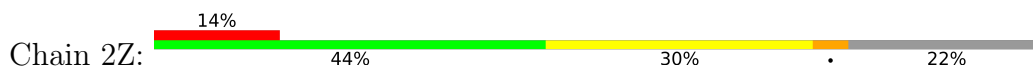
- Molecule 21: 50S ribosomal protein L25



ALA
GLY
VAL
VAL
ARG
ALA
GLY
GLY
VAL
LEU
GLN
E119
I120
H121
V126
R131
F136
D140
V141
SER
GLY
LEU
GLU
I146
D148
A152
L155
K156
L157
P158
P159
G160
V161
I171
ALA
VAL
VAL
PRO
PRO
GLU
ASP
VAL
GLU
LYS
LEU
ALA
GLU
ALA
ALA
GLU

VAL
ALA
GLU
PRO
VAL
VAL
ILE
LYS
LYS
LYS
LYS
GLU
GLU
GLU
GLU
GLU

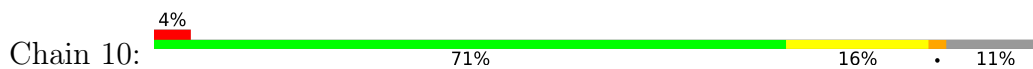
- Molecule 21: 50S ribosomal protein L25



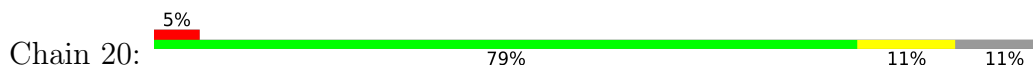
L91
S92
D93
E94
E97
M98
Y99
V100
P101
V105
G106
THR
PRO
ALA
VAL
VAL
ARG
ALA
VAL
GLY
GLY
VAL
LEU
GLN
GLU
ILE
H121
R122
D123
I124
L125
V126
K127
V128
S129
P130
R131
M132
I133
P134
E135
F136
S142
G143
L144
E145
I146
G147
D148
S149
L150
H151
A152
S153
D154
L155
K156
L157

P158
V161
L163
A164
V165
S166
P167
E168
E169
T170
A173
V174
VAL
PRO
PRO
GLU
ASP
VAL
GLY
GLY
VAL
LEU
ALA
GLU
GLU
ALA
ALA
ALA
VAL
ALA
GLU
PRO
GLU
VAL
VAL
GLY
LYS
LYS
GLY
GLY
GLU
GLU
GLU

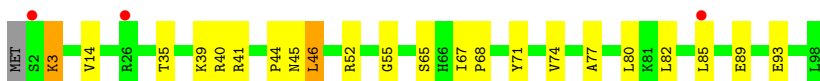
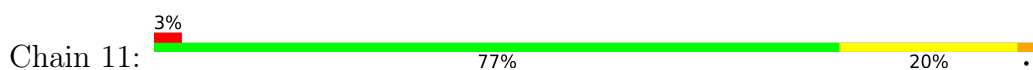
- Molecule 22: 50S ribosomal protein L27



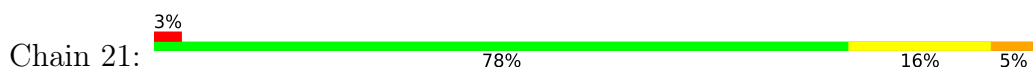
- Molecule 22: 50S ribosomal protein L27



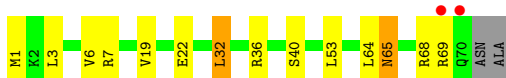
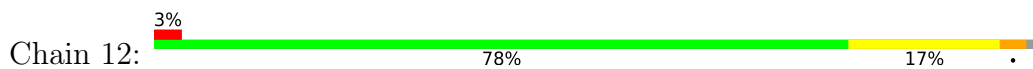
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



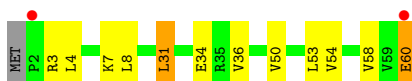
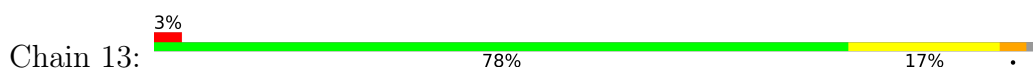
- Molecule 24: 50S ribosomal protein L29



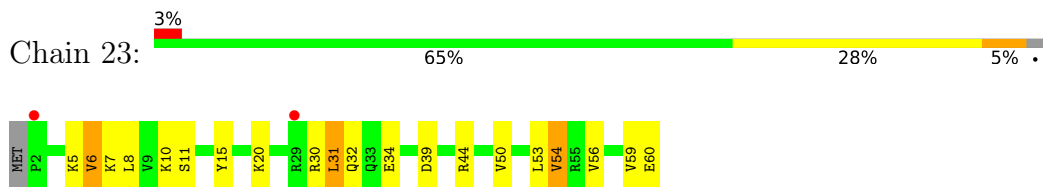
- Molecule 24: 50S ribosomal protein L29



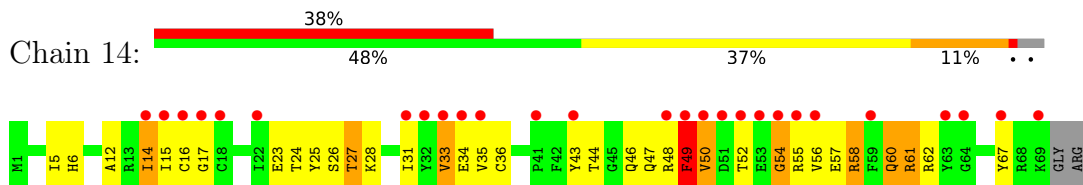
- Molecule 25: 50S ribosomal protein L30



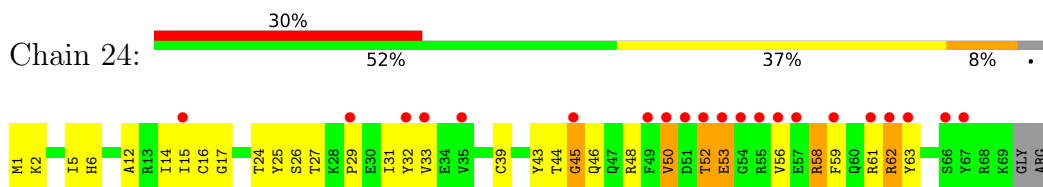
- Molecule 25: 50S ribosomal protein L30



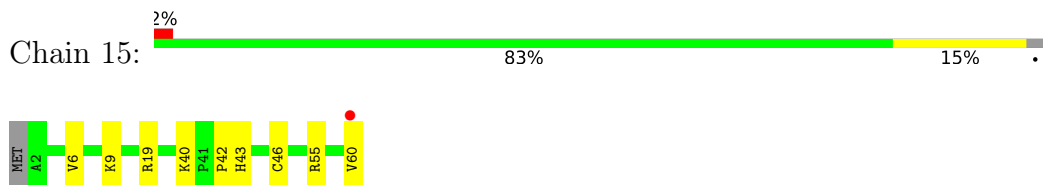
- Molecule 26: 50S ribosomal protein L31



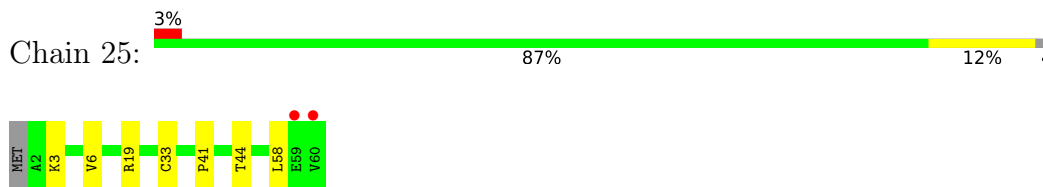
- Molecule 26: 50S ribosomal protein L31



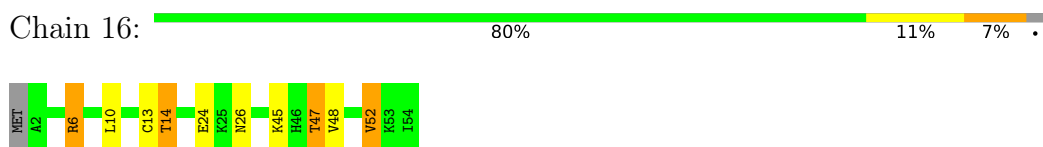
- Molecule 27: 50S ribosomal protein L32



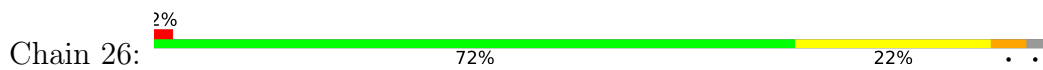
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33

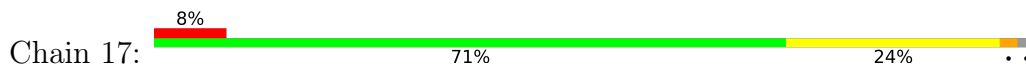


- Molecule 28: 50S ribosomal protein L33

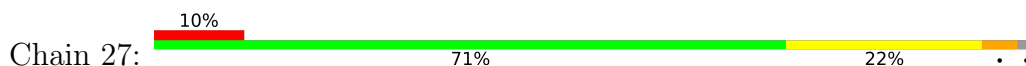




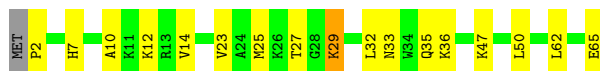
- Molecule 29: 50S ribosomal protein L34



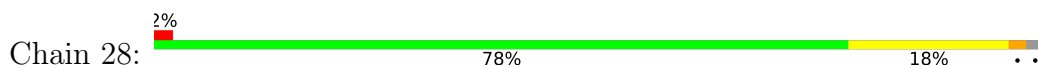
- Molecule 29: 50S ribosomal protein L34



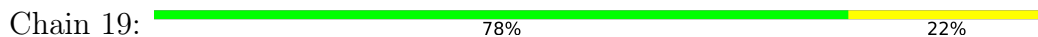
- Molecule 30: 50S ribosomal protein L35



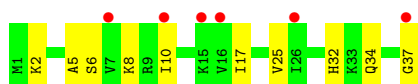
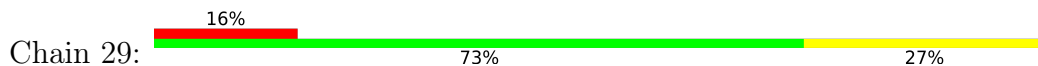
- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36

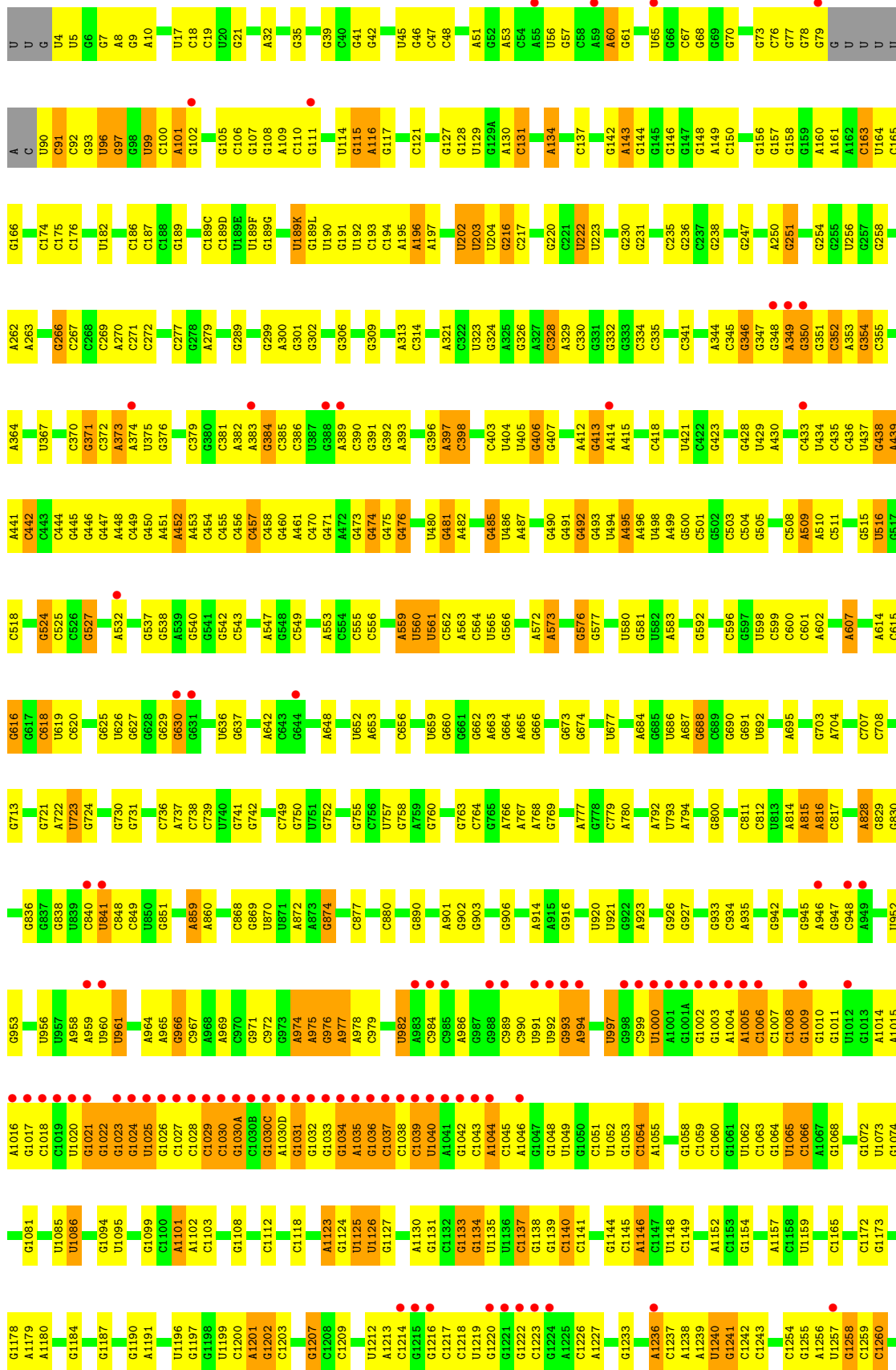


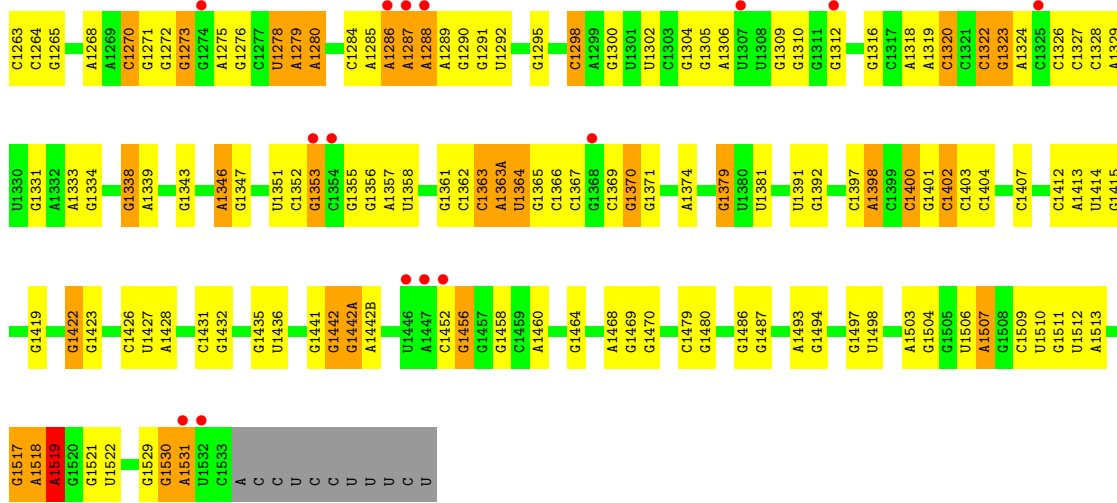
- Molecule 31: 50S ribosomal protein L36



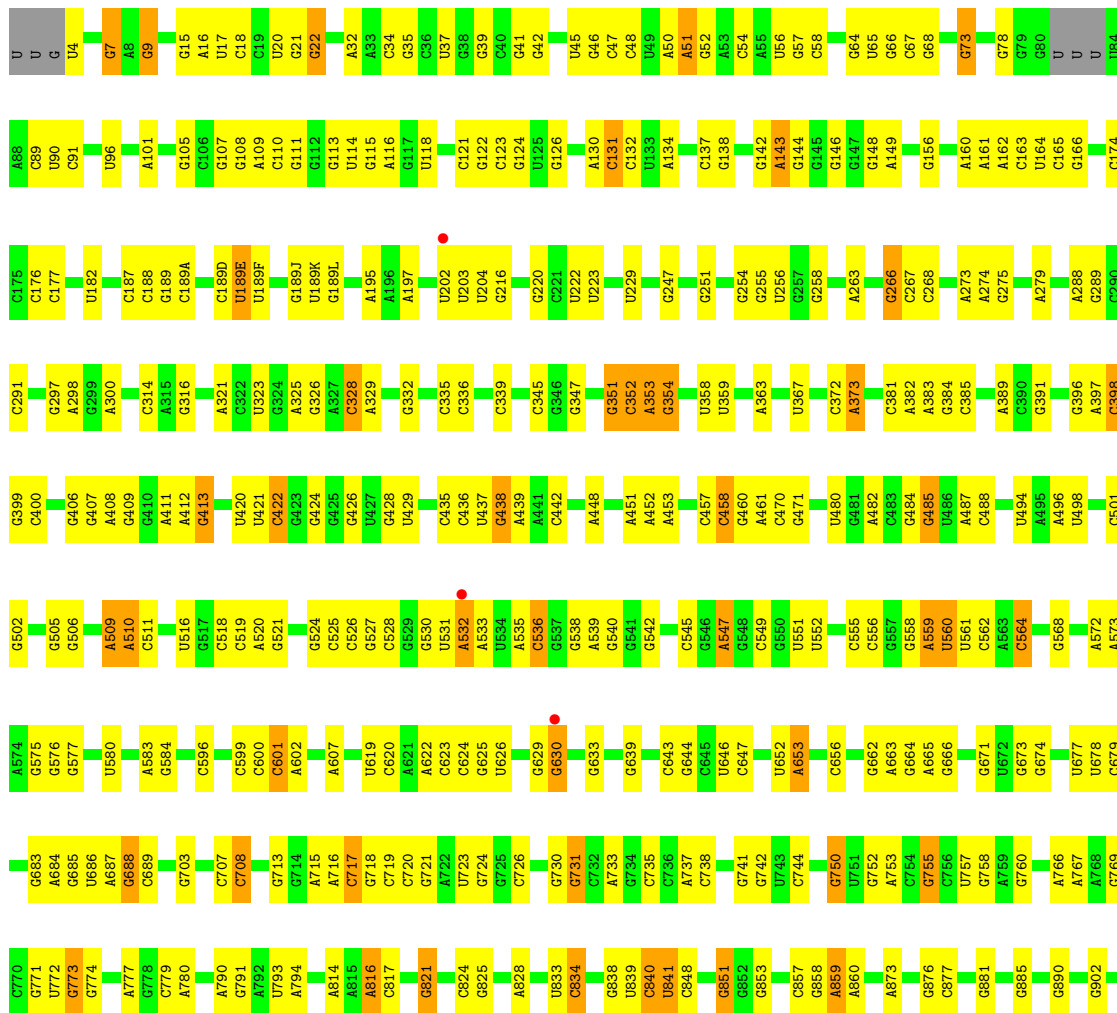
- Molecule 32: 16S Ribosomal RNA

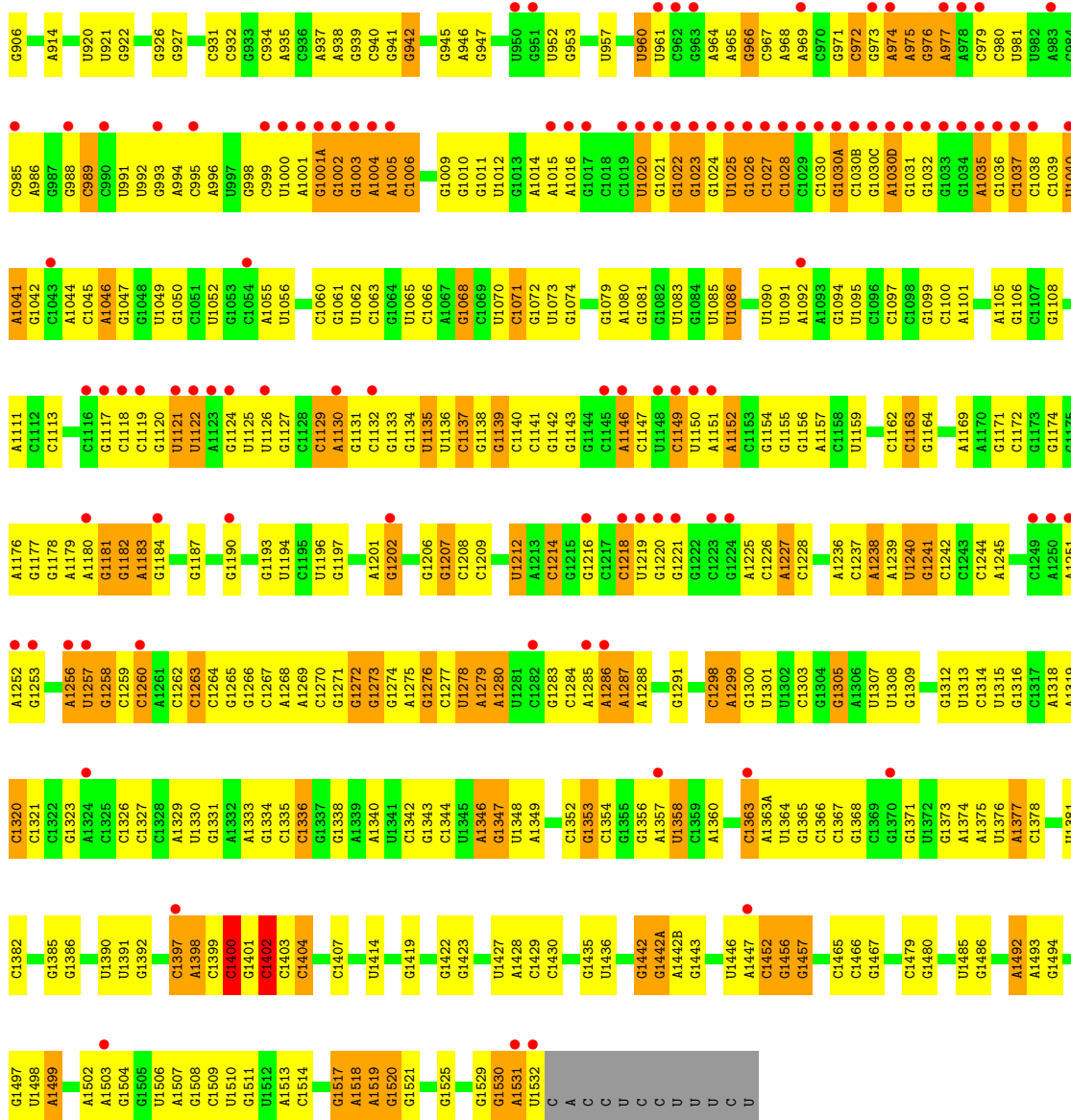




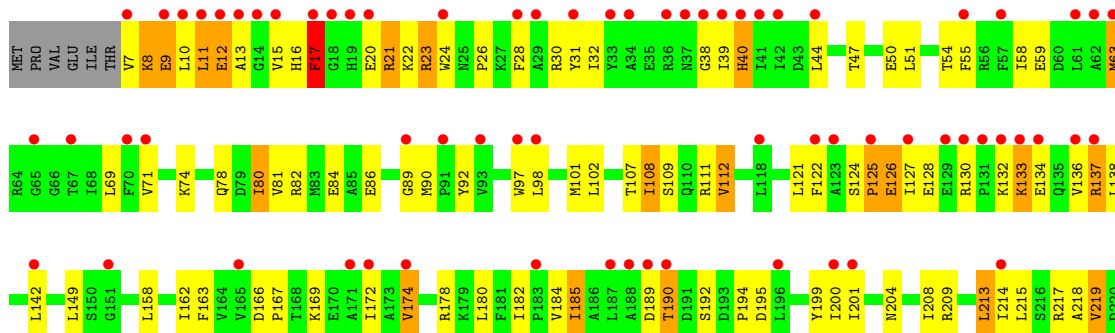


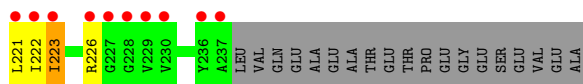
• Molecule 32: 16S Ribosomal RNA



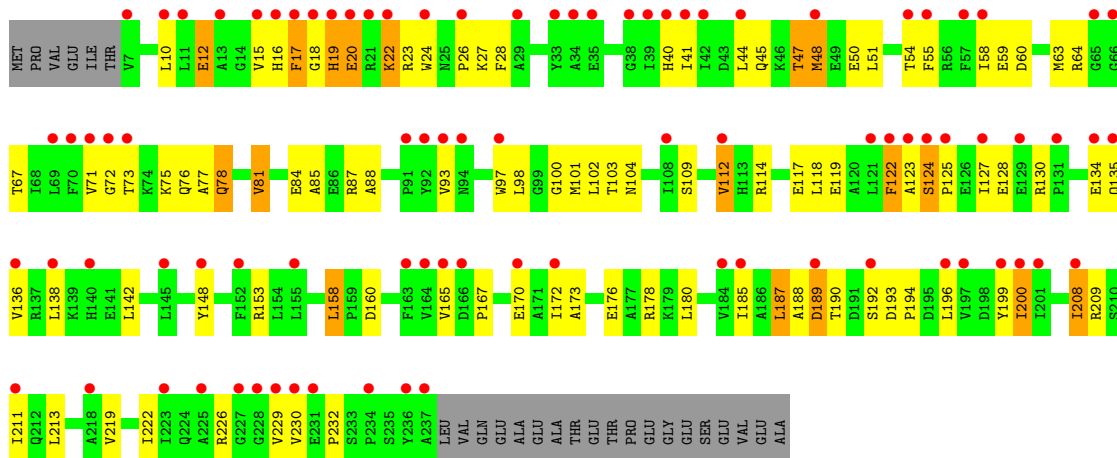


• Molecule 33: 30S ribosomal protein S2

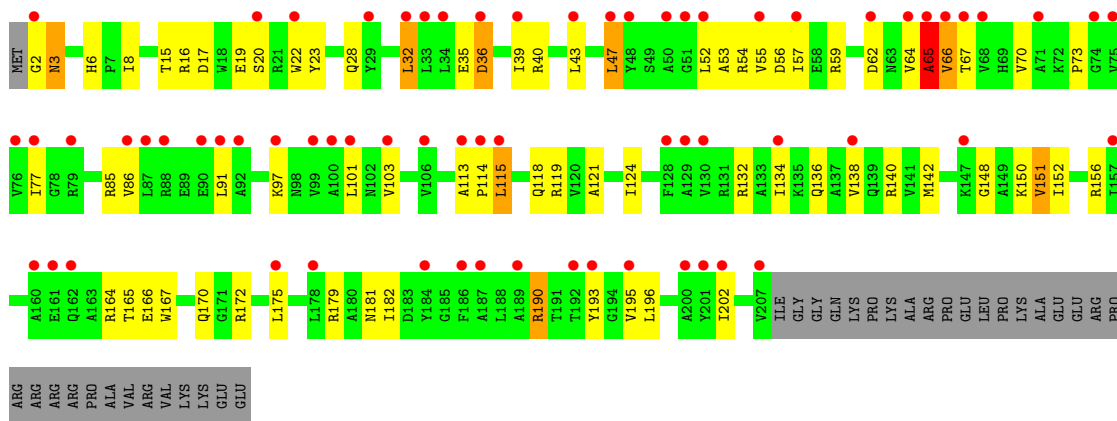




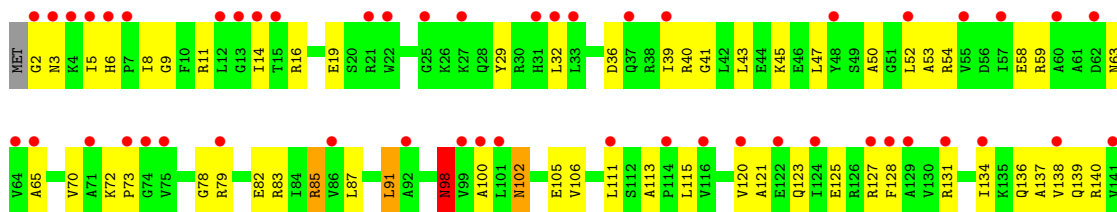
● Molecule 33: 30S ribosomal protein S2

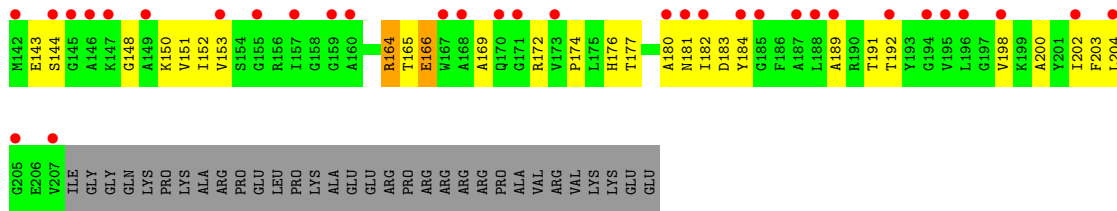


● Molecule 34: 30S ribosomal protein S3

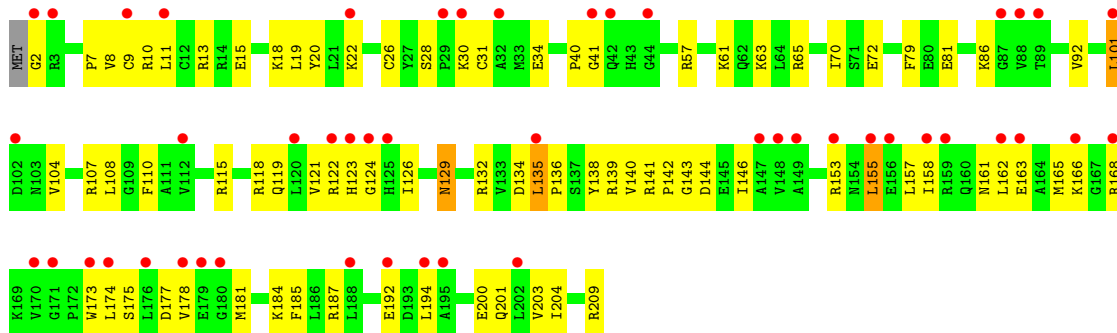


● Molecule 34: 30S ribosomal protein S3

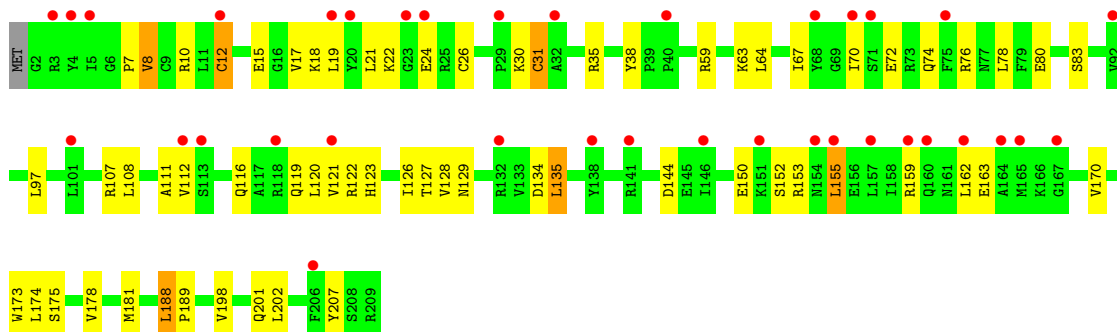




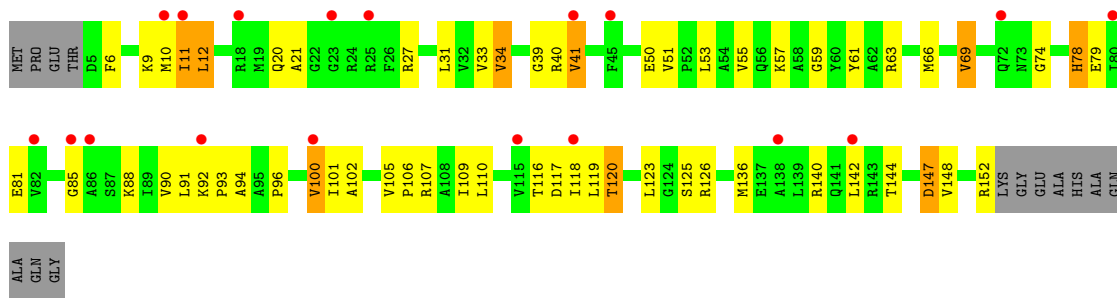
• Molecule 35: 30S ribosomal protein S4



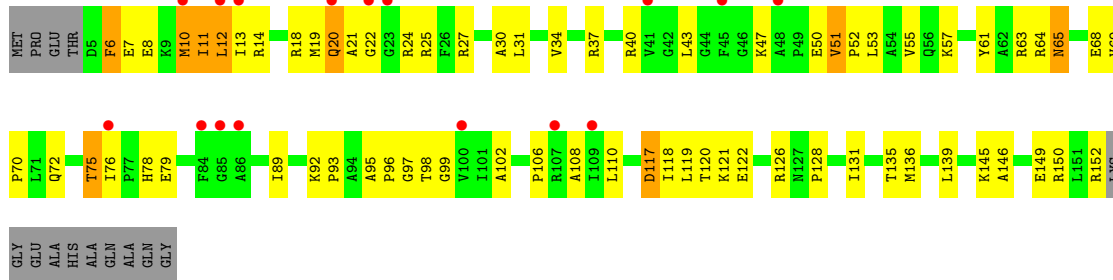
• Molecule 35: 30S ribosomal protein S4



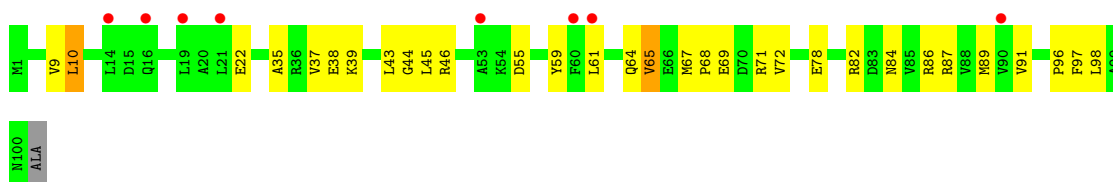
• Molecule 36: 30S ribosomal protein S5



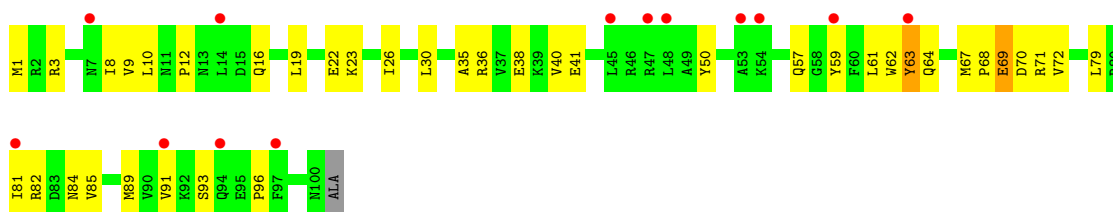
• Molecule 36: 30S ribosomal protein S5



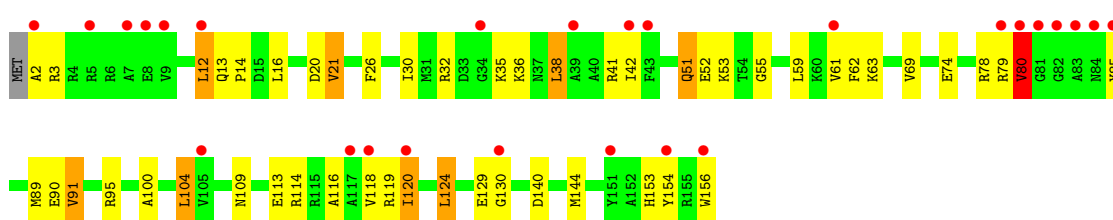
- Molecule 37: 30S ribosomal protein S6



- Molecule 37: 30S ribosomal protein S6

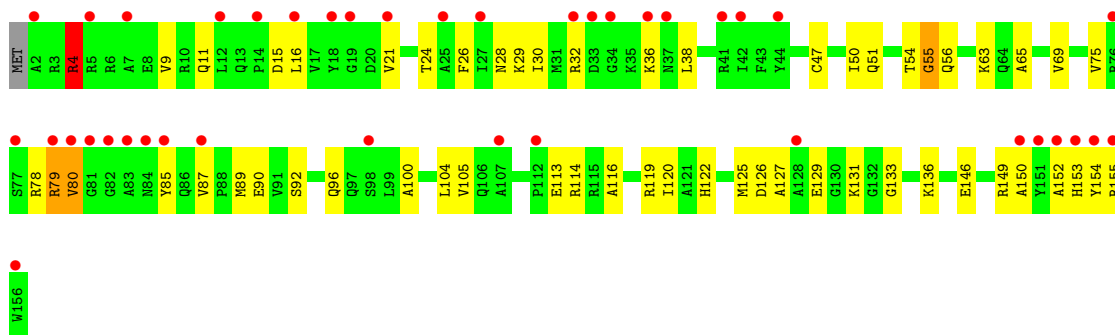


- Molecule 38: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S7

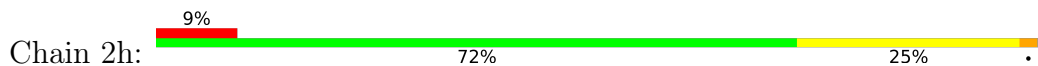




- Molecule 39: 30S ribosomal protein S8



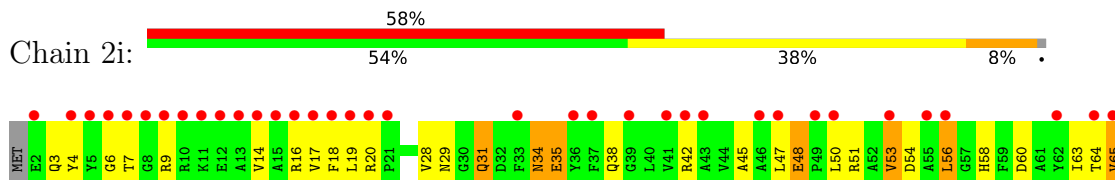
- Molecule 39: 30S ribosomal protein S8



- Molecule 40: 30S ribosomal protein S9

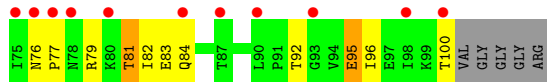
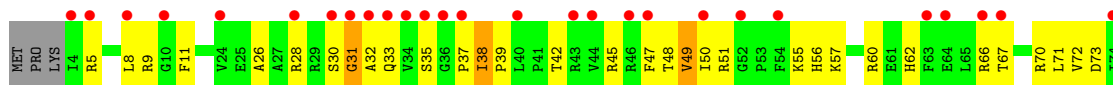


- Molecule 40: 30S ribosomal protein S9

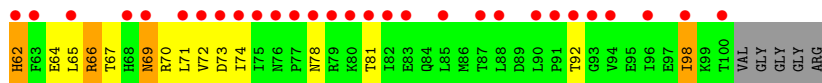
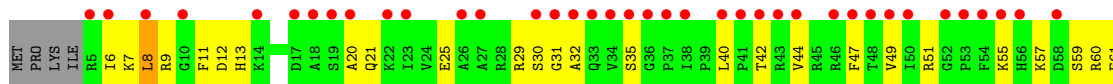




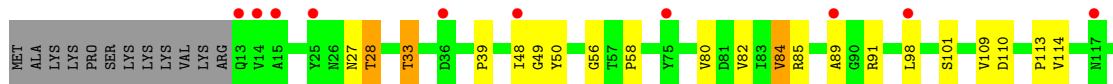
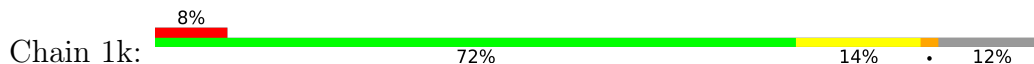
• Molecule 41: 30S ribosomal protein S10



• Molecule 41: 30S ribosomal protein S10



• Molecule 42: 30S ribosomal protein S11

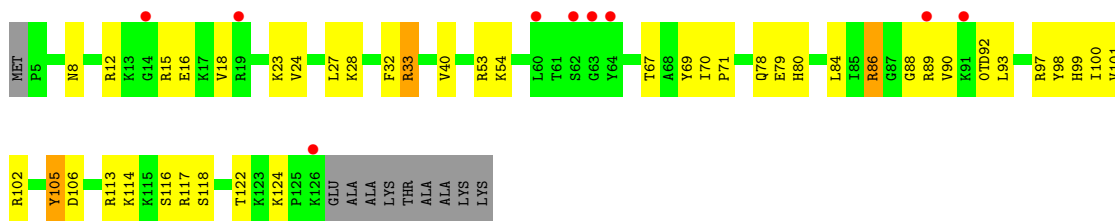


• Molecule 42: 30S ribosomal protein S11



• Molecule 43: 30S ribosomal protein S12

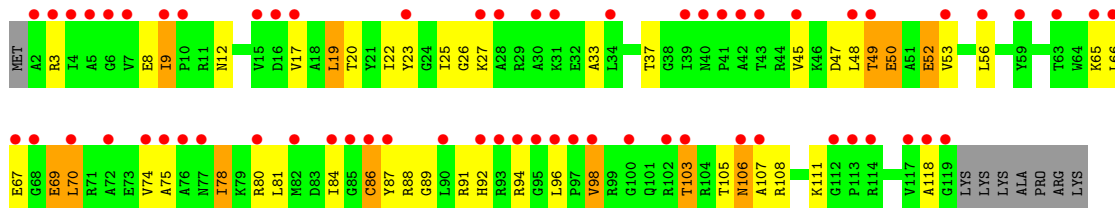




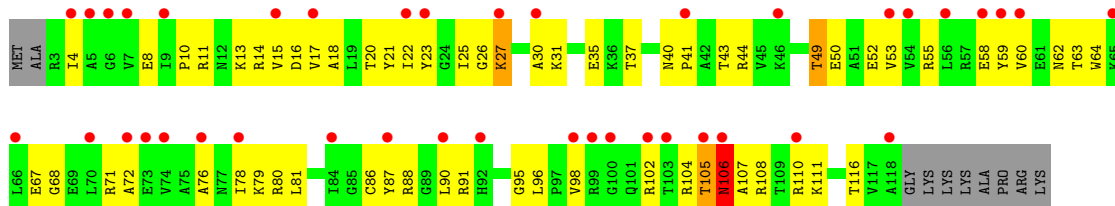
- Molecule 43: 30S ribosomal protein S12



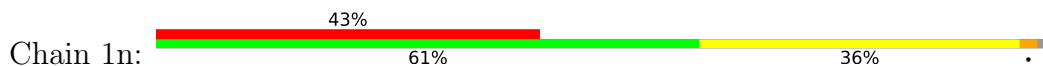
- Molecule 44: 30S ribosomal protein S13



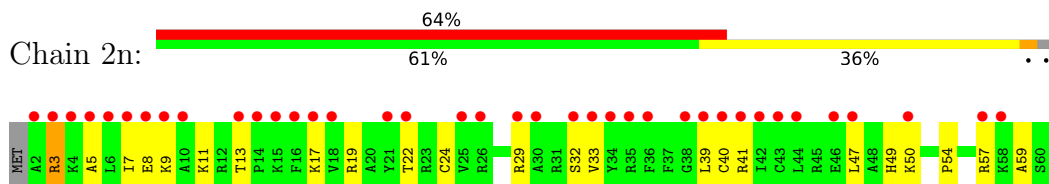
- Molecule 44: 30S ribosomal protein S13



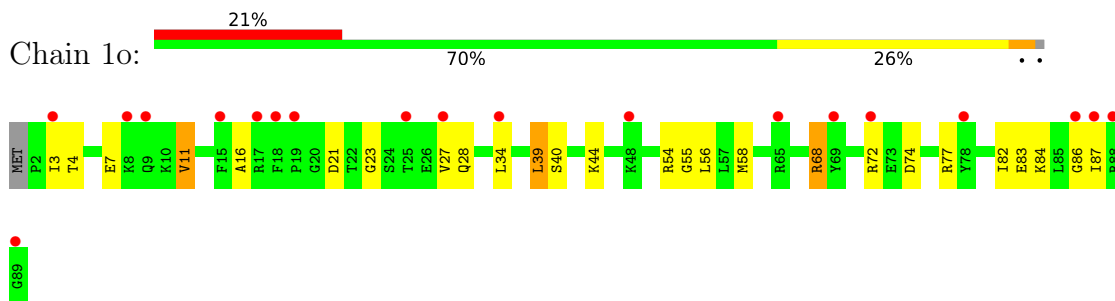
- Molecule 45: 30S ribosomal protein S14 type Z



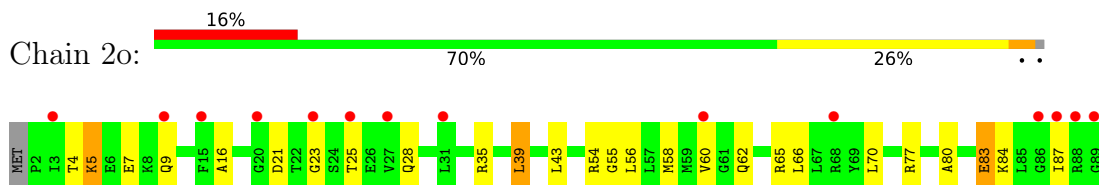
- Molecule 45: 30S ribosomal protein S14 type Z



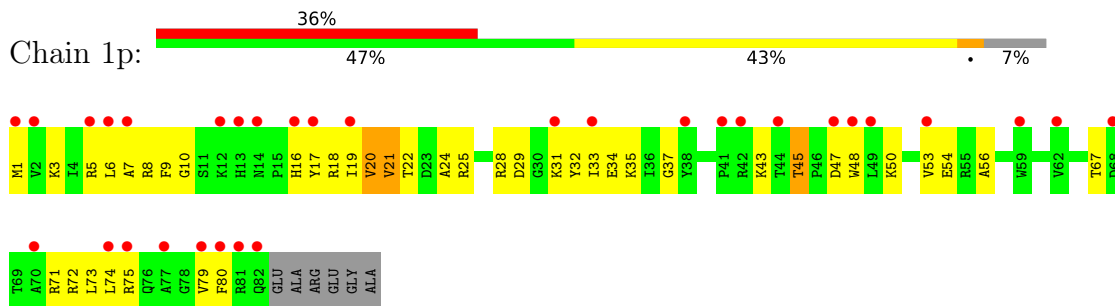
• Molecule 46: 30S ribosomal protein S15



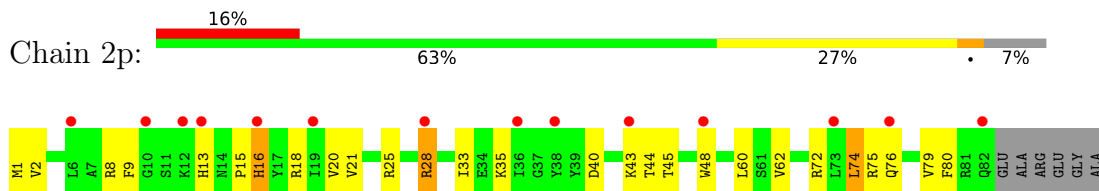
• Molecule 46: 30S ribosomal protein S15



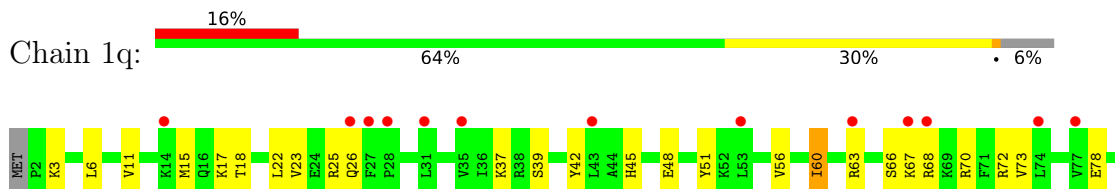
• Molecule 47: 30S ribosomal protein S16

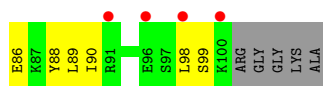


• Molecule 47: 30S ribosomal protein S16

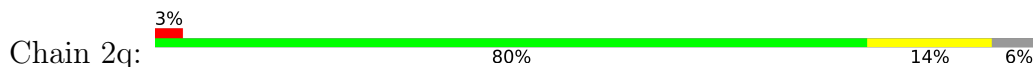


• Molecule 48: 30S ribosomal protein S17





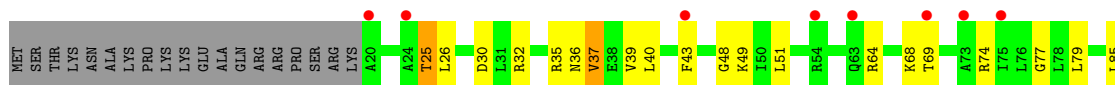
• Molecule 48: 30S ribosomal protein S17



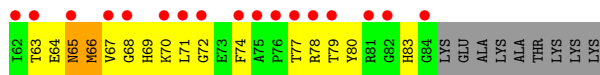
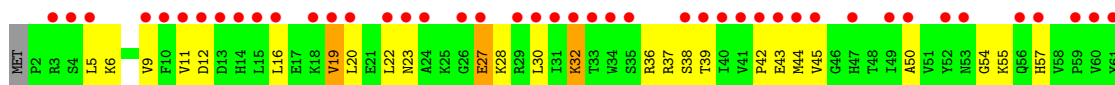
• Molecule 49: 30S ribosomal protein S18



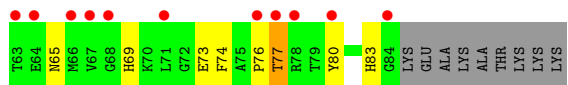
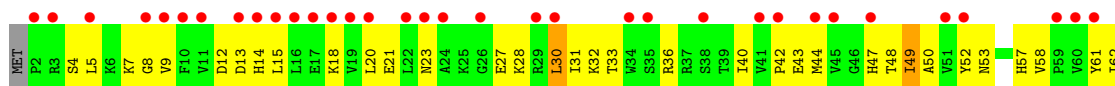
• Molecule 49: 30S ribosomal protein S18



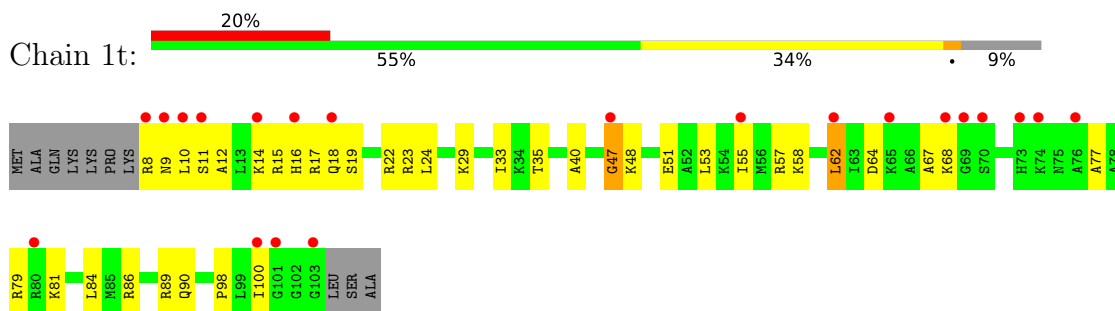
• Molecule 50: 30S ribosomal protein S19



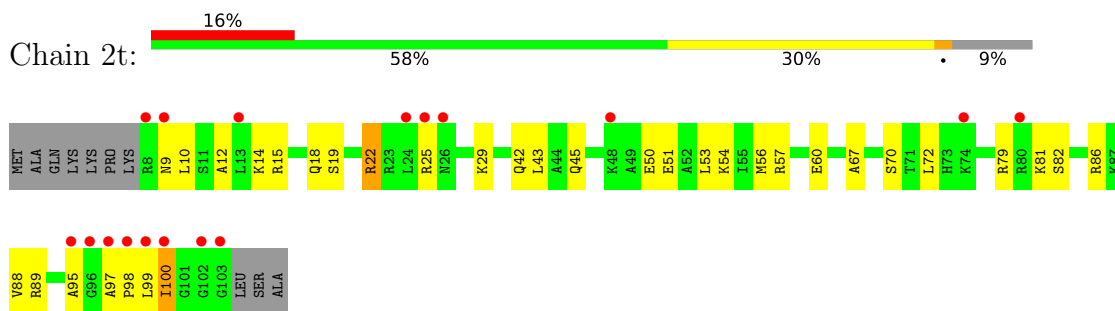
• Molecule 50: 30S ribosomal protein S19



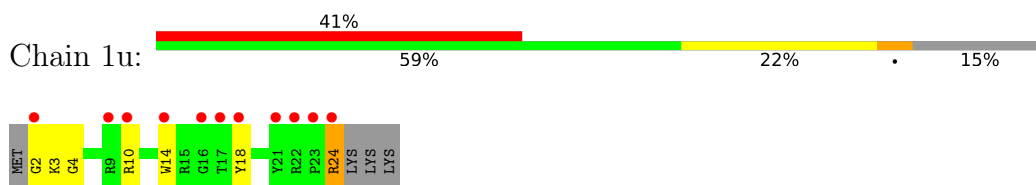
- Molecule 51: 30S ribosomal protein S20



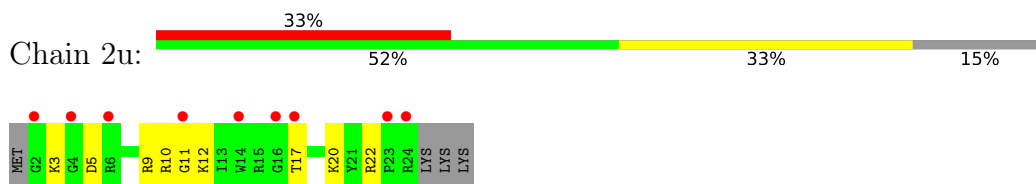
- Molecule 51: 30S ribosomal protein S20



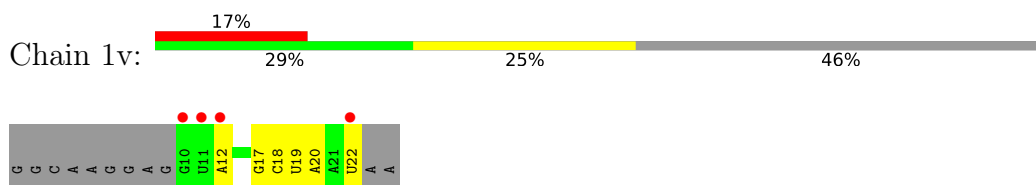
- Molecule 52: 30S ribosomal protein Thx



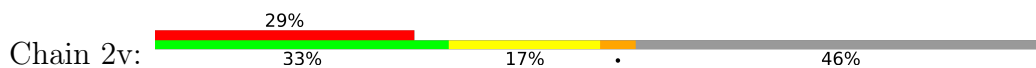
- Molecule 52: 30S ribosomal protein Thx

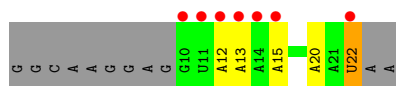


- Molecule 53: CYS-Stop mRNA

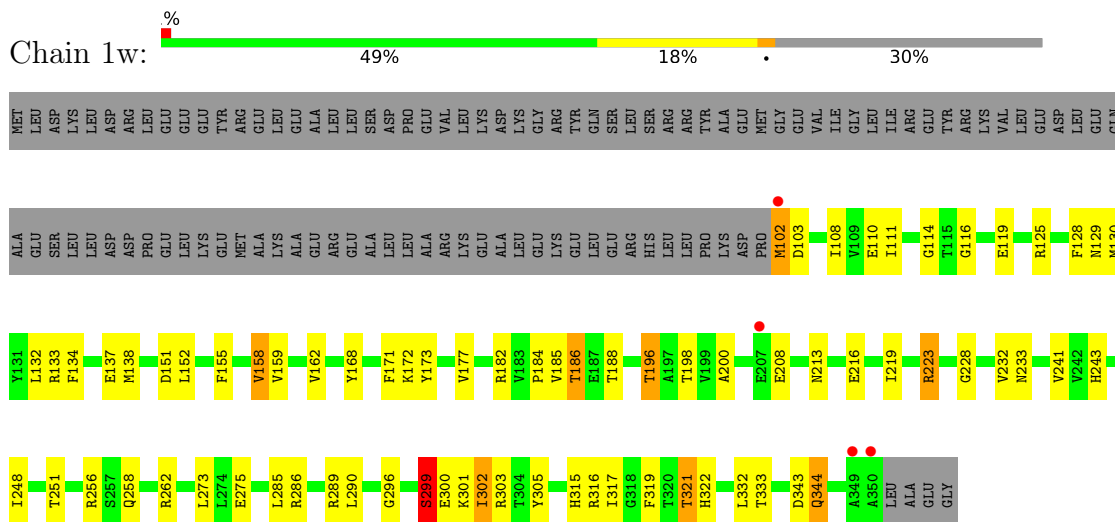


- Molecule 53: CYS-Stop mRNA

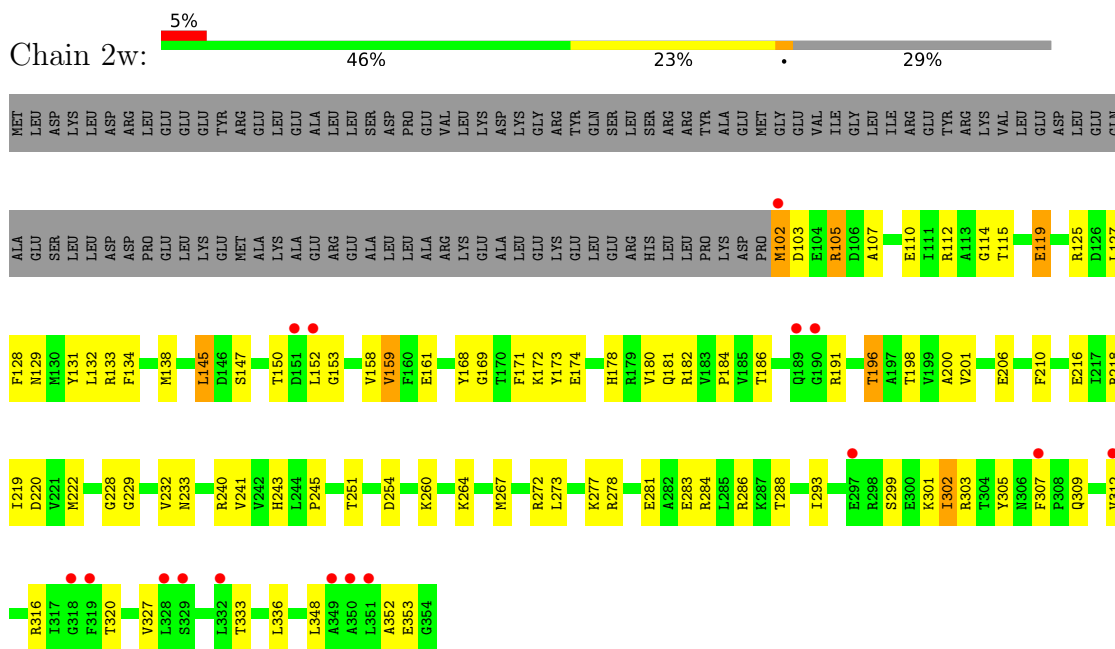




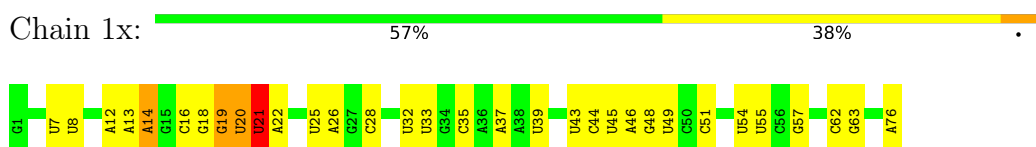
- Molecule 54: Peptide chain release factor 1



- Molecule 54: Peptide chain release factor 1



- Molecule 55: P-site Peptidyl-tRNA fMEAAAKC-tRNAcys RNA-part



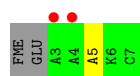
- Molecule 55: P-site Peptidyl-tRNA fMEAAAKC-tRNAcys RNA-part

Chain 2x:  66% 26% 8%



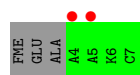
- Molecule 56: P-site Peptidyl-tRNA fMEAAAKC-tRNA_{cys} Peptide-part

Chain 1z:  29% 57% 14% 29%



- Molecule 56: P-site Peptidyl-tRNA fMEAAAKC-tRNA_{cys} Peptide-part

Chain 2z:  29% 57% 43%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.96Å 448.05Å 615.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.56 – 2.55 122.56 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.6 (122.56-2.55) 98.6 (122.56-2.55)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.55Å)	Xtrriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.216 , 0.257 0.218 , 0.258	Depositor DCC
R_{free} test set	91629 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtrriage
Anisotropy	0.153	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	297259	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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, ZN, OMG, 4OC, K, 2MA, OMU, 5MC, M2G, MA6, SF4, MG, UR3, MIA, 0TD, 8AN, H2U, PSU, G7M, 2MG, 4SU, 5MU

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	0.29	0/69011	0.47	1/107720 (0.0%)
1	2A	0.23	0/67295	0.41	1/105042 (0.0%)
2	1B	0.22	0/2882	0.40	0/4494
2	2B	0.19	0/2879	0.36	0/4487
3	1D	0.28	0/2186	0.52	0/2944
3	2D	0.23	0/2186	0.47	1/2944 (0.0%)
4	1E	0.26	0/1592	0.52	0/2149
4	2E	0.22	0/1592	0.44	0/2149
5	1F	0.26	0/1619	0.49	0/2193
5	2F	0.21	0/1615	0.43	0/2188
6	1G	0.20	0/1448	0.43	0/1957
6	2G	0.19	0/1453	0.43	0/1963
7	1H	0.21	0/1356	0.42	0/1834
7	2H	0.19	0/1356	0.38	0/1834
8	1I	0.19	0/1112	0.42	0/1514
8	2I	0.19	0/1079	0.39	0/1475
9	1N	0.27	0/1144	0.45	0/1543
9	2N	0.20	0/1144	0.41	0/1543
10	1O	0.26	0/943	0.46	0/1269
10	2O	0.21	0/943	0.44	0/1269
11	1P	0.27	0/1152	0.50	0/1533
11	2P	0.21	0/1152	0.46	0/1533
12	1Q	0.27	0/1143	0.50	0/1527
12	2Q	0.22	0/1143	0.43	0/1527
13	1R	0.26	0/982	0.50	0/1312
13	2R	0.22	0/982	0.43	0/1312
14	1S	0.23	0/883	0.45	0/1176
14	2S	0.19	0/880	0.43	0/1172
15	1T	0.25	0/1105	0.46	0/1477
15	2T	0.21	0/1097	0.43	0/1468
16	1U	0.27	0/977	0.47	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.19	0/977	0.40	0/1301
17	1V	0.24	0/782	0.45	0/1049
17	2V	0.17	0/782	0.38	0/1049
18	1W	0.28	0/897	0.46	0/1205
18	2W	0.21	0/897	0.42	0/1205
19	1X	0.26	0/764	0.53	2/1025 (0.2%)
19	2X	0.19	0/764	0.48	2/1025 (0.2%)
20	1Y	0.23	0/819	0.47	0/1095
20	2Y	0.20	0/819	0.42	0/1095
21	1Z	0.22	0/1267	0.50	0/1717
21	2Z	0.21	0/1299	0.45	0/1763
22	10	0.27	0/612	0.47	0/816
22	20	0.22	0/612	0.45	0/816
23	11	0.27	0/762	0.45	0/1014
23	21	0.23	0/762	0.40	0/1014
24	12	0.23	0/590	0.45	0/781
24	22	0.19	0/590	0.38	0/781
25	13	0.25	0/474	0.47	0/635
25	23	0.20	0/469	0.42	0/630
26	14	0.24	0/565	0.59	2/761 (0.3%)
26	24	0.24	0/545	0.55	0/737
27	15	0.24	0/469	0.50	0/635
27	25	0.22	0/469	0.44	0/635
28	16	0.27	0/460	0.50	0/613
28	26	0.21	0/456	0.46	0/608
29	17	0.32	0/426	0.56	0/561
29	27	0.24	0/426	0.48	0/561
30	18	0.27	0/525	0.48	0/691
30	28	0.21	0/525	0.38	0/691
31	19	0.30	0/310	0.51	0/407
31	29	0.19	0/310	0.44	0/407
32	1a	0.20	0/35795	0.39	1/55864 (0.0%)
32	2a	0.20	1/35886 (0.0%)	0.38	3/56005 (0.0%)
33	1b	0.22	0/1881	0.51	0/2542
33	2b	0.23	0/1860	0.47	0/2518
34	1c	0.21	0/1572	0.46	2/2126 (0.1%)
34	2c	0.21	0/1566	0.43	0/2119
35	1d	0.20	0/1685	0.42	0/2262
35	2d	0.20	0/1704	0.44	0/2284
36	1e	0.20	0/1145	0.45	0/1543
36	2e	0.21	0/1149	0.45	0/1548
37	1f	0.18	0/823	0.42	0/1115
37	2f	0.18	0/829	0.40	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.18	0/1250	0.43	0/1679
38	2g	0.21	0/1254	0.43	0/1683
39	1h	0.18	0/1108	0.40	0/1494
39	2h	0.18	0/1108	0.41	0/1494
40	1i	0.19	0/1002	0.44	0/1346
40	2i	0.21	0/997	0.45	0/1343
41	1j	0.25	0/722	0.47	0/982
41	2j	0.22	0/727	0.48	0/988
42	1k	0.19	0/844	0.41	0/1145
42	2k	0.18	0/848	0.40	0/1149
43	1l	0.20	0/937	0.45	0/1260
43	2l	0.19	0/937	0.44	0/1260
44	1m	0.21	0/929	0.50	0/1250
44	2m	0.22	0/917	0.45	0/1234
45	1n	0.19	0/501	0.48	0/664
45	2n	0.19	0/501	0.44	0/664
46	1o	0.19	0/739	0.38	0/985
46	2o	0.18	0/739	0.43	0/985
47	1p	0.19	0/697	0.44	0/939
47	2p	0.18	0/693	0.45	0/935
48	1q	0.20	0/836	0.41	0/1117
48	2q	0.17	0/836	0.40	0/1117
49	1r	0.20	0/560	0.41	0/746
49	2r	0.18	0/560	0.38	0/746
50	1s	0.22	0/667	0.52	0/900
50	2s	0.21	0/661	0.51	0/893
51	1t	0.20	0/730	0.43	0/965
51	2t	0.20	0/729	0.45	0/965
52	1u	0.22	0/203	0.43	0/266
52	2u	0.22	0/203	0.46	0/266
53	1v	0.25	0/310	0.44	0/480
53	2v	0.24	0/310	0.45	0/480
54	1w	0.22	0/1965	0.44	0/2648
54	2w	0.20	0/1983	0.39	0/2671
55	1x	0.23	0/1555	0.36	0/2419
55	2x	0.23	1/1555 (0.1%)	0.37	0/2419
56	1z	0.35	0/29	0.60	0/37
56	2z	0.30	0/24	0.51	0/30
All	All	0.24	2/313816 (0.0%)	0.43	15/468865 (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
11	1P	0	1
11	2P	0	1
21	1Z	0	2
26	14	0	1
33	1b	0	2
33	2b	0	2
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	527	G7M	O3'-P	5.13	1.61	1.56
55	2x	8	4SU	O3'-P	5.02	1.61	1.56

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1992	G	C2'-C3'-O3'	7.29	120.44	109.50
1	2A	1992	G	C2'-C3'-O3'	6.52	119.28	109.50
32	2a	1272	G	N1-C2-N2	-6.18	97.66	116.20
32	2a	1263	C	N1-C2-O2	5.99	136.85	118.90
34	1c	65	ALA	CA-C-N	5.83	132.46	121.97

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	52	THR	Peptide
11	1P	35	HIS	Peptide
21	1Z	136	PHE	Peptide
21	1Z	146	ILE	Peptide
33	1b	9	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31196	617	0
1	2A	60322	0	30426	647	0
2	1B	2577	0	1305	26	0
2	2B	2575	0	1303	26	0
3	1D	2136	0	2218	41	0
3	2D	2136	0	2218	49	0
4	1E	1559	0	1618	22	0
4	2E	1559	0	1618	21	0
5	1F	1584	0	1625	40	0
5	2F	1580	0	1619	46	0
6	1G	1423	0	1436	53	0
6	2G	1428	0	1438	47	0
7	1H	1330	0	1407	25	0
7	2H	1330	0	1407	40	0
8	1I	1097	0	1140	24	0
8	2I	1064	0	1082	37	0
9	1N	1117	0	1184	10	0
9	2N	1117	0	1184	19	0
10	1O	933	0	996	16	0
10	2O	933	0	996	18	0
11	1P	1135	0	1212	22	0
11	2P	1135	0	1212	24	0
12	1Q	1122	0	1179	12	0
12	2Q	1122	0	1179	24	0
13	1R	968	0	1033	14	0
13	2R	968	0	1033	16	0
14	1S	873	0	927	21	0
14	2S	870	0	923	20	0
15	1T	1091	0	1151	18	0
15	2T	1083	0	1136	30	0
16	1U	959	0	1019	12	0
16	2U	959	0	1019	19	0
17	1V	771	0	830	11	0
17	2V	771	0	830	11	0
18	1W	886	0	940	8	0
18	2W	886	0	940	12	0
19	1X	750	0	814	16	0
19	2X	750	0	814	12	0
20	1Y	806	0	881	17	0
20	2Y	806	0	881	20	0
21	1Z	1240	0	1240	29	0
21	2Z	1271	0	1273	43	0
22	10	604	0	619	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	604	0	619	7	0
23	11	755	0	826	15	0
23	21	755	0	826	18	0
24	12	588	0	643	8	0
24	22	588	0	643	13	0
25	13	469	0	518	5	0
25	23	464	0	514	12	0
26	14	552	0	533	29	0
26	24	532	0	503	27	0
27	15	455	0	465	4	0
27	25	455	0	465	4	0
28	16	453	0	473	6	0
28	26	449	0	469	6	0
29	17	418	0	467	9	0
29	27	418	0	467	9	0
30	18	517	0	582	13	0
30	28	517	0	582	14	0
31	19	307	0	335	5	0
31	29	307	0	335	8	0
32	1a	32246	0	16292	494	0
32	2a	32327	0	16338	500	0
33	1b	1846	0	1867	77	0
33	2b	1825	0	1828	59	0
34	1c	1548	0	1535	44	0
34	2c	1542	0	1517	57	0
35	1d	1655	0	1672	61	0
35	2d	1674	0	1714	42	0
36	1e	1129	0	1185	44	0
36	2e	1133	0	1191	50	0
37	1f	810	0	804	17	0
37	2f	816	0	808	24	0
38	1g	1231	0	1238	40	0
38	2g	1235	0	1249	37	0
39	1h	1088	0	1126	37	0
39	2h	1088	0	1126	28	0
40	1i	983	0	986	40	0
40	2i	978	0	966	41	0
41	1j	709	0	650	34	0
41	2j	714	0	672	32	0
42	1k	829	0	825	13	0
42	2k	833	0	836	30	0
43	1l	932	0	981	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	2l	932	0	981	19	0
44	1m	919	0	951	41	0
44	2m	907	0	934	49	0
45	1n	492	0	529	16	0
45	2n	492	0	529	24	0
46	1o	728	0	760	14	0
46	2o	728	0	760	17	0
47	1p	681	0	697	35	0
47	2p	677	0	686	15	0
48	1q	823	0	891	23	0
48	2q	823	0	891	10	0
49	1r	555	0	618	8	0
49	2r	555	0	618	15	0
50	1s	652	0	662	36	0
50	2s	646	0	644	37	0
51	1t	728	0	798	27	0
51	2t	727	0	796	25	0
52	1u	199	0	208	6	0
52	2u	199	0	208	8	0
53	1v	277	0	140	4	0
53	2v	277	0	140	3	0
54	1w	1937	0	1919	45	0
54	2w	1955	0	1927	50	0
55	1x	1577	0	801	14	0
55	2x	1577	0	801	11	0
56	1z	30	0	32	1	0
56	2z	25	0	27	0	0
57	10	8	0	0	0	0
57	11	4	0	0	0	0
57	12	2	0	0	0	0
57	13	4	0	0	0	0
57	15	8	0	0	0	0
57	16	1	0	0	0	0
57	17	6	0	0	0	0
57	18	4	0	0	0	0
57	19	1	0	0	0	0
57	1A	1088	0	0	0	0
57	1B	36	0	0	0	0
57	1D	13	0	0	0	0
57	1E	15	0	0	0	0
57	1F	15	0	0	0	0
57	1G	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1I	1	0	0	0	0
57	1N	6	0	0	0	0
57	1O	4	0	0	0	0
57	1P	4	0	0	0	0
57	1Q	8	0	0	0	0
57	1R	5	0	0	0	0
57	1S	3	0	0	0	0
57	1T	2	0	0	0	0
57	1U	10	0	0	0	0
57	1V	6	0	0	0	0
57	1W	6	0	0	0	0
57	1X	5	0	0	0	0
57	1Y	4	0	0	0	0
57	1Z	2	0	0	0	0
57	1a	223	0	0	0	0
57	1b	1	0	0	0	0
57	1d	1	0	0	0	0
57	1e	3	0	0	0	0
57	1f	1	0	0	0	0
57	1l	2	0	0	0	0
57	1m	1	0	0	0	0
57	1n	1	0	0	0	0
57	1p	1	0	0	0	0
57	1r	1	0	0	0	0
57	1t	1	0	0	0	0
57	1v	1	0	0	0	0
57	1w	2	0	0	0	0
57	1x	13	0	0	0	0
57	20	2	0	0	0	0
57	21	1	0	0	0	0
57	23	3	0	0	0	0
57	25	7	0	0	0	0
57	26	1	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	853	0	0	0	0
57	2B	22	0	0	0	0
57	2D	9	0	0	0	0
57	2E	9	0	0	0	0
57	2F	9	0	0	0	0
57	2G	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2N	1	0	0	0	0
57	2O	2	0	0	0	0
57	2P	1	0	0	0	0
57	2Q	4	0	0	0	0
57	2R	2	0	0	0	0
57	2T	3	0	0	0	0
57	2U	2	0	0	0	0
57	2V	2	0	0	0	0
57	2W	2	0	0	0	0
57	2X	2	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	176	0	0	0	0
57	2d	2	0	0	0	0
57	2e	1	0	0	0	0
57	2f	3	0	0	0	0
57	2g	1	0	0	0	0
57	2i	1	0	0	0	0
57	2j	1	0	0	0	0
57	2k	1	0	0	0	0
57	2l	2	0	0	0	0
57	2q	3	0	0	0	0
57	2t	1	0	0	0	0
57	2v	2	0	0	0	0
57	2w	1	0	0	0	0
57	2x	10	0	0	0	0
58	1A	1	0	0	0	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	0	0
61	10	9	0	0	0	0
61	11	10	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	12	3	0	0	0	0
61	13	4	0	0	0	0
61	15	5	0	0	0	0
61	16	1	0	0	0	0
61	17	6	0	0	0	0
61	18	10	0	0	0	0
61	1A	2032	0	0	76	0
61	1B	62	0	0	0	0
61	1D	24	0	0	1	0
61	1E	31	0	0	4	0
61	1F	15	0	0	0	0
61	1G	7	0	0	2	0
61	1H	2	0	0	0	0
61	1I	1	0	0	0	0
61	1N	5	0	0	0	0
61	1O	7	0	0	0	0
61	1P	20	0	0	1	0
61	1Q	7	0	0	0	0
61	1R	15	0	0	2	0
61	1S	4	0	0	0	0
61	1T	9	0	0	0	0
61	1U	13	0	0	1	0
61	1V	9	0	0	0	0
61	1W	11	0	0	0	0
61	1X	4	0	0	0	0
61	1Y	2	0	0	0	0
61	1Z	1	0	0	0	0
61	1a	289	0	0	25	0
61	1d	1	0	0	0	0
61	1j	1	0	0	0	0
61	1l	4	0	0	0	0
61	1q	2	0	0	0	0
61	1v	5	0	0	0	0
61	1w	5	0	0	1	0
61	1x	24	0	0	3	0
61	20	2	0	0	0	0
61	21	7	0	0	1	0
61	22	1	0	0	0	0
61	23	2	0	0	0	0
61	25	1	0	0	0	0
61	27	3	0	0	0	0
61	28	2	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	29	1	0	0	0	0
61	2A	1200	0	0	76	0
61	2B	20	0	0	1	0
61	2D	23	0	0	1	0
61	2E	12	0	0	0	0
61	2F	15	0	0	1	0
61	2I	2	0	0	0	0
61	2O	3	0	0	0	0
61	2P	14	0	0	0	0
61	2Q	1	0	0	0	0
61	2R	3	0	0	2	0
61	2T	4	0	0	0	0
61	2U	3	0	0	0	0
61	2W	2	0	0	0	0
61	2X	3	0	0	0	0
61	2Z	1	0	0	0	0
61	2a	152	0	0	9	0
61	2e	2	0	0	0	0
61	2j	1	0	0	0	0
61	2l	5	0	0	1	0
61	2o	1	0	0	0	0
61	2q	2	0	0	0	0
61	2t	1	0	0	0	0
61	2v	1	0	0	0	0
61	2w	3	0	0	0	0
61	2x	28	0	0	3	0
61	2z	1	0	0	0	0
All	All	297259	0	197120	4158	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 4158 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	1.33	1.26
32:1a:1035:A:H2'	32:1a:1036:G:H21	1.21	1.04
1:1A:1082:U:O4	1:1A:1086:A:N1	1.95	0.99
1:2A:2589:A:OP1	61:2A:3903:HOH:O	1.83	0.94
10:2O:48:PRO:HB3	32:2a:1422:G:H5''	1.50	0.94

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	262 (96%)	11 (4%)	0	100	100
3	2D	273/276 (99%)	257 (94%)	15 (6%)	1 (0%)	30	39
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	24	34
4	2E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	24	34
5	1F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	24	34
5	2F	201/210 (96%)	187 (93%)	11 (6%)	3 (2%)	8	10
6	1G	179/182 (98%)	167 (93%)	10 (6%)	2 (1%)	11	15
6	2G	179/182 (98%)	154 (86%)	21 (12%)	4 (2%)	5	5
7	1H	172/180 (96%)	162 (94%)	10 (6%)	0	100	100
7	2H	172/180 (96%)	157 (91%)	13 (8%)	2 (1%)	10	13
8	1I	144/148 (97%)	129 (90%)	14 (10%)	1 (1%)	18	25
8	2I	144/148 (97%)	125 (87%)	17 (12%)	2 (1%)	9	11
9	1N	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16	22
11	1P	147/150 (98%)	141 (96%)	4 (3%)	2 (1%)	9	11
11	2P	147/150 (98%)	136 (92%)	9 (6%)	2 (1%)	9	11
12	1Q	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	18	25
12	2Q	139/141 (99%)	131 (94%)	5 (4%)	3 (2%)	5	5
13	1R	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	95 (96%)	2 (2%)	2 (2%)	6	6
17	2V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	12	17
18	1W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
18	2W	110/113 (97%)	103 (94%)	7 (6%)	0	100	100
19	1X	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
19	2X	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
20	1Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
20	2Y	105/110 (96%)	96 (91%)	7 (7%)	2 (2%)	6	7
21	1Z	148/206 (72%)	132 (89%)	13 (9%)	3 (2%)	6	6
21	2Z	156/206 (76%)	140 (90%)	14 (9%)	2 (1%)	9	12
22	10	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
22	20	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
23	11	95/98 (97%)	91 (96%)	2 (2%)	2 (2%)	5	5
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	54 (81%)	11 (16%)	2 (3%)	3	2
26	24	67/71 (94%)	52 (78%)	8 (12%)	7 (10%)	0	0
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	51 (100%)	0	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	197 (86%)	25 (11%)	7 (3%)	3	2
33	2b	229/256 (90%)	199 (87%)	24 (10%)	6 (3%)	4	3
34	1c	204/239 (85%)	174 (85%)	28 (14%)	2 (1%)	12	17
34	2c	204/239 (85%)	178 (87%)	23 (11%)	3 (2%)	8	10
35	1d	206/209 (99%)	184 (89%)	22 (11%)	0	100	100
35	2d	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
36	1e	146/162 (90%)	133 (91%)	11 (8%)	2 (1%)	9	11
36	2e	146/162 (90%)	131 (90%)	12 (8%)	3 (2%)	5	5
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/101 (97%)	93 (95%)	4 (4%)	1 (1%)	12	17
38	1g	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	9	12
38	2g	153/156 (98%)	134 (88%)	17 (11%)	2 (1%)	9	12
39	1h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
39	2h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
40	1i	125/128 (98%)	107 (86%)	16 (13%)	2 (2%)	7	9
40	2i	125/128 (98%)	108 (86%)	15 (12%)	2 (2%)	7	9
41	1j	95/105 (90%)	78 (82%)	11 (12%)	6 (6%)	1	0
41	2j	94/105 (90%)	81 (86%)	11 (12%)	2 (2%)	5	5
42	1k	112/129 (87%)	99 (88%)	12 (11%)	1 (1%)	14	20
42	2k	112/129 (87%)	98 (88%)	12 (11%)	2 (2%)	6	7
43	1l	119/132 (90%)	111 (93%)	7 (6%)	1 (1%)	16	22
43	2l	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
44	1m	116/126 (92%)	104 (90%)	10 (9%)	2 (2%)	7	8
44	2m	114/126 (90%)	100 (88%)	13 (11%)	1 (1%)	14	20
45	1n	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7	8
45	2n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	1o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
46	2o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
47	1p	80/88 (91%)	66 (82%)	14 (18%)	0	100	100
47	2p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
48	1q	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
49	1r	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	8	10
50	1s	81/93 (87%)	70 (86%)	11 (14%)	0	100	100
50	2s	81/93 (87%)	73 (90%)	5 (6%)	3 (4%)	2	1
51	1t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	5	5
51	2t	94/106 (89%)	88 (94%)	5 (5%)	1 (1%)	11	15
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	16 (76%)	5 (24%)	0	100	100
54	1w	247/354 (70%)	238 (96%)	6 (2%)	3 (1%)	10	13
54	2w	251/354 (71%)	234 (93%)	16 (6%)	1 (0%)	30	39
56	1z	3/7 (43%)	3 (100%)	0	0	100	100
56	2z	2/7 (29%)	2 (100%)	0	0	100	100
All	All	11848/12850 (92%)	10976 (93%)	765 (6%)	107 (1%)	14	20

5 of 107 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
23	11	3	LYS
26	14	55	ARG
33	1b	10	LEU
33	1b	17	PHE

5.3.2 Protein sidechains [i](#)

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%)	205 (95%)	10 (5%)	23	36
3	2D	215/218 (99%)	200 (93%)	15 (7%)	14	19
4	1E	164/166 (99%)	153 (93%)	11 (7%)	15	21
4	2E	164/166 (99%)	155 (94%)	9 (6%)	19	29
5	1F	160/166 (96%)	147 (92%)	13 (8%)	11	15
5	2F	159/166 (96%)	140 (88%)	19 (12%)	5	5
6	1G	143/156 (92%)	134 (94%)	9 (6%)	16	23
6	2G	143/156 (92%)	122 (85%)	21 (15%)	3	2
7	1H	144/148 (97%)	136 (94%)	8 (6%)	19	29
7	2H	144/148 (97%)	131 (91%)	13 (9%)	9	11
8	1I	113/124 (91%)	97 (86%)	16 (14%)	3	3
8	2I	105/124 (85%)	88 (84%)	17 (16%)	2	2
9	1N	118/119 (99%)	109 (92%)	9 (8%)	12	17
9	2N	118/119 (99%)	110 (93%)	8 (7%)	14	20
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28	42
10	2O	100/100 (100%)	96 (96%)	4 (4%)	28	42
11	1P	115/116 (99%)	109 (95%)	6 (5%)	21	32
11	2P	115/116 (99%)	110 (96%)	5 (4%)	26	39
12	1Q	111/111 (100%)	108 (97%)	3 (3%)	39	58
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	24	38
13	1R	101/101 (100%)	99 (98%)	2 (2%)	48	67
13	2R	101/101 (100%)	99 (98%)	2 (2%)	48	67
14	1S	86/88 (98%)	79 (92%)	7 (8%)	11	15
14	2S	85/88 (97%)	73 (86%)	12 (14%)	3	3
15	1T	115/127 (91%)	107 (93%)	8 (7%)	14	19
15	2T	113/127 (89%)	102 (90%)	11 (10%)	8	9
16	1U	93/94 (99%)	90 (97%)	3 (3%)	34	51
16	2U	93/94 (99%)	88 (95%)	5 (5%)	20	30
17	1V	80/82 (98%)	78 (98%)	2 (2%)	42	60
17	2V	80/82 (98%)	73 (91%)	7 (9%)	9	12
18	1W	90/92 (98%)	88 (98%)	2 (2%)	45	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	2W	90/92 (98%)	86 (96%)	4 (4%)	25	38
19	1X	77/78 (99%)	73 (95%)	4 (5%)	21	32
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28	43
20	1Y	85/91 (93%)	76 (89%)	9 (11%)	6	7
20	2Y	85/91 (93%)	76 (89%)	9 (11%)	6	7
21	1Z	135/179 (75%)	123 (91%)	12 (9%)	9	12
21	2Z	137/179 (76%)	119 (87%)	18 (13%)	4	4
22	10	61/67 (91%)	59 (97%)	2 (3%)	33	50
22	20	61/67 (91%)	60 (98%)	1 (2%)	55	73
23	11	80/83 (96%)	77 (96%)	3 (4%)	29	44
23	21	80/83 (96%)	73 (91%)	7 (9%)	9	12
24	12	65/67 (97%)	61 (94%)	4 (6%)	16	24
24	22	65/67 (97%)	61 (94%)	4 (6%)	16	24
25	13	51/52 (98%)	47 (92%)	4 (8%)	11	16
25	23	50/52 (96%)	47 (94%)	3 (6%)	17	26
26	14	59/63 (94%)	49 (83%)	10 (17%)	2	2
26	24	53/63 (84%)	47 (89%)	6 (11%)	5	6
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	26
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	26
28	16	51/52 (98%)	46 (90%)	5 (10%)	7	9
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	9
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	18
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	9
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	29
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	29
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	55
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	55
33	1b	192/220 (87%)	161 (84%)	31 (16%)	2	2
33	2b	187/220 (85%)	159 (85%)	28 (15%)	3	2
34	1c	142/188 (76%)	129 (91%)	13 (9%)	8	10
34	2c	140/188 (74%)	128 (91%)	12 (9%)	10	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	1d	169/181 (93%)	155 (92%)	14 (8%)	10	14
35	2d	173/181 (96%)	155 (90%)	18 (10%)	7	8
36	1e	113/123 (92%)	101 (89%)	12 (11%)	6	7
36	2e	114/123 (93%)	102 (90%)	12 (10%)	6	8
37	1f	84/90 (93%)	77 (92%)	7 (8%)	10	14
37	2f	85/90 (94%)	81 (95%)	4 (5%)	23	36
38	1g	119/127 (94%)	100 (84%)	19 (16%)	2	2
38	2g	120/127 (94%)	109 (91%)	11 (9%)	8	10
39	1h	114/119 (96%)	106 (93%)	8 (7%)	14	19
39	2h	114/119 (96%)	104 (91%)	10 (9%)	9	12
40	1i	90/99 (91%)	76 (84%)	14 (16%)	2	2
40	2i	89/99 (90%)	71 (80%)	18 (20%)	1	1
41	1j	66/92 (72%)	56 (85%)	10 (15%)	3	2
41	2j	69/92 (75%)	61 (88%)	8 (12%)	5	6
42	1k	82/99 (83%)	76 (93%)	6 (7%)	13	18
42	2k	83/99 (84%)	76 (92%)	7 (8%)	10	14
43	1l	96/108 (89%)	88 (92%)	8 (8%)	10	14
43	2l	96/108 (89%)	91 (95%)	5 (5%)	21	32
44	1m	89/101 (88%)	72 (81%)	17 (19%)	1	1
44	2m	88/101 (87%)	78 (89%)	10 (11%)	5	6
45	1n	49/50 (98%)	42 (86%)	7 (14%)	3	3
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	8
46	1o	78/80 (98%)	70 (90%)	8 (10%)	7	8
46	2o	78/80 (98%)	73 (94%)	5 (6%)	16	23
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7	8
47	2p	68/74 (92%)	57 (84%)	11 (16%)	2	2
48	1q	94/97 (97%)	90 (96%)	4 (4%)	26	39
48	2q	94/97 (97%)	93 (99%)	1 (1%)	65	79
49	1r	59/77 (77%)	57 (97%)	2 (3%)	32	48
49	2r	59/77 (77%)	57 (97%)	2 (3%)	32	48
50	1s	69/80 (86%)	56 (81%)	13 (19%)	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	2s	67/80 (84%)	62 (92%)	5 (8%)	12	17
51	1t	70/82 (85%)	66 (94%)	4 (6%)	18	28
51	2t	70/82 (85%)	66 (94%)	4 (6%)	18	28
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	29
52	2u	18/22 (82%)	18 (100%)	0	100	100
54	1w	204/299 (68%)	186 (91%)	18 (9%)	9	12
54	2w	204/299 (68%)	185 (91%)	19 (9%)	8	10
56	1z	2/3 (67%)	2 (100%)	0	100	100
56	2z	2/3 (67%)	2 (100%)	0	100	100
All	All	9699/10668 (91%)	8881 (92%)	818 (8%)	10	14

5 of 818 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	2H	13	LYS
21	2Z	70	LEU
54	2w	102	MET
8	2I	20	ASP
6	2G	175	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 143 such sidechains are listed below:

Mol	Chain	Res	Type
36	2e	65	ASN
38	2g	153	HIS
44	2m	106	ASN
38	1g	28	ASN
38	1g	13	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	438 (15%)	31 (1%)
1	2A	2791/2915 (95%)	437 (15%)	26 (0%)
2	1B	119/121 (98%)	12 (10%)	0
2	2B	118/121 (97%)	19 (16%)	0
32	1a	1497/1521 (98%)	295 (19%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	2a	1501/1521 (98%)	299 (19%)	0
53	1v	10/24 (41%)	2 (20%)	0
53	2v	10/24 (41%)	3 (30%)	0
55	1x	72/74 (97%)	9 (12%)	0
55	2x	72/74 (97%)	8 (11%)	0
All	All	9054/9310 (97%)	1522 (16%)	57 (0%)

5 of 1522 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	36	G
1	1A	45	C

5 of 57 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2601	C
1	2A	2430	A
1	2A	528	A
1	2A	2406	U
1	2A	1653	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	2A	2552	57,1	19,22,23	1.18	2 (10%)	25,31,34	1.74	5 (20%)
1	5MC	1A	1962	57,1	19,22,23	2.01	3 (15%)	26,32,35	1.18	3 (11%)
32	2MG	1a	1207	32	23,26,27	1.28	4 (17%)	33,38,41	2.10	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	8AN	2x	76	56,57,55	21,24,25	1.34	3 (14%)	26,35,38	2.38	10 (38%)
55	4SU	1x	8	55	18,21,22	2.07	4 (22%)	25,30,33	1.94	4 (16%)
1	PSU	2A	1917	1	18,21,22	1.38	2 (11%)	21,30,33	2.09	4 (19%)
32	4OC	1a	1402	32,57	20,23,24	0.73	0	25,32,35	1.07	1 (4%)
1	5MU	2A	1915	57,1	19,22,23	1.49	4 (21%)	27,32,35	2.04	5 (18%)
32	M2G	2a	966	32	24,27,28	1.31	3 (12%)	33,40,43	1.91	6 (18%)
32	5MC	2a	967	32	19,22,23	1.74	3 (15%)	26,32,35	1.18	3 (11%)
55	8AN	1x	76	56,57,55	21,24,25	1.35	3 (14%)	26,35,38	2.22	10 (38%)
1	5MU	2A	1939	1	19,22,23	1.48	5 (26%)	27,32,35	2.23	6 (22%)
1	OMU	1A	2552	57,1	19,22,23	1.16	1 (5%)	25,31,34	1.90	6 (24%)
32	5MC	2a	1407	32,57	19,22,23	1.61	2 (10%)	26,32,35	1.23	3 (11%)
1	OMC	2A	1920	1	19,22,23	0.80	0	25,31,34	0.86	0
1	2MA	2A	2503	57,1	22,25,26	1.49	4 (18%)	32,37,40	2.40	9 (28%)
1	PSU	1A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	1.91	4 (19%)
32	MA6	2a	1519	32	23,26,27	0.41	0	33,38,41	2.17	10 (30%)
1	OMC	1A	1920	1	19,22,23	0.82	0	25,31,34	0.97	1 (4%)
55	H2U	1x	21	55	18,21,22	1.04	2 (11%)	19,30,33	1.73	3 (15%)
32	UR3	1a	1498	32	19,22,23	1.04	1 (5%)	26,32,35	1.75	5 (19%)
55	H2U	1x	20	55	18,21,22	0.93	2 (11%)	19,30,33	1.03	2 (10%)
32	2MG	2a	1207	32	23,26,27	1.26	3 (13%)	33,38,41	2.06	5 (15%)
32	M2G	1a	966	32	24,27,28	1.28	4 (16%)	33,40,43	1.90	6 (18%)
1	OMG	1A	2251	57,55,1	23,26,27	1.21	3 (13%)	32,38,41	2.01	7 (21%)
55	PSU	1x	32	55	18,21,22	1.33	2 (11%)	21,30,33	2.02	4 (19%)
43	0TD	1l	92	43	8,9,10	4.53	2 (25%)	6,11,13	8.06	2 (33%)
32	MA6	1a	1518	32	23,26,27	0.42	0	33,38,41	2.05	9 (27%)
1	5MC	2A	1942	1	19,22,23	1.56	3 (15%)	26,32,35	1.18	2 (7%)
1	5MC	2A	1962	1	19,22,23	1.52	3 (15%)	26,32,35	1.15	2 (7%)
55	PSU	2x	39	55	18,21,22	1.46	3 (16%)	21,30,33	1.64	3 (14%)
1	PSU	1A	1917	1	18,21,22	1.40	3 (16%)	21,30,33	2.12	5 (23%)
1	5MU	1A	1915	1	19,22,23	1.39	6 (31%)	27,32,35	2.22	6 (22%)
55	PSU	2x	32	55	18,21,22	1.32	2 (11%)	21,30,33	2.07	3 (14%)
32	4OC	2a	1402	32,57	20,23,24	0.78	0	25,32,35	1.11	3 (12%)
32	5MC	1a	1404	32	19,22,23	1.86	3 (15%)	26,32,35	1.18	4 (15%)
55	4SU	2x	8	55	18,21,22	1.81	5 (27%)	25,30,33	2.07	5 (20%)
32	5MC	1a	1400	32	19,22,23	1.83	3 (15%)	26,32,35	1.19	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	1A	1942	57,1	19,22,23	1.56	3 (15%)	26,32,35	1.25	4 (15%)
32	G7M	2a	527	32,57	23,26,27	1.55	3 (13%)	34,39,42	1.74	5 (14%)
55	PSU	1x	39	55	18,21,22	1.55	3 (16%)	21,30,33	1.74	3 (14%)
32	UR3	2a	1498	32	19,22,23	1.02	2 (10%)	26,32,35	1.69	3 (11%)
1	2MA	1A	2503	57,1	22,25,26	1.39	4 (18%)	32,37,40	2.35	10 (31%)
32	5MC	1a	967	32	19,22,23	1.62	2 (10%)	26,32,35	1.10	2 (7%)
1	PSU	2A	1911	1	18,21,22	1.40	3 (16%)	21,30,33	2.14	4 (19%)
55	5MU	1x	54	57,55	19,22,23	1.44	5 (26%)	27,32,35	1.78	5 (18%)
43	0TD	2l	92	43	8,9,10	4.62	1 (12%)	6,11,13	4.83	3 (50%)
55	5MU	2x	54	55	19,22,23	1.43	5 (26%)	27,32,35	1.83	6 (22%)
1	PSU	1A	2605	57,1	18,21,22	1.37	2 (11%)	21,30,33	2.15	4 (19%)
32	PSU	1a	516	32,57	18,21,22	1.37	2 (11%)	21,30,33	2.17	4 (19%)
1	5MU	1A	1939	1	19,22,23	1.52	4 (21%)	27,32,35	2.22	6 (22%)
55	H2U	2x	20	55	18,21,22	0.90	1 (5%)	19,30,33	1.04	1 (5%)
55	PSU	2x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.13	4 (19%)
32	5MC	1a	1407	32	19,22,23	1.73	3 (15%)	26,32,35	1.12	4 (15%)
55	PSU	1x	55	55	18,21,22	1.32	2 (11%)	21,30,33	2.16	4 (19%)
1	OMG	2A	2251	57,55,1	23,26,27	1.19	3 (13%)	32,38,41	1.91	6 (18%)
1	PSU	2A	2605	1	18,21,22	1.41	3 (16%)	21,30,33	2.08	5 (23%)
32	G7M	1a	527	32,57	23,26,27	1.56	4 (17%)	34,39,42	1.70	5 (14%)
32	5MC	2a	1400	32	19,22,23	1.73	3 (15%)	26,32,35	1.22	2 (7%)
32	MA6	2a	1518	32	23,26,27	0.41	0	33,38,41	2.07	9 (27%)
55	MIA	2x	37	55	21,24,32	1.59	3 (14%)	30,35,47	2.10	9 (30%)
32	5MC	2a	1404	32	19,22,23	1.74	3 (15%)	26,32,35	1.12	2 (7%)
55	MIA	1x	37	55	21,24,32	1.54	4 (19%)	30,35,47	2.11	10 (33%)
32	MA6	1a	1519	32	23,26,27	0.41	0	33,38,41	1.97	9 (27%)
32	PSU	2a	516	32,57	18,21,22	1.35	3 (16%)	21,30,33	1.98	5 (23%)
55	H2U	2x	21	55	18,21,22	0.85	2 (11%)	19,30,33	0.85	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	2A	2552	57,1	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1A	1962	57,1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
55	8AN	2x	76	56,57,55	-	1/7/25/26	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32,57	-	2/9/29/30	0/2/2/2
1	5MU	2A	1915	57,1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
55	8AN	1x	76	56,57,55	-	1/7/25/26	0/3/3/3
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	57,1	-	0/9/27/28	0/2/2/2
32	5MC	2a	1407	32,57	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
1	2MA	2A	2503	57,1	-	1/7/25/26	0/3/3/3
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	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
55	H2U	1x	21	55	-	6/7/38/39	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
55	H2U	1x	20	55	-	2/7/38/39	0/2/2/2
32	2MG	2a	1207	32	-	2/9/27/28	0/3/3/3
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	OMG	1A	2251	57,55,1	-	0/9/27/28	0/3/3/3
55	PSU	1x	32	55	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1	-	0/7/25/26	0/2/2/2
55	PSU	2x	39	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
55	PSU	2x	32	55	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,57	-	2/9/29/30	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	57,1	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32,57	-	2/7/25/26	0/3/3/3
55	PSU	1x	39	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	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	57,1	-	1/7/25/26	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	57,55	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	57,1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,57	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
55	H2U	2x	20	55	-	2/7/38/39	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	57,55,1	-	1/9/27/28	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,57	-	3/7/25/26	0/3/3/3
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
55	MIA	2x	37	55	-	2/7/25/34	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
55	MIA	1x	37	55	-	1/7/25/34	0/3/3/3
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
32	PSU	2a	516	32,57	-	2/7/25/26	0/2/2/2
55	H2U	2x	21	55	-	4/7/38/39	0/2/2/2

The worst 5 of 170 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.57	1.69	1.82
43	1l	92	0TD	CB-SB	-12.15	1.70	1.82
1	1A	1962	5MC	C5-C4	7.66	1.49	1.44
32	1a	1404	5MC	C5-C4	6.88	1.49	1.44
32	1a	1400	5MC	C5-C4	6.79	1.49	1.44

The worst 5 of 309 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-19.33	67.63	102.36
43	2l	92	0TD	CSB-SB-CB	-11.05	82.50	102.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2503	2MA	C5-C4-N3	-8.54	118.18	127.18
1	1A	2503	2MA	C5-C4-N3	-7.46	119.33	127.18
32	1a	516	PSU	N1-C2-N3	6.91	122.45	115.17

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
1	2A	2251	OMG	C1'-C2'-O2'-CM2
32	2a	1207	2MG	N1-C2-N2-CM2

There are no ring outliers.

27 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	2552	OMU	2	0
55	2x	76	8AN	2	0
1	2A	1917	PSU	1	0
32	1a	1402	4OC	4	0
32	2a	966	M2G	1	0
1	2A	1939	5MU	1	0
1	2A	1920	OMC	1	0
32	2a	1519	MA6	2	0
1	1A	1920	OMC	2	0
55	1x	21	H2U	1	0
55	1x	20	H2U	1	0
32	2a	1207	2MG	1	0
32	1a	966	M2G	1	0
1	1A	2251	OMG	1	0
32	1a	1518	MA6	1	0
1	2A	1942	5MC	1	0
1	1A	1917	PSU	1	0
1	1A	1915	5MU	1	0
32	2a	1402	4OC	1	0
32	1a	1400	5MC	1	0
32	1a	516	PSU	1	0
1	1A	1939	5MU	1	0
1	2A	2251	OMG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1400	5MC	1	0
32	2a	1518	MA6	3	0
32	2a	1404	5MC	1	0
32	1a	1519	MA6	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2693 ligands modelled in this entry, 2691 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	SF4	2d	303	35	0,12,12	-	-	-		
60	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
60	SF4	2d	303	35	-	-	0/6/5/5
60	SF4	1d	302	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	1A	2860/2915 (98%)	-0.40	157 (5%) 30 30	20, 36, 93, 105	0
1	2A	2789/2915 (95%)	-0.04	123 (4%) 39 39	30, 53, 89, 105	0
2	1B	120/121 (99%)	-0.27	0 100 100	29, 50, 61, 83	0
2	2B	120/121 (99%)	0.67	3 (2%) 58 59	55, 73, 79, 91	0
3	1D	275/276 (99%)	-0.13	3 (1%) 78 79	21, 35, 52, 77	0
3	2D	275/276 (99%)	0.21	3 (1%) 78 79	28, 46, 59, 75	0
4	1E	204/206 (99%)	-0.05	5 (2%) 58 59	20, 40, 58, 75	0
4	2E	204/206 (99%)	0.46	5 (2%) 58 59	30, 54, 67, 74	0
5	1F	203/210 (96%)	-0.06	1 (0%) 87 89	19, 41, 65, 80	0
5	2F	203/210 (96%)	0.57	4 (1%) 65 65	33, 62, 75, 86	0
6	1G	181/182 (99%)	1.26	31 (17%) 4 3	49, 67, 77, 84	0
6	2G	181/182 (99%)	1.46	34 (18%) 3 2	62, 76, 83, 91	0
7	1H	174/180 (96%)	0.48	3 (1%) 69 69	36, 52, 64, 75	0
7	2H	174/180 (96%)	1.52	49 (28%) 1 1	65, 78, 85, 91	0
8	1I	146/148 (98%)	1.08	15 (10%) 12 11	44, 70, 78, 81	0
8	2I	146/148 (98%)	1.51	32 (21%) 2 2	53, 74, 81, 86	0
9	1N	140/140 (100%)	-0.03	1 (0%) 84 86	26, 39, 59, 75	0
9	2N	140/140 (100%)	0.68	6 (4%) 40 40	44, 60, 73, 82	0
10	1O	122/122 (100%)	-0.02	0 100 100	26, 39, 59, 66	0
10	2O	122/122 (100%)	0.26	0 100 100	41, 50, 65, 70	0
11	1P	149/150 (99%)	0.14	1 (0%) 84 86	20, 42, 63, 75	0
11	2P	149/150 (99%)	0.65	3 (2%) 65 65	33, 62, 77, 84	0
12	1Q	141/141 (100%)	0.15	5 (3%) 47 48	26, 39, 54, 61	0
12	2Q	141/141 (100%)	0.80	9 (6%) 25 24	42, 59, 68, 72	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%)	-0.16	0 100 100	26, 35, 50, 59	0
13	2R	118/118 (100%)	0.22	0 100 100	36, 50, 59, 70	0
14	1S	110/112 (98%)	0.35	3 (2%) 56 57	37, 48, 60, 67	0
14	2S	110/112 (98%)	1.25	14 (12%) 8 7	55, 67, 75, 77	0
15	1T	131/146 (89%)	0.19	2 (1%) 72 73	32, 45, 70, 80	0
15	2T	131/146 (89%)	0.51	6 (4%) 37 38	46, 55, 72, 79	0
16	1U	116/118 (98%)	-0.34	0 100 100	21, 30, 48, 56	0
16	2U	116/118 (98%)	0.47	1 (0%) 81 83	38, 55, 68, 76	0
17	1V	101/101 (100%)	-0.19	0 100 100	21, 41, 56, 65	0
17	2V	101/101 (100%)	0.83	4 (3%) 42 43	40, 65, 76, 83	0
18	1W	112/113 (99%)	-0.21	0 100 100	23, 32, 53, 75	0
18	2W	112/113 (99%)	0.35	3 (2%) 56 57	37, 47, 62, 83	0
19	1X	95/96 (98%)	0.02	1 (1%) 78 79	25, 37, 58, 74	0
19	2X	95/96 (98%)	0.75	7 (7%) 20 19	46, 56, 73, 81	0
20	1Y	107/110 (97%)	0.44	2 (1%) 66 66	34, 48, 66, 76	0
20	2Y	107/110 (97%)	1.16	12 (11%) 10 9	57, 67, 78, 82	0
21	1Z	154/206 (74%)	0.74	10 (6%) 25 24	38, 57, 70, 75	0
21	2Z	160/206 (77%)	1.45	28 (17%) 4 3	58, 72, 79, 83	0
22	10	76/85 (89%)	0.03	3 (3%) 43 44	26, 37, 57, 63	0
22	20	76/85 (89%)	0.83	4 (5%) 32 31	45, 58, 69, 73	0
23	11	97/98 (98%)	0.29	3 (3%) 51 52	27, 42, 66, 71	0
23	21	97/98 (98%)	0.58	3 (3%) 51 52	37, 52, 70, 76	0
24	12	70/72 (97%)	0.23	2 (2%) 53 55	33, 48, 59, 75	0
24	22	70/72 (97%)	1.04	6 (8%) 16 15	58, 67, 73, 81	0
25	13	59/60 (98%)	-0.10	2 (3%) 48 49	25, 34, 56, 71	0
25	23	59/60 (98%)	0.64	2 (3%) 48 49	48, 57, 68, 74	0
26	14	69/71 (97%)	1.75	27 (39%) 1 0	59, 81, 90, 91	0
26	24	69/71 (97%)	1.73	21 (30%) 1 0	72, 82, 90, 91	0
27	15	59/60 (98%)	-0.23	1 (1%) 69 69	22, 35, 50, 61	0
27	25	59/60 (98%)	0.36	2 (3%) 48 49	31, 49, 65, 78	0
28	16	53/54 (98%)	-0.14	0 100 100	31, 41, 52, 55	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%)	0.62	1 (1%) 66 66	47, 56, 64, 67	0
29	17	48/49 (97%)	-0.08	4 (8%) 17 17	21, 26, 55, 62	0
29	27	48/49 (97%)	0.09	5 (10%) 11 11	30, 39, 62, 73	0
30	18	64/65 (98%)	-0.16	0 100 100	27, 33, 39, 51	0
30	28	64/65 (98%)	0.37	1 (1%) 70 71	41, 50, 57, 63	0
31	19	37/37 (100%)	0.15	0 100 100	31, 41, 53, 55	0
31	29	37/37 (100%)	1.11	6 (16%) 4 3	50, 63, 72, 74	0
32	1a	1488/1521 (97%)	0.76	105 (7%) 22 21	35, 72, 93, 104	0
32	2a	1491/1521 (98%)	0.65	107 (7%) 21 20	43, 72, 92, 104	0
33	1b	231/256 (90%)	1.77	78 (33%) 1 0	67, 78, 85, 88	0
33	2b	231/256 (90%)	1.85	88 (38%) 1 0	69, 80, 87, 91	0
34	1c	206/239 (86%)	1.78	67 (32%) 1 0	65, 78, 85, 88	0
34	2c	206/239 (86%)	1.82	83 (40%) 0 0	69, 80, 85, 88	0
35	1d	208/209 (99%)	1.53	48 (23%) 2 1	60, 75, 82, 84	0
35	2d	208/209 (99%)	1.36	36 (17%) 4 3	56, 70, 78, 83	0
36	1e	148/162 (91%)	1.11	18 (12%) 8 7	54, 68, 77, 82	0
36	2e	148/162 (91%)	1.13	16 (10%) 11 10	58, 70, 77, 80	0
37	1f	100/101 (99%)	0.95	8 (8%) 18 18	56, 68, 75, 77	0
37	2f	100/101 (99%)	1.17	13 (13%) 7 6	61, 72, 78, 81	0
38	1g	155/156 (99%)	1.30	26 (16%) 4 3	66, 75, 83, 89	0
38	2g	155/156 (99%)	1.59	40 (25%) 1 1	70, 79, 85, 90	0
39	1h	137/138 (99%)	1.13	16 (11%) 9 8	58, 71, 78, 80	0
39	2h	137/138 (99%)	1.13	12 (8%) 15 15	63, 70, 76, 81	0
40	1i	127/128 (99%)	1.63	30 (23%) 2 1	61, 77, 83, 87	0
40	2i	127/128 (99%)	2.42	74 (58%) 0 0	69, 82, 88, 90	0
41	1j	97/105 (92%)	1.91	38 (39%) 1 0	65, 79, 85, 87	0
41	2j	96/105 (91%)	2.49	67 (69%) 0 0	71, 83, 88, 91	0
42	1k	114/129 (88%)	1.01	10 (8%) 15 15	45, 67, 77, 82	0
42	2k	114/129 (88%)	1.21	14 (12%) 8 7	56, 72, 81, 84	0
43	1l	121/132 (91%)	0.99	9 (7%) 20 19	51, 59, 69, 75	0
43	2l	121/132 (91%)	0.81	7 (5%) 29 28	52, 60, 68, 74	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	118/126 (93%)	2.19	64 (54%) 0 0	71, 80, 84, 87	0
44	2m	116/126 (92%)	1.79	40 (34%) 1 0	72, 80, 85, 86	0
45	1n	60/61 (98%)	2.03	26 (43%) 0 0	67, 77, 83, 86	0
45	2n	60/61 (98%)	2.50	39 (65%) 0 0	73, 81, 85, 87	0
46	1o	88/89 (98%)	1.29	19 (21%) 2 2	50, 68, 77, 79	0
46	2o	88/89 (98%)	1.26	14 (15%) 5 4	59, 70, 76, 78	0
47	1p	82/88 (93%)	1.90	32 (39%) 1 0	63, 74, 81, 85	0
47	2p	82/88 (93%)	1.48	14 (17%) 4 3	58, 68, 75, 79	0
48	1q	99/105 (94%)	1.38	17 (17%) 4 3	56, 67, 76, 79	0
48	2q	99/105 (94%)	0.97	3 (3%) 52 54	58, 65, 75, 79	0
49	1r	68/88 (77%)	0.92	5 (7%) 20 19	56, 67, 74, 80	0
49	2r	68/88 (77%)	1.20	8 (11%) 9 8	63, 70, 80, 83	0
50	1s	83/93 (89%)	2.55	61 (73%) 0 0	72, 83, 87, 91	0
50	2s	83/93 (89%)	2.12	45 (54%) 0 0	70, 83, 88, 90	0
51	1t	96/106 (90%)	1.54	21 (21%) 2 2	63, 72, 78, 82	0
51	2t	96/106 (90%)	1.25	17 (17%) 4 3	56, 66, 77, 80	0
52	1u	23/27 (85%)	2.27	11 (47%) 0 0	73, 78, 81, 85	0
52	2u	23/27 (85%)	1.98	9 (39%) 1 0	74, 79, 82, 83	0
53	1v	13/24 (54%)	1.35	4 (30%) 1 0	47, 58, 94, 96	0
53	2v	13/24 (54%)	1.62	7 (53%) 0 0	57, 65, 96, 98	0
54	1w	249/354 (70%)	0.44	4 (1%) 70 71	22, 57, 77, 87	0
54	2w	253/354 (71%)	0.74	16 (6%) 26 25	38, 66, 80, 93	0
55	1x	65/74 (87%)	0.02	0 100 100	26, 60, 80, 83	0
55	2x	65/74 (87%)	0.24	0 100 100	40, 70, 84, 85	0
56	1z	5/7 (71%)	2.13	2 (40%) 1 0	31, 32, 56, 72	0
56	2z	4/7 (57%)	1.59	2 (50%) 0 0	42, 45, 48, 54	0
All	All	21082/22160 (95%)	0.56	2169 (10%) 12 11	19, 61, 85, 105	0

The worst 5 of 2169 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2A	2147	G	9.2
1	1A	2113	U	7.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	174	VAL	7.5
1	1A	2116	G	7.0
38	2g	83	ALA	6.9

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
55	H2U	1x	21	20/21	0.66	0.16	75,86,98,108	0
55	H2U	2x	21	20/21	0.73	0.15	84,92,97,105	0
55	H2U	2x	20	20/21	0.76	0.13	73,86,95,98	0
32	2MG	1a	1207	24/25	0.81	0.16	76,86,93,95	0
55	PSU	2x	55	20/21	0.84	0.11	74,77,87,91	0
55	5MU	2x	54	21/22	0.85	0.12	72,77,85,95	0
32	2MG	2a	1207	24/25	0.85	0.13	74,81,85,87	0
55	PSU	1x	55	20/21	0.86	0.12	69,75,80,85	0
43	0TD	1l	92	10/11	0.86	0.14	51,60,64,72	0
55	5MU	1x	54	21/22	0.87	0.12	69,76,83,86	0
55	H2U	1x	20	20/21	0.87	0.11	67,79,86,91	0
32	M2G	2a	966	25/26	0.90	0.15	50,63,77,85	0
32	PSU	2a	516	20/21	0.90	0.12	54,69,77,77	0
32	M2G	1a	966	25/26	0.91	0.12	51,57,71,83	0
43	0TD	2l	92	10/11	0.91	0.12	53,57,60,78	0
1	5MU	2A	1915	21/22	0.91	0.11	59,63,71,76	0
55	PSU	2x	32	20/21	0.91	0.11	61,68,73,78	0
32	G7M	2a	527	24/25	0.92	0.13	56,62,66,71	0
55	MIA	2x	37	22/30	0.92	0.10	55,65,69,72	0
55	PSU	1x	32	20/21	0.93	0.10	56,61,65,75	0
55	PSU	2x	39	20/21	0.93	0.10	57,67,70,74	0
32	PSU	1a	516	20/21	0.93	0.12	57,67,71,72	0
1	PSU	2A	1911	20/21	0.94	0.09	51,58,61,71	0
32	5MC	2a	1400	21/22	0.94	0.12	62,66,70,74	0
55	MIA	1x	37	22/30	0.94	0.10	50,57,60,60	0
32	5MC	2a	1404	21/22	0.94	0.11	45,52,56,61	0
1	5MU	1A	1915	21/22	0.94	0.10	46,52,58,60	0
32	5MC	1a	967	21/22	0.94	0.11	54,58,66,68	0
1	PSU	1A	1911	20/21	0.94	0.11	43,49,56,61	0
32	G7M	1a	527	24/25	0.94	0.12	53,58,62,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	5MC	2a	967	21/22	0.94	0.12	59,66,74,82	0
32	MA6	2a	1518	24/25	0.95	0.11	45,56,61,62	0
1	PSU	2A	1917	20/21	0.95	0.09	53,60,67,67	0
55	4SU	2x	8	20/21	0.95	0.08	66,71,76,77	0
32	5MC	1a	1400	21/22	0.95	0.10	45,51,55,57	0
32	4OC	1a	1402	22/23	0.95	0.11	42,47,55,57	0
32	4OC	2a	1402	22/23	0.95	0.10	47,56,61,67	0
32	5MC	1a	1404	21/22	0.95	0.11	36,42,46,52	0
32	UR3	2a	1498	21/22	0.95	0.09	47,55,60,62	0
32	MA6	1a	1518	24/25	0.96	0.13	35,42,44,50	0
55	4SU	1x	8	20/21	0.96	0.09	46,55,62,69	0
32	MA6	1a	1519	24/25	0.96	0.11	35,40,44,60	0
55	PSU	1x	39	20/21	0.96	0.08	46,50,56,56	0
1	PSU	1A	1917	20/21	0.96	0.08	43,49,56,56	0
32	5MC	2a	1407	21/22	0.96	0.10	39,49,52,55	0
1	OMC	2A	1920	21/22	0.96	0.10	48,55,59,64	0
1	5MC	2A	1962	21/22	0.96	0.08	37,43,48,54	0
32	MA6	2a	1519	24/25	0.96	0.10	48,58,63,64	0
1	OMG	2A	2251	24/25	0.97	0.08	33,36,42,43	0
1	2MA	2A	2503	23/24	0.97	0.07	28,34,38,40	0
1	PSU	2A	2605	20/21	0.97	0.07	30,34,39,40	0
1	5MC	1A	1962	21/22	0.97	0.07	27,33,37,39	0
1	OMC	1A	1920	21/22	0.97	0.08	34,43,46,47	0
1	5MC	1A	1942	21/22	0.97	0.07	25,32,36,39	0
1	5MC	2A	1942	21/22	0.97	0.08	34,45,50,52	0
32	UR3	1a	1498	21/22	0.97	0.08	38,43,45,46	0
55	8AN	2x	76	22/23	0.97	0.08	30,40,44,46	0
1	OMU	2A	2552	21/22	0.98	0.07	31,36,41,42	0
1	OMU	1A	2552	21/22	0.98	0.07	24,28,33,35	0
1	PSU	1A	2605	20/21	0.98	0.07	22,25,31,33	0
1	5MU	2A	1939	21/22	0.98	0.08	27,34,37,39	0
1	5MU	1A	1939	21/22	0.98	0.06	21,26,29,32	0
1	OMG	1A	2251	24/25	0.98	0.07	22,26,30,39	0
1	2MA	1A	2503	23/24	0.98	0.06	18,21,23,25	0
55	8AN	1x	76	22/23	0.98	0.06	21,25,29,30	0
32	5MC	1a	1407	21/22	0.98	0.07	31,41,44,45	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands i

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1A	3961	1/1	-0.04	0.37	87,87,87,87	0
57	MG	2j	201	1/1	0.19	0.26	88,88,88,88	0
57	MG	1l	201	1/1	0.38	0.16	75,75,75,75	0
57	MG	1a	1819	1/1	0.48	0.29	74,74,74,74	0
57	MG	2A	3650	1/1	0.50	0.35	76,76,76,76	0
57	MG	2A	3259	1/1	0.52	0.40	77,77,77,77	0
57	MG	1A	3981	1/1	0.52	0.22	70,70,70,70	0
57	MG	1a	1786	1/1	0.52	0.18	86,86,86,86	0
57	MG	1a	1783	1/1	0.53	0.27	91,91,91,91	0
57	MG	2A	3699	1/1	0.54	0.26	70,70,70,70	0
57	MG	1a	1667	1/1	0.54	0.19	82,82,82,82	0
57	MG	2A	3435	1/1	0.55	0.44	84,84,84,84	0
57	MG	1a	1778	1/1	0.55	0.28	88,88,88,88	0
57	MG	2a	1729	1/1	0.58	0.30	83,83,83,83	0
57	MG	1A	3966	1/1	0.59	0.23	71,71,71,71	0
57	MG	1A	3400	1/1	0.59	0.19	63,63,63,63	0
57	MG	2A	3714	1/1	0.61	0.23	46,46,46,46	0
57	MG	2A	3845	1/1	0.61	0.30	63,63,63,63	0
57	MG	1A	3930	1/1	0.61	0.24	71,71,71,71	0
57	MG	1A	3928	1/1	0.61	0.32	38,38,38,38	0
57	MG	2a	1760	1/1	0.62	0.21	74,74,74,74	0
57	MG	2B	205	1/1	0.65	0.33	76,76,76,76	0
57	MG	1A	3996	1/1	0.65	0.13	77,77,77,77	0
57	MG	2A	3050	1/1	0.66	0.31	76,76,76,76	0
57	MG	1a	1677	1/1	0.67	0.18	71,71,71,71	0
57	MG	2A	3532	1/1	0.67	0.23	46,46,46,46	0
57	MG	2a	1731	1/1	0.67	0.28	70,70,70,70	0
57	MG	2A	3757	1/1	0.67	0.19	79,79,79,79	0
57	MG	1B	231	1/1	0.67	0.26	69,69,69,69	0
57	MG	2A	3682	1/1	0.68	0.21	55,55,55,55	0
57	MG	2A	3193	1/1	0.68	0.35	78,78,78,78	0
57	MG	2a	1759	1/1	0.68	0.23	71,71,71,71	0
57	MG	2A	3239	1/1	0.68	0.44	81,81,81,81	0
57	MG	2a	1656	1/1	0.68	0.26	83,83,83,83	0
57	MG	1A	3963	1/1	0.69	0.17	69,69,69,69	0
57	MG	2a	1722	1/1	0.69	0.21	86,86,86,86	0
57	MG	2A	3316	1/1	0.69	0.16	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	1665	1/1	0.69	0.19	78,78,78,78	0
57	MG	1A	4018	1/1	0.69	0.14	67,67,67,67	0
57	MG	1A	4025	1/1	0.69	0.19	49,49,49,49	0
57	MG	2A	3674	1/1	0.69	0.26	77,77,77,77	0
57	MG	1A	4034	1/1	0.70	0.21	62,62,62,62	0
57	MG	2A	3372	1/1	0.70	0.25	74,74,74,74	0
57	MG	2A	3430	1/1	0.70	0.38	70,70,70,70	0
57	MG	1A	3793	1/1	0.70	0.30	66,66,66,66	0
57	MG	2A	3687	1/1	0.70	0.17	79,79,79,79	0
57	MG	2A	3693	1/1	0.70	0.18	65,65,65,65	0
57	MG	1a	1758	1/1	0.71	0.21	82,82,82,82	0
57	MG	1a	1763	1/1	0.71	0.24	66,66,66,66	0
57	MG	2A	3761	1/1	0.71	0.15	81,81,81,81	0
57	MG	2x	110	1/1	0.71	0.30	76,76,76,76	0
57	MG	2A	3364	1/1	0.72	0.27	61,61,61,61	0
57	MG	2A	3085	1/1	0.72	0.38	78,78,78,78	0
57	MG	1A	4068	1/1	0.72	0.23	50,50,50,50	0
57	MG	1A	3820	1/1	0.72	0.22	74,74,74,74	0
57	MG	1a	1625	1/1	0.72	0.31	70,70,70,70	0
57	MG	2A	3560	1/1	0.72	0.25	73,73,73,73	0
57	MG	2A	3590	1/1	0.72	0.23	73,73,73,73	0
57	MG	1a	1732	1/1	0.72	0.29	82,82,82,82	0
57	MG	2A	3669	1/1	0.72	0.14	64,64,64,64	0
57	MG	2A	3227	1/1	0.73	0.21	79,79,79,79	0
57	MG	2a	1732	1/1	0.73	0.17	84,84,84,84	0
57	MG	2A	3244	1/1	0.73	0.12	69,69,69,69	0
57	MG	1B	230	1/1	0.74	0.17	76,76,76,76	0
57	MG	2A	3755	1/1	0.74	0.25	73,73,73,73	0
57	MG	1A	3985	1/1	0.74	0.18	52,52,52,52	0
57	MG	2a	1769	1/1	0.74	0.34	73,73,73,73	0
57	MG	2A	3242	1/1	0.74	0.27	74,74,74,74	0
57	MG	1W	206	1/1	0.74	0.19	58,58,58,58	0
57	MG	2A	3087	1/1	0.75	0.19	80,80,80,80	0
57	MG	2B	203	1/1	0.75	0.20	69,69,69,69	0
57	MG	2A	3274	1/1	0.75	0.29	64,64,64,64	0
57	MG	2A	3169	1/1	0.75	0.26	72,72,72,72	0
57	MG	1A	3225	1/1	0.75	0.20	52,52,52,52	0
57	MG	2A	3200	1/1	0.75	0.20	74,74,74,74	0
57	MG	2A	3373	1/1	0.75	0.20	67,67,67,67	0
57	MG	1A	3232	1/1	0.75	0.33	68,68,68,68	0
57	MG	1A	3330	1/1	0.75	0.19	63,63,63,63	0
57	MG	2A	3727	1/1	0.75	0.17	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	3074	1/1	0.75	0.27	65,65,65,65	0
57	MG	2A	3243	1/1	0.75	0.23	78,78,78,78	0
57	MG	1G	203	1/1	0.75	0.14	58,58,58,58	0
57	MG	1A	3816	1/1	0.76	0.17	58,58,58,58	0
57	MG	1A	4054	1/1	0.76	0.15	71,71,71,71	0
57	MG	2A	3235	1/1	0.76	0.27	66,66,66,66	0
57	MG	2a	1755	1/1	0.76	0.26	73,73,73,73	0
57	MG	1A	3734	1/1	0.76	0.20	62,62,62,62	0
57	MG	1a	1706	1/1	0.76	0.25	67,67,67,67	0
57	MG	2R	202	1/1	0.76	0.22	62,62,62,62	0
57	MG	1a	1709	1/1	0.76	0.17	70,70,70,70	0
57	MG	1A	3699	1/1	0.76	0.28	68,68,68,68	0
57	MG	1a	1654	1/1	0.77	0.27	76,76,76,76	0
57	MG	2B	212	1/1	0.77	0.25	74,74,74,74	0
57	MG	2B	220	1/1	0.77	0.18	75,75,75,75	0
57	MG	1A	3865	1/1	0.77	0.17	27,27,27,27	0
57	MG	1A	3882	1/1	0.77	0.12	58,58,58,58	0
57	MG	1G	204	1/1	0.77	0.16	67,67,67,67	0
57	MG	1A	3785	1/1	0.77	0.14	58,58,58,58	0
57	MG	1a	1805	1/1	0.77	0.24	63,63,63,63	0
57	MG	2A	3586	1/1	0.77	0.16	49,49,49,49	0
57	MG	2A	3749	1/1	0.77	0.13	73,73,73,73	0
57	MG	1a	1620	1/1	0.77	0.17	74,74,74,74	0
57	MG	2A	3632	1/1	0.77	0.14	74,74,74,74	0
57	MG	2A	3330	1/1	0.77	0.23	66,66,66,66	0
57	MG	2a	1771	1/1	0.77	0.21	79,79,79,79	0
57	MG	2A	3661	1/1	0.77	0.27	52,52,52,52	0
57	MG	1A	3821	1/1	0.77	0.18	50,50,50,50	0
57	MG	1A	3603	1/1	0.78	0.15	53,53,53,53	0
57	MG	1A	3364	1/1	0.78	0.15	49,49,49,49	0
57	MG	1T	201	1/1	0.78	0.25	60,60,60,60	0
57	MG	1a	1810	1/1	0.78	0.15	76,76,76,76	0
57	MG	2B	214	1/1	0.78	0.18	69,69,69,69	0
57	MG	1a	1699	1/1	0.78	0.32	69,69,69,69	0
57	MG	2E	305	1/1	0.78	0.25	70,70,70,70	0
57	MG	1A	3708	1/1	0.78	0.16	58,58,58,58	0
57	MG	2a	1648	1/1	0.78	0.29	63,63,63,63	0
57	MG	1A	3405	1/1	0.78	0.14	69,69,69,69	0
57	MG	2a	1711	1/1	0.78	0.19	68,68,68,68	0
57	MG	1a	1726	1/1	0.78	0.33	75,75,75,75	0
57	MG	1A	4001	1/1	0.78	0.15	36,36,36,36	0
57	MG	2A	3341	1/1	0.78	0.32	79,79,79,79	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	2A	3167	1/1	0.78	0.19	74,74,74,74	0
57	MG	2a	1745	1/1	0.78	0.23	73,73,73,73	0
57	MG	1a	1753	1/1	0.78	0.18	81,81,81,81	0
57	MG	2A	3179	1/1	0.78	0.27	60,60,60,60	0
57	MG	2A	3421	1/1	0.78	0.22	65,65,65,65	0
57	MG	1a	1628	1/1	0.78	0.35	69,69,69,69	0
57	MG	1a	1640	1/1	0.78	0.21	76,76,76,76	0
57	MG	2A	3480	1/1	0.78	0.19	57,57,57,57	0
57	MG	2x	109	1/1	0.78	0.27	70,70,70,70	0
57	MG	1A	3593	1/1	0.78	0.14	30,30,30,30	0
57	MG	2A	3371	1/1	0.79	0.30	60,60,60,60	0
57	MG	2A	3164	1/1	0.79	0.21	67,67,67,67	0
57	MG	2A	3662	1/1	0.79	0.18	69,69,69,69	0
57	MG	1a	1749	1/1	0.79	0.21	69,69,69,69	0
57	MG	2A	3382	1/1	0.79	0.17	50,50,50,50	0
57	MG	2a	1617	1/1	0.79	0.22	62,62,62,62	0
57	MG	2a	1645	1/1	0.79	0.40	66,66,66,66	0
57	MG	2A	3390	1/1	0.79	0.20	73,73,73,73	0
57	MG	1A	3035	1/1	0.79	0.20	51,51,51,51	0
57	MG	2A	3249	1/1	0.79	0.14	57,57,57,57	0
57	MG	2a	1720	1/1	0.79	0.20	54,54,54,54	0
57	MG	1a	1636	1/1	0.79	0.21	69,69,69,69	0
57	MG	2A	3704	1/1	0.79	0.15	56,56,56,56	0
57	MG	2A	3273	1/1	0.79	0.29	63,63,63,63	0
57	MG	1A	3940	1/1	0.79	0.35	70,70,70,70	0
57	MG	2A	3539	1/1	0.79	0.12	40,40,40,40	0
57	MG	19	101	1/1	0.79	0.23	59,59,59,59	0
57	MG	1A	3809	1/1	0.79	0.15	39,39,39,39	0
57	MG	1R	205	1/1	0.79	0.17	45,45,45,45	0
57	MG	2A	3611	1/1	0.79	0.18	41,41,41,41	0
57	MG	2A	3847	1/1	0.79	0.22	69,69,69,69	0
57	MG	2A	3848	1/1	0.79	0.20	58,58,58,58	0
57	MG	2A	3094	1/1	0.79	0.18	77,77,77,77	0
57	MG	2A	3633	1/1	0.79	0.21	66,66,66,66	0
57	MG	1A	3706	1/1	0.80	0.14	50,50,50,50	0
57	MG	2A	3290	1/1	0.80	0.21	76,76,76,76	0
57	MG	2A	3299	1/1	0.80	0.26	65,65,65,65	0
57	MG	2B	215	1/1	0.80	0.17	77,77,77,77	0
57	MG	2A	3301	1/1	0.80	0.21	57,57,57,57	0
57	MG	1a	1647	1/1	0.80	0.38	77,77,77,77	0
57	MG	1A	3982	1/1	0.80	0.18	72,72,72,72	0
57	MG	2A	3667	1/1	0.80	0.27	71,71,71,71	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	3948	1/1	0.80	0.14	64,64,64,64	0
57	MG	1A	4055	1/1	0.80	0.17	56,56,56,56	0
57	MG	2A	3180	1/1	0.80	0.16	58,58,58,58	0
57	MG	2a	1672	1/1	0.80	0.19	75,75,75,75	0
57	MG	1A	3592	1/1	0.80	0.14	56,56,56,56	0
57	MG	1a	1682	1/1	0.80	0.24	70,70,70,70	0
57	MG	2A	3212	1/1	0.80	0.20	61,61,61,61	0
57	MG	1a	1796	1/1	0.80	0.20	74,74,74,74	0
57	MG	1a	1690	1/1	0.80	0.14	63,63,63,63	0
57	MG	1a	1610	1/1	0.80	0.38	83,83,83,83	0
57	MG	1B	220	1/1	0.80	0.14	65,65,65,65	0
57	MG	1A	3496	1/1	0.80	0.12	63,63,63,63	0
57	MG	2A	3004	1/1	0.80	0.28	71,71,71,71	0
57	MG	2A	3246	1/1	0.80	0.16	60,60,60,60	0
57	MG	1A	4005	1/1	0.80	0.11	39,39,39,39	0
57	MG	2A	3575	1/1	0.80	0.25	63,63,63,63	0
57	MG	1A	3854	1/1	0.80	0.27	41,41,41,41	0
57	MG	2A	3853	1/1	0.80	0.41	74,74,74,74	0
57	MG	1a	1734	1/1	0.80	0.28	70,70,70,70	0
57	MG	1A	3984	1/1	0.81	0.14	58,58,58,58	0
57	MG	1A	4037	1/1	0.81	0.21	48,48,48,48	0
57	MG	2A	3321	1/1	0.81	0.17	69,69,69,69	0
57	MG	1a	1817	1/1	0.81	0.18	64,64,64,64	0
57	MG	1a	1818	1/1	0.81	0.18	70,70,70,70	0
57	MG	1A	3777	1/1	0.81	0.22	57,57,57,57	0
57	MG	1a	1757	1/1	0.81	0.37	79,79,79,79	0
57	MG	1n	101	1/1	0.81	0.11	69,69,69,69	0
57	MG	1a	1697	1/1	0.81	0.34	62,62,62,62	0
57	MG	2a	1616	1/1	0.81	0.19	56,56,56,56	0
57	MG	2A	3030	1/1	0.81	0.16	72,72,72,72	0
57	MG	1A	3516	1/1	0.81	0.17	67,67,67,67	0
57	MG	1A	3918	1/1	0.81	0.15	61,61,61,61	0
57	MG	1a	1781	1/1	0.81	0.21	69,69,69,69	0
57	MG	2A	3090	1/1	0.81	0.26	53,53,53,53	0
57	MG	2a	1676	1/1	0.81	0.13	72,72,72,72	0
57	MG	1a	1782	1/1	0.81	0.18	79,79,79,79	0
57	MG	2a	1718	1/1	0.81	0.20	68,68,68,68	0
57	MG	2A	3529	1/1	0.81	0.16	40,40,40,40	0
57	MG	2A	3734	1/1	0.81	0.25	77,77,77,77	0
57	MG	2A	3262	1/1	0.81	0.14	68,68,68,68	0
57	MG	2A	3119	1/1	0.81	0.23	63,63,63,63	0
57	MG	1A	3349	1/1	0.81	0.20	56,56,56,56	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	3275	1/1	0.81	0.18	59,59,59,59	0
57	MG	2A	3772	1/1	0.81	0.12	72,72,72,72	0
57	MG	2A	3813	1/1	0.81	0.14	45,45,45,45	0
57	MG	2A	3815	1/1	0.81	0.23	58,58,58,58	0
57	MG	2a	1766	1/1	0.81	0.27	71,71,71,71	0
57	MG	2A	3826	1/1	0.81	0.14	55,55,55,55	0
57	MG	1A	3828	1/1	0.81	0.26	63,63,63,63	0
57	MG	2A	3587	1/1	0.81	0.15	51,51,51,51	0
57	MG	2x	104	1/1	0.81	0.42	87,87,87,87	0
57	MG	1A	3756	1/1	0.81	0.09	20,20,20,20	0
57	MG	2A	3850	1/1	0.81	0.18	53,53,53,53	0
57	MG	1A	3698	1/1	0.82	0.11	68,68,68,68	0
57	MG	1a	1808	1/1	0.82	0.25	77,77,77,77	0
57	MG	1A	3421	1/1	0.82	0.19	61,61,61,61	0
57	MG	1a	1708	1/1	0.82	0.16	82,82,82,82	0
57	MG	1A	3986	1/1	0.82	0.11	36,36,36,36	0
57	MG	2A	3380	1/1	0.82	0.27	60,60,60,60	0
57	MG	2a	1637	1/1	0.82	0.24	61,61,61,61	0
57	MG	1A	3424	1/1	0.82	0.15	53,53,53,53	0
57	MG	1A	3450	1/1	0.82	0.25	71,71,71,71	0
57	MG	1A	3210	1/1	0.82	0.16	72,72,72,72	0
57	MG	2A	3725	1/1	0.82	0.16	63,63,63,63	0
57	MG	1a	1648	1/1	0.82	0.13	68,68,68,68	0
57	MG	2a	1679	1/1	0.82	0.31	63,63,63,63	0
57	MG	2a	1706	1/1	0.82	0.18	57,57,57,57	0
57	MG	2A	3022	1/1	0.82	0.31	71,71,71,71	0
57	MG	1A	4015	1/1	0.82	0.14	64,64,64,64	0
57	MG	1A	4017	1/1	0.82	0.15	69,69,69,69	0
57	MG	1A	3361	1/1	0.82	0.24	57,57,57,57	0
57	MG	1A	3328	1/1	0.82	0.24	56,56,56,56	0
57	MG	2A	3542	1/1	0.82	0.11	78,78,78,78	0
57	MG	2A	3265	1/1	0.82	0.21	71,71,71,71	0
57	MG	2a	1742	1/1	0.82	0.23	71,71,71,71	0
57	MG	2A	3088	1/1	0.82	0.16	63,63,63,63	0
57	MG	2a	1746	1/1	0.82	0.22	76,76,76,76	0
57	MG	1a	1775	1/1	0.82	0.19	69,69,69,69	0
57	MG	1a	1678	1/1	0.82	0.16	67,67,67,67	0
57	MG	2A	3278	1/1	0.82	0.15	68,68,68,68	0
57	MG	1a	1680	1/1	0.82	0.20	69,69,69,69	0
57	MG	2A	3136	1/1	0.82	0.25	71,71,71,71	0
57	MG	2a	1770	1/1	0.82	0.26	80,80,80,80	0
57	MG	1A	3329	1/1	0.82	0.19	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	2a	1773	1/1	0.82	0.15	64,64,64,64	0
57	MG	2A	3639	1/1	0.82	0.14	68,68,68,68	0
57	MG	1a	1688	1/1	0.82	0.32	70,70,70,70	0
57	MG	1A	3145	1/1	0.82	0.11	52,52,52,52	0
57	MG	1A	4038	1/1	0.82	0.11	54,54,54,54	0
57	MG	1A	3627	1/1	0.83	0.12	72,72,72,72	0
57	MG	2A	3842	1/1	0.83	0.12	30,30,30,30	0
57	MG	2A	3843	1/1	0.83	0.21	60,60,60,60	0
57	MG	1A	3648	1/1	0.83	0.15	57,57,57,57	0
57	MG	2A	3442	1/1	0.83	0.10	61,61,61,61	0
57	MG	2A	3460	1/1	0.83	0.18	72,72,72,72	0
57	MG	1a	1705	1/1	0.83	0.24	74,74,74,74	0
57	MG	1A	3671	1/1	0.83	0.15	58,58,58,58	0
57	MG	1A	3515	1/1	0.83	0.26	45,45,45,45	0
57	MG	1A	3350	1/1	0.83	0.22	66,66,66,66	0
57	MG	1A	3580	1/1	0.83	0.12	40,40,40,40	0
57	MG	2A	3252	1/1	0.83	0.18	58,58,58,58	0
57	MG	1A	3971	1/1	0.83	0.14	64,64,64,64	0
57	MG	2B	219	1/1	0.83	0.17	71,71,71,71	0
57	MG	1A	3972	1/1	0.83	0.12	48,48,48,48	0
57	MG	1A	3006	1/1	0.83	0.23	58,58,58,58	0
57	MG	1a	1642	1/1	0.83	0.28	70,70,70,70	0
57	MG	23	101	1/1	0.83	0.22	64,64,64,64	0
57	MG	1a	1646	1/1	0.83	0.13	87,87,87,87	0
57	MG	2A	3620	1/1	0.83	0.13	48,48,48,48	0
57	MG	2a	1633	1/1	0.83	0.40	70,70,70,70	0
57	MG	1A	4065	1/1	0.83	0.20	65,65,65,65	0
57	MG	2a	1643	1/1	0.83	0.20	77,77,77,77	0
57	MG	1A	3263	1/1	0.83	0.24	80,80,80,80	0
57	MG	2A	3638	1/1	0.83	0.23	73,73,73,73	0
57	MG	2A	3288	1/1	0.83	0.09	72,72,72,72	0
57	MG	2a	1669	1/1	0.83	0.34	63,63,63,63	0
57	MG	2A	3111	1/1	0.83	0.38	60,60,60,60	0
57	MG	2A	3653	1/1	0.83	0.14	66,66,66,66	0
57	MG	2A	3658	1/1	0.83	0.12	54,54,54,54	0
57	MG	2a	1681	1/1	0.83	0.21	61,61,61,61	0
57	MG	2A	3296	1/1	0.83	0.15	56,56,56,56	0
57	MG	1A	4070	1/1	0.83	0.15	61,61,61,61	0
57	MG	2A	3300	1/1	0.83	0.43	45,45,45,45	0
57	MG	1B	208	1/1	0.83	0.17	63,63,63,63	0
57	MG	2A	3305	1/1	0.83	0.16	70,70,70,70	0
57	MG	2A	3314	1/1	0.83	0.27	68,68,68,68	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	3737	1/1	0.83	0.11	49,49,49,49	0
57	MG	2A	3165	1/1	0.83	0.26	68,68,68,68	0
57	MG	2a	1738	1/1	0.83	0.31	68,68,68,68	0
57	MG	2a	1740	1/1	0.83	0.19	75,75,75,75	0
57	MG	2A	3329	1/1	0.83	0.30	69,69,69,69	0
57	MG	1A	3751	1/1	0.83	0.11	32,32,32,32	0
57	MG	1A	3915	1/1	0.83	0.14	46,46,46,46	0
57	MG	2a	1747	1/1	0.83	0.15	74,74,74,74	0
57	MG	2A	3355	1/1	0.83	0.25	67,67,67,67	0
57	MG	1D	310	1/1	0.83	0.19	48,48,48,48	0
57	MG	1a	1794	1/1	0.83	0.17	45,45,45,45	0
57	MG	1A	3505	1/1	0.83	0.31	69,69,69,69	0
57	MG	1a	1687	1/1	0.83	0.23	66,66,66,66	0
57	MG	1A	3623	1/1	0.83	0.18	53,53,53,53	0
57	MG	2A	3216	1/1	0.83	0.20	69,69,69,69	0
57	MG	2A	3223	1/1	0.83	0.35	50,50,50,50	0
57	MG	2A	3777	1/1	0.83	0.16	63,63,63,63	0
57	MG	2q	203	1/1	0.83	0.30	75,75,75,75	0
57	MG	2A	3792	1/1	0.83	0.18	54,54,54,54	0
57	MG	1A	3929	1/1	0.83	0.17	31,31,31,31	0
57	MG	2A	3426	1/1	0.83	0.26	65,65,65,65	0
57	MG	1E	312	1/1	0.84	0.16	59,59,59,59	0
57	MG	2B	213	1/1	0.84	0.26	70,70,70,70	0
57	MG	1a	1674	1/1	0.84	0.19	77,77,77,77	0
57	MG	1F	304	1/1	0.84	0.11	60,60,60,60	0
57	MG	1A	3864	1/1	0.84	0.32	66,66,66,66	0
57	MG	2A	3174	1/1	0.84	0.14	73,73,73,73	0
57	MG	2D	308	1/1	0.84	0.13	62,62,62,62	0
57	MG	2A	3307	1/1	0.84	0.33	50,50,50,50	0
57	MG	1A	4019	1/1	0.84	0.13	53,53,53,53	0
57	MG	2A	3315	1/1	0.84	0.12	64,64,64,64	0
57	MG	2a	1607	1/1	0.84	0.16	53,53,53,53	0
57	MG	2A	3651	1/1	0.84	0.23	61,61,61,61	0
57	MG	1A	3385	1/1	0.84	0.15	63,63,63,63	0
57	MG	2a	1632	1/1	0.84	0.14	65,65,65,65	0
57	MG	2A	3191	1/1	0.84	0.22	66,66,66,66	0
57	MG	1A	3876	1/1	0.84	0.14	23,23,23,23	0
57	MG	1a	1804	1/1	0.84	0.24	77,77,77,77	0
57	MG	2A	3332	1/1	0.84	0.16	55,55,55,55	0
57	MG	2A	3203	1/1	0.84	0.24	61,61,61,61	0
57	MG	2A	3353	1/1	0.84	0.12	71,71,71,71	0
57	MG	2a	1662	1/1	0.84	0.17	73,73,73,73	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	3026	1/1	0.84	0.19	59,59,59,59	0
57	MG	2A	3686	1/1	0.84	0.09	64,64,64,64	0
57	MG	2a	1675	1/1	0.84	0.29	67,67,67,67	0
57	MG	2A	3357	1/1	0.84	0.11	69,69,69,69	0
57	MG	1A	3894	1/1	0.84	0.15	32,32,32,32	0
57	MG	2A	3696	1/1	0.84	0.18	73,73,73,73	0
57	MG	1a	1691	1/1	0.84	0.47	64,64,64,64	0
57	MG	1a	1606	1/1	0.84	0.12	63,63,63,63	0
57	MG	1A	3899	1/1	0.84	0.21	48,48,48,48	0
57	MG	1a	1612	1/1	0.84	0.30	67,67,67,67	0
57	MG	1A	3901	1/1	0.84	0.23	53,53,53,53	0
57	MG	1A	4057	1/1	0.84	0.13	41,41,41,41	0
57	MG	2A	3411	1/1	0.84	0.23	57,57,57,57	0
57	MG	2A	3752	1/1	0.84	0.11	58,58,58,58	0
57	MG	2a	1737	1/1	0.84	0.19	77,77,77,77	0
57	MG	1A	3568	1/1	0.84	0.22	48,48,48,48	0
57	MG	1A	3487	1/1	0.84	0.22	67,67,67,67	0
57	MG	1a	1730	1/1	0.84	0.38	68,68,68,68	0
57	MG	1A	3669	1/1	0.84	0.10	48,48,48,48	0
57	MG	2A	3255	1/1	0.84	0.42	64,64,64,64	0
57	MG	2A	3790	1/1	0.84	0.17	51,51,51,51	0
57	MG	2A	3449	1/1	0.84	0.12	69,69,69,69	0
57	MG	1A	4085	1/1	0.84	0.19	54,54,54,54	0
57	MG	2A	3470	1/1	0.84	0.29	66,66,66,66	0
57	MG	2a	1765	1/1	0.84	0.21	80,80,80,80	0
57	MG	1A	3343	1/1	0.84	0.15	69,69,69,69	0
57	MG	1a	1752	1/1	0.84	0.17	68,68,68,68	0
57	MG	1A	3694	1/1	0.84	0.12	47,47,47,47	0
57	MG	1A	3837	1/1	0.84	0.13	64,64,64,64	0
57	MG	1A	3947	1/1	0.84	0.10	28,28,28,28	0
57	MG	2d	302	1/1	0.84	0.12	69,69,69,69	0
57	MG	2f	203	1/1	0.84	0.31	74,74,74,74	0
57	MG	2A	3552	1/1	0.84	0.17	70,70,70,70	0
57	MG	1a	1662	1/1	0.84	0.24	78,78,78,78	0
57	MG	2A	3280	1/1	0.84	0.10	59,59,59,59	0
57	MG	1A	3264	1/1	0.84	0.15	61,61,61,61	0
57	MG	2A	3146	1/1	0.84	0.24	65,65,65,65	0
57	MG	1A	3819	1/1	0.85	0.13	56,56,56,56	0
57	MG	1A	3967	1/1	0.85	0.16	61,61,61,61	0
57	MG	1A	3970	1/1	0.85	0.20	64,64,64,64	0
57	MG	1A	3422	1/1	0.85	0.15	48,48,48,48	0
57	MG	1Y	202	1/1	0.85	0.29	51,51,51,51	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	2A	3622	1/1	0.85	0.34	63,63,63,63	0
57	MG	1a	1686	1/1	0.85	0.33	74,74,74,74	0
57	MG	1A	3254	1/1	0.85	0.14	57,57,57,57	0
57	MG	1A	3973	1/1	0.85	0.14	29,29,29,29	0
57	MG	2A	3322	1/1	0.85	0.37	73,73,73,73	0
57	MG	25	102	1/1	0.85	0.17	57,57,57,57	0
57	MG	2a	1605	1/1	0.85	0.31	67,67,67,67	0
57	MG	2A	3643	1/1	0.85	0.18	64,64,64,64	0
57	MG	2a	1609	1/1	0.85	0.15	67,67,67,67	0
57	MG	1A	3974	1/1	0.85	0.12	39,39,39,39	0
57	MG	2A	3205	1/1	0.85	0.11	75,75,75,75	0
57	MG	2A	3331	1/1	0.85	0.21	73,73,73,73	0
57	MG	2A	3207	1/1	0.85	0.19	69,69,69,69	0
57	MG	2a	1636	1/1	0.85	0.20	63,63,63,63	0
57	MG	1A	3912	1/1	0.85	0.12	47,47,47,47	0
57	MG	1a	1692	1/1	0.85	0.23	73,73,73,73	0
57	MG	1A	3822	1/1	0.85	0.13	46,46,46,46	0
57	MG	2a	1646	1/1	0.85	0.28	72,72,72,72	0
57	MG	1A	3170	1/1	0.85	0.29	58,58,58,58	0
57	MG	2a	1650	1/1	0.85	0.25	66,66,66,66	0
57	MG	1A	3578	1/1	0.85	0.21	55,55,55,55	0
57	MG	2a	1658	1/1	0.85	0.32	62,62,62,62	0
57	MG	2A	3370	1/1	0.85	0.27	66,66,66,66	0
57	MG	1A	3853	1/1	0.85	0.10	38,38,38,38	0
57	MG	1l	202	1/1	0.85	0.12	62,62,62,62	0
57	MG	1A	3460	1/1	0.85	0.20	67,67,67,67	0
57	MG	1x	106	1/1	0.85	0.15	57,57,57,57	0
57	MG	2a	1678	1/1	0.85	0.36	73,73,73,73	0
57	MG	1A	3858	1/1	0.85	0.27	46,46,46,46	0
57	MG	2A	3387	1/1	0.85	0.13	67,67,67,67	0
57	MG	2A	3712	1/1	0.85	0.12	64,64,64,64	0
57	MG	1a	1721	1/1	0.85	0.19	55,55,55,55	0
57	MG	2A	3721	1/1	0.85	0.10	61,61,61,61	0
57	MG	1A	3101	1/1	0.85	0.31	72,72,72,72	0
57	MG	2A	3415	1/1	0.85	0.34	60,60,60,60	0
57	MG	2A	3254	1/1	0.85	0.18	58,58,58,58	0
57	MG	2A	3424	1/1	0.85	0.18	72,72,72,72	0
57	MG	1A	3412	1/1	0.85	0.09	56,56,56,56	0
57	MG	1D	313	1/1	0.85	0.13	39,39,39,39	0
57	MG	1a	1733	1/1	0.85	0.15	76,76,76,76	0
57	MG	1a	1652	1/1	0.85	0.15	56,56,56,56	0
57	MG	2A	3763	1/1	0.85	0.10	73,73,73,73	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	1745	1/1	0.85	0.13	59,59,59,59	0
57	MG	1A	3957	1/1	0.85	0.23	66,66,66,66	0
57	MG	1a	1657	1/1	0.85	0.11	75,75,75,75	0
57	MG	2a	1751	1/1	0.85	0.14	59,59,59,59	0
57	MG	1a	1658	1/1	0.85	0.16	58,58,58,58	0
57	MG	2a	1758	1/1	0.85	0.16	74,74,74,74	0
57	MG	2A	3809	1/1	0.85	0.13	42,42,42,42	0
57	MG	2A	3503	1/1	0.85	0.19	64,64,64,64	0
57	MG	2A	3510	1/1	0.85	0.14	64,64,64,64	0
57	MG	2A	3514	1/1	0.85	0.12	38,38,38,38	0
57	MG	2A	3840	1/1	0.85	0.11	40,40,40,40	0
57	MG	2A	3522	1/1	0.85	0.14	56,56,56,56	0
57	MG	2A	3123	1/1	0.85	0.10	53,53,53,53	0
57	MG	2A	3281	1/1	0.85	0.32	76,76,76,76	0
57	MG	1A	3295	1/1	0.85	0.34	74,74,74,74	0
57	MG	1F	315	1/1	0.85	0.22	54,54,54,54	0
57	MG	2i	201	1/1	0.85	0.32	76,76,76,76	0
57	MG	2A	3549	1/1	0.85	0.19	51,51,51,51	0
57	MG	2A	3295	1/1	0.85	0.09	52,52,52,52	0
57	MG	1A	3507	1/1	0.85	0.15	61,61,61,61	0
57	MG	1a	1672	1/1	0.85	0.14	63,63,63,63	0
57	MG	2B	207	1/1	0.85	0.20	64,64,64,64	0
57	MG	1V	206	1/1	0.86	0.08	59,59,59,59	0
57	MG	1A	3812	1/1	0.86	0.12	43,43,43,43	0
57	MG	2A	3456	1/1	0.86	0.38	60,60,60,60	0
57	MG	1A	3626	1/1	0.86	0.19	60,60,60,60	0
57	MG	17	105	1/1	0.86	0.33	70,70,70,70	0
57	MG	2A	3471	1/1	0.86	0.14	63,63,63,63	0
57	MG	1a	1823	1/1	0.86	0.23	74,74,74,74	0
57	MG	2A	3486	1/1	0.86	0.19	52,52,52,52	0
57	MG	1e	202	1/1	0.86	0.13	64,64,64,64	0
57	MG	1A	3185	1/1	0.86	0.17	61,61,61,61	0
57	MG	1a	1601	1/1	0.86	0.21	59,59,59,59	0
57	MG	1A	3631	1/1	0.86	0.08	27,27,27,27	0
57	MG	2B	204	1/1	0.86	0.18	72,72,72,72	0
57	MG	2A	3526	1/1	0.86	0.12	67,67,67,67	0
57	MG	1A	3300	1/1	0.86	0.25	63,63,63,63	0
57	MG	1x	110	1/1	0.86	0.14	67,67,67,67	0
57	MG	1A	3366	1/1	0.86	0.33	63,63,63,63	0
57	MG	2A	3269	1/1	0.86	0.39	62,62,62,62	0
57	MG	2A	3544	1/1	0.86	0.21	69,69,69,69	0
57	MG	2A	3545	1/1	0.86	0.12	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	3007	1/1	0.86	0.24	58,58,58,58	0
57	MG	1A	3378	1/1	0.86	0.20	55,55,55,55	0
57	MG	2A	3023	1/1	0.86	0.27	68,68,68,68	0
57	MG	1A	3233	1/1	0.86	0.16	55,55,55,55	0
57	MG	2A	3585	1/1	0.86	0.13	31,31,31,31	0
57	MG	1a	1627	1/1	0.86	0.14	55,55,55,55	0
57	MG	27	102	1/1	0.86	0.30	68,68,68,68	0
57	MG	1A	3204	1/1	0.86	0.11	47,47,47,47	0
57	MG	1A	3968	1/1	0.86	0.13	60,60,60,60	0
57	MG	2A	3601	1/1	0.86	0.14	38,38,38,38	0
57	MG	2a	1613	1/1	0.86	0.26	62,62,62,62	0
57	MG	1A	3262	1/1	0.86	0.28	62,62,62,62	0
57	MG	2A	3613	1/1	0.86	0.20	62,62,62,62	0
57	MG	2a	1626	1/1	0.86	0.32	69,69,69,69	0
57	MG	2A	3293	1/1	0.86	0.21	59,59,59,59	0
57	MG	1A	3533	1/1	0.86	0.20	67,67,67,67	0
57	MG	1A	4079	1/1	0.86	0.20	55,55,55,55	0
57	MG	2A	3097	1/1	0.86	0.25	72,72,72,72	0
57	MG	2A	3099	1/1	0.86	0.29	66,66,66,66	0
57	MG	1a	1737	1/1	0.86	0.17	67,67,67,67	0
57	MG	2A	3642	1/1	0.86	0.15	52,52,52,52	0
57	MG	1A	3566	1/1	0.86	0.15	61,61,61,61	0
57	MG	2A	3646	1/1	0.86	0.11	55,55,55,55	0
57	MG	2a	1654	1/1	0.86	0.33	58,58,58,58	0
57	MG	1A	3728	1/1	0.86	0.10	22,22,22,22	0
57	MG	2A	3133	1/1	0.86	0.11	53,53,53,53	0
57	MG	1A	3335	1/1	0.86	0.32	57,57,57,57	0
57	MG	1B	221	1/1	0.86	0.13	56,56,56,56	0
57	MG	1A	3050	1/1	0.86	0.29	58,58,58,58	0
57	MG	1A	3183	1/1	0.86	0.26	51,51,51,51	0
57	MG	1A	3267	1/1	0.86	0.17	46,46,46,46	0
57	MG	1a	1766	1/1	0.86	0.20	70,70,70,70	0
57	MG	2A	3172	1/1	0.86	0.16	53,53,53,53	0
57	MG	2A	3677	1/1	0.86	0.13	54,54,54,54	0
57	MG	2A	3681	1/1	0.86	0.16	59,59,59,59	0
57	MG	1A	3900	1/1	0.86	0.27	38,38,38,38	0
57	MG	1A	3445	1/1	0.86	0.17	60,60,60,60	0
57	MG	2A	3352	1/1	0.86	0.21	68,68,68,68	0
57	MG	2A	3690	1/1	0.86	0.16	69,69,69,69	0
57	MG	2A	3692	1/1	0.86	0.13	56,56,56,56	0
57	MG	1a	1668	1/1	0.86	0.10	62,62,62,62	0
57	MG	2A	3185	1/1	0.86	0.24	70,70,70,70	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	3186	1/1	0.86	0.48	70,70,70,70	0
57	MG	2A	3701	1/1	0.86	0.12	56,56,56,56	0
57	MG	2A	3189	1/1	0.86	0.16	61,61,61,61	0
57	MG	2A	3707	1/1	0.86	0.10	38,38,38,38	0
57	MG	2a	1743	1/1	0.86	0.29	54,54,54,54	0
57	MG	2A	3708	1/1	0.86	0.20	59,59,59,59	0
57	MG	2A	3711	1/1	0.86	0.15	73,73,73,73	0
57	MG	1A	3782	1/1	0.86	0.11	20,20,20,20	0
57	MG	2A	3192	1/1	0.86	0.21	55,55,55,55	0
57	MG	2a	1753	1/1	0.86	0.34	68,68,68,68	0
57	MG	1a	1673	1/1	0.86	0.30	69,69,69,69	0
57	MG	2A	3197	1/1	0.86	0.15	63,63,63,63	0
57	MG	1A	3360	1/1	0.86	0.18	62,62,62,62	0
57	MG	1a	1790	1/1	0.86	0.18	61,61,61,61	0
57	MG	1a	1793	1/1	0.86	0.15	69,69,69,69	0
57	MG	2A	3389	1/1	0.86	0.25	78,78,78,78	0
57	MG	1A	3609	1/1	0.86	0.09	45,45,45,45	0
57	MG	2A	3402	1/1	0.86	0.19	42,42,42,42	0
57	MG	1A	4010	1/1	0.86	0.14	66,66,66,66	0
57	MG	2a	1772	1/1	0.86	0.14	76,76,76,76	0
57	MG	2A	3213	1/1	0.86	0.13	58,58,58,58	0
57	MG	2A	3764	1/1	0.86	0.15	51,51,51,51	0
57	MG	2f	202	1/1	0.86	0.17	75,75,75,75	0
57	MG	2A	3770	1/1	0.86	0.16	49,49,49,49	0
57	MG	1a	1797	1/1	0.86	0.17	56,56,56,56	0
57	MG	1A	3457	1/1	0.86	0.14	63,63,63,63	0
57	MG	2l	201	1/1	0.86	0.15	62,62,62,62	0
57	MG	1A	3811	1/1	0.86	0.19	55,55,55,55	0
57	MG	1U	210	1/1	0.86	0.25	47,47,47,47	0
57	MG	2A	3795	1/1	0.86	0.13	57,57,57,57	0
57	MG	2A	3238	1/1	0.86	0.22	71,71,71,71	0
57	MG	2A	3824	1/1	0.87	0.12	73,73,73,73	0
57	MG	1A	3683	1/1	0.87	0.12	39,39,39,39	0
57	MG	2A	3836	1/1	0.87	0.21	70,70,70,70	0
57	MG	2A	3263	1/1	0.87	0.20	62,62,62,62	0
57	MG	1a	1603	1/1	0.87	0.18	58,58,58,58	0
57	MG	1a	1605	1/1	0.87	0.15	74,74,74,74	0
57	MG	2A	3043	1/1	0.87	0.13	71,71,71,71	0
57	MG	1A	3442	1/1	0.87	0.20	59,59,59,59	0
57	MG	1a	1714	1/1	0.87	0.11	73,73,73,73	0
57	MG	1A	3339	1/1	0.87	0.22	70,70,70,70	0
57	MG	2A	3852	1/1	0.87	0.14	53,53,53,53	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	3373	1/1	0.87	0.17	61,61,61,61	0
57	MG	1a	1613	1/1	0.87	0.11	68,68,68,68	0
57	MG	2A	3286	1/1	0.87	0.22	61,61,61,61	0
57	MG	1A	3835	1/1	0.87	0.19	55,55,55,55	0
57	MG	1A	3296	1/1	0.87	0.35	65,65,65,65	0
57	MG	1A	3849	1/1	0.87	0.14	50,50,50,50	0
57	MG	2A	3562	1/1	0.87	0.21	60,60,60,60	0
57	MG	2A	3104	1/1	0.87	0.32	57,57,57,57	0
57	MG	2A	3581	1/1	0.87	0.19	61,61,61,61	0
57	MG	2B	216	1/1	0.87	0.20	67,67,67,67	0
57	MG	1a	1736	1/1	0.87	0.38	72,72,72,72	0
57	MG	1A	3046	1/1	0.87	0.09	28,28,28,28	0
57	MG	1A	3392	1/1	0.87	0.20	36,36,36,36	0
57	MG	1A	4073	1/1	0.87	0.14	73,73,73,73	0
57	MG	2A	3598	1/1	0.87	0.18	66,66,66,66	0
57	MG	2W	201	1/1	0.87	0.23	65,65,65,65	0
57	MG	1a	1750	1/1	0.87	0.13	64,64,64,64	0
57	MG	2A	3602	1/1	0.87	0.13	59,59,59,59	0
57	MG	25	104	1/1	0.87	0.17	53,53,53,53	0
57	MG	1A	3489	1/1	0.87	0.10	51,51,51,51	0
57	MG	28	102	1/1	0.87	0.21	57,57,57,57	0
57	MG	29	101	1/1	0.87	0.22	65,65,65,65	0
57	MG	1A	3615	1/1	0.87	0.10	29,29,29,29	0
57	MG	2A	3615	1/1	0.87	0.15	70,70,70,70	0
57	MG	1B	202	1/1	0.87	0.25	59,59,59,59	0
57	MG	1B	205	1/1	0.87	0.29	70,70,70,70	0
57	MG	2A	3630	1/1	0.87	0.17	60,60,60,60	0
57	MG	1a	1649	1/1	0.87	0.26	63,63,63,63	0
57	MG	2a	1619	1/1	0.87	0.14	63,63,63,63	0
57	MG	1a	1650	1/1	0.87	0.18	72,72,72,72	0
57	MG	2A	3634	1/1	0.87	0.20	64,64,64,64	0
57	MG	2A	3323	1/1	0.87	0.18	59,59,59,59	0
57	MG	2A	3326	1/1	0.87	0.17	75,75,75,75	0
57	MG	2A	3327	1/1	0.87	0.11	73,73,73,73	0
57	MG	2A	3328	1/1	0.87	0.17	70,70,70,70	0
57	MG	2A	3644	1/1	0.87	0.20	66,66,66,66	0
57	MG	1a	1651	1/1	0.87	0.29	67,67,67,67	0
57	MG	1A	3616	1/1	0.87	0.09	26,26,26,26	0
57	MG	1a	1653	1/1	0.87	0.23	69,69,69,69	0
57	MG	2a	1651	1/1	0.87	0.20	68,68,68,68	0
57	MG	1A	3393	1/1	0.87	0.15	53,53,53,53	0
57	MG	2A	3339	1/1	0.87	0.14	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	3980	1/1	0.87	0.13	62,62,62,62	0
57	MG	1A	3877	1/1	0.87	0.13	71,71,71,71	0
57	MG	2a	1667	1/1	0.87	0.27	66,66,66,66	0
57	MG	2A	3190	1/1	0.87	0.34	68,68,68,68	0
57	MG	2a	1671	1/1	0.87	0.21	67,67,67,67	0
57	MG	1a	1787	1/1	0.87	0.19	70,70,70,70	0
57	MG	1a	1788	1/1	0.87	0.22	68,68,68,68	0
57	MG	2A	3676	1/1	0.87	0.12	59,59,59,59	0
57	MG	2A	3359	1/1	0.87	0.21	75,75,75,75	0
57	MG	1A	3189	1/1	0.87	0.14	38,38,38,38	0
57	MG	2A	3369	1/1	0.87	0.29	61,61,61,61	0
57	MG	2a	1693	1/1	0.87	0.27	78,78,78,78	0
57	MG	1a	1792	1/1	0.87	0.14	65,65,65,65	0
57	MG	2A	3199	1/1	0.87	0.13	58,58,58,58	0
57	MG	1D	302	1/1	0.87	0.19	64,64,64,64	0
57	MG	1A	3351	1/1	0.87	0.22	66,66,66,66	0
57	MG	2A	3379	1/1	0.87	0.25	46,46,46,46	0
57	MG	1A	3359	1/1	0.87	0.10	49,49,49,49	0
57	MG	1E	308	1/1	0.87	0.21	60,60,60,60	0
57	MG	2A	3383	1/1	0.87	0.15	64,64,64,64	0
57	MG	2a	1733	1/1	0.87	0.12	55,55,55,55	0
57	MG	2A	3209	1/1	0.87	0.09	53,53,53,53	0
57	MG	2A	3705	1/1	0.87	0.15	49,49,49,49	0
57	MG	1A	3256	1/1	0.87	0.19	59,59,59,59	0
57	MG	1A	3989	1/1	0.87	0.14	46,46,46,46	0
57	MG	2A	3392	1/1	0.87	0.19	61,61,61,61	0
57	MG	2a	1744	1/1	0.87	0.23	74,74,74,74	0
57	MG	1A	3991	1/1	0.87	0.29	36,36,36,36	0
57	MG	1A	3794	1/1	0.87	0.18	56,56,56,56	0
57	MG	2A	3715	1/1	0.87	0.13	62,62,62,62	0
57	MG	1a	1679	1/1	0.87	0.13	66,66,66,66	0
57	MG	2A	3420	1/1	0.87	0.20	53,53,53,53	0
57	MG	1A	3911	1/1	0.87	0.13	29,29,29,29	0
57	MG	2a	1757	1/1	0.87	0.27	72,72,72,72	0
57	MG	1A	3795	1/1	0.87	0.13	45,45,45,45	0
57	MG	2A	3736	1/1	0.87	0.22	63,63,63,63	0
57	MG	2A	3745	1/1	0.87	0.11	68,68,68,68	0
57	MG	1A	3808	1/1	0.87	0.15	38,38,38,38	0
57	MG	1A	3655	1/1	0.87	0.11	40,40,40,40	0
57	MG	1A	3660	1/1	0.87	0.18	28,28,28,28	0
57	MG	1A	3294	1/1	0.87	0.16	56,56,56,56	0
57	MG	1A	3166	1/1	0.87	0.25	56,56,56,56	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	3453	1/1	0.87	0.14	69,69,69,69	0
57	MG	1x	104	1/1	0.87	0.17	65,65,65,65	0
57	MG	2A	3458	1/1	0.87	0.32	66,66,66,66	0
57	MG	1Y	203	1/1	0.87	0.14	62,62,62,62	0
57	MG	2A	3468	1/1	0.87	0.13	66,66,66,66	0
57	MG	2A	3779	1/1	0.87	0.08	46,46,46,46	0
57	MG	1A	3678	1/1	0.87	0.18	66,66,66,66	0
57	MG	1A	4033	1/1	0.87	0.14	59,59,59,59	0
57	MG	1a	1703	1/1	0.87	0.32	75,75,75,75	0
57	MG	2A	3482	1/1	0.87	0.26	55,55,55,55	0
57	MG	2A	3485	1/1	0.87	0.14	60,60,60,60	0
57	MG	2A	3261	1/1	0.87	0.10	68,68,68,68	0
57	MG	1A	3836	1/1	0.88	0.11	70,70,70,70	0
57	MG	2A	3294	1/1	0.88	0.23	64,64,64,64	0
57	MG	2A	3534	1/1	0.88	0.10	52,52,52,52	0
57	MG	2A	3124	1/1	0.88	0.10	66,66,66,66	0
57	MG	1A	4008	1/1	0.88	0.12	56,56,56,56	0
57	MG	2A	3298	1/1	0.88	0.20	60,60,60,60	0
57	MG	1D	312	1/1	0.88	0.24	41,41,41,41	0
57	MG	2A	3851	1/1	0.88	0.17	65,65,65,65	0
57	MG	1A	3427	1/1	0.88	0.12	61,61,61,61	0
57	MG	2A	3148	1/1	0.88	0.34	59,59,59,59	0
57	MG	2A	3303	1/1	0.88	0.14	60,60,60,60	0
57	MG	2A	3157	1/1	0.88	0.22	70,70,70,70	0
57	MG	2A	3563	1/1	0.88	0.20	58,58,58,58	0
57	MG	2B	206	1/1	0.88	0.29	67,67,67,67	0
57	MG	1a	1759	1/1	0.88	0.19	66,66,66,66	0
57	MG	2A	3310	1/1	0.88	0.17	56,56,56,56	0
57	MG	2A	3312	1/1	0.88	0.39	66,66,66,66	0
57	MG	1A	4013	1/1	0.88	0.08	59,59,59,59	0
57	MG	1A	3543	1/1	0.88	0.49	44,44,44,44	0
57	MG	1a	1774	1/1	0.88	0.11	61,61,61,61	0
57	MG	2B	218	1/1	0.88	0.21	70,70,70,70	0
57	MG	2A	3595	1/1	0.88	0.17	69,69,69,69	0
57	MG	2A	3319	1/1	0.88	0.20	55,55,55,55	0
57	MG	2B	222	1/1	0.88	0.21	73,73,73,73	0
57	MG	1A	3949	1/1	0.88	0.15	58,58,58,58	0
57	MG	2D	309	1/1	0.88	0.11	57,57,57,57	0
57	MG	1A	3612	1/1	0.88	0.09	32,32,32,32	0
57	MG	2E	306	1/1	0.88	0.10	30,30,30,30	0
57	MG	2O	201	1/1	0.88	0.10	60,60,60,60	0
57	MG	1A	3787	1/1	0.88	0.13	59,59,59,59	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	2V	201	1/1	0.88	0.20	52,52,52,52	0
57	MG	2A	3612	1/1	0.88	0.12	46,46,46,46	0
57	MG	2I	101	1/1	0.88	0.29	52,52,52,52	0
57	MG	1A	3962	1/1	0.88	0.12	39,39,39,39	0
57	MG	25	101	1/1	0.88	0.31	58,58,58,58	0
57	MG	1O	203	1/1	0.88	0.18	67,67,67,67	0
57	MG	2A	3619	1/1	0.88	0.34	47,47,47,47	0
57	MG	26	101	1/1	0.88	0.14	54,54,54,54	0
57	MG	1a	1671	1/1	0.88	0.18	65,65,65,65	0
57	MG	1O	204	1/1	0.88	0.11	60,60,60,60	0
57	MG	1A	3547	1/1	0.88	0.33	57,57,57,57	0
57	MG	2a	1603	1/1	0.88	0.12	63,63,63,63	0
57	MG	1A	3684	1/1	0.88	0.09	23,23,23,23	0
57	MG	1U	209	1/1	0.88	0.10	51,51,51,51	0
57	MG	1A	3548	1/1	0.88	0.27	51,51,51,51	0
57	MG	2A	3635	1/1	0.88	0.09	33,33,33,33	0
57	MG	2A	3340	1/1	0.88	0.12	58,58,58,58	0
57	MG	1A	3801	1/1	0.88	0.17	56,56,56,56	0
57	MG	2A	3641	1/1	0.88	0.26	68,68,68,68	0
57	MG	2a	1624	1/1	0.88	0.32	54,54,54,54	0
57	MG	2A	3348	1/1	0.88	0.18	65,65,65,65	0
57	MG	1A	4046	1/1	0.88	0.14	59,59,59,59	0
57	MG	1a	1681	1/1	0.88	0.17	68,68,68,68	0
57	MG	1A	4050	1/1	0.88	0.08	16,16,16,16	0
57	MG	2A	3649	1/1	0.88	0.14	53,53,53,53	0
57	MG	2A	3356	1/1	0.88	0.12	68,68,68,68	0
57	MG	1a	1684	1/1	0.88	0.26	60,60,60,60	0
57	MG	2A	3206	1/1	0.88	0.20	66,66,66,66	0
57	MG	2A	3363	1/1	0.88	0.26	62,62,62,62	0
57	MG	1A	4051	1/1	0.88	0.12	59,59,59,59	0
57	MG	1A	3695	1/1	0.88	0.13	62,62,62,62	0
57	MG	2A	3665	1/1	0.88	0.20	51,51,51,51	0
57	MG	1a	1815	1/1	0.88	0.09	68,68,68,68	0
57	MG	18	104	1/1	0.88	0.12	66,66,66,66	0
57	MG	2a	1660	1/1	0.88	0.50	71,71,71,71	0
57	MG	1A	3326	1/1	0.88	0.24	62,62,62,62	0
57	MG	2a	1666	1/1	0.88	0.13	66,66,66,66	0
57	MG	1A	3368	1/1	0.88	0.14	53,53,53,53	0
57	MG	2A	3225	1/1	0.88	0.20	59,59,59,59	0
57	MG	1a	1602	1/1	0.88	0.23	60,60,60,60	0
57	MG	2A	3232	1/1	0.88	0.25	61,61,61,61	0
57	MG	1A	4058	1/1	0.88	0.18	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	3898	1/1	0.88	0.12	25,25,25,25	0
57	MG	2a	1677	1/1	0.88	0.36	67,67,67,67	0
57	MG	1A	3577	1/1	0.88	0.19	56,56,56,56	0
57	MG	1A	3401	1/1	0.88	0.15	60,60,60,60	0
57	MG	1A	3720	1/1	0.88	0.11	49,49,49,49	0
57	MG	2a	1688	1/1	0.88	0.21	64,64,64,64	0
57	MG	1A	3903	1/1	0.88	0.12	40,40,40,40	0
57	MG	2A	3409	1/1	0.88	0.30	57,57,57,57	0
57	MG	2a	1709	1/1	0.88	0.20	63,63,63,63	0
57	MG	1A	4080	1/1	0.88	0.22	70,70,70,70	0
57	MG	1A	3633	1/1	0.88	0.16	50,50,50,50	0
57	MG	2A	3250	1/1	0.88	0.20	62,62,62,62	0
57	MG	1a	1718	1/1	0.88	0.24	73,73,73,73	0
57	MG	1a	1720	1/1	0.88	0.42	68,68,68,68	0
57	MG	1A	3456	1/1	0.88	0.10	56,56,56,56	0
57	MG	2A	3028	1/1	0.88	0.14	64,64,64,64	0
57	MG	2A	3431	1/1	0.88	0.38	70,70,70,70	0
57	MG	1a	1723	1/1	0.88	0.38	56,56,56,56	0
57	MG	2A	3437	1/1	0.88	0.28	65,65,65,65	0
57	MG	2A	3722	1/1	0.88	0.16	64,64,64,64	0
57	MG	2A	3438	1/1	0.88	0.20	65,65,65,65	0
57	MG	2A	3726	1/1	0.88	0.15	64,64,64,64	0
57	MG	1A	3423	1/1	0.88	0.17	58,58,58,58	0
57	MG	2A	3733	1/1	0.88	0.19	46,46,46,46	0
57	MG	2A	3446	1/1	0.88	0.29	65,65,65,65	0
57	MG	1a	1729	1/1	0.88	0.32	73,73,73,73	0
57	MG	2a	1750	1/1	0.88	0.14	62,62,62,62	0
57	MG	2A	3264	1/1	0.88	0.12	70,70,70,70	0
57	MG	2A	3084	1/1	0.88	0.14	49,49,49,49	0
57	MG	2A	3267	1/1	0.88	0.12	60,60,60,60	0
57	MG	1a	1635	1/1	0.88	0.27	68,68,68,68	0
57	MG	2A	3271	1/1	0.88	0.17	66,66,66,66	0
57	MG	2A	3758	1/1	0.88	0.13	68,68,68,68	0
57	MG	1A	3320	1/1	0.88	0.30	35,35,35,35	0
57	MG	1B	209	1/1	0.88	0.27	58,58,58,58	0
57	MG	2A	3479	1/1	0.88	0.18	52,52,52,52	0
57	MG	2a	1768	1/1	0.88	0.26	61,61,61,61	0
57	MG	1A	3831	1/1	0.88	0.18	56,56,56,56	0
57	MG	2A	3276	1/1	0.88	0.14	66,66,66,66	0
57	MG	1a	1643	1/1	0.88	0.32	64,64,64,64	0
57	MG	1A	3832	1/1	0.88	0.16	63,63,63,63	0
57	MG	2A	3780	1/1	0.88	0.09	75,75,75,75	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	2a	1776	1/1	0.88	0.14	68,68,68,68	0
57	MG	2A	3494	1/1	0.88	0.17	63,63,63,63	0
57	MG	2e	201	1/1	0.88	0.12	71,71,71,71	0
57	MG	2A	3500	1/1	0.88	0.14	44,44,44,44	0
57	MG	1a	1739	1/1	0.88	0.24	60,60,60,60	0
57	MG	2A	3800	1/1	0.88	0.10	46,46,46,46	0
57	MG	2A	3506	1/1	0.88	0.26	59,59,59,59	0
57	MG	2A	3282	1/1	0.88	0.29	69,69,69,69	0
57	MG	1B	223	1/1	0.88	0.13	53,53,53,53	0
57	MG	2v	101	1/1	0.88	0.33	63,63,63,63	0
57	MG	2A	3516	1/1	0.88	0.12	42,42,42,42	0
57	MG	1A	3664	1/1	0.88	0.19	56,56,56,56	0
57	MG	1A	4004	1/1	0.88	0.12	42,42,42,42	0
57	MG	2A	3617	1/1	0.89	0.10	59,59,59,59	0
57	MG	1A	3250	1/1	0.89	0.23	57,57,57,57	0
57	MG	1N	202	1/1	0.89	0.10	47,47,47,47	0
57	MG	1N	206	1/1	0.89	0.14	54,54,54,54	0
57	MG	1A	3024	1/1	0.89	0.30	56,56,56,56	0
57	MG	1A	3514	1/1	0.89	0.39	44,44,44,44	0
57	MG	1A	3091	1/1	0.89	0.12	48,48,48,48	0
57	MG	2A	3214	1/1	0.89	0.12	60,60,60,60	0
57	MG	2E	303	1/1	0.89	0.22	62,62,62,62	0
57	MG	2A	3215	1/1	0.89	0.10	59,59,59,59	0
57	MG	1a	1811	1/1	0.89	0.15	72,72,72,72	0
57	MG	2F	302	1/1	0.89	0.19	49,49,49,49	0
57	MG	2F	303	1/1	0.89	0.14	44,44,44,44	0
57	MG	1A	3645	1/1	0.89	0.08	23,23,23,23	0
57	MG	1A	3096	1/1	0.89	0.26	54,54,54,54	0
57	MG	1A	4022	1/1	0.89	0.18	63,63,63,63	0
57	MG	1A	3518	1/1	0.89	0.26	49,49,49,49	0
57	MG	2X	101	1/1	0.89	0.09	50,50,50,50	0
57	MG	1a	1820	1/1	0.89	0.17	66,66,66,66	0
57	MG	1A	3798	1/1	0.89	0.18	55,55,55,55	0
57	MG	1A	3923	1/1	0.89	0.13	61,61,61,61	0
57	MG	1a	1694	1/1	0.89	0.16	62,62,62,62	0
57	MG	1A	4035	1/1	0.89	0.09	39,39,39,39	0
57	MG	2A	3652	1/1	0.89	0.13	49,49,49,49	0
57	MG	1A	3306	1/1	0.89	0.20	45,45,45,45	0
57	MG	2A	3656	1/1	0.89	0.23	62,62,62,62	0
57	MG	1v	101	1/1	0.89	0.10	75,75,75,75	0
57	MG	2A	3391	1/1	0.89	0.30	71,71,71,71	0
57	MG	1A	3430	1/1	0.89	0.28	59,59,59,59	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	3663	1/1	0.89	0.10	68,68,68,68	0
57	MG	2a	1608	1/1	0.89	0.24	52,52,52,52	0
57	MG	1a	1704	1/1	0.89	0.16	62,62,62,62	0
57	MG	1A	4040	1/1	0.89	0.12	33,33,33,33	0
57	MG	2a	1615	1/1	0.89	0.14	58,58,58,58	0
57	MG	2A	3410	1/1	0.89	0.36	60,60,60,60	0
57	MG	1A	3431	1/1	0.89	0.24	47,47,47,47	0
57	MG	1A	3810	1/1	0.89	0.09	36,36,36,36	0
57	MG	2a	1620	1/1	0.89	0.19	47,47,47,47	0
57	MG	2a	1621	1/1	0.89	0.38	66,66,66,66	0
57	MG	2A	3416	1/1	0.89	0.23	60,60,60,60	0
57	MG	2A	3680	1/1	0.89	0.19	48,48,48,48	0
57	MG	1A	3441	1/1	0.89	0.13	58,58,58,58	0
57	MG	1A	3675	1/1	0.89	0.13	28,28,28,28	0
57	MG	1a	1716	1/1	0.89	0.23	67,67,67,67	0
57	MG	1A	3551	1/1	0.89	0.28	62,62,62,62	0
57	MG	2a	1642	1/1	0.89	0.23	56,56,56,56	0
57	MG	1a	1609	1/1	0.89	0.20	71,71,71,71	0
57	MG	2A	3045	1/1	0.89	0.29	59,59,59,59	0
57	MG	1A	3682	1/1	0.89	0.12	30,30,30,30	0
57	MG	2A	3268	1/1	0.89	0.13	61,61,61,61	0
57	MG	2A	3078	1/1	0.89	0.16	54,54,54,54	0
57	MG	1A	3959	1/1	0.89	0.11	76,76,76,76	0
57	MG	1A	3386	1/1	0.89	0.46	48,48,48,48	0
57	MG	1A	3309	1/1	0.89	0.30	55,55,55,55	0
57	MG	2a	1657	1/1	0.89	0.26	59,59,59,59	0
57	MG	1A	3690	1/1	0.89	0.10	31,31,31,31	0
57	MG	2a	1659	1/1	0.89	0.28	62,62,62,62	0
57	MG	2A	3454	1/1	0.89	0.19	63,63,63,63	0
57	MG	1a	1731	1/1	0.89	0.30	64,64,64,64	0
57	MG	2A	3093	1/1	0.89	0.14	69,69,69,69	0
57	MG	1A	3311	1/1	0.89	0.12	59,59,59,59	0
57	MG	1A	3451	1/1	0.89	0.18	62,62,62,62	0
57	MG	1A	3453	1/1	0.89	0.09	59,59,59,59	0
57	MG	1A	4084	1/1	0.89	0.23	63,63,63,63	0
57	MG	2a	1674	1/1	0.89	0.17	75,75,75,75	0
57	MG	2A	3723	1/1	0.89	0.15	68,68,68,68	0
57	MG	2A	3724	1/1	0.89	0.11	62,62,62,62	0
57	MG	1A	3397	1/1	0.89	0.12	43,43,43,43	0
57	MG	2A	3116	1/1	0.89	0.13	62,62,62,62	0
57	MG	2A	3118	1/1	0.89	0.19	51,51,51,51	0
57	MG	2A	3730	1/1	0.89	0.18	46,46,46,46	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	4086	1/1	0.89	0.18	70,70,70,70	0
57	MG	1a	1740	1/1	0.89	0.23	71,71,71,71	0
57	MG	2a	1698	1/1	0.89	0.25	72,72,72,72	0
57	MG	2A	3492	1/1	0.89	0.21	57,57,57,57	0
57	MG	2A	3737	1/1	0.89	0.10	62,62,62,62	0
57	MG	1a	1742	1/1	0.89	0.15	65,65,65,65	0
57	MG	2A	3747	1/1	0.89	0.12	50,50,50,50	0
57	MG	1A	3172	1/1	0.89	0.13	49,49,49,49	0
57	MG	2a	1721	1/1	0.89	0.16	59,59,59,59	0
57	MG	1A	3051	1/1	0.89	0.10	28,28,28,28	0
57	MG	2A	3140	1/1	0.89	0.12	46,46,46,46	0
57	MG	1A	3718	1/1	0.89	0.15	70,70,70,70	0
57	MG	1A	3851	1/1	0.89	0.14	42,42,42,42	0
57	MG	2A	3759	1/1	0.89	0.08	37,37,37,37	0
57	MG	1B	210	1/1	0.89	0.11	46,46,46,46	0
57	MG	2A	3162	1/1	0.89	0.28	57,57,57,57	0
57	MG	1A	3462	1/1	0.89	0.31	72,72,72,72	0
57	MG	2A	3311	1/1	0.89	0.20	57,57,57,57	0
57	MG	1A	3723	1/1	0.89	0.13	51,51,51,51	0
57	MG	2A	3773	1/1	0.89	0.09	62,62,62,62	0
57	MG	1A	3116	1/1	0.89	0.39	38,38,38,38	0
57	MG	1a	1762	1/1	0.89	0.14	70,70,70,70	0
57	MG	1A	3861	1/1	0.89	0.11	68,68,68,68	0
57	MG	2a	1748	1/1	0.89	0.15	65,65,65,65	0
57	MG	1A	3411	1/1	0.89	0.14	55,55,55,55	0
57	MG	1B	234	1/1	0.89	0.10	67,67,67,67	0
57	MG	1A	3736	1/1	0.89	0.11	43,43,43,43	0
57	MG	2A	3551	1/1	0.89	0.10	57,57,57,57	0
57	MG	1a	1661	1/1	0.89	0.32	62,62,62,62	0
57	MG	2A	3324	1/1	0.89	0.24	54,54,54,54	0
57	MG	1A	3495	1/1	0.89	0.18	57,57,57,57	0
57	MG	2A	3818	1/1	0.89	0.09	57,57,57,57	0
57	MG	2a	1762	1/1	0.89	0.10	71,71,71,71	0
57	MG	1A	3744	1/1	0.89	0.08	17,17,17,17	0
57	MG	2A	3566	1/1	0.89	0.10	65,65,65,65	0
57	MG	2A	3567	1/1	0.89	0.25	62,62,62,62	0
57	MG	1A	3995	1/1	0.89	0.09	64,64,64,64	0
57	MG	2A	3578	1/1	0.89	0.13	60,60,60,60	0
57	MG	1A	3879	1/1	0.89	0.14	35,35,35,35	0
57	MG	2A	3582	1/1	0.89	0.11	69,69,69,69	0
57	MG	1A	3617	1/1	0.89	0.12	54,54,54,54	0
57	MG	1A	3889	1/1	0.89	0.08	42,42,42,42	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	1F	311	1/1	0.89	0.11	47,47,47,47	0
57	MG	2A	3333	1/1	0.89	0.09	64,64,64,64	0
57	MG	2A	3592	1/1	0.89	0.15	66,66,66,66	0
57	MG	2A	3335	1/1	0.89	0.12	61,61,61,61	0
57	MG	2g	3101	1/1	0.89	0.18	76,76,76,76	0
57	MG	2A	3337	1/1	0.89	0.08	67,67,67,67	0
57	MG	1A	3752	1/1	0.89	0.11	28,28,28,28	0
57	MG	1a	1676	1/1	0.89	0.19	72,72,72,72	0
57	MG	2A	3610	1/1	0.89	0.15	44,44,44,44	0
57	MG	1A	3270	1/1	0.89	0.28	53,53,53,53	0
57	MG	2x	101	1/1	0.89	0.15	77,77,77,77	0
57	MG	2A	3204	1/1	0.89	0.24	57,57,57,57	0
57	MG	2A	3349	1/1	0.89	0.18	67,67,67,67	0
57	MG	2A	3350	1/1	0.89	0.18	62,62,62,62	0
57	MG	2B	211	1/1	0.90	0.18	60,60,60,60	0
57	MG	2A	3194	1/1	0.90	0.16	51,51,51,51	0
57	MG	1A	3952	1/1	0.90	0.14	38,38,38,38	0
57	MG	1A	3052	1/1	0.90	0.16	32,32,32,32	0
57	MG	1A	3667	1/1	0.90	0.09	60,60,60,60	0
57	MG	1a	1789	1/1	0.90	0.20	71,71,71,71	0
57	MG	1A	3324	1/1	0.90	0.10	49,49,49,49	0
57	MG	2A	3618	1/1	0.90	0.23	71,71,71,71	0
57	MG	1A	3171	1/1	0.90	0.36	42,42,42,42	0
57	MG	1A	3054	1/1	0.90	0.12	52,52,52,52	0
57	MG	1A	3815	1/1	0.90	0.13	50,50,50,50	0
57	MG	2A	3623	1/1	0.90	0.28	54,54,54,54	0
57	MG	2A	3629	1/1	0.90	0.25	68,68,68,68	0
57	MG	2A	3361	1/1	0.90	0.12	75,75,75,75	0
57	MG	2A	3631	1/1	0.90	0.18	64,64,64,64	0
57	MG	1A	3550	1/1	0.90	0.21	43,43,43,43	0
57	MG	2A	3210	1/1	0.90	0.09	54,54,54,54	0
57	MG	2G	201	1/1	0.90	0.11	60,60,60,60	0
57	MG	2A	3366	1/1	0.90	0.23	59,59,59,59	0
57	MG	1B	212	1/1	0.90	0.10	46,46,46,46	0
57	MG	1A	3818	1/1	0.90	0.09	38,38,38,38	0
57	MG	1A	3448	1/1	0.90	0.44	46,46,46,46	0
57	MG	2W	202	1/1	0.90	0.13	54,54,54,54	0
57	MG	1A	3564	1/1	0.90	0.19	67,67,67,67	0
57	MG	1B	225	1/1	0.90	0.10	52,52,52,52	0
57	MG	1A	3103	1/1	0.90	0.12	32,32,32,32	0
57	MG	1a	1812	1/1	0.90	0.14	55,55,55,55	0
57	MG	2A	3645	1/1	0.90	0.33	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	3069	1/1	0.90	0.07	46,46,46,46	0
57	MG	25	106	1/1	0.90	0.12	51,51,51,51	0
57	MG	2A	3230	1/1	0.90	0.40	68,68,68,68	0
57	MG	1A	3333	1/1	0.90	0.12	46,46,46,46	0
57	MG	2A	3388	1/1	0.90	0.17	72,72,72,72	0
57	MG	2A	3233	1/1	0.90	0.12	48,48,48,48	0
57	MG	1A	3830	1/1	0.90	0.15	50,50,50,50	0
57	MG	1A	3265	1/1	0.90	0.26	46,46,46,46	0
57	MG	2A	3657	1/1	0.90	0.14	53,53,53,53	0
57	MG	1A	3118	1/1	0.90	0.27	35,35,35,35	0
57	MG	2A	3393	1/1	0.90	0.24	63,63,63,63	0
57	MG	2a	1612	1/1	0.90	0.18	62,62,62,62	0
57	MG	2A	3394	1/1	0.90	0.11	57,57,57,57	0
57	MG	1A	3983	1/1	0.90	0.09	47,47,47,47	0
57	MG	2A	3408	1/1	0.90	0.15	54,54,54,54	0
57	MG	1A	3833	1/1	0.90	0.22	47,47,47,47	0
57	MG	1A	3581	1/1	0.90	0.20	44,44,44,44	0
57	MG	2A	3672	1/1	0.90	0.12	33,33,33,33	0
57	MG	1A	3703	1/1	0.90	0.15	69,69,69,69	0
57	MG	2A	3412	1/1	0.90	0.37	58,58,58,58	0
57	MG	2a	1625	1/1	0.90	0.25	67,67,67,67	0
57	MG	1m	201	1/1	0.90	0.08	68,68,68,68	0
57	MG	1A	3583	1/1	0.90	0.09	47,47,47,47	0
57	MG	1A	3990	1/1	0.90	0.09	16,16,16,16	0
57	MG	1A	3848	1/1	0.90	0.07	22,22,22,22	0
57	MG	1A	3992	1/1	0.90	0.09	20,20,20,20	0
57	MG	2a	1640	1/1	0.90	0.22	49,49,49,49	0
57	MG	1N	201	1/1	0.90	0.38	43,43,43,43	0
57	MG	1a	1693	1/1	0.90	0.10	76,76,76,76	0
57	MG	1A	3124	1/1	0.90	0.16	43,43,43,43	0
57	MG	1N	205	1/1	0.90	0.18	56,56,56,56	0
57	MG	1A	3709	1/1	0.90	0.15	49,49,49,49	0
57	MG	2A	3697	1/1	0.90	0.10	46,46,46,46	0
57	MG	1A	3714	1/1	0.90	0.13	59,59,59,59	0
57	MG	1A	3272	1/1	0.90	0.14	46,46,46,46	0
57	MG	1Q	205	1/1	0.90	0.24	67,67,67,67	0
57	MG	1A	3719	1/1	0.90	0.14	58,58,58,58	0
57	MG	1A	3464	1/1	0.90	0.30	58,58,58,58	0
57	MG	2A	3061	1/1	0.90	0.08	66,66,66,66	0
57	MG	2A	3076	1/1	0.90	0.19	56,56,56,56	0
57	MG	1A	3408	1/1	0.90	0.18	50,50,50,50	0
57	MG	2a	1665	1/1	0.90	0.29	69,69,69,69	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	3082	1/1	0.90	0.16	62,62,62,62	0
57	MG	1A	3725	1/1	0.90	0.12	50,50,50,50	0
57	MG	1A	3727	1/1	0.90	0.18	48,48,48,48	0
57	MG	1a	1717	1/1	0.90	0.10	69,69,69,69	0
57	MG	1A	4016	1/1	0.90	0.11	61,61,61,61	0
57	MG	1A	3134	1/1	0.90	0.13	39,39,39,39	0
57	MG	1A	3224	1/1	0.90	0.19	53,53,53,53	0
57	MG	2A	3483	1/1	0.90	0.15	74,74,74,74	0
57	MG	1A	3735	1/1	0.90	0.13	41,41,41,41	0
57	MG	1A	3417	1/1	0.90	0.17	62,62,62,62	0
57	MG	2A	3491	1/1	0.90	0.14	54,54,54,54	0
57	MG	1A	3893	1/1	0.90	0.10	49,49,49,49	0
57	MG	2A	3735	1/1	0.90	0.11	73,73,73,73	0
57	MG	2a	1692	1/1	0.90	0.17	53,53,53,53	0
57	MG	1A	4026	1/1	0.90	0.10	48,48,48,48	0
57	MG	2A	3107	1/1	0.90	0.27	56,56,56,56	0
57	MG	2a	1704	1/1	0.90	0.27	70,70,70,70	0
57	MG	1A	3504	1/1	0.90	0.12	57,57,57,57	0
57	MG	1A	3743	1/1	0.90	0.11	50,50,50,50	0
57	MG	1A	3355	1/1	0.90	0.10	49,49,49,49	0
57	MG	2a	1713	1/1	0.90	0.12	55,55,55,55	0
57	MG	1A	4036	1/1	0.90	0.08	32,32,32,32	0
57	MG	2A	3753	1/1	0.90	0.15	53,53,53,53	0
57	MG	1A	3745	1/1	0.90	0.13	47,47,47,47	0
57	MG	2A	3517	1/1	0.90	0.11	40,40,40,40	0
57	MG	2a	1725	1/1	0.90	0.34	70,70,70,70	0
57	MG	2a	1727	1/1	0.90	0.14	60,60,60,60	0
57	MG	1A	3625	1/1	0.90	0.08	15,15,15,15	0
57	MG	2a	1730	1/1	0.90	0.26	69,69,69,69	0
57	MG	2A	3525	1/1	0.90	0.21	51,51,51,51	0
57	MG	1a	1611	1/1	0.90	0.17	73,73,73,73	0
57	MG	2A	3308	1/1	0.90	0.28	62,62,62,62	0
57	MG	1A	3029	1/1	0.90	0.21	52,52,52,52	0
57	MG	2A	3769	1/1	0.90	0.20	63,63,63,63	0
57	MG	1A	3508	1/1	0.90	0.15	58,58,58,58	0
57	MG	2A	3771	1/1	0.90	0.10	56,56,56,56	0
57	MG	1a	1617	1/1	0.90	0.09	73,73,73,73	0
57	MG	2A	3313	1/1	0.90	0.29	68,68,68,68	0
57	MG	2A	3147	1/1	0.90	0.15	54,54,54,54	0
57	MG	1A	3630	1/1	0.90	0.07	32,32,32,32	0
57	MG	1A	3512	1/1	0.90	0.31	48,48,48,48	0
57	MG	2A	3787	1/1	0.90	0.10	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	3317	1/1	0.90	0.11	61,61,61,61	0
57	MG	2A	3160	1/1	0.90	0.12	45,45,45,45	0
57	MG	2A	3794	1/1	0.90	0.13	36,36,36,36	0
57	MG	1A	3783	1/1	0.90	0.11	35,35,35,35	0
57	MG	1A	3154	1/1	0.90	0.19	50,50,50,50	0
57	MG	1a	1630	1/1	0.90	0.21	58,58,58,58	0
57	MG	1A	3642	1/1	0.90	0.16	51,51,51,51	0
57	MG	1A	3165	1/1	0.90	0.09	41,41,41,41	0
57	MG	2A	3572	1/1	0.90	0.08	32,32,32,32	0
57	MG	2a	1764	1/1	0.90	0.24	75,75,75,75	0
57	MG	2A	3819	1/1	0.90	0.14	68,68,68,68	0
57	MG	1A	3247	1/1	0.90	0.12	63,63,63,63	0
57	MG	2A	3576	1/1	0.90	0.13	59,59,59,59	0
57	MG	2A	3827	1/1	0.90	0.11	64,64,64,64	0
57	MG	2A	3829	1/1	0.90	0.10	60,60,60,60	0
57	MG	2A	3173	1/1	0.90	0.17	72,72,72,72	0
57	MG	1A	3936	1/1	0.90	0.11	62,62,62,62	0
57	MG	1A	3049	1/1	0.90	0.07	20,20,20,20	0
57	MG	2a	1774	1/1	0.90	0.28	63,63,63,63	0
57	MG	2A	3584	1/1	0.90	0.07	34,34,34,34	0
57	MG	1a	1767	1/1	0.90	0.07	60,60,60,60	0
57	MG	1a	1769	1/1	0.90	0.11	78,78,78,78	0
57	MG	1A	3529	1/1	0.90	0.26	59,59,59,59	0
57	MG	1A	4074	1/1	0.90	0.17	38,38,38,38	0
57	MG	1A	4078	1/1	0.90	0.15	33,33,33,33	0
57	MG	2A	3338	1/1	0.90	0.26	60,60,60,60	0
57	MG	2A	3596	1/1	0.90	0.21	62,62,62,62	0
57	MG	2B	202	1/1	0.90	0.10	66,66,66,66	0
57	MG	1A	3662	1/1	0.90	0.09	29,29,29,29	0
57	MG	1A	3803	1/1	0.90	0.08	44,44,44,44	0
57	MG	1A	4083	1/1	0.90	0.16	48,48,48,48	0
57	MG	2x	103	1/1	0.90	0.15	35,35,35,35	0
57	MG	2A	3605	1/1	0.90	0.19	42,42,42,42	0
57	MG	2A	3608	1/1	0.90	0.13	41,41,41,41	0
57	MG	2B	208	1/1	0.90	0.18	57,57,57,57	0
57	MG	1A	3554	1/1	0.91	0.22	44,44,44,44	0
57	MG	2A	3226	1/1	0.91	0.27	62,62,62,62	0
57	MG	1A	4014	1/1	0.91	0.07	63,63,63,63	0
57	MG	1a	1773	1/1	0.91	0.10	58,58,58,58	0
57	MG	2A	3231	1/1	0.91	0.16	51,51,51,51	0
57	MG	1A	3063	1/1	0.91	0.16	52,52,52,52	0
57	MG	1A	3702	1/1	0.91	0.12	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	1776	1/1	0.91	0.22	71,71,71,71	0
57	MG	2A	3832	1/1	0.91	0.11	48,48,48,48	0
57	MG	2A	3834	1/1	0.91	0.13	46,46,46,46	0
57	MG	2A	3237	1/1	0.91	0.21	63,63,63,63	0
57	MG	1A	3317	1/1	0.91	0.13	55,55,55,55	0
57	MG	2A	3507	1/1	0.91	0.20	55,55,55,55	0
57	MG	1A	3705	1/1	0.91	0.15	53,53,53,53	0
57	MG	2A	3241	1/1	0.91	0.19	68,68,68,68	0
57	MG	1A	3227	1/1	0.91	0.11	48,48,48,48	0
57	MG	1A	3572	1/1	0.91	0.16	70,70,70,70	0
57	MG	1A	3575	1/1	0.91	0.17	55,55,55,55	0
57	MG	1A	3713	1/1	0.91	0.09	62,62,62,62	0
57	MG	1A	3321	1/1	0.91	0.10	56,56,56,56	0
57	MG	1A	3173	1/1	0.91	0.13	39,39,39,39	0
57	MG	2A	3530	1/1	0.91	0.10	48,48,48,48	0
57	MG	1A	3881	1/1	0.91	0.11	38,38,38,38	0
57	MG	2A	3533	1/1	0.91	0.18	65,65,65,65	0
57	MG	1a	1623	1/1	0.91	0.28	54,54,54,54	0
57	MG	2A	3536	1/1	0.91	0.15	55,55,55,55	0
57	MG	1A	3370	1/1	0.91	0.16	50,50,50,50	0
57	MG	1A	3886	1/1	0.91	0.10	39,39,39,39	0
57	MG	1A	3268	1/1	0.91	0.18	57,57,57,57	0
57	MG	1a	1629	1/1	0.91	0.23	60,60,60,60	0
57	MG	1a	1799	1/1	0.91	0.19	56,56,56,56	0
57	MG	1a	1800	1/1	0.91	0.11	66,66,66,66	0
57	MG	1A	4039	1/1	0.91	0.08	51,51,51,51	0
57	MG	1a	1634	1/1	0.91	0.27	65,65,65,65	0
57	MG	1A	3374	1/1	0.91	0.11	54,54,54,54	0
57	MG	1A	4043	1/1	0.91	0.30	54,54,54,54	0
57	MG	1a	1638	1/1	0.91	0.23	55,55,55,55	0
57	MG	1a	1639	1/1	0.91	0.22	81,81,81,81	0
57	MG	1A	3585	1/1	0.91	0.26	55,55,55,55	0
57	MG	1a	1641	1/1	0.91	0.12	59,59,59,59	0
57	MG	1A	3587	1/1	0.91	0.11	41,41,41,41	0
57	MG	1A	3589	1/1	0.91	0.12	26,26,26,26	0
57	MG	2A	3580	1/1	0.91	0.10	51,51,51,51	0
57	MG	2E	307	1/1	0.91	0.15	52,52,52,52	0
57	MG	1A	3269	1/1	0.91	0.14	55,55,55,55	0
57	MG	1A	3015	1/1	0.91	0.18	37,37,37,37	0
57	MG	2F	306	1/1	0.91	0.08	44,44,44,44	0
57	MG	1A	3597	1/1	0.91	0.12	56,56,56,56	0
57	MG	2A	3283	1/1	0.91	0.13	67,67,67,67	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	2R	201	1/1	0.91	0.14	54,54,54,54	0
57	MG	1f	201	1/1	0.91	0.21	58,58,58,58	0
57	MG	2T	3502	1/1	0.91	0.15	64,64,64,64	0
57	MG	2U	201	1/1	0.91	0.38	62,62,62,62	0
57	MG	2U	202	1/1	0.91	0.15	54,54,54,54	0
57	MG	2A	3287	1/1	0.91	0.31	70,70,70,70	0
57	MG	1A	3004	1/1	0.91	0.09	32,32,32,32	0
57	MG	1A	3742	1/1	0.91	0.14	46,46,46,46	0
57	MG	1A	3387	1/1	0.91	0.19	39,39,39,39	0
57	MG	2Z	301	1/1	0.91	0.12	60,60,60,60	0
57	MG	1A	4069	1/1	0.91	0.09	22,22,22,22	0
57	MG	1A	3470	1/1	0.91	0.15	49,49,49,49	0
57	MG	1A	3614	1/1	0.91	0.09	19,19,19,19	0
57	MG	1x	105	1/1	0.91	0.09	69,69,69,69	0
57	MG	1A	3747	1/1	0.91	0.13	22,22,22,22	0
57	MG	1A	4077	1/1	0.91	0.07	44,44,44,44	0
57	MG	1A	3474	1/1	0.91	0.10	57,57,57,57	0
57	MG	2A	3005	1/1	0.91	0.33	67,67,67,67	0
57	MG	2A	3304	1/1	0.91	0.14	66,66,66,66	0
57	MG	28	103	1/1	0.91	0.13	52,52,52,52	0
57	MG	1A	3331	1/1	0.91	0.18	55,55,55,55	0
57	MG	2A	3017	1/1	0.91	0.25	58,58,58,58	0
57	MG	2A	3019	1/1	0.91	0.13	59,59,59,59	0
57	MG	2A	3309	1/1	0.91	0.28	67,67,67,67	0
57	MG	1a	1663	1/1	0.91	0.15	66,66,66,66	0
57	MG	1A	3932	1/1	0.91	0.09	50,50,50,50	0
57	MG	1A	3332	1/1	0.91	0.17	56,56,56,56	0
57	MG	1A	3937	1/1	0.91	0.10	47,47,47,47	0
57	MG	2A	3626	1/1	0.91	0.15	55,55,55,55	0
57	MG	1A	3757	1/1	0.91	0.09	59,59,59,59	0
57	MG	2A	3044	1/1	0.91	0.09	45,45,45,45	0
57	MG	1A	3942	1/1	0.91	0.11	46,46,46,46	0
57	MG	1A	3762	1/1	0.91	0.07	45,45,45,45	0
57	MG	2A	3053	1/1	0.91	0.17	63,63,63,63	0
57	MG	2A	3057	1/1	0.91	0.15	63,63,63,63	0
57	MG	1A	3768	1/1	0.91	0.11	25,25,25,25	0
57	MG	2A	3064	1/1	0.91	0.40	55,55,55,55	0
57	MG	2a	1629	1/1	0.91	0.13	47,47,47,47	0
57	MG	2A	3069	1/1	0.91	0.18	49,49,49,49	0
57	MG	1a	1675	1/1	0.91	0.18	65,65,65,65	0
57	MG	1A	3619	1/1	0.91	0.08	29,29,29,29	0
57	MG	2A	3081	1/1	0.91	0.14	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	3950	1/1	0.91	0.10	35,35,35,35	0
57	MG	1A	3491	1/1	0.91	0.17	55,55,55,55	0
57	MG	1A	3953	1/1	0.91	0.08	41,41,41,41	0
57	MG	1B	218	1/1	0.91	0.21	51,51,51,51	0
57	MG	1A	3624	1/1	0.91	0.09	21,21,21,21	0
57	MG	1A	3494	1/1	0.91	0.21	56,56,56,56	0
57	MG	2a	1649	1/1	0.91	0.39	60,60,60,60	0
57	MG	2A	3091	1/1	0.91	0.13	45,45,45,45	0
57	MG	1A	3394	1/1	0.91	0.17	45,45,45,45	0
57	MG	2a	1652	1/1	0.91	0.12	57,57,57,57	0
57	MG	2A	3654	1/1	0.91	0.15	49,49,49,49	0
57	MG	2a	1655	1/1	0.91	0.13	56,56,56,56	0
57	MG	1A	3395	1/1	0.91	0.21	51,51,51,51	0
57	MG	1A	3628	1/1	0.91	0.11	24,24,24,24	0
57	MG	2A	3098	1/1	0.91	0.21	68,68,68,68	0
57	MG	2A	3659	1/1	0.91	0.10	45,45,45,45	0
57	MG	2A	3347	1/1	0.91	0.10	64,64,64,64	0
57	MG	2a	1661	1/1	0.91	0.28	62,62,62,62	0
57	MG	1A	3964	1/1	0.91	0.10	62,62,62,62	0
57	MG	2a	1664	1/1	0.91	0.19	53,53,53,53	0
57	MG	2A	3102	1/1	0.91	0.24	71,71,71,71	0
57	MG	1a	1689	1/1	0.91	0.09	75,75,75,75	0
57	MG	2A	3106	1/1	0.91	0.19	63,63,63,63	0
57	MG	1A	3501	1/1	0.91	0.14	53,53,53,53	0
57	MG	1A	3089	1/1	0.91	0.11	54,54,54,54	0
57	MG	1D	309	1/1	0.91	0.18	49,49,49,49	0
57	MG	2A	3675	1/1	0.91	0.22	60,60,60,60	0
57	MG	1A	3168	1/1	0.91	0.11	33,33,33,33	0
57	MG	1A	3640	1/1	0.91	0.16	43,43,43,43	0
57	MG	2A	3122	1/1	0.91	0.14	56,56,56,56	0
57	MG	2A	3362	1/1	0.91	0.12	60,60,60,60	0
57	MG	1A	3336	1/1	0.91	0.23	61,61,61,61	0
57	MG	2A	3683	1/1	0.91	0.21	62,62,62,62	0
57	MG	2A	3684	1/1	0.91	0.13	60,60,60,60	0
57	MG	2a	1689	1/1	0.91	0.20	54,54,54,54	0
57	MG	1E	306	1/1	0.91	0.15	61,61,61,61	0
57	MG	2A	3125	1/1	0.91	0.31	64,64,64,64	0
57	MG	1A	3337	1/1	0.91	0.13	48,48,48,48	0
57	MG	1A	3647	1/1	0.91	0.07	24,24,24,24	0
57	MG	2A	3137	1/1	0.91	0.22	53,53,53,53	0
57	MG	2A	3695	1/1	0.91	0.14	54,54,54,54	0
57	MG	2a	1710	1/1	0.91	0.19	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	1F	301	1/1	0.91	0.19	43,43,43,43	0
57	MG	1A	3001	1/1	0.91	0.11	38,38,38,38	0
57	MG	2A	3376	1/1	0.91	0.11	57,57,57,57	0
57	MG	2a	1719	1/1	0.91	0.17	68,68,68,68	0
57	MG	2A	3700	1/1	0.91	0.12	65,65,65,65	0
57	MG	1a	1707	1/1	0.91	0.23	64,64,64,64	0
57	MG	2A	3703	1/1	0.91	0.24	66,66,66,66	0
57	MG	2a	1723	1/1	0.91	0.16	62,62,62,62	0
57	MG	1A	3978	1/1	0.91	0.08	28,28,28,28	0
57	MG	2A	3149	1/1	0.91	0.11	60,60,60,60	0
57	MG	2A	3706	1/1	0.91	0.08	71,71,71,71	0
57	MG	1F	313	1/1	0.91	0.16	41,41,41,41	0
57	MG	2A	3385	1/1	0.91	0.13	57,57,57,57	0
57	MG	1a	1710	1/1	0.91	0.12	52,52,52,52	0
57	MG	2A	3161	1/1	0.91	0.36	64,64,64,64	0
57	MG	1a	1713	1/1	0.91	0.11	60,60,60,60	0
57	MG	1F	314	1/1	0.91	0.14	52,52,52,52	0
57	MG	1A	3297	1/1	0.91	0.13	51,51,51,51	0
57	MG	2a	1741	1/1	0.91	0.15	69,69,69,69	0
57	MG	1G	201	1/1	0.91	0.14	47,47,47,47	0
57	MG	2A	3168	1/1	0.91	0.11	53,53,53,53	0
57	MG	1A	3348	1/1	0.91	0.26	65,65,65,65	0
57	MG	2A	3396	1/1	0.91	0.20	52,52,52,52	0
57	MG	1A	3299	1/1	0.91	0.25	46,46,46,46	0
57	MG	2A	3403	1/1	0.91	0.18	53,53,53,53	0
57	MG	2A	3728	1/1	0.91	0.20	67,67,67,67	0
57	MG	1I	201	1/1	0.91	0.12	67,67,67,67	0
57	MG	1A	3259	1/1	0.91	0.09	36,36,36,36	0
57	MG	2a	1752	1/1	0.91	0.13	55,55,55,55	0
57	MG	1a	1724	1/1	0.91	0.10	52,52,52,52	0
57	MG	1A	3522	1/1	0.91	0.15	47,47,47,47	0
57	MG	1a	1728	1/1	0.91	0.15	53,53,53,53	0
57	MG	1A	3523	1/1	0.91	0.25	62,62,62,62	0
57	MG	2A	3738	1/1	0.91	0.08	59,59,59,59	0
57	MG	2A	3188	1/1	0.91	0.16	71,71,71,71	0
57	MG	1A	3526	1/1	0.91	0.24	49,49,49,49	0
57	MG	1O	201	1/1	0.91	0.15	59,59,59,59	0
57	MG	2A	3423	1/1	0.91	0.29	50,50,50,50	0
57	MG	1A	3988	1/1	0.91	0.09	41,41,41,41	0
57	MG	2a	1767	1/1	0.91	0.24	61,61,61,61	0
57	MG	1A	3214	1/1	0.91	0.09	42,42,42,42	0
57	MG	1A	3826	1/1	0.91	0.09	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	3352	1/1	0.91	0.27	43,43,43,43	0
57	MG	1S	203	1/1	0.91	0.09	65,65,65,65	0
57	MG	2A	3436	1/1	0.91	0.31	53,53,53,53	0
57	MG	1A	3681	1/1	0.91	0.09	35,35,35,35	0
57	MG	1A	3536	1/1	0.91	0.19	54,54,54,54	0
57	MG	2a	1775	1/1	0.91	0.13	63,63,63,63	0
57	MG	1A	3353	1/1	0.91	0.11	59,59,59,59	0
57	MG	1V	202	1/1	0.91	0.38	38,38,38,38	0
57	MG	1A	3999	1/1	0.91	0.09	28,28,28,28	0
57	MG	1W	201	1/1	0.91	0.27	55,55,55,55	0
57	MG	1A	3308	1/1	0.91	0.14	51,51,51,51	0
57	MG	1A	3356	1/1	0.91	0.13	61,61,61,61	0
57	MG	1A	3691	1/1	0.91	0.16	31,31,31,31	0
57	MG	15	108	1/1	0.91	0.07	40,40,40,40	0
57	MG	2k	201	1/1	0.91	0.13	61,61,61,61	0
57	MG	2A	3467	1/1	0.91	0.13	47,47,47,47	0
57	MG	2A	3788	1/1	0.91	0.09	33,33,33,33	0
57	MG	2t	201	1/1	0.91	0.20	51,51,51,51	0
57	MG	1A	3027	1/1	0.91	0.21	69,69,69,69	0
57	MG	17	106	1/1	0.91	0.09	43,43,43,43	0
57	MG	18	102	1/1	0.91	0.17	49,49,49,49	0
57	MG	1a	1765	1/1	0.91	0.08	62,62,62,62	0
57	MG	2x	105	1/1	0.91	0.11	64,64,64,64	0
57	MG	1A	3432	1/1	0.91	0.14	43,43,43,43	0
57	MG	2A	3481	1/1	0.91	0.14	32,32,32,32	0
57	MG	2A	3285	1/1	0.92	0.15	51,51,51,51	0
57	MG	2A	3058	1/1	0.92	0.20	48,48,48,48	0
57	MG	1A	3420	1/1	0.92	0.12	55,55,55,55	0
57	MG	2A	3550	1/1	0.92	0.09	44,44,44,44	0
57	MG	1A	3251	1/1	0.92	0.29	40,40,40,40	0
57	MG	2A	3289	1/1	0.92	0.21	68,68,68,68	0
57	MG	2A	3558	1/1	0.92	0.22	53,53,53,53	0
57	MG	2A	3065	1/1	0.92	0.27	65,65,65,65	0
57	MG	2A	3068	1/1	0.92	0.25	50,50,50,50	0
57	MG	1A	4027	1/1	0.92	0.09	41,41,41,41	0
57	MG	2A	3070	1/1	0.92	0.07	41,41,41,41	0
57	MG	1A	3252	1/1	0.92	0.08	67,67,67,67	0
57	MG	2A	3570	1/1	0.92	0.12	49,49,49,49	0
57	MG	2A	3297	1/1	0.92	0.09	77,77,77,77	0
57	MG	1A	3519	1/1	0.92	0.26	57,57,57,57	0
57	MG	2A	3079	1/1	0.92	0.16	52,52,52,52	0
57	MG	1A	3521	1/1	0.92	0.27	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	3253	1/1	0.92	0.17	51,51,51,51	0
57	MG	2B	217	1/1	0.92	0.31	65,65,65,65	0
57	MG	1A	3354	1/1	0.92	0.12	58,58,58,58	0
57	MG	1A	3909	1/1	0.92	0.11	59,59,59,59	0
57	MG	2A	3086	1/1	0.92	0.14	61,61,61,61	0
57	MG	2B	221	1/1	0.92	0.26	65,65,65,65	0
57	MG	1A	3637	1/1	0.92	0.11	53,53,53,53	0
57	MG	10	107	1/1	0.92	0.11	61,61,61,61	0
57	MG	11	104	1/1	0.92	0.14	63,63,63,63	0
57	MG	13	104	1/1	0.92	0.14	56,56,56,56	0
57	MG	15	104	1/1	0.92	0.33	43,43,43,43	0
57	MG	1A	3095	1/1	0.92	0.14	49,49,49,49	0
57	MG	1A	4041	1/1	0.92	0.08	29,29,29,29	0
57	MG	2E	309	1/1	0.92	0.14	61,61,61,61	0
57	MG	1A	3771	1/1	0.92	0.10	34,34,34,34	0
57	MG	1A	3773	1/1	0.92	0.07	39,39,39,39	0
57	MG	2F	305	1/1	0.92	0.10	56,56,56,56	0
57	MG	18	103	1/1	0.92	0.15	47,47,47,47	0
57	MG	1A	3527	1/1	0.92	0.06	60,60,60,60	0
57	MG	1A	3778	1/1	0.92	0.09	44,44,44,44	0
57	MG	1A	3781	1/1	0.92	0.09	19,19,19,19	0
57	MG	2A	3109	1/1	0.92	0.14	53,53,53,53	0
57	MG	2A	3110	1/1	0.92	0.16	57,57,57,57	0
57	MG	2T	3503	1/1	0.92	0.24	54,54,54,54	0
57	MG	1A	3209	1/1	0.92	0.12	53,53,53,53	0
57	MG	2A	3614	1/1	0.92	0.12	39,39,39,39	0
57	MG	2A	3112	1/1	0.92	0.34	62,62,62,62	0
57	MG	2A	3115	1/1	0.92	0.14	47,47,47,47	0
57	MG	1A	3532	1/1	0.92	0.22	58,58,58,58	0
57	MG	1A	3040	1/1	0.92	0.06	52,52,52,52	0
57	MG	1A	4059	1/1	0.92	0.07	40,40,40,40	0
57	MG	20	102	1/1	0.92	0.15	65,65,65,65	0
57	MG	2A	3120	1/1	0.92	0.10	47,47,47,47	0
57	MG	1A	4060	1/1	0.92	0.07	17,17,17,17	0
57	MG	1A	4063	1/1	0.92	0.12	52,52,52,52	0
57	MG	2A	3628	1/1	0.92	0.10	59,59,59,59	0
57	MG	1a	1743	1/1	0.92	0.11	59,59,59,59	0
57	MG	2A	3336	1/1	0.92	0.22	53,53,53,53	0
57	MG	25	107	1/1	0.92	0.11	49,49,49,49	0
57	MG	1A	3649	1/1	0.92	0.08	41,41,41,41	0
57	MG	2A	3126	1/1	0.92	0.10	56,56,56,56	0
57	MG	1A	3315	1/1	0.92	0.19	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	1A	3436	1/1	0.92	0.13	60,60,60,60	0
57	MG	1A	3260	1/1	0.92	0.06	39,39,39,39	0
57	MG	2A	3636	1/1	0.92	0.09	59,59,59,59	0
57	MG	1A	3318	1/1	0.92	0.11	52,52,52,52	0
57	MG	2A	3141	1/1	0.92	0.26	66,66,66,66	0
57	MG	2A	3144	1/1	0.92	0.27	48,48,48,48	0
57	MG	1A	3444	1/1	0.92	0.11	57,57,57,57	0
57	MG	2a	1610	1/1	0.92	0.09	52,52,52,52	0
57	MG	1A	3365	1/1	0.92	0.19	59,59,59,59	0
57	MG	1a	1626	1/1	0.92	0.18	63,63,63,63	0
57	MG	1A	3807	1/1	0.92	0.12	35,35,35,35	0
57	MG	1A	3211	1/1	0.92	0.08	34,34,34,34	0
57	MG	2A	3158	1/1	0.92	0.23	55,55,55,55	0
57	MG	2A	3358	1/1	0.92	0.09	45,45,45,45	0
57	MG	1A	3449	1/1	0.92	0.26	58,58,58,58	0
57	MG	1A	3146	1/1	0.92	0.09	38,38,38,38	0
57	MG	1a	1632	1/1	0.92	0.21	50,50,50,50	0
57	MG	1a	1768	1/1	0.92	0.33	67,67,67,67	0
57	MG	1a	1633	1/1	0.92	0.25	72,72,72,72	0
57	MG	1A	3323	1/1	0.92	0.11	48,48,48,48	0
57	MG	2a	1631	1/1	0.92	0.20	61,61,61,61	0
57	MG	2A	3367	1/1	0.92	0.09	48,48,48,48	0
57	MG	2A	3368	1/1	0.92	0.24	52,52,52,52	0
57	MG	2a	1635	1/1	0.92	0.17	63,63,63,63	0
57	MG	2A	3660	1/1	0.92	0.17	51,51,51,51	0
57	MG	1A	3372	1/1	0.92	0.14	48,48,48,48	0
57	MG	1A	3814	1/1	0.92	0.21	58,58,58,58	0
57	MG	2a	1641	1/1	0.92	0.27	61,61,61,61	0
57	MG	1A	4087	1/1	0.92	0.15	40,40,40,40	0
57	MG	1A	4089	1/1	0.92	0.10	64,64,64,64	0
57	MG	1a	1779	1/1	0.92	0.14	71,71,71,71	0
57	MG	2A	3175	1/1	0.92	0.10	41,41,41,41	0
57	MG	2A	3671	1/1	0.92	0.09	60,60,60,60	0
57	MG	2A	3377	1/1	0.92	0.16	61,61,61,61	0
57	MG	1A	3573	1/1	0.92	0.09	39,39,39,39	0
57	MG	1A	3965	1/1	0.92	0.11	65,65,65,65	0
57	MG	1A	3219	1/1	0.92	0.17	56,56,56,56	0
57	MG	1A	3325	1/1	0.92	0.20	57,57,57,57	0
57	MG	1A	3106	1/1	0.92	0.09	33,33,33,33	0
57	MG	2A	3386	1/1	0.92	0.12	63,63,63,63	0
57	MG	1A	3693	1/1	0.92	0.10	37,37,37,37	0
57	MG	1A	3579	1/1	0.92	0.28	70,70,70,70	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	3159	1/1	0.92	0.10	35,35,35,35	0
57	MG	1A	3463	1/1	0.92	0.18	46,46,46,46	0
57	MG	1A	3582	1/1	0.92	0.24	65,65,65,65	0
57	MG	2A	3689	1/1	0.92	0.15	35,35,35,35	0
57	MG	1A	3976	1/1	0.92	0.12	20,20,20,20	0
57	MG	1a	1795	1/1	0.92	0.14	58,58,58,58	0
57	MG	1A	3829	1/1	0.92	0.10	55,55,55,55	0
57	MG	2A	3395	1/1	0.92	0.18	46,46,46,46	0
57	MG	2a	1668	1/1	0.92	0.09	72,72,72,72	0
57	MG	1A	3182	1/1	0.92	0.25	50,50,50,50	0
57	MG	2A	3401	1/1	0.92	0.27	41,41,41,41	0
57	MG	2A	3202	1/1	0.92	0.12	66,66,66,66	0
57	MG	1a	1798	1/1	0.92	0.08	53,53,53,53	0
57	MG	1A	3469	1/1	0.92	0.24	59,59,59,59	0
57	MG	1A	3230	1/1	0.92	0.25	34,34,34,34	0
57	MG	1a	1660	1/1	0.92	0.16	64,64,64,64	0
57	MG	1A	3160	1/1	0.92	0.07	55,55,55,55	0
57	MG	1A	3184	1/1	0.92	0.11	54,54,54,54	0
57	MG	1A	3277	1/1	0.92	0.21	38,38,38,38	0
57	MG	2a	1684	1/1	0.92	0.08	59,59,59,59	0
57	MG	2a	1685	1/1	0.92	0.12	60,60,60,60	0
57	MG	2a	1686	1/1	0.92	0.18	58,58,58,58	0
57	MG	2A	3211	1/1	0.92	0.15	67,67,67,67	0
57	MG	1A	3594	1/1	0.92	0.12	45,45,45,45	0
57	MG	1A	3847	1/1	0.92	0.15	55,55,55,55	0
57	MG	1A	3285	1/1	0.92	0.13	45,45,45,45	0
57	MG	2a	1694	1/1	0.92	0.14	63,63,63,63	0
57	MG	2a	1695	1/1	0.92	0.20	50,50,50,50	0
57	MG	1E	309	1/1	0.92	0.10	25,25,25,25	0
57	MG	2a	1700	1/1	0.92	0.15	58,58,58,58	0
57	MG	2a	1701	1/1	0.92	0.15	49,49,49,49	0
57	MG	2a	1702	1/1	0.92	0.15	50,50,50,50	0
57	MG	2A	3717	1/1	0.92	0.11	35,35,35,35	0
57	MG	2A	3718	1/1	0.92	0.19	48,48,48,48	0
57	MG	1E	310	1/1	0.92	0.18	50,50,50,50	0
57	MG	2A	3428	1/1	0.92	0.11	57,57,57,57	0
57	MG	2A	3218	1/1	0.92	0.17	59,59,59,59	0
57	MG	1A	3598	1/1	0.92	0.08	23,23,23,23	0
57	MG	1A	3288	1/1	0.92	0.16	43,43,43,43	0
57	MG	1a	1822	1/1	0.92	0.18	75,75,75,75	0
57	MG	1A	3289	1/1	0.92	0.16	54,54,54,54	0
57	MG	1e	201	1/1	0.92	0.08	67,67,67,67	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	3729	1/1	0.92	0.14	65,65,65,65	0
57	MG	2A	3440	1/1	0.92	0.21	38,38,38,38	0
57	MG	2A	3441	1/1	0.92	0.13	54,54,54,54	0
57	MG	1F	305	1/1	0.92	0.12	57,57,57,57	0
57	MG	1A	3290	1/1	0.92	0.21	52,52,52,52	0
57	MG	1A	3613	1/1	0.92	0.07	31,31,31,31	0
57	MG	1A	3341	1/1	0.92	0.19	53,53,53,53	0
57	MG	2A	3236	1/1	0.92	0.12	60,60,60,60	0
57	MG	1A	3406	1/1	0.92	0.16	56,56,56,56	0
57	MG	1A	3732	1/1	0.92	0.13	64,64,64,64	0
57	MG	1p	101	1/1	0.92	0.12	63,63,63,63	0
57	MG	2A	3750	1/1	0.92	0.07	59,59,59,59	0
57	MG	2A	3461	1/1	0.92	0.07	43,43,43,43	0
57	MG	1r	101	1/1	0.92	0.29	60,60,60,60	0
57	MG	1G	202	1/1	0.92	0.17	57,57,57,57	0
57	MG	1A	3869	1/1	0.92	0.12	44,44,44,44	0
57	MG	1a	1685	1/1	0.92	0.09	53,53,53,53	0
57	MG	2A	3472	1/1	0.92	0.16	63,63,63,63	0
57	MG	2A	3476	1/1	0.92	0.12	54,54,54,54	0
57	MG	2A	3245	1/1	0.92	0.11	66,66,66,66	0
57	MG	1A	3872	1/1	0.92	0.10	24,24,24,24	0
57	MG	1A	3246	1/1	0.92	0.12	48,48,48,48	0
57	MG	1x	112	1/1	0.92	0.18	65,65,65,65	0
57	MG	2A	3001	1/1	0.92	0.30	55,55,55,55	0
57	MG	2a	1754	1/1	0.92	0.25	57,57,57,57	0
57	MG	1A	3130	1/1	0.92	0.16	51,51,51,51	0
57	MG	1A	3248	1/1	0.92	0.08	53,53,53,53	0
57	MG	2A	3257	1/1	0.92	0.10	65,65,65,65	0
57	MG	1A	3622	1/1	0.92	0.09	39,39,39,39	0
57	MG	1A	3741	1/1	0.92	0.15	51,51,51,51	0
57	MG	1A	3413	1/1	0.92	0.29	61,61,61,61	0
57	MG	1A	3888	1/1	0.92	0.14	55,55,55,55	0
57	MG	2A	3505	1/1	0.92	0.17	59,59,59,59	0
57	MG	1A	3132	1/1	0.92	0.06	60,60,60,60	0
57	MG	1a	1695	1/1	0.92	0.24	53,53,53,53	0
57	MG	2A	3508	1/1	0.92	0.15	45,45,45,45	0
57	MG	1a	1696	1/1	0.92	0.31	56,56,56,56	0
57	MG	2A	3807	1/1	0.92	0.14	66,66,66,66	0
57	MG	2A	3511	1/1	0.92	0.15	55,55,55,55	0
57	MG	2A	3033	1/1	0.92	0.07	42,42,42,42	0
57	MG	2A	3039	1/1	0.92	0.25	66,66,66,66	0
57	MG	2A	3817	1/1	0.92	0.08	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	2A	3041	1/1	0.92	0.38	58,58,58,58	0
57	MG	2A	3519	1/1	0.92	0.07	33,33,33,33	0
57	MG	2d	301	1/1	0.92	0.29	57,57,57,57	0
57	MG	2A	3821	1/1	0.92	0.11	59,59,59,59	0
57	MG	2A	3272	1/1	0.92	0.16	54,54,54,54	0
57	MG	2f	201	1/1	0.92	0.15	58,58,58,58	0
57	MG	1Q	201	1/1	0.92	0.27	48,48,48,48	0
57	MG	1A	3891	1/1	0.92	0.10	48,48,48,48	0
57	MG	2A	3828	1/1	0.92	0.11	30,30,30,30	0
57	MG	1a	1700	1/1	0.92	0.22	52,52,52,52	0
57	MG	2A	3830	1/1	0.92	0.26	65,65,65,65	0
57	MG	2A	3047	1/1	0.92	0.17	62,62,62,62	0
57	MG	2A	3048	1/1	0.92	0.15	48,48,48,48	0
57	MG	2A	3835	1/1	0.92	0.14	42,42,42,42	0
57	MG	1a	1701	1/1	0.92	0.33	57,57,57,57	0
57	MG	2A	3837	1/1	0.92	0.11	52,52,52,52	0
57	MG	1A	4023	1/1	0.92	0.12	39,39,39,39	0
57	MG	2A	3056	1/1	0.92	0.14	60,60,60,60	0
57	MG	1S	201	1/1	0.92	0.15	36,36,36,36	0
57	MG	2A	3541	1/1	0.92	0.14	48,48,48,48	0
57	MG	2x	107	1/1	0.92	0.12	74,74,74,74	0
57	MG	2A	3846	1/1	0.92	0.15	56,56,56,56	0
57	MG	2A	3284	1/1	0.92	0.33	55,55,55,55	0
57	MG	1A	3943	1/1	0.93	0.14	69,69,69,69	0
57	MG	2E	302	1/1	0.93	0.11	52,52,52,52	0
57	MG	2A	3624	1/1	0.93	0.16	64,64,64,64	0
57	MG	2A	3381	1/1	0.93	0.08	66,66,66,66	0
57	MG	2A	3627	1/1	0.93	0.12	51,51,51,51	0
57	MG	1a	1702	1/1	0.93	0.15	60,60,60,60	0
57	MG	2E	308	1/1	0.93	0.17	32,32,32,32	0
57	MG	1A	3946	1/1	0.93	0.07	52,52,52,52	0
57	MG	2A	3384	1/1	0.93	0.25	63,63,63,63	0
57	MG	1A	3092	1/1	0.93	0.20	55,55,55,55	0
57	MG	1A	3817	1/1	0.93	0.14	35,35,35,35	0
57	MG	10	103	1/1	0.93	0.12	52,52,52,52	0
57	MG	2F	307	1/1	0.93	0.15	58,58,58,58	0
57	MG	2A	3024	1/1	0.93	0.28	44,44,44,44	0
57	MG	1A	3314	1/1	0.93	0.25	53,53,53,53	0
57	MG	11	101	1/1	0.93	0.40	39,39,39,39	0
57	MG	2A	3637	1/1	0.93	0.12	62,62,62,62	0
57	MG	1A	4062	1/1	0.93	0.08	37,37,37,37	0
57	MG	12	101	1/1	0.93	0.09	49,49,49,49	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	3195	1/1	0.93	0.23	29,29,29,29	0
57	MG	1A	3534	1/1	0.93	0.08	61,61,61,61	0
57	MG	1a	1715	1/1	0.93	0.13	47,47,47,47	0
57	MG	2V	202	1/1	0.93	0.29	67,67,67,67	0
57	MG	1A	3316	1/1	0.93	0.09	45,45,45,45	0
57	MG	2A	3397	1/1	0.93	0.20	39,39,39,39	0
57	MG	1A	3724	1/1	0.93	0.08	52,52,52,52	0
57	MG	1A	3415	1/1	0.93	0.11	48,48,48,48	0
57	MG	1A	3102	1/1	0.93	0.15	47,47,47,47	0
57	MG	2A	3405	1/1	0.93	0.25	57,57,57,57	0
57	MG	2A	3406	1/1	0.93	0.17	34,34,34,34	0
57	MG	2A	3052	1/1	0.93	0.17	60,60,60,60	0
57	MG	1A	3419	1/1	0.93	0.21	68,68,68,68	0
57	MG	25	103	1/1	0.93	0.18	62,62,62,62	0
57	MG	1a	1722	1/1	0.93	0.12	54,54,54,54	0
57	MG	1A	3729	1/1	0.93	0.12	33,33,33,33	0
57	MG	2A	3248	1/1	0.93	0.26	63,63,63,63	0
57	MG	2A	3413	1/1	0.93	0.13	48,48,48,48	0
57	MG	2A	3414	1/1	0.93	0.19	60,60,60,60	0
57	MG	28	101	1/1	0.93	0.12	60,60,60,60	0
57	MG	1A	3207	1/1	0.93	0.12	59,59,59,59	0
57	MG	1A	3480	1/1	0.93	0.13	58,58,58,58	0
57	MG	2A	3063	1/1	0.93	0.21	55,55,55,55	0
57	MG	2A	3253	1/1	0.93	0.26	60,60,60,60	0
57	MG	1a	1727	1/1	0.93	0.29	69,69,69,69	0
57	MG	1A	3553	1/1	0.93	0.07	22,22,22,22	0
57	MG	2A	3425	1/1	0.93	0.35	56,56,56,56	0
57	MG	2A	3256	1/1	0.93	0.21	61,61,61,61	0
57	MG	1A	3481	1/1	0.93	0.25	43,43,43,43	0
57	MG	1A	3377	1/1	0.93	0.08	57,57,57,57	0
57	MG	1A	3738	1/1	0.93	0.09	54,54,54,54	0
57	MG	2A	3433	1/1	0.93	0.28	58,58,58,58	0
57	MG	1a	1607	1/1	0.93	0.12	51,51,51,51	0
57	MG	1A	3841	1/1	0.93	0.10	55,55,55,55	0
57	MG	1A	3843	1/1	0.93	0.09	44,44,44,44	0
57	MG	1A	3846	1/1	0.93	0.15	59,59,59,59	0
57	MG	1B	201	1/1	0.93	0.10	57,57,57,57	0
57	MG	1A	3643	1/1	0.93	0.14	47,47,47,47	0
57	MG	1a	1615	1/1	0.93	0.09	68,68,68,68	0
57	MG	2A	3443	1/1	0.93	0.13	56,56,56,56	0
57	MG	2A	3444	1/1	0.93	0.27	59,59,59,59	0
57	MG	2A	3445	1/1	0.93	0.10	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	1A	3975	1/1	0.93	0.11	39,39,39,39	0
57	MG	1a	1618	1/1	0.93	0.10	73,73,73,73	0
57	MG	2A	3450	1/1	0.93	0.14	61,61,61,61	0
57	MG	2A	3451	1/1	0.93	0.27	46,46,46,46	0
57	MG	2A	3698	1/1	0.93	0.18	72,72,72,72	0
57	MG	2a	1639	1/1	0.93	0.23	55,55,55,55	0
57	MG	1A	3093	1/1	0.93	0.15	55,55,55,55	0
57	MG	1A	3490	1/1	0.93	0.15	38,38,38,38	0
57	MG	1A	3850	1/1	0.93	0.10	48,48,48,48	0
57	MG	2A	3457	1/1	0.93	0.08	53,53,53,53	0
57	MG	2a	1644	1/1	0.93	0.18	57,57,57,57	0
57	MG	1a	1751	1/1	0.93	0.12	55,55,55,55	0
57	MG	2A	3277	1/1	0.93	0.10	65,65,65,65	0
57	MG	1B	211	1/1	0.93	0.11	53,53,53,53	0
57	MG	2A	3463	1/1	0.93	0.20	58,58,58,58	0
57	MG	2A	3465	1/1	0.93	0.23	61,61,61,61	0
57	MG	2A	3096	1/1	0.93	0.12	48,48,48,48	0
57	MG	1A	3380	1/1	0.93	0.12	47,47,47,47	0
57	MG	1B	213	1/1	0.93	0.20	59,59,59,59	0
57	MG	1B	214	1/1	0.93	0.07	50,50,50,50	0
57	MG	2A	3101	1/1	0.93	0.18	61,61,61,61	0
57	MG	2A	3473	1/1	0.93	0.09	53,53,53,53	0
57	MG	2A	3719	1/1	0.93	0.29	44,44,44,44	0
57	MG	1A	3492	1/1	0.93	0.10	38,38,38,38	0
57	MG	2A	3477	1/1	0.93	0.06	40,40,40,40	0
57	MG	1A	3383	1/1	0.93	0.29	29,29,29,29	0
57	MG	1A	3657	1/1	0.93	0.08	23,23,23,23	0
57	MG	1a	1764	1/1	0.93	0.17	52,52,52,52	0
57	MG	1B	222	1/1	0.93	0.10	64,64,64,64	0
57	MG	1A	3859	1/1	0.93	0.23	39,39,39,39	0
57	MG	2A	3484	1/1	0.93	0.06	29,29,29,29	0
57	MG	2A	3292	1/1	0.93	0.23	56,56,56,56	0
57	MG	1A	3425	1/1	0.93	0.23	50,50,50,50	0
57	MG	2a	1670	1/1	0.93	0.30	64,64,64,64	0
57	MG	2A	3488	1/1	0.93	0.10	40,40,40,40	0
57	MG	1A	3753	1/1	0.93	0.10	26,26,26,26	0
57	MG	1A	3234	1/1	0.93	0.23	48,48,48,48	0
57	MG	1B	232	1/1	0.93	0.08	60,60,60,60	0
57	MG	2A	3495	1/1	0.93	0.11	44,44,44,44	0
57	MG	1A	3244	1/1	0.93	0.22	44,44,44,44	0
57	MG	2A	3741	1/1	0.93	0.13	60,60,60,60	0
57	MG	2A	3502	1/1	0.93	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	1A	3758	1/1	0.93	0.11	23,23,23,23	0
57	MG	2a	1682	1/1	0.93	0.25	55,55,55,55	0
57	MG	2A	3748	1/1	0.93	0.13	62,62,62,62	0
57	MG	1D	308	1/1	0.93	0.14	38,38,38,38	0
57	MG	1A	3873	1/1	0.93	0.06	28,28,28,28	0
57	MG	1A	3875	1/1	0.93	0.09	25,25,25,25	0
57	MG	1a	1780	1/1	0.93	0.08	56,56,56,56	0
57	MG	2a	1691	1/1	0.93	0.20	56,56,56,56	0
57	MG	1A	3761	1/1	0.93	0.07	65,65,65,65	0
57	MG	2A	3756	1/1	0.93	0.07	62,62,62,62	0
57	MG	1A	3997	1/1	0.93	0.13	58,58,58,58	0
57	MG	1E	305	1/1	0.93	0.17	35,35,35,35	0
57	MG	1A	3665	1/1	0.93	0.11	53,53,53,53	0
57	MG	1A	3878	1/1	0.93	0.07	41,41,41,41	0
57	MG	2A	3518	1/1	0.93	0.08	45,45,45,45	0
57	MG	2A	3139	1/1	0.93	0.17	39,39,39,39	0
57	MG	2a	1703	1/1	0.93	0.16	41,41,41,41	0
57	MG	1A	3765	1/1	0.93	0.11	33,33,33,33	0
57	MG	1A	3503	1/1	0.93	0.11	50,50,50,50	0
57	MG	2a	1707	1/1	0.93	0.25	55,55,55,55	0
57	MG	2a	1708	1/1	0.93	0.21	56,56,56,56	0
57	MG	2A	3143	1/1	0.93	0.28	48,48,48,48	0
57	MG	2A	3527	1/1	0.93	0.08	45,45,45,45	0
57	MG	1a	1656	1/1	0.93	0.18	57,57,57,57	0
57	MG	2A	3774	1/1	0.93	0.13	77,77,77,77	0
57	MG	2a	1716	1/1	0.93	0.15	65,65,65,65	0
57	MG	1a	1791	1/1	0.93	0.10	52,52,52,52	0
57	MG	1A	3245	1/1	0.93	0.10	39,39,39,39	0
57	MG	1E	314	1/1	0.93	0.10	61,61,61,61	0
57	MG	1A	3389	1/1	0.93	0.11	62,62,62,62	0
57	MG	2A	3535	1/1	0.93	0.11	34,34,34,34	0
57	MG	2A	3151	1/1	0.93	0.08	40,40,40,40	0
57	MG	1A	3775	1/1	0.93	0.20	63,63,63,63	0
57	MG	1A	3131	1/1	0.93	0.16	45,45,45,45	0
57	MG	1A	3437	1/1	0.93	0.08	42,42,42,42	0
57	MG	2A	3543	1/1	0.93	0.07	35,35,35,35	0
57	MG	2A	3325	1/1	0.93	0.15	54,54,54,54	0
57	MG	1A	3509	1/1	0.93	0.17	62,62,62,62	0
57	MG	2A	3810	1/1	0.93	0.06	41,41,41,41	0
57	MG	2A	3812	1/1	0.93	0.07	50,50,50,50	0
57	MG	1a	1666	1/1	0.93	0.21	61,61,61,61	0
57	MG	2a	1739	1/1	0.93	0.21	60,60,60,60	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	3163	1/1	0.93	0.13	41,41,41,41	0
57	MG	1A	3588	1/1	0.93	0.10	55,55,55,55	0
57	MG	1A	3510	1/1	0.93	0.08	62,62,62,62	0
57	MG	2A	3557	1/1	0.93	0.21	61,61,61,61	0
57	MG	2A	3820	1/1	0.93	0.08	70,70,70,70	0
57	MG	1a	1669	1/1	0.93	0.11	75,75,75,75	0
57	MG	1A	3591	1/1	0.93	0.09	22,22,22,22	0
57	MG	1A	3511	1/1	0.93	0.18	52,52,52,52	0
57	MG	2A	3334	1/1	0.93	0.18	58,58,58,58	0
57	MG	1A	3792	1/1	0.93	0.31	31,31,31,31	0
57	MG	1A	3439	1/1	0.93	0.24	65,65,65,65	0
57	MG	1a	1813	1/1	0.93	0.10	53,53,53,53	0
57	MG	1A	3298	1/1	0.93	0.09	40,40,40,40	0
57	MG	2A	3833	1/1	0.93	0.09	43,43,43,43	0
57	MG	2A	3178	1/1	0.93	0.10	39,39,39,39	0
57	MG	1A	3020	1/1	0.93	0.11	42,42,42,42	0
57	MG	2A	3577	1/1	0.93	0.11	54,54,54,54	0
57	MG	1A	3109	1/1	0.93	0.27	31,31,31,31	0
57	MG	2A	3838	1/1	0.93	0.16	62,62,62,62	0
57	MG	2A	3183	1/1	0.93	0.06	57,57,57,57	0
57	MG	2A	3841	1/1	0.93	0.09	77,77,77,77	0
57	MG	1A	3914	1/1	0.93	0.08	48,48,48,48	0
57	MG	1A	3800	1/1	0.93	0.10	32,32,32,32	0
57	MG	1A	3396	1/1	0.93	0.16	46,46,46,46	0
57	MG	1A	3301	1/1	0.93	0.21	36,36,36,36	0
57	MG	1A	3520	1/1	0.93	0.20	40,40,40,40	0
57	MG	2A	3354	1/1	0.93	0.21	44,44,44,44	0
57	MG	2A	3849	1/1	0.93	0.13	63,63,63,63	0
57	MG	2A	3589	1/1	0.93	0.17	40,40,40,40	0
57	MG	1P	202	1/1	0.93	0.28	48,48,48,48	0
57	MG	2A	3591	1/1	0.93	0.10	48,48,48,48	0
57	MG	1e	203	1/1	0.93	0.14	77,77,77,77	0
57	MG	1A	3398	1/1	0.93	0.26	41,41,41,41	0
57	MG	1A	3167	1/1	0.93	0.17	41,41,41,41	0
57	MG	2A	3196	1/1	0.93	0.21	63,63,63,63	0
57	MG	2A	3599	1/1	0.93	0.12	50,50,50,50	0
57	MG	1R	204	1/1	0.93	0.20	38,38,38,38	0
57	MG	1A	3931	1/1	0.93	0.11	60,60,60,60	0
57	MG	1A	3220	1/1	0.93	0.14	39,39,39,39	0
57	MG	2B	209	1/1	0.93	0.16	57,57,57,57	0
57	MG	1S	202	1/1	0.93	0.12	53,53,53,53	0
57	MG	2A	3609	1/1	0.93	0.09	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	4045	1/1	0.93	0.10	35,35,35,35	0
57	MG	1A	3086	1/1	0.93	0.13	32,32,32,32	0
57	MG	2l	202	1/1	0.93	0.12	57,57,57,57	0
57	MG	2q	201	1/1	0.93	0.23	70,70,70,70	0
57	MG	1x	102	1/1	0.93	0.07	66,66,66,66	0
57	MG	1U	203	1/1	0.93	0.18	41,41,41,41	0
57	MG	1U	205	1/1	0.93	0.18	40,40,40,40	0
57	MG	1U	206	1/1	0.93	0.22	40,40,40,40	0
57	MG	1A	4049	1/1	0.93	0.11	66,66,66,66	0
57	MG	1A	3310	1/1	0.93	0.10	58,58,58,58	0
57	MG	1A	3710	1/1	0.93	0.14	57,57,57,57	0
57	MG	2A	3002	1/1	0.93	0.25	48,48,48,48	0
57	MG	2x	108	1/1	0.93	0.09	84,84,84,84	0
57	MG	2D	307	1/1	0.93	0.12	47,47,47,47	0
57	MG	1A	3528	1/1	0.93	0.34	63,63,63,63	0
57	MG	2D	306	1/1	0.94	0.28	41,41,41,41	0
57	MG	1A	3238	1/1	0.94	0.11	47,47,47,47	0
57	MG	1A	3088	1/1	0.94	0.15	37,37,37,37	0
57	MG	1a	1655	1/1	0.94	0.17	52,52,52,52	0
57	MG	2E	301	1/1	0.94	0.16	56,56,56,56	0
57	MG	2A	3184	1/1	0.94	0.27	61,61,61,61	0
57	MG	1A	3595	1/1	0.94	0.07	35,35,35,35	0
57	MG	1E	301	1/1	0.94	0.08	45,45,45,45	0
57	MG	2A	3187	1/1	0.94	0.09	60,60,60,60	0
57	MG	1A	3497	1/1	0.94	0.23	31,31,31,31	0
57	MG	1A	3057	1/1	0.94	0.17	43,43,43,43	0
57	MG	1A	3602	1/1	0.94	0.07	34,34,34,34	0
57	MG	1A	3416	1/1	0.94	0.09	45,45,45,45	0
57	MG	1A	3123	1/1	0.94	0.13	39,39,39,39	0
57	MG	1E	311	1/1	0.94	0.10	23,23,23,23	0
57	MG	1A	3852	1/1	0.94	0.08	39,39,39,39	0
57	MG	1A	3418	1/1	0.94	0.15	53,53,53,53	0
57	MG	2F	308	1/1	0.94	0.12	42,42,42,42	0
57	MG	1b	301	1/1	0.94	0.05	79,79,79,79	0
57	MG	2N	201	1/1	0.94	0.07	57,57,57,57	0
57	MG	2A	3198	1/1	0.94	0.18	62,62,62,62	0
57	MG	2P	201	1/1	0.94	0.24	48,48,48,48	0
57	MG	2Q	203	1/1	0.94	0.10	63,63,63,63	0
57	MG	1A	3506	1/1	0.94	0.10	51,51,51,51	0
57	MG	1F	303	1/1	0.94	0.21	35,35,35,35	0
57	MG	1a	1670	1/1	0.94	0.08	52,52,52,52	0
57	MG	1A	3855	1/1	0.94	0.20	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	4000	1/1	0.94	0.06	27,27,27,27	0
57	MG	1F	307	1/1	0.94	0.07	32,32,32,32	0
57	MG	1A	3060	1/1	0.94	0.55	64,64,64,64	0
57	MG	1A	3125	1/1	0.94	0.29	32,32,32,32	0
57	MG	1A	3357	1/1	0.94	0.07	57,57,57,57	0
57	MG	1A	4007	1/1	0.94	0.09	70,70,70,70	0
57	MG	1A	3863	1/1	0.94	0.08	43,43,43,43	0
57	MG	1x	101	1/1	0.94	0.20	57,57,57,57	0
57	MG	2A	3404	1/1	0.94	0.34	54,54,54,54	0
57	MG	2A	3655	1/1	0.94	0.16	67,67,67,67	0
57	MG	1A	3129	1/1	0.94	0.28	35,35,35,35	0
57	MG	23	102	1/1	0.94	0.09	55,55,55,55	0
57	MG	1x	103	1/1	0.94	0.35	56,56,56,56	0
57	MG	2A	3407	1/1	0.94	0.14	46,46,46,46	0
57	MG	1A	3061	1/1	0.94	0.09	36,36,36,36	0
57	MG	1A	3062	1/1	0.94	0.14	44,44,44,44	0
57	MG	1A	3363	1/1	0.94	0.14	40,40,40,40	0
57	MG	2A	3219	1/1	0.94	0.15	47,47,47,47	0
57	MG	2A	3220	1/1	0.94	0.11	59,59,59,59	0
57	MG	1x	107	1/1	0.94	0.10	52,52,52,52	0
57	MG	1A	3426	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	3016	1/1	0.94	0.33	51,51,51,51	0
57	MG	1N	204	1/1	0.94	0.50	48,48,48,48	0
57	MG	28	104	1/1	0.94	0.19	52,52,52,52	0
57	MG	2A	3228	1/1	0.94	0.14	48,48,48,48	0
57	MG	2A	3673	1/1	0.94	0.08	65,65,65,65	0
57	MG	2A	3229	1/1	0.94	0.16	45,45,45,45	0
57	MG	2A	3422	1/1	0.94	0.13	59,59,59,59	0
57	MG	1A	3312	1/1	0.94	0.20	53,53,53,53	0
57	MG	1A	3053	1/1	0.94	0.15	50,50,50,50	0
57	MG	2A	3679	1/1	0.94	0.13	35,35,35,35	0
57	MG	2a	1611	1/1	0.94	0.28	66,66,66,66	0
57	MG	1A	4021	1/1	0.94	0.08	43,43,43,43	0
57	MG	1A	3748	1/1	0.94	0.10	35,35,35,35	0
57	MG	2A	3234	1/1	0.94	0.20	47,47,47,47	0
57	MG	2A	3011	1/1	0.94	0.07	40,40,40,40	0
57	MG	1A	3200	1/1	0.94	0.09	33,33,33,33	0
57	MG	1A	3369	1/1	0.94	0.16	48,48,48,48	0
57	MG	1A	3257	1/1	0.94	0.09	64,64,64,64	0
57	MG	1Q	202	1/1	0.94	0.43	50,50,50,50	0
57	MG	2A	3240	1/1	0.94	0.28	57,57,57,57	0
57	MG	1A	3884	1/1	0.94	0.18	46,46,46,46	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	201	1/1	0.94	0.10	44,44,44,44	0
57	MG	2a	1628	1/1	0.94	0.28	63,63,63,63	0
57	MG	1A	4030	1/1	0.94	0.10	66,66,66,66	0
57	MG	2A	3031	1/1	0.94	0.08	47,47,47,47	0
57	MG	1A	4032	1/1	0.94	0.08	58,58,58,58	0
57	MG	2A	3034	1/1	0.94	0.15	52,52,52,52	0
57	MG	2A	3247	1/1	0.94	0.12	59,59,59,59	0
57	MG	2A	3036	1/1	0.94	0.09	55,55,55,55	0
57	MG	2A	3037	1/1	0.94	0.10	42,42,42,42	0
57	MG	2A	3702	1/1	0.94	0.12	53,53,53,53	0
57	MG	1A	3754	1/1	0.94	0.11	28,28,28,28	0
57	MG	1A	3887	1/1	0.94	0.24	26,26,26,26	0
57	MG	1A	3138	1/1	0.94	0.17	34,34,34,34	0
57	MG	1A	3634	1/1	0.94	0.11	40,40,40,40	0
57	MG	1A	3524	1/1	0.94	0.30	51,51,51,51	0
57	MG	2A	3046	1/1	0.94	0.09	55,55,55,55	0
57	MG	2A	3710	1/1	0.94	0.11	54,54,54,54	0
57	MG	1A	3638	1/1	0.94	0.10	65,65,65,65	0
57	MG	2A	3258	1/1	0.94	0.17	61,61,61,61	0
57	MG	1A	3639	1/1	0.94	0.10	30,30,30,30	0
57	MG	1A	3205	1/1	0.94	0.13	21,21,21,21	0
57	MG	1A	3261	1/1	0.94	0.10	51,51,51,51	0
57	MG	1A	3376	1/1	0.94	0.21	38,38,38,38	0
57	MG	2A	3055	1/1	0.94	0.08	48,48,48,48	0
57	MG	1A	4044	1/1	0.94	0.08	61,61,61,61	0
57	MG	1A	3772	1/1	0.94	0.07	42,42,42,42	0
57	MG	1A	3144	1/1	0.94	0.08	49,49,49,49	0
57	MG	1X	102	1/1	0.94	0.45	43,43,43,43	0
57	MG	2A	3475	1/1	0.94	0.10	45,45,45,45	0
57	MG	2A	3270	1/1	0.94	0.10	57,57,57,57	0
57	MG	2A	3062	1/1	0.94	0.09	67,67,67,67	0
57	MG	1Y	201	1/1	0.94	0.12	63,63,63,63	0
57	MG	1A	4047	1/1	0.94	0.09	48,48,48,48	0
57	MG	1A	3908	1/1	0.94	0.07	60,60,60,60	0
57	MG	2A	3731	1/1	0.94	0.11	40,40,40,40	0
57	MG	2A	3067	1/1	0.94	0.14	39,39,39,39	0
57	MG	1Z	302	1/1	0.94	0.20	54,54,54,54	0
57	MG	1A	3774	1/1	0.94	0.08	20,20,20,20	0
57	MG	10	104	1/1	0.94	0.35	43,43,43,43	0
57	MG	2A	3279	1/1	0.94	0.13	64,64,64,64	0
57	MG	2A	3072	1/1	0.94	0.09	53,53,53,53	0
57	MG	2A	3740	1/1	0.94	0.17	67,67,67,67	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	10	105	1/1	0.94	0.27	68,68,68,68	0
57	MG	2A	3743	1/1	0.94	0.12	51,51,51,51	0
57	MG	10	106	1/1	0.94	0.07	59,59,59,59	0
57	MG	1A	3646	1/1	0.94	0.07	20,20,20,20	0
57	MG	2a	1680	1/1	0.94	0.13	57,57,57,57	0
57	MG	1A	4052	1/1	0.94	0.10	49,49,49,49	0
57	MG	2A	3497	1/1	0.94	0.09	35,35,35,35	0
57	MG	2A	3499	1/1	0.94	0.09	33,33,33,33	0
57	MG	2A	3751	1/1	0.94	0.08	32,32,32,32	0
57	MG	1A	3531	1/1	0.94	0.21	54,54,54,54	0
57	MG	2A	3083	1/1	0.94	0.09	57,57,57,57	0
57	MG	1A	3100	1/1	0.94	0.09	43,43,43,43	0
57	MG	13	103	1/1	0.94	0.09	45,45,45,45	0
57	MG	1A	3379	1/1	0.94	0.18	52,52,52,52	0
57	MG	1A	3653	1/1	0.94	0.07	23,23,23,23	0
57	MG	2A	3291	1/1	0.94	0.11	71,71,71,71	0
57	MG	15	106	1/1	0.94	0.12	33,33,33,33	0
57	MG	2a	1696	1/1	0.94	0.09	50,50,50,50	0
57	MG	1A	3043	1/1	0.94	0.24	37,37,37,37	0
57	MG	2a	1699	1/1	0.94	0.18	61,61,61,61	0
57	MG	1a	1735	1/1	0.94	0.26	58,58,58,58	0
57	MG	2A	3765	1/1	0.94	0.14	79,79,79,79	0
57	MG	2A	3766	1/1	0.94	0.12	54,54,54,54	0
57	MG	17	101	1/1	0.94	0.12	39,39,39,39	0
57	MG	1A	3149	1/1	0.94	0.10	39,39,39,39	0
57	MG	1A	3539	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	3788	1/1	0.94	0.07	22,22,22,22	0
57	MG	2A	3521	1/1	0.94	0.09	35,35,35,35	0
57	MG	1A	3150	1/1	0.94	0.29	42,42,42,42	0
57	MG	2A	3775	1/1	0.94	0.11	64,64,64,64	0
57	MG	2A	3776	1/1	0.94	0.09	56,56,56,56	0
57	MG	1A	3663	1/1	0.94	0.05	24,24,24,24	0
57	MG	2a	1714	1/1	0.94	0.15	59,59,59,59	0
57	MG	1a	1744	1/1	0.94	0.15	59,59,59,59	0
57	MG	2A	3302	1/1	0.94	0.13	63,63,63,63	0
57	MG	2A	3781	1/1	0.94	0.13	45,45,45,45	0
57	MG	2A	3784	1/1	0.94	0.16	63,63,63,63	0
57	MG	2A	3528	1/1	0.94	0.14	36,36,36,36	0
57	MG	1A	3546	1/1	0.94	0.17	27,27,27,27	0
57	MG	2A	3103	1/1	0.94	0.12	58,58,58,58	0
57	MG	1a	1747	1/1	0.94	0.14	38,38,38,38	0
57	MG	2a	1726	1/1	0.94	0.20	68,68,68,68	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	3306	1/1	0.94	0.10	65,65,65,65	0
57	MG	1A	3455	1/1	0.94	0.15	43,43,43,43	0
57	MG	2A	3796	1/1	0.94	0.08	75,75,75,75	0
57	MG	1A	3939	1/1	0.94	0.08	50,50,50,50	0
57	MG	2A	3805	1/1	0.94	0.09	55,55,55,55	0
57	MG	1A	3666	1/1	0.94	0.09	32,32,32,32	0
57	MG	2a	1734	1/1	0.94	0.13	53,53,53,53	0
57	MG	1A	4075	1/1	0.94	0.15	55,55,55,55	0
57	MG	1A	3215	1/1	0.94	0.12	43,43,43,43	0
57	MG	1A	3216	1/1	0.94	0.10	47,47,47,47	0
57	MG	1A	3945	1/1	0.94	0.06	35,35,35,35	0
57	MG	1A	3458	1/1	0.94	0.13	59,59,59,59	0
57	MG	1A	3805	1/1	0.94	0.07	27,27,27,27	0
57	MG	2A	3548	1/1	0.94	0.06	27,27,27,27	0
57	MG	1A	3388	1/1	0.94	0.11	70,70,70,70	0
57	MG	1A	3676	1/1	0.94	0.10	24,24,24,24	0
57	MG	2A	3121	1/1	0.94	0.23	60,60,60,60	0
57	MG	1A	3461	1/1	0.94	0.24	73,73,73,73	0
57	MG	2A	3555	1/1	0.94	0.22	55,55,55,55	0
57	MG	1A	3151	1/1	0.94	0.19	32,32,32,32	0
57	MG	1A	3082	1/1	0.94	0.12	42,42,42,42	0
57	MG	1A	3275	1/1	0.94	0.07	41,41,41,41	0
57	MG	1a	1622	1/1	0.94	0.08	65,65,65,65	0
57	MG	2A	3130	1/1	0.94	0.08	44,44,44,44	0
57	MG	1a	1770	1/1	0.94	0.14	60,60,60,60	0
57	MG	1A	3958	1/1	0.94	0.13	46,46,46,46	0
57	MG	1A	3465	1/1	0.94	0.20	47,47,47,47	0
57	MG	2A	3571	1/1	0.94	0.16	55,55,55,55	0
57	MG	1A	3157	1/1	0.94	0.06	32,32,32,32	0
57	MG	1A	3334	1/1	0.94	0.20	49,49,49,49	0
57	MG	1a	1777	1/1	0.94	0.11	69,69,69,69	0
57	MG	1A	3473	1/1	0.94	0.26	64,64,64,64	0
57	MG	1A	3281	1/1	0.94	0.20	33,33,33,33	0
57	MG	1A	3475	1/1	0.94	0.11	45,45,45,45	0
57	MG	1A	3696	1/1	0.94	0.17	51,51,51,51	0
57	MG	1A	3477	1/1	0.94	0.13	47,47,47,47	0
57	MG	1B	217	1/1	0.94	0.09	49,49,49,49	0
57	MG	1a	1784	1/1	0.94	0.12	66,66,66,66	0
57	MG	2A	3152	1/1	0.94	0.12	56,56,56,56	0
57	MG	2A	3155	1/1	0.94	0.07	53,53,53,53	0
57	MG	2A	3345	1/1	0.94	0.13	58,58,58,58	0
57	MG	2A	3346	1/1	0.94	0.08	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	2A	3156	1/1	0.94	0.14	52,52,52,52	0
57	MG	2B	201	1/1	0.94	0.12	67,67,67,67	0
57	MG	1A	3478	1/1	0.94	0.20	59,59,59,59	0
57	MG	1A	3823	1/1	0.94	0.07	38,38,38,38	0
57	MG	1A	3825	1/1	0.94	0.09	45,45,45,45	0
57	MG	1A	3701	1/1	0.94	0.12	57,57,57,57	0
57	MG	1A	3083	1/1	0.94	0.17	36,36,36,36	0
57	MG	1A	3226	1/1	0.94	0.19	50,50,50,50	0
57	MG	1B	229	1/1	0.94	0.08	64,64,64,64	0
57	MG	1A	3584	1/1	0.94	0.09	37,37,37,37	0
57	MG	2A	3607	1/1	0.94	0.08	28,28,28,28	0
57	MG	1a	1645	1/1	0.94	0.39	64,64,64,64	0
57	MG	1A	3104	1/1	0.94	0.22	35,35,35,35	0
57	MG	1A	3084	1/1	0.94	0.15	40,40,40,40	0
57	MG	2A	3360	1/1	0.94	0.08	48,48,48,48	0
57	MG	2A	3170	1/1	0.94	0.09	60,60,60,60	0
57	MG	1A	3291	1/1	0.94	0.19	55,55,55,55	0
57	MG	2v	102	1/1	0.94	0.13	45,45,45,45	0
57	MG	1B	235	1/1	0.94	0.09	39,39,39,39	0
57	MG	1A	3055	1/1	0.94	0.07	44,44,44,44	0
57	MG	1A	3111	1/1	0.94	0.10	41,41,41,41	0
57	MG	2A	3176	1/1	0.94	0.14	57,57,57,57	0
57	MG	1A	3115	1/1	0.94	0.08	38,38,38,38	0
57	MG	2D	301	1/1	0.94	0.23	44,44,44,44	0
57	MG	2D	303	1/1	0.94	0.24	46,46,46,46	0
57	MG	2D	304	1/1	0.94	0.08	51,51,51,51	0
57	MG	1A	3338	1/1	0.95	0.07	52,52,52,52	0
57	MG	1A	3384	1/1	0.95	0.25	30,30,30,30	0
57	MG	2T	3501	1/1	0.95	0.07	51,51,51,51	0
57	MG	1A	3567	1/1	0.95	0.07	45,45,45,45	0
57	MG	1A	3222	1/1	0.95	0.07	37,37,37,37	0
57	MG	1A	3569	1/1	0.95	0.21	52,52,52,52	0
57	MG	2A	3455	1/1	0.95	0.14	40,40,40,40	0
57	MG	1A	3979	1/1	0.95	0.06	49,49,49,49	0
57	MG	1A	3493	1/1	0.95	0.07	46,46,46,46	0
57	MG	1a	1631	1/1	0.95	0.23	64,64,64,64	0
57	MG	1a	1772	1/1	0.95	0.12	62,62,62,62	0
57	MG	1B	233	1/1	0.95	0.08	46,46,46,46	0
57	MG	2X	102	1/1	0.95	0.11	49,49,49,49	0
57	MG	1A	3749	1/1	0.95	0.06	25,25,25,25	0
57	MG	1A	3651	1/1	0.95	0.07	27,27,27,27	0
57	MG	2A	3688	1/1	0.95	0.08	38,38,38,38	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	2A	3466	1/1	0.95	0.13	40,40,40,40	0
57	MG	1D	301	1/1	0.95	0.07	30,30,30,30	0
57	MG	1A	3433	1/1	0.95	0.20	54,54,54,54	0
57	MG	1A	3574	1/1	0.95	0.15	53,53,53,53	0
57	MG	1A	3857	1/1	0.95	0.29	36,36,36,36	0
57	MG	1A	3304	1/1	0.95	0.10	32,32,32,32	0
57	MG	1A	3342	1/1	0.95	0.28	51,51,51,51	0
57	MG	1A	3860	1/1	0.95	0.11	28,28,28,28	0
57	MG	1A	3438	1/1	0.95	0.08	49,49,49,49	0
57	MG	1A	3498	1/1	0.95	0.29	29,29,29,29	0
57	MG	2A	3478	1/1	0.95	0.14	55,55,55,55	0
57	MG	1a	1785	1/1	0.95	0.06	66,66,66,66	0
57	MG	1A	3181	1/1	0.95	0.08	32,32,32,32	0
57	MG	1A	3307	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3868	1/1	0.95	0.12	24,24,24,24	0
57	MG	2a	1601	1/1	0.95	0.07	54,54,54,54	0
57	MG	2a	1602	1/1	0.95	0.18	53,53,53,53	0
57	MG	1A	3073	1/1	0.95	0.11	13,13,13,13	0
57	MG	2a	1604	1/1	0.95	0.13	57,57,57,57	0
57	MG	1A	3766	1/1	0.95	0.15	56,56,56,56	0
57	MG	2a	1606	1/1	0.95	0.18	60,60,60,60	0
57	MG	1A	3767	1/1	0.95	0.11	54,54,54,54	0
57	MG	1E	313	1/1	0.95	0.25	43,43,43,43	0
57	MG	2A	3487	1/1	0.95	0.14	39,39,39,39	0
57	MG	1A	3034	1/1	0.95	0.24	33,33,33,33	0
57	MG	2A	3489	1/1	0.95	0.15	59,59,59,59	0
57	MG	1A	3769	1/1	0.95	0.08	64,64,64,64	0
57	MG	2A	3716	1/1	0.95	0.11	62,62,62,62	0
57	MG	2a	1614	1/1	0.95	0.15	55,55,55,55	0
57	MG	2A	3135	1/1	0.95	0.10	43,43,43,43	0
57	MG	2A	3493	1/1	0.95	0.07	39,39,39,39	0
57	MG	1A	3153	1/1	0.95	0.11	36,36,36,36	0
57	MG	2a	1618	1/1	0.95	0.19	59,59,59,59	0
57	MG	2A	3720	1/1	0.95	0.10	50,50,50,50	0
57	MG	1A	3446	1/1	0.95	0.14	51,51,51,51	0
57	MG	2A	3496	1/1	0.95	0.07	52,52,52,52	0
57	MG	1A	3674	1/1	0.95	0.09	37,37,37,37	0
57	MG	1A	3880	1/1	0.95	0.10	51,51,51,51	0
57	MG	1a	1659	1/1	0.95	0.11	46,46,46,46	0
57	MG	1A	4011	1/1	0.95	0.09	67,67,67,67	0
57	MG	1F	312	1/1	0.95	0.09	41,41,41,41	0
57	MG	1A	3127	1/1	0.95	0.31	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	1806	1/1	0.95	0.07	60,60,60,60	0
57	MG	1A	3231	1/1	0.95	0.12	57,57,57,57	0
57	MG	2a	1634	1/1	0.95	0.15	63,63,63,63	0
57	MG	1a	1809	1/1	0.95	0.07	69,69,69,69	0
57	MG	2A	3732	1/1	0.95	0.11	34,34,34,34	0
57	MG	2A	3509	1/1	0.95	0.15	52,52,52,52	0
57	MG	1A	3883	1/1	0.95	0.07	47,47,47,47	0
57	MG	1A	3677	1/1	0.95	0.09	24,24,24,24	0
57	MG	2A	3513	1/1	0.95	0.15	56,56,56,56	0
57	MG	2A	3318	1/1	0.95	0.20	52,52,52,52	0
57	MG	2A	3515	1/1	0.95	0.10	55,55,55,55	0
57	MG	2A	3153	1/1	0.95	0.12	38,38,38,38	0
57	MG	1A	3313	1/1	0.95	0.15	42,42,42,42	0
57	MG	1A	3590	1/1	0.95	0.09	39,39,39,39	0
57	MG	1A	3156	1/1	0.95	0.20	37,37,37,37	0
57	MG	2A	3746	1/1	0.95	0.09	62,62,62,62	0
57	MG	1A	3190	1/1	0.95	0.20	35,35,35,35	0
57	MG	1A	3108	1/1	0.95	0.24	39,39,39,39	0
57	MG	1A	3892	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	3786	1/1	0.95	0.06	41,41,41,41	0
57	MG	1a	1821	1/1	0.95	0.14	60,60,60,60	0
57	MG	1A	3686	1/1	0.95	0.10	29,29,29,29	0
57	MG	1A	3895	1/1	0.95	0.25	36,36,36,36	0
57	MG	1A	3897	1/1	0.95	0.05	29,29,29,29	0
57	MG	2A	3531	1/1	0.95	0.09	33,33,33,33	0
57	MG	1A	3689	1/1	0.95	0.09	53,53,53,53	0
57	MG	1A	3199	1/1	0.95	0.20	42,42,42,42	0
57	MG	1A	3097	1/1	0.95	0.15	34,34,34,34	0
57	MG	2A	3171	1/1	0.95	0.16	39,39,39,39	0
57	MG	1A	3407	1/1	0.95	0.37	49,49,49,49	0
57	MG	1A	3459	1/1	0.95	0.08	71,71,71,71	0
57	MG	1A	3904	1/1	0.95	0.05	77,77,77,77	0
57	MG	1a	1683	1/1	0.95	0.19	60,60,60,60	0
57	MG	1A	3905	1/1	0.95	0.10	67,67,67,67	0
57	MG	1A	3276	1/1	0.95	0.11	45,45,45,45	0
57	MG	2A	3343	1/1	0.95	0.15	69,69,69,69	0
57	MG	2A	3344	1/1	0.95	0.09	58,58,58,58	0
57	MG	1A	3799	1/1	0.95	0.18	65,65,65,65	0
57	MG	1A	3910	1/1	0.95	0.09	63,63,63,63	0
57	MG	1A	3098	1/1	0.95	0.07	37,37,37,37	0
57	MG	1A	3697	1/1	0.95	0.15	55,55,55,55	0
57	MG	2A	3554	1/1	0.95	0.06	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	1A	3802	1/1	0.95	0.40	30,30,30,30	0
57	MG	1A	3606	1/1	0.95	0.11	26,26,26,26	0
57	MG	1U	204	1/1	0.95	0.11	34,34,34,34	0
57	MG	2A	3782	1/1	0.95	0.11	75,75,75,75	0
57	MG	2a	1683	1/1	0.95	0.13	59,59,59,59	0
57	MG	1A	3916	1/1	0.95	0.10	52,52,52,52	0
57	MG	1A	3607	1/1	0.95	0.08	36,36,36,36	0
57	MG	1A	3919	1/1	0.95	0.12	54,54,54,54	0
57	MG	1A	3806	1/1	0.95	0.08	32,32,32,32	0
57	MG	2A	3791	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3926	1/1	0.95	0.07	51,51,51,51	0
57	MG	2A	3568	1/1	0.95	0.10	54,54,54,54	0
57	MG	2A	3569	1/1	0.95	0.12	60,60,60,60	0
57	MG	1a	1698	1/1	0.95	0.28	52,52,52,52	0
57	MG	2A	3797	1/1	0.95	0.17	30,30,30,30	0
57	MG	1A	3927	1/1	0.95	0.07	55,55,55,55	0
57	MG	2a	1697	1/1	0.95	0.17	63,63,63,63	0
57	MG	2A	3803	1/1	0.95	0.08	69,69,69,69	0
57	MG	2A	3195	1/1	0.95	0.12	65,65,65,65	0
57	MG	1A	3077	1/1	0.95	0.20	45,45,45,45	0
57	MG	1A	3065	1/1	0.95	0.10	36,36,36,36	0
57	MG	2A	3009	1/1	0.95	0.13	63,63,63,63	0
57	MG	2A	3811	1/1	0.95	0.09	33,33,33,33	0
57	MG	2A	3010	1/1	0.95	0.20	39,39,39,39	0
57	MG	1A	3117	1/1	0.95	0.24	42,42,42,42	0
57	MG	2A	3014	1/1	0.95	0.19	39,39,39,39	0
57	MG	2A	3015	1/1	0.95	0.17	64,64,64,64	0
57	MG	2A	3016	1/1	0.95	0.16	50,50,50,50	0
57	MG	1X	104	1/1	0.95	0.08	42,42,42,42	0
57	MG	1A	3367	1/1	0.95	0.26	57,57,57,57	0
57	MG	2a	1712	1/1	0.95	0.08	51,51,51,51	0
57	MG	2A	3021	1/1	0.95	0.31	42,42,42,42	0
57	MG	2A	3823	1/1	0.95	0.10	21,21,21,21	0
57	MG	1A	3140	1/1	0.95	0.10	37,37,37,37	0
57	MG	2a	1717	1/1	0.95	0.12	54,54,54,54	0
57	MG	2A	3374	1/1	0.95	0.11	67,67,67,67	0
57	MG	1A	3935	1/1	0.95	0.07	66,66,66,66	0
57	MG	1Z	301	1/1	0.95	0.07	60,60,60,60	0
57	MG	2A	3593	1/1	0.95	0.11	29,29,29,29	0
57	MG	2A	3378	1/1	0.95	0.07	50,50,50,50	0
57	MG	2A	3025	1/1	0.95	0.19	45,45,45,45	0
57	MG	2A	3597	1/1	0.95	0.08	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	3027	1/1	0.95	0.17	45,45,45,45	0
57	MG	1A	3066	1/1	0.95	0.08	50,50,50,50	0
57	MG	2A	3029	1/1	0.95	0.07	37,37,37,37	0
57	MG	1A	3813	1/1	0.95	0.14	48,48,48,48	0
57	MG	2A	3603	1/1	0.95	0.21	58,58,58,58	0
57	MG	1A	4066	1/1	0.95	0.17	15,15,15,15	0
57	MG	1A	3938	1/1	0.95	0.05	58,58,58,58	0
57	MG	1A	3471	1/1	0.95	0.24	37,37,37,37	0
57	MG	2a	1735	1/1	0.95	0.15	52,52,52,52	0
57	MG	2A	3221	1/1	0.95	0.08	39,39,39,39	0
57	MG	2A	3035	1/1	0.95	0.13	37,37,37,37	0
57	MG	2A	3224	1/1	0.95	0.26	42,42,42,42	0
57	MG	1A	3472	1/1	0.95	0.08	48,48,48,48	0
57	MG	1A	3711	1/1	0.95	0.20	61,61,61,61	0
57	MG	11	103	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3120	1/1	0.95	0.13	47,47,47,47	0
57	MG	2A	3042	1/1	0.95	0.29	59,59,59,59	0
57	MG	1A	3944	1/1	0.95	0.06	45,45,45,45	0
57	MG	1A	3293	1/1	0.95	0.06	44,44,44,44	0
57	MG	1A	3121	1/1	0.95	0.13	38,38,38,38	0
57	MG	2A	3621	1/1	0.95	0.08	65,65,65,65	0
57	MG	2A	3400	1/1	0.95	0.23	52,52,52,52	0
57	MG	1A	3535	1/1	0.95	0.10	63,63,63,63	0
57	MG	1A	3009	1/1	0.95	0.06	22,22,22,22	0
57	MG	1A	4082	1/1	0.95	0.06	51,51,51,51	0
57	MG	2A	3049	1/1	0.95	0.10	33,33,33,33	0
57	MG	1A	3537	1/1	0.95	0.28	32,32,32,32	0
57	MG	2a	1756	1/1	0.95	0.24	62,62,62,62	0
57	MG	2A	3051	1/1	0.95	0.11	43,43,43,43	0
57	MG	2B	210	1/1	0.95	0.10	70,70,70,70	0
57	MG	17	103	1/1	0.95	0.14	55,55,55,55	0
57	MG	1A	3255	1/1	0.95	0.23	47,47,47,47	0
57	MG	2a	1761	1/1	0.95	0.07	53,53,53,53	0
57	MG	1A	3951	1/1	0.95	0.10	24,24,24,24	0
57	MG	2a	1763	1/1	0.95	0.16	52,52,52,52	0
57	MG	18	101	1/1	0.95	0.18	42,42,42,42	0
57	MG	1A	3824	1/1	0.95	0.14	52,52,52,52	0
57	MG	1A	3175	1/1	0.95	0.24	31,31,31,31	0
57	MG	2A	3059	1/1	0.95	0.09	49,49,49,49	0
57	MG	1A	4088	1/1	0.95	0.05	40,40,40,40	0
57	MG	1A	3954	1/1	0.95	0.14	51,51,51,51	0
57	MG	1A	3177	1/1	0.95	0.09	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	3417	1/1	0.95	0.19	56,56,56,56	0
57	MG	2A	3418	1/1	0.95	0.40	56,56,56,56	0
57	MG	1A	3632	1/1	0.95	0.04	24,24,24,24	0
57	MG	1B	203	1/1	0.95	0.24	68,68,68,68	0
57	MG	2A	3251	1/1	0.95	0.07	52,52,52,52	0
57	MG	2A	3066	1/1	0.95	0.20	55,55,55,55	0
57	MG	1B	204	1/1	0.95	0.07	41,41,41,41	0
57	MG	1A	3484	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	3730	1/1	0.95	0.06	30,30,30,30	0
57	MG	1A	3485	1/1	0.95	0.23	32,32,32,32	0
57	MG	2A	3071	1/1	0.95	0.05	51,51,51,51	0
57	MG	1A	3733	1/1	0.95	0.07	45,45,45,45	0
57	MG	1A	3636	1/1	0.95	0.07	39,39,39,39	0
57	MG	2A	3077	1/1	0.95	0.11	42,42,42,42	0
57	MG	1A	3834	1/1	0.95	0.08	19,19,19,19	0
57	MG	1A	3486	1/1	0.95	0.06	41,41,41,41	0
57	MG	1A	3258	1/1	0.95	0.13	27,27,27,27	0
57	MG	2A	3439	1/1	0.95	0.10	62,62,62,62	0
57	MG	1a	1616	1/1	0.95	0.08	73,73,73,73	0
57	MG	2q	202	1/1	0.95	0.06	72,72,72,72	0
57	MG	2F	304	1/1	0.95	0.07	53,53,53,53	0
57	MG	1A	3488	1/1	0.95	0.09	60,60,60,60	0
57	MG	1A	3838	1/1	0.95	0.09	20,20,20,20	0
57	MG	1a	1619	1/1	0.95	0.21	52,52,52,52	0
57	MG	1A	3221	1/1	0.95	0.17	42,42,42,42	0
57	MG	2A	3668	1/1	0.95	0.10	65,65,65,65	0
57	MG	1a	1760	1/1	0.95	0.06	46,46,46,46	0
57	MG	2A	3670	1/1	0.95	0.05	43,43,43,43	0
57	MG	1A	3560	1/1	0.95	0.12	52,52,52,52	0
57	MG	2Q	201	1/1	0.95	0.15	57,57,57,57	0
57	MG	2A	3448	1/1	0.95	0.11	55,55,55,55	0
57	MG	2Q	204	1/1	0.95	0.07	45,45,45,45	0
58	K	1A	3549	1/1	0.95	0.11	73,73,73,73	0
59	ZN	14	501	1/1	0.95	0.11	117,117,117,117	0
59	ZN	24	501	1/1	0.95	0.11	127,127,127,127	0
57	MG	15	102	1/1	0.96	0.24	33,33,33,33	0
57	MG	2A	3664	1/1	0.96	0.08	58,58,58,58	0
57	MG	15	103	1/1	0.96	0.23	35,35,35,35	0
57	MG	2A	3666	1/1	0.96	0.09	54,54,54,54	0
57	MG	1A	3763	1/1	0.96	0.10	31,31,31,31	0
57	MG	1A	3499	1/1	0.96	0.22	41,41,41,41	0
57	MG	2A	3054	1/1	0.96	0.07	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	1A	3862	1/1	0.96	0.06	31,31,31,31	0
57	MG	16	101	1/1	0.96	0.08	57,57,57,57	0
57	MG	1A	3243	1/1	0.96	0.18	35,35,35,35	0
57	MG	1A	3502	1/1	0.96	0.18	38,38,38,38	0
57	MG	17	104	1/1	0.96	0.11	34,34,34,34	0
57	MG	1A	3381	1/1	0.96	0.14	43,43,43,43	0
57	MG	1a	1738	1/1	0.96	0.06	50,50,50,50	0
57	MG	1A	3866	1/1	0.96	0.06	27,27,27,27	0
57	MG	1A	3440	1/1	0.96	0.25	41,41,41,41	0
57	MG	1a	1741	1/1	0.96	0.15	58,58,58,58	0
57	MG	1A	3197	1/1	0.96	0.09	48,48,48,48	0
57	MG	2A	3452	1/1	0.96	0.23	42,42,42,42	0
57	MG	1A	3871	1/1	0.96	0.08	44,44,44,44	0
57	MG	1A	3112	1/1	0.96	0.20	34,34,34,34	0
57	MG	1A	3443	1/1	0.96	0.13	56,56,56,56	0
57	MG	2A	3260	1/1	0.96	0.17	50,50,50,50	0
57	MG	1a	1746	1/1	0.96	0.06	36,36,36,36	0
57	MG	25	105	1/1	0.96	0.13	51,51,51,51	0
57	MG	1A	3114	1/1	0.96	0.08	34,34,34,34	0
57	MG	1A	3203	1/1	0.96	0.08	29,29,29,29	0
57	MG	2A	3074	1/1	0.96	0.06	43,43,43,43	0
57	MG	2A	3075	1/1	0.96	0.07	24,24,24,24	0
57	MG	2A	3694	1/1	0.96	0.05	38,38,38,38	0
57	MG	2A	3266	1/1	0.96	0.15	68,68,68,68	0
57	MG	1A	3776	1/1	0.96	0.14	59,59,59,59	0
57	MG	1A	3002	1/1	0.96	0.08	40,40,40,40	0
57	MG	1A	3680	1/1	0.96	0.08	43,43,43,43	0
57	MG	2A	3469	1/1	0.96	0.16	50,50,50,50	0
57	MG	1B	226	1/1	0.96	0.08	56,56,56,56	0
57	MG	2A	3080	1/1	0.96	0.12	51,51,51,51	0
57	MG	1a	1755	1/1	0.96	0.09	44,44,44,44	0
57	MG	1B	228	1/1	0.96	0.06	38,38,38,38	0
57	MG	1A	3779	1/1	0.96	0.05	24,24,24,24	0
57	MG	1A	3249	1/1	0.96	0.17	44,44,44,44	0
57	MG	1A	3994	1/1	0.96	0.06	67,67,67,67	0
57	MG	1A	3162	1/1	0.96	0.23	28,28,28,28	0
57	MG	1a	1614	1/1	0.96	0.11	30,30,30,30	0
57	MG	1A	3391	1/1	0.96	0.17	34,34,34,34	0
57	MG	2A	3089	1/1	0.96	0.15	38,38,38,38	0
57	MG	1A	3025	1/1	0.96	0.14	36,36,36,36	0
57	MG	1A	3685	1/1	0.96	0.06	56,56,56,56	0
57	MG	2A	3092	1/1	0.96	0.11	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	1B	236	1/1	0.96	0.08	37,37,37,37	0
57	MG	1A	3208	1/1	0.96	0.19	36,36,36,36	0
57	MG	2A	3095	1/1	0.96	0.11	43,43,43,43	0
57	MG	1A	3688	1/1	0.96	0.06	13,13,13,13	0
57	MG	1D	304	1/1	0.96	0.12	40,40,40,40	0
57	MG	2A	3490	1/1	0.96	0.08	51,51,51,51	0
57	MG	1a	1771	1/1	0.96	0.06	60,60,60,60	0
57	MG	1D	306	1/1	0.96	0.06	35,35,35,35	0
57	MG	1a	1624	1/1	0.96	0.10	57,57,57,57	0
57	MG	2a	1627	1/1	0.96	0.23	53,53,53,53	0
57	MG	1A	3517	1/1	0.96	0.26	48,48,48,48	0
57	MG	1A	3135	1/1	0.96	0.05	38,38,38,38	0
57	MG	1A	3344	1/1	0.96	0.26	56,56,56,56	0
57	MG	1A	3600	1/1	0.96	0.11	15,15,15,15	0
57	MG	1A	3796	1/1	0.96	0.16	43,43,43,43	0
57	MG	1A	3797	1/1	0.96	0.08	58,58,58,58	0
57	MG	2A	3501	1/1	0.96	0.08	27,27,27,27	0
57	MG	1E	302	1/1	0.96	0.09	39,39,39,39	0
57	MG	1A	3347	1/1	0.96	0.14	41,41,41,41	0
57	MG	2a	1638	1/1	0.96	0.17	53,53,53,53	0
57	MG	1A	3136	1/1	0.96	0.07	32,32,32,32	0
57	MG	2A	3113	1/1	0.96	0.19	51,51,51,51	0
57	MG	2A	3114	1/1	0.96	0.07	49,49,49,49	0
57	MG	1A	3604	1/1	0.96	0.08	36,36,36,36	0
57	MG	1A	3067	1/1	0.96	0.07	35,35,35,35	0
57	MG	2A	3739	1/1	0.96	0.13	57,57,57,57	0
57	MG	1A	3302	1/1	0.96	0.33	48,48,48,48	0
57	MG	1a	1637	1/1	0.96	0.15	28,28,28,28	0
57	MG	2A	3742	1/1	0.96	0.06	49,49,49,49	0
57	MG	2A	3512	1/1	0.96	0.07	49,49,49,49	0
57	MG	1A	3902	1/1	0.96	0.13	55,55,55,55	0
57	MG	1A	3303	1/1	0.96	0.18	50,50,50,50	0
57	MG	1A	4020	1/1	0.96	0.05	71,71,71,71	0
57	MG	2a	1653	1/1	0.96	0.11	48,48,48,48	0
57	MG	1A	3804	1/1	0.96	0.07	40,40,40,40	0
57	MG	1A	3525	1/1	0.96	0.13	26,26,26,26	0
57	MG	1F	302	1/1	0.96	0.13	36,36,36,36	0
57	MG	1a	1644	1/1	0.96	0.19	58,58,58,58	0
57	MG	2A	3520	1/1	0.96	0.10	36,36,36,36	0
57	MG	2A	3127	1/1	0.96	0.05	46,46,46,46	0
57	MG	2A	3754	1/1	0.96	0.06	60,60,60,60	0
57	MG	2A	3129	1/1	0.96	0.07	61,61,61,61	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	3402	1/1	0.96	0.10	53,53,53,53	0
57	MG	2A	3131	1/1	0.96	0.15	41,41,41,41	0
57	MG	2A	3132	1/1	0.96	0.08	41,41,41,41	0
57	MG	1A	4024	1/1	0.96	0.05	48,48,48,48	0
57	MG	2A	3134	1/1	0.96	0.14	34,34,34,34	0
57	MG	1A	3139	1/1	0.96	0.29	33,33,33,33	0
57	MG	1A	3059	1/1	0.96	0.07	44,44,44,44	0
57	MG	1F	308	1/1	0.96	0.07	36,36,36,36	0
57	MG	2A	3138	1/1	0.96	0.21	49,49,49,49	0
57	MG	2A	3767	1/1	0.96	0.06	52,52,52,52	0
57	MG	2a	1673	1/1	0.96	0.14	47,47,47,47	0
57	MG	1F	309	1/1	0.96	0.16	22,22,22,22	0
57	MG	1F	310	1/1	0.96	0.12	27,27,27,27	0
57	MG	1a	1802	1/1	0.96	0.14	58,58,58,58	0
57	MG	2A	3537	1/1	0.96	0.07	33,33,33,33	0
57	MG	2A	3142	1/1	0.96	0.20	56,56,56,56	0
57	MG	1a	1803	1/1	0.96	0.07	50,50,50,50	0
57	MG	1A	3141	1/1	0.96	0.16	37,37,37,37	0
57	MG	1A	3530	1/1	0.96	0.12	55,55,55,55	0
57	MG	1A	4031	1/1	0.96	0.09	51,51,51,51	0
57	MG	1A	3466	1/1	0.96	0.08	42,42,42,42	0
57	MG	2A	3546	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	3620	1/1	0.96	0.06	46,46,46,46	0
57	MG	2A	3150	1/1	0.96	0.08	55,55,55,55	0
57	MG	2a	1687	1/1	0.96	0.08	53,53,53,53	0
57	MG	1A	3218	1/1	0.96	0.21	38,38,38,38	0
57	MG	2A	3785	1/1	0.96	0.06	48,48,48,48	0
57	MG	2a	1690	1/1	0.96	0.17	58,58,58,58	0
57	MG	1A	3410	1/1	0.96	0.10	53,53,53,53	0
57	MG	1A	3143	1/1	0.96	0.06	16,16,16,16	0
57	MG	1A	3715	1/1	0.96	0.08	38,38,38,38	0
57	MG	1A	3019	1/1	0.96	0.16	52,52,52,52	0
57	MG	2A	3342	1/1	0.96	0.08	66,66,66,66	0
57	MG	2A	3793	1/1	0.96	0.11	48,48,48,48	0
57	MG	1A	3041	1/1	0.96	0.07	28,28,28,28	0
57	MG	1A	3122	1/1	0.96	0.14	42,42,42,42	0
57	MG	2A	3159	1/1	0.96	0.16	54,54,54,54	0
57	MG	1a	1664	1/1	0.96	0.08	57,57,57,57	0
57	MG	2A	3798	1/1	0.96	0.11	29,29,29,29	0
57	MG	2A	3799	1/1	0.96	0.06	48,48,48,48	0
57	MG	1A	3538	1/1	0.96	0.21	34,34,34,34	0
57	MG	2A	3801	1/1	0.96	0.10	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	2a	1705	1/1	0.96	0.08	52,52,52,52	0
57	MG	1A	3105	1/1	0.96	0.08	49,49,49,49	0
57	MG	1A	3362	1/1	0.96	0.24	41,41,41,41	0
57	MG	1A	3007	1/1	0.96	0.12	36,36,36,36	0
57	MG	2A	3808	1/1	0.96	0.08	54,54,54,54	0
57	MG	2A	3351	1/1	0.96	0.16	54,54,54,54	0
57	MG	1A	3080	1/1	0.96	0.07	62,62,62,62	0
57	MG	2A	3166	1/1	0.96	0.19	66,66,66,66	0
57	MG	2A	3574	1/1	0.96	0.09	47,47,47,47	0
57	MG	1A	3152	1/1	0.96	0.17	36,36,36,36	0
57	MG	2a	1715	1/1	0.96	0.15	49,49,49,49	0
57	MG	1A	4048	1/1	0.96	0.08	21,21,21,21	0
57	MG	2A	3816	1/1	0.96	0.10	69,69,69,69	0
57	MG	1P	203	1/1	0.96	0.28	31,31,31,31	0
57	MG	1A	3635	1/1	0.96	0.09	37,37,37,37	0
57	MG	2A	3579	1/1	0.96	0.06	57,57,57,57	0
57	MG	1A	3186	1/1	0.96	0.08	36,36,36,36	0
57	MG	1Q	203	1/1	0.96	0.08	31,31,31,31	0
57	MG	1A	3022	1/1	0.96	0.07	44,44,44,44	0
57	MG	1Q	206	1/1	0.96	0.10	47,47,47,47	0
57	MG	1Q	207	1/1	0.96	0.08	47,47,47,47	0
57	MG	1Q	208	1/1	0.96	0.13	35,35,35,35	0
57	MG	2a	1728	1/1	0.96	0.12	60,60,60,60	0
57	MG	1t	201	1/1	0.96	0.11	58,58,58,58	0
57	MG	2A	3588	1/1	0.96	0.12	38,38,38,38	0
57	MG	1A	3271	1/1	0.96	0.08	32,32,32,32	0
57	MG	1w	402	1/1	0.96	0.07	49,49,49,49	0
57	MG	2A	3181	1/1	0.96	0.12	57,57,57,57	0
57	MG	2A	3182	1/1	0.96	0.08	56,56,56,56	0
57	MG	1A	4053	1/1	0.96	0.06	40,40,40,40	0
57	MG	2a	1736	1/1	0.96	0.15	56,56,56,56	0
57	MG	2A	3594	1/1	0.96	0.05	32,32,32,32	0
57	MG	1A	3941	1/1	0.96	0.09	56,56,56,56	0
57	MG	1A	3128	1/1	0.96	0.17	28,28,28,28	0
57	MG	1A	3556	1/1	0.96	0.07	41,41,41,41	0
57	MG	1A	3558	1/1	0.96	0.21	37,37,37,37	0
57	MG	1A	3274	1/1	0.96	0.20	33,33,33,33	0
57	MG	2A	3600	1/1	0.96	0.15	57,57,57,57	0
57	MG	1A	3739	1/1	0.96	0.11	46,46,46,46	0
57	MG	1x	108	1/1	0.96	0.12	55,55,55,55	0
57	MG	1A	4061	1/1	0.96	0.07	52,52,52,52	0
57	MG	1A	3644	1/1	0.96	0.07	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	113	1/1	0.96	0.12	50,50,50,50	0
57	MG	1A	3371	1/1	0.96	0.20	47,47,47,47	0
57	MG	1U	207	1/1	0.96	0.25	33,33,33,33	0
57	MG	1A	4064	1/1	0.96	0.08	50,50,50,50	0
57	MG	1A	3194	1/1	0.96	0.39	34,34,34,34	0
57	MG	2A	3006	1/1	0.96	0.15	43,43,43,43	0
57	MG	1A	3839	1/1	0.96	0.10	26,26,26,26	0
57	MG	1V	204	1/1	0.96	0.18	54,54,54,54	0
57	MG	2A	3201	1/1	0.96	0.12	53,53,53,53	0
57	MG	2A	3616	1/1	0.96	0.07	35,35,35,35	0
57	MG	1A	3840	1/1	0.96	0.14	33,33,33,33	0
57	MG	1A	3429	1/1	0.96	0.24	40,40,40,40	0
57	MG	2A	3013	1/1	0.96	0.07	40,40,40,40	0
57	MG	1W	205	1/1	0.96	0.13	35,35,35,35	0
57	MG	1A	3842	1/1	0.96	0.26	37,37,37,37	0
57	MG	1X	101	1/1	0.96	0.04	29,29,29,29	0
57	MG	2A	3208	1/1	0.96	0.13	51,51,51,51	0
57	MG	1A	3064	1/1	0.96	0.15	38,38,38,38	0
57	MG	2A	3398	1/1	0.96	0.19	42,42,42,42	0
57	MG	2A	3399	1/1	0.96	0.22	45,45,45,45	0
57	MG	1A	3955	1/1	0.96	0.13	47,47,47,47	0
57	MG	1X	105	1/1	0.96	0.18	37,37,37,37	0
57	MG	1A	3236	1/1	0.96	0.22	30,30,30,30	0
57	MG	1A	3570	1/1	0.96	0.09	41,41,41,41	0
57	MG	1A	3652	1/1	0.96	0.07	28,28,28,28	0
57	MG	1Y	204	1/1	0.96	0.23	43,43,43,43	0
57	MG	1A	3960	1/1	0.96	0.11	49,49,49,49	0
57	MG	1A	3279	1/1	0.96	0.18	35,35,35,35	0
57	MG	1A	4081	1/1	0.96	0.17	46,46,46,46	0
57	MG	1a	1711	1/1	0.96	0.06	51,51,51,51	0
57	MG	2D	305	1/1	0.96	0.09	29,29,29,29	0
57	MG	1a	1712	1/1	0.96	0.09	52,52,52,52	0
57	MG	2A	3222	1/1	0.96	0.14	46,46,46,46	0
57	MG	2A	3640	1/1	0.96	0.06	35,35,35,35	0
57	MG	2A	3032	1/1	0.96	0.08	37,37,37,37	0
57	MG	1A	3196	1/1	0.96	0.23	29,29,29,29	0
57	MG	1A	3656	1/1	0.96	0.12	42,42,42,42	0
57	MG	1A	3435	1/1	0.96	0.16	33,33,33,33	0
57	MG	1A	3659	1/1	0.96	0.05	20,20,20,20	0
57	MG	10	108	1/1	0.96	0.10	45,45,45,45	0
57	MG	2A	3647	1/1	0.96	0.07	51,51,51,51	0
57	MG	2A	3038	1/1	0.96	0.11	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	1A	3242	1/1	0.96	0.36	35,35,35,35	0
57	MG	2F	301	1/1	0.96	0.13	48,48,48,48	0
57	MG	2A	3040	1/1	0.96	0.10	52,52,52,52	0
57	MG	1a	1719	1/1	0.96	0.12	60,60,60,60	0
57	MG	2w	401	1/1	0.96	0.06	44,44,44,44	0
57	MG	1l	102	1/1	0.96	0.07	60,60,60,60	0
57	MG	2x	102	1/1	0.96	0.17	65,65,65,65	0
57	MG	1A	3661	1/1	0.96	0.06	22,22,22,22	0
57	MG	1A	3759	1/1	0.96	0.08	22,22,22,22	0
57	MG	1A	3969	1/1	0.96	0.16	57,57,57,57	0
57	MG	2x	106	1/1	0.96	0.12	57,57,57,57	0
57	MG	13	102	1/1	0.96	0.06	41,41,41,41	0
57	MG	2F	309	1/1	0.96	0.18	38,38,38,38	0
57	MG	1a	1725	1/1	0.96	0.08	53,53,53,53	0
57	MG	1A	3576	1/1	0.96	0.17	32,32,32,32	0
57	MG	2A	3432	1/1	0.96	0.27	53,53,53,53	0
57	MG	1A	3286	1/1	0.96	0.10	32,32,32,32	0
59	ZN	1n	102	1/1	0.96	0.05	85,85,85,85	0
57	MG	2A	3434	1/1	0.96	0.37	65,65,65,65	0
57	MG	1A	3404	1/1	0.97	0.13	41,41,41,41	0
57	MG	1A	3178	1/1	0.97	0.15	29,29,29,29	0
57	MG	1A	3028	1/1	0.97	0.14	26,26,26,26	0
57	MG	2a	1647	1/1	0.97	0.17	32,32,32,32	0
57	MG	1A	3217	1/1	0.97	0.19	36,36,36,36	0
57	MG	2A	3060	1/1	0.97	0.05	38,38,38,38	0
57	MG	1A	4071	1/1	0.97	0.06	46,46,46,46	0
57	MG	1A	3467	1/1	0.97	0.09	51,51,51,51	0
57	MG	1A	3113	1/1	0.97	0.10	37,37,37,37	0
57	MG	1A	3081	1/1	0.97	0.15	32,32,32,32	0
57	MG	1A	4076	1/1	0.97	0.04	36,36,36,36	0
57	MG	1A	3038	1/1	0.97	0.18	32,32,32,32	0
57	MG	1A	3305	1/1	0.97	0.08	19,19,19,19	0
57	MG	1R	203	1/1	0.97	0.12	39,39,39,39	0
57	MG	1A	3780	1/1	0.97	0.05	21,21,21,21	0
57	MG	1A	3692	1/1	0.97	0.06	54,54,54,54	0
57	MG	1A	3133	1/1	0.97	0.07	38,38,38,38	0
57	MG	1A	3874	1/1	0.97	0.11	26,26,26,26	0
57	MG	2A	3839	1/1	0.97	0.04	58,58,58,58	0
57	MG	2a	1663	1/1	0.97	0.17	55,55,55,55	0
57	MG	2A	3504	1/1	0.97	0.04	30,30,30,30	0
57	MG	2A	3073	1/1	0.97	0.16	52,52,52,52	0
57	MG	1A	3358	1/1	0.97	0.09	53,53,53,53	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	2A	3217	1/1	0.97	0.27	35,35,35,35	0
57	MG	1A	3784	1/1	0.97	0.07	35,35,35,35	0
57	MG	1T	202	1/1	0.97	0.07	54,54,54,54	0
57	MG	1U	201	1/1	0.97	0.20	37,37,37,37	0
57	MG	1A	3012	1/1	0.97	0.04	26,26,26,26	0
57	MG	1A	3618	1/1	0.97	0.10	26,26,26,26	0
57	MG	1A	3187	1/1	0.97	0.07	43,43,43,43	0
57	MG	1A	3188	1/1	0.97	0.07	37,37,37,37	0
57	MG	1A	3789	1/1	0.97	0.07	16,16,16,16	0
57	MG	1U	208	1/1	0.97	0.17	32,32,32,32	0
57	MG	1A	3479	1/1	0.97	0.12	39,39,39,39	0
57	MG	1A	3700	1/1	0.97	0.04	16,16,16,16	0
57	MG	1V	201	1/1	0.97	0.33	29,29,29,29	0
57	MG	1A	3541	1/1	0.97	0.20	32,32,32,32	0
57	MG	1A	3068	1/1	0.97	0.04	33,33,33,33	0
57	MG	1A	3987	1/1	0.97	0.05	50,50,50,50	0
57	MG	1a	1801	1/1	0.97	0.06	52,52,52,52	0
57	MG	1B	206	1/1	0.97	0.08	39,39,39,39	0
57	MG	2A	3375	1/1	0.97	0.21	57,57,57,57	0
57	MG	1W	202	1/1	0.97	0.16	52,52,52,52	0
57	MG	1W	203	1/1	0.97	0.13	37,37,37,37	0
57	MG	1W	204	1/1	0.97	0.21	37,37,37,37	0
57	MG	1B	207	1/1	0.97	0.16	40,40,40,40	0
57	MG	1A	3030	1/1	0.97	0.13	33,33,33,33	0
57	MG	1A	3704	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3483	1/1	0.97	0.22	30,30,30,30	0
57	MG	1X	103	1/1	0.97	0.10	42,42,42,42	0
57	MG	2A	3100	1/1	0.97	0.08	25,25,25,25	0
57	MG	1A	3228	1/1	0.97	0.19	29,29,29,29	0
57	MG	1A	3266	1/1	0.97	0.14	38,38,38,38	0
57	MG	2A	3540	1/1	0.97	0.05	32,32,32,32	0
57	MG	1A	3629	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3229	1/1	0.97	0.12	29,29,29,29	0
57	MG	1B	215	1/1	0.97	0.06	50,50,50,50	0
57	MG	1A	3193	1/1	0.97	0.04	38,38,38,38	0
57	MG	2A	3709	1/1	0.97	0.14	33,33,33,33	0
57	MG	1A	3137	1/1	0.97	0.12	36,36,36,36	0
57	MG	1B	219	1/1	0.97	0.10	36,36,36,36	0
57	MG	2A	3547	1/1	0.97	0.05	30,30,30,30	0
57	MG	2A	3713	1/1	0.97	0.07	50,50,50,50	0
57	MG	10	101	1/1	0.97	0.06	47,47,47,47	0
57	MG	10	102	1/1	0.97	0.20	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	1A	3161	1/1	0.97	0.26	30,30,30,30	0
57	MG	1d	301	1/1	0.97	0.28	48,48,48,48	0
57	MG	1A	3557	1/1	0.97	0.20	38,38,38,38	0
57	MG	1A	3087	1/1	0.97	0.26	36,36,36,36	0
57	MG	1A	4002	1/1	0.97	0.10	22,22,22,22	0
57	MG	1A	3428	1/1	0.97	0.16	41,41,41,41	0
57	MG	1A	3561	1/1	0.97	0.20	34,34,34,34	0
57	MG	1B	227	1/1	0.97	0.05	41,41,41,41	0
57	MG	1A	3721	1/1	0.97	0.06	46,46,46,46	0
57	MG	1A	3722	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	4009	1/1	0.97	0.04	41,41,41,41	0
57	MG	1A	3562	1/1	0.97	0.15	38,38,38,38	0
57	MG	1A	3907	1/1	0.97	0.05	40,40,40,40	0
57	MG	1A	3319	1/1	0.97	0.13	32,32,32,32	0
57	MG	2A	3128	1/1	0.97	0.15	47,47,47,47	0
57	MG	2a	1724	1/1	0.97	0.14	47,47,47,47	0
57	MG	1A	3163	1/1	0.97	0.10	26,26,26,26	0
57	MG	15	101	1/1	0.97	0.07	37,37,37,37	0
57	MG	2A	3573	1/1	0.97	0.13	64,64,64,64	0
57	MG	1A	3726	1/1	0.97	0.06	48,48,48,48	0
57	MG	1A	3641	1/1	0.97	0.11	37,37,37,37	0
57	MG	2Q	202	1/1	0.97	0.23	50,50,50,50	0
57	MG	1A	3235	1/1	0.97	0.09	62,62,62,62	0
57	MG	1A	3198	1/1	0.97	0.08	40,40,40,40	0
57	MG	1D	303	1/1	0.97	0.11	49,49,49,49	0
57	MG	1A	3237	1/1	0.97	0.07	24,24,24,24	0
57	MG	1A	3434	1/1	0.97	0.16	26,26,26,26	0
57	MG	2A	3419	1/1	0.97	0.24	49,49,49,49	0
57	MG	1x	109	1/1	0.97	0.13	58,58,58,58	0
57	MG	17	102	1/1	0.97	0.12	28,28,28,28	0
57	MG	1A	3917	1/1	0.97	0.05	12,12,12,12	0
57	MG	1A	3072	1/1	0.97	0.21	30,30,30,30	0
57	MG	1A	3278	1/1	0.97	0.14	26,26,26,26	0
57	MG	1D	311	1/1	0.97	0.14	31,31,31,31	0
57	MG	2A	3003	1/1	0.97	0.30	52,52,52,52	0
57	MG	2A	3427	1/1	0.97	0.08	30,30,30,30	0
57	MG	1A	3239	1/1	0.97	0.13	34,34,34,34	0
57	MG	2A	3429	1/1	0.97	0.17	38,38,38,38	0
57	MG	20	101	1/1	0.97	0.05	57,57,57,57	0
57	MG	1A	3924	1/1	0.97	0.09	42,42,42,42	0
57	MG	2a	1749	1/1	0.97	0.18	68,68,68,68	0
57	MG	1A	3925	1/1	0.97	0.05	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	1A	3280	1/1	0.97	0.39	39,39,39,39	0
57	MG	1E	303	1/1	0.97	0.07	28,28,28,28	0
57	MG	23	103	1/1	0.97	0.05	41,41,41,41	0
57	MG	1A	3240	1/1	0.97	0.06	30,30,30,30	0
57	MG	1A	3283	1/1	0.97	0.26	35,35,35,35	0
57	MG	2A	3012	1/1	0.97	0.08	47,47,47,47	0
57	MG	2A	3154	1/1	0.97	0.08	50,50,50,50	0
57	MG	2A	3762	1/1	0.97	0.06	57,57,57,57	0
57	MG	1E	307	1/1	0.97	0.09	23,23,23,23	0
57	MG	1A	3284	1/1	0.97	0.08	38,38,38,38	0
57	MG	1A	3740	1/1	0.97	0.06	25,25,25,25	0
57	MG	1A	3241	1/1	0.97	0.26	37,37,37,37	0
57	MG	1a	1608	1/1	0.97	0.06	74,74,74,74	0
57	MG	2A	3018	1/1	0.97	0.07	38,38,38,38	0
57	MG	1A	3032	1/1	0.97	0.16	24,24,24,24	0
57	MG	2A	3020	1/1	0.97	0.04	25,25,25,25	0
57	MG	1A	3933	1/1	0.97	0.04	45,45,45,45	0
57	MG	1A	3287	1/1	0.97	0.20	45,45,45,45	0
57	MG	1A	3658	1/1	0.97	0.09	24,24,24,24	0
57	MG	1A	3090	1/1	0.97	0.15	41,41,41,41	0
57	MG	1A	3142	1/1	0.97	0.07	33,33,33,33	0
57	MG	1A	3390	1/1	0.97	0.17	30,30,30,30	0
57	MG	2A	3778	1/1	0.97	0.07	61,61,61,61	0
57	MG	1A	4042	1/1	0.97	0.09	21,21,21,21	0
57	MG	1A	3169	1/1	0.97	0.25	42,42,42,42	0
57	MG	1A	3513	1/1	0.97	0.10	32,32,32,32	0
57	MG	1A	3008	1/1	0.97	0.15	22,22,22,22	0
57	MG	1A	3340	1/1	0.97	0.07	29,29,29,29	0
57	MG	1a	1621	1/1	0.97	0.07	47,47,47,47	0
57	MG	2A	3459	1/1	0.97	0.11	23,23,23,23	0
57	MG	1A	3292	1/1	0.97	0.17	31,31,31,31	0
57	MG	1A	3755	1/1	0.97	0.09	32,32,32,32	0
57	MG	1A	3075	1/1	0.97	0.10	31,31,31,31	0
57	MG	2A	3464	1/1	0.97	0.07	28,28,28,28	0
57	MG	1a	1748	1/1	0.97	0.12	36,36,36,36	0
57	MG	1A	3845	1/1	0.97	0.10	49,49,49,49	0
57	MG	1A	3668	1/1	0.97	0.05	19,19,19,19	0
57	MG	2A	3320	1/1	0.97	0.09	60,60,60,60	0
57	MG	2a	1623	1/1	0.97	0.10	59,59,59,59	0
57	MG	1A	3126	1/1	0.97	0.19	35,35,35,35	0
57	MG	1A	3047	1/1	0.97	0.04	34,34,34,34	0
57	MG	1A	3673	1/1	0.97	0.06	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	1A	3346	1/1	0.97	0.11	39,39,39,39	0
57	MG	1A	3148	1/1	0.97	0.20	32,32,32,32	0
57	MG	2A	3474	1/1	0.97	0.06	58,58,58,58	0
57	MG	2a	1630	1/1	0.97	0.12	55,55,55,55	0
57	MG	2A	3804	1/1	0.97	0.05	48,48,48,48	0
57	MG	1A	3764	1/1	0.97	0.10	21,21,21,21	0
57	MG	1A	3596	1/1	0.97	0.12	50,50,50,50	0
57	MG	1A	3956	1/1	0.97	0.10	53,53,53,53	0
57	MG	1a	1761	1/1	0.97	0.09	66,66,66,66	0
57	MG	1N	203	1/1	0.97	0.08	35,35,35,35	0
57	MG	1A	3212	1/1	0.97	0.14	38,38,38,38	0
57	MG	1A	3094	1/1	0.97	0.15	22,22,22,22	0
57	MG	1A	3599	1/1	0.97	0.07	36,36,36,36	0
57	MG	1A	3403	1/1	0.97	0.23	40,40,40,40	0
57	MG	2A	3648	1/1	0.97	0.09	71,71,71,71	0
57	MG	1O	202	1/1	0.97	0.10	42,42,42,42	0
57	MG	1A	3770	1/1	0.97	0.08	41,41,41,41	0
59	ZN	2n	501	1/1	0.97	0.05	87,87,87,87	0
60	SF4	1d	302	8/8	0.97	0.06	68,73,83,92	0
60	SF4	2d	303	8/8	0.97	0.06	60,71,82,89	0
57	MG	1A	3670	1/1	0.98	0.03	27,27,27,27	0
57	MG	1A	3544	1/1	0.98	0.10	33,33,33,33	0
57	MG	1A	3672	1/1	0.98	0.05	24,24,24,24	0
57	MG	1A	3545	1/1	0.98	0.19	40,40,40,40	0
57	MG	1A	3608	1/1	0.98	0.07	56,56,56,56	0
57	MG	1A	3079	1/1	0.98	0.05	26,26,26,26	0
57	MG	1A	3610	1/1	0.98	0.07	20,20,20,20	0
57	MG	2E	304	1/1	0.98	0.13	30,30,30,30	0
57	MG	1A	3750	1/1	0.98	0.06	35,35,35,35	0
57	MG	1A	3147	1/1	0.98	0.15	31,31,31,31	0
57	MG	2A	3498	1/1	0.98	0.10	44,44,44,44	0
57	MG	1A	3282	1/1	0.98	0.19	32,32,32,32	0
57	MG	2A	3625	1/1	0.98	0.17	55,55,55,55	0
57	MG	1A	3906	1/1	0.98	0.10	43,43,43,43	0
57	MG	1a	1604	1/1	0.98	0.08	57,57,57,57	0
57	MG	1A	3679	1/1	0.98	0.11	24,24,24,24	0
57	MG	1A	3827	1/1	0.98	0.04	56,56,56,56	0
57	MG	1A	3174	1/1	0.98	0.07	34,34,34,34	0
57	MG	1A	3993	1/1	0.98	0.04	40,40,40,40	0
57	MG	1A	3322	1/1	0.98	0.12	42,42,42,42	0
57	MG	1A	3552	1/1	0.98	0.17	36,36,36,36	0
57	MG	1A	3023	1/1	0.98	0.06	16,16,16,16	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	3177	1/1	0.98	0.06	48,48,48,48	0
57	MG	1P	201	1/1	0.98	0.21	28,28,28,28	0
57	MG	1A	3913	1/1	0.98	0.11	43,43,43,43	0
57	MG	2O	202	1/1	0.98	0.10	43,43,43,43	0
57	MG	1a	1816	1/1	0.98	0.04	58,58,58,58	0
57	MG	2A	3768	1/1	0.98	0.07	41,41,41,41	0
57	MG	1A	3998	1/1	0.98	0.04	32,32,32,32	0
57	MG	1P	204	1/1	0.98	0.23	25,25,25,25	0
57	MG	1A	3500	1/1	0.98	0.20	32,32,32,32	0
57	MG	1A	3555	1/1	0.98	0.23	45,45,45,45	0
57	MG	1A	3760	1/1	0.98	0.05	31,31,31,31	0
57	MG	1Q	204	1/1	0.98	0.06	43,43,43,43	0
57	MG	1A	3452	1/1	0.98	0.08	38,38,38,38	0
57	MG	1A	4003	1/1	0.98	0.03	28,28,28,28	0
57	MG	1A	3687	1/1	0.98	0.03	20,20,20,20	0
57	MG	1A	3621	1/1	0.98	0.10	45,45,45,45	0
57	MG	2A	3523	1/1	0.98	0.09	29,29,29,29	0
57	MG	1A	4006	1/1	0.98	0.10	36,36,36,36	0
57	MG	1A	3921	1/1	0.98	0.05	30,30,30,30	0
57	MG	1A	3922	1/1	0.98	0.05	33,33,33,33	0
57	MG	2A	3783	1/1	0.98	0.06	50,50,50,50	0
57	MG	1A	3176	1/1	0.98	0.09	33,33,33,33	0
57	MG	1A	3454	1/1	0.98	0.15	38,38,38,38	0
57	MG	2A	3786	1/1	0.98	0.09	44,44,44,44	0
57	MG	1A	3409	1/1	0.98	0.16	45,45,45,45	0
57	MG	1A	4012	1/1	0.98	0.04	40,40,40,40	0
57	MG	2A	3789	1/1	0.98	0.03	36,36,36,36	0
57	MG	1B	216	1/1	0.98	0.12	48,48,48,48	0
57	MG	1A	3044	1/1	0.98	0.06	33,33,33,33	0
57	MG	1A	3213	1/1	0.98	0.18	33,33,33,33	0
57	MG	1U	202	1/1	0.98	0.21	25,25,25,25	0
57	MG	1w	401	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3327	1/1	0.98	0.29	50,50,50,50	0
57	MG	2A	3538	1/1	0.98	0.07	38,38,38,38	0
57	MG	1A	3844	1/1	0.98	0.07	46,46,46,46	0
57	MG	1A	3565	1/1	0.98	0.15	34,34,34,34	0
57	MG	1A	3045	1/1	0.98	0.09	40,40,40,40	0
57	MG	27	101	1/1	0.98	0.17	35,35,35,35	0
57	MG	1A	3414	1/1	0.98	0.30	42,42,42,42	0
57	MG	1A	3179	1/1	0.98	0.12	19,19,19,19	0
57	MG	1A	3934	1/1	0.98	0.04	61,61,61,61	0
57	MG	1A	3180	1/1	0.98	0.06	32,32,32,32	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	3031	1/1	0.98	0.14	31,31,31,31	0
57	MG	1A	3571	1/1	0.98	0.08	33,33,33,33	0
57	MG	1A	3011	1/1	0.98	0.08	40,40,40,40	0
57	MG	1V	205	1/1	0.98	0.09	39,39,39,39	0
57	MG	2A	3105	1/1	0.98	0.07	49,49,49,49	0
57	MG	1A	3107	1/1	0.98	0.09	28,28,28,28	0
57	MG	1A	3048	1/1	0.98	0.10	30,30,30,30	0
57	MG	2A	3553	1/1	0.98	0.09	23,23,23,23	0
57	MG	2A	3108	1/1	0.98	0.17	40,40,40,40	0
57	MG	1A	3155	1/1	0.98	0.09	35,35,35,35	0
57	MG	2A	3556	1/1	0.98	0.10	59,59,59,59	0
57	MG	1A	3856	1/1	0.98	0.21	36,36,36,36	0
57	MG	1A	3468	1/1	0.98	0.08	44,44,44,44	0
57	MG	2A	3685	1/1	0.98	0.08	44,44,44,44	0
57	MG	2A	3559	1/1	0.98	0.06	34,34,34,34	0
57	MG	2A	3822	1/1	0.98	0.04	52,52,52,52	0
57	MG	1A	3707	1/1	0.98	0.05	21,21,21,21	0
57	MG	2A	3561	1/1	0.98	0.08	53,53,53,53	0
57	MG	2A	3825	1/1	0.98	0.04	48,48,48,48	0
57	MG	1A	3033	1/1	0.98	0.27	33,33,33,33	0
57	MG	1A	3223	1/1	0.98	0.16	30,30,30,30	0
57	MG	2A	3691	1/1	0.98	0.08	34,34,34,34	0
57	MG	2A	3564	1/1	0.98	0.07	30,30,30,30	0
57	MG	2a	1622	1/1	0.98	0.04	56,56,56,56	0
57	MG	2A	3565	1/1	0.98	0.04	31,31,31,31	0
57	MG	2A	3831	1/1	0.98	0.08	28,28,28,28	0
57	MG	2A	3008	1/1	0.98	0.04	35,35,35,35	0
57	MG	1a	1754	1/1	0.98	0.10	58,58,58,58	0
57	MG	2A	3117	1/1	0.98	0.08	29,29,29,29	0
57	MG	2A	3447	1/1	0.98	0.12	23,23,23,23	0
57	MG	1A	3017	1/1	0.98	0.07	57,57,57,57	0
57	MG	1a	1756	1/1	0.98	0.06	37,37,37,37	0
57	MG	1A	3158	1/1	0.98	0.21	39,39,39,39	0
57	MG	1D	305	1/1	0.98	0.07	16,16,16,16	0
57	MG	1A	3712	1/1	0.98	0.08	52,52,52,52	0
57	MG	1D	307	1/1	0.98	0.11	36,36,36,36	0
57	MG	1A	3018	1/1	0.98	0.05	16,16,16,16	0
57	MG	1A	3003	1/1	0.98	0.04	25,25,25,25	0
57	MG	2A	3844	1/1	0.98	0.03	49,49,49,49	0
57	MG	1A	3790	1/1	0.98	0.04	43,43,43,43	0
57	MG	1A	3191	1/1	0.98	0.14	27,27,27,27	0
57	MG	1A	3192	1/1	0.98	0.19	31,31,31,31	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	3039	1/1	0.98	0.14	34,34,34,34	0
57	MG	1A	3586	1/1	0.98	0.07	22,22,22,22	0
57	MG	2A	3583	1/1	0.98	0.05	53,53,53,53	0
57	MG	1A	3650	1/1	0.98	0.07	36,36,36,36	0
57	MG	2A	3462	1/1	0.98	0.17	49,49,49,49	0
57	MG	1A	3070	1/1	0.98	0.10	22,22,22,22	0
57	MG	1A	3013	1/1	0.98	0.09	29,29,29,29	0
57	MG	2A	3026	1/1	0.98	0.07	40,40,40,40	0
57	MG	1A	3164	1/1	0.98	0.16	29,29,29,29	0
57	MG	1A	3654	1/1	0.98	0.08	29,29,29,29	0
57	MG	1A	3482	1/1	0.98	0.19	36,36,36,36	0
57	MG	1A	3005	1/1	0.98	0.06	40,40,40,40	0
57	MG	1A	3056	1/1	0.98	0.13	32,32,32,32	0
57	MG	1A	3119	1/1	0.98	0.10	35,35,35,35	0
57	MG	1A	3273	1/1	0.98	0.09	38,38,38,38	0
57	MG	1A	4056	1/1	0.98	0.08	23,23,23,23	0
57	MG	12	102	1/1	0.98	0.13	41,41,41,41	0
57	MG	1A	3042	1/1	0.98	0.10	28,28,28,28	0
57	MG	1A	3202	1/1	0.98	0.07	40,40,40,40	0
57	MG	2A	3365	1/1	0.98	0.05	41,41,41,41	0
57	MG	1A	3885	1/1	0.98	0.09	33,33,33,33	0
57	MG	1A	3076	1/1	0.98	0.07	23,23,23,23	0
57	MG	1A	3058	1/1	0.98	0.06	33,33,33,33	0
57	MG	2A	3604	1/1	0.98	0.08	36,36,36,36	0
57	MG	1A	3399	1/1	0.98	0.31	56,56,56,56	0
57	MG	1F	306	1/1	0.98	0.12	30,30,30,30	0
57	MG	1A	3540	1/1	0.98	0.07	28,28,28,28	0
57	MG	1A	3078	1/1	0.98	0.06	30,30,30,30	0
57	MG	1A	3542	1/1	0.98	0.15	30,30,30,30	0
57	MG	2D	302	1/1	0.98	0.21	39,39,39,39	0
59	ZN	26	102	1/1	0.98	0.03	53,53,53,53	0
57	MG	1A	3206	1/1	0.98	0.09	36,36,36,36	0
57	MG	1A	3977	1/1	0.98	0.07	27,27,27,27	0
57	MG	1A	3605	1/1	0.98	0.07	41,41,41,41	0
57	MG	2A	3678	1/1	0.99	0.05	29,29,29,29	0
57	MG	1A	3085	1/1	0.99	0.10	24,24,24,24	0
57	MG	1A	3037	1/1	0.99	0.04	20,20,20,20	0
57	MG	1A	3746	1/1	0.99	0.08	40,40,40,40	0
57	MG	1A	3791	1/1	0.99	0.03	20,20,20,20	0
57	MG	1A	3110	1/1	0.99	0.20	30,30,30,30	0
57	MG	1E	304	1/1	0.99	0.17	31,31,31,31	0
57	MG	2A	3145	1/1	0.99	0.10	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	3201	1/1	0.99	0.09	21,21,21,21	0
57	MG	1A	3611	1/1	0.99	0.05	52,52,52,52	0
57	MG	1B	224	1/1	0.99	0.04	43,43,43,43	0
57	MG	1A	3559	1/1	0.99	0.20	29,29,29,29	0
57	MG	1A	3890	1/1	0.99	0.05	41,41,41,41	0
57	MG	1A	3375	1/1	0.99	0.09	25,25,25,25	0
57	MG	1A	3021	1/1	0.99	0.04	22,22,22,22	0
57	MG	2A	3606	1/1	0.99	0.04	42,42,42,42	0
57	MG	1A	4029	1/1	0.99	0.04	49,49,49,49	0
57	MG	13	101	1/1	0.99	0.11	28,28,28,28	0
57	MG	2A	3524	1/1	0.99	0.08	29,29,29,29	0
57	MG	1V	203	1/1	0.99	0.16	28,28,28,28	0
57	MG	1a	1807	1/1	0.99	0.04	48,48,48,48	0
57	MG	1A	3920	1/1	0.99	0.08	26,26,26,26	0
57	MG	2A	3744	1/1	0.99	0.06	50,50,50,50	0
57	MG	1A	3867	1/1	0.99	0.09	30,30,30,30	0
57	MG	1x	111	1/1	0.99	0.05	49,49,49,49	0
57	MG	1E	315	1/1	0.99	0.06	40,40,40,40	0
57	MG	1A	3731	1/1	0.99	0.03	13,13,13,13	0
57	MG	1A	3010	1/1	0.99	0.08	35,35,35,35	0
57	MG	1A	3870	1/1	0.99	0.09	48,48,48,48	0
57	MG	15	105	1/1	0.99	0.17	28,28,28,28	0
57	MG	1A	3563	1/1	0.99	0.15	32,32,32,32	0
57	MG	15	107	1/1	0.99	0.05	40,40,40,40	0
57	MG	1A	3014	1/1	0.99	0.05	28,28,28,28	0
57	MG	1A	3345	1/1	0.99	0.18	33,33,33,33	0
57	MG	2A	3802	1/1	0.99	0.04	35,35,35,35	0
57	MG	1A	3071	1/1	0.99	0.04	15,15,15,15	0
57	MG	1A	4067	1/1	0.99	0.09	29,29,29,29	0
57	MG	1A	3601	1/1	0.99	0.11	34,34,34,34	0
57	MG	2A	3806	1/1	0.99	0.03	40,40,40,40	0
57	MG	1A	3716	1/1	0.99	0.07	26,26,26,26	0
57	MG	2A	3760	1/1	0.99	0.03	49,49,49,49	0
57	MG	1R	202	1/1	0.99	0.20	35,35,35,35	0
59	ZN	1Y	205	1/1	0.99	0.03	60,60,60,60	0
57	MG	1A	3036	1/1	0.99	0.12	28,28,28,28	0
59	ZN	15	109	1/1	0.99	0.03	44,44,44,44	0
59	ZN	16	102	1/1	0.99	0.05	44,44,44,44	0
59	ZN	19	102	1/1	0.99	0.06	44,44,44,44	0
57	MG	1A	3447	1/1	0.99	0.15	47,47,47,47	0
59	ZN	2Y	501	1/1	0.99	0.03	82,82,82,82	0
57	MG	1A	4072	1/1	0.99	0.07	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
59	ZN	25	108	1/1	0.99	0.02	56,56,56,56	0
57	MG	1A	3476	1/1	0.99	0.18	33,33,33,33	0
59	ZN	29	102	1/1	0.99	0.05	65,65,65,65	0
57	MG	2A	3814	1/1	0.99	0.03	25,25,25,25	0
57	MG	1A	3382	1/1	0.99	0.31	27,27,27,27	0
57	MG	1A	3099	1/1	0.99	0.08	19,19,19,19	0
57	MG	1A	4028	1/1	1.00	0.05	24,24,24,24	0
57	MG	1A	3896	1/1	1.00	0.04	27,27,27,27	0
57	MG	1A	3717	1/1	1.00	0.07	20,20,20,20	0
57	MG	1a	1814	1/1	1.00	0.08	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.