



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2025 – 11:48 PM EDT

PDB ID : 9MTP / pdb_00009mtp
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with mRNA, A-site Q230-N5-methylated Release Factor 1, and P-site fM EAAAKC-peptidyl-tRNA_{cys} at 2.40Å 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 : 2.40 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 Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

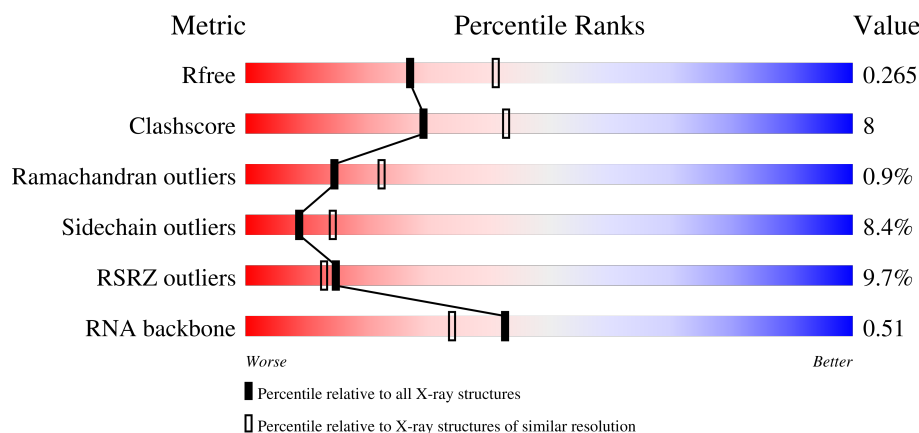
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.











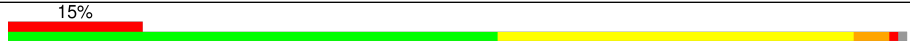

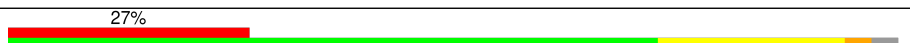


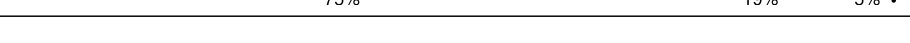
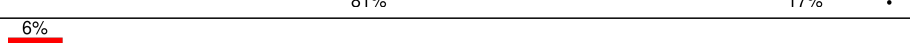
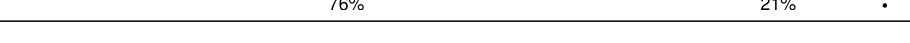
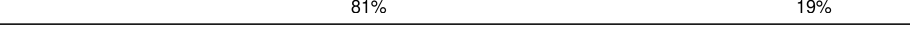
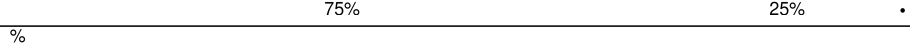
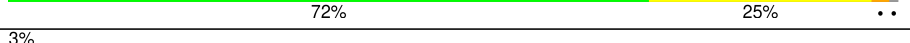






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)
RNA backbone	3690	1084 (2.70-2.10)

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	 6% 64% 28% 7% •
1	2A	2915	 5% 59% 32% 6% •
2	1B	121	 74% 22% ••





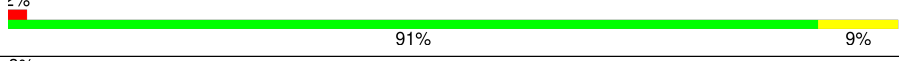
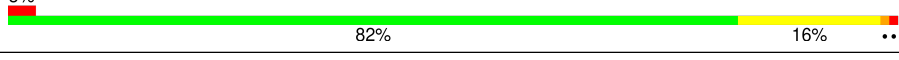


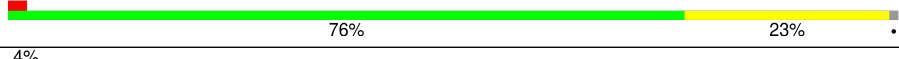







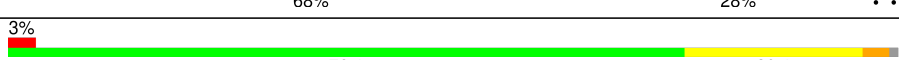

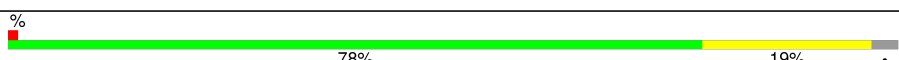

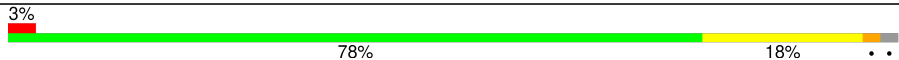




Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	25	60	
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	

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	1U	211	-	-	-	X
57	MG	1a	1640	-	-	-	X
57	MG	1a	1716	-	-	-	X
57	MG	2A	3263	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 297056 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	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
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called CYS-Stop mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	9	Total	C	N	O	P	0	0	0
			191	86	34	62	9			
53	2v	9	Total	C	N	O	P	0	0	0
			191	86	34	62	9			

- 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
			1939	1199	360	371	9			
54	2w	253	Total	C	N	O	S	0	0	0
			1957	1210	361	377	9			

- 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	1101	Total	Mg	0	0
			1101	1101		
57	1B	38	Total	Mg	0	0
			38	38		
57	1D	14	Total	Mg	0	0
			14	14		
57	1E	13	Total	Mg	0	0
			13	13		
57	1F	16	Total	Mg	0	0
			16	16		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1G	5	Total 5	Mg 5	0	0
57	1I	1	Total 1	Mg 1	0	0
57	1N	4	Total 4	Mg 4	0	0
57	1O	4	Total 4	Mg 4	0	0
57	1P	7	Total 7	Mg 7	0	0
57	1Q	7	Total 7	Mg 7	0	0
57	1R	4	Total 4	Mg 4	0	0
57	1S	3	Total 3	Mg 3	0	0
57	1T	3	Total 3	Mg 3	0	0
57	1U	11	Total 11	Mg 11	0	0
57	1V	7	Total 7	Mg 7	0	0
57	1W	5	Total 5	Mg 5	0	0
57	1X	5	Total 5	Mg 5	0	0
57	1Y	4	Total 4	Mg 4	0	0
57	1Z	2	Total 2	Mg 2	0	0
57	10	7	Total 7	Mg 7	0	0
57	11	4	Total 4	Mg 4	0	0
57	12	2	Total 2	Mg 2	0	0
57	13	3	Total 3	Mg 3	0	0
57	15	9	Total 9	Mg 9	0	0
57	16	2	Total 2	Mg 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	17	5	Total 5	Mg 5	0	0
57	18	4	Total 4	Mg 4	0	0
57	19	1	Total 1	Mg 1	0	0
57	1a	215	Total 215	Mg 215	0	0
57	1b	2	Total 2	Mg 2	0	0
57	1d	1	Total 1	Mg 1	0	0
57	1e	3	Total 3	Mg 3	0	0
57	1f	1	Total 1	Mg 1	0	0
57	1k	1	Total 1	Mg 1	0	0
57	1l	2	Total 2	Mg 2	0	0
57	1m	1	Total 1	Mg 1	0	0
57	1n	2	Total 2	Mg 2	0	0
57	1r	1	Total 1	Mg 1	0	0
57	1t	1	Total 1	Mg 1	0	0
57	1v	4	Total 4	Mg 4	0	0
57	1w	1	Total 1	Mg 1	0	0
57	1x	12	Total 12	Mg 12	0	0
57	2A	852	Total 852	Mg 852	0	0
57	2B	19	Total 19	Mg 19	0	0
57	2D	7	Total 7	Mg 7	0	0
57	2E	8	Total 8	Mg 8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2F	7	Total 7	Mg 7	0	0
57	2G	1	Total 1	Mg 1	0	0
57	2N	1	Total 1	Mg 1	0	0
57	2O	2	Total 2	Mg 2	0	0
57	2P	2	Total 2	Mg 2	0	0
57	2Q	4	Total 4	Mg 4	0	0
57	2R	1	Total 1	Mg 1	0	0
57	2T	3	Total 3	Mg 3	0	0
57	2U	2	Total 2	Mg 2	0	0
57	2V	2	Total 2	Mg 2	0	0
57	2W	2	Total 2	Mg 2	0	0
57	2Z	1	Total 1	Mg 1	0	0
57	20	1	Total 1	Mg 1	0	0
57	21	2	Total 2	Mg 2	0	0
57	23	4	Total 4	Mg 4	0	0
57	25	7	Total 7	Mg 7	0	0
57	26	1	Total 1	Mg 1	0	0
57	28	3	Total 3	Mg 3	0	0
57	29	1	Total 1	Mg 1	0	0
57	2a	185	Total 185	Mg 185	0	0
57	2d	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2e	2	Total 2	Mg 2	0	0
57	2f	1	Total 1	Mg 1	0	0
57	2g	1	Total 1	Mg 1	0	0
57	2i	1	Total 1	Mg 1	0	0
57	2j	1	Total 1	Mg 1	0	0
57	2l	2	Total 2	Mg 2	0	0
57	2n	1	Total 1	Mg 1	0	0
57	2q	2	Total 2	Mg 2	0	0
57	2r	1	Total 1	Mg 1	0	0
57	2t	1	Total 1	Mg 1	0	0
57	2v	1	Total 1	Mg 1	0	0
57	2x	5	Total 5	Mg 5	0	0

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

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

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

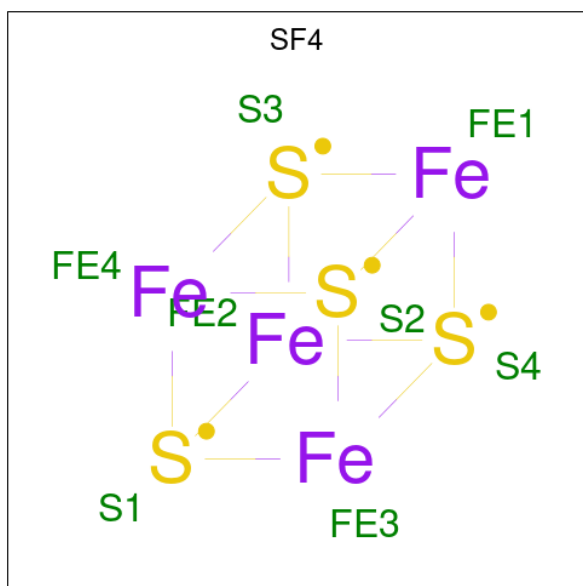
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total 1	Zn 1	0	0
59	14	1	Total 1	Zn 1	0	0
59	15	1	Total 1	Zn 1	0	0
59	16	1	Total 1	Zn 1	0	0

Continued on next page...

Continued from previous page...

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

- 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	2078	Total 2078	O 2078	0	0
61	1B	64	Total 64	O 64	0	0
61	1D	26	Total 26	O 26	0	0
61	1E	25	Total 25	O 25	0	0
61	1F	14	Total 14	O 14	0	0
61	1G	3	Total 3	O 3	0	0
61	1H	4	Total 4	O 4	0	0
61	1I	1	Total 1	O 1	0	0
61	1N	3	Total 3	O 3	0	0
61	1O	8	Total 8	O 8	0	0
61	1P	22	Total 22	O 22	0	0
61	1Q	10	Total 10	O 10	0	0
61	1R	14	Total 14	O 14	0	0
61	1S	4	Total 4	O 4	0	0
61	1T	5	Total 5	O 5	0	0
61	1U	12	Total 12	O 12	0	0
61	1V	9	Total 9	O 9	0	0
61	1W	12	Total 12	O 12	0	0
61	1X	2	Total 2	O 2	0	0
61	1Y	3	Total 3	O 3	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	10	Total 10	O 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	11	10	Total 10	O 10	0	0
61	12	4	Total 4	O 4	0	0
61	13	5	Total 5	O 5	0	0
61	15	6	Total 6	O 6	0	0
61	16	2	Total 2	O 2	0	0
61	17	8	Total 8	O 8	0	0
61	18	13	Total 13	O 13	0	0
61	1a	287	Total 287	O 287	0	0
61	1d	1	Total 1	O 1	0	0
61	1e	1	Total 1	O 1	0	0
61	1f	2	Total 2	O 2	0	0
61	1j	1	Total 1	O 1	0	0
61	1l	3	Total 3	O 3	0	0
61	1q	1	Total 1	O 1	0	0
61	1v	7	Total 7	O 7	0	0
61	1w	1	Total 1	O 1	0	0
61	1x	19	Total 19	O 19	0	0
61	2A	1124	Total 1124	O 1124	0	0
61	2B	19	Total 19	O 19	0	0
61	2D	23	Total 23	O 23	0	0
61	2E	17	Total 17	O 17	0	0

Continued on next page...

Continued from previous page...

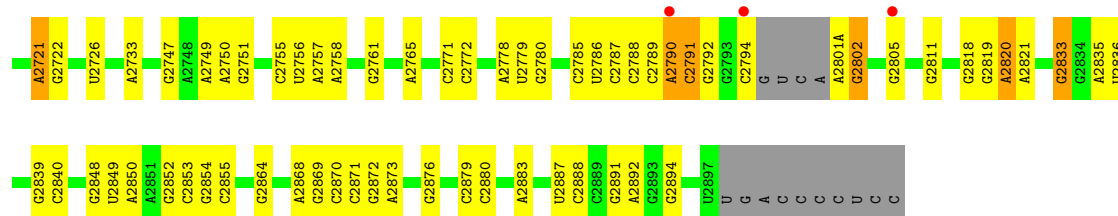
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2F	14	Total 14	O 14	0	0
61	2I	1	Total 1	O 1	0	0
61	2N	2	Total 2	O 2	0	0
61	2O	2	Total 2	O 2	0	0
61	2P	13	Total 13	O 13	0	0
61	2Q	2	Total 2	O 2	0	0
61	2R	4	Total 4	O 4	0	0
61	2T	3	Total 3	O 3	0	0
61	2U	2	Total 2	O 2	0	0
61	2V	1	Total 1	O 1	0	0
61	2W	2	Total 2	O 2	0	0
61	2X	4	Total 4	O 4	0	0
61	2Y	1	Total 1	O 1	0	0
61	2Z	1	Total 1	O 1	0	0
61	20	5	Total 5	O 5	0	0
61	21	9	Total 9	O 9	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	4	Total 4	O 4	0	0

Continued on next page...

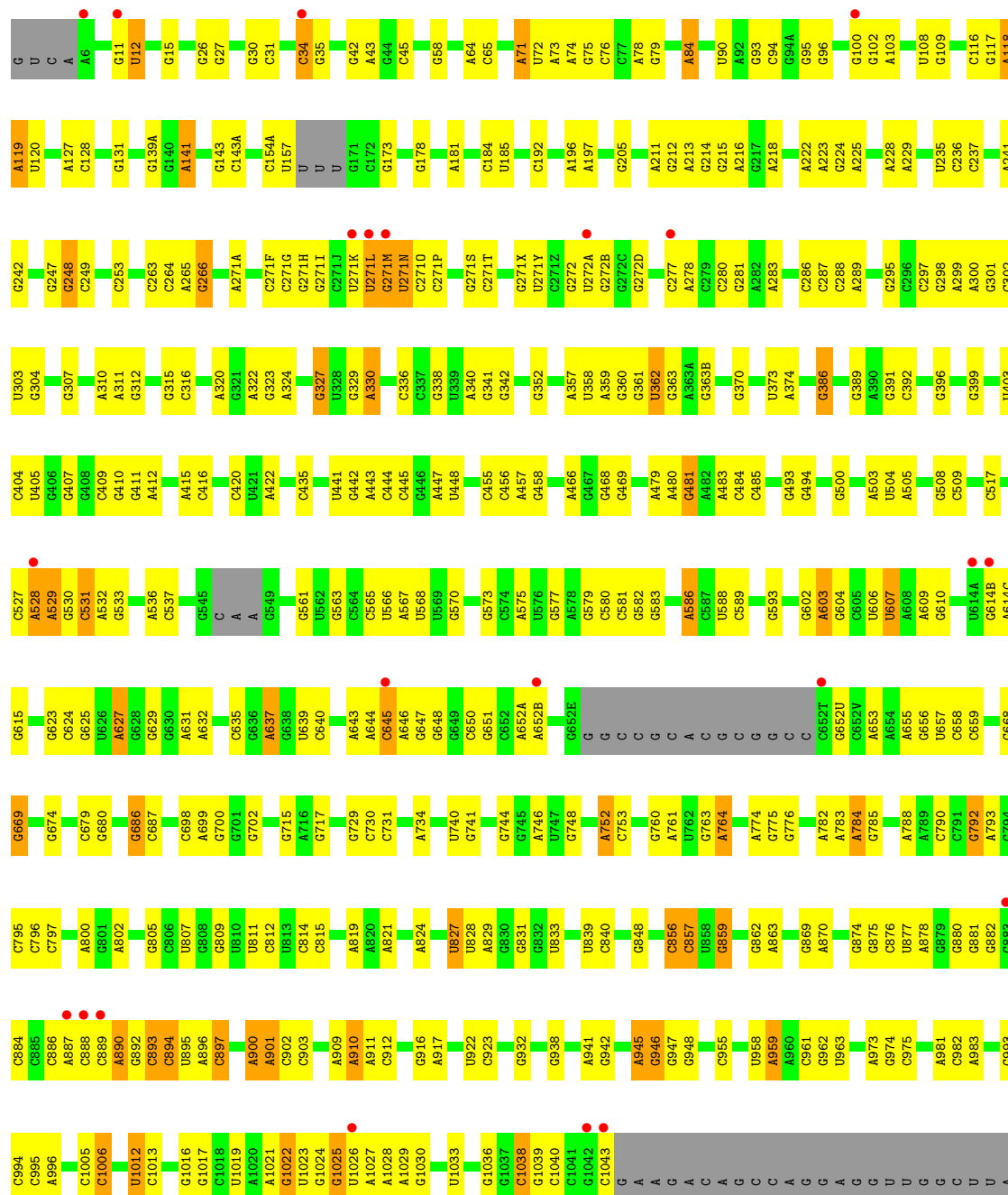
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	29	1	Total 1	O 1	0	0
61	2a	144	Total 144	O 144	0	0
61	2d	3	Total 3	O 3	0	0
61	2e	1	Total 1	O 1	0	0
61	2g	1	Total 1	O 1	0	0
61	2i	2	Total 2	O 2	0	0
61	2j	2	Total 2	O 2	0	0
61	2l	4	Total 4	O 4	0	0
61	2q	2	Total 2	O 2	0	0
61	2r	1	Total 1	O 1	0	0
61	2t	3	Total 3	O 3	0	0
61	2v	2	Total 2	O 2	0	0
61	2w	5	Total 5	O 5	0	0
61	2x	17	Total 17	O 17	0	0

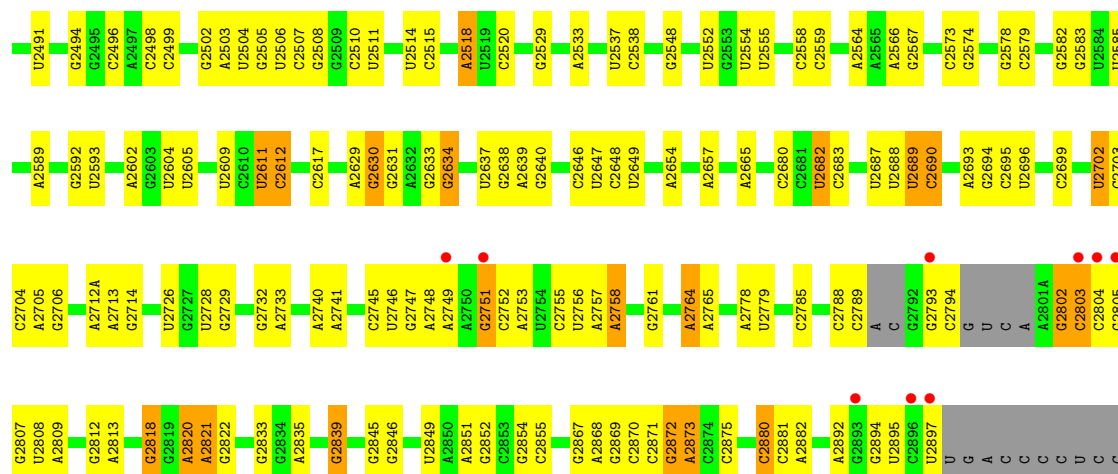
A2602	G2603	U2604	U2605	U2609	C2610	U2611	C2612	U2615	C2616	C2617	A2629	C2630	C2646	U2647	C2648	U2649	U2650	A2654	A2657	C2658	C2663	U2664	U2665	U2667	C2668	C2673	C2678	U2679	C2683	U2684	C2685	U2686	C2687	U2688	C2689	C2690	C2691	C2692	A2693	C2694	U2702	C2703	U2706	A2711	U2712	A2712A	A2713	C2714	U2716					
U2491	G2494	G2502	A2503	U2504	C2505	U2506	C2507	C2512	G2513	A2518	G2525	U2529	G2532	G2535	U2536	U2537	C2538	G2549	C2550	C2551	U2552	U2553	U2554	U2555	U2556	U2557	C2558	U2563	A2564	U2565	C2566	C2567	C2568	C2573	C2574	A2577	C2578	U2581	U2585	C2591	C2592	C2593	C2594	U2702	C2703	U2706	A2711	U2712	A2712A	A2713	C2714	U2716		
C2359	A2360	A2366	G2375	A2376	A2377	A2378	C2379	G2382	C2383	C2384	C2385	U2390	U2399	U2406	G2407	G2410	A2422	U2423	A2424	A2425	A2426	C2427	C2428	C2429	A2430	U2431	A2435	A2436	A2439	C2440	C2441	G2447	A2448	A2451	C2461	U2462	C2463	C2464	A2468	U2469	A2476	C2477	A2478	C2483										
G2250	G2251	A2268	G2271	U2272	A2273	A2274	G2277	G2280	C2283	A2286	A2287	A2288	G2289	U2290	U2291	C2292	G2302	G2303	A2304	A2305	C2306	C2307	C2308	U2312	G2319	A2320	G2321	G2325	C2326	A2327	A2328	C2329	G2330	G2331	G2334	A2335	A2336	C2347	U2348	C2349	C2350	C2351	A2352	G2353	C2354	C2355								
G2159	G2160	C2161	G2162	C2163	C2164	G2165	U2166	C2167	C2168	A2169	A2170	A2171	U2172	A2173	C2174	C2175	A2176	C2177	C2178	C2179	U2180	G2181	C2182	C2183	C2184	C2185	C2186	C2187	C2188	U2189	C2190	C2191	A2198	A2199	C2200	U2203	C2205	G2206	C2207	A2208	U2218	G2224	A2225	C2226	U2233	C2234	G2235	C2236	G2237	C2238	C2239	U2243	U2244	U2245
U2099	G2100	U2102	C2103	C2104	C2105	C2106	C2107	C2108	U2109	C2110	C2111	G2112	U2113	G2115	A2116	U2117	U2118	G2119	C2120	G2121	U2122	C2123	G2124	G2125	A2126	C2127	C2128	C2129	U2130	G2131	U2132	A2133	A2134	A2135	C2136	C2137	C2138	C2139	C2055	C2056	A2059	A2060	A2062	C2069	G2070	U2079	G1963	C1965	A1966	C1967	A1970	A1971		
A1972	U1991	C1992	U1993	C1996	G1997	G1998	A2001	G2002	C2006	G2010	A2013	A2014	A2020	C2021	C2022	G2023	G2029	A2030	A2031	C2032	A2033	C2040	U2041	C2042	C2043	G2049	C2050	G2052	C2055	C2056	A2059	A2060	A2062	C2069	G2070	U2079	G1963	C1965	A1966	C1967	A1970	A1971												
A1859	G1865	C1866	C1867	A1876	A1877	G1878	C1882	G1883	A1889	G1891	C1892	G1899	U1911	C1914	U1915	A1916	U1917	C1920	C1921	G1922	U1923	C1924	G1929	A1802	C1803	C1804	U1805	A1810	G1811	A1812	G1813	A1815	G1816	G1817	G1822	A1829	C1837	G1838	G1839	G1840	A1847	A1848	A1741											
C1745A	G1746	G1753	C1754	A1755	G1756	A1759	C1760	G1761	A1762	G1763	G1764	G1769	A1773	A1780	C1781	C1782	A1783	A1786	A1791	U1796	C1797	U1798	C1800	G1801	A1802	C1803	C1804	U1805	A1810	G1811	A1812	G1813	A1815	G1816	G1817	G1822	A1829	C1837	G1838	G1839	G1840	A1847	A1848	A1741										
A1580	G1581	C1582	A1583	C1584	A1586	C1607	A1608	A1609	A1610	G1622	C1636	A1637	A1641	G1642	G1645	C1646	U1647	C1648	G1653	A1654	U1659	A1665	G1666	G1667	A1668	A1669	C1670	U1673	G1674	C1683	C1684	U1688	U1693	G1696	A1700	A1701	G1702	U1720	G1721	A1722	U1739	A1740	A1741											
G1319	G1332	G1339	G1342	U1352	A1353	A1354	G1355	A1359	A1360	G1364	A1365	C1370	G1371	U1372	A1373	A1379	G1380	A1384	G1385	U1396	U1405	U1406	C1407	A1412	G1413	G1416	C1417	G1418	A1419	U1420	G1421	G1425	U1426	A1427	G1428	G1429	U1431	G1437	A1445	C1445A														
C1180	G1187	U1188	G1191	G1195	C1196	U1197	U1198	C1201	U1205	A1210	U1211	G1212	C1218	G1219	A1220	G1239	U1240	A1242	G1243	U1250	A1253	G1256	G1266	U1267	A1268	A1269	G1270	G1271	A1272	U1273	G1299	U1300	A1301	A1302	G1303	A1308	G1309	G1310	G1311	U1312	U1313	C1315												
U1081	U1082	A1083	A1084	A1085	A1086	G1087	A1088	U1089	U1090	U1091	C1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	U1104	U1105	G1106	G1110	A1111	G1112	U1113	G1114	C1115	C1116	A1128	C1135	G1136	G1139	A1142A	C1153	G1154	A1155	G1164	U1165	C1166	G1171	G1173	A1174	U1175	G1176	A1177	C1178	C1179			



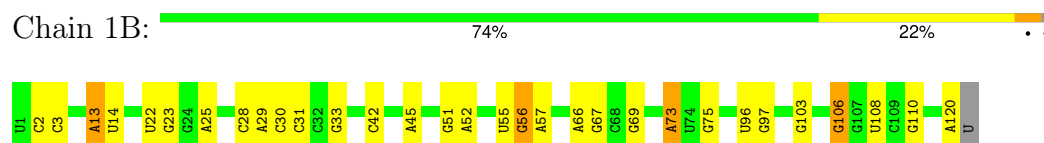
• Molecule 1: 23S Ribosomal RNA



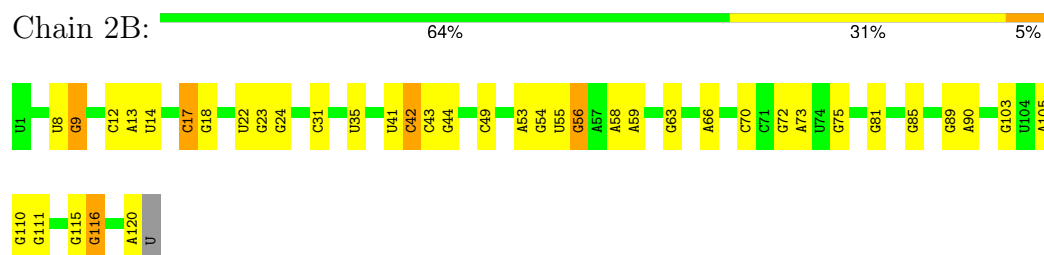
C2386	C2306	C2188	C2128	C2043	A1938	A1812	A1693	A1554	U1453	G1364	A1247	G1136	G
U2387	G2307	U2189	C2129	G2049	U1939	A1815	U1693	C1557	G1455	A1365	A1247	G1139	A
A2388	G2308	G2190	U2130	C2050	C1942	G1816	A1698	A1558	G1456	A1366	A1253	C1140	A
G2389	G2191	G2192	U2131	A2051	U1943	G1817	G1699	G1559	A1460	A1367	A1254	U1141	C
U2390	C2312	C2193	U2132	G2052	A1952	G1822	A1700	A1566	G1465	C1370	U1255	U1142	A
G2391	C2313	A2134	C2133	G2053	A1952	G1822	U1709	A1566	G1466	G1371	G1256	A1142A	C
G2396	C2314	A2135	A2136	A2054	U1955	C1827	U1710	A1569	C1467	U1372	C1261	A1143	C
C2404	C2316	C2137	C2137	G2056	U1956	G1828	G1721	A1570	G1470	A1262	U1263	G1144	C
G2405	G2317	A2208	C2138	G2056	C1957	A1929	A1722	A1571	G1471	C1376	G1264	G1149	A
U2406	G2319	U2218	C2139	A2060	C1958	U1833	U1739	A1572	A1472	A1379	C1150	C1150	C
G2410	A2320	G2219	C2140	A2061	C1958	U1833	U1739	A1572	A1472	G1380	G1154	C1150	C
G2410	G2321	A2225	G2141	A2062	C1962	U1834	G1740	U1578	G1473	A1268	G1154	G1154	U
A2422	A2322	C2226	C2142	A2062	U1963	G1835	G1741	A1579	A1477	A1269	A1155	A1155	U
U2423	G2325	A2227	C2143	C2064	C1963	G1836	G1742	A1580	G1478	C1270	A1155	A1155	U
C2424	G2326	A2227	U2144	C2065	C1967	C1837	C1743	A1583	G1482	A1271	G1169	G1169	A
A2425	G2327	G2234	C2145	C2066	A1969	G1838	G1746	C1584	A1490	U1272	G1170	G1170	A
A2426	A2328	G2234	C2146	C2069	A1970	G1839	G1766	A1586	A1490	U1273	G1171	G1171	A
G2427	G2329	G2238	G2147	G2070	A1971	A1847	G1796	A1587	A1490	A1274	G	G	G
G2428	G2239	G2239	G2149	A2071	A1972	A1848	A1762	A1593	U1405	A1275	U	U	A
G2429	G2240	G2240	U2150	A2071	A1972	A1848	G1763	G1594	U1406	A1276	U	U	A
A2430	A2335	G2248	G2151	G2080	A1981	G1858	A1762	C1493	U1407	A1284	A	A	C
U2431	A2336	G2250	G2152	G2086	G1984	A1859	G1764	A1494	C1407	C1297	C1178	C1178	C
A2434	C2343	G2251	G2153	U2086	G1984	C1866	G1765	A1495	C1408	C1297	C1179	C1179	G
A2435	U2344	G2255	G2155	U2096	G1991	A1876	U1766	A1496	C1409	U1300	C1180	C1180	U
G2443	G2345	G2255	U2156	U2096	U1991	A1877	C1767	U1497	G1410	A1301	G1184	G1184	A
G2445	A2346	G2257	G2157	U2097	G1992	A1878	U1768	U1503	C1411	A1302	G1184	G1184	A
G2446	C2347	G2258	U2158	U2098	U1993	G1878	G1769	C1504	A1412	G1303	G1187	G1187	U
C2441	C2348	G2259	A2159	U2099	G1983	G1883	A1773	A1507	G1413	G1303	G1187	G1187	A
G2442	C2349	G2260	G2160	G2100	G1997	G1883	A1773	A1507	G1414	G1303	G1187	G1187	A
G2443	C2350	G2261	G2161	G2101	A2001	A1889	U1778	A1508	U1415	G1310	U1188	U1188	G
G2444	A2351	G2262	G2162	U2102	G2002	A1890	U1779	C1509	G1416	G1311	A1189	A1189	C
G2445	C2355	C2163	C2163	C2103	C2002	A1890	U1780	A1509A	C1417	G1311	A1189	A1189	U
G2446	G2358	C2164	C2164	C2104	G2010	G1999	G1781	A1509B	G1418	C1314	G1191	G1191	C
G2447	A2274	G2165	C2165	C2105	G2011	A1900	C1782	G1510	A1419	C1314	G1191	G1191	A
A2448	G2275	G2166	G2166	G2106	U2011	A1901	C1783	G1510	U1420	U1316	C1200	C1200	C
U2449	G2276	U2167	C2167	C2107	G2012	C1902	A1784	U1514	G1421	A1317	C1201	C1201	U
A2450	G2277	C2168	C2168	C2108	A2013	G1906	A1785	G1515	G1426	C1318	C1202	C1202	G
U2457	G2364	A2169	A2169	U2109	A2014	G1907	A1786	G1529	A1427	G1319	A1204	A1204	U
U2462	G2365	A2170	A2170	C2110	A2015	G1907	A1786	G1529	A1427	C1320	U1205	U1205	C
U2462	A2366	A2171	A2171	C2111	A2015	C1908	A1786	G1529	A1427	G1324	A1210	A1210	A
C2465	A2369	U2172	U2172	G2112	A2019	U1911	A1791	C1643	G1428	G1324	U1211	U1211	A
C2465	G2370	A2173	A2173	U2113	A2020	U1911	A1791	C1643	G1428	G1324	U1211	U1211	A
G2468	G2371	C2174	C2174	A2114	C2021	U1914	U1794	A1652	C1531	G1339	G1114	G1114	U
A2469	G2372	A2175	A2175	G2115	U2022	C1914	U1796	A1653	C1532	A1342	A1220	A1220	A
U2476	A2376	C2176	C2176	G2116	G2023	U1915	C1797	A1654	G1435	A1342	A1220	A1220	A
A2476	A2377	C2177	C2177	A2117	G2027	A1916	U1798	G1667	G1537	G1346	C1221A	C1221A	G
C2477	A2378	C2178	C2178	U2118	G2027	U1917	U1798	G1667	G1538	G1346	C1222	C1222	G
U2477	G2379	U2180	U2180	A2119	A2030	C1920	U1799	G1667	G1539	U1362	G1223	G1223	U
C2480	G2380	G2181	G2181	G2120	A2031	C1920	U1799	G1667	G1539	U1362	G1223	G1223	U
C2480	G2381	G2182	G2182	G2121	A2031	C1920	U1799	G1667	G1539	U1362	G1223	G1223	U
C2483	G2382	G2183	G2183	U2122	G2032	G1929	U1799	G1667	G1539	U1362	G1223	G1223	U
G2484	G2383	G2184	G2184	G2123	A2033	G1930	U1799	G1667	G1539	U1362	G1223	G1223	U
G2484	G2384	G2185	G2185	G2124	A2033	U1931	U1799	G1667	G1539	U1362	G1223	G1223	U
G2486	G2385	C2186	C2186	G2125	C2040	A1932	U1799	G1667	G1539	U1362	G1223	G1223	U
G2486	G2385	A2187	A2187	A2126	U2041	G1933	U1799	G1667	G1539	U1362	G1223	G1223	U
G2486	G2385	G2187	G2187	G2127	A2042	G1933	U1799	G1667	G1539	U1362	G1223	G1223	U



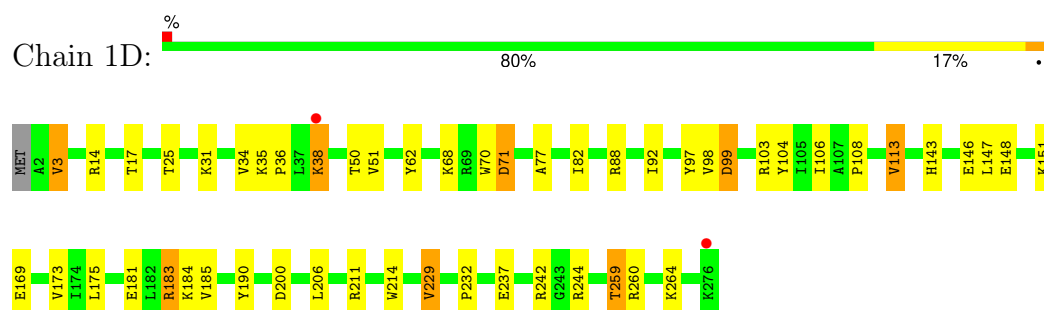
• Molecule 2: 5S Ribosomal RNA



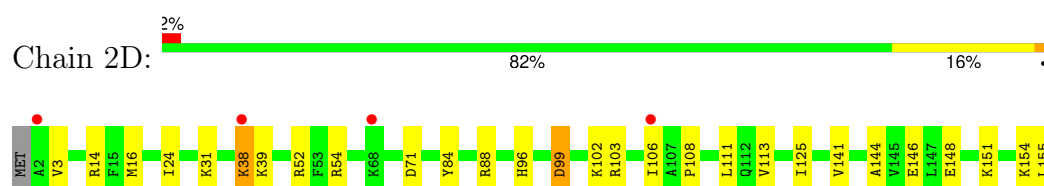
• Molecule 2: 5S Ribosomal RNA



• Molecule 3: 50S ribosomal protein L2

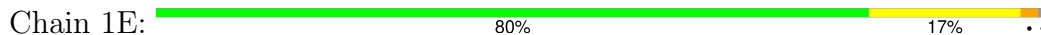


• Molecule 3: 50S ribosomal protein L2

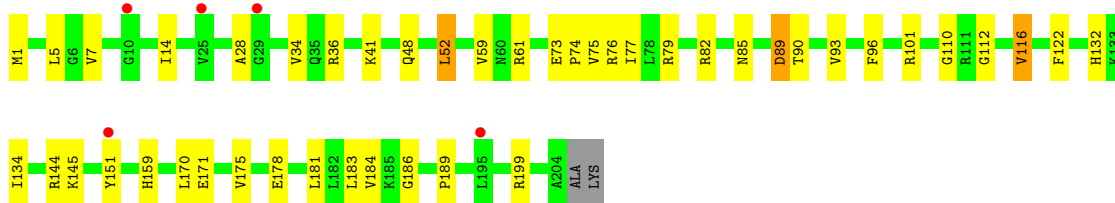
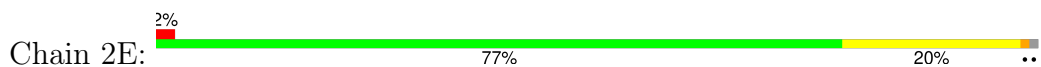




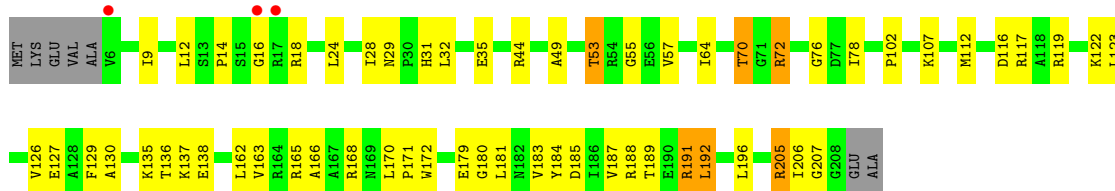
• Molecule 4: 50S ribosomal protein L3



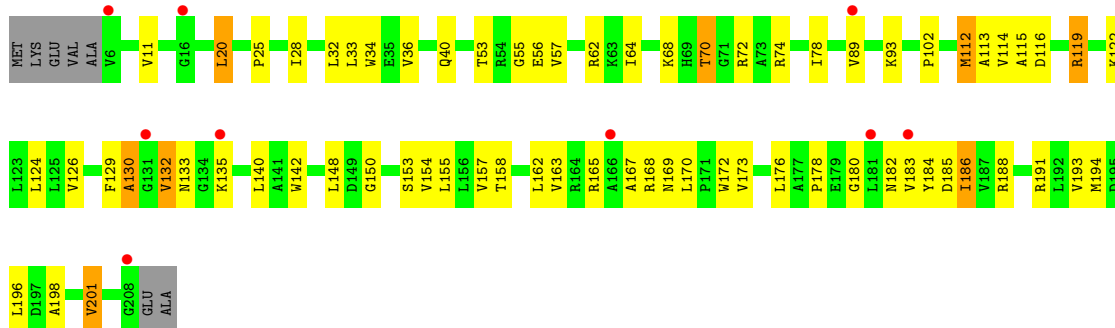
• Molecule 4: 50S ribosomal protein L3



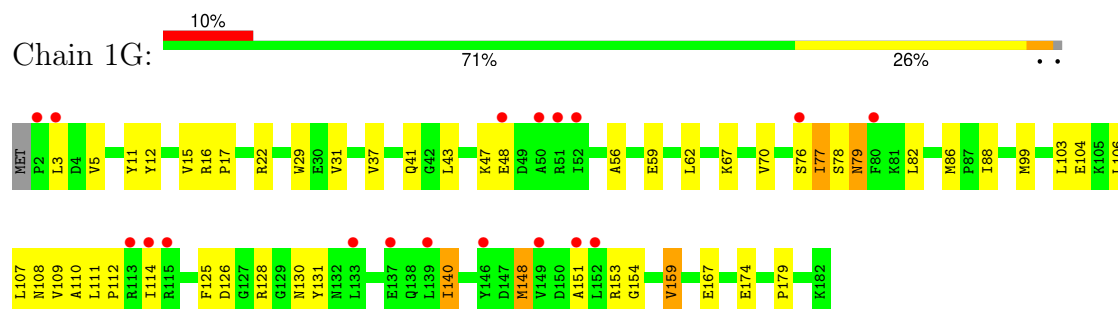
• Molecule 5: 50S ribosomal protein L4



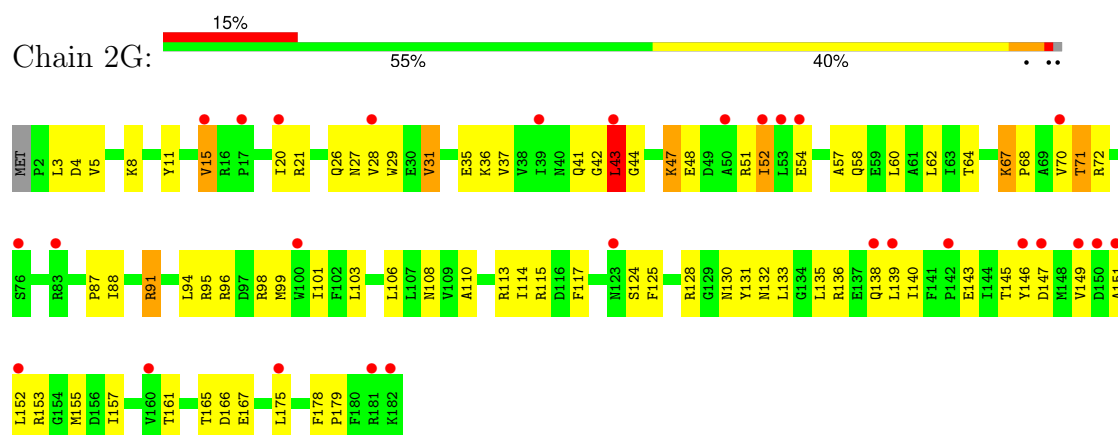
• Molecule 5: 50S ribosomal protein L4



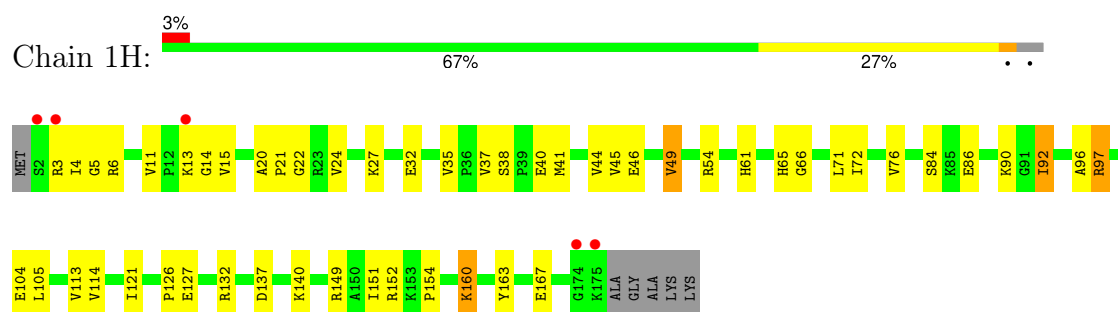
- Molecule 6: 50S ribosomal protein L5



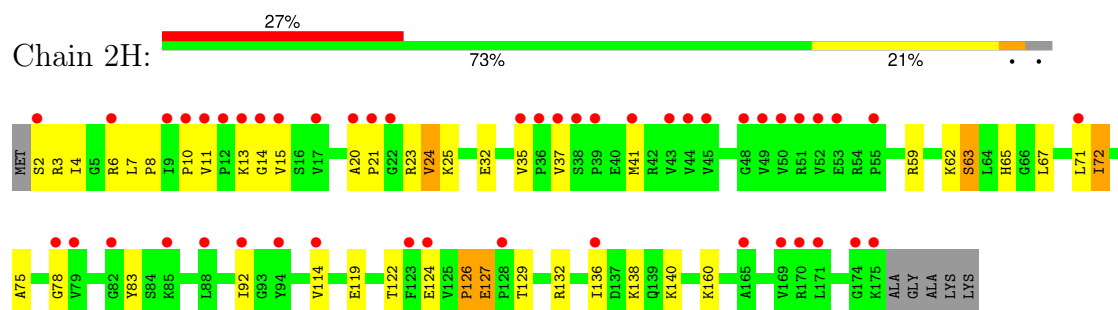
- Molecule 6: 50S ribosomal protein L5



- Molecule 7: 50S ribosomal protein L6

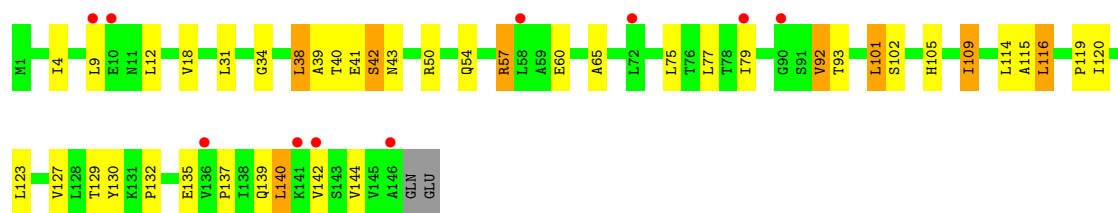


- Molecule 7: 50S ribosomal protein L6

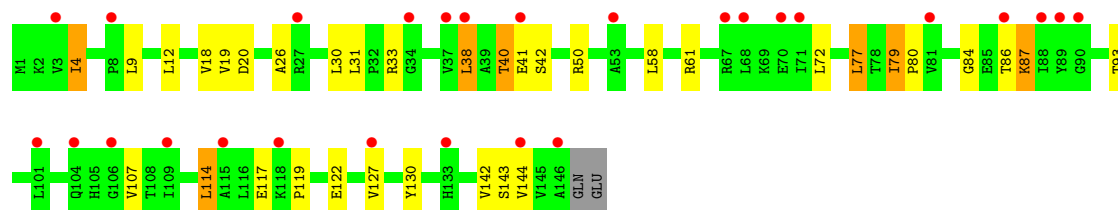
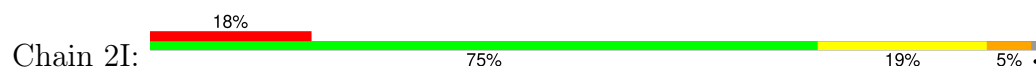


- Molecule 8: 50S ribosomal protein L9

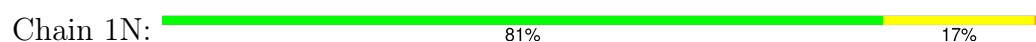




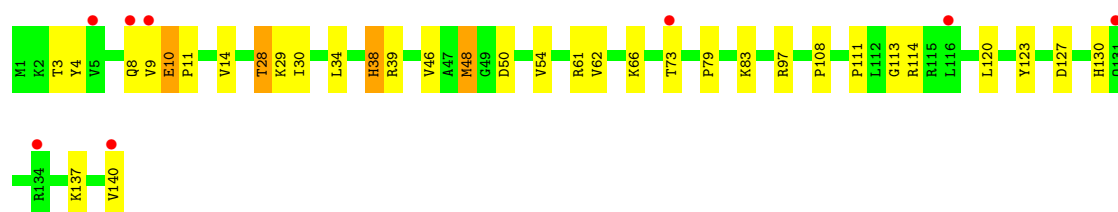
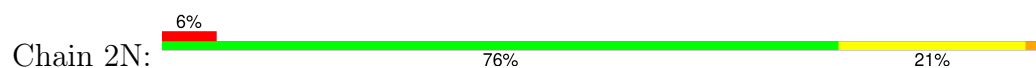
• Molecule 8: 50S ribosomal protein L9



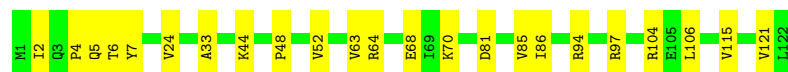
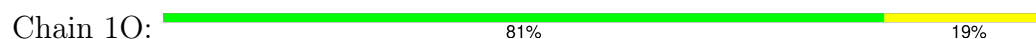
• Molecule 9: 50S ribosomal protein L13



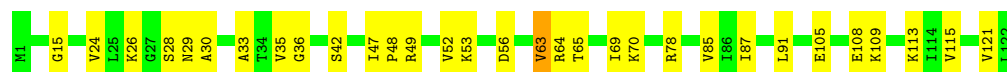
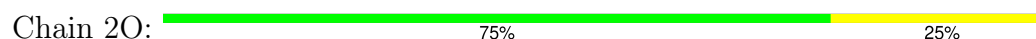
• Molecule 9: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L14



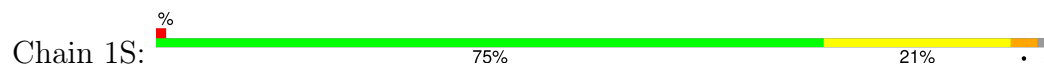
• Molecule 10: 50S ribosomal protein L14



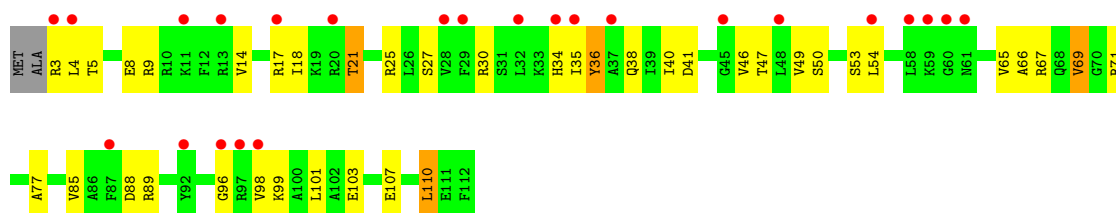
- Chain 2R: 75% 25%



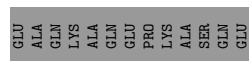
- Molecule 14: 50S ribosomal protein L18



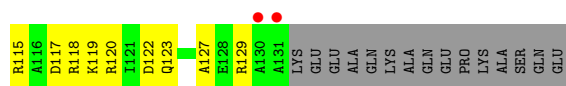
- Molecule 14: 50S ribosomal protein L18



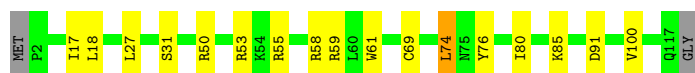
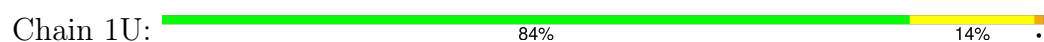
- Molecule 15: 50S ribosomal protein L19



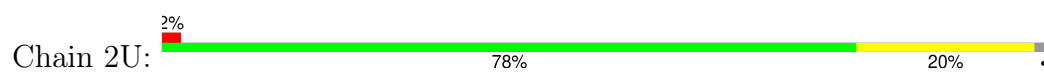
- Molecule 15: 50S ribosomal protein L19



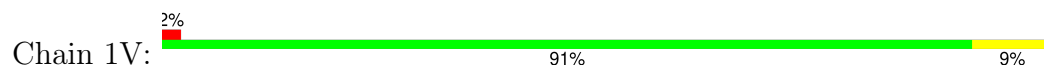
- Molecule 16: 50S ribosomal protein L20



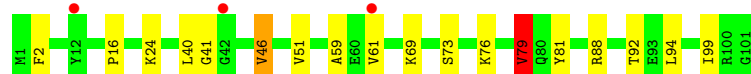
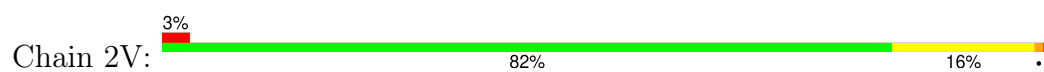
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



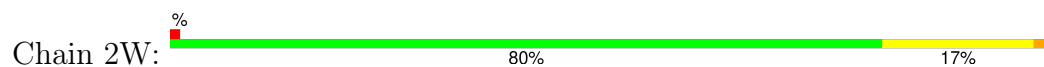
- Molecule 17: 50S ribosomal protein L21



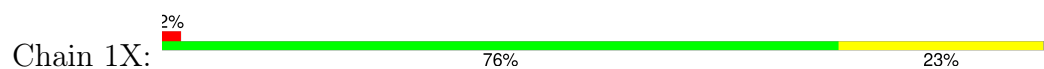
- Molecule 18: 50S ribosomal protein L22



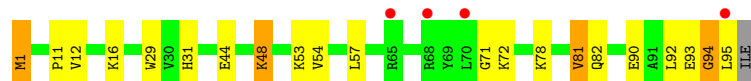
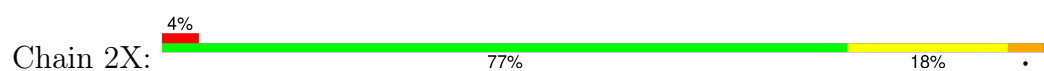
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



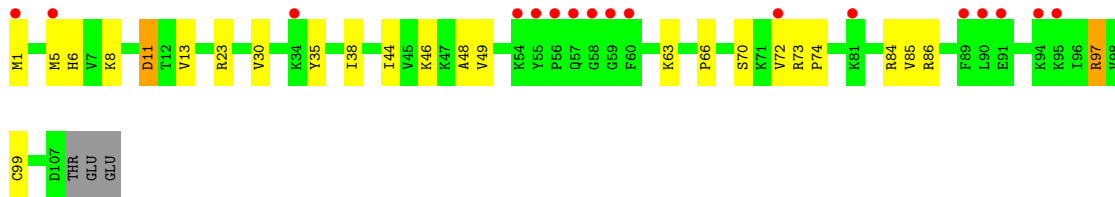
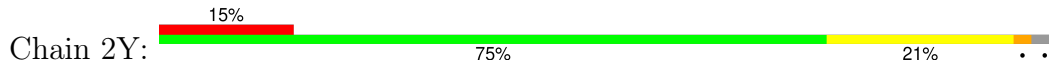
- Molecule 19: 50S ribosomal protein L23



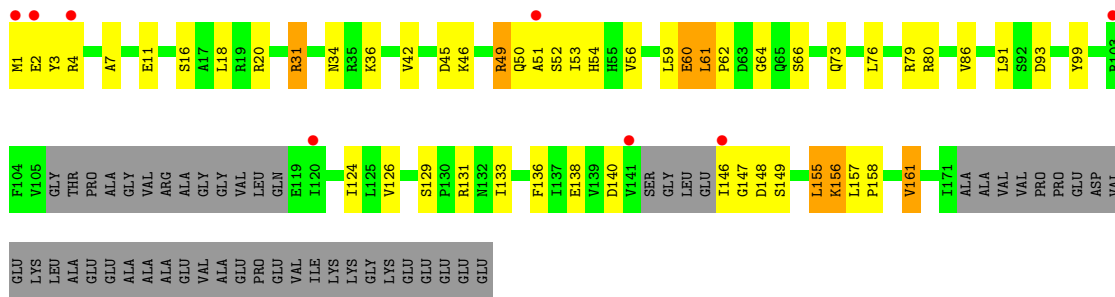
- Molecule 20: 50S ribosomal protein L24



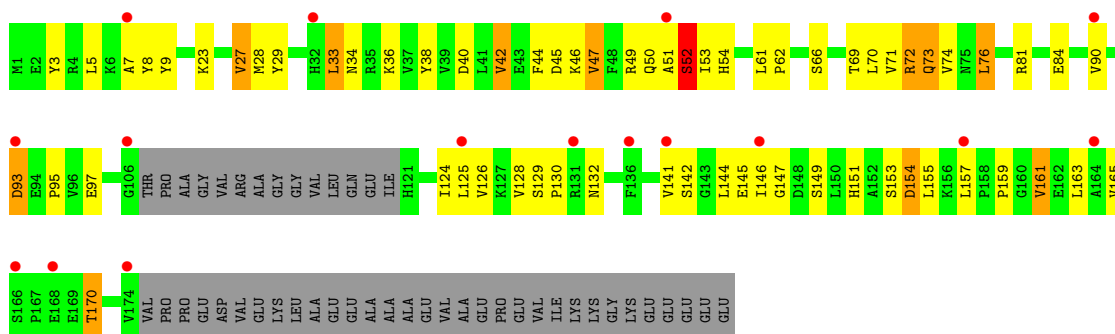
- Molecule 20: 50S ribosomal protein L24



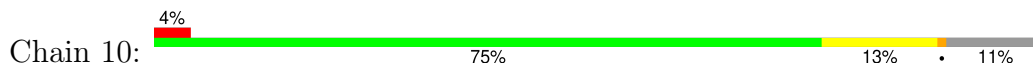
- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25

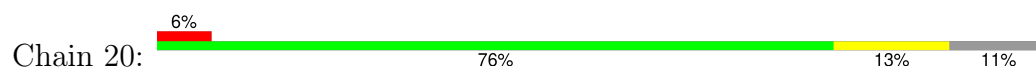


- Molecule 22: 50S ribosomal protein L27





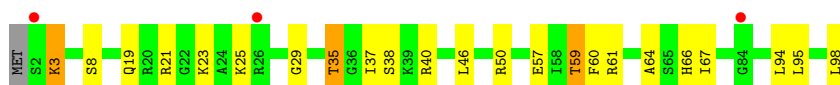
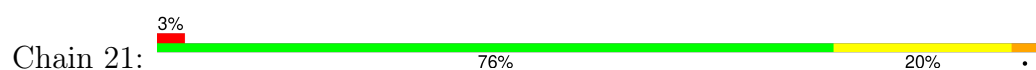
- Molecule 22: 50S ribosomal protein L27



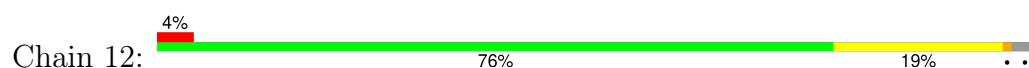
- Molecule 23: 50S ribosomal protein L28



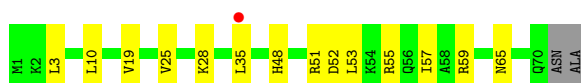
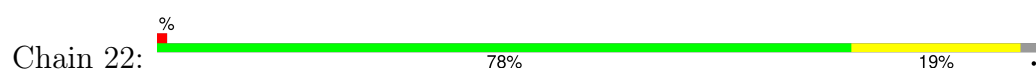
- Molecule 23: 50S ribosomal protein L28



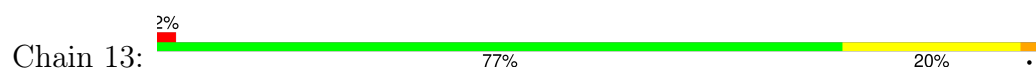
- Molecule 24: 50S ribosomal protein L29



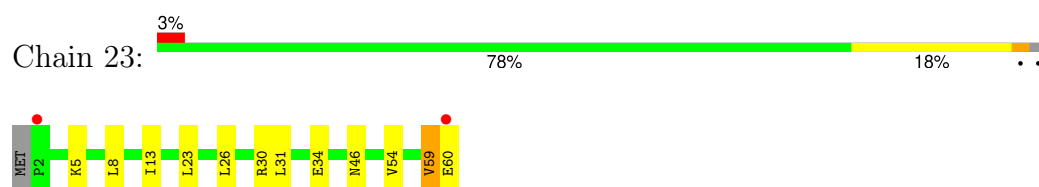
- Molecule 24: 50S ribosomal protein L29



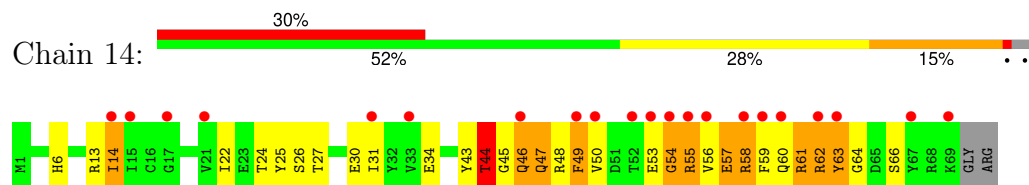
- Molecule 25: 50S ribosomal protein L30



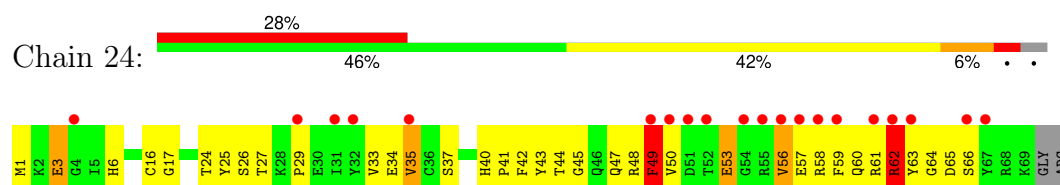
- Molecule 25: 50S ribosomal protein L30



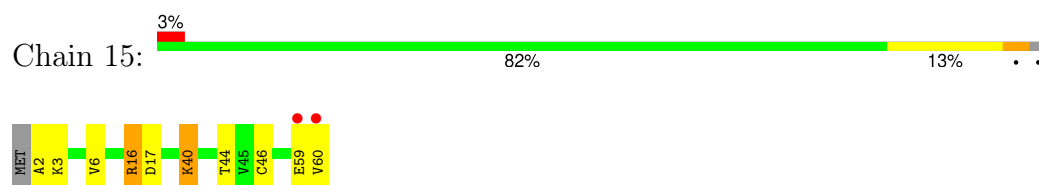
- Molecule 26: 50S ribosomal protein L31



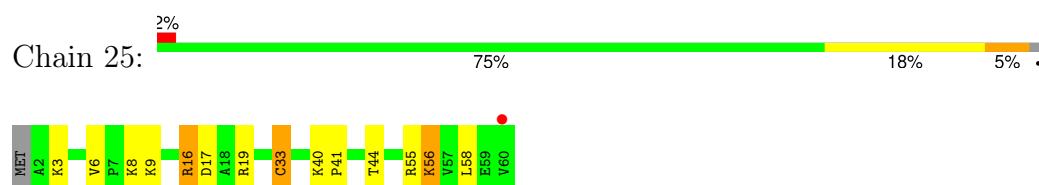
- Molecule 26: 50S ribosomal protein L31



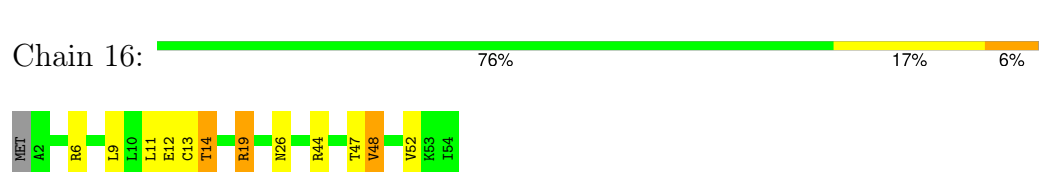
- Molecule 27: 50S ribosomal protein L32



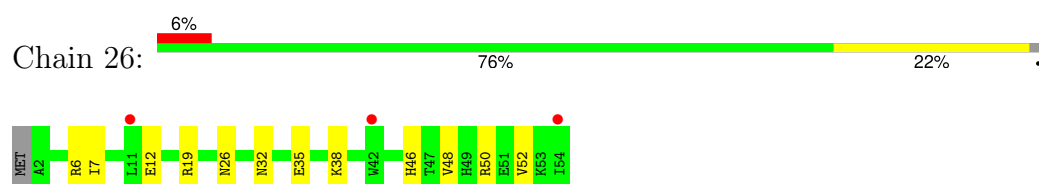
- Molecule 27: 50S ribosomal protein L32



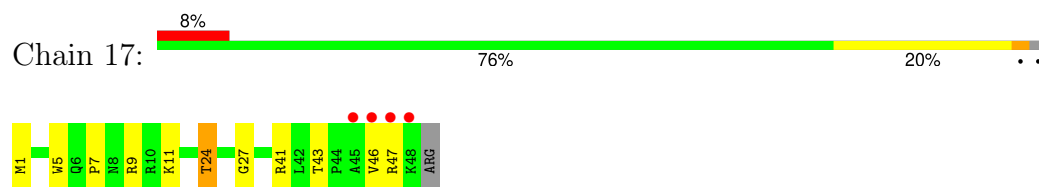
- Molecule 28: 50S ribosomal protein L33



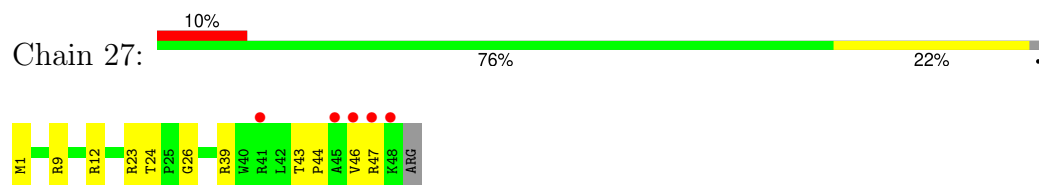
- Molecule 28: 50S ribosomal protein L33



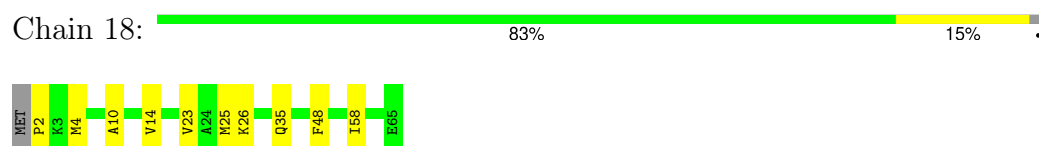
- Molecule 29: 50S ribosomal protein L34



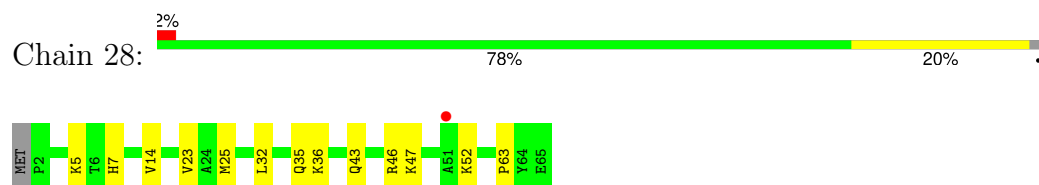
- Molecule 29: 50S ribosomal protein L34



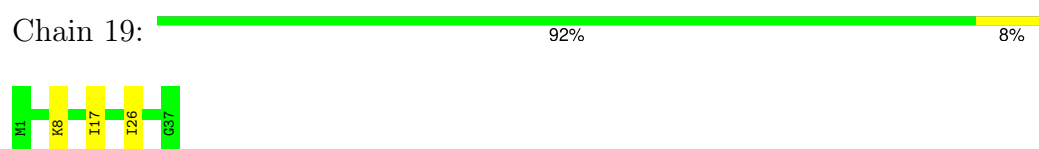
- Molecule 30: 50S ribosomal protein L35



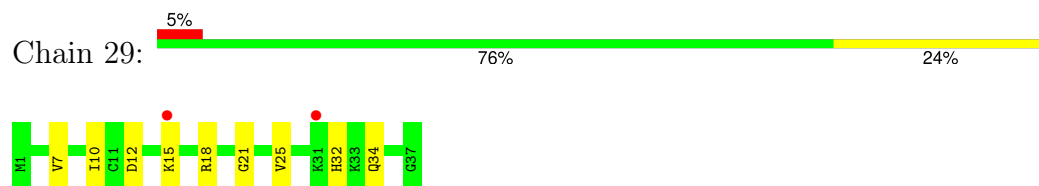
- Molecule 30: 50S ribosomal protein L35



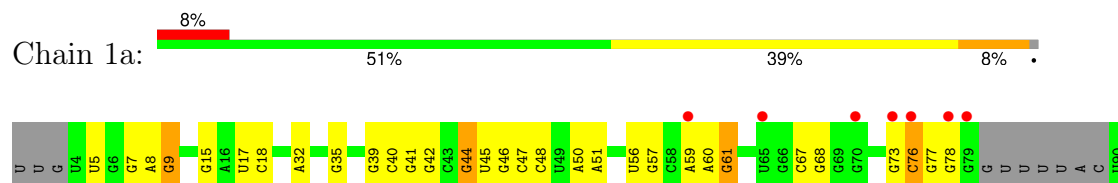
- Molecule 31: 50S ribosomal protein L36



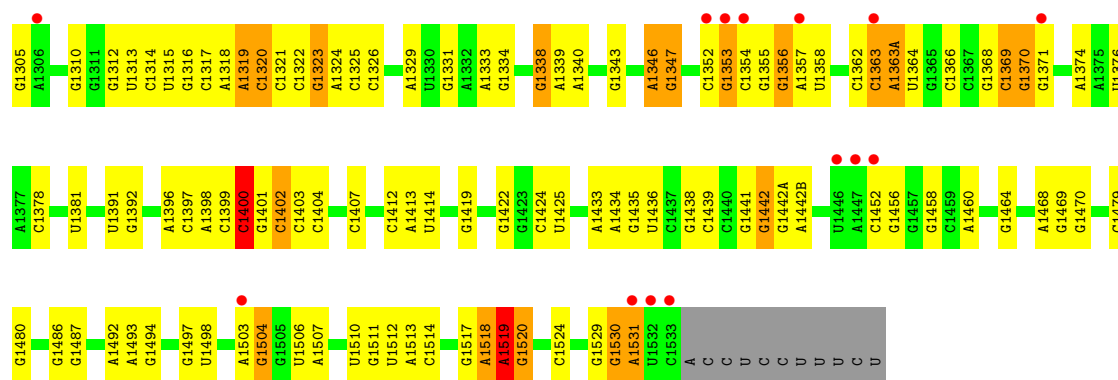
- Molecule 31: 50S ribosomal protein L36



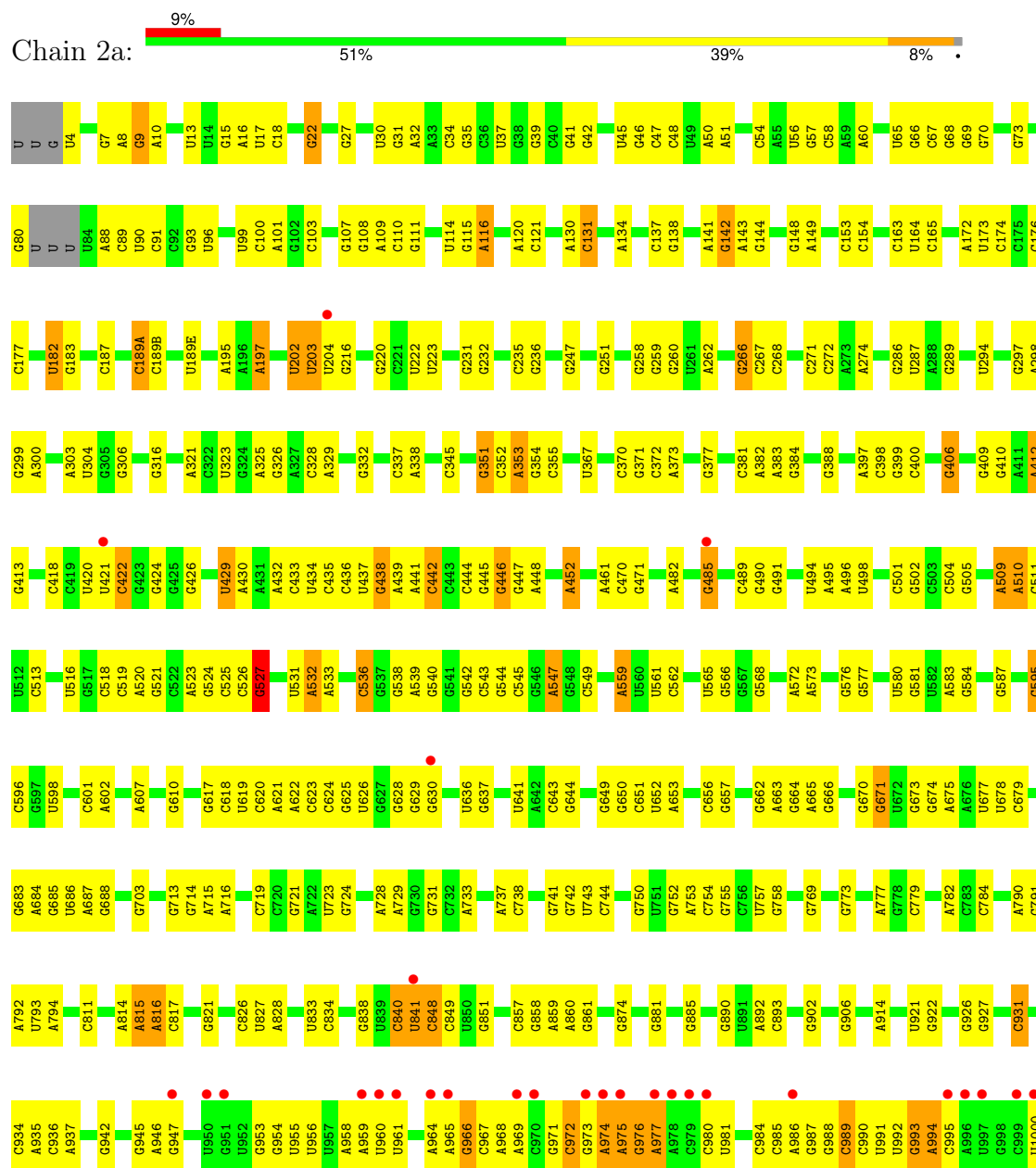
- Molecule 32: 16S Ribosomal RNA

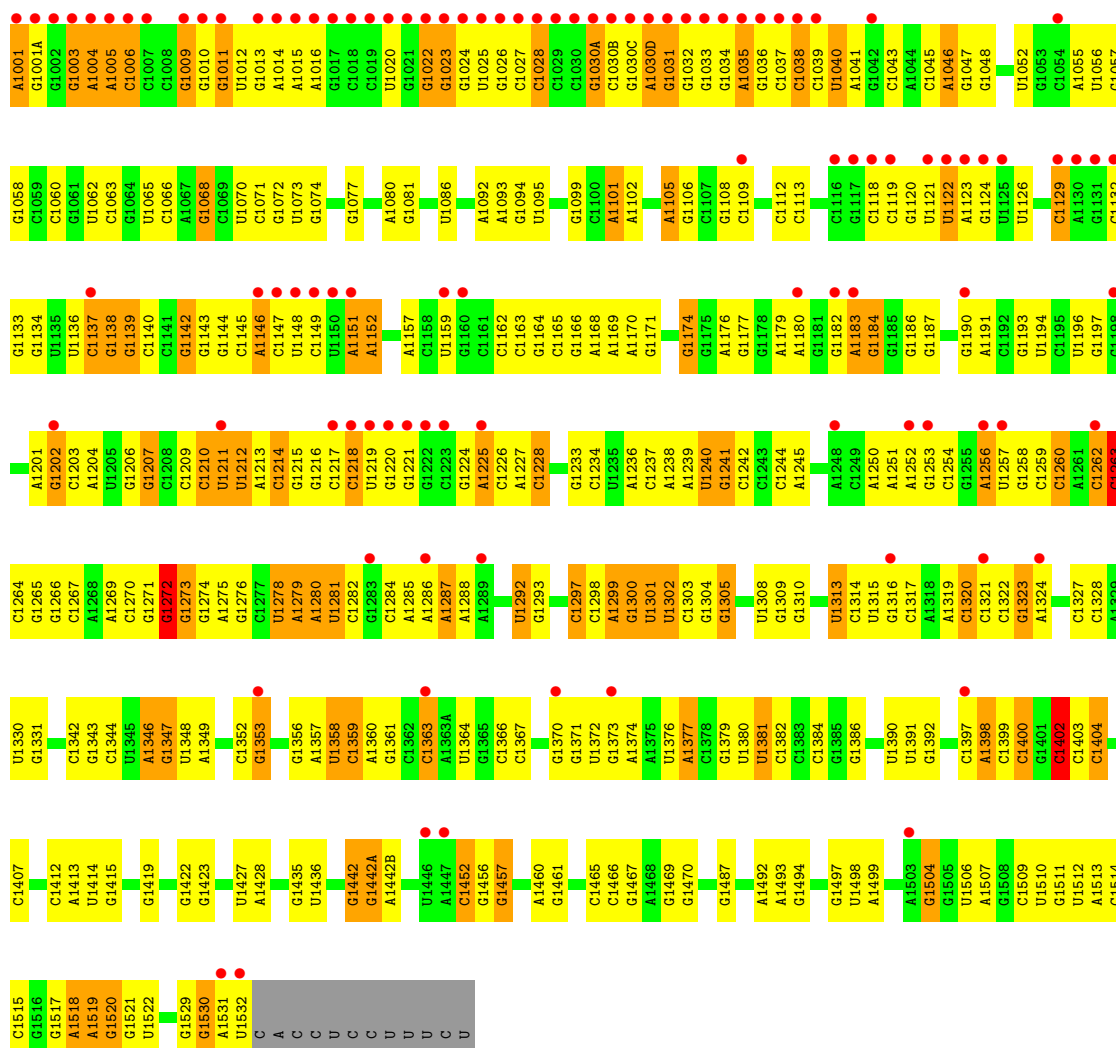




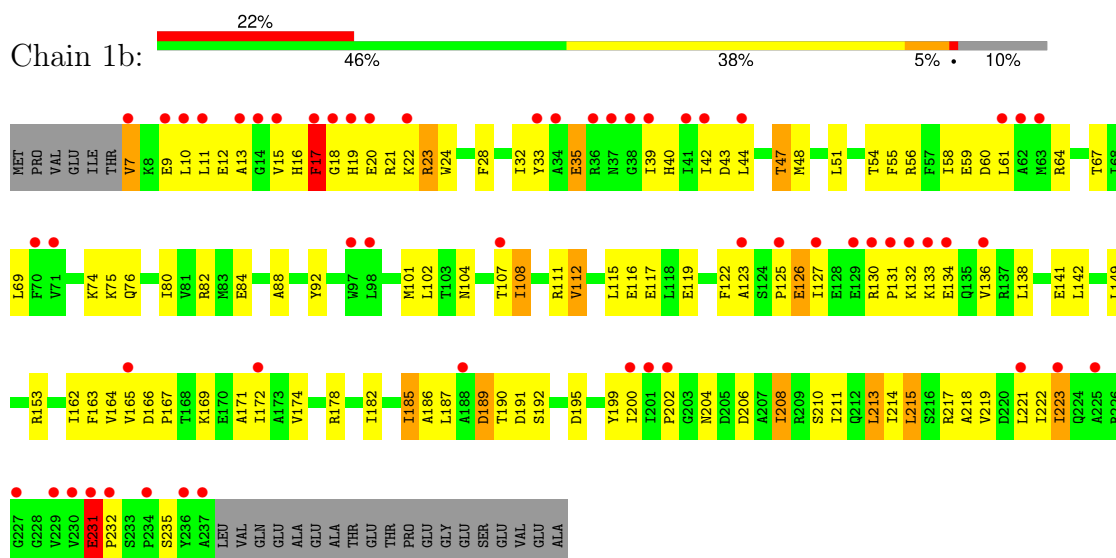


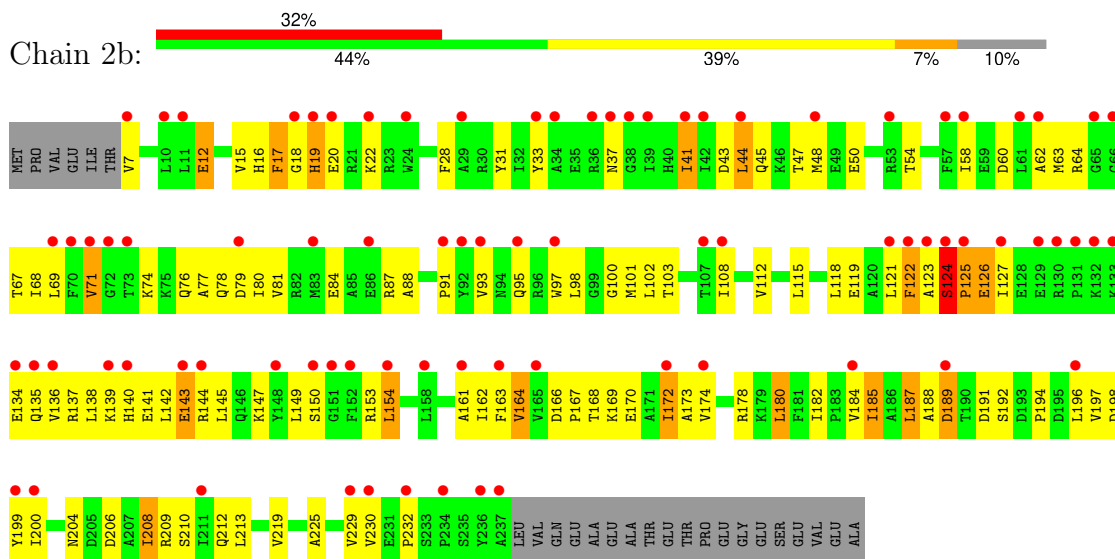
• Molecule 32: 16S Ribosomal RNA



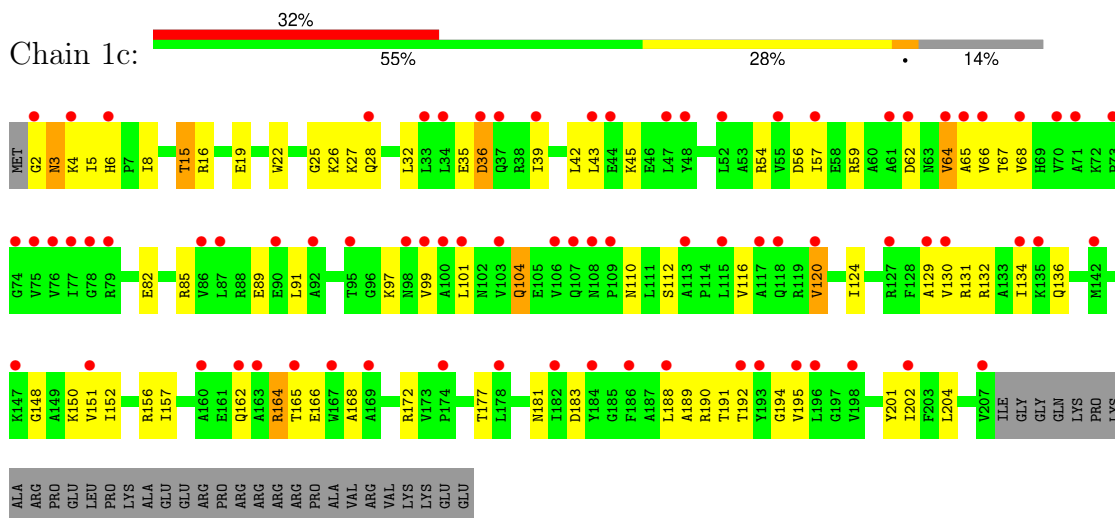


• Molecule 33: 30S ribosomal protein S2

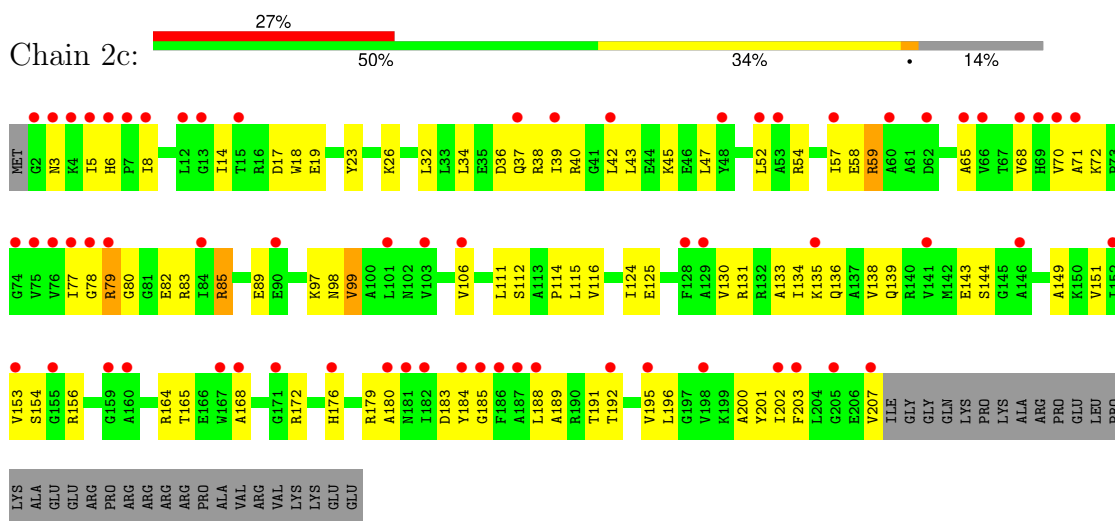




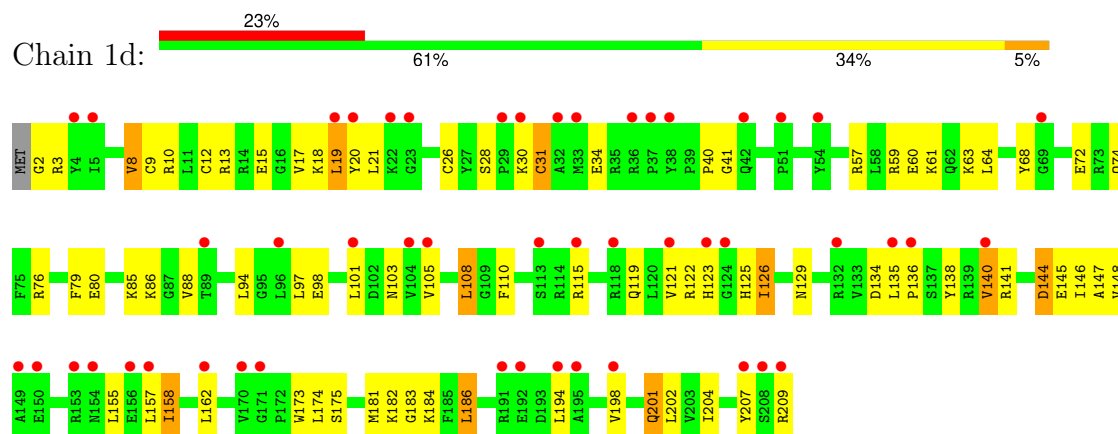
- Molecule 34: 30S ribosomal protein S3



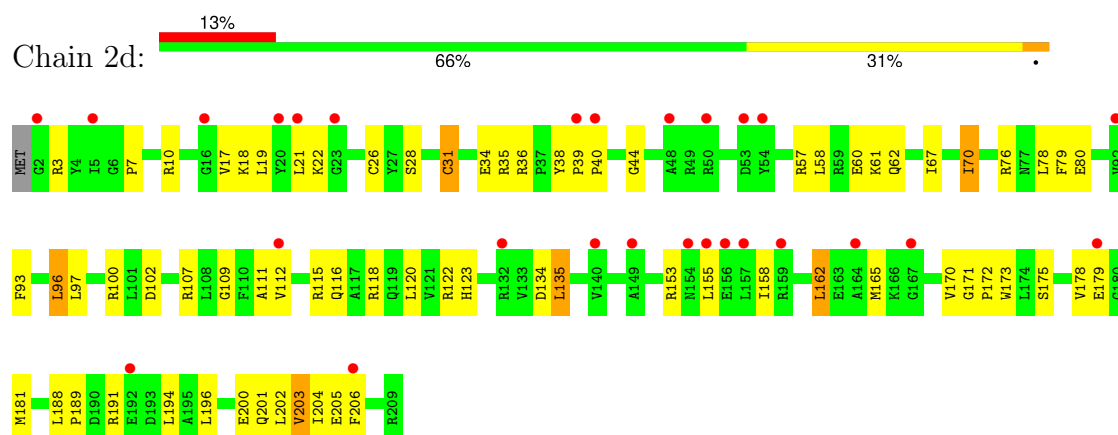
- Molecule 34: 30S ribosomal protein S3



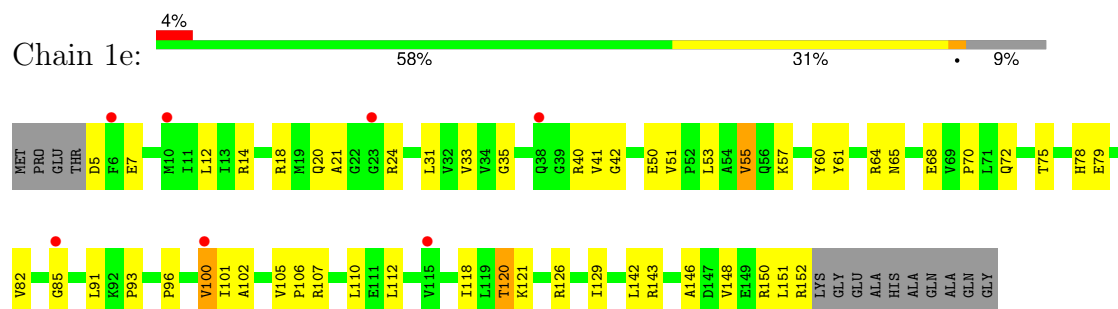
- Molecule 35: 30S ribosomal protein S4



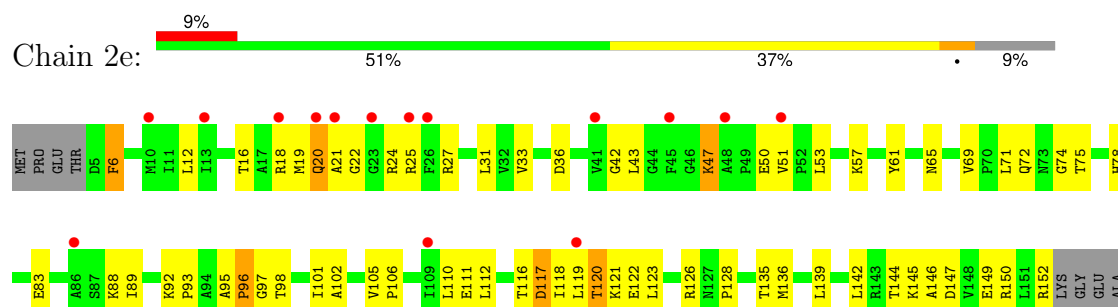
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5




- Molecule 36: 30S ribosomal protein S5



HIS
ALA
GLN
ALA
GLN
GLY

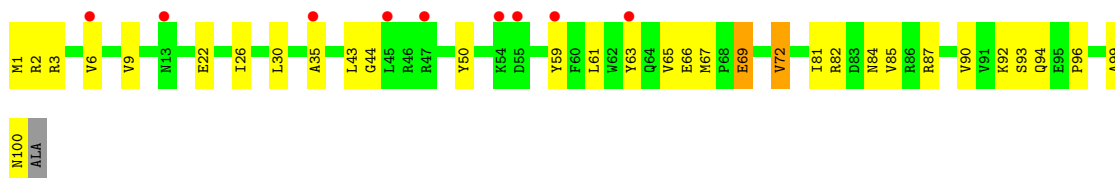
• Molecule 37: 30S ribosomal protein S6

Chain 1f:  7% 79% 19% ..



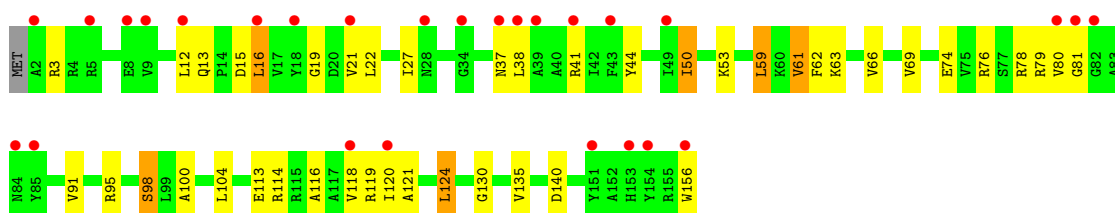
• Molecule 37: 30S ribosomal protein S6

Chain 2f:  9% 67% 30% ..



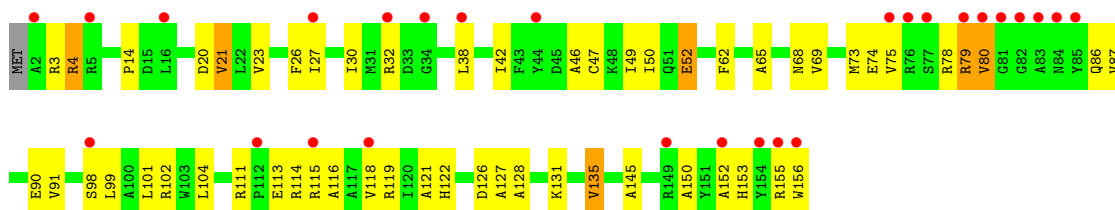
• Molecule 38: 30S ribosomal protein S7

Chain 1g:  17% 71% 24% ..




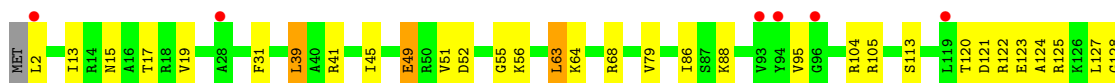
• Molecule 38: 30S ribosomal protein S7

Chain 2g:  17% 63% 32% ..



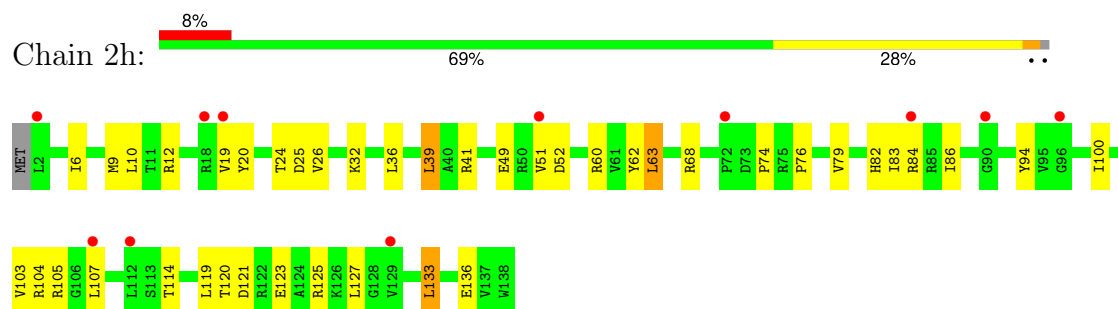
• Molecule 39: 30S ribosomal protein S8

Chain 1h:  4% 74% 22% ..

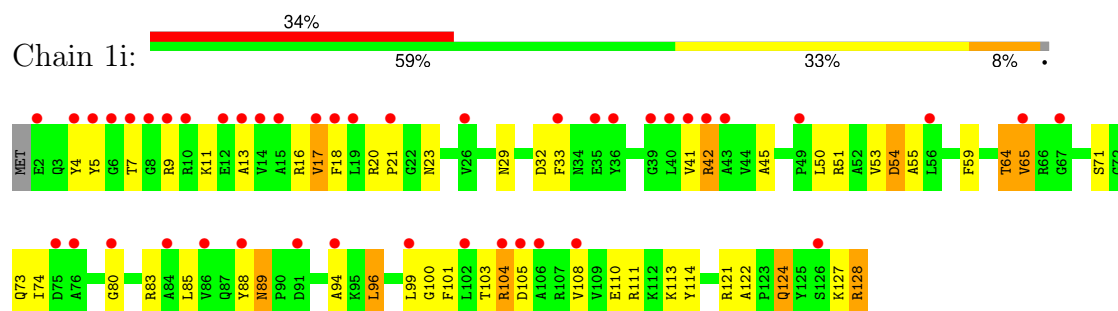




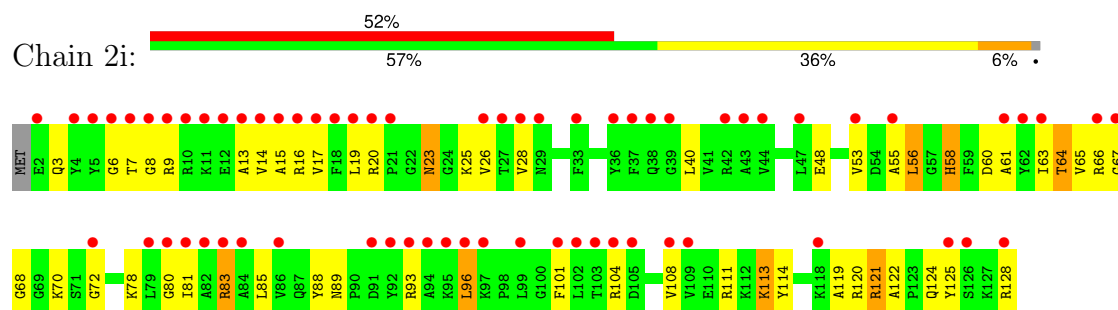
- Molecule 39: 30S ribosomal protein S8



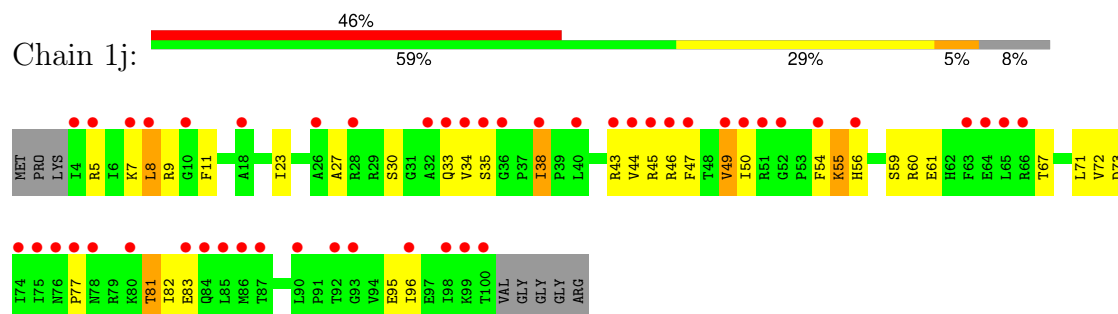
- Molecule 40: 30S ribosomal protein S9



- Molecule 40: 30S ribosomal protein S9

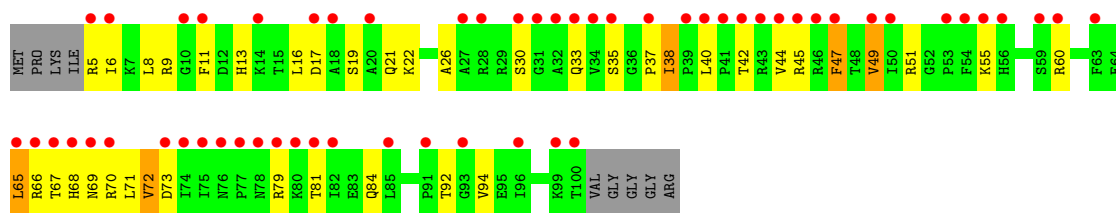


- Molecule 41: 30S ribosomal protein S10

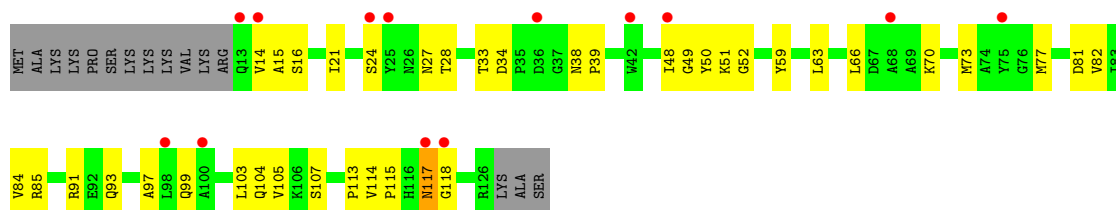


- Molecule 41: 30S ribosomal protein S10

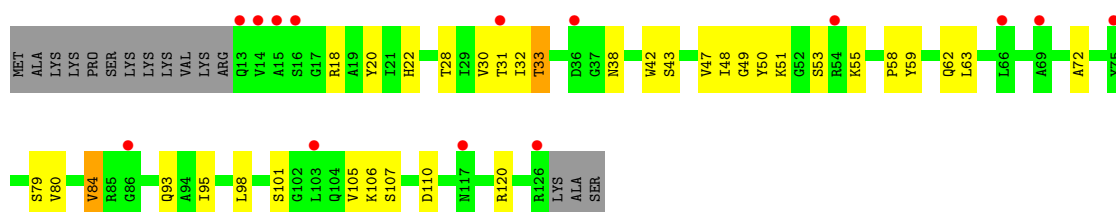




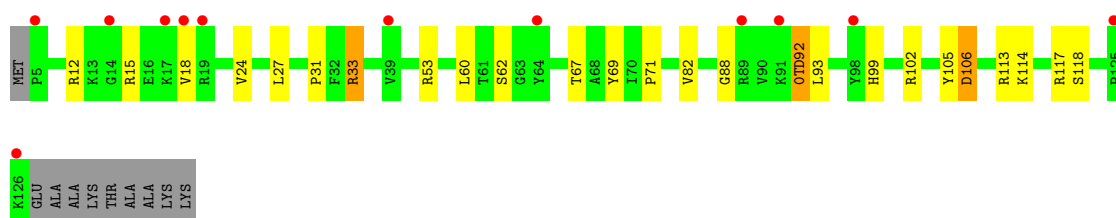
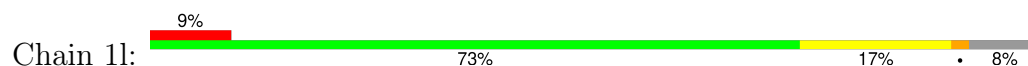
• Molecule 42: 30S ribosomal protein S11



• Molecule 42: 30S ribosomal protein S11



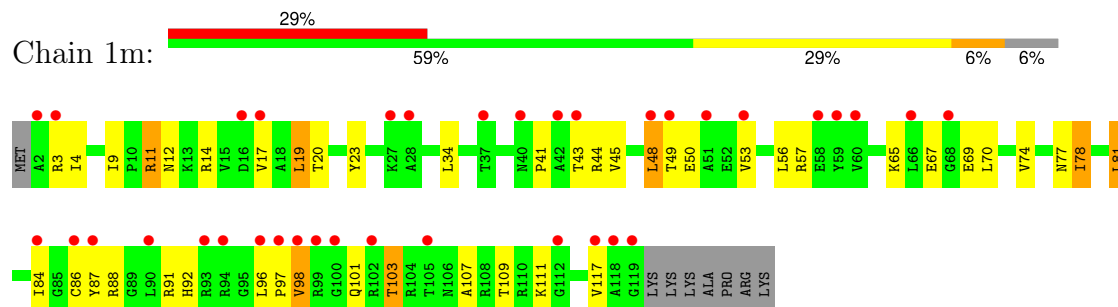
• Molecule 43: 30S ribosomal protein S12



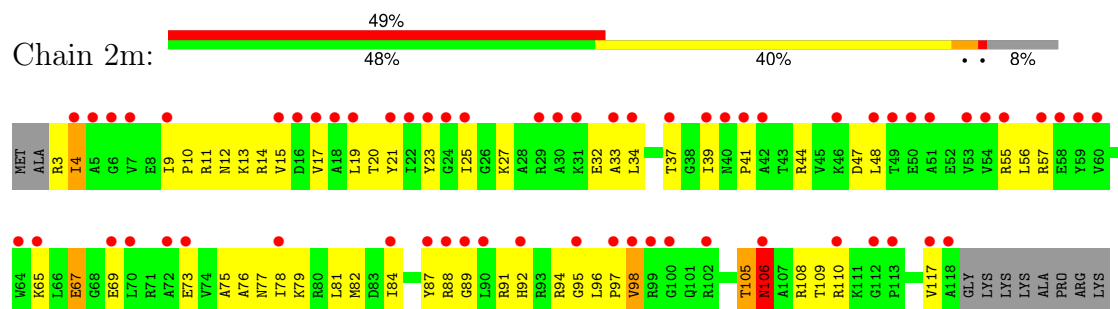
• Molecule 43: 30S ribosomal protein S12



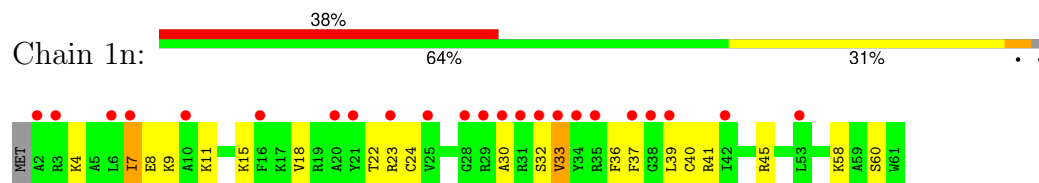
- Molecule 44: 30S ribosomal protein S13



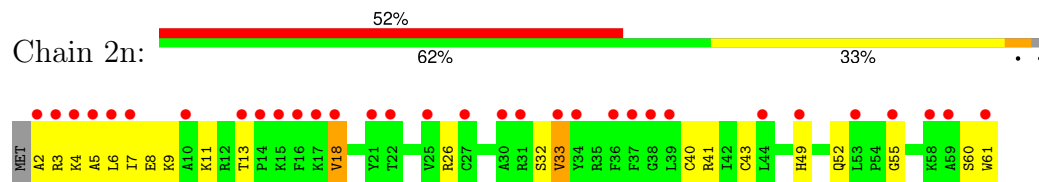
- Molecule 44: 30S ribosomal protein S13



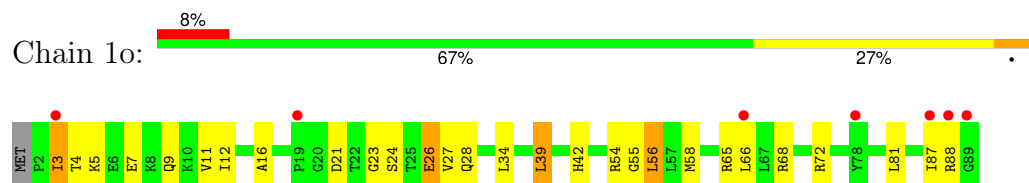
- Molecule 45: 30S ribosomal protein S14 type Z



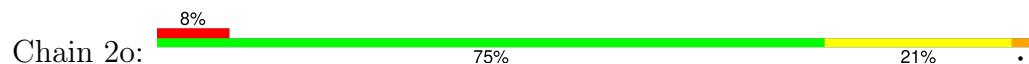
- Molecule 45: 30S ribosomal protein S14 type Z

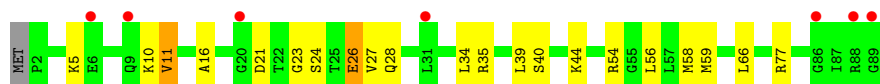


- Molecule 46: 30S ribosomal protein S15

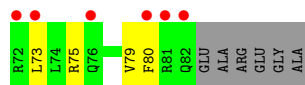


- Molecule 46: 30S ribosomal protein S15

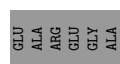
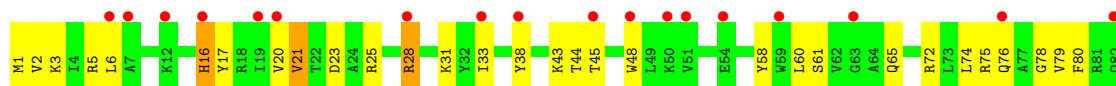




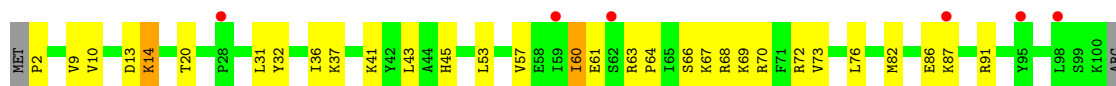
- Molecule 47: 30S ribosomal protein S16



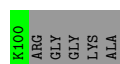
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17

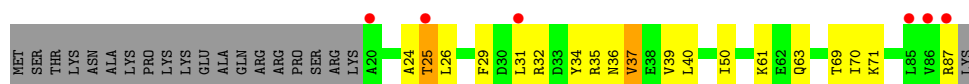


- Molecule 48: 30S ribosomal protein S17

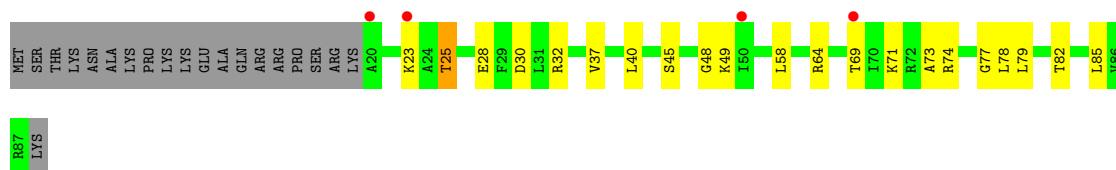


- Molecule 49: 30S ribosomal protein S18

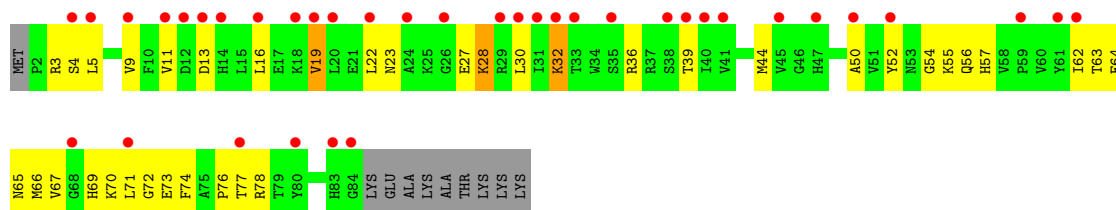
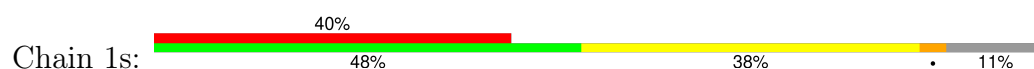




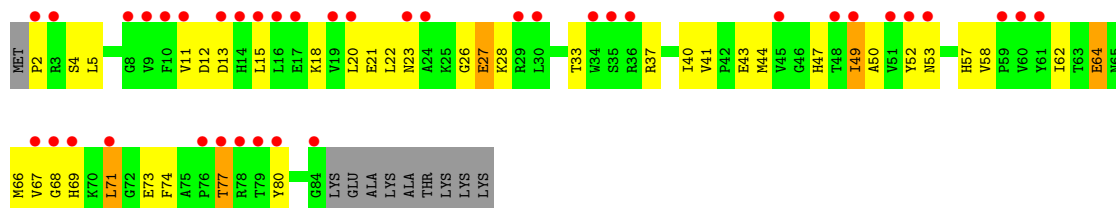
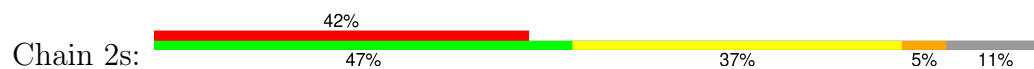
- Molecule 49: 30S ribosomal protein S18



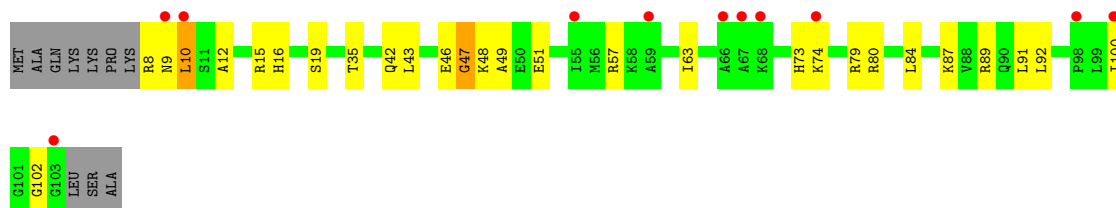
- Molecule 50: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S19

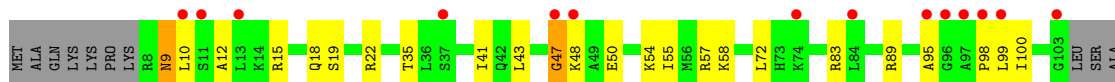


- Molecule 51: 30S ribosomal protein S20

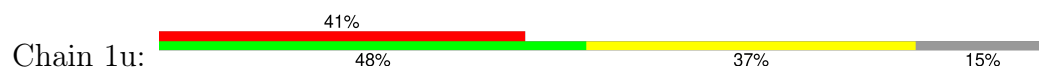


- Molecule 51: 30S ribosomal protein S20

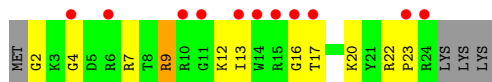
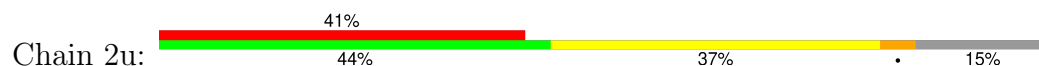




- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



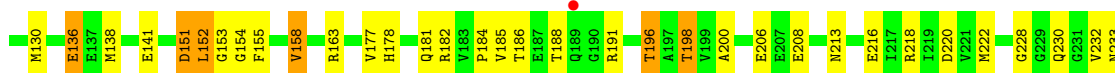
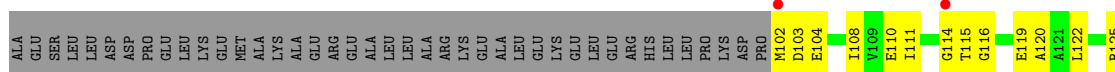
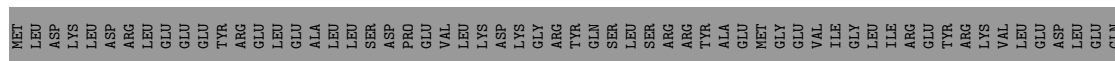
- Molecule 53: CYS-Stop mRNA



- Molecule 53: CYS-Stop mRNA



- Molecule 54: Peptide chain release factor 1



FMG		
GLU		
ALA		
A4		
A5		
K6		
C7		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.40Å 447.21Å 624.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.08 – 2.40 107.08 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.3 (107.08-2.40) 94.3 (107.08-2.40)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.223 , 0.263 0.224 , 0.265	Depositor DCC
R_{free} test set	112284 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	297056	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% 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, 5MC, M2G, H2U, K, MEQ, SF4, UR3, 8AN, 5MU, 4OC, G7M, PSU, 4SU, ZN, 2MG, MIA, OMG, 2MA, MG, MA6, 0TD, OMU

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	0.30	0/69011	0.48	3/107720 (0.0%)
1	2A	0.22	1/67295 (0.0%)	0.41	1/105042 (0.0%)
2	1B	0.21	0/2882	0.40	0/4494
2	2B	0.18	0/2879	0.35	0/4487
3	1D	0.27	0/2186	0.52	1/2944 (0.0%)
3	2D	0.24	0/2186	0.46	0/2944
4	1E	0.28	0/1592	0.53	0/2149
4	2E	0.21	0/1592	0.45	0/2149
5	1F	0.27	0/1619	0.51	0/2193
5	2F	0.20	0/1615	0.41	0/2188
6	1G	0.20	0/1448	0.43	0/1957
6	2G	0.19	0/1453	0.42	0/1963
7	1H	0.21	0/1356	0.45	2/1834 (0.1%)
7	2H	0.18	0/1356	0.37	0/1834
8	1I	0.18	0/1112	0.41	0/1514
8	2I	0.19	0/1079	0.41	0/1475
9	1N	0.25	0/1144	0.45	0/1543
9	2N	0.19	0/1144	0.41	0/1543
10	1O	0.25	0/943	0.47	0/1269
10	2O	0.20	0/943	0.43	0/1269
11	1P	0.27	0/1152	0.53	0/1533
11	2P	0.21	0/1152	0.45	0/1533
12	1Q	0.29	0/1143	0.52	0/1527
12	2Q	0.20	0/1143	0.44	0/1527
13	1R	0.28	0/982	0.52	0/1312
13	2R	0.22	0/982	0.46	0/1312
14	1S	0.23	0/883	0.47	0/1176
14	2S	0.21	0/880	0.45	0/1172
15	1T	0.26	0/1105	0.46	0/1477
15	2T	0.21	0/1097	0.45	0/1468
16	1U	0.30	0/977	0.49	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.39	0/1301
17	1V	0.27	0/782	0.48	0/1049
17	2V	0.18	0/782	0.38	0/1049
18	1W	0.28	0/897	0.45	0/1205
18	2W	0.21	0/897	0.41	0/1205
19	1X	0.27	0/764	0.54	0/1025
19	2X	0.20	0/764	0.49	2/1025 (0.2%)
20	1Y	0.23	0/819	0.47	0/1095
20	2Y	0.19	0/819	0.41	0/1095
21	1Z	0.22	0/1267	0.50	0/1717
21	2Z	0.21	0/1299	0.46	0/1763
22	10	0.27	0/612	0.50	0/816
22	20	0.20	0/612	0.44	0/816
23	11	0.26	0/762	0.44	0/1014
23	21	0.21	0/762	0.40	0/1014
24	12	0.23	0/590	0.44	0/781
24	22	0.19	0/590	0.37	0/781
25	13	0.27	0/474	0.52	0/635
25	23	0.20	0/469	0.48	0/630
26	14	0.24	0/565	0.62	2/761 (0.3%)
26	24	0.24	0/545	0.56	0/737
27	15	0.28	0/469	0.54	0/635
27	25	0.24	0/469	0.53	0/635
28	16	0.27	0/460	0.52	0/613
28	26	0.18	0/456	0.42	0/608
29	17	0.33	0/426	0.53	0/561
29	27	0.23	0/426	0.48	0/561
30	18	0.26	0/525	0.50	0/691
30	28	0.20	0/525	0.40	0/691
31	19	0.29	0/310	0.48	0/407
31	29	0.19	0/310	0.43	0/407
32	1a	0.20	0/35795	0.39	0/55864
32	2a	0.20	0/35886	0.38	5/56005 (0.0%)
33	1b	0.23	0/1881	0.53	0/2542
33	2b	0.23	0/1860	0.46	0/2518
34	1c	0.21	0/1572	0.44	0/2126
34	2c	0.19	0/1566	0.42	0/2119
35	1d	0.19	0/1685	0.43	0/2262
35	2d	0.18	0/1704	0.41	0/2284
36	1e	0.20	0/1145	0.46	0/1543
36	2e	0.19	0/1149	0.44	0/1548
37	1f	0.20	0/823	0.41	0/1115
37	2f	0.19	0/829	0.39	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1250	0.47	0/1679
38	2g	0.18	0/1254	0.43	0/1683
39	1h	0.18	0/1108	0.41	0/1494
39	2h	0.20	0/1108	0.46	1/1494 (0.1%)
40	1i	0.20	0/1002	0.46	0/1346
40	2i	0.21	0/997	0.45	0/1343
41	1j	0.19	0/722	0.47	0/982
41	2j	0.25	0/727	0.48	0/988
42	1k	0.21	0/844	0.46	1/1145 (0.1%)
42	2k	0.19	0/848	0.40	0/1149
43	1l	0.21	0/937	0.45	0/1260
43	2l	0.19	0/937	0.42	0/1260
44	1m	0.20	0/929	0.49	0/1250
44	2m	0.21	0/917	0.44	0/1234
45	1n	0.17	0/501	0.46	0/664
45	2n	0.19	0/501	0.43	0/664
46	1o	0.20	0/739	0.39	0/985
46	2o	0.19	0/739	0.39	0/985
47	1p	0.19	0/697	0.42	0/939
47	2p	0.19	0/693	0.45	0/935
48	1q	0.19	0/836	0.41	0/1117
48	2q	0.18	0/836	0.40	0/1117
49	1r	0.18	0/560	0.38	0/746
49	2r	0.16	0/560	0.38	0/746
50	1s	0.21	0/667	0.50	0/900
50	2s	0.20	0/661	0.42	0/893
51	1t	0.19	0/730	0.48	0/965
51	2t	0.20	0/729	0.45	0/965
52	1u	0.21	0/203	0.44	0/266
52	2u	0.20	0/203	0.43	0/266
53	1v	0.22	0/213	0.46	0/329
53	2v	0.21	0/213	0.39	0/329
54	1w	0.21	0/1956	0.42	0/2634
54	2w	0.20	0/1974	0.44	0/2657
55	1x	0.22	1/1555 (0.1%)	0.36	0/2419
55	2x	0.21	0/1555	0.36	0/2419
56	1z	0.30	0/29	0.45	0/37
56	2z	0.28	0/24	0.48	0/30
All	All	0.24	2/313604 (0.0%)	0.43	18/468535 (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	1
33	1b	0	2
33	2b	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	8	4SU	O3'-P	5.13	1.61	1.56
1	2A	2552	OMU	O3'-P	5.05	1.61	1.56

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1992	G	C2'-C3'-O3'	7.85	121.28	109.50
32	2a	1272	G	N1-C2-N2	-7.14	94.78	116.20
32	2a	1263	C	N1-C2-O2	6.83	139.38	118.90
1	2A	1992	G	C2'-C3'-O3'	6.82	119.73	109.50
32	2a	1272	G	N3-C2-N2	6.49	139.38	119.90

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
21	1Z	136	PHE	Peptide
33	1b	122	PHE	Peptide
33	1b	9	GLU	Peptide
11	2P	35	HIS	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	31195	622	0
1	2A	60322	0	30427	647	0
2	1B	2577	0	1304	20	0
2	2B	2575	0	1303	25	0
3	1D	2136	0	2218	45	0
3	2D	2136	0	2218	38	0
4	1E	1559	0	1618	24	0
4	2E	1559	0	1618	26	0
5	1F	1584	0	1625	37	0
5	2F	1580	0	1619	49	0
6	1G	1423	0	1436	35	0
6	2G	1428	0	1438	54	0
7	1H	1330	0	1407	33	0
7	2H	1330	0	1407	23	0
8	1I	1097	0	1140	27	0
8	2I	1064	0	1082	18	0
9	1N	1117	0	1184	18	0
9	2N	1117	0	1184	21	0
10	1O	933	0	996	15	0
10	2O	933	0	996	18	0
11	1P	1135	0	1212	32	0
11	2P	1135	0	1212	23	0
12	1Q	1122	0	1179	18	0
12	2Q	1122	0	1179	26	0
13	1R	968	0	1033	14	0
13	2R	968	0	1033	19	0
14	1S	873	0	927	18	0
14	2S	870	0	923	26	0
15	1T	1091	0	1151	23	0
15	2T	1083	0	1136	25	0
16	1U	959	0	1019	12	0
16	2U	959	0	1019	13	0
17	1V	771	0	830	6	0
17	2V	771	0	830	10	0
18	1W	886	0	939	6	0
18	2W	886	0	940	14	0
19	1X	750	0	814	13	0
19	2X	750	0	814	12	0
20	1Y	806	0	881	18	0
20	2Y	806	0	881	22	0
21	1Z	1240	0	1240	31	0
21	2Z	1271	0	1273	33	0
22	10	604	0	619	13	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	9	0
23	11	755	0	826	20	0
23	21	755	0	826	14	0
24	12	588	0	643	11	0
24	22	588	0	643	5	0
25	13	469	0	518	6	0
25	23	464	0	514	6	0
26	14	552	0	533	28	0
26	24	532	0	503	31	0
27	15	455	0	465	6	0
27	25	455	0	465	10	0
28	16	453	0	473	7	0
28	26	449	0	469	7	0
29	17	418	0	467	8	0
29	27	418	0	467	7	0
30	18	517	0	582	7	0
30	28	517	0	582	9	0
31	19	307	0	335	1	0
31	29	307	0	335	6	0
32	1a	32246	0	16294	484	0
32	2a	32327	0	16338	495	0
33	1b	1846	0	1867	70	0
33	2b	1825	0	1828	73	0
34	1c	1548	0	1535	53	0
34	2c	1542	0	1517	62	0
35	1d	1655	0	1672	61	0
35	2d	1674	0	1713	49	0
36	1e	1129	0	1185	45	0
36	2e	1133	0	1191	47	0
37	1f	810	0	804	11	0
37	2f	816	0	808	25	0
38	1g	1231	0	1238	32	0
38	2g	1235	0	1249	46	0
39	1h	1088	0	1126	23	0
39	2h	1088	0	1126	27	0
40	1i	983	0	986	40	0
40	2i	978	0	966	42	0
41	1j	709	0	650	29	0
41	2j	714	0	672	36	0
42	1k	829	0	825	18	0
42	2k	833	0	836	19	0
43	1l	932	0	981	18	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	18	0
44	1m	919	0	951	30	0
44	2m	907	0	934	40	0
45	1n	492	0	529	15	0
45	2n	492	0	529	21	0
46	1o	728	0	760	16	0
46	2o	728	0	760	14	0
47	1p	681	0	697	24	0
47	2p	677	0	686	20	0
48	1q	823	0	891	18	0
48	2q	823	0	891	17	0
49	1r	555	0	618	13	0
49	2r	555	0	618	15	0
50	1s	652	0	662	27	0
50	2s	646	0	644	32	0
51	1t	728	0	798	20	0
51	2t	727	0	796	18	0
52	1u	199	0	208	9	0
52	2u	199	0	208	11	0
53	1v	191	0	97	4	0
53	2v	191	0	97	2	0
54	1w	1939	0	1925	51	0
54	2w	1957	0	1935	39	0
55	1x	1577	0	801	10	0
55	2x	1577	0	802	17	0
56	1z	30	0	32	3	0
56	2z	25	0	27	1	0
57	10	7	0	0	0	0
57	11	4	0	0	0	0
57	12	2	0	0	0	0
57	13	3	0	0	0	0
57	15	9	0	0	0	0
57	16	2	0	0	0	0
57	17	5	0	0	0	0
57	18	4	0	0	0	0
57	19	1	0	0	0	0
57	1A	1101	0	0	0	0
57	1B	38	0	0	0	0
57	1D	14	0	0	0	0
57	1E	13	0	0	0	0
57	1F	16	0	0	0	0
57	1G	5	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	4	0	0	0	0
57	1O	4	0	0	0	0
57	1P	7	0	0	0	0
57	1Q	7	0	0	0	0
57	1R	4	0	0	0	0
57	1S	3	0	0	0	0
57	1T	3	0	0	0	0
57	1U	11	0	0	0	0
57	1V	7	0	0	0	0
57	1W	5	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	215	0	0	0	0
57	1b	2	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	1k	1	0	0	0	0
57	1l	2	0	0	0	0
57	1m	1	0	0	0	0
57	1n	2	0	0	0	0
57	1r	1	0	0	0	0
57	1t	1	0	0	0	0
57	1v	4	0	0	0	0
57	1w	1	0	0	0	0
57	1x	12	0	0	0	0
57	20	1	0	0	0	0
57	21	2	0	0	0	0
57	23	4	0	0	0	0
57	25	7	0	0	0	0
57	26	1	0	0	0	0
57	28	3	0	0	0	0
57	29	1	0	0	0	0
57	2A	852	0	0	0	0
57	2B	19	0	0	0	0
57	2D	7	0	0	0	0
57	2E	8	0	0	0	0
57	2F	7	0	0	0	0
57	2G	1	0	0	0	0
57	2N	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	2O	2	0	0	0	0
57	2P	2	0	0	0	0
57	2Q	4	0	0	0	0
57	2R	1	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	2Z	1	0	0	0	0
57	2a	185	0	0	0	0
57	2d	1	0	0	0	0
57	2e	2	0	0	0	0
57	2f	1	0	0	0	0
57	2g	1	0	0	0	0
57	2i	1	0	0	0	0
57	2j	1	0	0	0	0
57	2l	2	0	0	0	0
57	2n	1	0	0	0	0
57	2q	2	0	0	0	0
57	2r	1	0	0	0	0
57	2t	1	0	0	0	0
57	2v	1	0	0	0	0
57	2x	5	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	1	0
60	2d	8	0	0	0	0
61	10	10	0	0	0	0
61	11	10	0	0	0	0
61	12	4	0	0	0	0
61	13	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	15	6	0	0	0	0
61	16	2	0	0	0	0
61	17	8	0	0	0	0
61	18	13	0	0	0	0
61	1A	2078	0	0	73	0
61	1B	64	0	0	1	0
61	1D	26	0	0	1	0
61	1E	25	0	0	0	0
61	1F	14	0	0	1	0
61	1G	3	0	0	1	0
61	1H	4	0	0	0	0
61	1I	1	0	0	0	0
61	1N	3	0	0	0	0
61	1O	8	0	0	0	0
61	1P	22	0	0	2	0
61	1Q	10	0	0	0	0
61	1R	14	0	0	2	0
61	1S	4	0	0	0	0
61	1T	5	0	0	0	0
61	1U	12	0	0	0	0
61	1V	9	0	0	0	0
61	1W	12	0	0	1	0
61	1X	2	0	0	0	0
61	1Y	3	0	0	0	0
61	1Z	1	0	0	0	0
61	1a	287	0	0	20	0
61	1d	1	0	0	0	0
61	1e	1	0	0	0	0
61	1f	2	0	0	0	0
61	1j	1	0	0	0	0
61	1l	3	0	0	0	0
61	1q	1	0	0	0	0
61	1v	7	0	0	0	0
61	1w	1	0	0	0	0
61	1x	19	0	0	2	0
61	20	5	0	0	0	0
61	21	9	0	0	1	0
61	22	1	0	0	0	0
61	23	2	0	0	1	0
61	25	1	0	0	0	0
61	27	3	0	0	0	0
61	28	4	0	0	0	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	1124	0	0	67	0
61	2B	19	0	0	1	0
61	2D	23	0	0	0	0
61	2E	17	0	0	0	0
61	2F	14	0	0	0	0
61	2I	1	0	0	0	0
61	2N	2	0	0	0	0
61	2O	2	0	0	0	0
61	2P	13	0	0	1	0
61	2Q	2	0	0	0	0
61	2R	4	0	0	2	0
61	2T	3	0	0	0	0
61	2U	2	0	0	0	0
61	2V	1	0	0	0	0
61	2W	2	0	0	0	0
61	2X	4	0	0	0	0
61	2Y	1	0	0	0	0
61	2Z	1	0	0	0	0
61	2a	144	0	0	8	0
61	2d	3	0	0	0	0
61	2e	1	0	0	0	0
61	2g	1	0	0	0	0
61	2i	2	0	0	0	0
61	2j	2	0	0	0	0
61	2l	4	0	0	0	0
61	2q	2	0	0	0	0
61	2r	1	0	0	0	0
61	2t	3	0	0	0	0
61	2v	2	0	0	0	0
61	2w	5	0	0	0	0
61	2x	17	0	0	2	0
All	All	297056	0	197048	4059	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 8.

The worst 5 of 4059 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2104:G:H1	1:2A:2185:C:H42	1.03	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2129:C:H42	1:2A:2159:G:H1	1.11	0.96
32:1a:1035:A:H2'	32:1a:1036:G:H21	1.29	0.95
1:1A:1082:U:H3	1:1A:1086:A:N6	1.62	0.95
1:2A:1689:A:H62	1:2A:1698:A:H2	1.15	0.95

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	261 (96%)	12 (4%)	0	100	100
3	2D	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
4	1E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	25	38
4	2E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	25	38
5	1F	201/210 (96%)	193 (96%)	6 (3%)	2 (1%)	13	20
5	2F	201/210 (96%)	188 (94%)	12 (6%)	1 (0%)	25	38
6	1G	179/182 (98%)	166 (93%)	12 (7%)	1 (1%)	22	33
6	2G	179/182 (98%)	157 (88%)	18 (10%)	4 (2%)	5	6
7	1H	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	22	33
7	2H	172/180 (96%)	156 (91%)	15 (9%)	1 (1%)	22	33
8	1I	144/148 (97%)	125 (87%)	17 (12%)	2 (1%)	9	13
8	2I	144/148 (97%)	127 (88%)	15 (10%)	2 (1%)	9	13
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%)	115 (96%)	4 (3%)	1 (1%)	16	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	1P	147/150 (98%)	139 (95%)	7 (5%)	1 (1%)	19	29
11	2P	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	19	29
12	1Q	139/141 (99%)	128 (92%)	10 (7%)	1 (1%)	19	29
12	2Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	19	29
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	14	22
14	1S	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	14	22
14	2S	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	14	22
15	1T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	16	26
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
17	2V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	13	20
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	12	18
19	2X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	12	18
20	1Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
20	2Y	105/110 (96%)	94 (90%)	11 (10%)	0	100	100
21	1Z	148/206 (72%)	132 (89%)	13 (9%)	3 (2%)	6	8
21	2Z	156/206 (76%)	141 (90%)	12 (8%)	3 (2%)	6	8
22	10	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
22	20	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	12	18
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	12	18
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	14	67/71 (94%)	49 (73%)	11 (16%)	7 (10%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	24	67/71 (94%)	51 (76%)	9 (13%)	7 (10%)	0	0
27	15	57/60 (95%)	57 (100%)	0	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	61 (98%)	1 (2%)	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%)	194 (85%)	28 (12%)	7 (3%)	3	3
33	2b	229/256 (90%)	203 (89%)	19 (8%)	7 (3%)	3	3
34	1c	204/239 (85%)	176 (86%)	26 (13%)	2 (1%)	13	20
34	2c	204/239 (85%)	174 (85%)	27 (13%)	3 (2%)	8	12
35	1d	206/209 (99%)	185 (90%)	21 (10%)	0	100	100
35	2d	206/209 (99%)	187 (91%)	19 (9%)	0	100	100
36	1e	146/162 (90%)	129 (88%)	16 (11%)	1 (1%)	19	29
36	2e	146/162 (90%)	138 (94%)	6 (4%)	2 (1%)	9	13
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
37	2f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
38	1g	153/156 (98%)	134 (88%)	17 (11%)	2 (1%)	10	15
38	2g	153/156 (98%)	136 (89%)	14 (9%)	3 (2%)	6	8
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
40	1i	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	16	26
40	2i	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	16	26
41	1j	95/105 (90%)	82 (86%)	9 (10%)	4 (4%)	2	2
41	2j	94/105 (90%)	76 (81%)	16 (17%)	2 (2%)	5	7
42	1k	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	7	9
42	2k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	14	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	1l	119/132 (90%)	113 (95%)	5 (4%)	1 (1%)	16	26
43	2l	119/132 (90%)	112 (94%)	6 (5%)	1 (1%)	16	26
44	1m	116/126 (92%)	100 (86%)	14 (12%)	2 (2%)	7	10
44	2m	114/126 (90%)	94 (82%)	18 (16%)	2 (2%)	7	9
45	1n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
45	2n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
46	1o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
46	2o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
47	1p	80/88 (91%)	69 (86%)	11 (14%)	0	100	100
47	2p	80/88 (91%)	71 (89%)	9 (11%)	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%)	61 (92%)	3 (4%)	2 (3%)	3	3
49	2r	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	8	12
50	1s	81/93 (87%)	71 (88%)	10 (12%)	0	100	100
50	2s	81/93 (87%)	73 (90%)	7 (9%)	1 (1%)	11	16
51	1t	94/106 (89%)	83 (88%)	8 (8%)	3 (3%)	3	3
51	2t	94/106 (89%)	85 (90%)	7 (7%)	2 (2%)	5	7
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	16 (76%)	5 (24%)	0	100	100
54	1w	246/354 (70%)	228 (93%)	14 (6%)	4 (2%)	8	11
54	2w	250/354 (71%)	235 (94%)	13 (5%)	2 (1%)	16	26
56	1z	3/7 (43%)	3 (100%)	0	0	100	100
56	2z	2/7 (29%)	2 (100%)	0	0	100	100
All	All	11846/12850 (92%)	10950 (92%)	787 (7%)	109 (1%)	14	22

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	1Z	53	ILE
23	11	3	LYS
26	14	44	THR
26	14	55	ARG
26	14	62	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	203 (94%)	12 (6%)	17	30
3	2D	215/218 (99%)	206 (96%)	9 (4%)	25	43
4	1E	164/166 (99%)	152 (93%)	12 (7%)	11	20
4	2E	164/166 (99%)	152 (93%)	12 (7%)	11	20
5	1F	160/166 (96%)	148 (92%)	12 (8%)	11	18
5	2F	159/166 (96%)	143 (90%)	16 (10%)	6	9
6	1G	143/156 (92%)	131 (92%)	12 (8%)	9	14
6	2G	143/156 (92%)	125 (87%)	18 (13%)	3	4
7	1H	144/148 (97%)	133 (92%)	11 (8%)	11	18
7	2H	144/148 (97%)	128 (89%)	16 (11%)	5	7
8	1I	113/124 (91%)	100 (88%)	13 (12%)	4	6
8	2I	105/124 (85%)	90 (86%)	15 (14%)	2	3
9	1N	118/119 (99%)	110 (93%)	8 (7%)	13	22
9	2N	118/119 (99%)	106 (90%)	12 (10%)	6	9
10	1O	100/100 (100%)	99 (99%)	1 (1%)	73	86
10	2O	100/100 (100%)	93 (93%)	7 (7%)	12	21
11	1P	115/116 (99%)	108 (94%)	7 (6%)	15	27
11	2P	115/116 (99%)	110 (96%)	5 (4%)	25	42
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	18	32
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	23	40
13	1R	101/101 (100%)	94 (93%)	7 (7%)	13	22
13	2R	101/101 (100%)	98 (97%)	3 (3%)	36	57
14	1S	86/88 (98%)	77 (90%)	9 (10%)	5	8
14	2S	85/88 (97%)	78 (92%)	7 (8%)	9	15
15	1T	115/127 (91%)	107 (93%)	8 (7%)	12	21
15	2T	113/127 (89%)	104 (92%)	9 (8%)	10	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/94 (99%)	89 (96%)	4 (4%)	25	42
16	2U	93/94 (99%)	88 (95%)	5 (5%)	18	32
17	1V	80/82 (98%)	79 (99%)	1 (1%)	65	81
17	2V	80/82 (98%)	76 (95%)	4 (5%)	20	36
18	1W	90/92 (98%)	84 (93%)	6 (7%)	13	23
18	2W	90/92 (98%)	85 (94%)	5 (6%)	17	30
19	1X	77/78 (99%)	76 (99%)	1 (1%)	65	81
19	2X	77/78 (99%)	72 (94%)	5 (6%)	14	24
20	1Y	85/91 (93%)	75 (88%)	10 (12%)	4	6
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	12	20
21	1Z	135/179 (75%)	117 (87%)	18 (13%)	3	4
21	2Z	137/179 (76%)	113 (82%)	24 (18%)	1	2
22	10	61/67 (91%)	60 (98%)	1 (2%)	58	76
22	20	61/67 (91%)	61 (100%)	0	100	100
23	11	80/83 (96%)	75 (94%)	5 (6%)	15	25
23	21	80/83 (96%)	73 (91%)	7 (9%)	8	13
24	12	65/67 (97%)	63 (97%)	2 (3%)	35	56
24	22	65/67 (97%)	59 (91%)	6 (9%)	7	12
25	13	51/52 (98%)	47 (92%)	4 (8%)	10	17
25	23	50/52 (96%)	47 (94%)	3 (6%)	16	27
26	14	59/63 (94%)	52 (88%)	7 (12%)	4	6
26	24	53/63 (84%)	47 (89%)	6 (11%)	4	7
27	15	50/52 (96%)	45 (90%)	5 (10%)	6	9
27	25	50/52 (96%)	45 (90%)	5 (10%)	6	9
28	16	51/52 (98%)	46 (90%)	5 (10%)	6	10
28	26	50/52 (96%)	46 (92%)	4 (8%)	10	16
29	17	41/42 (98%)	38 (93%)	3 (7%)	11	20
29	27	41/42 (98%)	38 (93%)	3 (7%)	11	20
30	18	54/55 (98%)	51 (94%)	3 (6%)	17	30
30	28	54/55 (98%)	52 (96%)	2 (4%)	29	48
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	58
33	1b	192/220 (87%)	161 (84%)	31 (16%)	2	2
33	2b	187/220 (85%)	155 (83%)	32 (17%)	1	2
34	1c	142/188 (76%)	129 (91%)	13 (9%)	7	12
34	2c	140/188 (74%)	132 (94%)	8 (6%)	17	29
35	1d	169/181 (93%)	151 (89%)	18 (11%)	5	8
35	2d	173/181 (96%)	156 (90%)	17 (10%)	6	10
36	1e	113/123 (92%)	106 (94%)	7 (6%)	15	26
36	2e	114/123 (93%)	104 (91%)	10 (9%)	8	13
37	1f	84/90 (93%)	79 (94%)	5 (6%)	16	27
37	2f	85/90 (94%)	81 (95%)	4 (5%)	22	38
38	1g	119/127 (94%)	105 (88%)	14 (12%)	4	6
38	2g	120/127 (94%)	115 (96%)	5 (4%)	25	43
39	1h	114/119 (96%)	104 (91%)	10 (9%)	8	13
39	2h	114/119 (96%)	106 (93%)	8 (7%)	12	21
40	1i	90/99 (91%)	73 (81%)	17 (19%)	1	1
40	2i	89/99 (90%)	79 (89%)	10 (11%)	5	7
41	1j	66/92 (72%)	59 (89%)	7 (11%)	5	8
41	2j	69/92 (75%)	61 (88%)	8 (12%)	4	6
42	1k	82/99 (83%)	76 (93%)	6 (7%)	11	20
42	2k	83/99 (84%)	78 (94%)	5 (6%)	16	27
43	1l	96/108 (89%)	91 (95%)	5 (5%)	19	34
43	2l	96/108 (89%)	90 (94%)	6 (6%)	15	25
44	1m	89/101 (88%)	76 (85%)	13 (15%)	2	3
44	2m	88/101 (87%)	77 (88%)	11 (12%)	3	5
45	1n	49/50 (98%)	45 (92%)	4 (8%)	9	15
45	2n	49/50 (98%)	45 (92%)	4 (8%)	9	15
46	1o	78/80 (98%)	68 (87%)	10 (13%)	3	4
46	2o	78/80 (98%)	72 (92%)	6 (8%)	10	17
47	1p	69/74 (93%)	61 (88%)	8 (12%)	4	6
47	2p	68/74 (92%)	59 (87%)	9 (13%)	3	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/97 (97%)	85 (90%)	9 (10%)	7	10
48	2q	94/97 (97%)	90 (96%)	4 (4%)	25	42
49	1r	59/77 (77%)	56 (95%)	3 (5%)	20	35
49	2r	59/77 (77%)	54 (92%)	5 (8%)	8	14
50	1s	69/80 (86%)	61 (88%)	8 (12%)	4	6
50	2s	67/80 (84%)	59 (88%)	8 (12%)	4	6
51	1t	70/82 (85%)	69 (99%)	1 (1%)	62	79
51	2t	70/82 (85%)	67 (96%)	3 (4%)	25	42
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	16 (89%)	2 (11%)	5	7
54	1w	203/298 (68%)	184 (91%)	19 (9%)	7	11
54	2w	203/298 (68%)	180 (89%)	23 (11%)	4	7
56	1z	2/3 (67%)	2 (100%)	0	100	100
56	2z	2/3 (67%)	2 (100%)	0	100	100
All	All	9697/10666 (91%)	8887 (92%)	810 (8%)	9	14

5 of 810 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	2H	62	LYS
21	2Z	73	GLN
54	2w	258	GLN
8	2I	38	LEU
7	2H	41	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

Mol	Chain	Res	Type
44	2m	12	ASN
46	2o	62	GLN
41	1j	56	HIS
40	1i	124	GLN
49	2r	63	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	437 (15%)	33 (1%)
1	2A	2791/2915 (95%)	450 (16%)	24 (0%)
2	1B	119/121 (98%)	12 (10%)	0
2	2B	118/121 (97%)	17 (14%)	0
32	1a	1497/1521 (98%)	288 (19%)	0
32	2a	1501/1521 (98%)	295 (19%)	0
53	1v	8/24 (33%)	1 (12%)	0
53	2v	8/24 (33%)	1 (12%)	0
55	1x	72/74 (97%)	11 (15%)	0
55	2x	72/74 (97%)	7 (9%)	0
All	All	9050/9310 (97%)	1519 (16%)	57 (0%)

5 of 1519 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	14	A
1	1A	15	G
1	1A	34	C
1	1A	45	C

5 of 57 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2430	A
1	2A	2689	U
1	2A	266	G
1	2A	2406	U
1	2A	1420	U

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

68 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
32	5MC	1a	967	32	19,22,23	1.48	3 (15%)	26,32,35	1.10	3 (11%)
1	2MA	2A	2503	57,1	18,25,26	0.72	0	20,37,40	1.88	3 (15%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	21,30,33	2.00	5 (23%)
55	H2U	1x	21	55	18,21,22	0.99	1 (5%)	19,30,33	1.60	2 (10%)
32	2MG	1a	1207	32	18,26,27	0.92	1 (5%)	16,38,41	1.27	1 (6%)
55	H2U	2x	20	55	18,21,22	0.99	2 (11%)	19,30,33	1.12	1 (5%)
1	5MU	2A	1939	57,1	19,22,23	1.46	5 (26%)	27,32,35	2.17	8 (29%)
55	PSU	1x	39	55	18,21,22	1.42	3 (16%)	21,30,33	1.90	3 (14%)
55	MIA	1x	37	55	17,24,32	0.98	1 (5%)	16,35,47	1.33	2 (12%)
32	5MC	1a	1407	32	19,22,23	1.80	3 (15%)	26,32,35	1.15	4 (15%)
1	PSU	1A	1917	1	18,21,22	1.49	3 (16%)	21,30,33	2.00	5 (23%)
1	PSU	2A	2605	1	18,21,22	1.33	2 (11%)	21,30,33	1.96	5 (23%)
32	4OC	1a	1402	57,32	20,23,24	0.76	0	25,32,35	1.08	2 (8%)
32	MA6	2a	1519	32	19,26,27	1.04	2 (10%)	18,38,41	1.94	3 (16%)
1	OMU	2A	2552	57,1	19,22,23	1.17	2 (10%)	25,31,34	1.76	5 (20%)
32	5MC	2a	1404	32	19,22,23	1.61	3 (15%)	26,32,35	1.14	2 (7%)
1	PSU	1A	2605	57,1	18,21,22	1.35	2 (11%)	21,30,33	2.22	4 (19%)
1	OMG	1A	2251	57,55,1	19,26,27	1.00	1 (5%)	21,38,41	1.11	3 (14%)
32	MA6	2a	1518	32	19,26,27	1.02	2 (10%)	18,38,41	1.89	3 (16%)
32	UR3	1a	1498	32	19,22,23	0.98	0	26,32,35	1.71	3 (11%)
1	PSU	2A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	1.97	4 (19%)
1	5MU	2A	1915	57,1	19,22,23	1.49	6 (31%)	27,32,35	2.22	7 (25%)
55	8AN	1x	76	57,56,55	17,24,25	1.15	2 (11%)	13,35,38	2.91	2 (15%)
32	G7M	2a	527	57,32	20,26,27	1.20	2 (10%)	16,39,42	0.64	0
55	PSU	1x	55	55	18,21,22	1.31	2 (11%)	21,30,33	2.10	4 (19%)
1	5MC	1A	1962	57,1	19,22,23	1.68	3 (15%)	26,32,35	1.09	3 (11%)
1	5MC	1A	1942	57,1	19,22,23	1.59	3 (15%)	26,32,35	1.26	4 (15%)
32	PSU	1a	516	57,32	18,21,22	1.40	2 (11%)	21,30,33	2.10	4 (19%)
32	MA6	1a	1519	32	19,26,27	1.03	1 (5%)	18,38,41	1.92	3 (16%)
55	5MU	2x	54	55	19,22,23	1.42	4 (21%)	27,32,35	2.18	8 (29%)
1	5MC	2A	1942	1	19,22,23	1.70	2 (10%)	26,32,35	1.15	3 (11%)
32	5MC	1a	1400	32	19,22,23	1.69	3 (15%)	26,32,35	1.17	2 (7%)
1	OMG	2A	2251	57,55,1	19,26,27	0.89	1 (5%)	21,38,41	1.14	3 (14%)
54	MEQ	2w	230	54	8,9,10	0.84	0	5,10,12	0.83	0
32	5MC	2a	1400	32	19,22,23	1.72	3 (15%)	26,32,35	1.15	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	G7M	1a	527	57,32	20,26,27	1.21	2 (10%)	16,39,42	0.58	0
1	OMC	2A	1920	57,1	19,22,23	0.82	0	25,31,34	0.93	1 (4%)
43	0TD	2l	92	43	8,9,10	4.64	1 (12%)	6,11,13	6.71	3 (50%)
55	H2U	1x	20	55	18,21,22	0.88	2 (11%)	19,30,33	1.08	1 (5%)
1	5MC	2A	1962	57,1	19,22,23	1.78	3 (15%)	26,32,35	1.16	3 (11%)
55	PSU	2x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.17	4 (19%)
1	PSU	1A	1911	1	18,21,22	1.40	3 (16%)	21,30,33	1.98	4 (19%)
1	OMU	1A	2552	57,1	19,22,23	1.23	3 (15%)	25,31,34	1.68	5 (20%)
32	MA6	1a	1518	32	19,26,27	1.03	2 (10%)	18,38,41	1.95	3 (16%)
55	H2U	2x	21	55	18,21,22	1.02	2 (11%)	19,30,33	1.28	3 (15%)
32	5MC	2a	967	32	19,22,23	1.73	3 (15%)	26,32,35	1.10	2 (7%)
32	2MG	2a	1207	32	18,26,27	0.90	1 (5%)	16,38,41	1.19	1 (6%)
55	4SU	1x	8	55	18,21,22	1.87	5 (27%)	25,30,33	2.03	4 (16%)
32	5MC	1a	1404	32	19,22,23	1.75	3 (15%)	26,32,35	1.15	2 (7%)
1	PSU	2A	1917	1	18,21,22	1.38	2 (11%)	21,30,33	2.19	4 (19%)
32	5MC	2a	1407	57,32	19,22,23	1.64	3 (15%)	26,32,35	1.23	3 (11%)
32	M2G	1a	966	32	20,27,28	1.45	3 (15%)	19,40,43	0.98	2 (10%)
1	2MA	1A	2503	57,1	18,25,26	0.72	0	20,37,40	1.92	2 (10%)
55	8AN	2x	76	57,56,55	17,24,25	1.11	2 (11%)	13,35,38	2.72	2 (15%)
43	0TD	1l	92	43	8,9,10	4.56	2 (25%)	6,11,13	8.74	3 (50%)
32	4OC	2a	1402	57,32	20,23,24	0.78	0	25,32,35	0.97	1 (4%)
55	PSU	2x	39	55	18,21,22	1.41	3 (16%)	21,30,33	1.74	4 (19%)
32	M2G	2a	966	32	20,27,28	1.36	2 (10%)	19,40,43	1.02	1 (5%)
55	4SU	2x	8	55	18,21,22	1.83	4 (22%)	25,30,33	1.88	5 (20%)
55	MIA	2x	37	55	17,24,32	0.99	1 (5%)	16,35,47	1.54	3 (18%)
54	MEQ	1w	230	54	8,9,10	0.96	0	5,10,12	0.32	0
55	PSU	1x	32	57,55	18,21,22	1.33	2 (11%)	21,30,33	2.04	3 (14%)
32	UR3	2a	1498	32	19,22,23	0.94	1 (5%)	26,32,35	1.72	3 (11%)
55	5MU	1x	54	57,55	19,22,23	1.37	4 (21%)	27,32,35	1.87	6 (22%)
55	PSU	2x	32	55	18,21,22	1.35	2 (11%)	21,30,33	2.02	4 (19%)
1	5MU	1A	1939	57,1	19,22,23	1.49	5 (26%)	27,32,35	2.10	6 (22%)
1	5MU	1A	1915	1	19,22,23	1.38	5 (26%)	27,32,35	2.31	6 (22%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	1.04	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	57,1	-	1/3/25/26	0/3/3/3
32	PSU	2a	516	32	-	2/7/25/26	0/2/2/2
55	H2U	1x	21	55	-	4/7/38/39	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
55	H2U	2x	20	55	-	4/7/38/39	0/2/2/2
1	5MU	2A	1939	57,1	-	0/7/25/26	0/2/2/2
55	PSU	1x	39	55	-	0/7/25/26	0/2/2/2
55	MIA	1x	37	55	-	2/3/25/34	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	57,32	-	2/9/29/30	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
1	OMU	2A	2552	57,1	-	0/9/27/28	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	57,1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	57,55,1	-	0/5/27/28	0/3/3/3
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	57,1	-	0/7/25/26	0/2/2/2
55	8AN	1x	76	57,56,55	-	1/3/25/26	0/3/3/3
32	G7M	2a	527	57,32	-	3/3/25/26	0/3/3/3
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	57,1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	57,1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	57,32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
1	OMG	2A	2251	57,55,1	-	0/5/27/28	0/3/3/3
54	MEQ	2w	230	54	-	2/8/9/11	-
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	57,32	-	2/3/25/26	0/3/3/3
1	OMC	2A	1920	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
43	0TD	2l	92	43	-	2/7/12/14	-
55	H2U	1x	20	55	-	2/7/38/39	0/2/2/2
1	5MC	2A	1962	57,1	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	57,1	-	0/9/27/28	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
55	H2U	2x	21	55	-	5/7/38/39	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	57,32	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	2MA	1A	2503	57,1	-	1/3/25/26	0/3/3/3
55	8AN	2x	76	57,56,55	-	1/3/25/26	0/3/3/3
43	0TD	1l	92	43	-	2/7/12/14	-
32	4OC	2a	1402	57,32	-	4/9/29/30	0/2/2/2
55	PSU	2x	39	55	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
55	MIA	2x	37	55	-	2/3/25/34	0/3/3/3
54	MEQ	1w	230	54	-	4/8/9/11	-
55	PSU	1x	32	57,55	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	57,55	-	2/7/25/26	0/2/2/2
55	PSU	2x	32	55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	57,1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2

The worst 5 of 147 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.77	1.69	1.82
43	1l	92	0TD	CB-SB	-12.31	1.69	1.82
32	1a	1407	5MC	C5-C4	6.64	1.49	1.44
1	2A	1962	5MC	C5-C4	6.63	1.49	1.44
32	1a	1404	5MC	C5-C4	6.45	1.49	1.44

The worst 5 of 212 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-20.98	64.66	102.36
43	2l	92	0TD	CSB-SB-CB	-15.79	73.98	102.36
55	1x	76	8AN	C4'-O4'-C1'	-8.16	102.45	109.92
55	2x	76	8AN	C4'-O4'-C1'	-7.26	103.27	109.92
32	2a	1498	UR3	C4-N3-C2	-7.10	118.86	124.58

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	O-C-CA-CB
54	1w	230	MEQ	C-CA-CB-CG

There are no ring outliers.

34 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	967	5MC	1	0
55	1x	21	H2U	1	0
55	2x	20	H2U	1	0
1	2A	1939	5MU	1	0
1	1A	1917	PSU	1	0
32	1a	1402	4OC	2	0
32	2a	1519	MA6	3	0
32	2a	1404	5MC	2	0
1	1A	2251	OMG	1	0
32	2a	1518	MA6	1	0
1	2A	1915	5MU	2	0
55	1x	76	8AN	2	0
32	2a	527	G7M	1	0
32	1a	516	PSU	1	0
32	1a	1519	MA6	2	0
1	2A	1942	5MC	1	0
32	1a	1400	5MC	2	0
32	2a	1400	5MC	1	0
43	2l	92	0TD	1	0
55	1x	20	H2U	1	0
1	1A	2552	OMU	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1518	MA6	1	0
32	2a	1207	2MG	1	0
55	1x	8	4SU	1	0
32	1a	966	M2G	2	0
55	2x	76	8AN	1	0
43	1l	92	0TD	1	0
32	2a	1402	4OC	1	0
32	2a	966	M2G	1	0
55	2x	8	4SU	1	0
54	1w	230	MEQ	2	0
1	1A	1939	5MU	1	0
1	1A	1915	5MU	1	0
1	1A	1920	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2691 ligands modelled in this entry, 2689 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	1d	302	35	0,12,12	-	-	-		
60	SF4	2d	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	1d	302	35	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	2d	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	1d	302	SF4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	-0.32	170 (5%)	29	27	22, 38, 91, 104	0
1	2A	2789/2915 (95%)	0.12	134 (4%)	36	34	33, 57, 88, 101	0
2	1B	120/121 (99%)	-0.14	0	100	100	32, 53, 65, 80	0
2	2B	120/121 (99%)	0.77	0	100	100	58, 75, 82, 91	0
3	1D	275/276 (99%)	-0.21	2 (0%)	84	81	23, 39, 53, 77	0
3	2D	275/276 (99%)	0.25	6 (2%)	62	59	30, 50, 62, 76	0
4	1E	204/206 (99%)	-0.09	0	100	100	21, 41, 61, 72	0
4	2E	204/206 (99%)	0.41	5 (2%)	58	55	34, 57, 70, 77	0
5	1F	203/210 (96%)	-0.07	3 (1%)	71	68	19, 42, 67, 80	0
5	2F	203/210 (96%)	0.73	9 (4%)	39	37	36, 65, 77, 84	0
6	1G	181/182 (99%)	0.93	18 (9%)	14	12	51, 66, 76, 84	0
6	2G	181/182 (99%)	1.36	28 (15%)	6	6	69, 77, 82, 87	0
7	1H	174/180 (96%)	0.33	5 (2%)	54	50	39, 55, 65, 76	0
7	2H	174/180 (96%)	1.60	48 (27%)	2	2	68, 78, 85, 88	0
8	1I	146/148 (98%)	0.93	10 (6%)	25	22	48, 70, 77, 81	0
8	2I	146/148 (98%)	1.40	27 (18%)	4	4	58, 73, 79, 84	0
9	1N	140/140 (100%)	-0.15	0	100	100	28, 40, 59, 76	0
9	2N	140/140 (100%)	0.77	8 (5%)	30	28	45, 63, 74, 78	0
10	1O	122/122 (100%)	-0.00	0	100	100	32, 43, 59, 64	0
10	2O	122/122 (100%)	0.25	0	100	100	45, 54, 66, 71	0
11	1P	149/150 (99%)	0.02	1 (0%)	84	81	22, 44, 64, 72	0
11	2P	149/150 (99%)	0.77	4 (2%)	56	53	38, 66, 79, 84	0
12	1Q	141/141 (100%)	0.02	4 (2%)	55	51	28, 42, 53, 67	0
12	2Q	141/141 (100%)	0.85	12 (8%)	18	17	49, 62, 72, 78	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%)	-0.24	0 100 100	26, 37, 50, 62	0
13	2R	118/118 (100%)	0.29	0 100 100	41, 52, 61, 70	0
14	1S	110/112 (98%)	0.26	1 (0%) 81 78	40, 53, 65, 70	0
14	2S	110/112 (98%)	1.48	24 (21%) 3 3	62, 70, 78, 84	0
15	1T	131/146 (89%)	0.09	2 (1%) 71 68	34, 46, 67, 74	0
15	2T	131/146 (89%)	0.49	3 (2%) 61 58	49, 58, 72, 79	0
16	1U	116/118 (98%)	-0.40	0 100 100	23, 33, 46, 58	0
16	2U	116/118 (98%)	0.57	2 (1%) 69 65	43, 58, 70, 76	0
17	1V	101/101 (100%)	-0.15	2 (1%) 64 61	22, 42, 58, 77	0
17	2V	101/101 (100%)	0.72	3 (2%) 52 49	45, 66, 75, 79	0
18	1W	112/113 (99%)	-0.30	0 100 100	25, 33, 53, 74	0
18	2W	112/113 (99%)	0.28	1 (0%) 81 78	41, 51, 66, 78	0
19	1X	95/96 (98%)	0.08	2 (2%) 63 60	32, 40, 62, 75	0
19	2X	95/96 (98%)	0.49	4 (4%) 41 38	48, 61, 71, 77	0
20	1Y	107/110 (97%)	0.48	4 (3%) 45 43	39, 50, 64, 77	0
20	2Y	107/110 (97%)	1.18	17 (15%) 6 5	59, 69, 77, 82	0
21	1Z	154/206 (74%)	0.69	8 (5%) 34 31	42, 59, 72, 81	0
21	2Z	160/206 (77%)	1.22	16 (10%) 14 12	62, 73, 80, 85	0
22	10	76/85 (89%)	-0.01	3 (3%) 44 41	30, 40, 57, 65	0
22	20	76/85 (89%)	0.84	5 (6%) 26 23	48, 62, 71, 76	0
23	11	97/98 (98%)	0.09	2 (2%) 63 60	32, 44, 68, 75	0
23	21	97/98 (98%)	0.46	3 (3%) 51 48	43, 57, 72, 78	0
24	12	70/72 (97%)	0.18	3 (4%) 40 38	35, 50, 62, 72	0
24	22	70/72 (97%)	0.88	1 (1%) 73 70	61, 69, 75, 76	0
25	13	59/60 (98%)	-0.22	1 (1%) 69 65	29, 36, 58, 71	0
25	23	59/60 (98%)	0.50	2 (3%) 48 45	53, 59, 72, 75	0
26	14	69/71 (97%)	1.53	21 (30%) 1 1	61, 78, 86, 90	0
26	24	69/71 (97%)	1.73	20 (28%) 1 1	72, 82, 88, 90	0
27	15	59/60 (98%)	-0.22	2 (3%) 48 45	22, 36, 56, 70	0
27	25	59/60 (98%)	0.29	1 (1%) 69 65	37, 54, 65, 78	0
28	16	53/54 (98%)	-0.11	0 100 100	36, 43, 56, 62	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.61	3 (5%) 30 28	50, 60, 67, 71	0
29	17	48/49 (97%)	-0.03	4 (8%) 19 17	22, 29, 64, 69	0
29	27	48/49 (97%)	0.25	5 (10%) 13 11	34, 45, 67, 74	0
30	18	64/65 (98%)	-0.30	0 100 100	28, 35, 43, 54	0
30	28	64/65 (98%)	0.49	1 (1%) 70 67	44, 54, 61, 64	0
31	19	37/37 (100%)	-0.05	0 100 100	31, 41, 52, 58	0
31	29	37/37 (100%)	0.89	2 (5%) 32 30	54, 64, 72, 73	0
32	1a	1488/1521 (97%)	0.77	121 (8%) 19 17	39, 73, 91, 100	0
32	2a	1491/1521 (98%)	0.77	132 (8%) 17 15	48, 74, 90, 100	0
33	1b	231/256 (90%)	1.43	56 (24%) 2 2	68, 77, 84, 87	0
33	2b	231/256 (90%)	1.69	82 (35%) 1 1	68, 79, 85, 88	0
34	1c	206/239 (86%)	1.75	77 (37%) 1 1	68, 77, 84, 89	0
34	2c	206/239 (86%)	1.67	65 (31%) 1 1	69, 79, 84, 87	0
35	1d	208/209 (99%)	1.40	49 (23%) 2 2	60, 73, 80, 85	0
35	2d	208/209 (99%)	1.25	27 (12%) 9 7	61, 70, 77, 83	0
36	1e	148/162 (91%)	0.84	7 (4%) 37 34	50, 67, 75, 82	0
36	2e	148/162 (91%)	1.12	15 (10%) 14 12	58, 71, 77, 80	0
37	1f	100/101 (99%)	0.98	7 (7%) 24 22	60, 70, 76, 78	0
37	2f	100/101 (99%)	1.01	9 (9%) 17 15	63, 71, 77, 80	0
38	1g	155/156 (99%)	1.25	27 (17%) 5 4	66, 74, 82, 87	0
38	2g	155/156 (99%)	1.43	27 (17%) 5 4	70, 77, 86, 89	0
39	1h	137/138 (99%)	0.90	6 (4%) 39 37	58, 69, 76, 80	0
39	2h	137/138 (99%)	0.96	11 (8%) 20 18	65, 72, 76, 79	0
40	1i	127/128 (99%)	1.76	44 (34%) 1 1	64, 78, 82, 83	0
40	2i	127/128 (99%)	2.27	66 (51%) 0 0	71, 81, 86, 88	0
41	1j	97/105 (92%)	2.13	48 (49%) 0 0	66, 80, 85, 87	0
41	2j	96/105 (91%)	2.29	57 (59%) 0 0	72, 82, 88, 90	0
42	1k	114/129 (88%)	0.98	13 (11%) 11 10	48, 68, 77, 80	0
42	2k	114/129 (88%)	1.09	14 (12%) 9 8	56, 72, 81, 85	0
43	1l	121/132 (91%)	1.07	12 (9%) 14 12	50, 62, 70, 72	0
43	2l	121/132 (91%)	0.92	8 (6%) 26 23	56, 63, 71, 76	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%)	1.66	36 (30%) 1 1	68, 78, 81, 85	0
44	2m	116/126 (92%)	2.10	62 (53%) 0 0	72, 80, 84, 85	0
45	1n	60/61 (98%)	1.91	23 (38%) 1 1	70, 76, 82, 85	0
45	2n	60/61 (98%)	2.07	32 (53%) 0 0	74, 80, 83, 84	0
46	1o	88/89 (98%)	0.99	7 (7%) 20 18	51, 67, 75, 77	0
46	2o	88/89 (98%)	1.06	7 (7%) 20 18	60, 70, 77, 79	0
47	1p	82/88 (93%)	1.62	24 (29%) 1 1	64, 73, 80, 83	0
47	2p	82/88 (93%)	1.43	18 (21%) 3 3	63, 70, 75, 78	0
48	1q	99/105 (94%)	1.08	6 (6%) 28 26	58, 68, 75, 79	0
48	2q	99/105 (94%)	0.87	8 (8%) 19 17	60, 68, 75, 81	0
49	1r	68/88 (77%)	0.86	6 (8%) 17 16	59, 68, 76, 80	0
49	2r	68/88 (77%)	1.02	4 (5%) 29 27	62, 71, 78, 82	0
50	1s	83/93 (89%)	1.99	37 (44%) 1 1	72, 80, 85, 85	0
50	2s	83/93 (89%)	2.08	39 (46%) 0 0	71, 83, 86, 91	0
51	1t	96/106 (90%)	1.23	11 (11%) 11 9	61, 70, 78, 82	0
51	2t	96/106 (90%)	1.12	14 (14%) 7 6	59, 69, 77, 80	0
52	1u	23/27 (85%)	2.03	11 (47%) 0 0	71, 77, 80, 82	0
52	2u	23/27 (85%)	2.00	11 (47%) 0 0	74, 78, 80, 81	0
53	1v	9/24 (37%)	0.99	3 (33%) 1 1	55, 58, 82, 87	0
53	2v	9/24 (37%)	1.30	3 (33%) 1 1	64, 66, 86, 86	0
54	1w	248/354 (70%)	0.59	11 (4%) 39 37	35, 64, 78, 84	0
54	2w	252/354 (71%)	0.88	24 (9%) 15 13	52, 71, 83, 91	0
55	1x	65/74 (87%)	0.25	0 100 100	36, 66, 80, 83	0
55	2x	65/74 (87%)	0.54	1 (1%) 71 68	53, 76, 83, 86	0
56	1z	5/7 (71%)	1.77	2 (40%) 1 1	42, 46, 55, 68	0
56	2z	4/7 (57%)	2.71	2 (50%) 0 0	59, 64, 65, 66	0
All	All	21072/22160 (95%)	0.57	2044 (9%) 15 13	19, 64, 84, 104	0

The worst 5 of 2044 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2A	2147	G	9.3
1	1A	2114	A	9.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2113	U	8.1
1	1A	2178	C	7.9
1	2A	2105	C	7.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	H2U	2x	20	20/21	0.66	0.17	81,91,97,105	0
55	H2U	2x	21	20/21	0.71	0.17	82,92,100,106	0
55	H2U	1x	21	20/21	0.76	0.15	79,87,97,116	0
55	5MU	2x	54	21/22	0.81	0.14	78,82,88,99	0
55	PSU	2x	55	20/21	0.81	0.12	74,78,89,91	0
32	2MG	2a	1207	24/25	0.87	0.12	76,82,85,91	0
32	2MG	1a	1207	24/25	0.87	0.14	72,81,87,92	0
43	0TD	1l	92	10/11	0.88	0.14	56,59,63,79	0
55	PSU	1x	55	20/21	0.89	0.12	69,74,83,84	0
55	H2U	1x	20	20/21	0.89	0.10	72,79,85,90	0
55	5MU	1x	54	21/22	0.90	0.12	65,74,80,87	0
32	PSU	2a	516	20/21	0.90	0.13	59,69,78,79	0
55	PSU	2x	32	20/21	0.90	0.12	68,73,78,82	0
55	MIA	2x	37	22/30	0.90	0.12	62,70,72,75	0
1	5MU	2A	1915	21/22	0.91	0.11	66,70,77,78	0
43	0TD	2l	92	10/11	0.91	0.14	58,63,68,87	0
32	G7M	2a	527	24/25	0.91	0.14	61,65,71,73	0
32	PSU	1a	516	20/21	0.92	0.13	64,72,77,78	0
32	M2G	2a	966	25/26	0.92	0.15	54,68,75,82	0
55	PSU	1x	32	20/21	0.92	0.11	60,66,73,74	0
32	5MC	2a	1404	21/22	0.93	0.11	46,54,59,61	0
32	G7M	1a	527	24/25	0.93	0.13	51,60,66,68	0
55	MIA	1x	37	22/30	0.93	0.10	55,64,68,72	0
55	4SU	2x	8	20/21	0.93	0.10	74,80,83,84	0
32	M2G	1a	966	25/26	0.93	0.12	56,59,72,76	0
32	5MC	1a	967	21/22	0.93	0.12	58,63,72,75	0
32	5MC	2a	967	21/22	0.93	0.13	60,67,73,80	0
1	PSU	2A	1917	20/21	0.93	0.08	57,63,68,74	0
55	PSU	2x	39	20/21	0.94	0.09	59,71,75,77	0
32	4OC	2a	1402	22/23	0.94	0.11	50,62,63,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	PSU	2A	1911	20/21	0.94	0.09	54,62,65,68	0
1	5MU	1A	1915	21/22	0.94	0.10	49,57,60,66	0
32	5MC	2a	1400	21/22	0.94	0.12	61,68,73,75	0
55	8AN	2x	76	22/23	0.94	0.10	45,56,63,66	0
1	PSU	1A	1911	20/21	0.95	0.09	46,54,61,62	0
54	MEQ	2w	230	10/11	0.95	0.13	52,55,57,64	0
55	4SU	1x	8	20/21	0.95	0.08	55,62,67,77	0
32	MA6	2a	1518	24/25	0.96	0.11	49,58,64,65	0
32	MA6	2a	1519	24/25	0.96	0.10	51,60,64,65	0
32	5MC	1a	1400	21/22	0.96	0.11	49,58,62,64	0
32	5MC	1a	1404	21/22	0.96	0.10	42,46,51,52	0
55	PSU	1x	39	20/21	0.96	0.09	56,59,62,63	0
32	MA6	1a	1519	24/25	0.96	0.10	43,47,51,52	0
1	OMC	2A	1920	21/22	0.96	0.08	50,60,63,64	0
1	5MC	2A	1942	21/22	0.96	0.09	46,51,53,55	0
1	OMG	2A	2251	24/25	0.96	0.09	33,45,48,49	0
1	PSU	1A	1917	20/21	0.96	0.08	49,54,59,59	0
55	8AN	1x	76	22/23	0.96	0.08	31,40,46,47	0
32	UR3	2a	1498	21/22	0.96	0.10	52,57,64,65	0
1	PSU	2A	2605	20/21	0.97	0.08	31,38,41,42	0
32	4OC	1a	1402	22/23	0.97	0.09	45,50,53,56	0
1	5MC	1A	1942	21/22	0.97	0.08	31,37,44,49	0
32	5MC	1a	1407	21/22	0.97	0.08	35,44,49,51	0
1	5MC	1A	1962	21/22	0.97	0.08	33,38,45,55	0
1	5MU	2A	1939	21/22	0.97	0.08	33,40,43,45	0
1	PSU	1A	2605	20/21	0.97	0.08	24,29,33,37	0
1	5MC	2A	1962	21/22	0.97	0.08	37,45,50,59	0
54	MEQ	1w	230	10/11	0.97	0.09	32,39,43,44	0
32	5MC	2a	1407	21/22	0.97	0.09	46,51,57,63	0
1	2MA	2A	2503	23/24	0.97	0.08	31,39,44,45	0
32	MA6	1a	1518	24/25	0.98	0.10	38,45,51,52	0
1	OMC	1A	1920	21/22	0.98	0.07	40,47,52,55	0
1	5MU	1A	1939	21/22	0.98	0.07	24,29,34,34	0
1	OMG	1A	2251	24/25	0.98	0.06	27,30,35,37	0
1	2MA	1A	2503	23/24	0.98	0.05	20,24,26,27	0
1	OMU	1A	2552	21/22	0.98	0.06	26,31,35,35	0
1	OMU	2A	2552	21/22	0.98	0.06	38,43,44,46	0
32	UR3	1a	1498	21/22	0.98	0.08	41,48,53,56	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1A	3952	1/1	0.39	0.27	83,83,83,83	0
57	MG	1A	4056	1/1	0.57	0.20	63,63,63,63	0
57	MG	1A	4059	1/1	0.57	0.18	62,62,62,62	0
57	MG	1A	4000	1/1	0.59	0.17	89,89,89,89	0
57	MG	2A	3714	1/1	0.61	0.20	43,43,43,43	0
57	MG	2A	3425	1/1	0.62	0.39	82,82,82,82	0
57	MG	1a	1762	1/1	0.62	0.23	81,81,81,81	0
57	MG	2A	3586	1/1	0.63	0.21	50,50,50,50	0
57	MG	1A	3592	1/1	0.65	0.23	61,61,61,61	0
57	MG	1A	3921	1/1	0.65	0.19	41,41,41,41	0
57	MG	1O	204	1/1	0.66	0.30	67,67,67,67	0
57	MG	1a	1771	1/1	0.67	0.18	82,82,82,82	0
57	MG	1A	3629	1/1	0.67	0.25	60,60,60,60	0
57	MG	2a	1771	1/1	0.67	0.18	79,79,79,79	0
57	MG	1A	3922	1/1	0.68	0.24	66,66,66,66	0
57	MG	2A	3838	1/1	0.69	0.27	80,80,80,80	0
57	MG	1a	1675	1/1	0.70	0.21	87,87,87,87	0
57	MG	1E	310	1/1	0.70	0.23	72,72,72,72	0
57	MG	2A	3624	1/1	0.70	0.22	68,68,68,68	0
57	MG	1a	1768	1/1	0.70	0.17	73,73,73,73	0
57	MG	1A	3512	1/1	0.70	0.24	74,74,74,74	0
57	MG	2A	3190	1/1	0.70	0.30	77,77,77,77	0
57	MG	1U	211	1/1	0.71	0.51	74,74,74,74	0
57	MG	1A	3404	1/1	0.71	0.21	61,61,61,61	0
57	MG	1A	3500	1/1	0.72	0.35	70,70,70,70	0
57	MG	1l	202	1/1	0.72	0.11	80,80,80,80	0
57	MG	2a	1724	1/1	0.72	0.26	68,68,68,68	0
57	MG	2A	3651	1/1	0.72	0.23	76,76,76,76	0
57	MG	2a	1777	1/1	0.72	0.23	73,73,73,73	0
57	MG	2r	101	1/1	0.72	0.29	82,82,82,82	0
57	MG	2A	3258	1/1	0.73	0.14	90,90,90,90	0
57	MG	2a	1741	1/1	0.73	0.25	78,78,78,78	0
57	MG	2A	3380	1/1	0.73	0.21	63,63,63,63	0
57	MG	1A	3613	1/1	0.73	0.21	65,65,65,65	0
57	MG	15	109	1/1	0.73	0.17	61,61,61,61	0
57	MG	28	103	1/1	0.74	0.18	69,69,69,69	0
57	MG	2A	3437	1/1	0.74	0.27	77,77,77,77	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	4026	1/1	0.74	0.20	57,57,57,57	0
57	MG	2a	1762	1/1	0.74	0.28	69,69,69,69	0
57	MG	2A	3755	1/1	0.74	0.14	84,84,84,84	0
57	MG	2A	3834	1/1	0.74	0.20	79,79,79,79	0
57	MG	1A	3851	1/1	0.74	0.19	72,72,72,72	0
57	MG	2A	3824	1/1	0.75	0.16	39,39,39,39	0
57	MG	2A	3578	1/1	0.75	0.24	67,67,67,67	0
57	MG	1a	1714	1/1	0.75	0.24	82,82,82,82	0
57	MG	1A	4102	1/1	0.75	0.28	105,105,105,105	0
57	MG	1x	110	1/1	0.75	0.33	79,79,79,79	0
57	MG	1A	3773	1/1	0.75	0.13	53,53,53,53	0
57	MG	2A	3472	1/1	0.75	0.24	75,75,75,75	0
57	MG	2A	3808	1/1	0.75	0.14	54,54,54,54	0
57	MG	2a	1772	1/1	0.75	0.21	74,74,74,74	0
57	MG	2A	3813	1/1	0.75	0.17	72,72,72,72	0
57	MG	2A	3820	1/1	0.75	0.21	53,53,53,53	0
57	MG	2x	101	1/1	0.75	0.14	81,81,81,81	0
57	MG	2a	1757	1/1	0.76	0.28	68,68,68,68	0
57	MG	1B	230	1/1	0.76	0.24	83,83,83,83	0
57	MG	1a	1640	1/1	0.76	0.42	74,74,74,74	0
57	MG	2B	202	1/1	0.76	0.20	76,76,76,76	0
57	MG	1A	3873	1/1	0.76	0.22	63,63,63,63	0
57	MG	1A	4003	1/1	0.76	0.27	71,71,71,71	0
57	MG	1A	3348	1/1	0.76	0.21	65,65,65,65	0
57	MG	2A	3788	1/1	0.77	0.21	70,70,70,70	0
57	MG	2A	3085	1/1	0.77	0.23	69,69,69,69	0
57	MG	2A	3189	1/1	0.77	0.21	60,60,60,60	0
57	MG	1a	1661	1/1	0.77	0.21	73,73,73,73	0
57	MG	1A	3955	1/1	0.77	0.16	68,68,68,68	0
57	MG	2A	3277	1/1	0.77	0.18	78,78,78,78	0
57	MG	1A	3683	1/1	0.77	0.18	61,61,61,61	0
57	MG	1a	1716	1/1	0.77	0.45	75,75,75,75	0
57	MG	1a	1750	1/1	0.77	0.26	73,73,73,73	0
57	MG	2a	1651	1/1	0.77	0.33	71,71,71,71	0
57	MG	2a	1675	1/1	0.77	0.31	70,70,70,70	0
57	MG	2a	1684	1/1	0.77	0.30	71,71,71,71	0
57	MG	2A	3451	1/1	0.77	0.35	75,75,75,75	0
57	MG	2a	1731	1/1	0.77	0.21	71,71,71,71	0
57	MG	1A	3900	1/1	0.77	0.21	74,74,74,74	0
57	MG	1A	3332	1/1	0.77	0.24	68,68,68,68	0
57	MG	1A	3817	1/1	0.77	0.19	65,65,65,65	0
57	MG	2A	3611	1/1	0.77	0.19	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	1812	1/1	0.77	0.37	71,71,71,71	0
57	MG	1A	3681	1/1	0.77	0.16	49,49,49,49	0
57	MG	2a	1780	1/1	0.77	0.22	73,73,73,73	0
57	MG	1A	4093	1/1	0.77	0.19	74,74,74,74	0
57	MG	2A	3003	1/1	0.77	0.21	69,69,69,69	0
57	MG	2A	3757	1/1	0.78	0.14	49,49,49,49	0
57	MG	2A	3759	1/1	0.78	0.17	74,74,74,74	0
57	MG	2a	1694	1/1	0.78	0.36	75,75,75,75	0
57	MG	1A	3893	1/1	0.78	0.23	47,47,47,47	0
57	MG	2A	3293	1/1	0.78	0.28	70,70,70,70	0
57	MG	2A	3059	1/1	0.78	0.24	71,71,71,71	0
57	MG	1a	1781	1/1	0.78	0.18	71,71,71,71	0
57	MG	2A	3639	1/1	0.78	0.18	69,69,69,69	0
57	MG	2A	3642	1/1	0.78	0.27	62,62,62,62	0
57	MG	1A	3782	1/1	0.78	0.22	56,56,56,56	0
57	MG	2A	3660	1/1	0.78	0.15	60,60,60,60	0
57	MG	1A	3818	1/1	0.78	0.15	55,55,55,55	0
57	MG	2a	1605	1/1	0.78	0.22	75,75,75,75	0
57	MG	1A	3982	1/1	0.78	0.23	46,46,46,46	0
57	MG	1A	3023	1/1	0.79	0.17	56,56,56,56	0
57	MG	1A	3763	1/1	0.79	0.28	77,77,77,77	0
57	MG	1B	222	1/1	0.79	0.24	61,61,61,61	0
57	MG	1B	223	1/1	0.79	0.15	65,65,65,65	0
57	MG	1a	1740	1/1	0.79	0.27	70,70,70,70	0
57	MG	2a	1756	1/1	0.79	0.25	78,78,78,78	0
57	MG	2A	3471	1/1	0.79	0.18	72,72,72,72	0
57	MG	1a	1744	1/1	0.79	0.21	82,82,82,82	0
57	MG	2E	301	1/1	0.79	0.29	73,73,73,73	0
57	MG	2A	3511	1/1	0.79	0.13	67,67,67,67	0
57	MG	2A	3532	1/1	0.79	0.17	52,52,52,52	0
57	MG	2a	1644	1/1	0.79	0.39	74,74,74,74	0
57	MG	2A	3263	1/1	0.79	0.60	78,78,78,78	0
57	MG	1A	3974	1/1	0.79	0.21	73,73,73,73	0
57	MG	1A	3866	1/1	0.80	0.20	39,39,39,39	0
57	MG	2A	3590	1/1	0.80	0.26	70,70,70,70	0
57	MG	1a	1660	1/1	0.80	0.26	77,77,77,77	0
57	MG	2P	201	1/1	0.80	0.15	70,70,70,70	0
57	MG	1A	3801	1/1	0.80	0.23	59,59,59,59	0
57	MG	2A	3626	1/1	0.80	0.22	64,64,64,64	0
57	MG	2a	1606	1/1	0.80	0.23	77,77,77,77	0
57	MG	2a	1634	1/1	0.80	0.23	70,70,70,70	0
57	MG	1A	4009	1/1	0.80	0.17	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	2A	3321	1/1	0.80	0.25	68,68,68,68	0
57	MG	2a	1660	1/1	0.80	0.20	81,81,81,81	0
57	MG	2A	3323	1/1	0.80	0.15	57,57,57,57	0
57	MG	1a	1676	1/1	0.80	0.37	74,74,74,74	0
57	MG	2A	3685	1/1	0.80	0.18	64,64,64,64	0
57	MG	2a	1717	1/1	0.80	0.27	66,66,66,66	0
57	MG	1a	1683	1/1	0.80	0.20	83,83,83,83	0
57	MG	2A	3715	1/1	0.80	0.20	76,76,76,76	0
57	MG	2A	3728	1/1	0.80	0.24	74,74,74,74	0
57	MG	1a	1700	1/1	0.80	0.16	81,81,81,81	0
57	MG	2A	3440	1/1	0.80	0.15	69,69,69,69	0
57	MG	1A	4025	1/1	0.80	0.17	69,69,69,69	0
57	MG	1A	3091	1/1	0.80	0.19	56,56,56,56	0
57	MG	1A	3715	1/1	0.80	0.10	25,25,25,25	0
57	MG	2A	3509	1/1	0.80	0.20	62,62,62,62	0
57	MG	2A	3164	1/1	0.80	0.19	77,77,77,77	0
57	MG	1A	3977	1/1	0.80	0.24	76,76,76,76	0
57	MG	1A	3719	1/1	0.80	0.21	73,73,73,73	0
57	MG	2A	3260	1/1	0.81	0.25	68,68,68,68	0
57	MG	1a	1794	1/1	0.81	0.17	74,74,74,74	0
57	MG	1A	3950	1/1	0.81	0.15	71,71,71,71	0
57	MG	2A	3722	1/1	0.81	0.13	66,66,66,66	0
57	MG	2A	3534	1/1	0.81	0.14	57,57,57,57	0
57	MG	1a	1659	1/1	0.81	0.20	80,80,80,80	0
57	MG	1a	1725	1/1	0.81	0.30	75,75,75,75	0
57	MG	2a	1682	1/1	0.81	0.42	73,73,73,73	0
57	MG	1E	308	1/1	0.81	0.11	24,24,24,24	0
57	MG	1A	3867	1/1	0.81	0.13	70,70,70,70	0
57	MG	1a	1662	1/1	0.81	0.24	71,71,71,71	0
57	MG	2A	3094	1/1	0.81	0.28	73,73,73,73	0
57	MG	2A	3632	1/1	0.81	0.17	66,66,66,66	0
57	MG	2A	3633	1/1	0.81	0.24	70,70,70,70	0
57	MG	1A	3854	1/1	0.81	0.20	59,59,59,59	0
57	MG	1A	4037	1/1	0.81	0.11	45,45,45,45	0
57	MG	2A	3851	1/1	0.81	0.13	64,64,64,64	0
57	MG	1A	3811	1/1	0.81	0.20	54,54,54,54	0
57	MG	2B	205	1/1	0.81	0.20	77,77,77,77	0
57	MG	2B	217	1/1	0.81	0.17	75,75,75,75	0
57	MG	2a	1779	1/1	0.81	0.33	78,78,78,78	0
57	MG	18	104	1/1	0.81	0.12	68,68,68,68	0
57	MG	2a	1782	1/1	0.81	0.26	68,68,68,68	0
57	MG	2a	1784	1/1	0.81	0.18	86,86,86,86	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	3672	1/1	0.81	0.21	70,70,70,70	0
57	MG	2A	3676	1/1	0.81	0.21	75,75,75,75	0
57	MG	1A	3019	1/1	0.82	0.15	48,48,48,48	0
57	MG	1A	4084	1/1	0.82	0.14	70,70,70,70	0
57	MG	1A	4013	1/1	0.82	0.25	63,63,63,63	0
57	MG	1A	3582	1/1	0.82	0.13	34,34,34,34	0
57	MG	2A	3716	1/1	0.82	0.17	67,67,67,67	0
57	MG	2A	3504	1/1	0.82	0.21	71,71,71,71	0
57	MG	1B	217	1/1	0.82	0.17	55,55,55,55	0
57	MG	2a	1671	1/1	0.82	0.28	80,80,80,80	0
57	MG	2A	3733	1/1	0.82	0.15	49,49,49,49	0
57	MG	1A	3821	1/1	0.82	0.16	67,67,67,67	0
57	MG	1a	1774	1/1	0.82	0.21	72,72,72,72	0
57	MG	1a	1698	1/1	0.82	0.19	74,74,74,74	0
57	MG	1a	1612	1/1	0.82	0.17	75,75,75,75	0
57	MG	2A	3791	1/1	0.82	0.14	54,54,54,54	0
57	MG	1a	1623	1/1	0.82	0.30	74,74,74,74	0
57	MG	2A	3285	1/1	0.82	0.13	64,64,64,64	0
57	MG	1b	302	1/1	0.82	0.15	80,80,80,80	0
57	MG	2A	3306	1/1	0.82	0.45	76,76,76,76	0
57	MG	2A	3320	1/1	0.82	0.26	80,80,80,80	0
57	MG	1A	3830	1/1	0.82	0.14	54,54,54,54	0
57	MG	1v	102	1/1	0.82	0.23	77,77,77,77	0
57	MG	2A	3346	1/1	0.82	0.21	69,69,69,69	0
57	MG	2B	203	1/1	0.82	0.12	64,64,64,64	0
57	MG	2A	3361	1/1	0.82	0.29	67,67,67,67	0
57	MG	1A	3956	1/1	0.82	0.20	67,67,67,67	0
57	MG	1a	1730	1/1	0.82	0.25	74,74,74,74	0
57	MG	2i	201	1/1	0.82	0.17	78,78,78,78	0
57	MG	2G	201	1/1	0.82	0.22	79,79,79,79	0
57	MG	2A	3020	1/1	0.82	0.33	69,69,69,69	0
57	MG	2x	105	1/1	0.82	0.12	71,71,71,71	0
57	MG	1A	3810	1/1	0.83	0.20	57,57,57,57	0
57	MG	1A	4043	1/1	0.83	0.28	85,85,85,85	0
57	MG	1a	1728	1/1	0.83	0.21	59,59,59,59	0
57	MG	2A	3234	1/1	0.83	0.42	76,76,76,76	0
57	MG	2A	3701	1/1	0.83	0.21	68,68,68,68	0
57	MG	2A	3709	1/1	0.83	0.18	73,73,73,73	0
57	MG	2A	3710	1/1	0.83	0.12	71,71,71,71	0
57	MG	1a	1803	1/1	0.83	0.14	72,72,72,72	0
57	MG	1A	3603	1/1	0.83	0.09	35,35,35,35	0
57	MG	1A	3781	1/1	0.83	0.23	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	1a	1622	1/1	0.83	0.12	62,62,62,62	0
57	MG	2A	3278	1/1	0.83	0.45	75,75,75,75	0
57	MG	1a	1747	1/1	0.83	0.25	67,67,67,67	0
57	MG	2A	3746	1/1	0.83	0.12	72,72,72,72	0
57	MG	2A	3560	1/1	0.83	0.23	73,73,73,73	0
57	MG	2A	3563	1/1	0.83	0.30	68,68,68,68	0
57	MG	1A	3895	1/1	0.83	0.12	75,75,75,75	0
57	MG	2A	3784	1/1	0.83	0.11	47,47,47,47	0
57	MG	2A	3582	1/1	0.83	0.13	68,68,68,68	0
57	MG	1A	4028	1/1	0.83	0.14	48,48,48,48	0
57	MG	2A	3310	1/1	0.83	0.26	64,64,64,64	0
57	MG	2A	3599	1/1	0.83	0.22	47,47,47,47	0
57	MG	2A	3814	1/1	0.83	0.14	68,68,68,68	0
57	MG	2A	3816	1/1	0.83	0.12	60,60,60,60	0
57	MG	2A	3818	1/1	0.83	0.23	73,73,73,73	0
57	MG	2A	3017	1/1	0.83	0.17	61,61,61,61	0
57	MG	1a	1649	1/1	0.83	0.21	81,81,81,81	0
57	MG	1A	4035	1/1	0.83	0.29	56,56,56,56	0
57	MG	2A	3060	1/1	0.83	0.24	68,68,68,68	0
57	MG	1a	1772	1/1	0.83	0.17	74,74,74,74	0
57	MG	2A	3366	1/1	0.83	0.28	70,70,70,70	0
57	MG	1a	1773	1/1	0.83	0.27	79,79,79,79	0
57	MG	2A	3102	1/1	0.83	0.42	68,68,68,68	0
57	MG	2B	210	1/1	0.83	0.14	75,75,75,75	0
57	MG	1A	3918	1/1	0.84	0.11	58,58,58,58	0
57	MG	2A	3470	1/1	0.84	0.22	70,70,70,70	0
57	MG	1A	3447	1/1	0.84	0.20	61,61,61,61	0
57	MG	2T	202	1/1	0.84	0.17	66,66,66,66	0
57	MG	1A	4042	1/1	0.84	0.28	61,61,61,61	0
57	MG	2A	3484	1/1	0.84	0.21	54,54,54,54	0
57	MG	2A	3253	1/1	0.84	0.25	61,61,61,61	0
57	MG	2a	1610	1/1	0.84	0.24	69,69,69,69	0
57	MG	1A	3988	1/1	0.84	0.15	66,66,66,66	0
57	MG	1A	4049	1/1	0.84	0.14	57,57,57,57	0
57	MG	1a	1805	1/1	0.84	0.23	71,71,71,71	0
57	MG	1a	1807	1/1	0.84	0.23	73,73,73,73	0
57	MG	2a	1664	1/1	0.84	0.25	71,71,71,71	0
57	MG	1a	1708	1/1	0.84	0.15	69,69,69,69	0
57	MG	1A	3997	1/1	0.84	0.10	41,41,41,41	0
57	MG	1A	3690	1/1	0.84	0.10	53,53,53,53	0
57	MG	2A	3296	1/1	0.84	0.25	61,61,61,61	0
57	MG	2a	1691	1/1	0.84	0.29	75,75,75,75	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	1n	102	1/1	0.84	0.20	68,68,68,68	0
57	MG	1a	1613	1/1	0.84	0.10	83,83,83,83	0
57	MG	2A	3795	1/1	0.84	0.12	56,56,56,56	0
57	MG	1A	4073	1/1	0.84	0.16	73,73,73,73	0
57	MG	1A	3218	1/1	0.84	0.25	61,61,61,61	0
57	MG	1A	3883	1/1	0.84	0.17	64,64,64,64	0
57	MG	1A	3506	1/1	0.84	0.12	72,72,72,72	0
57	MG	1A	4014	1/1	0.84	0.18	68,68,68,68	0
57	MG	2A	3365	1/1	0.84	0.23	68,68,68,68	0
57	MG	1A	3597	1/1	0.84	0.16	56,56,56,56	0
57	MG	2A	3378	1/1	0.84	0.37	73,73,73,73	0
57	MG	2A	3650	1/1	0.84	0.28	80,80,80,80	0
57	MG	2A	3847	1/1	0.84	0.19	73,73,73,73	0
57	MG	1A	3965	1/1	0.84	0.13	39,39,39,39	0
57	MG	2A	3390	1/1	0.84	0.19	48,48,48,48	0
57	MG	2A	3670	1/1	0.84	0.16	77,77,77,77	0
57	MG	1A	3770	1/1	0.84	0.11	27,27,27,27	0
57	MG	1a	1666	1/1	0.84	0.15	72,72,72,72	0
57	MG	1a	1668	1/1	0.84	0.10	76,76,76,76	0
57	MG	1l	201	1/1	0.85	0.22	72,72,72,72	0
57	MG	1A	3574	1/1	0.85	0.32	50,50,50,50	0
57	MG	1A	3738	1/1	0.85	0.10	28,28,28,28	0
57	MG	1A	3576	1/1	0.85	0.10	36,36,36,36	0
57	MG	2A	3752	1/1	0.85	0.13	64,64,64,64	0
57	MG	2A	3379	1/1	0.85	0.11	68,68,68,68	0
57	MG	1a	1688	1/1	0.85	0.26	60,60,60,60	0
57	MG	1B	231	1/1	0.85	0.25	67,67,67,67	0
57	MG	2A	3767	1/1	0.85	0.15	53,53,53,53	0
57	MG	2A	3412	1/1	0.85	0.25	67,67,67,67	0
57	MG	1A	3877	1/1	0.85	0.25	29,29,29,29	0
57	MG	1A	3630	1/1	0.85	0.13	42,42,42,42	0
57	MG	2A	3036	1/1	0.85	0.37	74,74,74,74	0
57	MG	2A	3042	1/1	0.85	0.29	73,73,73,73	0
57	MG	1A	4030	1/1	0.85	0.11	51,51,51,51	0
57	MG	1S	203	1/1	0.85	0.13	73,73,73,73	0
57	MG	1a	1723	1/1	0.85	0.32	71,71,71,71	0
57	MG	1A	3966	1/1	0.85	0.11	42,42,42,42	0
57	MG	2A	3501	1/1	0.85	0.12	49,49,49,49	0
57	MG	2A	3097	1/1	0.85	0.27	71,71,71,71	0
57	MG	1A	3969	1/1	0.85	0.12	32,32,32,32	0
57	MG	2A	3837	1/1	0.85	0.15	40,40,40,40	0
57	MG	2A	3119	1/1	0.85	0.12	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3124	1/1	0.85	0.15	66,66,66,66	0
57	MG	2A	3141	1/1	0.85	0.28	61,61,61,61	0
57	MG	2A	3546	1/1	0.85	0.15	58,58,58,58	0
57	MG	2A	3555	1/1	0.85	0.28	61,61,61,61	0
57	MG	1A	3888	1/1	0.85	0.14	31,31,31,31	0
57	MG	2A	3166	1/1	0.85	0.21	74,74,74,74	0
57	MG	2A	3572	1/1	0.85	0.10	45,45,45,45	0
57	MG	1a	1739	1/1	0.85	0.15	64,64,64,64	0
57	MG	2E	302	1/1	0.85	0.29	63,63,63,63	0
57	MG	1A	3349	1/1	0.85	0.22	53,53,53,53	0
57	MG	1A	4045	1/1	0.85	0.25	66,66,66,66	0
57	MG	2R	201	1/1	0.85	0.15	54,54,54,54	0
57	MG	2T	201	1/1	0.85	0.15	59,59,59,59	0
57	MG	2A	3589	1/1	0.85	0.18	59,59,59,59	0
57	MG	2I	101	1/1	0.85	0.37	59,59,59,59	0
57	MG	2A	3235	1/1	0.85	0.31	59,59,59,59	0
57	MG	2A	3598	1/1	0.85	0.19	71,71,71,71	0
57	MG	2A	3247	1/1	0.85	0.26	64,64,64,64	0
57	MG	1a	1614	1/1	0.85	0.31	67,67,67,67	0
57	MG	2a	1616	1/1	0.85	0.14	73,73,73,73	0
57	MG	2A	3612	1/1	0.85	0.22	62,62,62,62	0
57	MG	2A	3257	1/1	0.85	0.27	69,69,69,69	0
57	MG	2a	1646	1/1	0.85	0.32	75,75,75,75	0
57	MG	1a	1621	1/1	0.85	0.34	73,73,73,73	0
57	MG	2A	3259	1/1	0.85	0.11	73,73,73,73	0
57	MG	1A	3894	1/1	0.85	0.08	81,81,81,81	0
57	MG	2A	3637	1/1	0.85	0.22	71,71,71,71	0
57	MG	1A	3826	1/1	0.85	0.12	66,66,66,66	0
57	MG	1a	1627	1/1	0.85	0.18	58,58,58,58	0
57	MG	2A	3646	1/1	0.85	0.14	54,54,54,54	0
57	MG	1A	3994	1/1	0.85	0.13	30,30,30,30	0
57	MG	2A	3282	1/1	0.85	0.16	62,62,62,62	0
57	MG	1a	1646	1/1	0.85	0.29	61,61,61,61	0
57	MG	2A	3662	1/1	0.85	0.21	61,61,61,61	0
57	MG	2A	3663	1/1	0.85	0.10	79,79,79,79	0
57	MG	2a	1732	1/1	0.85	0.20	77,77,77,77	0
57	MG	2A	3666	1/1	0.85	0.18	56,56,56,56	0
57	MG	2a	1742	1/1	0.85	0.28	68,68,68,68	0
57	MG	2a	1744	1/1	0.85	0.17	74,74,74,74	0
57	MG	2a	1754	1/1	0.85	0.15	77,77,77,77	0
57	MG	1A	4069	1/1	0.85	0.12	47,47,47,47	0
57	MG	1a	1655	1/1	0.85	0.21	77,77,77,77	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	3504	1/1	0.85	0.31	80,80,80,80	0
57	MG	1A	4077	1/1	0.85	0.16	66,66,66,66	0
57	MG	2A	3687	1/1	0.85	0.18	62,62,62,62	0
57	MG	2A	3700	1/1	0.85	0.14	58,58,58,58	0
57	MG	1A	3191	1/1	0.85	0.17	57,57,57,57	0
57	MG	2A	3708	1/1	0.85	0.13	65,65,65,65	0
57	MG	1A	3085	1/1	0.85	0.15	43,43,43,43	0
57	MG	1A	3864	1/1	0.85	0.12	30,30,30,30	0
57	MG	2A	3711	1/1	0.85	0.12	69,69,69,69	0
57	MG	2A	3341	1/1	0.85	0.26	73,73,73,73	0
57	MG	1A	4012	1/1	0.85	0.24	69,69,69,69	0
57	MG	2A	3355	1/1	0.85	0.16	67,67,67,67	0
57	MG	1A	4086	1/1	0.86	0.19	71,71,71,71	0
57	MG	2A	3554	1/1	0.86	0.15	68,68,68,68	0
57	MG	1A	3707	1/1	0.86	0.15	51,51,51,51	0
57	MG	1A	4095	1/1	0.86	0.15	59,59,59,59	0
57	MG	1A	3896	1/1	0.86	0.12	51,51,51,51	0
57	MG	1A	3711	1/1	0.86	0.14	62,62,62,62	0
57	MG	2A	3835	1/1	0.86	0.15	43,43,43,43	0
57	MG	2A	3262	1/1	0.86	0.15	68,68,68,68	0
57	MG	1A	3910	1/1	0.86	0.10	70,70,70,70	0
57	MG	2A	3840	1/1	0.86	0.23	70,70,70,70	0
57	MG	2A	3265	1/1	0.86	0.14	71,71,71,71	0
57	MG	2A	3267	1/1	0.86	0.21	64,64,64,64	0
57	MG	2A	3274	1/1	0.86	0.14	72,72,72,72	0
57	MG	1a	1667	1/1	0.86	0.28	70,70,70,70	0
57	MG	1A	3397	1/1	0.86	0.16	63,63,63,63	0
57	MG	2A	3279	1/1	0.86	0.15	77,77,77,77	0
57	MG	2B	212	1/1	0.86	0.18	85,85,85,85	0
57	MG	2A	3281	1/1	0.86	0.20	68,68,68,68	0
57	MG	1A	3356	1/1	0.86	0.26	63,63,63,63	0
57	MG	1A	3416	1/1	0.86	0.32	64,64,64,64	0
57	MG	2A	3631	1/1	0.86	0.36	81,81,81,81	0
57	MG	1A	3940	1/1	0.86	0.16	63,63,63,63	0
57	MG	1A	3836	1/1	0.86	0.14	54,54,54,54	0
57	MG	1a	1696	1/1	0.86	0.24	72,72,72,72	0
57	MG	1A	3739	1/1	0.86	0.12	33,33,33,33	0
57	MG	2A	3319	1/1	0.86	0.20	74,74,74,74	0
57	MG	1x	101	1/1	0.86	0.20	69,69,69,69	0
57	MG	1A	4031	1/1	0.86	0.14	51,51,51,51	0
57	MG	1A	3743	1/1	0.86	0.11	25,25,25,25	0
57	MG	2A	3333	1/1	0.86	0.20	75,75,75,75	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	1614	1/1	0.86	0.13	69,69,69,69	0
57	MG	2A	3661	1/1	0.86	0.11	46,46,46,46	0
57	MG	2a	1629	1/1	0.86	0.18	58,58,58,58	0
57	MG	2a	1632	1/1	0.86	0.23	64,64,64,64	0
57	MG	2A	3336	1/1	0.86	0.31	74,74,74,74	0
57	MG	1Y	202	1/1	0.86	0.14	62,62,62,62	0
57	MG	1A	3750	1/1	0.86	0.10	39,39,39,39	0
57	MG	1a	1718	1/1	0.86	0.22	73,73,73,73	0
57	MG	1A	3530	1/1	0.86	0.19	60,60,60,60	0
57	MG	2A	3058	1/1	0.86	0.12	64,64,64,64	0
57	MG	1a	1724	1/1	0.86	0.34	72,72,72,72	0
57	MG	2a	1672	1/1	0.86	0.25	58,58,58,58	0
57	MG	2A	3370	1/1	0.86	0.13	72,72,72,72	0
57	MG	2a	1678	1/1	0.86	0.25	73,73,73,73	0
57	MG	2A	3697	1/1	0.86	0.19	71,71,71,71	0
57	MG	2a	1683	1/1	0.86	0.20	71,71,71,71	0
57	MG	1A	3379	1/1	0.86	0.20	57,57,57,57	0
57	MG	1A	3634	1/1	0.86	0.07	29,29,29,29	0
57	MG	1a	1729	1/1	0.86	0.22	63,63,63,63	0
57	MG	2a	1709	1/1	0.86	0.15	55,55,55,55	0
57	MG	2a	1713	1/1	0.86	0.17	65,65,65,65	0
57	MG	2a	1715	1/1	0.86	0.22	50,50,50,50	0
57	MG	1A	3876	1/1	0.86	0.18	49,49,49,49	0
57	MG	2a	1721	1/1	0.86	0.18	61,61,61,61	0
57	MG	2a	1722	1/1	0.86	0.24	80,80,80,80	0
57	MG	1a	1731	1/1	0.86	0.09	64,64,64,64	0
57	MG	2A	3413	1/1	0.86	0.36	62,62,62,62	0
57	MG	2A	3420	1/1	0.86	0.37	69,69,69,69	0
57	MG	2a	1733	1/1	0.86	0.18	49,49,49,49	0
57	MG	2a	1739	1/1	0.86	0.10	66,66,66,66	0
57	MG	2A	3111	1/1	0.86	0.30	80,80,80,80	0
57	MG	1A	3467	1/1	0.86	0.19	54,54,54,54	0
57	MG	1A	3979	1/1	0.86	0.11	44,44,44,44	0
57	MG	1A	4065	1/1	0.86	0.14	39,39,39,39	0
57	MG	2A	3143	1/1	0.86	0.13	77,77,77,77	0
57	MG	1a	1746	1/1	0.86	0.22	66,66,66,66	0
57	MG	1A	3482	1/1	0.86	0.24	71,71,71,71	0
57	MG	2A	3483	1/1	0.86	0.12	42,42,42,42	0
57	MG	1a	1748	1/1	0.86	0.25	68,68,68,68	0
57	MG	1A	3686	1/1	0.86	0.24	62,62,62,62	0
57	MG	2A	3760	1/1	0.86	0.21	71,71,71,71	0
57	MG	2A	3503	1/1	0.86	0.23	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	3193	1/1	0.86	0.27	71,71,71,71	0
57	MG	2A	3507	1/1	0.86	0.18	56,56,56,56	0
57	MG	2g	201	1/1	0.86	0.12	75,75,75,75	0
57	MG	2A	3212	1/1	0.86	0.17	62,62,62,62	0
57	MG	1A	3380	1/1	0.86	0.14	63,63,63,63	0
57	MG	1a	1648	1/1	0.86	0.18	68,68,68,68	0
57	MG	1A	3706	1/1	0.86	0.17	61,61,61,61	0
57	MG	2A	3852	1/1	0.87	0.16	73,73,73,73	0
57	MG	1A	3487	1/1	0.87	0.12	54,54,54,54	0
57	MG	1A	3748	1/1	0.87	0.10	58,58,58,58	0
57	MG	2B	204	1/1	0.87	0.13	67,67,67,67	0
57	MG	2A	3362	1/1	0.87	0.29	74,74,74,74	0
57	MG	2A	3140	1/1	0.87	0.20	68,68,68,68	0
57	MG	1A	3442	1/1	0.87	0.20	71,71,71,71	0
57	MG	1F	305	1/1	0.87	0.17	48,48,48,48	0
57	MG	2D	307	1/1	0.87	0.14	59,59,59,59	0
57	MG	2A	3373	1/1	0.87	0.15	59,59,59,59	0
57	MG	2A	3374	1/1	0.87	0.12	58,58,58,58	0
57	MG	2E	308	1/1	0.87	0.23	72,72,72,72	0
57	MG	2A	3160	1/1	0.87	0.17	70,70,70,70	0
57	MG	2A	3658	1/1	0.87	0.19	58,58,58,58	0
57	MG	1a	1665	1/1	0.87	0.12	64,64,64,64	0
57	MG	1A	3620	1/1	0.87	0.14	60,60,60,60	0
57	MG	1A	3246	1/1	0.87	0.22	76,76,76,76	0
57	MG	1A	3183	1/1	0.87	0.13	45,45,45,45	0
57	MG	1A	3417	1/1	0.87	0.15	56,56,56,56	0
57	MG	10	104	1/1	0.87	0.25	66,66,66,66	0
57	MG	10	105	1/1	0.87	0.13	64,64,64,64	0
57	MG	2A	3675	1/1	0.87	0.13	40,40,40,40	0
57	MG	2A	3432	1/1	0.87	0.31	69,69,69,69	0
57	MG	1A	4015	1/1	0.87	0.10	36,36,36,36	0
57	MG	1a	1692	1/1	0.87	0.20	58,58,58,58	0
57	MG	1A	3656	1/1	0.87	0.18	48,48,48,48	0
57	MG	2A	3467	1/1	0.87	0.29	71,71,71,71	0
57	MG	2a	1643	1/1	0.87	0.19	65,65,65,65	0
57	MG	1a	1605	1/1	0.87	0.13	72,72,72,72	0
57	MG	1A	3972	1/1	0.87	0.15	51,51,51,51	0
57	MG	1a	1701	1/1	0.87	0.10	62,62,62,62	0
57	MG	1A	4091	1/1	0.87	0.24	63,63,63,63	0
57	MG	1A	4092	1/1	0.87	0.17	53,53,53,53	0
57	MG	2A	3489	1/1	0.87	0.16	48,48,48,48	0
57	MG	1a	1620	1/1	0.87	0.36	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1x	106	1/1	0.87	0.18	83,83,83,83	0
57	MG	2a	1677	1/1	0.87	0.14	77,77,77,77	0
57	MG	1A	3904	1/1	0.87	0.11	43,43,43,43	0
57	MG	2A	3727	1/1	0.87	0.12	69,69,69,69	0
57	MG	1a	1721	1/1	0.87	0.24	69,69,69,69	0
57	MG	2A	3013	1/1	0.87	0.38	78,78,78,78	0
57	MG	2A	3739	1/1	0.87	0.32	70,70,70,70	0
57	MG	1A	3662	1/1	0.87	0.11	26,26,26,26	0
57	MG	2a	1695	1/1	0.87	0.28	70,70,70,70	0
57	MG	2A	3529	1/1	0.87	0.21	46,46,46,46	0
57	MG	1A	3978	1/1	0.87	0.15	44,44,44,44	0
57	MG	2A	3533	1/1	0.87	0.16	79,79,79,79	0
57	MG	2A	3021	1/1	0.87	0.12	58,58,58,58	0
57	MG	2A	3029	1/1	0.87	0.12	53,53,53,53	0
57	MG	1a	1626	1/1	0.87	0.12	61,61,61,61	0
57	MG	1B	210	1/1	0.87	0.25	49,49,49,49	0
57	MG	2A	3786	1/1	0.87	0.16	52,52,52,52	0
57	MG	2A	3556	1/1	0.87	0.16	61,61,61,61	0
57	MG	1a	1635	1/1	0.87	0.20	74,74,74,74	0
57	MG	1a	1637	1/1	0.87	0.26	73,73,73,73	0
57	MG	2A	3804	1/1	0.87	0.15	42,42,42,42	0
57	MG	2A	3805	1/1	0.87	0.11	50,50,50,50	0
57	MG	1B	213	1/1	0.87	0.18	55,55,55,55	0
57	MG	2a	1751	1/1	0.87	0.42	74,74,74,74	0
57	MG	2a	1752	1/1	0.87	0.24	71,71,71,71	0
57	MG	2A	3810	1/1	0.87	0.18	74,74,74,74	0
57	MG	2A	3812	1/1	0.87	0.14	70,70,70,70	0
57	MG	2A	3076	1/1	0.87	0.32	65,65,65,65	0
57	MG	2A	3580	1/1	0.87	0.09	51,51,51,51	0
57	MG	2a	1770	1/1	0.87	0.15	77,77,77,77	0
57	MG	2A	3083	1/1	0.87	0.15	66,66,66,66	0
57	MG	2A	3084	1/1	0.87	0.15	75,75,75,75	0
57	MG	1A	3734	1/1	0.87	0.12	27,27,27,27	0
57	MG	2A	3331	1/1	0.87	0.18	61,61,61,61	0
57	MG	2A	3825	1/1	0.87	0.15	68,68,68,68	0
57	MG	1A	3920	1/1	0.87	0.18	38,38,38,38	0
57	MG	1A	3678	1/1	0.87	0.12	38,38,38,38	0
57	MG	1A	3523	1/1	0.87	0.24	62,62,62,62	0
57	MG	1a	1657	1/1	0.87	0.17	73,73,73,73	0
57	MG	2q	202	1/1	0.87	0.21	72,72,72,72	0
57	MG	2A	3622	1/1	0.87	0.36	66,66,66,66	0
57	MG	2A	3348	1/1	0.87	0.10	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	2A	3350	1/1	0.87	0.18	71,71,71,71	0
57	MG	2A	3091	1/1	0.88	0.21	69,69,69,69	0
57	MG	1A	3971	1/1	0.88	0.10	56,56,56,56	0
57	MG	1A	3891	1/1	0.88	0.10	52,52,52,52	0
57	MG	1A	3343	1/1	0.88	0.21	75,75,75,75	0
57	MG	2A	3107	1/1	0.88	0.39	72,72,72,72	0
57	MG	2A	3638	1/1	0.88	0.14	70,70,70,70	0
57	MG	1a	1765	1/1	0.88	0.15	68,68,68,68	0
57	MG	2B	209	1/1	0.88	0.27	73,73,73,73	0
57	MG	1A	3976	1/1	0.88	0.12	56,56,56,56	0
57	MG	2A	3643	1/1	0.88	0.15	65,65,65,65	0
57	MG	2A	3644	1/1	0.88	0.17	69,69,69,69	0
57	MG	2B	219	1/1	0.88	0.23	73,73,73,73	0
57	MG	2A	3120	1/1	0.88	0.14	60,60,60,60	0
57	MG	1a	1672	1/1	0.88	0.10	60,60,60,60	0
57	MG	1A	3345	1/1	0.88	0.24	65,65,65,65	0
57	MG	2A	3654	1/1	0.88	0.14	69,69,69,69	0
57	MG	2A	3655	1/1	0.88	0.11	42,42,42,42	0
57	MG	1A	3455	1/1	0.88	0.11	53,53,53,53	0
57	MG	1a	1678	1/1	0.88	0.22	60,60,60,60	0
57	MG	2A	3377	1/1	0.88	0.16	64,64,64,64	0
57	MG	1a	1776	1/1	0.88	0.24	57,57,57,57	0
57	MG	2Z	301	1/1	0.88	0.12	74,74,74,74	0
57	MG	1a	1779	1/1	0.88	0.14	50,50,50,50	0
57	MG	23	102	1/1	0.88	0.23	61,61,61,61	0
57	MG	1A	3204	1/1	0.88	0.12	73,73,73,73	0
57	MG	2A	3170	1/1	0.88	0.18	74,74,74,74	0
57	MG	1a	1790	1/1	0.88	0.20	79,79,79,79	0
57	MG	1a	1684	1/1	0.88	0.14	69,69,69,69	0
57	MG	2A	3418	1/1	0.88	0.20	67,67,67,67	0
57	MG	1a	1801	1/1	0.88	0.13	63,63,63,63	0
57	MG	1a	1686	1/1	0.88	0.17	79,79,79,79	0
57	MG	2A	3217	1/1	0.88	0.22	66,66,66,66	0
57	MG	2A	3233	1/1	0.88	0.14	73,73,73,73	0
57	MG	2a	1641	1/1	0.88	0.24	70,70,70,70	0
57	MG	1A	3025	1/1	0.88	0.14	59,59,59,59	0
57	MG	2A	3446	1/1	0.88	0.14	52,52,52,52	0
57	MG	1a	1806	1/1	0.88	0.12	62,62,62,62	0
57	MG	2A	3237	1/1	0.88	0.13	74,74,74,74	0
57	MG	2A	3468	1/1	0.88	0.14	54,54,54,54	0
57	MG	2A	3469	1/1	0.88	0.18	57,57,57,57	0
57	MG	2A	3245	1/1	0.88	0.19	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3246	1/1	0.88	0.14	60,60,60,60	0
57	MG	2a	1673	1/1	0.88	0.37	73,73,73,73	0
57	MG	1A	3732	1/1	0.88	0.14	54,54,54,54	0
57	MG	2A	3725	1/1	0.88	0.21	72,72,72,72	0
57	MG	2A	3726	1/1	0.88	0.17	65,65,65,65	0
57	MG	2A	3249	1/1	0.88	0.17	70,70,70,70	0
57	MG	1a	1808	1/1	0.88	0.16	66,66,66,66	0
57	MG	1A	3827	1/1	0.88	0.14	31,31,31,31	0
57	MG	2A	3736	1/1	0.88	0.13	66,66,66,66	0
57	MG	1A	3097	1/1	0.88	0.27	67,67,67,67	0
57	MG	2A	3741	1/1	0.88	0.14	48,48,48,48	0
57	MG	2a	1698	1/1	0.88	0.23	69,69,69,69	0
57	MG	2a	1708	1/1	0.88	0.17	63,63,63,63	0
57	MG	1A	3376	1/1	0.88	0.19	41,41,41,41	0
57	MG	1A	3290	1/1	0.88	0.27	60,60,60,60	0
57	MG	1a	1707	1/1	0.88	0.15	64,64,64,64	0
57	MG	1A	3638	1/1	0.88	0.08	33,33,33,33	0
57	MG	1A	3929	1/1	0.88	0.11	48,48,48,48	0
57	MG	1A	3939	1/1	0.88	0.14	74,74,74,74	0
57	MG	1B	203	1/1	0.88	0.18	64,64,64,64	0
57	MG	2A	3769	1/1	0.88	0.12	74,74,74,74	0
57	MG	2A	3771	1/1	0.88	0.20	77,77,77,77	0
57	MG	2A	3275	1/1	0.88	0.10	66,66,66,66	0
57	MG	1A	3298	1/1	0.88	0.23	61,61,61,61	0
57	MG	1a	1722	1/1	0.88	0.14	68,68,68,68	0
57	MG	1A	3947	1/1	0.88	0.22	65,65,65,65	0
57	MG	2A	3792	1/1	0.88	0.21	40,40,40,40	0
57	MG	2a	1746	1/1	0.88	0.14	61,61,61,61	0
57	MG	2a	1747	1/1	0.88	0.25	62,62,62,62	0
57	MG	2A	3793	1/1	0.88	0.12	42,42,42,42	0
57	MG	1A	3323	1/1	0.88	0.26	58,58,58,58	0
57	MG	1a	1642	1/1	0.88	0.10	80,80,80,80	0
57	MG	1A	3326	1/1	0.88	0.15	56,56,56,56	0
57	MG	2A	3286	1/1	0.88	0.24	74,74,74,74	0
57	MG	2a	1760	1/1	0.88	0.19	68,68,68,68	0
57	MG	1A	3954	1/1	0.88	0.11	65,65,65,65	0
57	MG	2A	3576	1/1	0.88	0.22	71,71,71,71	0
57	MG	1A	3412	1/1	0.88	0.23	63,63,63,63	0
57	MG	2A	3051	1/1	0.88	0.10	64,64,64,64	0
57	MG	2A	3308	1/1	0.88	0.21	54,54,54,54	0
57	MG	1A	3331	1/1	0.88	0.30	72,72,72,72	0
57	MG	1a	1733	1/1	0.88	0.15	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3822	1/1	0.88	0.11	75,75,75,75	0
57	MG	1E	306	1/1	0.88	0.19	58,58,58,58	0
57	MG	2f	201	1/1	0.88	0.16	59,59,59,59	0
57	MG	2A	3061	1/1	0.88	0.21	57,57,57,57	0
57	MG	1A	4033	1/1	0.88	0.12	38,38,38,38	0
57	MG	2A	3324	1/1	0.88	0.11	69,69,69,69	0
57	MG	1A	3198	1/1	0.88	0.10	43,43,43,43	0
57	MG	1A	3439	1/1	0.88	0.48	46,46,46,46	0
57	MG	1A	3698	1/1	0.88	0.15	62,62,62,62	0
57	MG	1a	1759	1/1	0.89	0.10	60,60,60,60	0
57	MG	2A	3581	1/1	0.89	0.17	62,62,62,62	0
57	MG	1A	3444	1/1	0.89	0.25	49,49,49,49	0
57	MG	2A	3096	1/1	0.89	0.23	74,74,74,74	0
57	MG	2A	3828	1/1	0.89	0.10	56,56,56,56	0
57	MG	1A	3852	1/1	0.89	0.10	32,32,32,32	0
57	MG	1A	3948	1/1	0.89	0.18	61,61,61,61	0
57	MG	2A	3595	1/1	0.89	0.15	71,71,71,71	0
57	MG	2A	3104	1/1	0.89	0.21	62,62,62,62	0
57	MG	2A	3329	1/1	0.89	0.17	71,71,71,71	0
57	MG	2A	3842	1/1	0.89	0.18	58,58,58,58	0
57	MG	2A	3844	1/1	0.89	0.21	73,73,73,73	0
57	MG	2A	3846	1/1	0.89	0.14	57,57,57,57	0
57	MG	2A	3610	1/1	0.89	0.16	54,54,54,54	0
57	MG	2A	3849	1/1	0.89	0.16	50,50,50,50	0
57	MG	2A	3330	1/1	0.89	0.14	63,63,63,63	0
57	MG	1a	1769	1/1	0.89	0.18	64,64,64,64	0
57	MG	2A	3110	1/1	0.89	0.16	50,50,50,50	0
57	MG	1A	3136	1/1	0.89	0.12	42,42,42,42	0
57	MG	1A	3855	1/1	0.89	0.11	28,28,28,28	0
57	MG	2A	3628	1/1	0.89	0.13	70,70,70,70	0
57	MG	2A	3342	1/1	0.89	0.15	60,60,60,60	0
57	MG	2A	3343	1/1	0.89	0.22	66,66,66,66	0
57	MG	1A	3953	1/1	0.89	0.14	52,52,52,52	0
57	MG	1G	202	1/1	0.89	0.17	66,66,66,66	0
57	MG	1O	203	1/1	0.89	0.10	59,59,59,59	0
57	MG	2D	303	1/1	0.89	0.17	65,65,65,65	0
57	MG	2A	3352	1/1	0.89	0.13	76,76,76,76	0
57	MG	2A	3641	1/1	0.89	0.19	73,73,73,73	0
57	MG	2A	3354	1/1	0.89	0.33	73,73,73,73	0
57	MG	1A	3367	1/1	0.89	0.18	53,53,53,53	0
57	MG	1A	3765	1/1	0.89	0.14	57,57,57,57	0
57	MG	2A	3156	1/1	0.89	0.31	76,76,76,76	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	3648	1/1	0.89	0.17	84,84,84,84	0
57	MG	1a	1785	1/1	0.89	0.17	70,70,70,70	0
57	MG	1A	3611	1/1	0.89	0.09	22,22,22,22	0
57	MG	2W	201	1/1	0.89	0.15	58,58,58,58	0
57	MG	2A	3653	1/1	0.89	0.09	61,61,61,61	0
57	MG	1A	3958	1/1	0.89	0.11	74,74,74,74	0
57	MG	1a	1800	1/1	0.89	0.19	57,57,57,57	0
57	MG	2A	3180	1/1	0.89	0.13	73,73,73,73	0
57	MG	1A	3514	1/1	0.89	0.25	58,58,58,58	0
57	MG	1A	3462	1/1	0.89	0.13	63,63,63,63	0
57	MG	1A	3524	1/1	0.89	0.30	59,59,59,59	0
57	MG	2a	1611	1/1	0.89	0.23	67,67,67,67	0
57	MG	2A	3201	1/1	0.89	0.15	61,61,61,61	0
57	MG	2A	3202	1/1	0.89	0.11	68,68,68,68	0
57	MG	2a	1624	1/1	0.89	0.28	71,71,71,71	0
57	MG	2a	1626	1/1	0.89	0.32	67,67,67,67	0
57	MG	2A	3391	1/1	0.89	0.21	59,59,59,59	0
57	MG	2A	3392	1/1	0.89	0.49	65,65,65,65	0
57	MG	2A	3402	1/1	0.89	0.27	60,60,60,60	0
57	MG	2a	1636	1/1	0.89	0.22	67,67,67,67	0
57	MG	2a	1638	1/1	0.89	0.23	69,69,69,69	0
57	MG	2A	3203	1/1	0.89	0.26	71,71,71,71	0
57	MG	1A	3793	1/1	0.89	0.10	32,32,32,32	0
57	MG	1a	1601	1/1	0.89	0.17	63,63,63,63	0
57	MG	2A	3689	1/1	0.89	0.10	60,60,60,60	0
57	MG	2A	3693	1/1	0.89	0.15	67,67,67,67	0
57	MG	2A	3695	1/1	0.89	0.10	47,47,47,47	0
57	MG	2A	3696	1/1	0.89	0.19	65,65,65,65	0
57	MG	1A	3800	1/1	0.89	0.19	55,55,55,55	0
57	MG	2A	3698	1/1	0.89	0.12	56,56,56,56	0
57	MG	2A	3421	1/1	0.89	0.26	59,59,59,59	0
57	MG	1A	4064	1/1	0.89	0.10	58,58,58,58	0
57	MG	2A	3428	1/1	0.89	0.22	59,59,59,59	0
57	MG	1A	3071	1/1	0.89	0.23	66,66,66,66	0
57	MG	2a	1679	1/1	0.89	0.20	60,60,60,60	0
57	MG	2a	1681	1/1	0.89	0.36	66,66,66,66	0
57	MG	2A	3435	1/1	0.89	0.13	69,69,69,69	0
57	MG	1A	3975	1/1	0.89	0.14	42,42,42,42	0
57	MG	2A	3239	1/1	0.89	0.20	62,62,62,62	0
57	MG	1A	3803	1/1	0.89	0.39	64,64,64,64	0
57	MG	1a	1717	1/1	0.89	0.16	53,53,53,53	0
57	MG	2A	3717	1/1	0.89	0.11	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3572	1/1	0.89	0.28	62,62,62,62	0
57	MG	1A	4079	1/1	0.89	0.12	66,66,66,66	0
57	MG	1x	105	1/1	0.89	0.22	74,74,74,74	0
57	MG	1A	3721	1/1	0.89	0.16	50,50,50,50	0
57	MG	1x	109	1/1	0.89	0.13	55,55,55,55	0
57	MG	1A	3027	1/1	0.89	0.13	41,41,41,41	0
57	MG	2A	3734	1/1	0.89	0.13	63,63,63,63	0
57	MG	2A	3477	1/1	0.89	0.15	54,54,54,54	0
57	MG	2A	3480	1/1	0.89	0.16	61,61,61,61	0
57	MG	2a	1726	1/1	0.89	0.14	58,58,58,58	0
57	MG	2A	3740	1/1	0.89	0.14	78,78,78,78	0
57	MG	1A	4089	1/1	0.89	0.13	58,58,58,58	0
57	MG	2A	3261	1/1	0.89	0.14	76,76,76,76	0
57	MG	1A	3317	1/1	0.89	0.20	53,53,53,53	0
57	MG	2A	3493	1/1	0.89	0.18	69,69,69,69	0
57	MG	2A	3756	1/1	0.89	0.14	70,70,70,70	0
57	MG	1A	3736	1/1	0.89	0.07	26,26,26,26	0
57	MG	1A	3822	1/1	0.89	0.12	58,58,58,58	0
57	MG	1A	3353	1/1	0.89	0.13	45,45,45,45	0
57	MG	2a	1750	1/1	0.89	0.14	73,73,73,73	0
57	MG	1A	3587	1/1	0.89	0.12	31,31,31,31	0
57	MG	2A	3768	1/1	0.89	0.10	59,59,59,59	0
57	MG	1A	4001	1/1	0.89	0.17	50,50,50,50	0
57	MG	1a	1738	1/1	0.89	0.15	66,66,66,66	0
57	MG	2A	3780	1/1	0.89	0.14	63,63,63,63	0
57	MG	2A	3047	1/1	0.89	0.24	69,69,69,69	0
57	MG	1A	3588	1/1	0.89	0.08	38,38,38,38	0
57	MG	2a	1768	1/1	0.89	0.33	70,70,70,70	0
57	MG	1a	1653	1/1	0.89	0.17	66,66,66,66	0
57	MG	1A	3745	1/1	0.89	0.12	26,26,26,26	0
57	MG	2A	3539	1/1	0.89	0.15	39,39,39,39	0
57	MG	2a	1775	1/1	0.89	0.25	59,59,59,59	0
57	MG	1B	214	1/1	0.89	0.07	59,59,59,59	0
57	MG	1A	3837	1/1	0.89	0.15	56,56,56,56	0
57	MG	2A	3800	1/1	0.89	0.12	66,66,66,66	0
57	MG	1A	3938	1/1	0.89	0.08	26,26,26,26	0
57	MG	2A	3295	1/1	0.89	0.22	58,58,58,58	0
57	MG	1A	3841	1/1	0.89	0.12	58,58,58,58	0
57	MG	2A	3297	1/1	0.89	0.12	64,64,64,64	0
57	MG	2A	3571	1/1	0.89	0.21	61,61,61,61	0
57	MG	2n	101	1/1	0.89	0.19	77,77,77,77	0
57	MG	2A	3301	1/1	0.89	0.14	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	3573	1/1	0.89	0.18	61,61,61,61	0
57	MG	1a	1756	1/1	0.89	0.19	75,75,75,75	0
57	MG	2x	102	1/1	0.89	0.19	65,65,65,65	0
57	MG	1a	1758	1/1	0.89	0.10	69,69,69,69	0
57	MG	2A	3634	1/1	0.90	0.16	69,69,69,69	0
57	MG	2A	3376	1/1	0.90	0.10	66,66,66,66	0
57	MG	1a	1796	1/1	0.90	0.14	71,71,71,71	0
57	MG	1B	235	1/1	0.90	0.17	81,81,81,81	0
57	MG	1D	312	1/1	0.90	0.25	63,63,63,63	0
57	MG	1A	3934	1/1	0.90	0.14	61,61,61,61	0
57	MG	2A	3382	1/1	0.90	0.13	69,69,69,69	0
57	MG	2A	3386	1/1	0.90	0.23	49,49,49,49	0
57	MG	1A	4022	1/1	0.90	0.16	65,65,65,65	0
57	MG	2A	3230	1/1	0.90	0.15	65,65,65,65	0
57	MG	2B	216	1/1	0.90	0.11	72,72,72,72	0
57	MG	1A	3315	1/1	0.90	0.22	52,52,52,52	0
57	MG	2A	3396	1/1	0.90	0.23	72,72,72,72	0
57	MG	2D	302	1/1	0.90	0.22	56,56,56,56	0
57	MG	2A	3652	1/1	0.90	0.16	48,48,48,48	0
57	MG	2A	3400	1/1	0.90	0.15	56,56,56,56	0
57	MG	1A	3120	1/1	0.90	0.19	56,56,56,56	0
57	MG	2A	3406	1/1	0.90	0.29	58,58,58,58	0
57	MG	2A	3408	1/1	0.90	0.38	64,64,64,64	0
57	MG	1F	312	1/1	0.90	0.13	58,58,58,58	0
57	MG	2N	201	1/1	0.90	0.14	63,63,63,63	0
57	MG	1a	1687	1/1	0.90	0.14	69,69,69,69	0
57	MG	2A	3414	1/1	0.90	0.13	71,71,71,71	0
57	MG	2A	3415	1/1	0.90	0.32	64,64,64,64	0
57	MG	1F	315	1/1	0.90	0.14	58,58,58,58	0
57	MG	2A	3241	1/1	0.90	0.21	68,68,68,68	0
57	MG	1a	1689	1/1	0.90	0.25	59,59,59,59	0
57	MG	1A	3541	1/1	0.90	0.33	59,59,59,59	0
57	MG	1G	205	1/1	0.90	0.22	65,65,65,65	0
57	MG	2A	3682	1/1	0.90	0.11	59,59,59,59	0
57	MG	2A	3683	1/1	0.90	0.12	57,57,57,57	0
57	MG	1A	3560	1/1	0.90	0.10	62,62,62,62	0
57	MG	2A	3433	1/1	0.90	0.18	60,60,60,60	0
57	MG	2A	3250	1/1	0.90	0.17	59,59,59,59	0
57	MG	2A	3691	1/1	0.90	0.17	75,75,75,75	0
57	MG	2a	1615	1/1	0.90	0.13	66,66,66,66	0
57	MG	1A	3669	1/1	0.90	0.13	40,40,40,40	0
57	MG	2a	1619	1/1	0.90	0.15	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	3439	1/1	0.90	0.15	58,58,58,58	0
57	MG	2a	1625	1/1	0.90	0.24	70,70,70,70	0
57	MG	1Q	206	1/1	0.90	0.13	58,58,58,58	0
57	MG	2a	1628	1/1	0.90	0.13	57,57,57,57	0
57	MG	2A	3445	1/1	0.90	0.11	68,68,68,68	0
57	MG	2a	1630	1/1	0.90	0.18	59,59,59,59	0
57	MG	1A	3843	1/1	0.90	0.09	41,41,41,41	0
57	MG	1T	203	1/1	0.90	0.20	64,64,64,64	0
57	MG	1a	1711	1/1	0.90	0.19	63,63,63,63	0
57	MG	2a	1637	1/1	0.90	0.34	67,67,67,67	0
57	MG	2A	3002	1/1	0.90	0.34	71,71,71,71	0
57	MG	1A	3844	1/1	0.90	0.21	40,40,40,40	0
57	MG	1A	3322	1/1	0.90	0.12	47,47,47,47	0
57	MG	10	102	1/1	0.90	0.12	54,54,54,54	0
57	MG	1A	3755	1/1	0.90	0.09	24,24,24,24	0
57	MG	2a	1648	1/1	0.90	0.23	69,69,69,69	0
57	MG	2A	3473	1/1	0.90	0.26	69,69,69,69	0
57	MG	1A	3369	1/1	0.90	0.14	56,56,56,56	0
57	MG	1l	102	1/1	0.90	0.11	62,62,62,62	0
57	MG	2a	1666	1/1	0.90	0.21	66,66,66,66	0
57	MG	2a	1667	1/1	0.90	0.17	60,60,60,60	0
57	MG	1A	4044	1/1	0.90	0.07	23,23,23,23	0
57	MG	2A	3723	1/1	0.90	0.12	70,70,70,70	0
57	MG	1A	3243	1/1	0.90	0.19	54,54,54,54	0
57	MG	1A	3038	1/1	0.90	0.15	58,58,58,58	0
57	MG	1a	1726	1/1	0.90	0.20	58,58,58,58	0
57	MG	2A	3500	1/1	0.90	0.12	39,39,39,39	0
57	MG	1a	1602	1/1	0.90	0.26	78,78,78,78	0
57	MG	1A	3961	1/1	0.90	0.13	52,52,52,52	0
57	MG	1A	3276	1/1	0.90	0.14	59,59,59,59	0
57	MG	1A	3468	1/1	0.90	0.15	59,59,59,59	0
57	MG	1A	3967	1/1	0.90	0.13	25,25,25,25	0
57	MG	2a	1688	1/1	0.90	0.24	73,73,73,73	0
57	MG	1A	3394	1/1	0.90	0.13	58,58,58,58	0
57	MG	2a	1692	1/1	0.90	0.14	71,71,71,71	0
57	MG	2A	3513	1/1	0.90	0.16	64,64,64,64	0
57	MG	2A	3751	1/1	0.90	0.13	41,41,41,41	0
57	MG	2a	1697	1/1	0.90	0.09	70,70,70,70	0
57	MG	2A	3515	1/1	0.90	0.09	64,64,64,64	0
57	MG	2A	3517	1/1	0.90	0.12	46,46,46,46	0
57	MG	2A	3526	1/1	0.90	0.12	71,71,71,71	0
57	MG	1A	3594	1/1	0.90	0.08	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3795	1/1	0.90	0.13	38,38,38,38	0
57	MG	2A	3303	1/1	0.90	0.18	64,64,64,64	0
57	MG	2A	3761	1/1	0.90	0.16	48,48,48,48	0
57	MG	2A	3089	1/1	0.90	0.12	47,47,47,47	0
57	MG	1A	3796	1/1	0.90	0.18	43,43,43,43	0
57	MG	1A	3885	1/1	0.90	0.28	42,42,42,42	0
57	MG	2A	3313	1/1	0.90	0.39	70,70,70,70	0
57	MG	1A	3799	1/1	0.90	0.10	42,42,42,42	0
57	MG	1a	1629	1/1	0.90	0.43	77,77,77,77	0
57	MG	2A	3557	1/1	0.90	0.15	58,58,58,58	0
57	MG	1A	3889	1/1	0.90	0.13	35,35,35,35	0
57	MG	1a	1753	1/1	0.90	0.11	81,81,81,81	0
57	MG	2A	3567	1/1	0.90	0.23	55,55,55,55	0
57	MG	1A	3710	1/1	0.90	0.10	53,53,53,53	0
57	MG	2A	3794	1/1	0.90	0.09	54,54,54,54	0
57	MG	1A	3278	1/1	0.90	0.13	50,50,50,50	0
57	MG	1A	3287	1/1	0.90	0.10	53,53,53,53	0
57	MG	2A	3803	1/1	0.90	0.15	59,59,59,59	0
57	MG	2A	3114	1/1	0.90	0.15	73,73,73,73	0
57	MG	1A	3809	1/1	0.90	0.12	54,54,54,54	0
57	MG	1A	3289	1/1	0.90	0.31	60,60,60,60	0
57	MG	2a	1759	1/1	0.90	0.22	80,80,80,80	0
57	MG	1A	3165	1/1	0.90	0.23	63,63,63,63	0
57	MG	1B	209	1/1	0.90	0.36	67,67,67,67	0
57	MG	2a	1767	1/1	0.90	0.34	71,71,71,71	0
57	MG	1A	3724	1/1	0.90	0.12	46,46,46,46	0
57	MG	2a	1769	1/1	0.90	0.20	59,59,59,59	0
57	MG	1A	3175	1/1	0.90	0.14	40,40,40,40	0
57	MG	1A	3819	1/1	0.90	0.14	53,53,53,53	0
57	MG	1A	4006	1/1	0.90	0.09	61,61,61,61	0
57	MG	1A	3429	1/1	0.90	0.12	65,65,65,65	0
57	MG	1a	1778	1/1	0.90	0.15	75,75,75,75	0
57	MG	2A	3609	1/1	0.90	0.14	37,37,37,37	0
57	MG	1A	3430	1/1	0.90	0.21	59,59,59,59	0
57	MG	2a	1781	1/1	0.90	0.20	82,82,82,82	0
57	MG	2A	3176	1/1	0.90	0.23	58,58,58,58	0
57	MG	2A	3830	1/1	0.90	0.14	54,54,54,54	0
57	MG	1B	225	1/1	0.90	0.09	66,66,66,66	0
57	MG	2A	3617	1/1	0.90	0.11	57,57,57,57	0
57	MG	1B	229	1/1	0.90	0.09	61,61,61,61	0
57	MG	2l	201	1/1	0.90	0.14	65,65,65,65	0
57	MG	1A	3825	1/1	0.90	0.10	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3369	1/1	0.90	0.23	50,50,50,50	0
57	MG	2A	3192	1/1	0.90	0.23	71,71,71,71	0
57	MG	1A	3737	1/1	0.90	0.11	43,43,43,43	0
57	MG	2A	3200	1/1	0.90	0.27	66,66,66,66	0
57	MG	2x	103	1/1	0.90	0.12	68,68,68,68	0
57	MG	2x	104	1/1	0.90	0.15	69,69,69,69	0
57	MG	2A	3375	1/1	0.90	0.12	73,73,73,73	0
58	K	1A	3543	1/1	0.90	0.12	81,81,81,81	0
57	MG	1A	3557	1/1	0.91	0.11	40,40,40,40	0
57	MG	1A	3831	1/1	0.91	0.20	35,35,35,35	0
57	MG	2A	3831	1/1	0.91	0.12	39,39,39,39	0
57	MG	2A	3832	1/1	0.91	0.21	56,56,56,56	0
57	MG	1a	1673	1/1	0.91	0.19	64,64,64,64	0
57	MG	1a	1674	1/1	0.91	0.16	77,77,77,77	0
57	MG	1A	3284	1/1	0.91	0.15	59,59,59,59	0
57	MG	1A	3712	1/1	0.91	0.12	55,55,55,55	0
57	MG	2A	3284	1/1	0.91	0.26	66,66,66,66	0
57	MG	1a	1677	1/1	0.91	0.22	64,64,64,64	0
57	MG	1A	3567	1/1	0.91	0.20	77,77,77,77	0
57	MG	1A	3973	1/1	0.91	0.14	59,59,59,59	0
57	MG	2A	3005	1/1	0.91	0.24	60,60,60,60	0
57	MG	1A	3432	1/1	0.91	0.13	65,65,65,65	0
57	MG	2A	3850	1/1	0.91	0.10	72,72,72,72	0
57	MG	1A	3285	1/1	0.91	0.33	66,66,66,66	0
57	MG	2A	3300	1/1	0.91	0.26	65,65,65,65	0
57	MG	1A	3440	1/1	0.91	0.21	59,59,59,59	0
57	MG	2A	3302	1/1	0.91	0.36	70,70,70,70	0
57	MG	1A	3725	1/1	0.91	0.08	55,55,55,55	0
57	MG	2A	3026	1/1	0.91	0.14	64,64,64,64	0
57	MG	2B	206	1/1	0.91	0.24	75,75,75,75	0
57	MG	2B	208	1/1	0.91	0.20	63,63,63,63	0
57	MG	2A	3027	1/1	0.91	0.20	56,56,56,56	0
57	MG	2A	3028	1/1	0.91	0.10	58,58,58,58	0
57	MG	2B	211	1/1	0.91	0.22	68,68,68,68	0
57	MG	1A	3728	1/1	0.91	0.17	61,61,61,61	0
57	MG	2A	3317	1/1	0.91	0.11	69,69,69,69	0
57	MG	1a	1690	1/1	0.91	0.31	57,57,57,57	0
57	MG	1A	3731	1/1	0.91	0.09	17,17,17,17	0
57	MG	2A	3043	1/1	0.91	0.08	60,60,60,60	0
57	MG	2A	3615	1/1	0.91	0.09	66,66,66,66	0
57	MG	2A	3044	1/1	0.91	0.35	62,62,62,62	0
57	MG	1A	3580	1/1	0.91	0.07	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	3048	1/1	0.91	0.10	54,54,54,54	0
57	MG	2E	305	1/1	0.91	0.10	36,36,36,36	0
57	MG	1A	3054	1/1	0.91	0.08	32,32,32,32	0
57	MG	2F	302	1/1	0.91	0.20	44,44,44,44	0
57	MG	2A	3055	1/1	0.91	0.14	53,53,53,53	0
57	MG	2A	3629	1/1	0.91	0.12	76,76,76,76	0
57	MG	2A	3056	1/1	0.91	0.13	56,56,56,56	0
57	MG	1A	3057	1/1	0.91	0.47	59,59,59,59	0
57	MG	1A	3872	1/1	0.91	0.11	68,68,68,68	0
57	MG	1A	3354	1/1	0.91	0.18	53,53,53,53	0
57	MG	2U	201	1/1	0.91	0.16	59,59,59,59	0
57	MG	1A	3589	1/1	0.91	0.14	18,18,18,18	0
57	MG	1a	1709	1/1	0.91	0.14	69,69,69,69	0
57	MG	2A	3078	1/1	0.91	0.17	62,62,62,62	0
57	MG	1A	3452	1/1	0.91	0.27	62,62,62,62	0
57	MG	2A	3351	1/1	0.91	0.24	68,68,68,68	0
57	MG	2a	1602	1/1	0.91	0.22	64,64,64,64	0
57	MG	1a	1712	1/1	0.91	0.12	51,51,51,51	0
57	MG	1A	3879	1/1	0.91	0.08	43,43,43,43	0
57	MG	1F	316	1/1	0.91	0.15	47,47,47,47	0
57	MG	1A	3151	1/1	0.91	0.30	44,44,44,44	0
57	MG	2A	3649	1/1	0.91	0.12	51,51,51,51	0
57	MG	1A	3160	1/1	0.91	0.13	61,61,61,61	0
57	MG	2A	3363	1/1	0.91	0.10	63,63,63,63	0
57	MG	2a	1618	1/1	0.91	0.30	65,65,65,65	0
57	MG	1I	201	1/1	0.91	0.12	68,68,68,68	0
57	MG	1A	3299	1/1	0.91	0.22	54,54,54,54	0
57	MG	2A	3368	1/1	0.91	0.12	64,64,64,64	0
57	MG	1A	3314	1/1	0.91	0.12	57,57,57,57	0
57	MG	1Q	204	1/1	0.91	0.08	52,52,52,52	0
57	MG	2A	3106	1/1	0.91	0.29	60,60,60,60	0
57	MG	1A	3890	1/1	0.91	0.29	37,37,37,37	0
57	MG	2A	3108	1/1	0.91	0.32	66,66,66,66	0
57	MG	1A	4017	1/1	0.91	0.15	54,54,54,54	0
57	MG	1A	3469	1/1	0.91	0.33	67,67,67,67	0
57	MG	1A	3614	1/1	0.91	0.15	64,64,64,64	0
57	MG	2A	3671	1/1	0.91	0.11	57,57,57,57	0
57	MG	2a	1640	1/1	0.91	0.32	70,70,70,70	0
57	MG	2A	3116	1/1	0.91	0.32	69,69,69,69	0
57	MG	1A	3474	1/1	0.91	0.10	63,63,63,63	0
57	MG	1Z	301	1/1	0.91	0.09	62,62,62,62	0
57	MG	2A	3385	1/1	0.91	0.33	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	4027	1/1	0.91	0.09	47,47,47,47	0
57	MG	2a	1649	1/1	0.91	0.16	59,59,59,59	0
57	MG	1A	3623	1/1	0.91	0.18	49,49,49,49	0
57	MG	2a	1656	1/1	0.91	0.26	58,58,58,58	0
57	MG	1A	3220	1/1	0.91	0.20	61,61,61,61	0
57	MG	2A	3142	1/1	0.91	0.25	65,65,65,65	0
57	MG	2A	3394	1/1	0.91	0.23	42,42,42,42	0
57	MG	1A	3240	1/1	0.91	0.33	40,40,40,40	0
57	MG	2a	1669	1/1	0.91	0.29	60,60,60,60	0
57	MG	2A	3144	1/1	0.91	0.15	66,66,66,66	0
57	MG	1A	3491	1/1	0.91	0.12	68,68,68,68	0
57	MG	1A	3784	1/1	0.91	0.13	47,47,47,47	0
57	MG	19	101	1/1	0.91	0.14	54,54,54,54	0
57	MG	2A	3410	1/1	0.91	0.20	64,64,64,64	0
57	MG	1A	4036	1/1	0.91	0.09	70,70,70,70	0
57	MG	1A	3791	1/1	0.91	0.08	33,33,33,33	0
57	MG	1a	1603	1/1	0.91	0.16	71,71,71,71	0
57	MG	1A	3392	1/1	0.91	0.20	65,65,65,65	0
57	MG	2A	3185	1/1	0.91	0.12	71,71,71,71	0
57	MG	2A	3188	1/1	0.91	0.18	62,62,62,62	0
57	MG	2a	1687	1/1	0.91	0.26	67,67,67,67	0
57	MG	1A	3642	1/1	0.91	0.09	52,52,52,52	0
57	MG	1A	3651	1/1	0.91	0.15	57,57,57,57	0
57	MG	1A	3503	1/1	0.91	0.11	71,71,71,71	0
57	MG	1A	3931	1/1	0.91	0.10	55,55,55,55	0
57	MG	2A	3194	1/1	0.91	0.23	60,60,60,60	0
57	MG	1A	4053	1/1	0.91	0.10	42,42,42,42	0
57	MG	1A	3319	1/1	0.91	0.15	50,50,50,50	0
57	MG	2a	1700	1/1	0.91	0.21	63,63,63,63	0
57	MG	2a	1701	1/1	0.91	0.32	71,71,71,71	0
57	MG	1a	1770	1/1	0.91	0.15	73,73,73,73	0
57	MG	1A	3161	1/1	0.91	0.17	64,64,64,64	0
57	MG	2A	3204	1/1	0.91	0.15	69,69,69,69	0
57	MG	2A	3209	1/1	0.91	0.08	65,65,65,65	0
57	MG	2a	1716	1/1	0.91	0.21	52,52,52,52	0
57	MG	2A	3735	1/1	0.91	0.17	59,59,59,59	0
57	MG	2a	1719	1/1	0.91	0.14	49,49,49,49	0
57	MG	1A	3245	1/1	0.91	0.12	58,58,58,58	0
57	MG	2A	3463	1/1	0.91	0.14	45,45,45,45	0
57	MG	2A	3216	1/1	0.91	0.17	57,57,57,57	0
57	MG	1A	3411	1/1	0.91	0.12	58,58,58,58	0
57	MG	2a	1727	1/1	0.91	0.21	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1730	1/1	0.91	0.23	61,61,61,61	0
57	MG	1A	4066	1/1	0.91	0.12	56,56,56,56	0
57	MG	2A	3747	1/1	0.91	0.12	54,54,54,54	0
57	MG	2A	3750	1/1	0.91	0.13	75,75,75,75	0
57	MG	2a	1735	1/1	0.91	0.23	80,80,80,80	0
57	MG	2a	1736	1/1	0.91	0.20	56,56,56,56	0
57	MG	1a	1631	1/1	0.91	0.17	60,60,60,60	0
57	MG	1A	3945	1/1	0.91	0.16	59,59,59,59	0
57	MG	2A	3754	1/1	0.91	0.19	71,71,71,71	0
57	MG	1A	4072	1/1	0.91	0.10	47,47,47,47	0
57	MG	1A	3682	1/1	0.91	0.14	60,60,60,60	0
57	MG	1a	1641	1/1	0.91	0.19	70,70,70,70	0
57	MG	1A	3053	1/1	0.91	0.11	52,52,52,52	0
57	MG	2A	3243	1/1	0.91	0.16	63,63,63,63	0
57	MG	1a	1791	1/1	0.91	0.09	66,66,66,66	0
57	MG	2a	1753	1/1	0.91	0.18	68,68,68,68	0
57	MG	2A	3763	1/1	0.91	0.13	53,53,53,53	0
57	MG	2A	3485	1/1	0.91	0.09	33,33,33,33	0
57	MG	1A	3812	1/1	0.91	0.07	46,46,46,46	0
57	MG	2A	3492	1/1	0.91	0.15	57,57,57,57	0
57	MG	1A	4080	1/1	0.91	0.17	58,58,58,58	0
57	MG	2a	1761	1/1	0.91	0.26	67,67,67,67	0
57	MG	2A	3774	1/1	0.91	0.09	66,66,66,66	0
57	MG	2a	1765	1/1	0.91	0.28	68,68,68,68	0
57	MG	2a	1766	1/1	0.91	0.25	66,66,66,66	0
57	MG	2A	3495	1/1	0.91	0.13	54,54,54,54	0
57	MG	2A	3248	1/1	0.91	0.12	64,64,64,64	0
57	MG	1A	4081	1/1	0.91	0.17	50,50,50,50	0
57	MG	1A	3685	1/1	0.91	0.09	63,63,63,63	0
57	MG	1A	3254	1/1	0.91	0.27	57,57,57,57	0
57	MG	1A	3688	1/1	0.91	0.18	74,74,74,74	0
57	MG	1A	3528	1/1	0.91	0.09	56,56,56,56	0
57	MG	1A	3098	1/1	0.91	0.12	55,55,55,55	0
57	MG	2a	1778	1/1	0.91	0.24	62,62,62,62	0
57	MG	1A	3705	1/1	0.91	0.20	82,82,82,82	0
57	MG	1a	1809	1/1	0.91	0.16	76,76,76,76	0
57	MG	1A	3099	1/1	0.91	0.21	72,72,72,72	0
57	MG	2A	3525	1/1	0.91	0.19	52,52,52,52	0
57	MG	1a	1813	1/1	0.91	0.12	77,77,77,77	0
57	MG	2A	3527	1/1	0.91	0.11	51,51,51,51	0
57	MG	2A	3528	1/1	0.91	0.16	43,43,43,43	0
57	MG	1A	4100	1/1	0.91	0.18	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	2j	201	1/1	0.91	0.13	75,75,75,75	0
57	MG	2A	3530	1/1	0.91	0.10	41,41,41,41	0
57	MG	1A	3549	1/1	0.91	0.16	62,62,62,62	0
57	MG	2A	3268	1/1	0.91	0.33	72,72,72,72	0
57	MG	2A	3269	1/1	0.91	0.34	57,57,57,57	0
57	MG	2A	3819	1/1	0.91	0.09	62,62,62,62	0
57	MG	2A	3536	1/1	0.91	0.21	67,67,67,67	0
57	MG	2A	3821	1/1	0.91	0.25	65,65,65,65	0
57	MG	2A	3271	1/1	0.91	0.24	61,61,61,61	0
57	MG	1B	202	1/1	0.91	0.19	58,58,58,58	0
57	MG	2A	3553	1/1	0.91	0.13	70,70,70,70	0
57	MG	2A	3427	1/1	0.92	0.11	73,73,73,73	0
57	MG	1a	1702	1/1	0.92	0.18	63,63,63,63	0
57	MG	2A	3776	1/1	0.92	0.11	74,74,74,74	0
57	MG	2A	3778	1/1	0.92	0.08	56,56,56,56	0
57	MG	2A	3429	1/1	0.92	0.15	60,60,60,60	0
57	MG	2A	3783	1/1	0.92	0.11	65,65,65,65	0
57	MG	1A	3464	1/1	0.92	0.16	43,43,43,43	0
57	MG	1A	3942	1/1	0.92	0.13	30,30,30,30	0
57	MG	1A	3612	1/1	0.92	0.08	17,17,17,17	0
57	MG	2A	3436	1/1	0.92	0.13	62,62,62,62	0
57	MG	1B	220	1/1	0.92	0.12	60,60,60,60	0
57	MG	2A	3150	1/1	0.92	0.10	58,58,58,58	0
57	MG	2A	3151	1/1	0.92	0.15	67,67,67,67	0
57	MG	2A	3442	1/1	0.92	0.16	62,62,62,62	0
57	MG	1A	3775	1/1	0.92	0.10	53,53,53,53	0
57	MG	2A	3802	1/1	0.92	0.18	66,66,66,66	0
57	MG	1A	3237	1/1	0.92	0.18	60,60,60,60	0
57	MG	2A	3448	1/1	0.92	0.25	66,66,66,66	0
57	MG	2A	3161	1/1	0.92	0.16	71,71,71,71	0
57	MG	2A	3807	1/1	0.92	0.24	57,57,57,57	0
57	MG	2A	3454	1/1	0.92	0.18	66,66,66,66	0
57	MG	2A	3163	1/1	0.92	0.19	60,60,60,60	0
57	MG	2A	3811	1/1	0.92	0.11	67,67,67,67	0
57	MG	2A	3466	1/1	0.92	0.10	44,44,44,44	0
57	MG	1a	1715	1/1	0.92	0.09	54,54,54,54	0
57	MG	1A	3358	1/1	0.92	0.18	48,48,48,48	0
57	MG	1A	3129	1/1	0.92	0.26	40,40,40,40	0
57	MG	1A	3786	1/1	0.92	0.20	52,52,52,52	0
57	MG	1a	1719	1/1	0.92	0.44	73,73,73,73	0
57	MG	2A	3182	1/1	0.92	0.11	59,59,59,59	0
57	MG	1A	3788	1/1	0.92	0.15	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	1B	233	1/1	0.92	0.16	72,72,72,72	0
57	MG	2A	3823	1/1	0.92	0.14	57,57,57,57	0
57	MG	1A	3472	1/1	0.92	0.15	63,63,63,63	0
57	MG	1A	3627	1/1	0.92	0.13	50,50,50,50	0
57	MG	2A	3191	1/1	0.92	0.17	55,55,55,55	0
57	MG	1A	3311	1/1	0.92	0.13	66,66,66,66	0
57	MG	1A	3480	1/1	0.92	0.09	66,66,66,66	0
57	MG	2A	3491	1/1	0.92	0.15	60,60,60,60	0
57	MG	1A	3798	1/1	0.92	0.11	36,36,36,36	0
57	MG	2A	3196	1/1	0.92	0.09	57,57,57,57	0
57	MG	1A	3631	1/1	0.92	0.07	31,31,31,31	0
57	MG	2A	3497	1/1	0.92	0.10	62,62,62,62	0
57	MG	1F	306	1/1	0.92	0.17	63,63,63,63	0
57	MG	1F	307	1/1	0.92	0.13	63,63,63,63	0
57	MG	1a	1732	1/1	0.92	0.13	65,65,65,65	0
57	MG	1A	3374	1/1	0.92	0.08	45,45,45,45	0
57	MG	2A	3506	1/1	0.92	0.16	57,57,57,57	0
57	MG	2A	3207	1/1	0.92	0.15	62,62,62,62	0
57	MG	2A	3508	1/1	0.92	0.17	52,52,52,52	0
57	MG	2A	3208	1/1	0.92	0.13	63,63,63,63	0
57	MG	1A	3635	1/1	0.92	0.10	57,57,57,57	0
57	MG	2A	3211	1/1	0.92	0.28	64,64,64,64	0
57	MG	1A	3970	1/1	0.92	0.23	75,75,75,75	0
57	MG	1A	3486	1/1	0.92	0.10	52,52,52,52	0
57	MG	1G	203	1/1	0.92	0.09	70,70,70,70	0
57	MG	2A	3227	1/1	0.92	0.26	68,68,68,68	0
57	MG	2B	207	1/1	0.92	0.11	64,64,64,64	0
57	MG	1G	204	1/1	0.92	0.10	58,58,58,58	0
57	MG	1A	3241	1/1	0.92	0.20	55,55,55,55	0
57	MG	1A	3490	1/1	0.92	0.23	61,61,61,61	0
57	MG	1O	202	1/1	0.92	0.23	72,72,72,72	0
57	MG	1A	3377	1/1	0.92	0.12	54,54,54,54	0
57	MG	2B	213	1/1	0.92	0.15	62,62,62,62	0
57	MG	1A	3658	1/1	0.92	0.14	59,59,59,59	0
57	MG	1P	203	1/1	0.92	0.22	39,39,39,39	0
57	MG	1Q	201	1/1	0.92	0.36	43,43,43,43	0
57	MG	1a	1760	1/1	0.92	0.15	68,68,68,68	0
57	MG	2A	3540	1/1	0.92	0.17	59,59,59,59	0
57	MG	2A	3544	1/1	0.92	0.09	48,48,48,48	0
57	MG	1A	3166	1/1	0.92	0.24	40,40,40,40	0
57	MG	2A	3552	1/1	0.92	0.24	61,61,61,61	0
57	MG	1A	3663	1/1	0.92	0.10	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3316	1/1	0.92	0.20	61,61,61,61	0
57	MG	1T	201	1/1	0.92	0.08	48,48,48,48	0
57	MG	1A	3820	1/1	0.92	0.13	51,51,51,51	0
57	MG	2A	3252	1/1	0.92	0.12	51,51,51,51	0
57	MG	2O	201	1/1	0.92	0.12	68,68,68,68	0
57	MG	1A	3981	1/1	0.92	0.10	36,36,36,36	0
57	MG	2P	202	1/1	0.92	0.14	58,58,58,58	0
57	MG	1V	204	1/1	0.92	0.18	55,55,55,55	0
57	MG	1V	207	1/1	0.92	0.08	70,70,70,70	0
57	MG	2A	3570	1/1	0.92	0.16	56,56,56,56	0
57	MG	1A	3060	1/1	0.92	0.12	45,45,45,45	0
57	MG	2U	202	1/1	0.92	0.20	61,61,61,61	0
57	MG	1A	3318	1/1	0.92	0.16	47,47,47,47	0
57	MG	1A	3177	1/1	0.92	0.18	50,50,50,50	0
57	MG	1A	3398	1/1	0.92	0.20	58,58,58,58	0
57	MG	23	101	1/1	0.92	0.14	61,61,61,61	0
57	MG	2A	3577	1/1	0.92	0.17	64,64,64,64	0
57	MG	25	107	1/1	0.92	0.10	58,58,58,58	0
57	MG	28	102	1/1	0.92	0.20	60,60,60,60	0
57	MG	1A	3684	1/1	0.92	0.11	53,53,53,53	0
57	MG	29	101	1/1	0.92	0.17	62,62,62,62	0
57	MG	2A	3264	1/1	0.92	0.11	58,58,58,58	0
57	MG	1A	3516	1/1	0.92	0.12	70,70,70,70	0
57	MG	15	103	1/1	0.92	0.14	40,40,40,40	0
57	MG	2A	3584	1/1	0.92	0.08	40,40,40,40	0
57	MG	15	108	1/1	0.92	0.15	51,51,51,51	0
57	MG	2a	1612	1/1	0.92	0.15	61,61,61,61	0
57	MG	1a	1792	1/1	0.92	0.07	65,65,65,65	0
57	MG	1A	3522	1/1	0.92	0.07	56,56,56,56	0
57	MG	2A	3273	1/1	0.92	0.10	68,68,68,68	0
57	MG	2A	3597	1/1	0.92	0.09	39,39,39,39	0
57	MG	1a	1795	1/1	0.92	0.07	62,62,62,62	0
57	MG	2a	1620	1/1	0.92	0.20	53,53,53,53	0
57	MG	2a	1622	1/1	0.92	0.15	70,70,70,70	0
57	MG	17	103	1/1	0.92	0.17	43,43,43,43	0
57	MG	2A	3602	1/1	0.92	0.13	56,56,56,56	0
57	MG	2A	3605	1/1	0.92	0.19	46,46,46,46	0
57	MG	2A	3276	1/1	0.92	0.13	72,72,72,72	0
57	MG	1A	3832	1/1	0.92	0.14	55,55,55,55	0
57	MG	1A	3833	1/1	0.92	0.09	50,50,50,50	0
57	MG	2a	1631	1/1	0.92	0.26	72,72,72,72	0
57	MG	1A	4010	1/1	0.92	0.09	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3614	1/1	0.92	0.12	51,51,51,51	0
57	MG	1A	3320	1/1	0.92	0.28	65,65,65,65	0
57	MG	1A	3407	1/1	0.92	0.13	55,55,55,55	0
57	MG	2A	3618	1/1	0.92	0.19	70,70,70,70	0
57	MG	1a	1604	1/1	0.92	0.09	60,60,60,60	0
57	MG	1A	3693	1/1	0.92	0.10	42,42,42,42	0
57	MG	1A	3695	1/1	0.92	0.14	65,65,65,65	0
57	MG	1A	3140	1/1	0.92	0.12	55,55,55,55	0
57	MG	1A	3702	1/1	0.92	0.11	43,43,43,43	0
57	MG	2A	3630	1/1	0.92	0.21	55,55,55,55	0
57	MG	1A	3529	1/1	0.92	0.18	60,60,60,60	0
57	MG	2a	1650	1/1	0.92	0.24	61,61,61,61	0
57	MG	1e	202	1/1	0.92	0.11	73,73,73,73	0
57	MG	2A	3299	1/1	0.92	0.13	64,64,64,64	0
57	MG	1f	201	1/1	0.92	0.23	57,57,57,57	0
57	MG	1A	3853	1/1	0.92	0.09	47,47,47,47	0
57	MG	1A	3256	1/1	0.92	0.15	52,52,52,52	0
57	MG	1A	3537	1/1	0.92	0.24	50,50,50,50	0
57	MG	1A	3858	1/1	0.92	0.11	32,32,32,32	0
57	MG	1v	104	1/1	0.92	0.14	60,60,60,60	0
57	MG	1A	3324	1/1	0.92	0.30	55,55,55,55	0
57	MG	1A	3190	1/1	0.92	0.20	37,37,37,37	0
57	MG	1a	1630	1/1	0.92	0.29	69,69,69,69	0
57	MG	1A	3553	1/1	0.92	0.32	39,39,39,39	0
57	MG	1A	3330	1/1	0.92	0.13	45,45,45,45	0
57	MG	1A	3146	1/1	0.92	0.10	37,37,37,37	0
57	MG	1a	1639	1/1	0.92	0.27	72,72,72,72	0
57	MG	2A	3004	1/1	0.92	0.16	54,54,54,54	0
57	MG	2A	3326	1/1	0.92	0.17	69,69,69,69	0
57	MG	1A	3564	1/1	0.92	0.13	48,48,48,48	0
57	MG	2A	3007	1/1	0.92	0.20	53,53,53,53	0
57	MG	1A	3723	1/1	0.92	0.07	38,38,38,38	0
57	MG	2a	1690	1/1	0.92	0.16	70,70,70,70	0
57	MG	1A	3565	1/1	0.92	0.13	38,38,38,38	0
57	MG	2A	3335	1/1	0.92	0.20	59,59,59,59	0
57	MG	2a	1693	1/1	0.92	0.50	72,72,72,72	0
57	MG	1a	1643	1/1	0.92	0.30	79,79,79,79	0
57	MG	1a	1645	1/1	0.92	0.12	57,57,57,57	0
57	MG	1A	3150	1/1	0.92	0.08	42,42,42,42	0
57	MG	2A	3669	1/1	0.92	0.13	60,60,60,60	0
57	MG	1A	3436	1/1	0.92	0.24	60,60,60,60	0
57	MG	1A	3336	1/1	0.92	0.25	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	1704	1/1	0.92	0.16	60,60,60,60	0
57	MG	1a	1651	1/1	0.92	0.20	59,59,59,59	0
57	MG	2A	3674	1/1	0.92	0.09	68,68,68,68	0
57	MG	2A	3349	1/1	0.92	0.15	49,49,49,49	0
57	MG	1A	4054	1/1	0.92	0.11	51,51,51,51	0
57	MG	1A	3201	1/1	0.92	0.12	57,57,57,57	0
57	MG	1A	3578	1/1	0.92	0.10	34,34,34,34	0
57	MG	2A	3684	1/1	0.92	0.19	56,56,56,56	0
57	MG	2A	3353	1/1	0.92	0.14	61,61,61,61	0
57	MG	1A	3735	1/1	0.92	0.11	37,37,37,37	0
57	MG	2a	1723	1/1	0.92	0.15	63,63,63,63	0
57	MG	1A	3286	1/1	0.92	0.15	54,54,54,54	0
57	MG	2A	3690	1/1	0.92	0.14	43,43,43,43	0
57	MG	2A	3359	1/1	0.92	0.19	55,55,55,55	0
57	MG	1A	3581	1/1	0.92	0.12	55,55,55,55	0
57	MG	1A	3112	1/1	0.92	0.20	50,50,50,50	0
57	MG	2A	3053	1/1	0.92	0.14	66,66,66,66	0
57	MG	1A	4070	1/1	0.92	0.12	34,34,34,34	0
57	MG	1A	3446	1/1	0.92	0.19	59,59,59,59	0
57	MG	1A	3114	1/1	0.92	0.25	37,37,37,37	0
57	MG	1A	3902	1/1	0.92	0.11	58,58,58,58	0
57	MG	2a	1740	1/1	0.92	0.12	64,64,64,64	0
57	MG	2A	3705	1/1	0.92	0.10	52,52,52,52	0
57	MG	2A	3706	1/1	0.92	0.08	75,75,75,75	0
57	MG	2a	1743	1/1	0.92	0.20	60,60,60,60	0
57	MG	1a	1669	1/1	0.92	0.13	79,79,79,79	0
57	MG	2A	3371	1/1	0.92	0.20	55,55,55,55	0
57	MG	1a	1671	1/1	0.92	0.25	66,66,66,66	0
57	MG	2A	3062	1/1	0.92	0.15	57,57,57,57	0
57	MG	2A	3712	1/1	0.92	0.09	68,68,68,68	0
57	MG	1A	3903	1/1	0.92	0.11	29,29,29,29	0
57	MG	1A	3450	1/1	0.92	0.26	65,65,65,65	0
57	MG	1A	3907	1/1	0.92	0.09	48,48,48,48	0
57	MG	1A	3351	1/1	0.92	0.14	54,54,54,54	0
57	MG	1A	3093	1/1	0.92	0.16	42,42,42,42	0
57	MG	1A	3752	1/1	0.92	0.11	47,47,47,47	0
57	MG	2A	3381	1/1	0.92	0.17	63,63,63,63	0
57	MG	2A	3090	1/1	0.92	0.16	65,65,65,65	0
57	MG	1A	3456	1/1	0.92	0.19	53,53,53,53	0
57	MG	2a	1763	1/1	0.92	0.23	59,59,59,59	0
57	MG	2a	1764	1/1	0.92	0.23	64,64,64,64	0
57	MG	1A	3758	1/1	0.92	0.07	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3730	1/1	0.92	0.16	59,59,59,59	0
57	MG	2A	3731	1/1	0.92	0.09	49,49,49,49	0
57	MG	2A	3387	1/1	0.92	0.22	53,53,53,53	0
57	MG	1A	3928	1/1	0.92	0.10	66,66,66,66	0
57	MG	1A	3759	1/1	0.92	0.08	52,52,52,52	0
57	MG	2A	3098	1/1	0.92	0.08	54,54,54,54	0
57	MG	2A	3737	1/1	0.92	0.17	67,67,67,67	0
57	MG	2A	3101	1/1	0.92	0.21	68,68,68,68	0
57	MG	1A	4096	1/1	0.92	0.17	46,46,46,46	0
57	MG	2A	3397	1/1	0.92	0.52	64,64,64,64	0
57	MG	2A	3743	1/1	0.92	0.09	51,51,51,51	0
57	MG	2A	3398	1/1	0.92	0.27	64,64,64,64	0
57	MG	1A	3761	1/1	0.92	0.06	36,36,36,36	0
57	MG	1A	3932	1/1	0.92	0.11	53,53,53,53	0
57	MG	2A	3403	1/1	0.92	0.23	61,61,61,61	0
57	MG	1B	201	1/1	0.92	0.12	54,54,54,54	0
57	MG	1a	1691	1/1	0.92	0.11	53,53,53,53	0
57	MG	1A	3601	1/1	0.92	0.07	38,38,38,38	0
57	MG	1A	3936	1/1	0.92	0.07	42,42,42,42	0
57	MG	1a	1697	1/1	0.92	0.16	58,58,58,58	0
57	MG	1A	3291	1/1	0.92	0.23	41,41,41,41	0
57	MG	2q	201	1/1	0.92	0.09	71,71,71,71	0
57	MG	1a	1699	1/1	0.92	0.23	61,61,61,61	0
57	MG	1A	3769	1/1	0.92	0.13	25,25,25,25	0
57	MG	2A	3762	1/1	0.92	0.14	72,72,72,72	0
57	MG	1B	212	1/1	0.92	0.18	50,50,50,50	0
57	MG	2A	3134	1/1	0.92	0.17	48,48,48,48	0
57	MG	2A	3138	1/1	0.92	0.20	48,48,48,48	0
57	MG	2A	3426	1/1	0.92	0.32	54,54,54,54	0
57	MG	2A	3770	1/1	0.92	0.12	60,60,60,60	0
57	MG	1A	3863	1/1	0.93	0.07	34,34,34,34	0
57	MG	2A	3088	1/1	0.93	0.11	48,48,48,48	0
57	MG	1A	3163	1/1	0.93	0.08	34,34,34,34	0
57	MG	2A	3340	1/1	0.93	0.13	60,60,60,60	0
57	MG	1A	3617	1/1	0.93	0.10	31,31,31,31	0
57	MG	1A	3618	1/1	0.93	0.06	30,30,30,30	0
57	MG	1A	3325	1/1	0.93	0.25	71,71,71,71	0
57	MG	2A	3345	1/1	0.93	0.16	55,55,55,55	0
57	MG	1A	3280	1/1	0.93	0.12	49,49,49,49	0
57	MG	2A	3613	1/1	0.93	0.09	41,41,41,41	0
57	MG	1A	3624	1/1	0.93	0.20	52,52,52,52	0
57	MG	1A	3746	1/1	0.93	0.09	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3747	1/1	0.93	0.08	37,37,37,37	0
57	MG	1A	4023	1/1	0.93	0.14	65,65,65,65	0
57	MG	1R	204	1/1	0.93	0.18	40,40,40,40	0
57	MG	2B	214	1/1	0.93	0.23	59,59,59,59	0
57	MG	2B	215	1/1	0.93	0.14	74,74,74,74	0
57	MG	1A	4024	1/1	0.93	0.10	68,68,68,68	0
57	MG	2A	3625	1/1	0.93	0.18	66,66,66,66	0
57	MG	1A	3881	1/1	0.93	0.11	55,55,55,55	0
57	MG	1A	3502	1/1	0.93	0.08	54,54,54,54	0
57	MG	1A	3283	1/1	0.93	0.06	36,36,36,36	0
57	MG	2A	3360	1/1	0.93	0.24	66,66,66,66	0
57	MG	1A	3413	1/1	0.93	0.13	46,46,46,46	0
57	MG	1A	3415	1/1	0.93	0.10	53,53,53,53	0
57	MG	1Y	201	1/1	0.93	0.19	58,58,58,58	0
57	MG	2E	307	1/1	0.93	0.18	39,39,39,39	0
57	MG	1A	3633	1/1	0.93	0.06	22,22,22,22	0
57	MG	2A	3635	1/1	0.93	0.09	41,41,41,41	0
57	MG	1A	3202	1/1	0.93	0.20	38,38,38,38	0
57	MG	1A	3059	1/1	0.93	0.17	45,45,45,45	0
57	MG	2A	3125	1/1	0.93	0.13	54,54,54,54	0
57	MG	2A	3131	1/1	0.93	0.18	68,68,68,68	0
57	MG	1A	3636	1/1	0.93	0.09	42,42,42,42	0
57	MG	2Q	203	1/1	0.93	0.09	62,62,62,62	0
57	MG	2A	3136	1/1	0.93	0.16	66,66,66,66	0
57	MG	1A	3764	1/1	0.93	0.10	54,54,54,54	0
57	MG	1A	3515	1/1	0.93	0.13	41,41,41,41	0
57	MG	2T	203	1/1	0.93	0.21	56,56,56,56	0
57	MG	1A	3897	1/1	0.93	0.14	64,64,64,64	0
57	MG	1A	3418	1/1	0.93	0.10	58,58,58,58	0
57	MG	1A	3649	1/1	0.93	0.10	30,30,30,30	0
57	MG	1A	4048	1/1	0.93	0.07	63,63,63,63	0
57	MG	1A	3771	1/1	0.93	0.07	41,41,41,41	0
57	MG	2I	102	1/1	0.93	0.09	52,52,52,52	0
57	MG	1A	3419	1/1	0.93	0.10	68,68,68,68	0
57	MG	2A	3153	1/1	0.93	0.16	56,56,56,56	0
57	MG	25	101	1/1	0.93	0.32	62,62,62,62	0
57	MG	25	105	1/1	0.93	0.14	55,55,55,55	0
57	MG	25	106	1/1	0.93	0.13	55,55,55,55	0
57	MG	1a	1757	1/1	0.93	0.15	69,69,69,69	0
57	MG	28	101	1/1	0.93	0.19	55,55,55,55	0
57	MG	1A	3654	1/1	0.93	0.11	70,70,70,70	0
57	MG	1A	3776	1/1	0.93	0.06	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3389	1/1	0.93	0.29	46,46,46,46	0
57	MG	2A	3162	1/1	0.93	0.13	67,67,67,67	0
57	MG	2a	1603	1/1	0.93	0.09	67,67,67,67	0
57	MG	2a	1604	1/1	0.93	0.35	63,63,63,63	0
57	MG	1A	3915	1/1	0.93	0.10	61,61,61,61	0
57	MG	1A	3917	1/1	0.93	0.14	58,58,58,58	0
57	MG	2a	1608	1/1	0.93	0.08	61,61,61,61	0
57	MG	2A	3667	1/1	0.93	0.13	61,61,61,61	0
57	MG	2A	3165	1/1	0.93	0.10	59,59,59,59	0
57	MG	1A	3422	1/1	0.93	0.13	47,47,47,47	0
57	MG	2A	3167	1/1	0.93	0.11	61,61,61,61	0
57	MG	1a	1606	1/1	0.93	0.37	76,76,76,76	0
57	MG	1a	1608	1/1	0.93	0.28	67,67,67,67	0
57	MG	2A	3177	1/1	0.93	0.15	61,61,61,61	0
57	MG	1A	3048	1/1	0.93	0.22	51,51,51,51	0
57	MG	2A	3677	1/1	0.93	0.18	55,55,55,55	0
57	MG	2a	1621	1/1	0.93	0.29	62,62,62,62	0
57	MG	2A	3681	1/1	0.93	0.12	44,44,44,44	0
57	MG	2A	3181	1/1	0.93	0.20	67,67,67,67	0
57	MG	1A	3219	1/1	0.93	0.20	44,44,44,44	0
57	MG	2A	3409	1/1	0.93	0.12	53,53,53,53	0
57	MG	1A	3026	1/1	0.93	0.16	71,71,71,71	0
57	MG	1a	1618	1/1	0.93	0.16	58,58,58,58	0
57	MG	2A	3688	1/1	0.93	0.07	64,64,64,64	0
57	MG	1A	3666	1/1	0.93	0.10	25,25,25,25	0
57	MG	1A	3433	1/1	0.93	0.17	49,49,49,49	0
57	MG	1A	4074	1/1	0.93	0.19	57,57,57,57	0
57	MG	1A	4076	1/1	0.93	0.10	47,47,47,47	0
57	MG	1a	1780	1/1	0.93	0.11	66,66,66,66	0
57	MG	1A	3675	1/1	0.93	0.06	16,16,16,16	0
57	MG	2a	1639	1/1	0.93	0.37	69,69,69,69	0
57	MG	2A	3422	1/1	0.93	0.31	59,59,59,59	0
57	MG	1a	1782	1/1	0.93	0.14	50,50,50,50	0
57	MG	2A	3699	1/1	0.93	0.14	64,64,64,64	0
57	MG	2A	3197	1/1	0.93	0.10	58,58,58,58	0
57	MG	2A	3198	1/1	0.93	0.19	64,64,64,64	0
57	MG	2a	1647	1/1	0.93	0.29	65,65,65,65	0
57	MG	2A	3703	1/1	0.93	0.12	54,54,54,54	0
57	MG	1a	1783	1/1	0.93	0.12	52,52,52,52	0
57	MG	1a	1784	1/1	0.93	0.12	76,76,76,76	0
57	MG	1A	4078	1/1	0.93	0.12	64,64,64,64	0
57	MG	2a	1655	1/1	0.93	0.32	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	3677	1/1	0.93	0.07	35,35,35,35	0
57	MG	2a	1657	1/1	0.93	0.19	75,75,75,75	0
57	MG	1A	3227	1/1	0.93	0.10	61,61,61,61	0
57	MG	1A	3935	1/1	0.93	0.06	43,43,43,43	0
57	MG	1a	1634	1/1	0.93	0.25	82,82,82,82	0
57	MG	1A	3176	1/1	0.93	0.26	57,57,57,57	0
57	MG	1A	3542	1/1	0.93	0.22	54,54,54,54	0
57	MG	1a	1798	1/1	0.93	0.16	66,66,66,66	0
57	MG	1a	1638	1/1	0.93	0.27	62,62,62,62	0
57	MG	2A	3719	1/1	0.93	0.21	47,47,47,47	0
57	MG	1A	3292	1/1	0.93	0.23	48,48,48,48	0
57	MG	2a	1676	1/1	0.93	0.16	68,68,68,68	0
57	MG	2A	3447	1/1	0.93	0.17	63,63,63,63	0
57	MG	2A	3224	1/1	0.93	0.19	41,41,41,41	0
57	MG	1A	3296	1/1	0.93	0.16	56,56,56,56	0
57	MG	2a	1680	1/1	0.93	0.27	57,57,57,57	0
57	MG	1A	3802	1/1	0.93	0.18	52,52,52,52	0
57	MG	2A	3461	1/1	0.93	0.23	65,65,65,65	0
57	MG	2A	3232	1/1	0.93	0.21	61,61,61,61	0
57	MG	1A	3016	1/1	0.93	0.30	51,51,51,51	0
57	MG	2a	1685	1/1	0.93	0.10	60,60,60,60	0
57	MG	1A	3805	1/1	0.93	0.09	55,55,55,55	0
57	MG	1a	1644	1/1	0.93	0.25	61,61,61,61	0
57	MG	2A	3236	1/1	0.93	0.10	63,63,63,63	0
57	MG	1A	3445	1/1	0.93	0.12	39,39,39,39	0
57	MG	2A	3238	1/1	0.93	0.07	75,75,75,75	0
57	MG	1a	1811	1/1	0.93	0.18	65,65,65,65	0
57	MG	1A	4097	1/1	0.93	0.15	57,57,57,57	0
57	MG	1A	3178	1/1	0.93	0.08	62,62,62,62	0
57	MG	2A	3478	1/1	0.93	0.13	52,52,52,52	0
57	MG	1a	1814	1/1	0.93	0.10	88,88,88,88	0
57	MG	1b	301	1/1	0.93	0.08	76,76,76,76	0
57	MG	2A	3748	1/1	0.93	0.09	68,68,68,68	0
57	MG	1A	4101	1/1	0.93	0.11	55,55,55,55	0
57	MG	2a	1705	1/1	0.93	0.17	61,61,61,61	0
57	MG	2a	1707	1/1	0.93	0.16	71,71,71,71	0
57	MG	1e	201	1/1	0.93	0.15	53,53,53,53	0
57	MG	2A	3486	1/1	0.93	0.10	58,58,58,58	0
57	MG	1A	3689	1/1	0.93	0.09	29,29,29,29	0
57	MG	1A	3300	1/1	0.93	0.11	56,56,56,56	0
57	MG	1A	3692	1/1	0.93	0.14	55,55,55,55	0
57	MG	1A	3361	1/1	0.93	0.10	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	1B	205	1/1	0.93	0.21	71,71,71,71	0
57	MG	1v	101	1/1	0.93	0.23	64,64,64,64	0
57	MG	1B	206	1/1	0.93	0.07	44,44,44,44	0
57	MG	1B	208	1/1	0.93	0.10	62,62,62,62	0
57	MG	1A	3363	1/1	0.93	0.09	47,47,47,47	0
57	MG	2A	3764	1/1	0.93	0.17	57,57,57,57	0
57	MG	1x	102	1/1	0.93	0.09	58,58,58,58	0
57	MG	1x	103	1/1	0.93	0.09	64,64,64,64	0
57	MG	1A	3696	1/1	0.93	0.07	47,47,47,47	0
57	MG	1B	211	1/1	0.93	0.10	52,52,52,52	0
57	MG	1A	3310	1/1	0.93	0.19	35,35,35,35	0
57	MG	2A	3773	1/1	0.93	0.09	66,66,66,66	0
57	MG	1A	3963	1/1	0.93	0.08	52,52,52,52	0
57	MG	1A	3179	1/1	0.93	0.16	65,65,65,65	0
57	MG	1A	3088	1/1	0.93	0.11	55,55,55,55	0
57	MG	2A	3516	1/1	0.93	0.09	49,49,49,49	0
57	MG	1A	3463	1/1	0.93	0.16	63,63,63,63	0
57	MG	2A	3519	1/1	0.93	0.11	42,42,42,42	0
57	MG	1A	3154	1/1	0.93	0.14	50,50,50,50	0
57	MG	2a	1745	1/1	0.93	0.10	53,53,53,53	0
57	MG	1A	3829	1/1	0.93	0.10	33,33,33,33	0
57	MG	1A	3465	1/1	0.93	0.21	47,47,47,47	0
57	MG	2a	1749	1/1	0.93	0.12	75,75,75,75	0
57	MG	2A	3015	1/1	0.93	0.22	60,60,60,60	0
57	MG	1B	226	1/1	0.93	0.11	55,55,55,55	0
57	MG	1A	3583	1/1	0.93	0.12	53,53,53,53	0
57	MG	2A	3280	1/1	0.93	0.25	64,64,64,64	0
57	MG	1A	3252	1/1	0.93	0.22	70,70,70,70	0
57	MG	1a	1682	1/1	0.93	0.41	68,68,68,68	0
57	MG	1A	3253	1/1	0.93	0.12	59,59,59,59	0
57	MG	1A	3716	1/1	0.93	0.07	31,31,31,31	0
57	MG	1A	3055	1/1	0.93	0.15	51,51,51,51	0
57	MG	1A	3390	1/1	0.93	0.28	43,43,43,43	0
57	MG	2A	3039	1/1	0.93	0.29	62,62,62,62	0
57	MG	2A	3040	1/1	0.93	0.09	61,61,61,61	0
57	MG	1E	302	1/1	0.93	0.21	56,56,56,56	0
57	MG	1A	3593	1/1	0.93	0.09	37,37,37,37	0
57	MG	1A	3193	1/1	0.93	0.24	45,45,45,45	0
57	MG	1A	3848	1/1	0.93	0.22	44,44,44,44	0
57	MG	1E	313	1/1	0.93	0.08	50,50,50,50	0
57	MG	1a	1694	1/1	0.93	0.32	59,59,59,59	0
57	MG	1A	3259	1/1	0.93	0.11	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3983	1/1	0.93	0.08	17,17,17,17	0
57	MG	1A	3268	1/1	0.93	0.19	38,38,38,38	0
57	MG	2A	3311	1/1	0.93	0.25	62,62,62,62	0
57	MG	2a	1776	1/1	0.93	0.21	70,70,70,70	0
57	MG	1F	308	1/1	0.93	0.12	44,44,44,44	0
57	MG	1A	3484	1/1	0.93	0.13	60,60,60,60	0
57	MG	2A	3575	1/1	0.93	0.07	54,54,54,54	0
57	MG	2A	3827	1/1	0.93	0.07	37,37,37,37	0
57	MG	1F	313	1/1	0.93	0.10	50,50,50,50	0
57	MG	1A	3485	1/1	0.93	0.30	61,61,61,61	0
57	MG	1a	1704	1/1	0.93	0.09	62,62,62,62	0
57	MG	2a	1785	1/1	0.93	0.09	66,66,66,66	0
57	MG	2e	202	1/1	0.93	0.22	69,69,69,69	0
57	MG	2A	3322	1/1	0.93	0.06	62,62,62,62	0
57	MG	2A	3833	1/1	0.93	0.12	65,65,65,65	0
57	MG	2A	3065	1/1	0.93	0.13	52,52,52,52	0
57	MG	1a	1706	1/1	0.93	0.29	74,74,74,74	0
57	MG	2A	3836	1/1	0.93	0.07	77,77,77,77	0
57	MG	2A	3325	1/1	0.93	0.19	52,52,52,52	0
57	MG	2A	3585	1/1	0.93	0.13	42,42,42,42	0
57	MG	1A	3006	1/1	0.93	0.12	53,53,53,53	0
57	MG	2A	3841	1/1	0.93	0.14	53,53,53,53	0
57	MG	2A	3081	1/1	0.93	0.16	61,61,61,61	0
57	MG	1A	3856	1/1	0.93	0.07	34,34,34,34	0
57	MG	2A	3845	1/1	0.93	0.13	57,57,57,57	0
57	MG	2A	3592	1/1	0.93	0.19	59,59,59,59	0
57	MG	1A	3401	1/1	0.93	0.11	52,52,52,52	0
57	MG	2A	3596	1/1	0.93	0.14	59,59,59,59	0
57	MG	2A	3569	1/1	0.94	0.10	55,55,55,55	0
57	MG	2A	3298	1/1	0.94	0.09	62,62,62,62	0
57	MG	2A	3054	1/1	0.94	0.17	64,64,64,64	0
57	MG	1A	3118	1/1	0.94	0.15	46,46,46,46	0
57	MG	1A	3668	1/1	0.94	0.08	38,38,38,38	0
57	MG	1N	202	1/1	0.94	0.08	45,45,45,45	0
57	MG	1O	201	1/1	0.94	0.13	57,57,57,57	0
57	MG	2A	3304	1/1	0.94	0.26	69,69,69,69	0
57	MG	1A	3391	1/1	0.94	0.23	53,53,53,53	0
57	MG	2A	3579	1/1	0.94	0.06	69,69,69,69	0
57	MG	1A	3078	1/1	0.94	0.10	44,44,44,44	0
57	MG	1A	3393	1/1	0.94	0.09	51,51,51,51	0
57	MG	2A	3063	1/1	0.94	0.12	57,57,57,57	0
57	MG	1A	3783	1/1	0.94	0.08	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3316	1/1	0.94	0.12	60,60,60,60	0
57	MG	2A	3067	1/1	0.94	0.07	47,47,47,47	0
57	MG	2A	3587	1/1	0.94	0.10	44,44,44,44	0
57	MG	2A	3069	1/1	0.94	0.08	61,61,61,61	0
57	MG	2A	3074	1/1	0.94	0.22	55,55,55,55	0
57	MG	2A	3591	1/1	0.94	0.14	59,59,59,59	0
57	MG	1P	206	1/1	0.94	0.06	39,39,39,39	0
57	MG	1A	3260	1/1	0.94	0.14	59,59,59,59	0
57	MG	2A	3079	1/1	0.94	0.16	51,51,51,51	0
57	MG	1A	3263	1/1	0.94	0.07	47,47,47,47	0
57	MG	1A	4034	1/1	0.94	0.10	23,23,23,23	0
57	MG	1A	3787	1/1	0.94	0.21	57,57,57,57	0
57	MG	2A	3327	1/1	0.94	0.24	53,53,53,53	0
57	MG	2A	3328	1/1	0.94	0.10	74,74,74,74	0
57	MG	1A	3571	1/1	0.94	0.18	56,56,56,56	0
57	MG	1A	3338	1/1	0.94	0.10	60,60,60,60	0
57	MG	1A	3302	1/1	0.94	0.23	53,53,53,53	0
57	MG	1A	3344	1/1	0.94	0.14	39,39,39,39	0
57	MG	2F	301	1/1	0.94	0.18	49,49,49,49	0
57	MG	2A	3334	1/1	0.94	0.14	56,56,56,56	0
57	MG	2F	307	1/1	0.94	0.20	54,54,54,54	0
57	MG	1A	3916	1/1	0.94	0.11	39,39,39,39	0
57	MG	1A	3406	1/1	0.94	0.09	45,45,45,45	0
57	MG	2A	3616	1/1	0.94	0.09	45,45,45,45	0
57	MG	2O	202	1/1	0.94	0.17	61,61,61,61	0
57	MG	2A	3337	1/1	0.94	0.11	66,66,66,66	0
57	MG	2A	3339	1/1	0.94	0.17	65,65,65,65	0
57	MG	2A	3621	1/1	0.94	0.10	56,56,56,56	0
57	MG	1A	4047	1/1	0.94	0.07	41,41,41,41	0
57	MG	2A	3623	1/1	0.94	0.19	55,55,55,55	0
57	MG	1A	3797	1/1	0.94	0.10	43,43,43,43	0
57	MG	1A	3919	1/1	0.94	0.11	58,58,58,58	0
57	MG	1A	4050	1/1	0.94	0.10	40,40,40,40	0
57	MG	2A	3344	1/1	0.94	0.09	56,56,56,56	0
57	MG	2V	201	1/1	0.94	0.11	53,53,53,53	0
57	MG	2V	202	1/1	0.94	0.21	67,67,67,67	0
57	MG	1A	3303	1/1	0.94	0.28	53,53,53,53	0
57	MG	1A	3476	1/1	0.94	0.14	32,32,32,32	0
57	MG	2O	101	1/1	0.94	0.08	62,62,62,62	0
57	MG	2A	3105	1/1	0.94	0.20	65,65,65,65	0
57	MG	1O	106	1/1	0.94	0.23	67,67,67,67	0
57	MG	1A	3479	1/1	0.94	0.23	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	11	104	1/1	0.94	0.17	58,58,58,58	0
57	MG	23	103	1/1	0.94	0.10	62,62,62,62	0
57	MG	12	101	1/1	0.94	0.08	53,53,53,53	0
57	MG	13	103	1/1	0.94	0.12	45,45,45,45	0
57	MG	1A	3923	1/1	0.94	0.10	62,62,62,62	0
57	MG	1A	3924	1/1	0.94	0.09	66,66,66,66	0
57	MG	26	101	1/1	0.94	0.11	61,61,61,61	0
57	MG	2A	3357	1/1	0.94	0.34	69,69,69,69	0
57	MG	2A	3118	1/1	0.94	0.07	53,53,53,53	0
57	MG	1A	3927	1/1	0.94	0.09	70,70,70,70	0
57	MG	17	101	1/1	0.94	0.09	34,34,34,34	0
57	MG	2A	3121	1/1	0.94	0.09	50,50,50,50	0
57	MG	2A	3647	1/1	0.94	0.08	62,62,62,62	0
57	MG	1a	1749	1/1	0.94	0.07	57,57,57,57	0
57	MG	1A	3410	1/1	0.94	0.10	51,51,51,51	0
57	MG	2A	3126	1/1	0.94	0.14	47,47,47,47	0
57	MG	2a	1607	1/1	0.94	0.14	61,61,61,61	0
57	MG	1a	1752	1/1	0.94	0.25	68,68,68,68	0
57	MG	2A	3133	1/1	0.94	0.18	52,52,52,52	0
57	MG	18	103	1/1	0.94	0.10	54,54,54,54	0
57	MG	1a	1754	1/1	0.94	0.15	56,56,56,56	0
57	MG	2A	3372	1/1	0.94	0.17	65,65,65,65	0
57	MG	1a	1755	1/1	0.94	0.10	61,61,61,61	0
57	MG	1A	4067	1/1	0.94	0.11	47,47,47,47	0
57	MG	2a	1617	1/1	0.94	0.21	67,67,67,67	0
57	MG	1A	3586	1/1	0.94	0.09	59,59,59,59	0
57	MG	1A	3304	1/1	0.94	0.24	57,57,57,57	0
57	MG	1A	3306	1/1	0.94	0.07	37,37,37,37	0
57	MG	2A	3664	1/1	0.94	0.08	59,59,59,59	0
57	MG	1A	3933	1/1	0.94	0.10	53,53,53,53	0
57	MG	2A	3149	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3806	1/1	0.94	0.20	63,63,63,63	0
57	MG	1a	1764	1/1	0.94	0.11	59,59,59,59	0
57	MG	1A	3234	1/1	0.94	0.17	42,42,42,42	0
57	MG	1a	1766	1/1	0.94	0.08	82,82,82,82	0
57	MG	1a	1767	1/1	0.94	0.14	84,84,84,84	0
57	MG	1A	3699	1/1	0.94	0.09	49,49,49,49	0
57	MG	2A	3388	1/1	0.94	0.22	50,50,50,50	0
57	MG	1A	3236	1/1	0.94	0.07	42,42,42,42	0
57	MG	2A	3679	1/1	0.94	0.09	57,57,57,57	0
57	MG	1a	1611	1/1	0.94	0.08	69,69,69,69	0
57	MG	1A	3149	1/1	0.94	0.11	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3355	1/1	0.94	0.11	49,49,49,49	0
57	MG	2A	3393	1/1	0.94	0.29	61,61,61,61	0
57	MG	1A	3595	1/1	0.94	0.11	45,45,45,45	0
57	MG	1a	1616	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	4083	1/1	0.94	0.08	45,45,45,45	0
57	MG	2A	3171	1/1	0.94	0.13	62,62,62,62	0
57	MG	2A	3173	1/1	0.94	0.08	52,52,52,52	0
57	MG	2A	3401	1/1	0.94	0.14	57,57,57,57	0
57	MG	1a	1777	1/1	0.94	0.10	67,67,67,67	0
57	MG	1A	3944	1/1	0.94	0.12	53,53,53,53	0
57	MG	2A	3405	1/1	0.94	0.36	67,67,67,67	0
57	MG	2a	1653	1/1	0.94	0.26	60,60,60,60	0
57	MG	1A	3279	1/1	0.94	0.08	49,49,49,49	0
57	MG	1A	4087	1/1	0.94	0.15	53,53,53,53	0
57	MG	1A	3600	1/1	0.94	0.06	30,30,30,30	0
57	MG	1a	1625	1/1	0.94	0.18	57,57,57,57	0
57	MG	2a	1662	1/1	0.94	0.14	60,60,60,60	0
57	MG	2A	3411	1/1	0.94	0.14	59,59,59,59	0
57	MG	2A	3187	1/1	0.94	0.23	54,54,54,54	0
57	MG	2A	3704	1/1	0.94	0.18	55,55,55,55	0
57	MG	1A	3496	1/1	0.94	0.10	42,42,42,42	0
57	MG	1A	3498	1/1	0.94	0.15	54,54,54,54	0
57	MG	1a	1628	1/1	0.94	0.54	74,74,74,74	0
57	MG	2A	3416	1/1	0.94	0.11	55,55,55,55	0
57	MG	2a	1674	1/1	0.94	0.35	60,60,60,60	0
57	MG	1a	1787	1/1	0.94	0.12	66,66,66,66	0
57	MG	1a	1788	1/1	0.94	0.10	70,70,70,70	0
57	MG	1A	3824	1/1	0.94	0.18	50,50,50,50	0
57	MG	2A	3713	1/1	0.94	0.10	59,59,59,59	0
57	MG	1A	3605	1/1	0.94	0.10	56,56,56,56	0
57	MG	2A	3423	1/1	0.94	0.35	65,65,65,65	0
57	MG	1A	3610	1/1	0.94	0.18	50,50,50,50	0
57	MG	1A	3499	1/1	0.94	0.08	51,51,51,51	0
57	MG	1A	4099	1/1	0.94	0.13	55,55,55,55	0
57	MG	1A	3722	1/1	0.94	0.13	41,41,41,41	0
57	MG	1A	3125	1/1	0.94	0.20	54,54,54,54	0
57	MG	1A	3959	1/1	0.94	0.13	62,62,62,62	0
57	MG	1A	3420	1/1	0.94	0.15	38,38,38,38	0
57	MG	1a	1802	1/1	0.94	0.17	63,63,63,63	0
57	MG	2A	3206	1/1	0.94	0.17	60,60,60,60	0
57	MG	1A	3359	1/1	0.94	0.10	43,43,43,43	0
57	MG	1A	3127	1/1	0.94	0.12	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	3732	1/1	0.94	0.14	40,40,40,40	0
57	MG	1A	3729	1/1	0.94	0.17	50,50,50,50	0
57	MG	2A	3210	1/1	0.94	0.27	58,58,58,58	0
57	MG	2A	3444	1/1	0.94	0.14	52,52,52,52	0
57	MG	1A	3730	1/1	0.94	0.10	51,51,51,51	0
57	MG	1A	3362	1/1	0.94	0.08	47,47,47,47	0
57	MG	2a	1702	1/1	0.94	0.18	64,64,64,64	0
57	MG	2A	3213	1/1	0.94	0.19	67,67,67,67	0
57	MG	2A	3215	1/1	0.94	0.12	59,59,59,59	0
57	MG	1A	3619	1/1	0.94	0.07	34,34,34,34	0
57	MG	1A	3508	1/1	0.94	0.25	52,52,52,52	0
57	MG	2A	3455	1/1	0.94	0.15	55,55,55,55	0
57	MG	2a	1710	1/1	0.94	0.10	56,56,56,56	0
57	MG	2A	3220	1/1	0.94	0.35	48,48,48,48	0
57	MG	2a	1714	1/1	0.94	0.15	52,52,52,52	0
57	MG	2A	3462	1/1	0.94	0.12	46,46,46,46	0
57	MG	2A	3749	1/1	0.94	0.09	77,77,77,77	0
57	MG	2A	3223	1/1	0.94	0.16	44,44,44,44	0
57	MG	1A	3845	1/1	0.94	0.14	39,39,39,39	0
57	MG	1A	3242	1/1	0.94	0.13	55,55,55,55	0
57	MG	1A	3365	1/1	0.94	0.21	51,51,51,51	0
57	MG	1a	1815	1/1	0.94	0.14	67,67,67,67	0
57	MG	1A	3366	1/1	0.94	0.07	68,68,68,68	0
57	MG	1a	1656	1/1	0.94	0.29	61,61,61,61	0
57	MG	1A	3113	1/1	0.94	0.21	47,47,47,47	0
57	MG	2a	1728	1/1	0.94	0.16	52,52,52,52	0
57	MG	1B	218	1/1	0.94	0.13	51,51,51,51	0
57	MG	1A	3521	1/1	0.94	0.22	58,58,58,58	0
57	MG	1B	221	1/1	0.94	0.21	51,51,51,51	0
57	MG	1A	3159	1/1	0.94	0.25	35,35,35,35	0
57	MG	2A	3240	1/1	0.94	0.12	60,60,60,60	0
57	MG	1a	1663	1/1	0.94	0.09	52,52,52,52	0
57	MG	1A	3744	1/1	0.94	0.08	55,55,55,55	0
57	MG	2A	3244	1/1	0.94	0.17	56,56,56,56	0
57	MG	2A	3487	1/1	0.94	0.10	24,24,24,24	0
57	MG	2A	3488	1/1	0.94	0.16	61,61,61,61	0
57	MG	2A	3772	1/1	0.94	0.12	64,64,64,64	0
57	MG	1A	3980	1/1	0.94	0.09	58,58,58,58	0
57	MG	1v	103	1/1	0.94	0.07	52,52,52,52	0
57	MG	1A	3632	1/1	0.94	0.07	22,22,22,22	0
57	MG	1B	228	1/1	0.94	0.09	40,40,40,40	0
57	MG	2a	1748	1/1	0.94	0.15	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	3441	1/1	0.94	0.11	62,62,62,62	0
57	MG	2A	3781	1/1	0.94	0.06	52,52,52,52	0
57	MG	1a	1670	1/1	0.94	0.14	73,73,73,73	0
57	MG	1A	3209	1/1	0.94	0.18	53,53,53,53	0
57	MG	1A	3865	1/1	0.94	0.07	26,26,26,26	0
57	MG	2A	3254	1/1	0.94	0.21	54,54,54,54	0
57	MG	2a	1755	1/1	0.94	0.23	46,46,46,46	0
57	MG	1x	108	1/1	0.94	0.19	53,53,53,53	0
57	MG	1A	3250	1/1	0.94	0.10	47,47,47,47	0
57	MG	2a	1758	1/1	0.94	0.12	65,65,65,65	0
57	MG	1A	3212	1/1	0.94	0.20	43,43,43,43	0
57	MG	1x	112	1/1	0.94	0.15	63,63,63,63	0
57	MG	1B	236	1/1	0.94	0.10	56,56,56,56	0
57	MG	2A	3798	1/1	0.94	0.11	58,58,58,58	0
57	MG	1D	310	1/1	0.94	0.09	47,47,47,47	0
57	MG	1A	3133	1/1	0.94	0.12	35,35,35,35	0
57	MG	2A	3514	1/1	0.94	0.08	35,35,35,35	0
57	MG	1D	313	1/1	0.94	0.15	45,45,45,45	0
57	MG	1a	1679	1/1	0.94	0.07	47,47,47,47	0
57	MG	1a	1680	1/1	0.94	0.22	68,68,68,68	0
57	MG	1A	3110	1/1	0.94	0.13	43,43,43,43	0
57	MG	1A	3874	1/1	0.94	0.14	45,45,45,45	0
57	MG	2A	3270	1/1	0.94	0.17	50,50,50,50	0
57	MG	1A	4005	1/1	0.94	0.07	48,48,48,48	0
57	MG	2A	3272	1/1	0.94	0.11	53,53,53,53	0
57	MG	1a	1685	1/1	0.94	0.21	65,65,65,65	0
57	MG	2A	3023	1/1	0.94	0.21	45,45,45,45	0
57	MG	1A	3538	1/1	0.94	0.21	37,37,37,37	0
57	MG	1A	4008	1/1	0.94	0.12	76,76,76,76	0
57	MG	1A	3386	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3878	1/1	0.94	0.16	62,62,62,62	0
57	MG	2A	3030	1/1	0.94	0.07	48,48,48,48	0
57	MG	2a	1783	1/1	0.94	0.08	73,73,73,73	0
57	MG	1A	3652	1/1	0.94	0.07	59,59,59,59	0
57	MG	2A	3542	1/1	0.94	0.20	63,63,63,63	0
57	MG	2d	301	1/1	0.94	0.09	69,69,69,69	0
57	MG	2e	201	1/1	0.94	0.12	72,72,72,72	0
57	MG	1A	3451	1/1	0.94	0.14	62,62,62,62	0
57	MG	1A	3544	1/1	0.94	0.09	49,49,49,49	0
57	MG	2A	3548	1/1	0.94	0.13	49,49,49,49	0
57	MG	2A	3550	1/1	0.94	0.17	54,54,54,54	0
57	MG	2A	3551	1/1	0.94	0.12	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	1a	1693	1/1	0.94	0.26	53,53,53,53	0
57	MG	2l	202	1/1	0.94	0.11	56,56,56,56	0
57	MG	1A	3546	1/1	0.94	0.09	35,35,35,35	0
57	MG	1A	4016	1/1	0.94	0.08	50,50,50,50	0
57	MG	2A	3289	1/1	0.94	0.08	53,53,53,53	0
57	MG	1A	3387	1/1	0.94	0.25	59,59,59,59	0
57	MG	2v	101	1/1	0.94	0.09	55,55,55,55	0
57	MG	2A	3294	1/1	0.94	0.12	61,61,61,61	0
57	MG	2A	3558	1/1	0.94	0.20	47,47,47,47	0
57	MG	1A	4021	1/1	0.94	0.11	53,53,53,53	0
57	MG	2A	3562	1/1	0.94	0.08	56,56,56,56	0
57	MG	1A	3550	1/1	0.94	0.15	46,46,46,46	0
57	MG	1A	3665	1/1	0.94	0.09	60,60,60,60	0
57	MG	1A	3670	1/1	0.95	0.12	41,41,41,41	0
57	MG	2A	3073	1/1	0.95	0.09	56,56,56,56	0
57	MG	1Q	205	1/1	0.95	0.11	53,53,53,53	0
57	MG	2A	3307	1/1	0.95	0.27	58,58,58,58	0
57	MG	2A	3075	1/1	0.95	0.16	49,49,49,49	0
57	MG	2A	3309	1/1	0.95	0.17	66,66,66,66	0
57	MG	2A	3574	1/1	0.95	0.19	62,62,62,62	0
57	MG	1A	3673	1/1	0.95	0.11	31,31,31,31	0
57	MG	2A	3077	1/1	0.95	0.17	49,49,49,49	0
57	MG	2A	3312	1/1	0.95	0.10	51,51,51,51	0
57	MG	1A	3471	1/1	0.95	0.10	39,39,39,39	0
57	MG	1S	202	1/1	0.95	0.10	58,58,58,58	0
57	MG	1A	4038	1/1	0.95	0.09	48,48,48,48	0
57	MG	2A	3082	1/1	0.95	0.14	60,60,60,60	0
57	MG	1A	4041	1/1	0.95	0.09	28,28,28,28	0
57	MG	1T	202	1/1	0.95	0.09	57,57,57,57	0
57	MG	1A	3912	1/1	0.95	0.14	36,36,36,36	0
57	MG	2A	3087	1/1	0.95	0.26	56,56,56,56	0
57	MG	1U	205	1/1	0.95	0.15	39,39,39,39	0
57	MG	1U	207	1/1	0.95	0.17	37,37,37,37	0
57	MG	1A	3568	1/1	0.95	0.20	42,42,42,42	0
57	MG	1A	3346	1/1	0.95	0.12	54,54,54,54	0
57	MG	2B	218	1/1	0.95	0.19	63,63,63,63	0
57	MG	1V	206	1/1	0.95	0.10	58,58,58,58	0
57	MG	2A	3593	1/1	0.95	0.14	43,43,43,43	0
57	MG	2A	3095	1/1	0.95	0.11	30,30,30,30	0
57	MG	2D	306	1/1	0.95	0.12	51,51,51,51	0
57	MG	1A	3347	1/1	0.95	0.07	45,45,45,45	0
57	MG	1W	201	1/1	0.95	0.11	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3332	1/1	0.95	0.08	64,64,64,64	0
57	MG	1W	205	1/1	0.95	0.09	30,30,30,30	0
57	MG	2E	306	1/1	0.95	0.07	53,53,53,53	0
57	MG	1X	102	1/1	0.95	0.09	50,50,50,50	0
57	MG	1X	104	1/1	0.95	0.16	41,41,41,41	0
57	MG	2A	3608	1/1	0.95	0.13	42,42,42,42	0
57	MG	1A	3573	1/1	0.95	0.11	50,50,50,50	0
57	MG	2F	304	1/1	0.95	0.09	46,46,46,46	0
57	MG	2F	305	1/1	0.95	0.11	55,55,55,55	0
57	MG	2F	306	1/1	0.95	0.12	44,44,44,44	0
57	MG	1a	1736	1/1	0.95	0.10	45,45,45,45	0
57	MG	2A	3338	1/1	0.95	0.07	65,65,65,65	0
57	MG	1a	1737	1/1	0.95	0.14	63,63,63,63	0
57	MG	1A	3475	1/1	0.95	0.25	53,53,53,53	0
57	MG	1A	3145	1/1	0.95	0.11	45,45,45,45	0
57	MG	1A	3577	1/1	0.95	0.11	57,57,57,57	0
57	MG	1a	1741	1/1	0.95	0.09	66,66,66,66	0
57	MG	2Q	202	1/1	0.95	0.23	57,57,57,57	0
57	MG	2A	3113	1/1	0.95	0.14	51,51,51,51	0
57	MG	2Q	204	1/1	0.95	0.13	50,50,50,50	0
57	MG	10	103	1/1	0.95	0.24	48,48,48,48	0
57	MG	2A	3619	1/1	0.95	0.18	47,47,47,47	0
57	MG	1A	4051	1/1	0.95	0.04	19,19,19,19	0
57	MG	2A	3347	1/1	0.95	0.07	70,70,70,70	0
57	MG	1A	4052	1/1	0.95	0.09	61,61,61,61	0
57	MG	1A	3478	1/1	0.95	0.08	51,51,51,51	0
57	MG	11	101	1/1	0.95	0.38	47,47,47,47	0
57	MG	1A	3579	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	3087	1/1	0.95	0.09	36,36,36,36	0
57	MG	2W	202	1/1	0.95	0.23	50,50,50,50	0
57	MG	1A	3305	1/1	0.95	0.18	50,50,50,50	0
57	MG	1A	3481	1/1	0.95	0.11	62,62,62,62	0
57	MG	2A	3128	1/1	0.95	0.13	51,51,51,51	0
57	MG	2A	3356	1/1	0.95	0.06	40,40,40,40	0
57	MG	2A	3129	1/1	0.95	0.18	46,46,46,46	0
57	MG	2A	3358	1/1	0.95	0.11	56,56,56,56	0
57	MG	1A	3264	1/1	0.95	0.16	48,48,48,48	0
57	MG	23	104	1/1	0.95	0.09	50,50,50,50	0
57	MG	2A	3132	1/1	0.95	0.24	64,64,64,64	0
57	MG	1A	3930	1/1	0.95	0.06	63,63,63,63	0
57	MG	1A	3483	1/1	0.95	0.08	63,63,63,63	0
57	MG	16	102	1/1	0.95	0.07	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	3364	1/1	0.95	0.13	64,64,64,64	0
57	MG	1A	3808	1/1	0.95	0.08	39,39,39,39	0
57	MG	1A	3307	1/1	0.95	0.12	54,54,54,54	0
57	MG	2A	3367	1/1	0.95	0.10	61,61,61,61	0
57	MG	1a	1761	1/1	0.95	0.18	70,70,70,70	0
57	MG	1A	3697	1/1	0.95	0.14	55,55,55,55	0
57	MG	1a	1763	1/1	0.95	0.12	59,59,59,59	0
57	MG	1A	3226	1/1	0.95	0.23	50,50,50,50	0
57	MG	2A	3145	1/1	0.95	0.11	36,36,36,36	0
57	MG	2A	3146	1/1	0.95	0.17	62,62,62,62	0
57	MG	1A	3061	1/1	0.95	0.20	51,51,51,51	0
57	MG	1A	3813	1/1	0.95	0.22	63,63,63,63	0
57	MG	1A	3815	1/1	0.95	0.11	62,62,62,62	0
57	MG	2A	3656	1/1	0.95	0.17	62,62,62,62	0
57	MG	2A	3657	1/1	0.95	0.25	57,57,57,57	0
57	MG	2a	1613	1/1	0.95	0.19	65,65,65,65	0
57	MG	1A	3357	1/1	0.95	0.13	62,62,62,62	0
57	MG	2A	3659	1/1	0.95	0.08	45,45,45,45	0
57	MG	2A	3154	1/1	0.95	0.14	48,48,48,48	0
57	MG	1A	3489	1/1	0.95	0.14	45,45,45,45	0
57	MG	2A	3158	1/1	0.95	0.15	43,43,43,43	0
57	MG	2A	3159	1/1	0.95	0.12	56,56,56,56	0
57	MG	1A	3943	1/1	0.95	0.10	43,43,43,43	0
57	MG	2A	3665	1/1	0.95	0.07	69,69,69,69	0
57	MG	2A	3383	1/1	0.95	0.07	47,47,47,47	0
57	MG	2a	1623	1/1	0.95	0.07	59,59,59,59	0
57	MG	1A	3228	1/1	0.95	0.22	36,36,36,36	0
57	MG	1a	1607	1/1	0.95	0.11	65,65,65,65	0
57	MG	1A	3116	1/1	0.95	0.16	49,49,49,49	0
57	MG	2a	1627	1/1	0.95	0.23	69,69,69,69	0
57	MG	1a	1610	1/1	0.95	0.08	72,72,72,72	0
57	MG	1a	1775	1/1	0.95	0.17	61,61,61,61	0
57	MG	2A	3673	1/1	0.95	0.06	59,59,59,59	0
57	MG	1A	3709	1/1	0.95	0.10	52,52,52,52	0
57	MG	1A	3235	1/1	0.95	0.12	45,45,45,45	0
57	MG	2a	1633	1/1	0.95	0.10	53,53,53,53	0
57	MG	2A	3169	1/1	0.95	0.19	44,44,44,44	0
57	MG	1A	3281	1/1	0.95	0.11	62,62,62,62	0
57	MG	2A	3678	1/1	0.95	0.16	64,64,64,64	0
57	MG	1A	3951	1/1	0.95	0.07	52,52,52,52	0
57	MG	1A	3282	1/1	0.95	0.17	40,40,40,40	0
57	MG	1a	1617	1/1	0.95	0.08	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3714	1/1	0.95	0.17	49,49,49,49	0
57	MG	2A	3399	1/1	0.95	0.38	56,56,56,56	0
57	MG	2A	3179	1/1	0.95	0.06	51,51,51,51	0
57	MG	2a	1645	1/1	0.95	0.16	63,63,63,63	0
57	MG	1A	3426	1/1	0.95	0.26	39,39,39,39	0
57	MG	1A	3063	1/1	0.95	0.09	56,56,56,56	0
57	MG	1A	3717	1/1	0.95	0.07	43,43,43,43	0
57	MG	2A	3404	1/1	0.95	0.30	69,69,69,69	0
57	MG	1A	3718	1/1	0.95	0.05	16,16,16,16	0
57	MG	2A	3692	1/1	0.95	0.07	39,39,39,39	0
57	MG	2a	1652	1/1	0.95	0.18	60,60,60,60	0
57	MG	1a	1624	1/1	0.95	0.18	60,60,60,60	0
57	MG	2a	1654	1/1	0.95	0.16	48,48,48,48	0
57	MG	2A	3407	1/1	0.95	0.19	58,58,58,58	0
57	MG	1a	1789	1/1	0.95	0.07	54,54,54,54	0
57	MG	1A	3609	1/1	0.95	0.06	36,36,36,36	0
57	MG	2a	1659	1/1	0.95	0.33	59,59,59,59	0
57	MG	1A	3185	1/1	0.95	0.12	37,37,37,37	0
57	MG	1A	3962	1/1	0.95	0.12	77,77,77,77	0
57	MG	1A	3835	1/1	0.95	0.21	65,65,65,65	0
57	MG	2a	1665	1/1	0.95	0.16	64,64,64,64	0
57	MG	1A	3964	1/1	0.95	0.12	32,32,32,32	0
57	MG	1A	3152	1/1	0.95	0.14	48,48,48,48	0
57	MG	2A	3195	1/1	0.95	0.19	58,58,58,58	0
57	MG	2a	1670	1/1	0.95	0.18	54,54,54,54	0
57	MG	1a	1797	1/1	0.95	0.09	70,70,70,70	0
57	MG	1A	3368	1/1	0.95	0.10	50,50,50,50	0
57	MG	1a	1632	1/1	0.95	0.10	31,31,31,31	0
57	MG	2A	3199	1/1	0.95	0.14	56,56,56,56	0
57	MG	1a	1633	1/1	0.95	0.14	59,59,59,59	0
57	MG	1A	3838	1/1	0.95	0.06	23,23,23,23	0
57	MG	2A	3424	1/1	0.95	0.13	59,59,59,59	0
57	MG	1A	3840	1/1	0.95	0.11	42,42,42,42	0
57	MG	1B	207	1/1	0.95	0.10	48,48,48,48	0
57	MG	1A	3507	1/1	0.95	0.33	57,57,57,57	0
57	MG	1A	3435	1/1	0.95	0.22	69,69,69,69	0
57	MG	1A	3616	1/1	0.95	0.07	36,36,36,36	0
57	MG	2A	3718	1/1	0.95	0.26	62,62,62,62	0
57	MG	1A	3510	1/1	0.95	0.30	35,35,35,35	0
57	MG	2A	3721	1/1	0.95	0.11	61,61,61,61	0
57	MG	1a	1810	1/1	0.95	0.20	59,59,59,59	0
57	MG	1A	3092	1/1	0.95	0.19	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	3513	1/1	0.95	0.27	48,48,48,48	0
57	MG	1A	3192	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	3066	1/1	0.95	0.06	47,47,47,47	0
57	MG	1A	3049	1/1	0.95	0.12	31,31,31,31	0
57	MG	2A	3729	1/1	0.95	0.11	63,63,63,63	0
57	MG	2A	3441	1/1	0.95	0.12	56,56,56,56	0
57	MG	2a	1696	1/1	0.95	0.14	61,61,61,61	0
57	MG	1a	1647	1/1	0.95	0.06	55,55,55,55	0
57	MG	1B	219	1/1	0.95	0.07	37,37,37,37	0
57	MG	2a	1699	1/1	0.95	0.19	62,62,62,62	0
57	MG	1A	3518	1/1	0.95	0.27	66,66,66,66	0
57	MG	1A	3378	1/1	0.95	0.08	57,57,57,57	0
57	MG	1e	203	1/1	0.95	0.13	62,62,62,62	0
57	MG	2a	1703	1/1	0.95	0.19	58,58,58,58	0
57	MG	2A	3225	1/1	0.95	0.17	54,54,54,54	0
57	MG	1a	1652	1/1	0.95	0.09	75,75,75,75	0
57	MG	2A	3229	1/1	0.95	0.14	56,56,56,56	0
57	MG	1A	3329	1/1	0.95	0.09	60,60,60,60	0
57	MG	2A	3231	1/1	0.95	0.09	62,62,62,62	0
57	MG	1A	3002	1/1	0.95	0.11	44,44,44,44	0
57	MG	1n	101	1/1	0.95	0.30	70,70,70,70	0
57	MG	1A	3740	1/1	0.95	0.07	30,30,30,30	0
57	MG	1A	3984	1/1	0.95	0.16	32,32,32,32	0
57	MG	1a	1658	1/1	0.95	0.08	64,64,64,64	0
57	MG	1A	3987	1/1	0.95	0.07	63,63,63,63	0
57	MG	2a	1718	1/1	0.95	0.14	65,65,65,65	0
57	MG	1A	3381	1/1	0.95	0.17	27,27,27,27	0
57	MG	1A	3989	1/1	0.95	0.08	82,82,82,82	0
57	MG	1A	3991	1/1	0.95	0.10	35,35,35,35	0
57	MG	1B	232	1/1	0.95	0.09	66,66,66,66	0
57	MG	2A	3242	1/1	0.95	0.12	53,53,53,53	0
57	MG	1x	104	1/1	0.95	0.39	73,73,73,73	0
57	MG	1a	1664	1/1	0.95	0.09	61,61,61,61	0
57	MG	2A	3482	1/1	0.95	0.11	58,58,58,58	0
57	MG	1A	3992	1/1	0.95	0.08	26,26,26,26	0
57	MG	1A	3382	1/1	0.95	0.16	39,39,39,39	0
57	MG	1A	3995	1/1	0.95	0.08	29,29,29,29	0
57	MG	1B	238	1/1	0.95	0.06	41,41,41,41	0
57	MG	2A	3766	1/1	0.95	0.20	67,67,67,67	0
57	MG	1D	302	1/1	0.95	0.20	42,42,42,42	0
57	MG	2a	1738	1/1	0.95	0.11	64,64,64,64	0
57	MG	2A	3001	1/1	0.95	0.10	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	3251	1/1	0.95	0.17	61,61,61,61	0
57	MG	1D	309	1/1	0.95	0.13	48,48,48,48	0
57	MG	1A	3449	1/1	0.95	0.12	73,73,73,73	0
57	MG	1A	3999	1/1	0.95	0.08	32,32,32,32	0
57	MG	2A	3256	1/1	0.95	0.09	67,67,67,67	0
57	MG	2A	3496	1/1	0.95	0.08	44,44,44,44	0
57	MG	1A	3870	1/1	0.95	0.11	50,50,50,50	0
57	MG	2A	3777	1/1	0.95	0.10	50,50,50,50	0
57	MG	1D	314	1/1	0.95	0.09	34,34,34,34	0
57	MG	2A	3779	1/1	0.95	0.09	56,56,56,56	0
57	MG	1A	3871	1/1	0.95	0.09	32,32,32,32	0
57	MG	2A	3014	1/1	0.95	0.16	53,53,53,53	0
57	MG	2A	3782	1/1	0.95	0.09	59,59,59,59	0
57	MG	1E	305	1/1	0.95	0.20	33,33,33,33	0
57	MG	2A	3505	1/1	0.95	0.05	34,34,34,34	0
57	MG	1A	3384	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3079	1/1	0.95	0.15	52,52,52,52	0
57	MG	2A	3790	1/1	0.95	0.08	40,40,40,40	0
57	MG	1A	3082	1/1	0.95	0.15	32,32,32,32	0
57	MG	1E	311	1/1	0.95	0.20	41,41,41,41	0
57	MG	2A	3266	1/1	0.95	0.20	54,54,54,54	0
57	MG	2A	3512	1/1	0.95	0.11	52,52,52,52	0
57	MG	2A	3025	1/1	0.95	0.20	51,51,51,51	0
57	MG	2A	3796	1/1	0.95	0.09	39,39,39,39	0
57	MG	2A	3797	1/1	0.95	0.08	41,41,41,41	0
57	MG	1E	312	1/1	0.95	0.12	63,63,63,63	0
57	MG	1A	4007	1/1	0.95	0.07	71,71,71,71	0
57	MG	1A	3875	1/1	0.95	0.12	45,45,45,45	0
57	MG	1A	3639	1/1	0.95	0.07	31,31,31,31	0
57	MG	1A	3641	1/1	0.95	0.12	36,36,36,36	0
57	MG	2A	3521	1/1	0.95	0.09	50,50,50,50	0
57	MG	2A	3523	1/1	0.95	0.11	41,41,41,41	0
57	MG	2A	3032	1/1	0.95	0.11	47,47,47,47	0
57	MG	2a	1774	1/1	0.95	0.11	68,68,68,68	0
57	MG	1A	3753	1/1	0.95	0.09	57,57,57,57	0
57	MG	2A	3037	1/1	0.95	0.13	66,66,66,66	0
57	MG	1A	3389	1/1	0.95	0.11	49,49,49,49	0
57	MG	1A	3646	1/1	0.95	0.05	21,21,21,21	0
57	MG	2A	3041	1/1	0.95	0.10	54,54,54,54	0
57	MG	1A	3647	1/1	0.95	0.10	22,22,22,22	0
57	MG	1A	3056	1/1	0.95	0.09	49,49,49,49	0
57	MG	1G	201	1/1	0.95	0.09	44,44,44,44	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	3457	1/1	0.95	0.19	44,44,44,44	0
57	MG	2A	3283	1/1	0.95	0.17	63,63,63,63	0
57	MG	1A	3337	1/1	0.95	0.09	54,54,54,54	0
57	MG	1a	1695	1/1	0.95	0.26	67,67,67,67	0
57	MG	2A	3543	1/1	0.95	0.20	68,68,68,68	0
57	MG	1A	3547	1/1	0.95	0.09	24,24,24,24	0
57	MG	2A	3826	1/1	0.95	0.12	56,56,56,56	0
57	MG	2A	3545	1/1	0.95	0.09	62,62,62,62	0
57	MG	2A	3287	1/1	0.95	0.13	60,60,60,60	0
57	MG	2A	3288	1/1	0.95	0.13	51,51,51,51	0
57	MG	2A	3549	1/1	0.95	0.12	33,33,33,33	0
57	MG	1A	3655	1/1	0.95	0.07	28,28,28,28	0
57	MG	2A	3291	1/1	0.95	0.11	63,63,63,63	0
57	MG	1A	3210	1/1	0.95	0.07	51,51,51,51	0
57	MG	1N	201	1/1	0.95	0.20	44,44,44,44	0
57	MG	1A	3342	1/1	0.95	0.11	61,61,61,61	0
57	MG	1A	3174	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3466	1/1	0.95	0.08	54,54,54,54	0
57	MG	1A	3301	1/1	0.95	0.12	51,51,51,51	0
57	MG	1A	3899	1/1	0.95	0.06	47,47,47,47	0
57	MG	1A	3562	1/1	0.95	0.10	53,53,53,53	0
57	MG	1A	3143	1/1	0.95	0.28	37,37,37,37	0
57	MG	1A	3399	1/1	0.95	0.12	43,43,43,43	0
57	MG	1A	3640	1/1	0.96	0.07	30,30,30,30	0
57	MG	1F	314	1/1	0.96	0.10	33,33,33,33	0
57	MG	1A	3090	1/1	0.96	0.13	29,29,29,29	0
57	MG	1A	3882	1/1	0.96	0.13	42,42,42,42	0
57	MG	1A	3754	1/1	0.96	0.16	73,73,73,73	0
57	MG	1A	3884	1/1	0.96	0.11	32,32,32,32	0
57	MG	2A	3668	1/1	0.96	0.10	66,66,66,66	0
57	MG	1A	3531	1/1	0.96	0.17	36,36,36,36	0
57	MG	1A	3644	1/1	0.96	0.08	20,20,20,20	0
57	MG	1A	3534	1/1	0.96	0.12	34,34,34,34	0
57	MG	1A	3536	1/1	0.96	0.25	33,33,33,33	0
57	MG	2A	3022	1/1	0.96	0.18	50,50,50,50	0
57	MG	1A	3312	1/1	0.96	0.14	49,49,49,49	0
57	MG	1A	3892	1/1	0.96	0.17	64,64,64,64	0
57	MG	1N	204	1/1	0.96	0.26	44,44,44,44	0
57	MG	1A	3372	1/1	0.96	0.25	32,32,32,32	0
57	MG	1A	3539	1/1	0.96	0.18	44,44,44,44	0
57	MG	1A	3767	1/1	0.96	0.08	30,30,30,30	0
57	MG	1A	3653	1/1	0.96	0.09	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3031	1/1	0.96	0.08	56,56,56,56	0
57	MG	1A	3313	1/1	0.96	0.08	43,43,43,43	0
57	MG	25	102	1/1	0.96	0.08	64,64,64,64	0
57	MG	25	104	1/1	0.96	0.11	45,45,45,45	0
57	MG	2A	3033	1/1	0.96	0.08	53,53,53,53	0
57	MG	1A	3041	1/1	0.96	0.24	36,36,36,36	0
57	MG	1A	4039	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	4040	1/1	0.96	0.07	52,52,52,52	0
57	MG	2A	3449	1/1	0.96	0.19	65,65,65,65	0
57	MG	1A	3772	1/1	0.96	0.06	45,45,45,45	0
57	MG	1A	3901	1/1	0.96	0.07	63,63,63,63	0
57	MG	1R	202	1/1	0.96	0.23	44,44,44,44	0
57	MG	2A	3456	1/1	0.96	0.09	48,48,48,48	0
57	MG	2A	3458	1/1	0.96	0.08	51,51,51,51	0
57	MG	1A	3255	1/1	0.96	0.13	46,46,46,46	0
57	MG	1S	201	1/1	0.96	0.10	43,43,43,43	0
57	MG	1A	3199	1/1	0.96	0.11	24,24,24,24	0
57	MG	2A	3465	1/1	0.96	0.07	45,45,45,45	0
57	MG	1A	3659	1/1	0.96	0.05	32,32,32,32	0
57	MG	2A	3050	1/1	0.96	0.10	65,65,65,65	0
57	MG	2A	3702	1/1	0.96	0.06	61,61,61,61	0
57	MG	1a	1703	1/1	0.96	0.09	60,60,60,60	0
57	MG	1A	4046	1/1	0.96	0.11	56,56,56,56	0
57	MG	1a	1705	1/1	0.96	0.06	59,59,59,59	0
57	MG	1A	3779	1/1	0.96	0.05	22,22,22,22	0
57	MG	1A	3780	1/1	0.96	0.30	33,33,33,33	0
57	MG	1U	204	1/1	0.96	0.14	50,50,50,50	0
57	MG	1A	3453	1/1	0.96	0.10	61,61,61,61	0
57	MG	1a	1710	1/1	0.96	0.10	60,60,60,60	0
57	MG	1A	3454	1/1	0.96	0.12	45,45,45,45	0
57	MG	2A	3481	1/1	0.96	0.13	54,54,54,54	0
57	MG	1U	209	1/1	0.96	0.31	44,44,44,44	0
57	MG	1A	3258	1/1	0.96	0.22	50,50,50,50	0
57	MG	2A	3064	1/1	0.96	0.06	37,37,37,37	0
57	MG	1V	202	1/1	0.96	0.35	35,35,35,35	0
57	MG	2A	3066	1/1	0.96	0.17	48,48,48,48	0
57	MG	1A	3044	1/1	0.96	0.05	23,23,23,23	0
57	MG	1A	3785	1/1	0.96	0.09	62,62,62,62	0
57	MG	1A	3147	1/1	0.96	0.16	38,38,38,38	0
57	MG	2A	3490	1/1	0.96	0.08	45,45,45,45	0
57	MG	2A	3724	1/1	0.96	0.09	61,61,61,61	0
57	MG	1A	3460	1/1	0.96	0.14	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1W	202	1/1	0.96	0.07	48,48,48,48	0
57	MG	1W	204	1/1	0.96	0.18	39,39,39,39	0
57	MG	1A	3203	1/1	0.96	0.11	50,50,50,50	0
57	MG	1X	101	1/1	0.96	0.24	37,37,37,37	0
57	MG	1A	4061	1/1	0.96	0.12	61,61,61,61	0
57	MG	2A	3498	1/1	0.96	0.14	43,43,43,43	0
57	MG	1X	103	1/1	0.96	0.17	42,42,42,42	0
57	MG	1a	1727	1/1	0.96	0.13	70,70,70,70	0
57	MG	2a	1642	1/1	0.96	0.16	48,48,48,48	0
57	MG	1A	3789	1/1	0.96	0.05	48,48,48,48	0
57	MG	1X	105	1/1	0.96	0.12	57,57,57,57	0
57	MG	1A	3671	1/1	0.96	0.08	24,24,24,24	0
57	MG	1A	3792	1/1	0.96	0.08	33,33,33,33	0
57	MG	2A	3292	1/1	0.96	0.14	61,61,61,61	0
57	MG	1Y	203	1/1	0.96	0.21	44,44,44,44	0
57	MG	1Y	204	1/1	0.96	0.12	63,63,63,63	0
57	MG	2A	3742	1/1	0.96	0.13	64,64,64,64	0
57	MG	1a	1735	1/1	0.96	0.14	44,44,44,44	0
57	MG	1A	3672	1/1	0.96	0.09	64,64,64,64	0
57	MG	1Z	302	1/1	0.96	0.06	42,42,42,42	0
57	MG	1A	3321	1/1	0.96	0.10	51,51,51,51	0
57	MG	1A	3385	1/1	0.96	0.11	49,49,49,49	0
57	MG	1A	3676	1/1	0.96	0.09	51,51,51,51	0
57	MG	1A	3046	1/1	0.96	0.07	37,37,37,37	0
57	MG	2A	3518	1/1	0.96	0.07	45,45,45,45	0
57	MG	2A	3099	1/1	0.96	0.16	53,53,53,53	0
57	MG	1A	3267	1/1	0.96	0.19	28,28,28,28	0
57	MG	2a	1663	1/1	0.96	0.34	65,65,65,65	0
57	MG	2A	3522	1/1	0.96	0.11	54,54,54,54	0
57	MG	10	107	1/1	0.96	0.10	46,46,46,46	0
57	MG	2A	3305	1/1	0.96	0.20	59,59,59,59	0
57	MG	2A	3103	1/1	0.96	0.17	50,50,50,50	0
57	MG	1A	3062	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	3270	1/1	0.96	0.19	37,37,37,37	0
57	MG	11	103	1/1	0.96	0.06	44,44,44,44	0
57	MG	1A	3271	1/1	0.96	0.21	30,30,30,30	0
57	MG	1A	3328	1/1	0.96	0.18	63,63,63,63	0
57	MG	12	102	1/1	0.96	0.16	54,54,54,54	0
57	MG	13	101	1/1	0.96	0.09	32,32,32,32	0
57	MG	2A	3535	1/1	0.96	0.09	36,36,36,36	0
57	MG	2A	3314	1/1	0.96	0.18	57,57,57,57	0
57	MG	1A	3272	1/1	0.96	0.18	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	15	101	1/1	0.96	0.17	42,42,42,42	0
57	MG	2A	3541	1/1	0.96	0.07	36,36,36,36	0
57	MG	2A	3318	1/1	0.96	0.12	59,59,59,59	0
57	MG	2A	3775	1/1	0.96	0.07	70,70,70,70	0
57	MG	1A	3274	1/1	0.96	0.07	56,56,56,56	0
57	MG	2A	3117	1/1	0.96	0.11	54,54,54,54	0
57	MG	15	104	1/1	0.96	0.28	33,33,33,33	0
57	MG	2a	1686	1/1	0.96	0.23	68,68,68,68	0
57	MG	1A	3395	1/1	0.96	0.07	42,42,42,42	0
57	MG	2A	3547	1/1	0.96	0.08	43,43,43,43	0
57	MG	1A	3010	1/1	0.96	0.04	33,33,33,33	0
57	MG	1A	4085	1/1	0.96	0.11	49,49,49,49	0
57	MG	2A	3123	1/1	0.96	0.23	48,48,48,48	0
57	MG	1A	3477	1/1	0.96	0.16	36,36,36,36	0
57	MG	2A	3785	1/1	0.96	0.05	49,49,49,49	0
57	MG	1A	3011	1/1	0.96	0.08	37,37,37,37	0
57	MG	17	105	1/1	0.96	0.13	43,43,43,43	0
57	MG	2A	3789	1/1	0.96	0.13	45,45,45,45	0
57	MG	1A	4088	1/1	0.96	0.17	50,50,50,50	0
57	MG	1A	3213	1/1	0.96	0.15	56,56,56,56	0
57	MG	2A	3130	1/1	0.96	0.10	41,41,41,41	0
57	MG	1A	4090	1/1	0.96	0.07	53,53,53,53	0
57	MG	1A	3101	1/1	0.96	0.27	45,45,45,45	0
57	MG	1A	3402	1/1	0.96	0.09	54,54,54,54	0
57	MG	1A	3816	1/1	0.96	0.05	59,59,59,59	0
57	MG	1A	3403	1/1	0.96	0.07	52,52,52,52	0
57	MG	2a	1706	1/1	0.96	0.18	55,55,55,55	0
57	MG	2A	3566	1/1	0.96	0.08	60,60,60,60	0
57	MG	2A	3137	1/1	0.96	0.13	50,50,50,50	0
57	MG	2A	3568	1/1	0.96	0.09	56,56,56,56	0
57	MG	1A	3105	1/1	0.96	0.22	33,33,33,33	0
57	MG	2a	1712	1/1	0.96	0.08	55,55,55,55	0
57	MG	1A	3341	1/1	0.96	0.10	56,56,56,56	0
57	MG	1A	3700	1/1	0.96	0.07	53,53,53,53	0
57	MG	2A	3806	1/1	0.96	0.08	44,44,44,44	0
57	MG	1A	3590	1/1	0.96	0.09	33,33,33,33	0
57	MG	1A	3069	1/1	0.96	0.11	33,33,33,33	0
57	MG	1A	3957	1/1	0.96	0.07	65,65,65,65	0
57	MG	1A	3823	1/1	0.96	0.10	20,20,20,20	0
57	MG	1A	3408	1/1	0.96	0.14	57,57,57,57	0
57	MG	2A	3147	1/1	0.96	0.15	36,36,36,36	0
57	MG	2A	3148	1/1	0.96	0.12	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	1A	3409	1/1	0.96	0.11	50,50,50,50	0
57	MG	1a	1615	1/1	0.96	0.09	65,65,65,65	0
57	MG	1A	3221	1/1	0.96	0.21	40,40,40,40	0
57	MG	1A	3225	1/1	0.96	0.07	57,57,57,57	0
57	MG	2a	1729	1/1	0.96	0.20	72,72,72,72	0
57	MG	1A	3598	1/1	0.96	0.08	25,25,25,25	0
57	MG	2A	3155	1/1	0.96	0.11	46,46,46,46	0
57	MG	1A	3070	1/1	0.96	0.10	15,15,15,15	0
57	MG	1A	3493	1/1	0.96	0.16	35,35,35,35	0
57	MG	1A	3051	1/1	0.96	0.14	45,45,45,45	0
57	MG	1A	3414	1/1	0.96	0.17	46,46,46,46	0
57	MG	1A	3074	1/1	0.96	0.30	50,50,50,50	0
57	MG	1A	3230	1/1	0.96	0.12	49,49,49,49	0
57	MG	1A	3231	1/1	0.96	0.18	34,34,34,34	0
57	MG	1a	1793	1/1	0.96	0.10	52,52,52,52	0
57	MG	1B	215	1/1	0.96	0.07	51,51,51,51	0
57	MG	1B	216	1/1	0.96	0.10	47,47,47,47	0
57	MG	1A	3232	1/1	0.96	0.07	32,32,32,32	0
57	MG	2A	3168	1/1	0.96	0.11	43,43,43,43	0
57	MG	2A	3601	1/1	0.96	0.15	40,40,40,40	0
57	MG	1A	3839	1/1	0.96	0.08	51,51,51,51	0
57	MG	2A	3604	1/1	0.96	0.09	37,37,37,37	0
57	MG	1A	3352	1/1	0.96	0.07	50,50,50,50	0
57	MG	2A	3607	1/1	0.96	0.07	31,31,31,31	0
57	MG	1A	3015	1/1	0.96	0.20	35,35,35,35	0
57	MG	2A	3172	1/1	0.96	0.17	53,53,53,53	0
57	MG	1A	3842	1/1	0.96	0.10	33,33,33,33	0
57	MG	1A	3615	1/1	0.96	0.10	22,22,22,22	0
57	MG	1A	3421	1/1	0.96	0.30	45,45,45,45	0
57	MG	2A	3848	1/1	0.96	0.07	57,57,57,57	0
57	MG	1B	224	1/1	0.96	0.11	50,50,50,50	0
57	MG	1A	3726	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	3004	1/1	0.96	0.07	32,32,32,32	0
57	MG	1A	3850	1/1	0.96	0.08	35,35,35,35	0
57	MG	2B	201	1/1	0.96	0.08	58,58,58,58	0
57	MG	2A	3184	1/1	0.96	0.30	63,63,63,63	0
57	MG	1A	3032	1/1	0.96	0.18	36,36,36,36	0
57	MG	1A	3511	1/1	0.96	0.35	44,44,44,44	0
57	MG	1A	3084	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	3621	1/1	0.96	0.08	47,47,47,47	0
57	MG	1A	3126	1/1	0.96	0.09	33,33,33,33	0
57	MG	1B	234	1/1	0.96	0.12	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	3384	1/1	0.96	0.25	60,60,60,60	0
57	MG	1A	3001	1/1	0.96	0.07	33,33,33,33	0
57	MG	1A	3128	1/1	0.96	0.10	46,46,46,46	0
57	MG	1A	3859	1/1	0.96	0.07	39,39,39,39	0
57	MG	2a	1773	1/1	0.96	0.18	62,62,62,62	0
57	MG	1a	1650	1/1	0.96	0.11	50,50,50,50	0
57	MG	1A	3860	1/1	0.96	0.10	54,54,54,54	0
57	MG	1D	304	1/1	0.96	0.12	41,41,41,41	0
57	MG	1D	306	1/1	0.96	0.06	39,39,39,39	0
57	MG	1a	1654	1/1	0.96	0.09	52,52,52,52	0
57	MG	1A	3861	1/1	0.96	0.06	50,50,50,50	0
57	MG	1A	3998	1/1	0.96	0.05	34,34,34,34	0
57	MG	1A	3862	1/1	0.96	0.11	26,26,26,26	0
57	MG	1t	201	1/1	0.96	0.15	53,53,53,53	0
57	MG	1A	3628	1/1	0.96	0.06	42,42,42,42	0
57	MG	1A	3434	1/1	0.96	0.12	50,50,50,50	0
57	MG	1A	3360	1/1	0.96	0.17	40,40,40,40	0
57	MG	1E	304	1/1	0.96	0.20	36,36,36,36	0
57	MG	2E	304	1/1	0.96	0.24	68,68,68,68	0
57	MG	2A	3645	1/1	0.96	0.23	36,36,36,36	0
57	MG	1A	3086	1/1	0.96	0.20	46,46,46,46	0
57	MG	1A	3741	1/1	0.96	0.09	32,32,32,32	0
57	MG	1A	3742	1/1	0.96	0.07	29,29,29,29	0
57	MG	1A	3039	1/1	0.96	0.07	36,36,36,36	0
57	MG	1A	3058	1/1	0.96	0.06	34,34,34,34	0
57	MG	1A	3248	1/1	0.96	0.06	29,29,29,29	0
57	MG	1x	107	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	4011	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3525	1/1	0.96	0.14	52,52,52,52	0
57	MG	2A	3221	1/1	0.96	0.21	48,48,48,48	0
57	MG	2t	201	1/1	0.96	0.20	55,55,55,55	0
57	MG	2A	3222	1/1	0.96	0.07	53,53,53,53	0
57	MG	1A	3526	1/1	0.96	0.13	66,66,66,66	0
57	MG	1A	3089	1/1	0.96	0.16	60,60,60,60	0
57	MG	1A	3749	1/1	0.96	0.04	38,38,38,38	0
57	MG	1A	3141	1/1	0.96	0.06	35,35,35,35	0
57	MG	2Q	201	1/1	0.96	0.14	50,50,50,50	0
57	MG	2A	3228	1/1	0.96	0.07	56,56,56,56	0
59	ZN	1n	103	1/1	0.96	0.06	89,89,89,89	0
59	ZN	24	501	1/1	0.96	0.09	112,112,112,112	0
57	MG	2A	3178	1/1	0.97	0.13	54,54,54,54	0
57	MG	1B	227	1/1	0.97	0.05	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	3075	1/1	0.97	0.06	36,36,36,36	0
57	MG	1A	3517	1/1	0.97	0.19	48,48,48,48	0
57	MG	2F	303	1/1	0.97	0.07	68,68,68,68	0
57	MG	1A	3985	1/1	0.97	0.10	23,23,23,23	0
57	MG	2A	3183	1/1	0.97	0.07	56,56,56,56	0
57	MG	2A	3636	1/1	0.97	0.07	54,54,54,54	0
57	MG	1A	3142	1/1	0.97	0.17	34,34,34,34	0
57	MG	1A	3622	1/1	0.97	0.08	40,40,40,40	0
57	MG	1A	3519	1/1	0.97	0.18	51,51,51,51	0
57	MG	2A	3640	1/1	0.97	0.07	38,38,38,38	0
57	MG	2A	3395	1/1	0.97	0.11	44,44,44,44	0
57	MG	1A	3040	1/1	0.97	0.09	34,34,34,34	0
57	MG	1A	3275	1/1	0.97	0.14	36,36,36,36	0
57	MG	1A	3993	1/1	0.97	0.05	25,25,25,25	0
57	MG	1B	237	1/1	0.97	0.08	45,45,45,45	0
57	MG	1a	1636	1/1	0.97	0.06	46,46,46,46	0
57	MG	1A	3448	1/1	0.97	0.14	49,49,49,49	0
57	MG	1d	301	1/1	0.97	0.30	50,50,50,50	0
57	MG	1D	301	1/1	0.97	0.15	32,32,32,32	0
57	MG	1A	3115	1/1	0.97	0.12	40,40,40,40	0
57	MG	1D	303	1/1	0.97	0.08	46,46,46,46	0
57	MG	1A	3229	1/1	0.97	0.07	29,29,29,29	0
57	MG	1A	3327	1/1	0.97	0.11	55,55,55,55	0
57	MG	1D	307	1/1	0.97	0.09	33,33,33,33	0
57	MG	1m	3001	1/1	0.97	0.08	70,70,70,70	0
57	MG	1D	308	1/1	0.97	0.05	40,40,40,40	0
57	MG	1A	3527	1/1	0.97	0.13	62,62,62,62	0
57	MG	1A	3064	1/1	0.97	0.08	33,33,33,33	0
57	MG	1A	3388	1/1	0.97	0.09	43,43,43,43	0
57	MG	1A	4002	1/1	0.97	0.05	52,52,52,52	0
57	MG	1A	3184	1/1	0.97	0.17	41,41,41,41	0
57	MG	1E	301	1/1	0.97	0.24	34,34,34,34	0
57	MG	1A	3033	1/1	0.97	0.06	42,42,42,42	0
57	MG	2A	3419	1/1	0.97	0.15	37,37,37,37	0
57	MG	1E	303	1/1	0.97	0.09	44,44,44,44	0
57	MG	1A	3532	1/1	0.97	0.13	34,34,34,34	0
57	MG	1A	3533	1/1	0.97	0.09	45,45,45,45	0
57	MG	1A	3187	1/1	0.97	0.07	38,38,38,38	0
57	MG	1A	3148	1/1	0.97	0.08	38,38,38,38	0
57	MG	1A	3458	1/1	0.97	0.05	40,40,40,40	0
57	MG	2A	3218	1/1	0.97	0.07	43,43,43,43	0
57	MG	2A	3219	1/1	0.97	0.15	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	3643	1/1	0.97	0.07	43,43,43,43	0
57	MG	1A	3459	1/1	0.97	0.07	53,53,53,53	0
57	MG	2A	3430	1/1	0.97	0.06	41,41,41,41	0
57	MG	2A	3431	1/1	0.97	0.16	37,37,37,37	0
57	MG	2a	1601	1/1	0.97	0.19	56,56,56,56	0
57	MG	1A	3756	1/1	0.97	0.04	62,62,62,62	0
57	MG	1x	111	1/1	0.97	0.11	56,56,56,56	0
57	MG	1F	301	1/1	0.97	0.12	41,41,41,41	0
57	MG	1F	303	1/1	0.97	0.16	32,32,32,32	0
57	MG	2A	3226	1/1	0.97	0.17	54,54,54,54	0
57	MG	1A	3757	1/1	0.97	0.04	41,41,41,41	0
57	MG	1A	3083	1/1	0.97	0.18	38,38,38,38	0
57	MG	1A	3461	1/1	0.97	0.12	49,49,49,49	0
57	MG	1A	3760	1/1	0.97	0.05	46,46,46,46	0
57	MG	2A	3443	1/1	0.97	0.14	41,41,41,41	0
57	MG	1F	311	1/1	0.97	0.10	34,34,34,34	0
57	MG	2A	3011	1/1	0.97	0.10	47,47,47,47	0
57	MG	2A	3012	1/1	0.97	0.11	50,50,50,50	0
57	MG	1A	4018	1/1	0.97	0.10	56,56,56,56	0
57	MG	1A	3648	1/1	0.97	0.04	28,28,28,28	0
57	MG	2A	3694	1/1	0.97	0.07	52,52,52,52	0
57	MG	1A	3762	1/1	0.97	0.07	21,21,21,21	0
57	MG	2A	3450	1/1	0.97	0.06	50,50,50,50	0
57	MG	1A	3037	1/1	0.97	0.22	32,32,32,32	0
57	MG	2A	3452	1/1	0.97	0.13	67,67,67,67	0
57	MG	2A	3453	1/1	0.97	0.06	44,44,44,44	0
57	MG	2A	3019	1/1	0.97	0.23	36,36,36,36	0
57	MG	1A	3238	1/1	0.97	0.14	46,46,46,46	0
57	MG	1A	3396	1/1	0.97	0.13	44,44,44,44	0
57	MG	1A	3766	1/1	0.97	0.07	49,49,49,49	0
57	MG	2A	3459	1/1	0.97	0.17	51,51,51,51	0
57	MG	1A	3339	1/1	0.97	0.12	62,62,62,62	0
57	MG	2A	3024	1/1	0.97	0.10	43,43,43,43	0
57	MG	2A	3707	1/1	0.97	0.06	33,33,33,33	0
57	MG	1A	3340	1/1	0.97	0.26	38,38,38,38	0
57	MG	2A	3464	1/1	0.97	0.09	44,44,44,44	0
57	MG	1A	4029	1/1	0.97	0.08	40,40,40,40	0
57	MG	1A	3239	1/1	0.97	0.06	53,53,53,53	0
57	MG	1A	3400	1/1	0.97	0.29	55,55,55,55	0
57	MG	1A	3554	1/1	0.97	0.13	38,38,38,38	0
57	MG	1a	1681	1/1	0.97	0.17	63,63,63,63	0
57	MG	1A	3556	1/1	0.97	0.07	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	3774	1/1	0.97	0.06	60,60,60,60	0
57	MG	1A	3898	1/1	0.97	0.10	41,41,41,41	0
57	MG	2A	3034	1/1	0.97	0.08	42,42,42,42	0
57	MG	2A	3474	1/1	0.97	0.10	69,69,69,69	0
57	MG	2A	3476	1/1	0.97	0.08	62,62,62,62	0
57	MG	1A	3660	1/1	0.97	0.07	26,26,26,26	0
57	MG	2A	3255	1/1	0.97	0.08	60,60,60,60	0
57	MG	2A	3479	1/1	0.97	0.04	43,43,43,43	0
57	MG	1A	3661	1/1	0.97	0.08	34,34,34,34	0
57	MG	2A	3038	1/1	0.97	0.22	54,54,54,54	0
57	MG	1P	202	1/1	0.97	0.18	32,32,32,32	0
57	MG	1A	3288	1/1	0.97	0.07	41,41,41,41	0
57	MG	1P	204	1/1	0.97	0.17	33,33,33,33	0
57	MG	1P	205	1/1	0.97	0.24	32,32,32,32	0
57	MG	1A	3558	1/1	0.97	0.11	36,36,36,36	0
57	MG	1P	207	1/1	0.97	0.24	35,35,35,35	0
57	MG	2A	3046	1/1	0.97	0.04	31,31,31,31	0
57	MG	2a	1658	1/1	0.97	0.19	52,52,52,52	0
57	MG	1A	3664	1/1	0.97	0.06	27,27,27,27	0
57	MG	1Q	202	1/1	0.97	0.10	31,31,31,31	0
57	MG	2a	1661	1/1	0.97	0.14	35,35,35,35	0
57	MG	1A	3559	1/1	0.97	0.07	38,38,38,38	0
57	MG	1A	3905	1/1	0.97	0.11	38,38,38,38	0
57	MG	2A	3738	1/1	0.97	0.05	56,56,56,56	0
57	MG	1A	3906	1/1	0.97	0.05	49,49,49,49	0
57	MG	2A	3494	1/1	0.97	0.09	39,39,39,39	0
57	MG	1Q	207	1/1	0.97	0.06	41,41,41,41	0
57	MG	2a	1668	1/1	0.97	0.15	60,60,60,60	0
57	MG	1R	201	1/1	0.97	0.06	42,42,42,42	0
57	MG	1A	3470	1/1	0.97	0.19	38,38,38,38	0
57	MG	2A	3744	1/1	0.97	0.14	58,58,58,58	0
57	MG	2A	3745	1/1	0.97	0.06	70,70,70,70	0
57	MG	1R	203	1/1	0.97	0.13	29,29,29,29	0
57	MG	1A	3667	1/1	0.97	0.12	40,40,40,40	0
57	MG	1A	3911	1/1	0.97	0.06	62,62,62,62	0
57	MG	1A	3029	1/1	0.97	0.09	38,38,38,38	0
57	MG	1A	3913	1/1	0.97	0.04	35,35,35,35	0
57	MG	1A	3914	1/1	0.97	0.03	36,36,36,36	0
57	MG	1A	3563	1/1	0.97	0.12	44,44,44,44	0
57	MG	2A	3753	1/1	0.97	0.09	44,44,44,44	0
57	MG	1A	3194	1/1	0.97	0.09	40,40,40,40	0
57	MG	1U	202	1/1	0.97	0.27	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1U	203	1/1	0.97	0.23	43,43,43,43	0
57	MG	2A	3510	1/1	0.97	0.18	58,58,58,58	0
57	MG	1A	3473	1/1	0.97	0.10	49,49,49,49	0
57	MG	2A	3070	1/1	0.97	0.10	51,51,51,51	0
57	MG	1A	3197	1/1	0.97	0.12	35,35,35,35	0
57	MG	1U	206	1/1	0.97	0.17	47,47,47,47	0
57	MG	2a	1689	1/1	0.97	0.13	47,47,47,47	0
57	MG	1A	4055	1/1	0.97	0.08	42,42,42,42	0
57	MG	1A	3790	1/1	0.97	0.45	27,27,27,27	0
57	MG	1U	210	1/1	0.97	0.11	34,34,34,34	0
57	MG	2A	3290	1/1	0.97	0.13	53,53,53,53	0
57	MG	1A	4057	1/1	0.97	0.10	16,16,16,16	0
57	MG	1V	201	1/1	0.97	0.25	30,30,30,30	0
57	MG	2A	3080	1/1	0.97	0.08	56,56,56,56	0
57	MG	1a	1720	1/1	0.97	0.16	44,44,44,44	0
57	MG	1A	3047	1/1	0.97	0.05	24,24,24,24	0
57	MG	1V	203	1/1	0.97	0.09	30,30,30,30	0
57	MG	1A	4060	1/1	0.97	0.05	22,22,22,22	0
57	MG	1V	205	1/1	0.97	0.11	37,37,37,37	0
57	MG	1A	3674	1/1	0.97	0.08	29,29,29,29	0
57	MG	1A	4062	1/1	0.97	0.05	40,40,40,40	0
57	MG	2A	3531	1/1	0.97	0.07	35,35,35,35	0
57	MG	1A	3293	1/1	0.97	0.12	40,40,40,40	0
57	MG	1A	3295	1/1	0.97	0.07	41,41,41,41	0
57	MG	1A	3102	1/1	0.97	0.10	33,33,33,33	0
57	MG	2A	3092	1/1	0.97	0.15	46,46,46,46	0
57	MG	2A	3093	1/1	0.97	0.09	58,58,58,58	0
57	MG	2A	3537	1/1	0.97	0.07	37,37,37,37	0
57	MG	2a	1711	1/1	0.97	0.11	60,60,60,60	0
57	MG	2A	3538	1/1	0.97	0.08	38,38,38,38	0
57	MG	1A	3925	1/1	0.97	0.07	41,41,41,41	0
57	MG	2A	3787	1/1	0.97	0.10	39,39,39,39	0
57	MG	1A	4068	1/1	0.97	0.05	44,44,44,44	0
57	MG	1A	3155	1/1	0.97	0.11	59,59,59,59	0
57	MG	1A	3072	1/1	0.97	0.05	30,30,30,30	0
57	MG	1A	3249	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3130	1/1	0.97	0.06	41,41,41,41	0
57	MG	2a	1720	1/1	0.97	0.22	57,57,57,57	0
57	MG	2A	3100	1/1	0.97	0.04	52,52,52,52	0
57	MG	1A	3251	1/1	0.97	0.11	60,60,60,60	0
57	MG	1A	3132	1/1	0.97	0.09	40,40,40,40	0
57	MG	1A	3208	1/1	0.97	0.06	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1725	1/1	0.97	0.08	53,53,53,53	0
57	MG	1A	3687	1/1	0.97	0.03	15,15,15,15	0
57	MG	1A	3162	1/1	0.97	0.09	38,38,38,38	0
57	MG	1a	1742	1/1	0.97	0.05	49,49,49,49	0
57	MG	1a	1743	1/1	0.97	0.06	44,44,44,44	0
57	MG	1A	3807	1/1	0.97	0.08	37,37,37,37	0
57	MG	2A	3109	1/1	0.97	0.14	51,51,51,51	0
57	MG	1A	3108	1/1	0.97	0.19	34,34,34,34	0
57	MG	1A	4082	1/1	0.97	0.11	45,45,45,45	0
57	MG	2a	1734	1/1	0.97	0.08	63,63,63,63	0
57	MG	1A	3584	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	3691	1/1	0.97	0.13	48,48,48,48	0
57	MG	2a	1737	1/1	0.97	0.12	73,73,73,73	0
57	MG	1A	3941	1/1	0.97	0.09	42,42,42,42	0
57	MG	1a	1751	1/1	0.97	0.04	58,58,58,58	0
57	MG	1A	3488	1/1	0.97	0.06	50,50,50,50	0
57	MG	1A	3211	1/1	0.97	0.21	37,37,37,37	0
57	MG	1A	3308	1/1	0.97	0.24	61,61,61,61	0
57	MG	2A	3815	1/1	0.97	0.10	65,65,65,65	0
57	MG	1A	3814	1/1	0.97	0.06	38,38,38,38	0
57	MG	2A	3122	1/1	0.97	0.07	57,57,57,57	0
57	MG	1A	3946	1/1	0.97	0.09	47,47,47,47	0
57	MG	1A	3309	1/1	0.97	0.06	33,33,33,33	0
57	MG	1A	3492	1/1	0.97	0.22	32,32,32,32	0
57	MG	1A	3949	1/1	0.97	0.05	57,57,57,57	0
57	MG	2A	3127	1/1	0.97	0.08	49,49,49,49	0
57	MG	13	102	1/1	0.97	0.10	45,45,45,45	0
57	MG	1A	4094	1/1	0.97	0.09	44,44,44,44	0
57	MG	1A	3257	1/1	0.97	0.16	41,41,41,41	0
57	MG	1A	3423	1/1	0.97	0.23	44,44,44,44	0
57	MG	1A	3135	1/1	0.97	0.17	45,45,45,45	0
57	MG	2A	3829	1/1	0.97	0.07	40,40,40,40	0
57	MG	15	107	1/1	0.97	0.11	34,34,34,34	0
57	MG	1A	4098	1/1	0.97	0.05	44,44,44,44	0
57	MG	1A	3701	1/1	0.97	0.07	42,42,42,42	0
57	MG	2A	3583	1/1	0.97	0.14	54,54,54,54	0
57	MG	1A	3427	1/1	0.97	0.10	64,64,64,64	0
57	MG	1A	3704	1/1	0.97	0.06	26,26,26,26	0
57	MG	1A	3596	1/1	0.97	0.06	45,45,45,45	0
57	MG	17	104	1/1	0.97	0.07	54,54,54,54	0
57	MG	2A	3588	1/1	0.97	0.09	42,42,42,42	0
57	MG	2A	3839	1/1	0.97	0.06	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3073	1/1	0.97	0.04	27,27,27,27	0
57	MG	18	101	1/1	0.97	0.10	45,45,45,45	0
57	MG	18	102	1/1	0.97	0.07	34,34,34,34	0
57	MG	1A	3501	1/1	0.97	0.07	51,51,51,51	0
57	MG	1A	3708	1/1	0.97	0.10	57,57,57,57	0
57	MG	2A	3594	1/1	0.97	0.05	37,37,37,37	0
57	MG	1B	204	1/1	0.97	0.12	51,51,51,51	0
57	MG	1A	3960	1/1	0.97	0.09	50,50,50,50	0
57	MG	1A	3214	1/1	0.97	0.05	32,32,32,32	0
57	MG	1A	3828	1/1	0.97	0.12	27,27,27,27	0
57	MG	1A	3431	1/1	0.97	0.16	40,40,40,40	0
57	MG	1A	3602	1/1	0.97	0.05	21,21,21,21	0
57	MG	1A	3262	1/1	0.97	0.05	33,33,33,33	0
57	MG	2A	3603	1/1	0.97	0.18	63,63,63,63	0
57	MG	1A	3604	1/1	0.97	0.04	22,22,22,22	0
57	MG	1A	3505	1/1	0.97	0.10	66,66,66,66	0
57	MG	2A	3606	1/1	0.97	0.14	52,52,52,52	0
57	MG	2A	3157	1/1	0.97	0.26	50,50,50,50	0
57	MG	1a	1786	1/1	0.97	0.08	52,52,52,52	0
57	MG	1a	1609	1/1	0.97	0.12	35,35,35,35	0
57	MG	1A	3606	1/1	0.97	0.09	26,26,26,26	0
57	MG	1A	3607	1/1	0.97	0.07	27,27,27,27	0
57	MG	1A	3608	1/1	0.97	0.10	47,47,47,47	0
57	MG	1A	3167	1/1	0.97	0.10	39,39,39,39	0
57	MG	1A	3370	1/1	0.97	0.15	45,45,45,45	0
57	MG	1A	3173	1/1	0.97	0.10	24,24,24,24	0
57	MG	1A	3509	1/1	0.97	0.13	36,36,36,36	0
57	MG	1A	3265	1/1	0.97	0.07	40,40,40,40	0
57	MG	1A	3375	1/1	0.97	0.36	47,47,47,47	0
57	MG	1a	1619	1/1	0.97	0.06	51,51,51,51	0
57	MG	2A	3620	1/1	0.97	0.12	54,54,54,54	0
57	MG	1A	3139	1/1	0.97	0.10	42,42,42,42	0
57	MG	1a	1799	1/1	0.97	0.07	58,58,58,58	0
57	MG	2D	305	1/1	0.97	0.13	42,42,42,42	0
57	MG	1A	3028	1/1	0.97	0.23	33,33,33,33	0
57	MG	1A	3846	1/1	0.97	0.15	38,38,38,38	0
57	MG	2A	3174	1/1	0.97	0.09	53,53,53,53	0
57	MG	2A	3175	1/1	0.97	0.14	43,43,43,43	0
57	MG	2E	303	1/1	0.97	0.17	44,44,44,44	0
57	MG	2A	3627	1/1	0.97	0.13	53,53,53,53	0
59	ZN	14	501	1/1	0.97	0.07	98,98,98,98	0
57	MG	1A	3222	1/1	0.97	0.22	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	ZN	2Y	501	1/1	0.97	0.06	91,91,91,91	0
57	MG	1A	3443	1/1	0.97	0.11	37,37,37,37	0
59	ZN	2n	102	1/1	0.97	0.06	88,88,88,88	0
60	SF4	1d	302	8/8	0.97	0.06	71,78,83,88	0
57	MG	2A	3035	1/1	0.98	0.13	33,33,33,33	0
57	MG	1A	3425	1/1	0.98	0.13	34,34,34,34	0
57	MG	1A	3494	1/1	0.98	0.21	42,42,42,42	0
57	MG	1A	4075	1/1	0.98	0.06	51,51,51,51	0
57	MG	2A	3186	1/1	0.98	0.05	56,56,56,56	0
57	MG	1A	3495	1/1	0.98	0.11	41,41,41,41	0
57	MG	1A	3188	1/1	0.98	0.20	28,28,28,28	0
57	MG	1A	3189	1/1	0.98	0.13	39,39,39,39	0
57	MG	1A	3005	1/1	0.98	0.06	43,43,43,43	0
57	MG	1A	3244	1/1	0.98	0.07	27,27,27,27	0
57	MG	1P	201	1/1	0.98	0.18	36,36,36,36	0
57	MG	1A	3968	1/1	0.98	0.05	28,28,28,28	0
57	MG	1A	3364	1/1	0.98	0.09	27,27,27,27	0
57	MG	1A	3111	1/1	0.98	0.07	41,41,41,41	0
57	MG	2A	3049	1/1	0.98	0.07	66,66,66,66	0
57	MG	1A	3585	1/1	0.98	0.07	48,48,48,48	0
57	MG	2A	3499	1/1	0.98	0.07	41,41,41,41	0
57	MG	1A	3144	1/1	0.98	0.05	35,35,35,35	0
57	MG	2A	3052	1/1	0.98	0.06	50,50,50,50	0
57	MG	2A	3502	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3768	1/1	0.98	0.04	27,27,27,27	0
57	MG	1A	3868	1/1	0.98	0.03	40,40,40,40	0
57	MG	1A	3869	1/1	0.98	0.07	41,41,41,41	0
57	MG	1Q	203	1/1	0.98	0.09	45,45,45,45	0
57	MG	2A	3057	1/1	0.98	0.07	42,42,42,42	0
57	MG	1A	3247	1/1	0.98	0.17	34,34,34,34	0
57	MG	1A	3045	1/1	0.98	0.04	32,32,32,32	0
57	MG	1A	3024	1/1	0.98	0.10	41,41,41,41	0
57	MG	1A	3438	1/1	0.98	0.23	55,55,55,55	0
57	MG	1A	3591	1/1	0.98	0.07	37,37,37,37	0
57	MG	1A	3679	1/1	0.98	0.05	43,43,43,43	0
57	MG	1A	3196	1/1	0.98	0.06	35,35,35,35	0
57	MG	1A	3036	1/1	0.98	0.26	35,35,35,35	0
57	MG	2A	3843	1/1	0.98	0.08	57,57,57,57	0
57	MG	2A	3214	1/1	0.98	0.52	44,44,44,44	0
57	MG	1A	3777	1/1	0.98	0.04	22,22,22,22	0
57	MG	1A	3778	1/1	0.98	0.05	45,45,45,45	0
57	MG	2A	3068	1/1	0.98	0.05	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3520	1/1	0.98	0.07	48,48,48,48	0
57	MG	1A	3373	1/1	0.98	0.18	29,29,29,29	0
57	MG	1A	3008	1/1	0.98	0.10	25,25,25,25	0
57	MG	2A	3071	1/1	0.98	0.05	40,40,40,40	0
57	MG	2A	3524	1/1	0.98	0.08	33,33,33,33	0
57	MG	1A	3017	1/1	0.98	0.06	27,27,27,27	0
57	MG	1A	3990	1/1	0.98	0.10	52,52,52,52	0
57	MG	1U	201	1/1	0.98	0.29	35,35,35,35	0
57	MG	1A	3200	1/1	0.98	0.07	34,34,34,34	0
57	MG	1A	3117	1/1	0.98	0.11	39,39,39,39	0
57	MG	1A	3886	1/1	0.98	0.05	35,35,35,35	0
57	MG	1A	3887	1/1	0.98	0.09	34,34,34,34	0
57	MG	1A	3599	1/1	0.98	0.05	50,50,50,50	0
57	MG	1A	3050	1/1	0.98	0.07	28,28,28,28	0
57	MG	1A	3119	1/1	0.98	0.24	38,38,38,38	0
57	MG	1A	3094	1/1	0.98	0.06	44,44,44,44	0
57	MG	1A	3205	1/1	0.98	0.08	38,38,38,38	0
57	MG	1A	3206	1/1	0.98	0.16	41,41,41,41	0
57	MG	1A	3694	1/1	0.98	0.03	28,28,28,28	0
57	MG	1A	3520	1/1	0.98	0.07	25,25,25,25	0
57	MG	1A	3383	1/1	0.98	0.13	30,30,30,30	0
57	MG	1A	3261	1/1	0.98	0.12	38,38,38,38	0
57	MG	1A	3207	1/1	0.98	0.15	32,32,32,32	0
57	MG	1A	3121	1/1	0.98	0.16	33,33,33,33	0
57	MG	2D	301	1/1	0.98	0.21	40,40,40,40	0
57	MG	1A	3156	1/1	0.98	0.18	31,31,31,31	0
57	MG	1A	3122	1/1	0.98	0.21	33,33,33,33	0
57	MG	2D	304	1/1	0.98	0.05	26,26,26,26	0
57	MG	1W	203	1/1	0.98	0.10	35,35,35,35	0
57	MG	1A	3266	1/1	0.98	0.12	39,39,39,39	0
57	MG	1A	3123	1/1	0.98	0.17	36,36,36,36	0
57	MG	1A	3124	1/1	0.98	0.11	36,36,36,36	0
57	MG	1a	1804	1/1	0.98	0.04	61,61,61,61	0
57	MG	1A	3095	1/1	0.98	0.05	16,16,16,16	0
57	MG	1A	3096	1/1	0.98	0.07	52,52,52,52	0
57	MG	1A	3804	1/1	0.98	0.07	42,42,42,42	0
57	MG	1A	3215	1/1	0.98	0.18	45,45,45,45	0
57	MG	1A	3273	1/1	0.98	0.07	44,44,44,44	0
57	MG	1A	4019	1/1	0.98	0.04	42,42,42,42	0
57	MG	1A	3164	1/1	0.98	0.17	43,43,43,43	0
57	MG	2A	3720	1/1	0.98	0.07	49,49,49,49	0
57	MG	1A	3535	1/1	0.98	0.05	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	2A	3559	1/1	0.98	0.06	39,39,39,39	0
57	MG	1A	3334	1/1	0.98	0.21	38,38,38,38	0
57	MG	2A	3561	1/1	0.98	0.12	59,59,59,59	0
57	MG	1A	3335	1/1	0.98	0.18	38,38,38,38	0
57	MG	10	101	1/1	0.98	0.04	45,45,45,45	0
57	MG	1A	3013	1/1	0.98	0.06	23,23,23,23	0
57	MG	2A	3112	1/1	0.98	0.11	33,33,33,33	0
57	MG	1A	3080	1/1	0.98	0.05	39,39,39,39	0
57	MG	1A	3625	1/1	0.98	0.08	57,57,57,57	0
57	MG	2A	3115	1/1	0.98	0.07	54,54,54,54	0
57	MG	1A	3626	1/1	0.98	0.10	43,43,43,43	0
57	MG	1A	3540	1/1	0.98	0.16	36,36,36,36	0
57	MG	1A	3720	1/1	0.98	0.06	53,53,53,53	0
57	MG	1A	3277	1/1	0.98	0.10	43,43,43,43	0
57	MG	1k	201	1/1	0.98	0.07	55,55,55,55	0
57	MG	1A	4032	1/1	0.98	0.08	27,27,27,27	0
57	MG	1A	3020	1/1	0.98	0.06	26,26,26,26	0
57	MG	2A	3417	1/1	0.98	0.10	38,38,38,38	0
57	MG	1A	3169	1/1	0.98	0.15	33,33,33,33	0
57	MG	1A	3545	1/1	0.98	0.17	38,38,38,38	0
57	MG	1D	305	1/1	0.98	0.05	20,20,20,20	0
57	MG	1r	101	1/1	0.98	0.10	65,65,65,65	0
57	MG	1A	3926	1/1	0.98	0.05	57,57,57,57	0
57	MG	1A	3223	1/1	0.98	0.23	30,30,30,30	0
57	MG	1A	3405	1/1	0.98	0.08	42,42,42,42	0
57	MG	1A	3727	1/1	0.98	0.06	27,27,27,27	0
57	MG	1A	3548	1/1	0.98	0.14	31,31,31,31	0
57	MG	1w	401	1/1	0.98	0.07	41,41,41,41	0
57	MG	1A	3224	1/1	0.98	0.17	51,51,51,51	0
57	MG	1A	3172	1/1	0.98	0.15	31,31,31,31	0
57	MG	2A	3135	1/1	0.98	0.15	57,57,57,57	0
57	MG	1A	3552	1/1	0.98	0.11	43,43,43,43	0
57	MG	1A	3100	1/1	0.98	0.05	33,33,33,33	0
57	MG	16	101	1/1	0.98	0.09	46,46,46,46	0
57	MG	25	103	1/1	0.98	0.13	46,46,46,46	0
57	MG	2A	3434	1/1	0.98	0.11	49,49,49,49	0
57	MG	2A	3139	1/1	0.98	0.08	36,36,36,36	0
57	MG	2A	3758	1/1	0.98	0.04	56,56,56,56	0
57	MG	1A	3131	1/1	0.98	0.08	38,38,38,38	0
57	MG	1A	3065	1/1	0.98	0.03	32,32,32,32	0
57	MG	17	102	1/1	0.98	0.07	30,30,30,30	0
57	MG	2A	3600	1/1	0.98	0.16	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3021	1/1	0.98	0.07	39,39,39,39	0
57	MG	1A	3134	1/1	0.98	0.20	34,34,34,34	0
57	MG	2A	3765	1/1	0.98	0.12	40,40,40,40	0
57	MG	1A	3104	1/1	0.98	0.14	42,42,42,42	0
57	MG	1E	307	1/1	0.98	0.06	24,24,24,24	0
57	MG	1A	3350	1/1	0.98	0.14	38,38,38,38	0
57	MG	1E	309	1/1	0.98	0.11	26,26,26,26	0
57	MG	1A	3561	1/1	0.98	0.11	39,39,39,39	0
57	MG	1A	3067	1/1	0.98	0.10	31,31,31,31	0
57	MG	1A	3233	1/1	0.98	0.12	33,33,33,33	0
57	MG	2a	1609	1/1	0.98	0.29	68,68,68,68	0
57	MG	2A	3152	1/1	0.98	0.17	47,47,47,47	0
57	MG	2A	3006	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3650	1/1	0.98	0.04	29,29,29,29	0
57	MG	2A	3008	1/1	0.98	0.14	45,45,45,45	0
57	MG	2A	3009	1/1	0.98	0.03	40,40,40,40	0
57	MG	2A	3010	1/1	0.98	0.06	45,45,45,45	0
57	MG	1A	3180	1/1	0.98	0.04	37,37,37,37	0
57	MG	1F	302	1/1	0.98	0.17	34,34,34,34	0
57	MG	2A	3457	1/1	0.98	0.06	25,25,25,25	0
57	MG	1A	3181	1/1	0.98	0.09	42,42,42,42	0
57	MG	1F	304	1/1	0.98	0.22	32,32,32,32	0
57	MG	1A	3566	1/1	0.98	0.11	46,46,46,46	0
57	MG	2A	3016	1/1	0.98	0.06	34,34,34,34	0
57	MG	1A	4058	1/1	0.98	0.10	32,32,32,32	0
57	MG	2A	3018	1/1	0.98	0.05	26,26,26,26	0
57	MG	1A	3137	1/1	0.98	0.12	34,34,34,34	0
57	MG	1A	3107	1/1	0.98	0.07	33,33,33,33	0
57	MG	2A	3315	1/1	0.98	0.11	47,47,47,47	0
57	MG	1F	309	1/1	0.98	0.03	36,36,36,36	0
57	MG	1F	310	1/1	0.98	0.25	28,28,28,28	0
57	MG	1A	3570	1/1	0.98	0.08	39,39,39,39	0
57	MG	1A	3657	1/1	0.98	0.04	34,34,34,34	0
57	MG	1A	3847	1/1	0.98	0.26	37,37,37,37	0
57	MG	1A	3751	1/1	0.98	0.07	27,27,27,27	0
57	MG	1A	3849	1/1	0.98	0.20	36,36,36,36	0
57	MG	2a	1635	1/1	0.98	0.05	47,47,47,47	0
57	MG	2A	3475	1/1	0.98	0.08	59,59,59,59	0
57	MG	2A	3799	1/1	0.98	0.05	52,52,52,52	0
57	MG	1A	3043	1/1	0.98	0.04	39,39,39,39	0
57	MG	1A	3186	1/1	0.98	0.10	39,39,39,39	0
57	MG	1A	3109	1/1	0.98	0.05	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1745	1/1	0.98	0.04	41,41,41,41	0
57	MG	1A	3424	1/1	0.98	0.18	47,47,47,47	0
57	MG	1A	4071	1/1	0.98	0.07	44,44,44,44	0
57	MG	1A	3575	1/1	0.98	0.05	22,22,22,22	0
60	SF4	2d	302	8/8	0.98	0.06	69,73,83,84	0
57	MG	1A	3713	1/1	0.99	0.04	44,44,44,44	0
57	MG	1A	3003	1/1	0.99	0.03	23,23,23,23	0
57	MG	1A	3857	1/1	0.99	0.11	37,37,37,37	0
57	MG	1N	203	1/1	0.99	0.03	34,34,34,34	0
57	MG	2A	3680	1/1	0.99	0.06	35,35,35,35	0
57	MG	2A	3460	1/1	0.99	0.04	28,28,28,28	0
57	MG	1A	3908	1/1	0.99	0.06	47,47,47,47	0
57	MG	1A	3909	1/1	0.99	0.02	14,14,14,14	0
57	MG	1A	3012	1/1	0.99	0.03	33,33,33,33	0
57	MG	1A	4020	1/1	0.99	0.03	26,26,26,26	0
57	MG	2A	3686	1/1	0.99	0.04	50,50,50,50	0
57	MG	2A	3045	1/1	0.99	0.11	42,42,42,42	0
57	MG	1A	3034	1/1	0.99	0.08	38,38,38,38	0
57	MG	1A	3294	1/1	0.99	0.07	23,23,23,23	0
57	MG	1A	3035	1/1	0.99	0.08	24,24,24,24	0
57	MG	1A	3018	1/1	0.99	0.05	43,43,43,43	0
57	MG	1A	3297	1/1	0.99	0.03	30,30,30,30	0
57	MG	1A	3076	1/1	0.99	0.06	27,27,27,27	0
57	MG	1A	3551	1/1	0.99	0.17	43,43,43,43	0
57	MG	1A	3437	1/1	0.99	0.07	49,49,49,49	0
57	MG	1A	3077	1/1	0.99	0.10	42,42,42,42	0
57	MG	1A	3333	1/1	0.99	0.18	38,38,38,38	0
57	MG	1A	3680	1/1	0.99	0.04	30,30,30,30	0
57	MG	1A	3637	1/1	0.99	0.09	37,37,37,37	0
57	MG	1A	3555	1/1	0.99	0.17	32,32,32,32	0
57	MG	1A	3153	1/1	0.99	0.19	35,35,35,35	0
57	MG	1D	311	1/1	0.99	0.10	30,30,30,30	0
57	MG	15	102	1/1	0.99	0.20	28,28,28,28	0
57	MG	1A	3009	1/1	0.99	0.04	30,30,30,30	0
57	MG	1A	3269	1/1	0.99	0.20	38,38,38,38	0
57	MG	15	105	1/1	0.99	0.12	29,29,29,29	0
57	MG	1a	1713	1/1	0.99	0.23	46,46,46,46	0
57	MG	15	106	1/1	0.99	0.11	38,38,38,38	0
57	MG	2A	3205	1/1	0.99	0.11	54,54,54,54	0
57	MG	1A	3371	1/1	0.99	0.20	28,28,28,28	0
57	MG	1A	3014	1/1	0.99	0.03	28,28,28,28	0
57	MG	1A	3182	1/1	0.99	0.09	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	3645	1/1	0.99	0.06	22,22,22,22	0
57	MG	2A	3564	1/1	0.99	0.03	29,29,29,29	0
57	MG	2A	3565	1/1	0.99	0.05	48,48,48,48	0
57	MG	1A	3007	1/1	0.99	0.03	36,36,36,36	0
57	MG	2A	3072	1/1	0.99	0.06	31,31,31,31	0
57	MG	1A	3880	1/1	0.99	0.07	45,45,45,45	0
57	MG	1A	3986	1/1	0.99	0.05	38,38,38,38	0
57	MG	1A	3157	1/1	0.99	0.08	31,31,31,31	0
57	MG	1A	3158	1/1	0.99	0.08	25,25,25,25	0
57	MG	1A	3081	1/1	0.99	0.05	29,29,29,29	0
57	MG	1A	3834	1/1	0.99	0.10	58,58,58,58	0
57	MG	1A	3937	1/1	0.99	0.04	52,52,52,52	0
57	MG	2A	3801	1/1	0.99	0.05	50,50,50,50	0
57	MG	1A	3052	1/1	0.99	0.05	49,49,49,49	0
57	MG	1A	3216	1/1	0.99	0.06	37,37,37,37	0
57	MG	1A	3217	1/1	0.99	0.08	33,33,33,33	0
57	MG	1U	208	1/1	0.99	0.08	36,36,36,36	0
57	MG	1A	3569	1/1	0.99	0.09	39,39,39,39	0
57	MG	1A	3996	1/1	0.99	0.02	33,33,33,33	0
57	MG	2A	3086	1/1	0.99	0.14	34,34,34,34	0
57	MG	2A	3809	1/1	0.99	0.04	38,38,38,38	0
57	MG	1A	3138	1/1	0.99	0.04	17,17,17,17	0
57	MG	1a	1734	1/1	0.99	0.06	42,42,42,42	0
57	MG	2A	3438	1/1	0.99	0.09	23,23,23,23	0
57	MG	1A	3022	1/1	0.99	0.05	17,17,17,17	0
57	MG	1A	3030	1/1	0.99	0.14	26,26,26,26	0
57	MG	1A	3794	1/1	0.99	0.03	24,24,24,24	0
57	MG	1A	3068	1/1	0.99	0.03	17,17,17,17	0
57	MG	2A	3817	1/1	0.99	0.04	25,25,25,25	0
57	MG	1A	3103	1/1	0.99	0.04	23,23,23,23	0
57	MG	1A	3703	1/1	0.99	0.07	26,26,26,26	0
57	MG	1A	4004	1/1	0.99	0.03	56,56,56,56	0
57	MG	1A	3042	1/1	0.99	0.11	42,42,42,42	0
57	MG	1A	4063	1/1	0.99	0.04	31,31,31,31	0
57	MG	1A	3031	1/1	0.99	0.12	31,31,31,31	0
59	ZN	1Y	205	1/1	0.99	0.03	58,58,58,58	0
57	MG	1A	3497	1/1	0.99	0.10	35,35,35,35	0
59	ZN	15	110	1/1	0.99	0.03	47,47,47,47	0
59	ZN	16	103	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	3195	1/1	0.99	0.15	25,25,25,25	0
57	MG	1A	3168	1/1	0.99	0.06	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3106	1/1	0.99	0.13	30,30,30,30	0
59	ZN	25	108	1/1	0.99	0.03	58,58,58,58	0
59	ZN	26	102	1/1	0.99	0.04	64,64,64,64	0
59	ZN	29	102	1/1	0.99	0.05	68,68,68,68	0
57	MG	1A	3170	1/1	0.99	0.07	37,37,37,37	0
57	MG	1A	3171	1/1	0.99	0.05	25,25,25,25	0
57	MG	1A	3428	1/1	0.99	0.05	43,43,43,43	0
57	MG	1A	3733	1/1	1.00	0.07	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.