



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 20, 2023 – 08:37 PM EST

PDB ID : 8G2C
Title : Crystal structure of the A2503-C2,C8-dimethylated *Thermus thermophilus* 70S ribosome in complex with tylosin, mRNA, aminoacylated A-site Phe-tRNA_{Phe}, aminoacylated P-site fMet-tRNA_{Met}, and deacylated E-site tRNA_{Phe} at 2.65Å resolution
Authors : Aleksandrova, E.V.; Wu, K.J.Y.; Tresco, B.I.C.; Syroegin, E.A.; Killeavy, E.E.; Balasanyants, S.M.; Svetlov, M.S.; Gregory, S.T.; Atkinson, G.C.; Myers, A.G.; Polikanov, Y.S.
Deposited on : 2023-02-03
Resolution : 2.65 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)

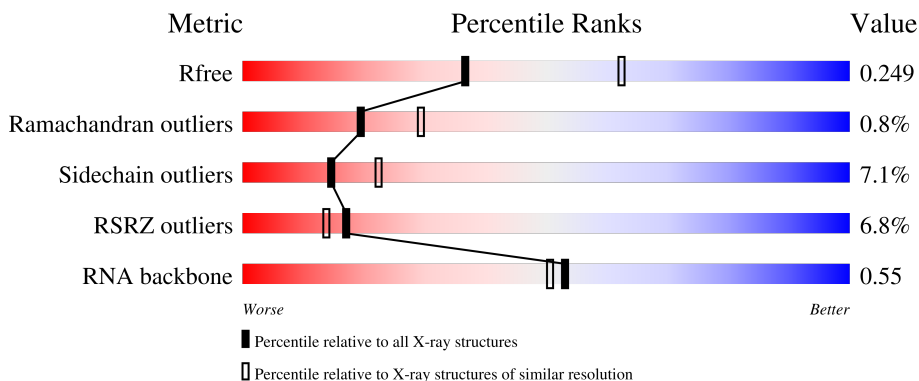
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


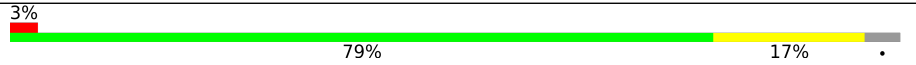
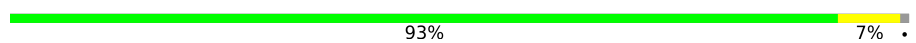
The reported resolution of this entry is 2.65 Å.

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}	130704	1332 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)
RNA backbone	3102	1010 (2.96-2.36)



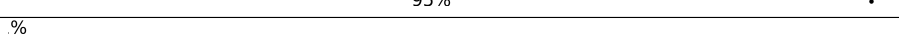
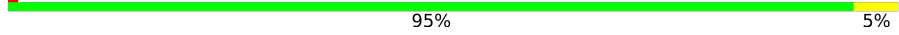

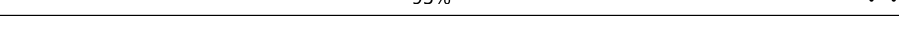
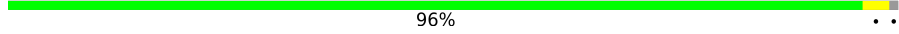

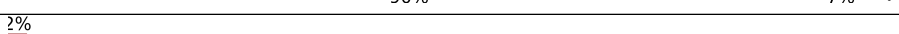


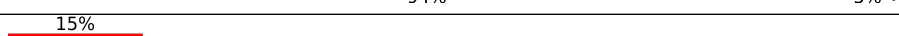


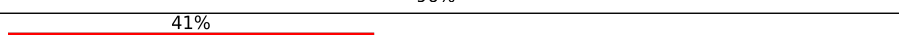





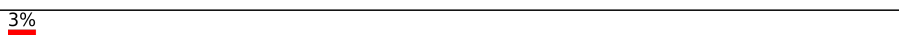
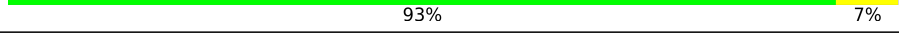
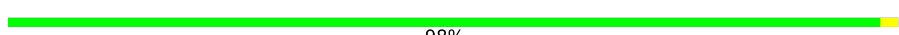
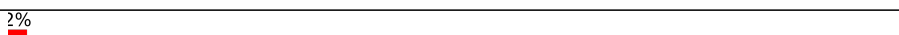
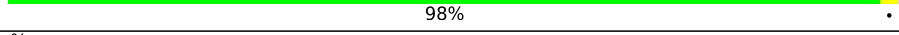
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	 5% 82% 16% .
1	2A	2915	 3% 79% 17% .
2	1B	121	 93% 7% .

Continued on next page...

Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.36

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	2B	121	 72% 27%
3	1D	276	 2% 95%
3	2D	276	 95% 5%
4	1E	206	 95%
4	2E	206	 96%
5	1F	210	 90% 7%
5	2F	210	 2% 91% 5%
6	1G	182	 94% 5%
6	2G	182	 15% 90% 9%
7	1H	180	 96%
7	2H	180	 41% 89% 8%
8	1I	148	 86% 13%
8	2I	148	 5% 89% 10%
9	1N	140	 94% 6%
9	2N	140	 3% 93% 7%
10	1O	122	 98%
10	2O	122	 2% 98%
11	1P	150	 92% 7%
11	2P	150	 21% 89% 9%
12	1Q	141	 98%
12	2Q	141	 98%
13	1R	118	 96%
13	2R	118	 3% 97%
14	1S	112	 91% 7%
14	2S	112	 2% 87% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	1T	146	% 86% 10%
15	2T	146	6% 87% 10%
16	1U	118	96%
16	2U	118	% 94%
17	1V	101	94% 5%
17	2V	101	4% 95%
18	1W	113	% 95%
18	2W	113	93% 6%
19	1X	96	% 96%
19	2X	96	3% 96%
20	1Y	110	92% 5%
20	2Y	110	5% 90% 7%
21	1Z	206	2% 69% 5% 25%
21	2Z	206	9% 71% 7% 22%
22	10	85	98%
22	20	85	95%
23	11	98	2% 98%
23	21	98	6% 94% 5%
24	12	72	94%
24	22	72	94%
25	13	60	2% 88% 10%
25	23	60	8% 95%
26	14	71	8% 89% 6%
26	24	71	23% 83% 14%
27	15	60	2% 93% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	25	60	5% 95% ..
28	16	54	91% 7% .
28	26	54	6% 85% 13% .
29	17	49	2% 90% 8% .
29	27	49	8% 92% 6% .
30	18	65	92% 6% .
30	28	65	5% 91% 8% .
31	19	37	100%
31	29	37	11% 95% 5%
32	1a	1521	2% 82% 16% ..
32	2a	1521	4% 80% 18% ..
33	1b	256	11% 82% 8% 10%
33	2b	256	32% 82% 7% 10%
34	1c	239	81% 5% 14%
34	2c	239	33% 81% 5% 14%
35	1d	209	5% 92% 7%
35	2d	209	6% 92% 8%
36	1e	162	83% 9% 9%
36	2e	162	14% 82% 9% 9%
37	1f	101	5% 94% 5% .
37	2f	101	% 95% ..
38	1g	156	6% 88% 11% .
38	2g	156	22% 93% 6% .
39	1h	138	10% 96% ..
39	2h	138	9% 95% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	1i	128	6% 91% 7% ..
40	2i	128	55% 88% 12% .
41	1j	105	13% 84% 9% 8%
41	2j	105	44% 81% 10% 9%
42	1k	129	6% 81% 8% 12%
42	2k	129	% 84% 5% 12%
43	1l	132	88% 5% 8%
43	2l	132	2% 88% 5% 8%
44	1m	126	2% 88% 10% .
44	2m	126	22% 87% 9% ..
45	1n	61	92% 7% .
45	2n	61	70% 87% 11% .
46	1o	89	6% 97% ..
46	2o	89	93% 6% .
47	1p	88	85% 8% 7%
47	2p	88	3% 85% 8% 7%
48	1q	105	14% 90% . 6%
48	2q	105	6% 86% 9% 6%
49	1r	88	19% 75% . 23%
49	2r	88	% 73% .. 23%
50	1s	93	3% 85% . 11%
50	2s	93	40% 83% 5% . 11%
51	1t	106	14% 84% 5% . 9%
51	2t	106	25% 84% 7% 9%
52	1u	27	81% . 15%

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	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1y	76	
56	2y	76	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	5MU	1y	54	-	-	-	X
56	PSU	1y	55	-	-	-	X
56	PSU	2y	32	-	-	-	X
56	MIA	2y	37	-	-	-	X
56	G7M	2y	46	-	-	-	X
56	5MU	2y	54	-	-	-	X
57	MG	18	107	-	-	-	X
57	MG	1A	3016	-	-	-	X
57	MG	1A	3327	-	-	-	X
57	MG	1A	3388	-	-	-	X
57	MG	1A	3427	-	-	-	X
57	MG	1A	3434	-	-	-	X
57	MG	1A	3467	-	-	-	X
57	MG	1A	3909	-	-	-	X
57	MG	1F	315	-	-	-	X
57	MG	1U	210	-	-	-	X
57	MG	2A	3077	-	-	-	X
57	MG	2A	3177	-	-	-	X
57	MG	2A	3199	-	-	-	X
57	MG	2A	3203	-	-	-	X
57	MG	2A	3359	-	-	-	X
57	MG	2A	3395	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	2A	3548	-	-	-	X
57	MG	2A	3662	-	-	-	X
57	MG	2A	3675	-	-	-	X
57	MG	2D	306	-	-	-	X
57	MG	2a	1795	-	-	-	X
57	MG	2v	102	-	-	-	X

2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 300115 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1A	2871	Total	C	N	O	P	0	0	0
			61853	27532	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60323	26849	11284	19390	2800			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
5	2F	202	Total	C	N	O	S	0	0	0
			1579	1007	296	274	2			

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called MF-mRNA.

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

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

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

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

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

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

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

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1099	Total	Mg	0	0
			1099	1099		
57	1B	34	Total	Mg	0	0
			34	34		
57	1D	12	Total	Mg	0	0
			12	12		
57	1E	10	Total	Mg	0	0
			10	10		
57	1F	15	Total	Mg	0	0
			15	15		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	15	6	Total Mg 6 6	0	0
57	16	1	Total Mg 1 1	0	0
57	17	5	Total Mg 5 5	0	0
57	18	7	Total Mg 7 7	0	0
57	19	1	Total Mg 1 1	0	0
57	1a	214	Total Mg 214 214	0	0
57	1b	1	Total Mg 1 1	0	0
57	1e	2	Total Mg 2 2	0	0
57	1f	1	Total Mg 1 1	0	0
57	1h	1	Total Mg 1 1	0	0
57	1l	2	Total Mg 2 2	0	0
57	1m	1	Total Mg 1 1	0	0
57	1n	1	Total Mg 1 1	0	0
57	1p	1	Total Mg 1 1	0	0
57	1r	1	Total Mg 1 1	0	0
57	1t	1	Total Mg 1 1	0	0
57	1v	1	Total Mg 1 1	0	0
57	1w	5	Total Mg 5 5	0	0
57	1x	13	Total Mg 13 13	0	0
57	1y	1	Total Mg 1 1	0	0
57	2A	797	Total Mg 797 797	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2B	19	Total Mg 19 19	0	0
57	2D	8	Total Mg 8 8	0	0
57	2E	9	Total Mg 9 9	0	0
57	2F	8	Total Mg 8 8	0	0
57	2G	1	Total Mg 1 1	0	0
57	2N	1	Total Mg 1 1	0	0
57	2O	1	Total Mg 1 1	0	0
57	2P	2	Total Mg 2 2	0	0
57	2Q	4	Total Mg 4 4	0	0
57	2R	2	Total Mg 2 2	0	0
57	2T	2	Total Mg 2 2	0	0
57	2U	1	Total Mg 1 1	0	0
57	2V	2	Total Mg 2 2	0	0
57	2W	2	Total Mg 2 2	0	0
57	2X	2	Total Mg 2 2	0	0
57	2Y	1	Total Mg 1 1	0	0
57	20	2	Total Mg 2 2	0	0
57	21	2	Total Mg 2 2	0	0
57	23	2	Total Mg 2 2	0	0
57	25	4	Total Mg 4 4	0	0
57	27	2	Total Mg 2 2	0	0

Continued on next page...

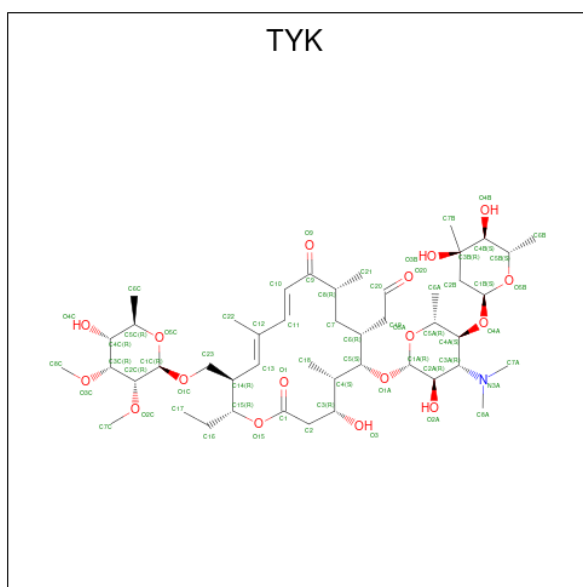
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	28	5	Total Mg 5 5	0	0
57	29	1	Total Mg 1 1	0	0
57	2a	221	Total Mg 221 221	0	0
57	2d	2	Total Mg 2 2	0	0
57	2e	1	Total Mg 1 1	0	0
57	2f	3	Total Mg 3 3	0	0
57	2j	1	Total Mg 1 1	0	0
57	2k	1	Total Mg 1 1	0	0
57	2l	1	Total Mg 1 1	0	0
57	2q	2	Total Mg 2 2	0	0
57	2t	1	Total Mg 1 1	0	0
57	2v	4	Total Mg 4 4	0	0
57	2w	7	Total Mg 7 7	0	0
57	2x	9	Total Mg 9 9	0	0
57	2y	2	Total Mg 2 2	0	0

- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 59 is TYLOSIN (three-letter code: TYK) (formula: C₄₆H₇₇NO₁₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
59	1A	1	Total	C	N	O	0	0
			64	46	1	17		
59	2A	1	Total	C	N	O	0	0
			64	46	1	17		

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

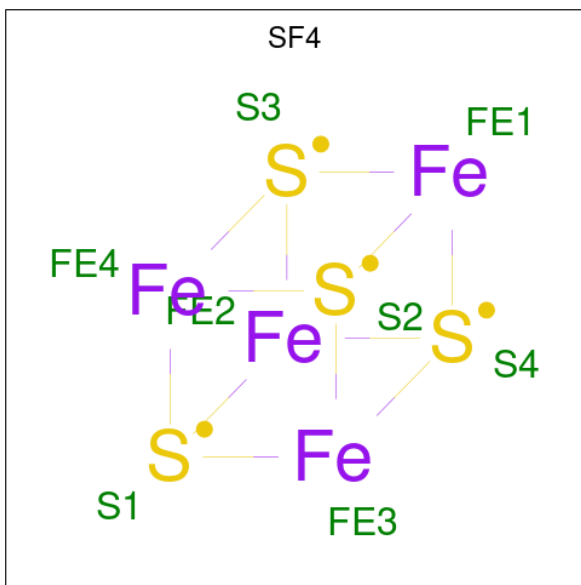
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1Y	1	Total	Zn	0	0
			1	1		
60	14	1	Total	Zn	0	0
			1	1		
60	15	1	Total	Zn	0	0
			1	1		
60	16	1	Total	Zn	0	0
			1	1		
60	19	1	Total	Zn	0	0
			1	1		
60	1n	1	Total	Zn	0	0
			1	1		
60	2Y	1	Total	Zn	0	0
			1	1		
60	24	1	Total	Zn	0	0
			1	1		
60	25	1	Total	Zn	0	0
			1	1		
60	26	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1A	1975	Total O 1975 1975	0	0
62	1B	59	Total O 59 59	0	0
62	1D	25	Total O 25 25	0	0
62	1E	25	Total O 25 25	0	0
62	1F	13	Total O 13 13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1G	2	Total O 2 2	0	0
62	1H	2	Total O 2 2	0	0
62	1N	5	Total O 5 5	0	0
62	1O	4	Total O 4 4	0	0
62	1P	23	Total O 23 23	0	0
62	1Q	6	Total O 6 6	0	0
62	1R	9	Total O 9 9	0	0
62	1S	2	Total O 2 2	0	0
62	1T	7	Total O 7 7	0	0
62	1U	11	Total O 11 11	0	0
62	1V	8	Total O 8 8	0	0
62	1W	7	Total O 7 7	0	0
62	1X	6	Total O 6 6	0	0
62	1Y	3	Total O 3 3	0	0
62	1Z	1	Total O 1 1	0	0
62	10	10	Total O 10 10	0	0
62	11	6	Total O 6 6	0	0
62	12	3	Total O 3 3	0	0
62	13	3	Total O 3 3	0	0
62	14	1	Total O 1 1	0	0
62	15	6	Total O 6 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	16	2	Total O 2 2	0	0
62	17	10	Total O 10 10	0	0
62	18	12	Total O 12 12	0	0
62	1a	377	Total O 377 377	0	0
62	1b	1	Total O 1 1	0	0
62	1e	2	Total O 2 2	0	0
62	1f	2	Total O 2 2	0	0
62	1l	6	Total O 6 6	0	0
62	1m	1	Total O 1 1	0	0
62	1o	1	Total O 1 1	0	0
62	1p	1	Total O 1 1	0	0
62	1q	2	Total O 2 2	0	0
62	1u	1	Total O 1 1	0	0
62	1v	5	Total O 5 5	0	0
62	1w	12	Total O 12 12	0	0
62	1x	15	Total O 15 15	0	0
62	1y	1	Total O 1 1	0	0
62	2A	1136	Total O 1136 1136	0	0
62	2B	22	Total O 22 22	0	0
62	2D	21	Total O 21 21	0	0
62	2E	16	Total O 16 16	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2F	13	Total 13	O 13	0	0
62	2O	2	Total 2	O 2	0	0
62	2P	5	Total 5	O 5	0	0
62	2Q	1	Total 1	O 1	0	0
62	2R	2	Total 2	O 2	0	0
62	2T	7	Total 7	O 7	0	0
62	2U	4	Total 4	O 4	0	0
62	2W	3	Total 3	O 3	0	0
62	2X	2	Total 2	O 2	0	0
62	2Z	1	Total 1	O 1	0	0
62	20	4	Total 4	O 4	0	0
62	21	7	Total 7	O 7	0	0
62	23	2	Total 2	O 2	0	0
62	25	1	Total 1	O 1	0	0
62	26	2	Total 2	O 2	0	0
62	27	4	Total 4	O 4	0	0
62	28	4	Total 4	O 4	0	0
62	29	1	Total 1	O 1	0	0
62	2a	254	Total 254	O 254	0	0
62	2c	1	Total 1	O 1	0	0
62	2d	1	Total 1	O 1	0	0

Continued on next page...

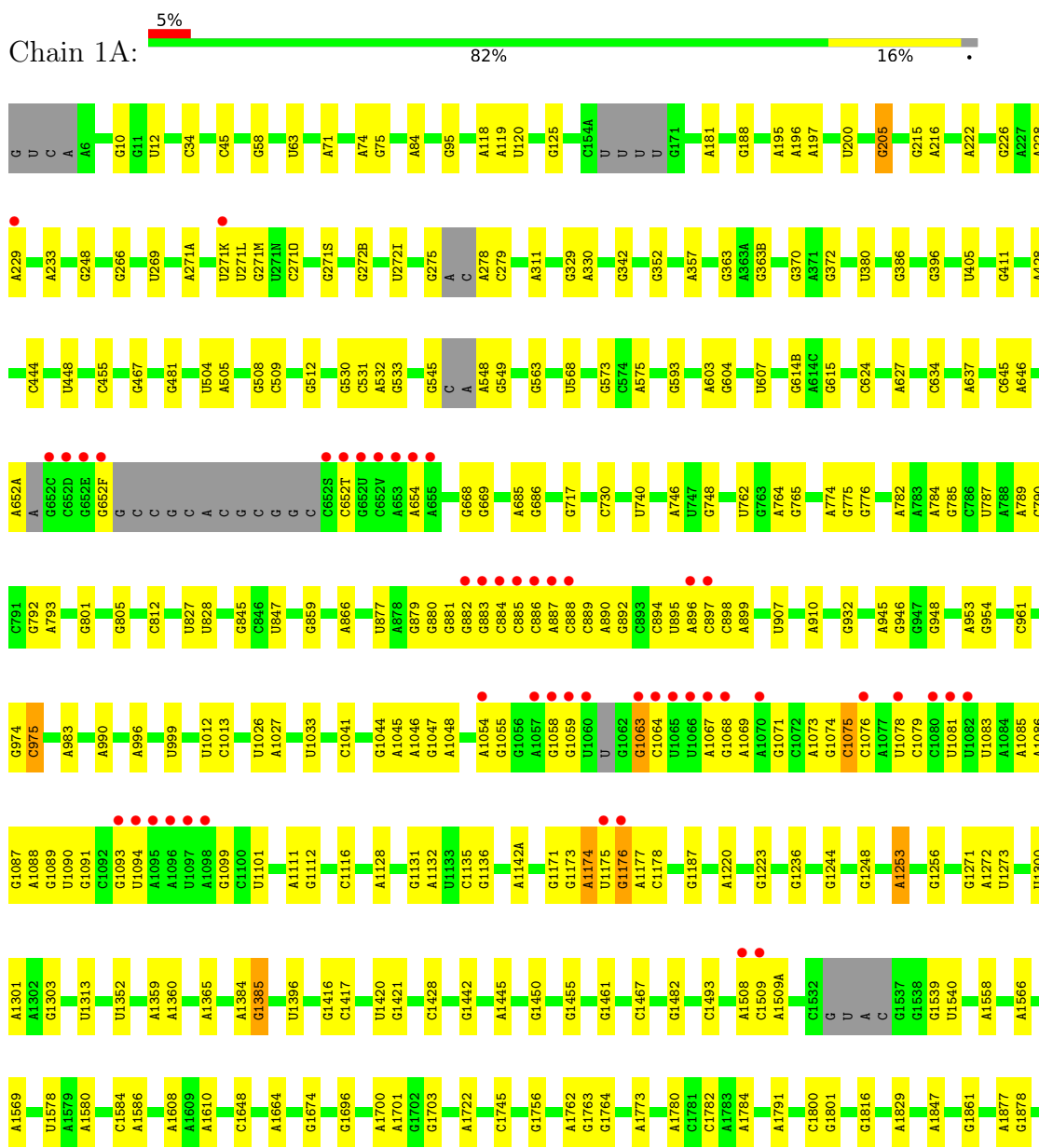
Continued from previous page...

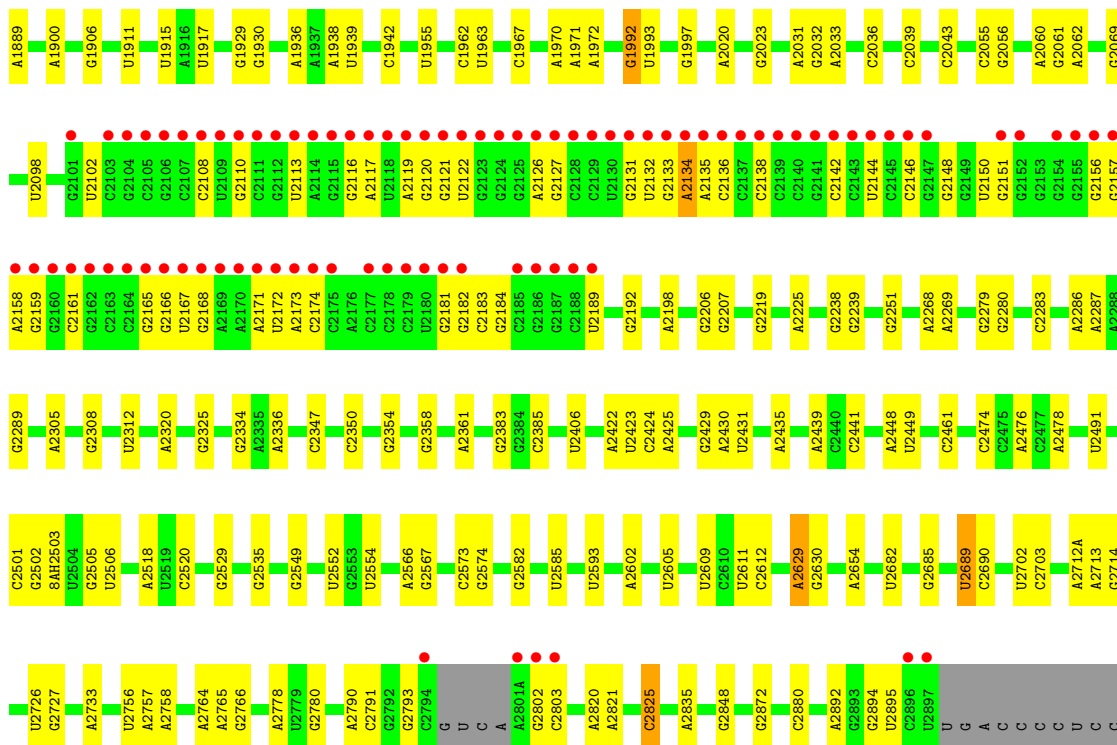
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2e	1	Total 1	O 1	0	0
62	2j	4	Total 4	O 4	0	0
62	2l	4	Total 4	O 4	0	0
62	2n	1	Total 1	O 1	0	0
62	2o	1	Total 1	O 1	0	0
62	2p	1	Total 1	O 1	0	0
62	2q	2	Total 2	O 2	0	0
62	2t	2	Total 2	O 2	0	0
62	2v	2	Total 2	O 2	0	0
62	2w	3	Total 3	O 3	0	0
62	2x	10	Total 10	O 10	0	0
62	2y	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

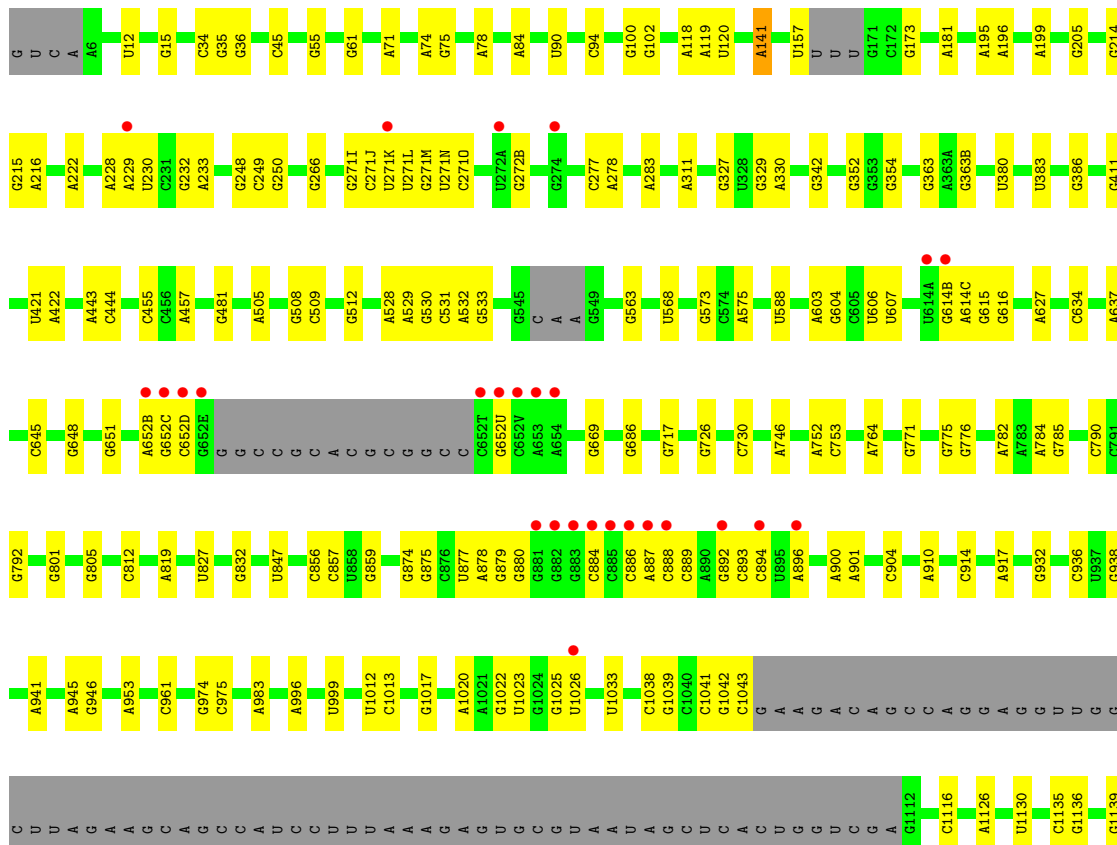
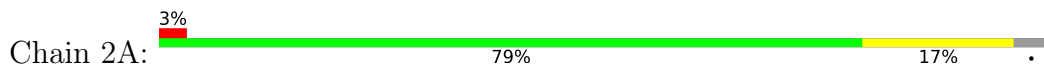
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

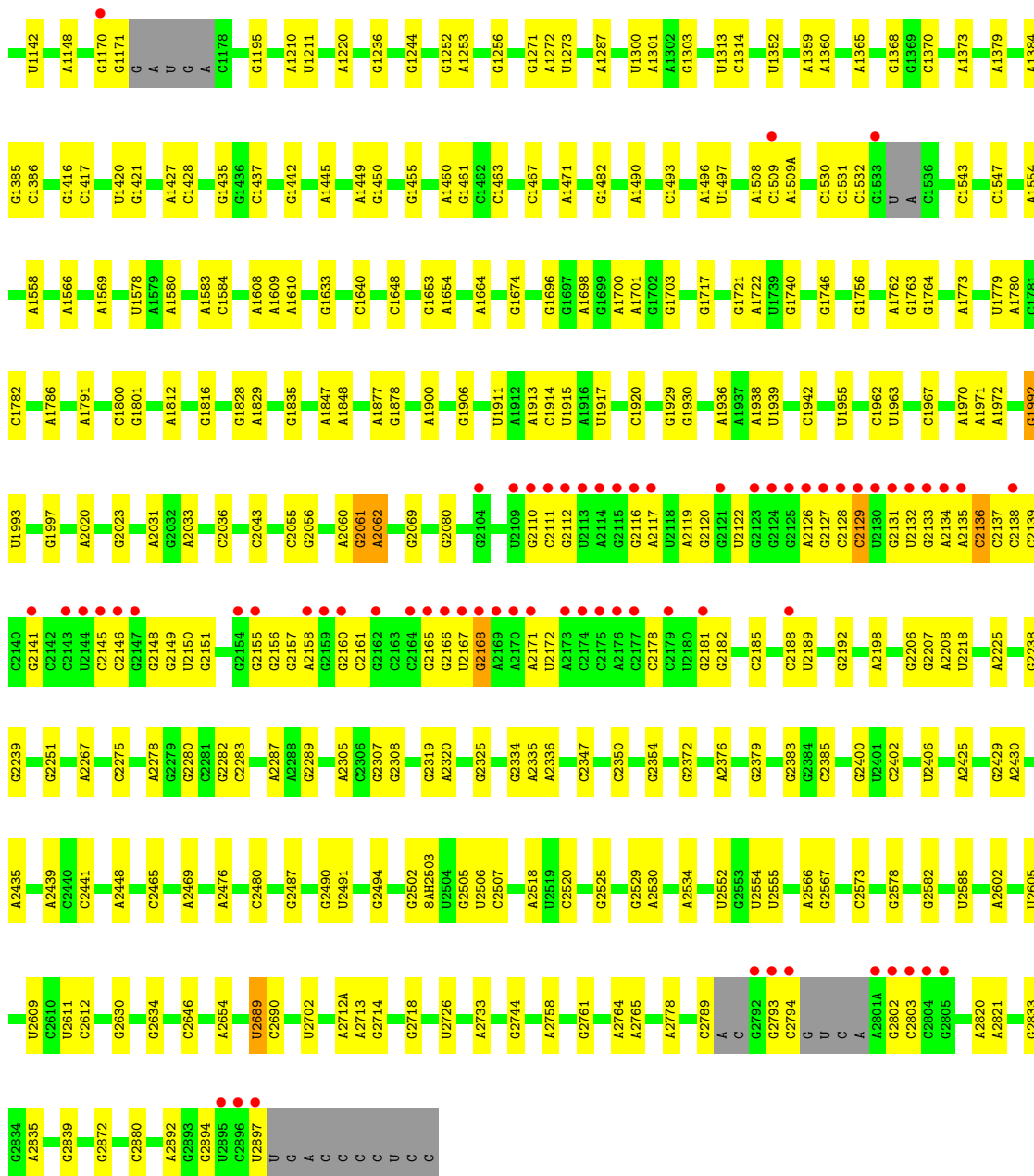
- Molecule 1: 23S Ribosomal RNA





• Molecule 1: 23S Ribosomal RNA





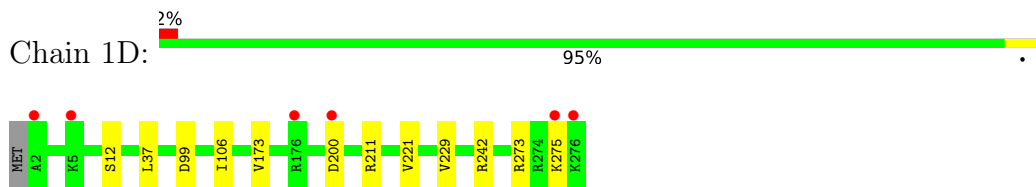
• Molecule 2: 5S Ribosomal RNA



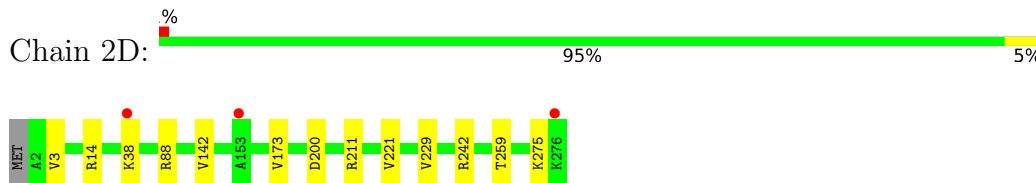
• Molecule 2: 5S Ribosomal RNA



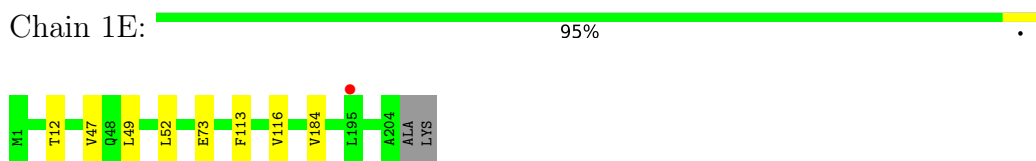
- Molecule 3: 50S ribosomal protein L2



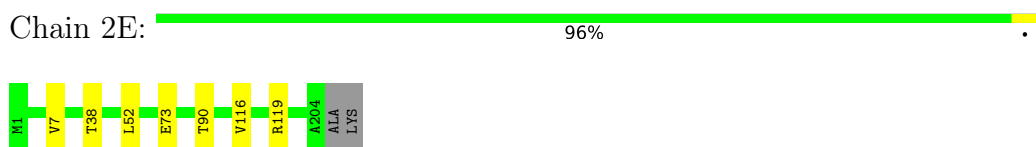
- Molecule 3: 50S ribosomal protein L2



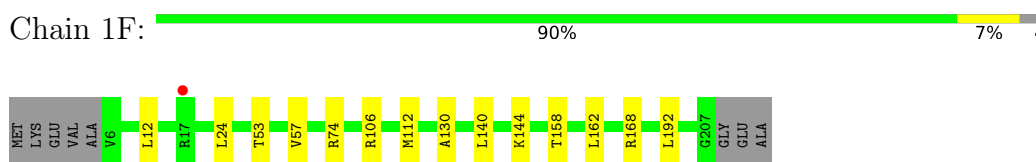
- Molecule 4: 50S ribosomal protein L3



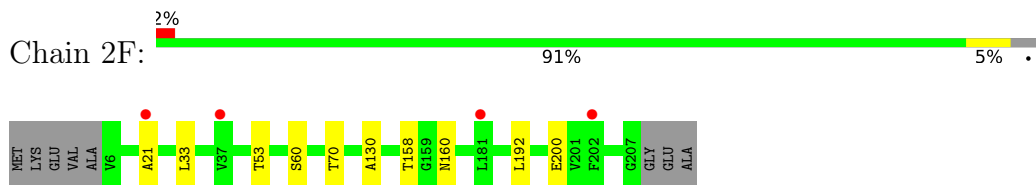
- Molecule 4: 50S ribosomal protein L3



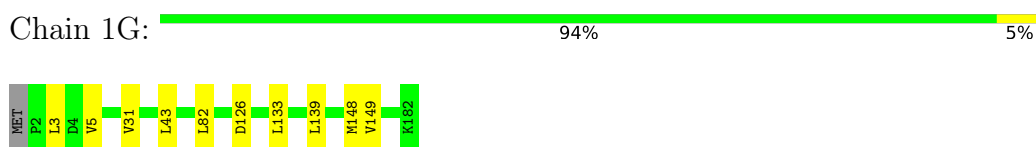
- Molecule 5: 50S ribosomal protein L4



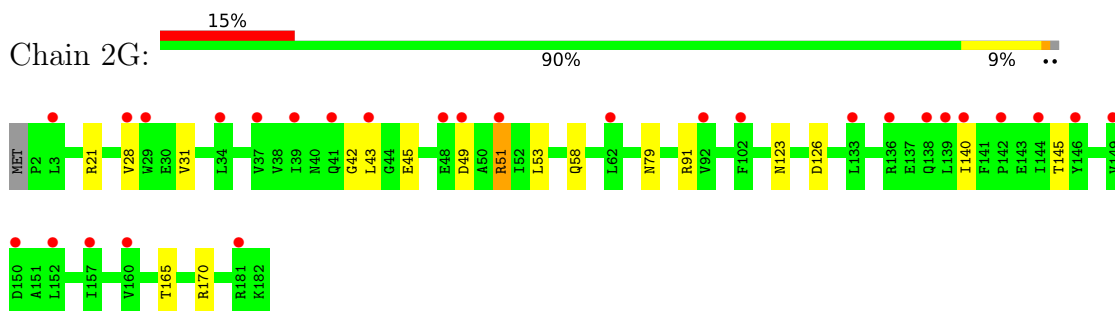
- Molecule 5: 50S ribosomal protein L4



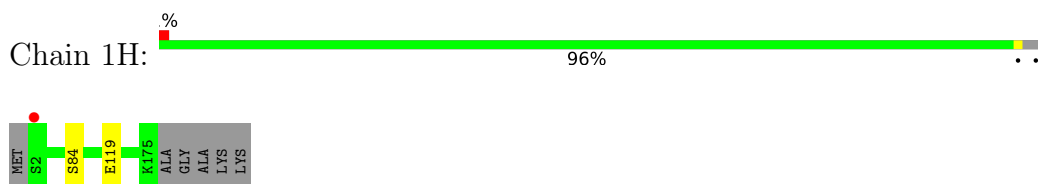
- Molecule 6: 50S ribosomal protein L5



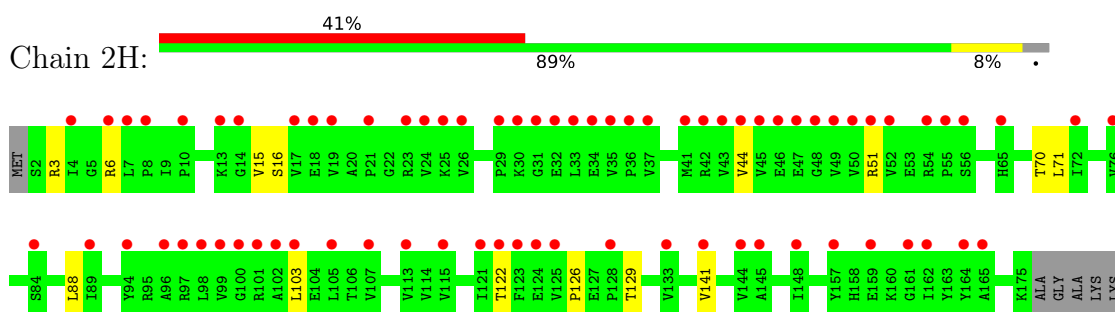
- Molecule 6: 50S ribosomal protein L5



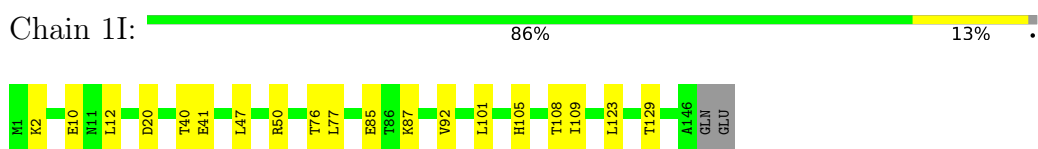
- Molecule 7: 50S ribosomal protein L6



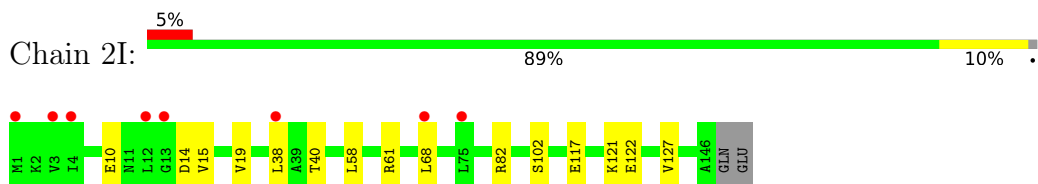
- Molecule 7: 50S ribosomal protein L6



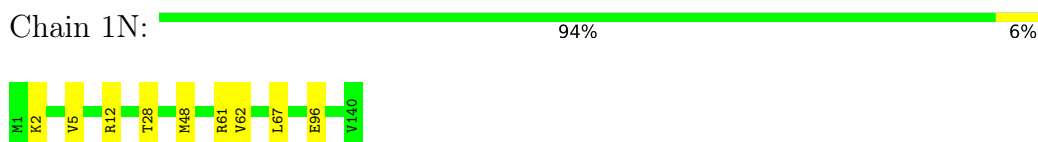
- Molecule 8: 50S ribosomal protein L9



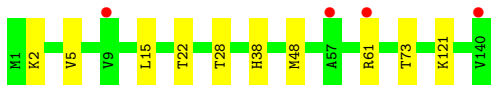
- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13



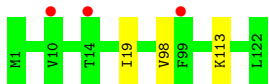
- Molecule 9: 50S ribosomal protein L13



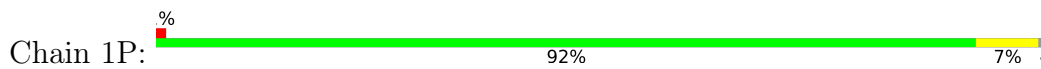
- Molecule 10: 50S ribosomal protein L14



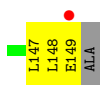
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15



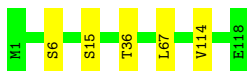
- Molecule 12: 50S ribosomal protein L16



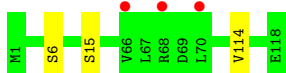
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



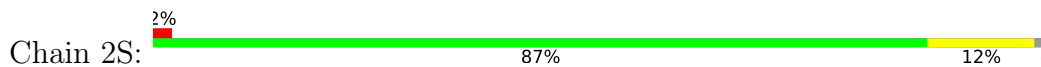
- Molecule 13: 50S ribosomal protein L17



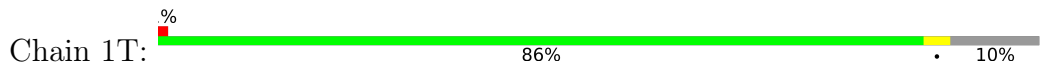
- Molecule 14: 50S ribosomal protein L18



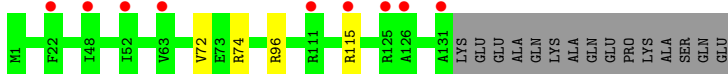
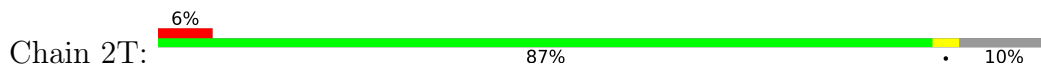
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20

Chain 1U:  96%



- Molecule 16: 50S ribosomal protein L20

Chain 2U:  94%



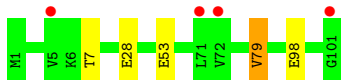
- Molecule 17: 50S ribosomal protein L21

Chain 1V:  94%



- Molecule 17: 50S ribosomal protein L21

Chain 2V:  95%



- Molecule 18: 50S ribosomal protein L22

Chain 1W:  95%



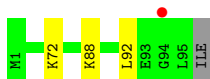
- Molecule 18: 50S ribosomal protein L22

Chain 2W:  93%

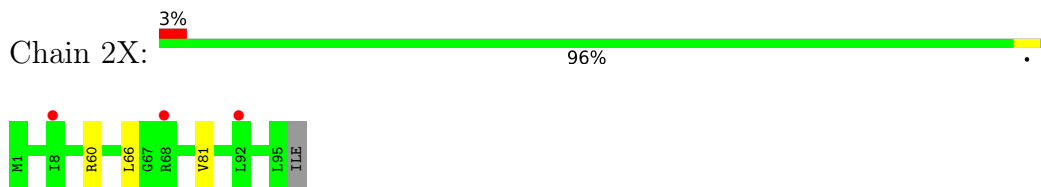


- Molecule 19: 50S ribosomal protein L23

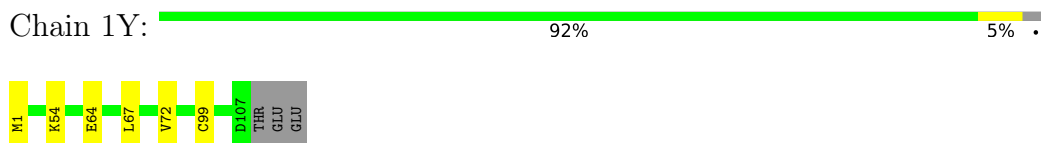
Chain 1X:  96%



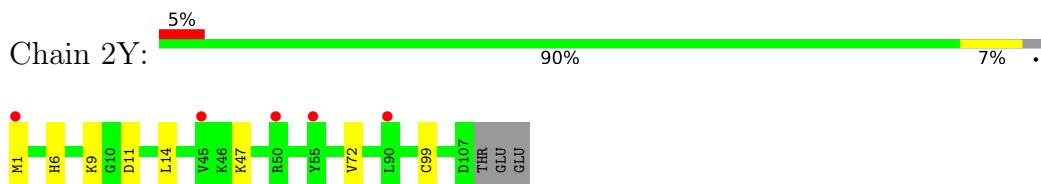
- Molecule 19: 50S ribosomal protein L23



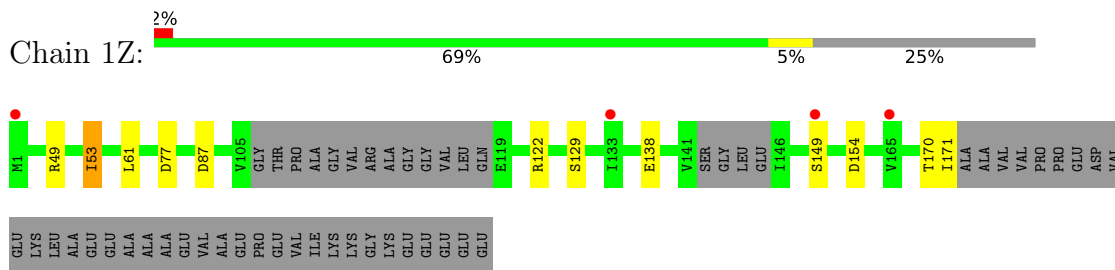
- Molecule 20: 50S ribosomal protein L24



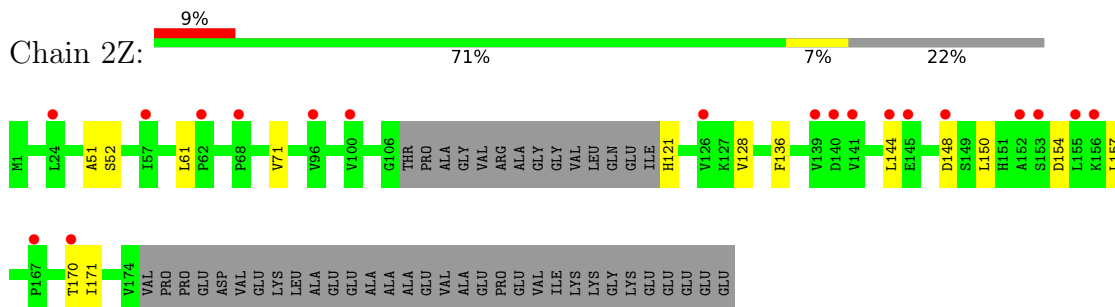
- Molecule 20: 50S ribosomal protein L24



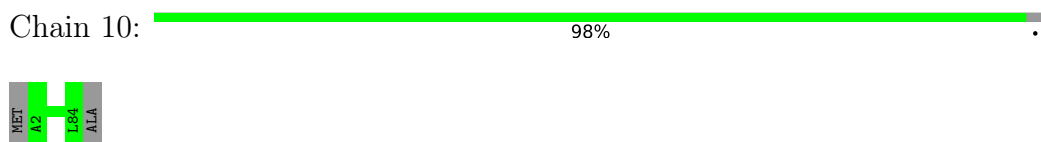
- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25



- Molecule 22: 50S ribosomal protein L27



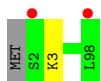
- Molecule 22: 50S ribosomal protein L27

Chain 20:  95%



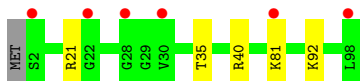
- Molecule 23: 50S ribosomal protein L28

Chain 11:  98%



- Molecule 23: 50S ribosomal protein L28

Chain 21:  94% 5%



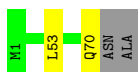
- Molecule 24: 50S ribosomal protein L29

Chain 12:  94%




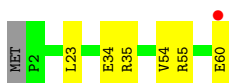
- Molecule 24: 50S ribosomal protein L29

Chain 22:  94%



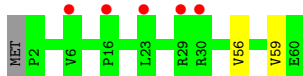
- Molecule 25: 50S ribosomal protein L30

Chain 13:  88% 10%

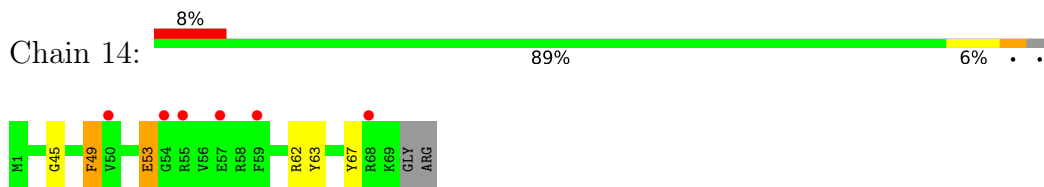


- Molecule 25: 50S ribosomal protein L30

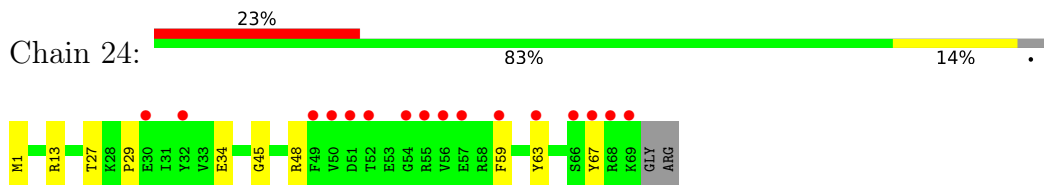
Chain 23:  95%



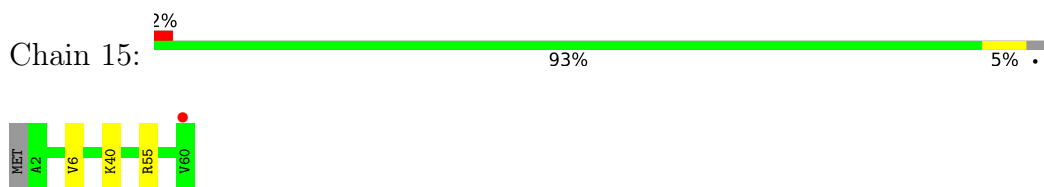
- Molecule 26: 50S ribosomal protein L31



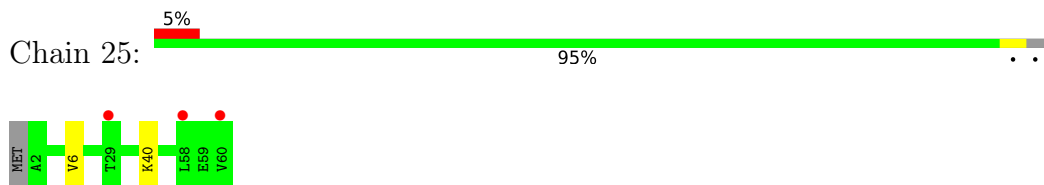
- Molecule 26: 50S ribosomal protein L31



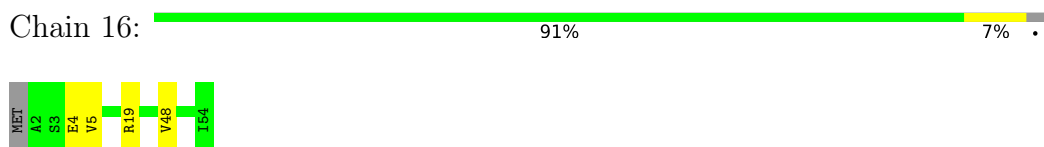
- Molecule 27: 50S ribosomal protein L32



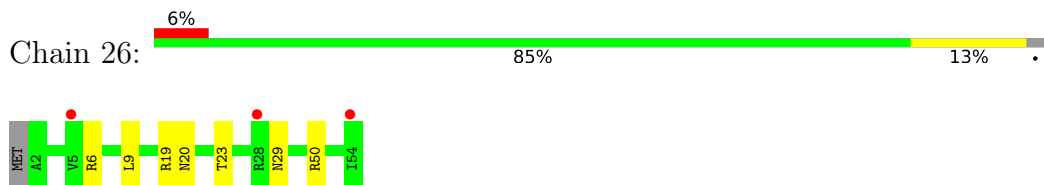
- Molecule 27: 50S ribosomal protein L32



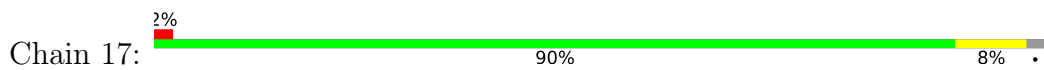
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34

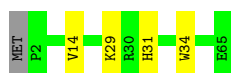




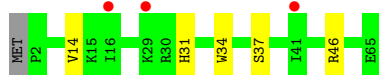
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35

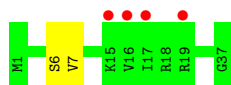


- Molecule 31: 50S ribosomal protein L36

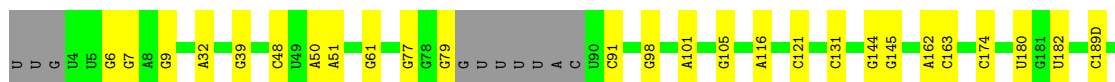
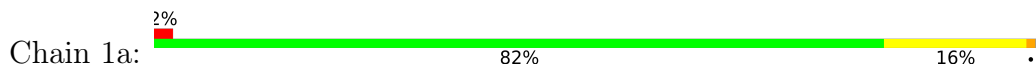


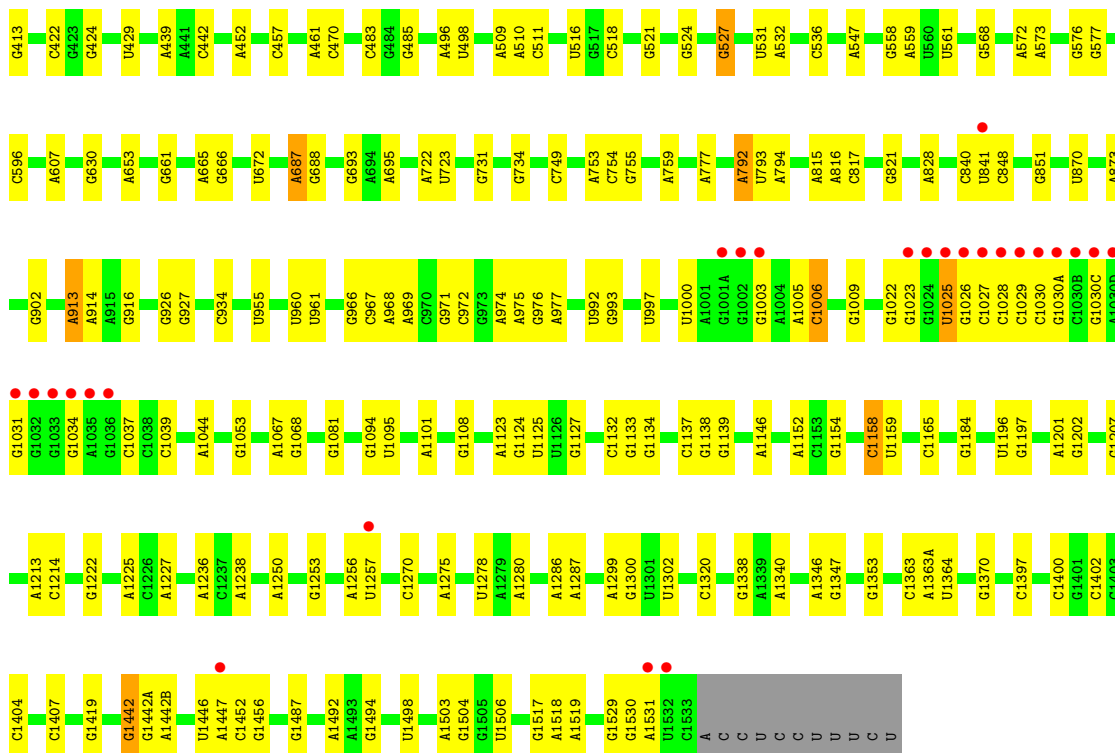
There are no outlier residues recorded for this chain.

- Molecule 31: 50S ribosomal protein L36

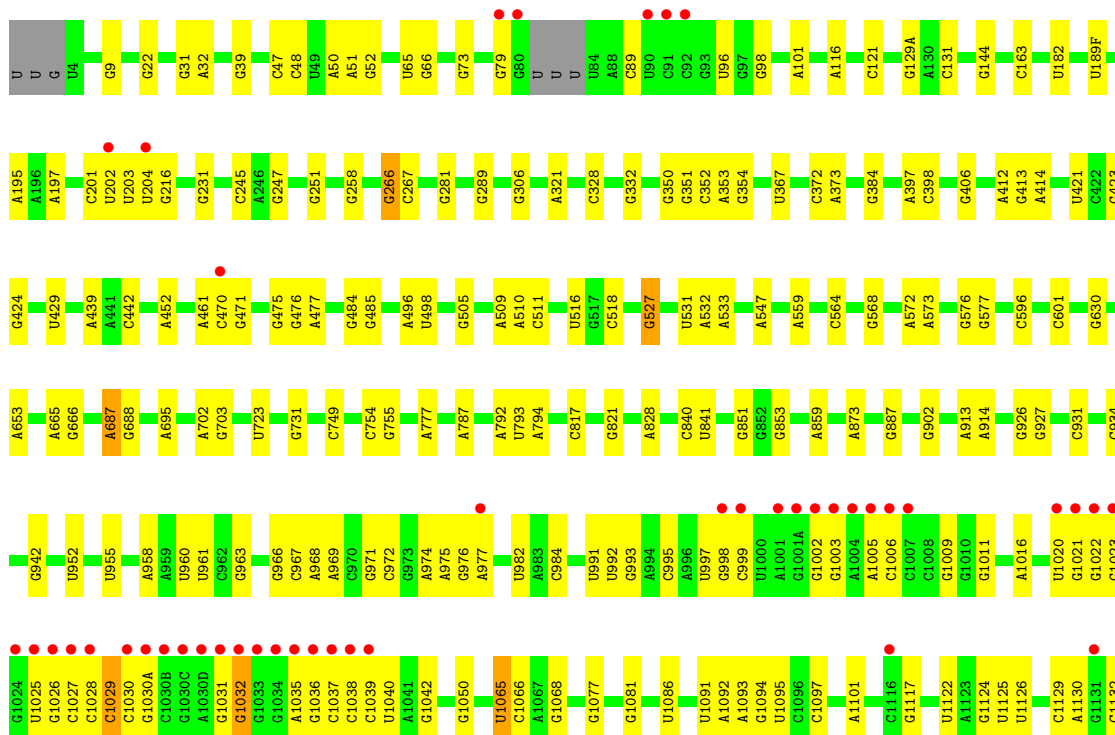
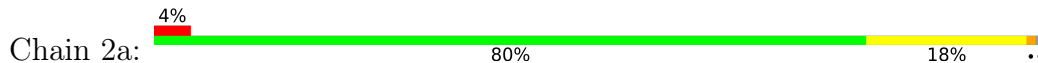


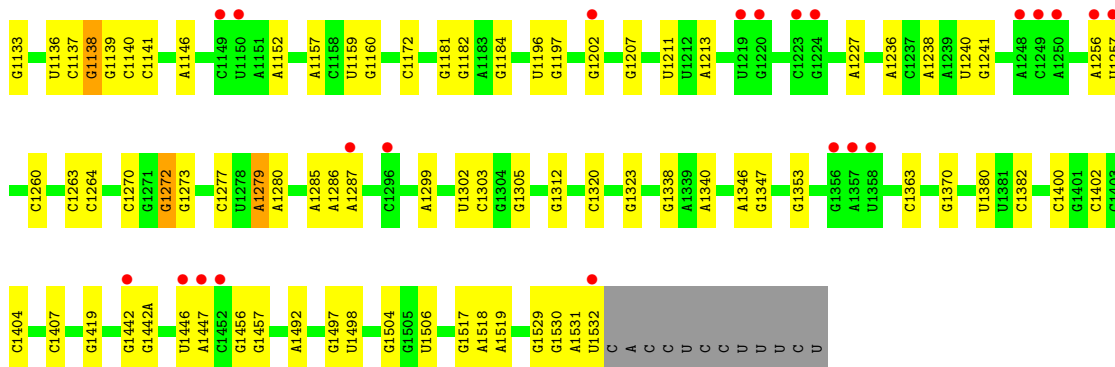
- Molecule 32: 16S Ribosomal RNA



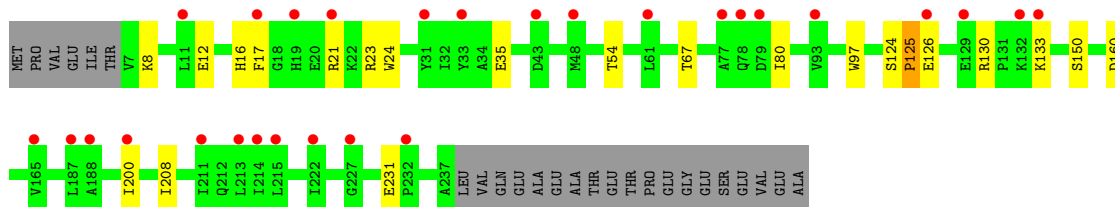
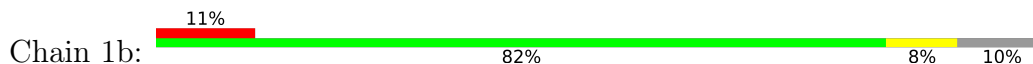


● Molecule 32: 16S Ribosomal RNA

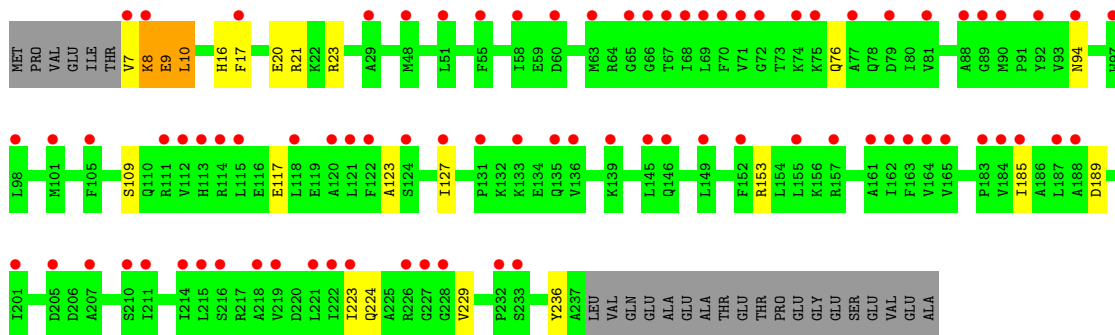
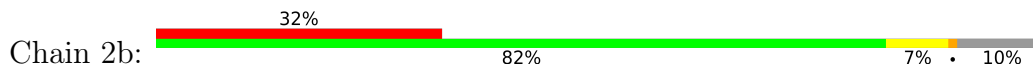




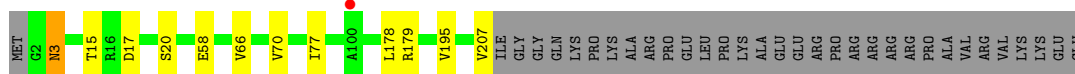
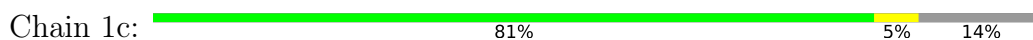
• Molecule 33: 30S ribosomal protein S2



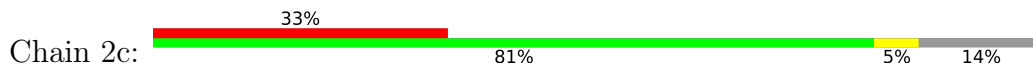
• Molecule 33: 30S ribosomal protein S2

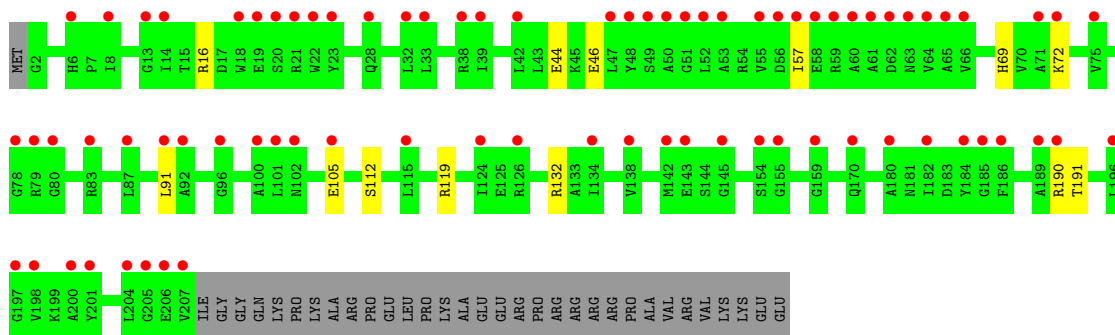


• Molecule 34: 30S ribosomal protein S3

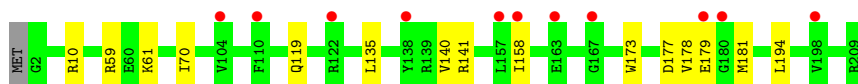


• Molecule 34: 30S ribosomal protein S3

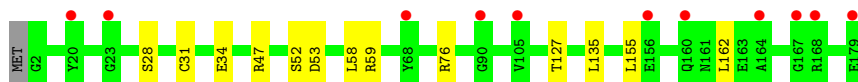
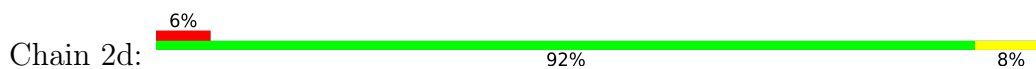




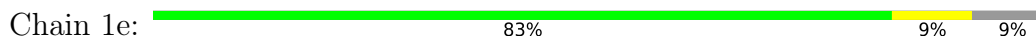
- Molecule 35: 30S ribosomal protein S4



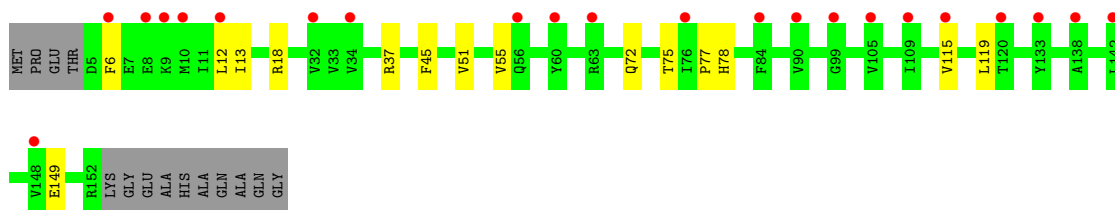
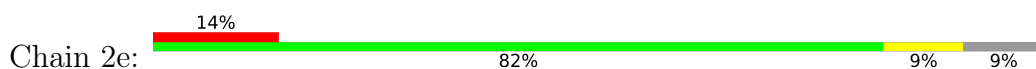
- Molecule 35: 30S ribosomal protein S4



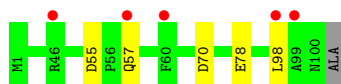
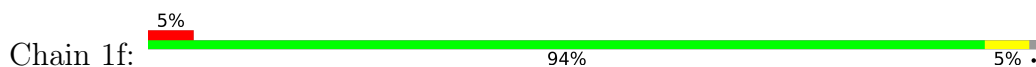
- Molecule 36: 30S ribosomal protein S5



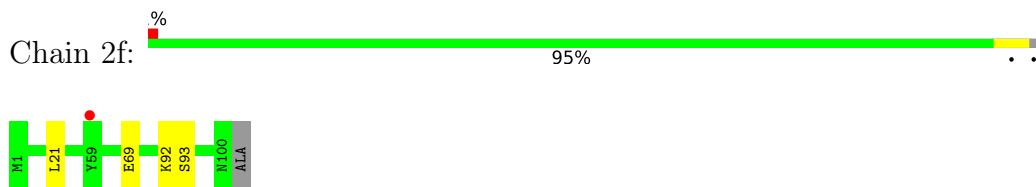
- Molecule 36: 30S ribosomal protein S5



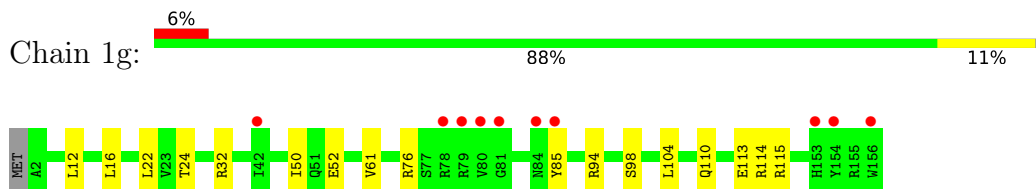
- Molecule 37: 30S ribosomal protein S6



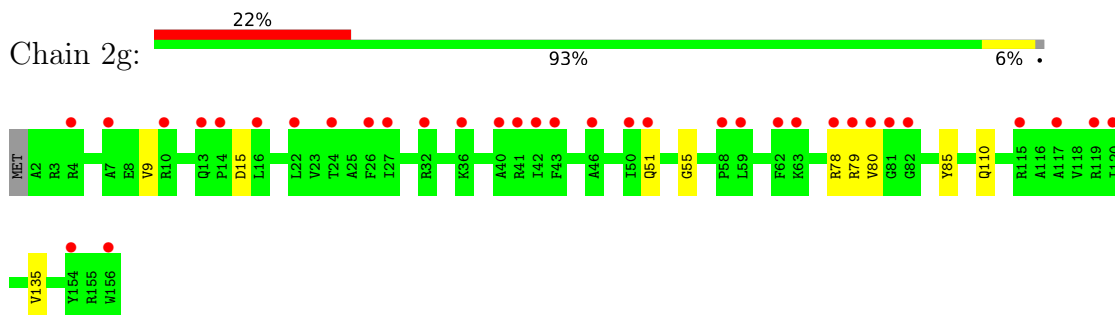
- Molecule 37: 30S ribosomal protein S6



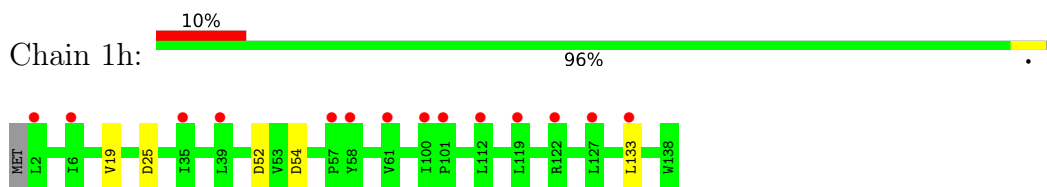
- Molecule 38: 30S ribosomal protein S7



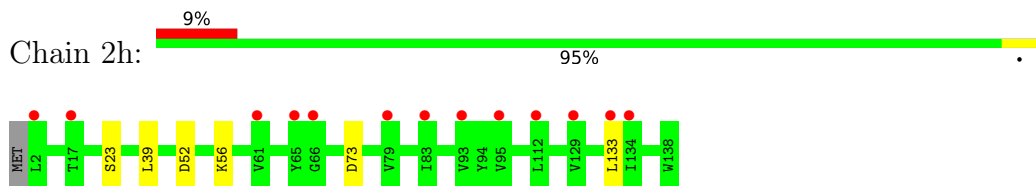
- Molecule 38: 30S ribosomal protein S7



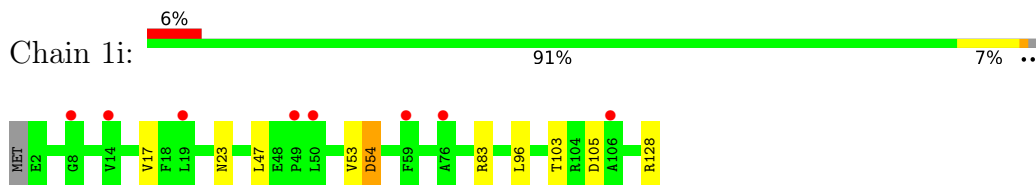
- Molecule 39: 30S ribosomal protein S8



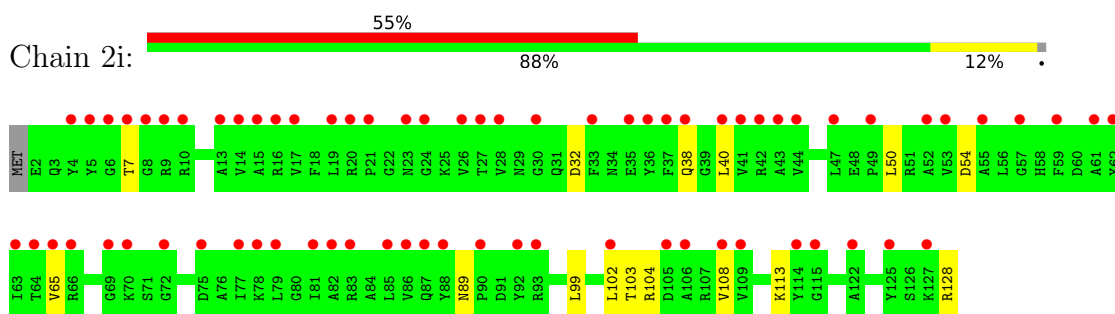
- Molecule 39: 30S ribosomal protein S8



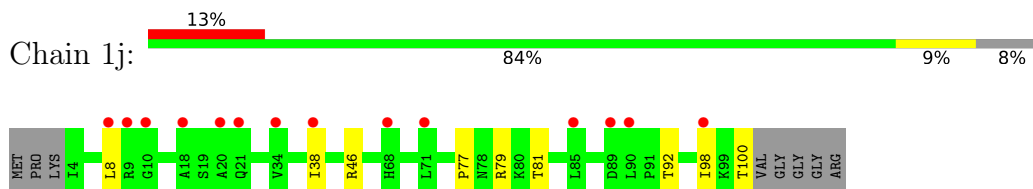
- Molecule 40: 30S ribosomal protein S9



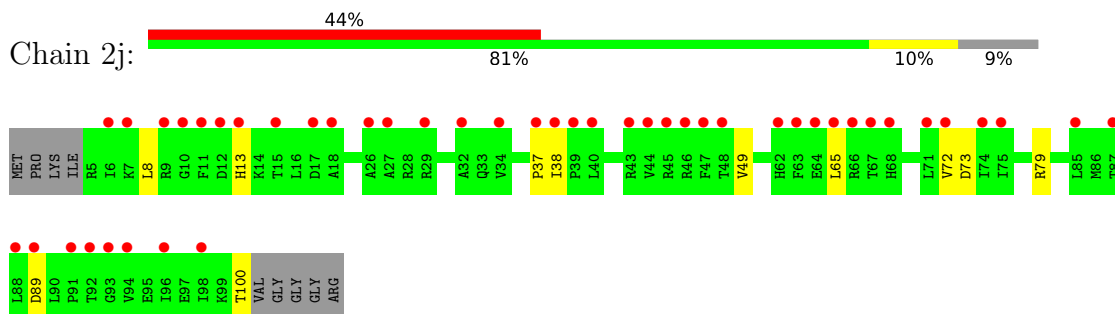
- Molecule 40: 30S ribosomal protein S9



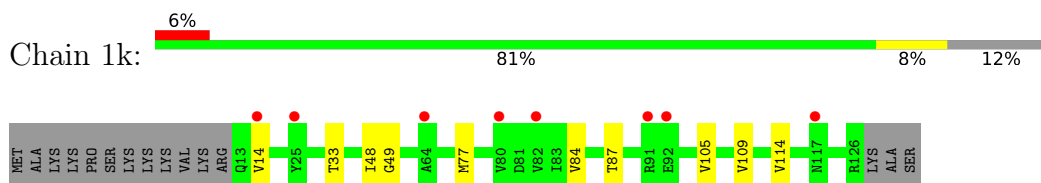
- Molecule 41: 30S ribosomal protein S10



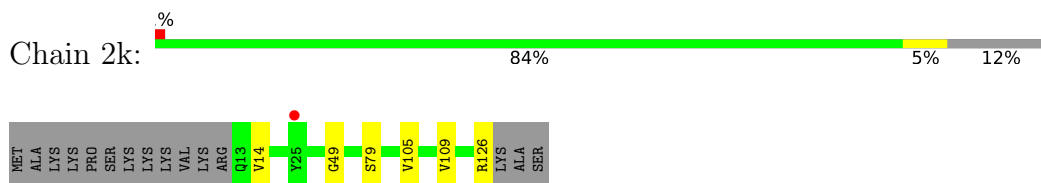
- Molecule 41: 30S ribosomal protein S10



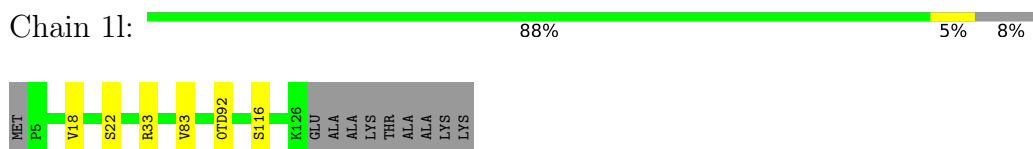
- Molecule 42: 30S ribosomal protein S11



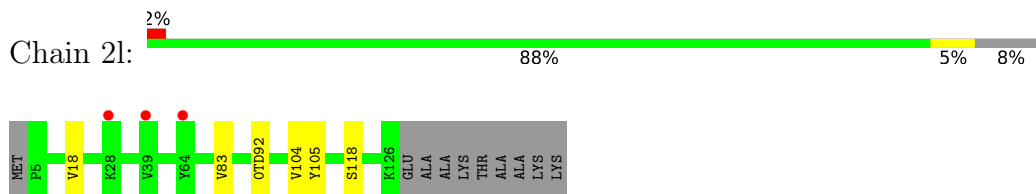
- Molecule 42: 30S ribosomal protein S11



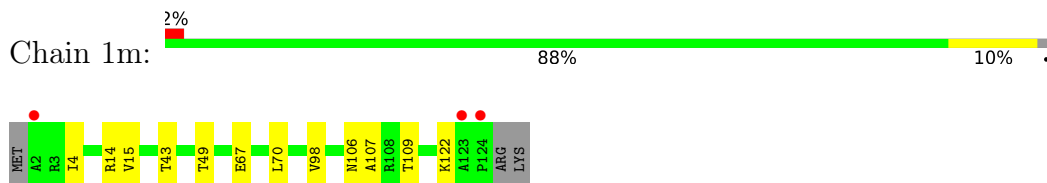
- Molecule 43: 30S ribosomal protein S12



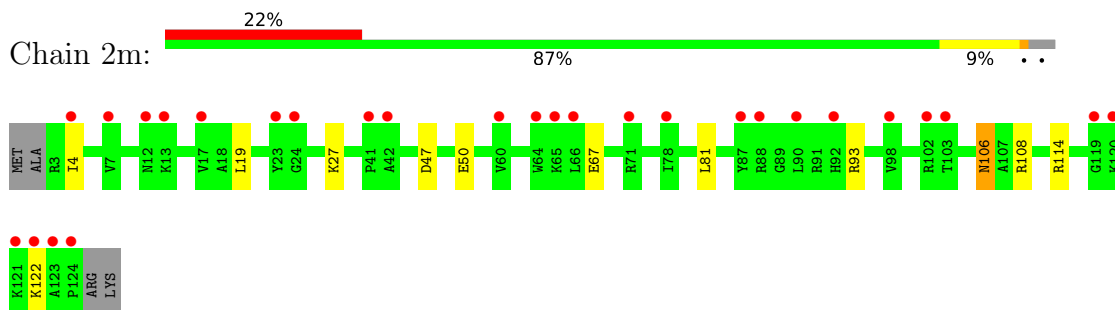
- Molecule 43: 30S ribosomal protein S12



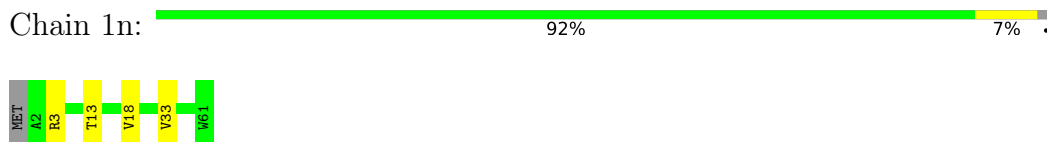
- Molecule 44: 30S ribosomal protein S13



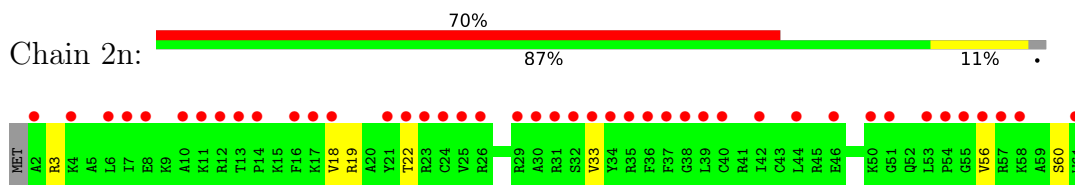
- Molecule 44: 30S ribosomal protein S13



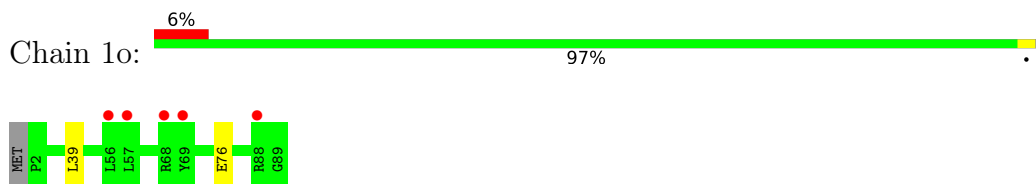
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15




- Molecule 46: 30S ribosomal protein S15

Chain 2o:  93% 6%




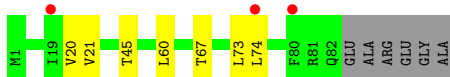
• Molecule 47: 30S ribosomal protein S16

Chain 1p:  85% 8% 7%




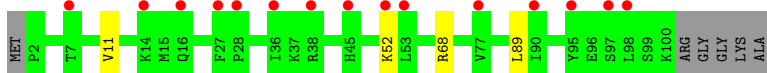
• Molecule 47: 30S ribosomal protein S16

Chain 2p:  3% 85% 8% 7%




• Molecule 48: 30S ribosomal protein S17

Chain 1q:  14% 90% 6%




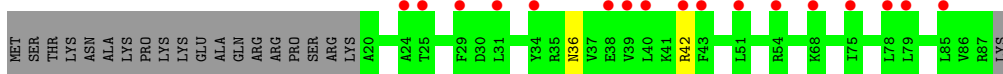
• Molecule 48: 30S ribosomal protein S17

Chain 2q:  6% 86% 9% 6%




• Molecule 49: 30S ribosomal protein S18

Chain 1r:  19% 75% 23%

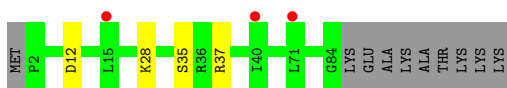
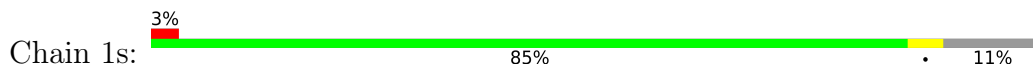


• Molecule 49: 30S ribosomal protein S18

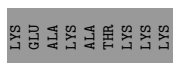
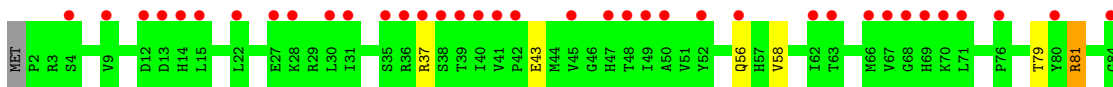
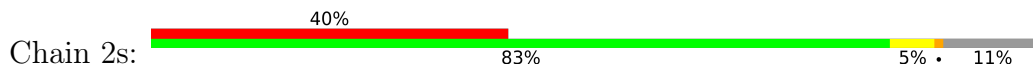
Chain 2r:  % 73% 23%



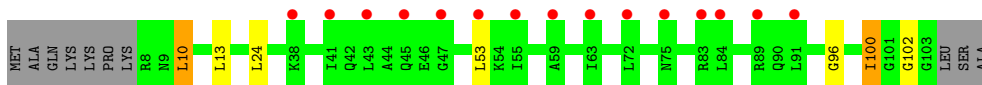
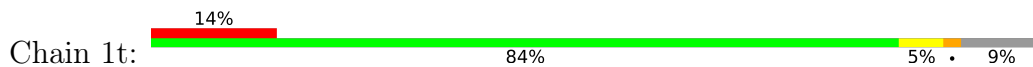
- Molecule 50: 30S ribosomal protein S19



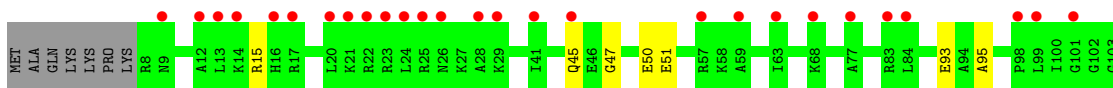
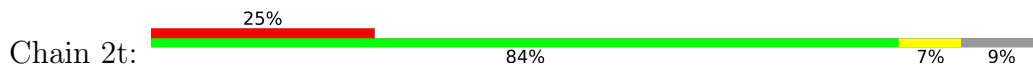
- Molecule 50: 30S ribosomal protein S19



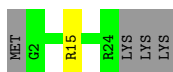
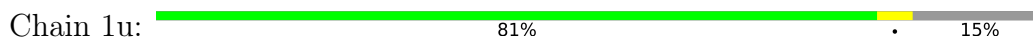
- Molecule 51: 30S ribosomal protein S20



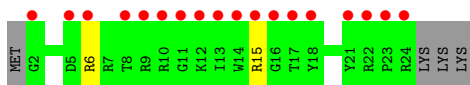
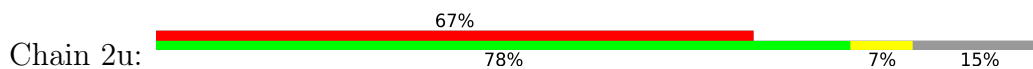
- Molecule 51: 30S ribosomal protein S20



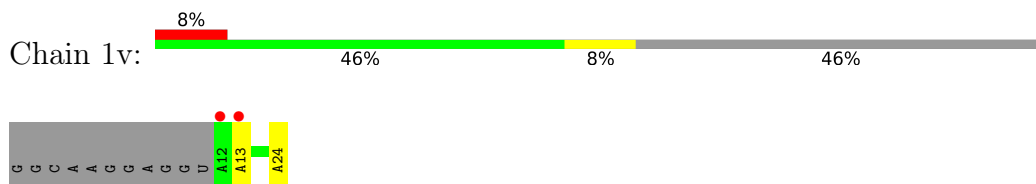
- Molecule 52: 30S ribosomal protein Thx



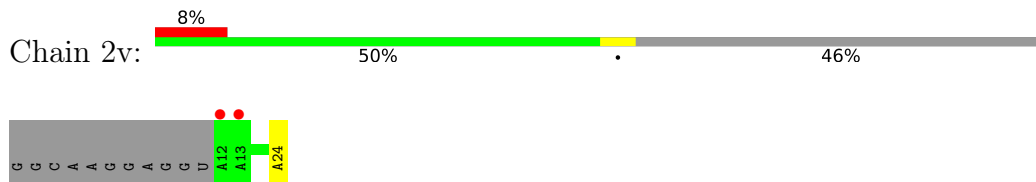
- Molecule 52: 30S ribosomal protein Thx



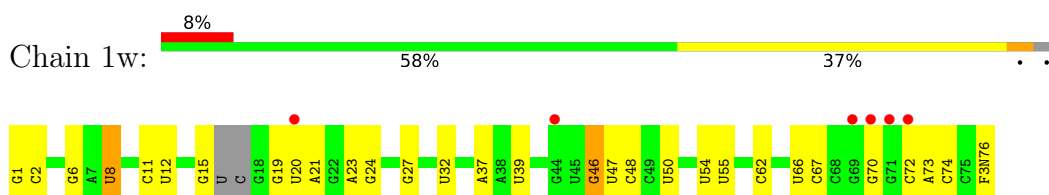
- Molecule 53: MF-mRNA



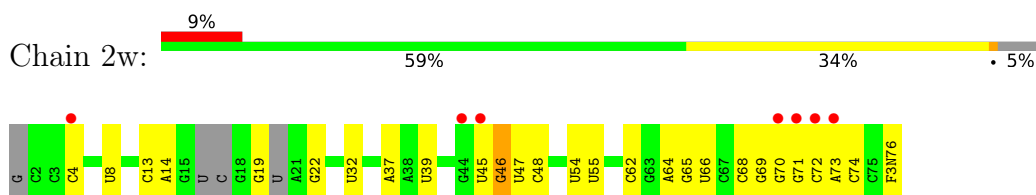
- Molecule 53: MF-mRNA



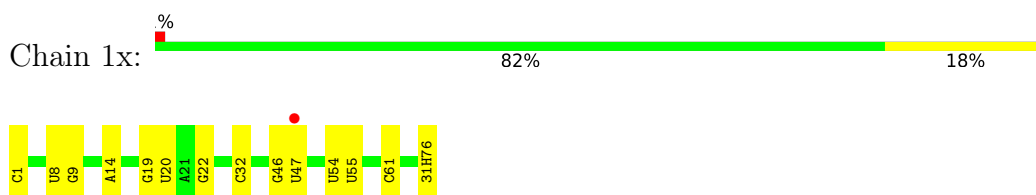
- Molecule 54: A-site Aminoacylated Phe-tRNAphe



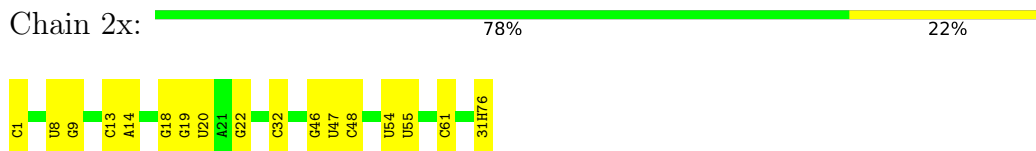
- Molecule 54: A-site Aminoacylated Phe-tRNAphe



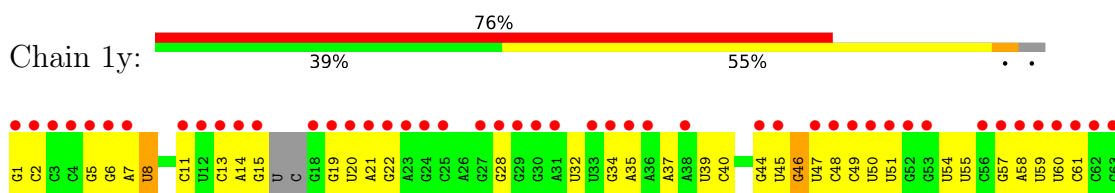
- Molecule 55: P-site Aminoacylated fMet-tRNAmet

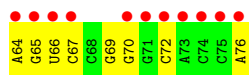


- Molecule 55: P-site Aminoacylated fMet-tRNAmet

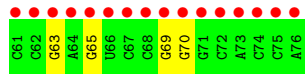
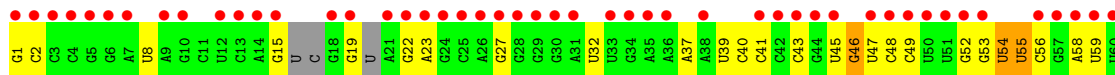
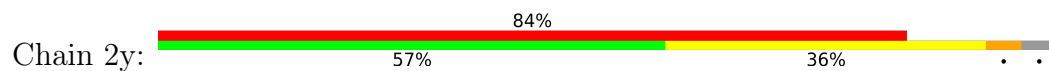


- Molecule 56: E-site Deacylated tRNAphe





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.65Å 448.12Å 621.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	162.05 – 2.65 162.05 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.7 (162.05-2.65) 98.7 (162.05-2.65)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.65Å)	Xtrriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.207 , 0.249 0.207 , 0.249	Depositor DCC
R_{free} test set	82773 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtrriage
Anisotropy	0.155	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	300115	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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: 8AH, M2G, MG, 5MC, 2MU, F3N, K, 0TD, SF4, 31H, 4OC, ZN, OMG, TYK, MA6, PSU, MIA, 2MG, 5MU, G7M, UR3, OMC, 4SU

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	0.49	0/69010	0.93	57/107716 (0.1%)
1	2A	0.37	0/67294	0.84	25/105038 (0.0%)
2	1B	0.43	1/2882 (0.0%)	0.85	0/4494
2	2B	0.37	1/2879 (0.0%)	0.82	1/4487 (0.0%)
3	1D	0.36	0/2186	0.56	0/2944
3	2D	0.31	0/2186	0.51	0/2944
4	1E	0.33	0/1592	0.55	0/2149
4	2E	0.30	0/1592	0.50	0/2149
5	1F	0.32	0/1618	0.53	0/2191
5	2F	0.30	0/1614	0.50	0/2186
6	1G	0.31	0/1448	0.50	0/1957
6	2G	0.28	0/1453	0.47	0/1963
7	1H	0.32	0/1356	0.51	0/1834
7	2H	0.29	0/1356	0.47	0/1834
8	1I	0.29	0/1112	0.49	0/1514
8	2I	0.29	0/1079	0.50	0/1475
9	1N	0.33	0/1144	0.51	0/1543
9	2N	0.27	0/1144	0.45	0/1543
10	1O	0.34	0/943	0.53	0/1269
10	2O	0.30	0/943	0.54	0/1269
11	1P	0.31	0/1152	0.61	0/1533
11	2P	0.29	0/1152	0.53	0/1533
12	1Q	0.35	0/1143	0.52	0/1527
12	2Q	0.30	0/1143	0.48	0/1527
13	1R	0.32	0/982	0.52	0/1312
13	2R	0.26	0/982	0.49	0/1312
14	1S	0.31	0/883	0.49	0/1176
14	2S	0.29	0/880	0.47	0/1172
15	1T	0.32	0/1105	0.50	0/1477
15	2T	0.29	0/1097	0.49	0/1468
16	1U	0.35	0/977	0.50	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.29	0/977	0.43	0/1301
17	1V	0.32	0/782	0.54	0/1049
17	2V	0.29	0/782	0.49	0/1049
18	1W	0.34	0/897	0.51	0/1205
18	2W	0.30	0/897	0.47	0/1205
19	1X	0.38	0/764	0.58	0/1025
19	2X	0.30	0/764	0.53	0/1025
20	1Y	0.32	0/819	0.54	0/1095
20	2Y	0.31	0/819	0.50	0/1095
21	1Z	0.28	0/1267	0.49	0/1717
21	2Z	0.29	0/1299	0.50	0/1763
22	10	0.35	0/662	0.56	0/881
22	20	0.30	0/662	0.49	0/881
23	11	0.32	0/762	0.50	0/1014
23	21	0.31	0/762	0.47	0/1014
24	12	0.30	0/590	0.44	0/781
24	22	0.28	0/590	0.41	0/781
25	13	0.31	0/474	0.51	0/635
25	23	0.29	0/469	0.44	0/630
26	14	0.32	0/565	0.56	0/761
26	24	0.32	0/545	0.47	0/737
27	15	0.34	0/469	0.54	0/635
27	25	0.30	0/469	0.50	0/635
28	16	0.34	0/460	0.51	0/613
28	26	0.29	0/456	0.48	0/608
29	17	0.34	0/426	0.54	0/561
29	27	0.28	0/426	0.50	0/561
30	18	0.33	0/525	0.53	0/691
30	28	0.29	0/525	0.49	0/691
31	19	0.31	0/310	0.52	0/407
31	29	0.30	0/310	0.52	0/407
32	1a	0.36	0/35795	0.85	21/55864 (0.0%)
32	2a	0.34	3/35886 (0.0%)	0.87	36/56005 (0.1%)
33	1b	0.30	0/1881	0.48	0/2542
33	2b	0.30	0/1860	0.47	0/2518
34	1c	0.29	0/1572	0.46	0/2126
34	2c	0.29	0/1566	0.47	0/2119
35	1d	0.28	0/1685	0.44	0/2262
35	2d	0.28	0/1704	0.46	0/2284
36	1e	0.30	0/1145	0.50	0/1543
36	2e	0.30	0/1149	0.49	0/1548
37	1f	0.28	0/823	0.46	0/1115
37	2f	0.30	0/829	0.49	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.28	0/1250	0.44	0/1679
38	2g	0.29	0/1254	0.43	0/1683
39	1h	0.29	0/1108	0.48	0/1494
39	2h	0.29	0/1108	0.47	0/1494
40	1i	0.30	0/1002	0.50	0/1346
40	2i	0.30	0/997	0.48	0/1343
41	1j	0.28	0/722	0.50	0/982
41	2j	0.27	0/727	0.54	0/988
42	1k	0.28	0/844	0.47	0/1145
42	2k	0.29	0/848	0.47	0/1149
43	1l	0.34	0/937	0.54	0/1260
43	2l	0.27	0/937	0.50	0/1260
44	1m	0.28	0/969	0.49	0/1302
44	2m	0.29	0/961	0.51	0/1291
45	1n	0.32	0/501	0.48	0/664
45	2n	0.30	0/501	0.47	0/664
46	1o	0.27	0/739	0.44	0/985
46	2o	0.26	0/739	0.43	0/985
47	1p	0.27	0/697	0.47	0/939
47	2p	0.28	0/693	0.51	0/935
48	1q	0.28	0/836	0.48	0/1117
48	2q	0.27	0/836	0.46	0/1117
49	1r	0.27	0/560	0.51	0/746
49	2r	0.27	0/560	0.49	1/746 (0.1%)
50	1s	0.28	0/667	0.51	0/900
50	2s	0.32	0/661	0.56	0/893
51	1t	0.28	0/730	0.43	0/965
51	2t	0.26	0/729	0.41	0/965
52	1u	0.25	0/203	0.44	0/266
52	2u	0.28	0/203	0.47	0/266
53	1v	0.45	0/310	0.92	0/480
53	2v	0.38	0/310	0.84	0/480
54	1w	0.50	1/1581 (0.1%)	1.00	0/2458
54	2w	0.41	0/1531	0.98	0/2379
55	1x	0.59	5/1723 (0.3%)	1.11	20/2684 (0.7%)
55	2x	0.53	1/1723 (0.1%)	1.05	13/2684 (0.5%)
56	1y	0.56	1/1606 (0.1%)	1.11	5/2497 (0.2%)
56	2y	0.52	1/1583 (0.1%)	0.98	1/2459 (0.0%)
All	All	0.38	14/316632 (0.0%)	0.80	180/474029 (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
33	1b	0	1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	1	C	OP3-P	-10.29	1.48	1.61
56	1y	1	G	OP3-P	-10.15	1.49	1.61
2	1B	1	U	OP3-P	-10.15	1.49	1.61
54	1w	1	G	OP3-P	-10.12	1.49	1.61
2	2B	1	U	OP3-P	-10.09	1.49	1.61

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	27.29	135.27	118.90
32	2a	1272	G	N3-C2-N2	24.11	136.78	119.90
32	2a	1272	G	C5-C6-O6	22.16	141.89	128.60
32	2a	1272	G	N1-C2-N2	-18.59	99.47	116.20
32	2a	1272	G	C6-N1-C2	16.24	134.84	125.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	125	PRO	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	255 (93%)	18 (7%)	0	100	100
4	1E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	29	43
4	2E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	29	43
5	1F	200/210 (95%)	195 (98%)	4 (2%)	1 (0%)	29	43
5	2F	200/210 (95%)	194 (97%)	4 (2%)	2 (1%)	15	23
6	1G	179/182 (98%)	168 (94%)	11 (6%)	0	100	100
6	2G	179/182 (98%)	159 (89%)	17 (10%)	3 (2%)	9	13
7	1H	172/180 (96%)	165 (96%)	7 (4%)	0	100	100
7	2H	172/180 (96%)	156 (91%)	15 (9%)	1 (1%)	25	37
8	1I	144/148 (97%)	124 (86%)	20 (14%)	0	100	100
8	2I	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	11	16
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	22	33
10	1O	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	19	29
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
11	1P	147/150 (98%)	133 (90%)	11 (8%)	3 (2%)	7	10
11	2P	147/150 (98%)	130 (88%)	11 (8%)	6 (4%)	3	3
12	1Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
12	2Q	139/141 (99%)	122 (88%)	17 (12%)	0	100	100
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	102 (94%)	4 (4%)	2 (2%)	8	11
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
15	2T	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	23
17	2V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	23
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	2 (2%)	1 (1%)	17	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	1Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	15	23
20	2Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
21	1Z	148/206 (72%)	135 (91%)	12 (8%)	1 (1%)	22	33
21	2Z	156/206 (76%)	130 (83%)	22 (14%)	4 (3%)	5	7
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	21
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	8	12
26	14	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	1
26	24	67/71 (94%)	52 (78%)	12 (18%)	3 (4%)	2	2
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	44 (96%)	2 (4%)	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%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	197 (86%)	27 (12%)	5 (2%)	6	9
33	2b	229/256 (90%)	194 (85%)	28 (12%)	7 (3%)	4	5
34	1c	204/239 (85%)	186 (91%)	17 (8%)	1 (0%)	29	43
34	2c	204/239 (85%)	180 (88%)	24 (12%)	0	100	100
35	1d	206/209 (99%)	191 (93%)	14 (7%)	1 (0%)	29	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/209 (99%)	193 (94%)	13 (6%)	0	100	100
36	1e	146/162 (90%)	133 (91%)	11 (8%)	2 (1%)	11	16
36	2e	146/162 (90%)	137 (94%)	7 (5%)	2 (1%)	11	16
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
37	2f	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
38	1g	153/156 (98%)	143 (94%)	9 (6%)	1 (1%)	22	33
38	2g	153/156 (98%)	133 (87%)	18 (12%)	2 (1%)	12	18
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	121 (90%)	13 (10%)	1 (1%)	22	33
40	1i	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	19	29
40	2i	125/128 (98%)	104 (83%)	21 (17%)	0	100	100
41	1j	95/105 (90%)	84 (88%)	9 (10%)	2 (2%)	7	10
41	2j	94/105 (90%)	82 (87%)	10 (11%)	2 (2%)	7	10
42	1k	112/129 (87%)	101 (90%)	8 (7%)	3 (3%)	5	6
42	2k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	17	26
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	111 (93%)	7 (6%)	1 (1%)	19	29
44	1m	121/126 (96%)	107 (88%)	12 (10%)	2 (2%)	9	13
44	2m	120/126 (95%)	103 (86%)	15 (12%)	2 (2%)	9	13
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	9	13
46	1o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
46	2o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
47	1p	80/88 (91%)	73 (91%)	7 (9%)	0	100	100
47	2p	80/88 (91%)	71 (89%)	9 (11%)	0	100	100
48	1q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	15	23
48	2q	97/105 (92%)	90 (93%)	5 (5%)	2 (2%)	7	10
49	1r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
49	2r	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	10	15
50	1s	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
50	2s	81/93 (87%)	66 (82%)	14 (17%)	1 (1%)	13	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2	3
51	2t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	7	10
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11368/12128 (94%)	10509 (92%)	769 (7%)	90 (1%)	19	29

5 of 90 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
11	1P	29	LYS
11	1P	36	LYS
21	1Z	53	ILE
26	14	45	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	203 (94%)	12 (6%)	21	33
3	2D	215/218 (99%)	202 (94%)	13 (6%)	19	30
4	1E	164/166 (99%)	157 (96%)	7 (4%)	29	44
4	2E	164/166 (99%)	158 (96%)	6 (4%)	34	50
5	1F	160/166 (96%)	147 (92%)	13 (8%)	11	17
5	2F	159/166 (96%)	151 (95%)	8 (5%)	24	38
6	1G	143/156 (92%)	133 (93%)	10 (7%)	15	23
6	2G	143/156 (92%)	127 (89%)	16 (11%)	6	8
7	1H	144/148 (97%)	142 (99%)	2 (1%)	67	81
7	2H	144/148 (97%)	131 (91%)	13 (9%)	9	14
8	1I	113/124 (91%)	94 (83%)	19 (17%)	2	2
8	2I	105/124 (85%)	92 (88%)	13 (12%)	4	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	1N	118/119 (99%)	109 (92%)	9 (8%)	13	21
9	2N	118/119 (99%)	109 (92%)	9 (8%)	13	21
10	1O	100/100 (100%)	98 (98%)	2 (2%)	55	73
10	2O	100/100 (100%)	97 (97%)	3 (3%)	41	59
11	1P	115/116 (99%)	107 (93%)	8 (7%)	15	23
11	2P	115/116 (99%)	105 (91%)	10 (9%)	10	15
12	1Q	111/111 (100%)	108 (97%)	3 (3%)	44	63
12	2Q	111/111 (100%)	108 (97%)	3 (3%)	44	63
13	1R	101/101 (100%)	96 (95%)	5 (5%)	24	38
13	2R	101/101 (100%)	98 (97%)	3 (3%)	41	59
14	1S	86/88 (98%)	78 (91%)	8 (9%)	9	13
14	2S	85/88 (97%)	74 (87%)	11 (13%)	4	5
15	1T	115/127 (91%)	110 (96%)	5 (4%)	29	44
15	2T	113/127 (89%)	109 (96%)	4 (4%)	36	52
16	1U	93/94 (99%)	90 (97%)	3 (3%)	39	56
16	2U	93/94 (99%)	88 (95%)	5 (5%)	22	34
17	1V	80/82 (98%)	74 (92%)	6 (8%)	13	21
17	2V	80/82 (98%)	75 (94%)	5 (6%)	18	28
18	1W	90/92 (98%)	85 (94%)	5 (6%)	21	33
18	2W	90/92 (98%)	84 (93%)	6 (7%)	16	25
19	1X	77/78 (99%)	74 (96%)	3 (4%)	32	48
19	2X	77/78 (99%)	74 (96%)	3 (4%)	32	48
20	1Y	85/91 (93%)	80 (94%)	5 (6%)	19	30
20	2Y	85/91 (93%)	77 (91%)	8 (9%)	8	13
21	1Z	135/179 (75%)	123 (91%)	12 (9%)	9	14
21	2Z	137/179 (76%)	127 (93%)	10 (7%)	14	21
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	63 (97%)	2 (3%)	40	57
23	11	80/83 (96%)	80 (100%)	0	100	100
23	21	80/83 (96%)	75 (94%)	5 (6%)	18	28
24	12	65/67 (97%)	63 (97%)	2 (3%)	40	57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	22	65/67 (97%)	63 (97%)	2 (3%)	40	57
25	13	51/52 (98%)	45 (88%)	6 (12%)	5	7
25	23	50/52 (96%)	49 (98%)	1 (2%)	55	73
26	14	59/63 (94%)	55 (93%)	4 (7%)	16	24
26	24	53/63 (84%)	46 (87%)	7 (13%)	4	5
27	15	50/52 (96%)	47 (94%)	3 (6%)	19	30
27	25	50/52 (96%)	48 (96%)	2 (4%)	31	47
28	16	51/52 (98%)	47 (92%)	4 (8%)	12	20
28	26	50/52 (96%)	43 (86%)	7 (14%)	3	4
29	17	41/42 (98%)	37 (90%)	4 (10%)	8	11
29	27	41/42 (98%)	38 (93%)	3 (7%)	14	21
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	21
30	28	54/55 (98%)	49 (91%)	5 (9%)	9	13
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	32 (94%)	2 (6%)	19	30
33	1b	192/220 (87%)	175 (91%)	17 (9%)	9	14
33	2b	187/220 (85%)	169 (90%)	18 (10%)	8	12
34	1c	142/188 (76%)	130 (92%)	12 (8%)	10	15
34	2c	140/188 (74%)	127 (91%)	13 (9%)	9	13
35	1d	169/181 (93%)	155 (92%)	14 (8%)	11	16
35	2d	173/181 (96%)	157 (91%)	16 (9%)	9	13
36	1e	113/123 (92%)	101 (89%)	12 (11%)	6	10
36	2e	114/123 (93%)	101 (89%)	13 (11%)	5	8
37	1f	84/90 (93%)	79 (94%)	5 (6%)	19	30
37	2f	85/90 (94%)	81 (95%)	4 (5%)	26	40
38	1g	119/127 (94%)	103 (87%)	16 (13%)	4	5
38	2g	120/127 (94%)	112 (93%)	8 (7%)	16	25
39	1h	114/119 (96%)	109 (96%)	5 (4%)	28	43
39	2h	114/119 (96%)	109 (96%)	5 (4%)	28	43
40	1i	90/99 (91%)	80 (89%)	10 (11%)	6	8
40	2i	89/99 (90%)	74 (83%)	15 (17%)	2	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	1j	66/92 (72%)	59 (89%)	7 (11%)	6	10
41	2j	69/92 (75%)	60 (87%)	9 (13%)	4	5
42	1k	82/99 (83%)	75 (92%)	7 (8%)	10	15
42	2k	83/99 (84%)	78 (94%)	5 (6%)	19	30
43	1l	96/108 (89%)	91 (95%)	5 (5%)	23	36
43	2l	96/108 (89%)	92 (96%)	4 (4%)	30	45
44	1m	93/101 (92%)	83 (89%)	10 (11%)	6	9
44	2m	92/101 (91%)	81 (88%)	11 (12%)	5	7
45	1n	49/50 (98%)	45 (92%)	4 (8%)	11	17
45	2n	49/50 (98%)	43 (88%)	6 (12%)	5	6
46	1o	78/80 (98%)	76 (97%)	2 (3%)	46	64
46	2o	78/80 (98%)	73 (94%)	5 (6%)	17	27
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7	10
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7	10
48	1q	94/97 (97%)	91 (97%)	3 (3%)	39	56
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13	21
49	1r	59/77 (77%)	57 (97%)	2 (3%)	37	53
49	2r	59/77 (77%)	56 (95%)	3 (5%)	24	37
50	1s	69/80 (86%)	65 (94%)	4 (6%)	20	31
50	2s	67/80 (84%)	61 (91%)	6 (9%)	9	14
51	1t	70/82 (85%)	65 (93%)	5 (7%)	14	22
51	2t	70/82 (85%)	65 (93%)	5 (7%)	14	22
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21	33
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	8
All	All	9303/10064 (92%)	8644 (93%)	659 (7%)	14	22

5 of 659 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	21	21	ARG
39	2h	133	LEU
26	24	63	TYR
22	20	74	ARG
34	2c	72	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
9	2N	56	ASN
21	2Z	73	GLN
44	2m	62	ASN
12	2Q	12	GLN
14	2S	84	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2862/2915 (98%)	430 (15%)	30 (1%)
1	2A	2789/2915 (95%)	462 (16%)	26 (0%)
2	1B	119/121 (98%)	7 (5%)	0
2	2B	118/121 (97%)	31 (26%)	0
32	1a	1494/1521 (98%)	241 (16%)	0
32	2a	1498/1521 (98%)	272 (18%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	1 (8%)	0
54	1w	70/76 (92%)	23 (32%)	0
54	2w	67/76 (88%)	20 (29%)	0
55	1x	75/77 (97%)	5 (6%)	0
55	2x	75/77 (97%)	8 (10%)	0
56	1y	71/76 (93%)	34 (47%)	0
56	2y	69/76 (90%)	24 (34%)	0
All	All	9331/9620 (96%)	1560 (16%)	56 (0%)

5 of 1560 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	58	G

5 of 56 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2689	U
1	2A	2689	U
1	2A	271(M)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2439	A
1	2A	1913	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	5MC	2A	1942	1	18,22,23	0.96	2 (11%)	26,32,35	1.12	2 (7%)
1	5MU	1A	1915	1	19,22,23	1.38	5 (26%)	28,32,35	2.18	7 (25%)
32	PSU	1a	516	32	18,21,22	1.34	2 (11%)	22,30,33	1.82	5 (22%)
55	5MU	1x	54	55,57	19,22,23	1.40	5 (26%)	28,32,35	1.99	6 (21%)
54	MIA	2w	37	54	20,27,32	1.83	3 (15%)	22,39,47	1.85	7 (31%)
1	PSU	2A	1911	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	4 (18%)
32	UR3	1a	1498	32	19,22,23	1.05	2 (10%)	26,32,35	1.50	2 (7%)
32	UR3	2a	1498	32	19,22,23	1.07	1 (5%)	26,32,35	1.45	1 (3%)
55	31H	2x	76	55,57	28,34,35	1.05	3 (10%)	23,47,50	1.58	4 (17%)
54	4SU	2w	8	54	18,21,22	1.63	3 (16%)	26,30,33	2.72	5 (19%)
56	PSU	1y	32	56	18,21,22	1.32	2 (11%)	22,30,33	1.81	3 (13%)
56	4SU	2y	8	56	18,21,22	1.63	4 (22%)	26,30,33	2.33	6 (23%)
54	PSU	2w	55	54	18,21,22	1.34	2 (11%)	22,30,33	1.83	3 (13%)
32	4OC	1a	1402	32	20,23,24	0.73	0	26,32,35	0.95	1 (3%)
56	PSU	1y	39	56	18,21,22	1.41	2 (11%)	22,30,33	1.68	3 (13%)
54	PSU	2w	32	54	18,21,22	1.35	2 (11%)	22,30,33	1.81	3 (13%)
56	4SU	1y	8	56	18,21,22	1.68	4 (22%)	26,30,33	2.04	5 (19%)
32	MA6	2a	1519	32	19,26,27	0.84	0	18,38,41	1.63	2 (11%)
1	8AH	1A	2503	1,57	20,26,27	0.82	1 (5%)	23,39,42	2.14	4 (17%)
55	4SU	1x	8	55	18,21,22	2.21	5 (27%)	26,30,33	1.72	6 (23%)
56	PSU	2y	39	56	18,21,22	1.38	2 (11%)	22,30,33	1.64	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	2A	2251	1,55	18,26,27	0.93	1 (5%)	19,38,41	1.14	3 (15%)
32	2MG	1a	1207	32	18,26,27	0.96	1 (5%)	16,38,41	1.09	2 (12%)
1	PSU	1A	1917	1	18,21,22	1.32	2 (11%)	22,30,33	1.89	3 (13%)
32	4OC	2a	1402	32	20,23,24	0.78	0	26,32,35	1.06	2 (7%)
1	5MU	1A	1939	1,57	19,22,23	1.35	5 (26%)	28,32,35	2.17	6 (21%)
1	PSU	1A	1911	1	18,21,22	1.41	2 (11%)	22,30,33	1.90	3 (13%)
56	MIA	1y	37	56	18,24,32	1.19	2 (11%)	18,35,47	1.21	2 (11%)
1	OMC	1A	1920	1	19,22,23	0.84	0	26,31,34	0.84	0
56	5MU	2y	54	56	19,22,23	1.48	4 (21%)	28,32,35	1.98	6 (21%)
1	OMC	2A	1920	1	19,22,23	0.82	0	26,31,34	0.91	1 (3%)
55	31H	1x	76	55,57	28,34,35	1.07	3 (10%)	23,47,50	1.64	4 (17%)
54	MIA	1w	37	54	24,31,32	2.23	3 (12%)	26,44,47	2.33	9 (34%)
32	PSU	2a	516	32	18,21,22	1.31	2 (11%)	22,30,33	1.83	3 (13%)
32	MA6	2a	1518	32	19,26,27	0.82	0	18,38,41	1.45	2 (11%)
54	PSU	1w	32	54,57	18,21,22	1.28	2 (11%)	22,30,33	1.81	3 (13%)
32	5MC	1a	1407	32	18,22,23	0.91	2 (11%)	26,32,35	1.07	3 (11%)
1	PSU	2A	2605	1	18,21,22	1.40	3 (16%)	22,30,33	1.92	4 (18%)
1	5MC	1A	1962	1	18,22,23	0.97	2 (11%)	26,32,35	1.19	2 (7%)
1	2MU	2A	2552	1	19,22,24	1.29	3 (15%)	26,31,36	1.77	6 (23%)
32	M2G	2a	966	32	20,27,28	1.35	3 (15%)	22,40,43	1.05	2 (9%)
54	G7M	2w	46	54	20,26,27	1.25	1 (5%)	17,39,42	0.63	0
54	PSU	2w	39	54	18,21,22	1.37	2 (11%)	22,30,33	1.58	3 (13%)
1	OMG	1A	2251	1,57,55	18,26,27	0.98	1 (5%)	19,38,41	1.08	3 (15%)
32	5MC	1a	967	32	18,22,23	0.97	2 (11%)	26,32,35	1.14	2 (7%)
32	5MC	1a	1404	32	18,22,23	1.05	2 (11%)	26,32,35	1.17	4 (15%)
55	4SU	2x	8	55	18,21,22	2.05	6 (33%)	26,30,33	1.42	5 (19%)
55	PSU	1x	55	55	18,21,22	1.32	2 (11%)	22,30,33	1.88	4 (18%)
32	MA6	1a	1518	32	19,26,27	0.83	0	18,38,41	1.48	2 (11%)
55	5MC	1x	32	55	18,22,23	0.98	2 (11%)	26,32,35	1.25	3 (11%)
55	PSU	2x	55	55	18,21,22	1.37	2 (11%)	22,30,33	1.91	4 (18%)
1	PSU	2A	1917	1	18,21,22	1.36	2 (11%)	22,30,33	1.82	3 (13%)
54	PSU	1w	55	54	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
32	5MC	2a	1404	32	18,22,23	0.99	2 (11%)	26,32,35	1.16	3 (11%)
56	PSU	2y	55	56	18,21,22	1.30	3 (16%)	22,30,33	1.85	4 (18%)
1	2MU	1A	2552	1,57	19,22,24	1.17	2 (10%)	26,31,36	1.88	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	1A	1942	1	18,22,23	0.93	2 (11%)	26,32,35	1.19	4 (15%)
54	5MU	1w	54	54	19,22,23	1.37	4 (21%)	28,32,35	1.92	6 (21%)
55	5MC	2x	32	55	18,22,23	0.97	2 (11%)	26,32,35	1.24	3 (11%)
1	5MU	2A	1915	1	19,22,23	1.46	6 (31%)	28,32,35	2.16	6 (21%)
43	0TD	1l	92	43	7,9,10	4.79	2 (28%)	6,11,13	7.46	2 (33%)
54	F3N	2w	76	1,54	30,36,37	1.45	5 (16%)	29,51,54	1.22	1 (3%)
32	5MC	2a	967	32	18,22,23	0.93	2 (11%)	26,32,35	1.19	3 (11%)
1	5MU	2A	1939	1,57	19,22,23	1.40	4 (21%)	28,32,35	2.28	6 (21%)
55	5MU	2x	54	55	19,22,23	1.41	6 (31%)	28,32,35	2.12	6 (21%)
56	G7M	2y	46	56	20,26,27	1.43	3 (15%)	17,39,42	0.83	1 (5%)
32	M2G	1a	966	32	20,27,28	1.38	3 (15%)	22,40,43	1.03	2 (9%)
32	5MC	1a	1400	32	18,22,23	0.94	2 (11%)	26,32,35	1.14	3 (11%)
32	G7M	1a	527	32,57	20,26,27	1.20	2 (10%)	17,39,42	0.68	0
32	5MC	2a	1400	32	18,22,23	0.97	2 (11%)	26,32,35	1.24	4 (15%)
1	5MC	2A	1962	1,57	18,22,23	0.96	2 (11%)	26,32,35	1.18	2 (7%)
54	4SU	1w	8	54	18,21,22	1.67	4 (22%)	26,30,33	1.84	4 (15%)
32	MA6	1a	1519	32	19,26,27	0.84	0	18,38,41	1.61	2 (11%)
56	PSU	1y	55	56	18,21,22	1.38	2 (11%)	22,30,33	1.92	4 (18%)
56	G7M	1y	46	56	20,26,27	1.43	2 (10%)	17,39,42	0.67	0
54	5MU	2w	54	54	19,22,23	1.36	4 (21%)	28,32,35	1.90	6 (21%)
32	2MG	2a	1207	32	18,26,27	0.96	1 (5%)	16,38,41	0.99	2 (12%)
54	G7M	1w	46	54	20,26,27	1.23	2 (10%)	17,39,42	0.70	0
32	5MC	2a	1407	32	18,22,23	0.97	2 (11%)	26,32,35	1.11	2 (7%)
1	8AH	2A	2503	1,57	20,26,27	0.85	1 (5%)	23,39,42	1.89	4 (17%)
43	0TD	2l	92	43	7,9,10	4.76	1 (14%)	6,11,13	1.91	2 (33%)
56	MIA	2y	37	56	18,24,32	1.16	2 (11%)	18,35,47	1.30	2 (11%)
54	PSU	1w	39	54	18,21,22	1.38	2 (11%)	22,30,33	1.69	3 (13%)
56	PSU	2y	32	56	18,21,22	1.30	2 (11%)	22,30,33	1.80	3 (13%)
56	5MU	1y	54	56	19,22,23	1.39	5 (26%)	28,32,35	2.14	7 (25%)
54	F3N	1w	76	1,54	30,36,37	1.57	6 (20%)	29,51,54	1.31	2 (6%)
32	G7M	2a	527	32,57	20,26,27	1.29	2 (10%)	17,39,42	0.47	0
1	PSU	1A	2605	1,57	18,21,22	1.32	2 (11%)	22,30,33	1.88	4 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	1/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55,57	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/7/29/34	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
55	31H	2x	76	55,57	-	3/18/40/41	0/3/3/3
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
56	4SU	2y	8	56	-	1/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
56	4SU	1y	8	56	-	2/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
1	8AH	1A	2503	1,57	-	2/3/25/26	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55	-	0/5/27/28	0/3/3/3
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
1	5MU	1A	1939	1,57	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
56	MIA	1y	37	56	-	2/3/25/34	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
56	5MU	2y	54	56	-	2/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
55	31H	1x	76	55,57	-	3/18/40/41	0/3/3/3
54	MIA	1w	37	54	-	3/11/33/34	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
54	PSU	1w	32	54,57	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MU	2A	2552	1	-	0/9/27/28	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	G7M	2w	46	54	-	1/3/25/26	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,57,55	-	0/5/27/28	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	6/7/25/26	0/2/2/2
1	2MU	1A	2552	1,57	-	0/9/27/28	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
54	F3N	2w	76	1,54	-	1/15/37/38	0/4/4/4
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,57	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
56	G7M	2y	46	56	-	2/3/25/26	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,57	-	3/3/25/26	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,57	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
56	PSU	1y	55	56	-	1/7/25/26	0/2/2/2
56	G7M	1y	46	56	-	2/3/25/26	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	1/5/27/28	0/3/3/3
54	G7M	1w	46	54	-	1/3/25/26	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	8AH	2A	2503	1,57	-	1/3/25/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	0TD	2l	92	43	-	3/7/12/14	-
56	MIA	2y	37	56	-	3/3/25/34	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	0/7/25/26	0/2/2/2
54	F3N	1w	76	1,54	-	2/15/37/38	0/4/4/4
32	G7M	2a	527	32,57	-	3/3/25/26	0/3/3/3
1	PSU	1A	2605	1,57	-	0/7/25/26	0/2/2/2

The worst 5 of 210 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.28	1.69	1.82
43	1l	92	0TD	CB-SB	-12.15	1.69	1.82
54	1w	37	MIA	C13-C14	7.34	1.53	1.32
54	2w	37	MIA	C2-S10	-6.77	1.70	1.75
54	1w	37	MIA	C2-S10	-6.57	1.70	1.75

The worst 5 of 293 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-17.74	70.35	102.44
54	2w	8	4SU	C4-N3-C2	-8.89	118.71	127.34
1	1A	2503	8AH	C2-N3-C4	7.29	121.44	115.52
56	2y	8	4SU	C4-N3-C2	-7.28	120.27	127.34
54	1w	37	MIA	C12-C13-C14	-6.97	113.57	127.14

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	527	G7M	C3'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C15
54	1w	76	F3N	C3'-C4'-C5'-O5'
55	1x	76	31H	C3'-C4'-C5'-O5'
56	1y	8	4SU	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2685 ligands modelled in this entry, 2681 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	TYK	2A	3798	1	67,67,67	1.81	8 (11%)	83,97,97	1.49	14 (16%)
59	TYK	1A	4101	1	67,67,67	1.74	6 (8%)	83,97,97	1.31	14 (16%)
61	SF4	2d	303	35	0,12,12	-	-	-	-	-
61	SF4	1d	501	35	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	TYK	2A	3798	1	-	4/67/126/126	1/3/4/4
59	TYK	1A	4101	1	-	2/67/126/126	1/3/4/4
61	SF4	2d	303	35	-	-	0/6/5/5
61	SF4	1d	501	35	-	-	0/6/5/5

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	2A	3798	TYK	C14-C13	-8.12	1.37	1.50
59	1A	4101	TYK	C8-C9	-7.66	1.38	1.51
59	2A	3798	TYK	C8-C9	-7.64	1.38	1.51
59	1A	4101	TYK	C14-C13	-7.46	1.39	1.50
59	2A	3798	TYK	C2-C1	-4.72	1.41	1.50

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	2A	3798	TYK	C10-C11-C12	-4.31	119.72	126.23
59	1A	4101	TYK	C3B-C2B-C1B	-4.24	106.69	114.82
59	2A	3798	TYK	C1B-O4A-C4A	3.81	122.36	114.66
59	2A	3798	TYK	C3B-C2B-C1B	-3.63	107.85	114.82
59	2A	3798	TYK	O4B-C4B-C5B	-3.62	103.04	109.39

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

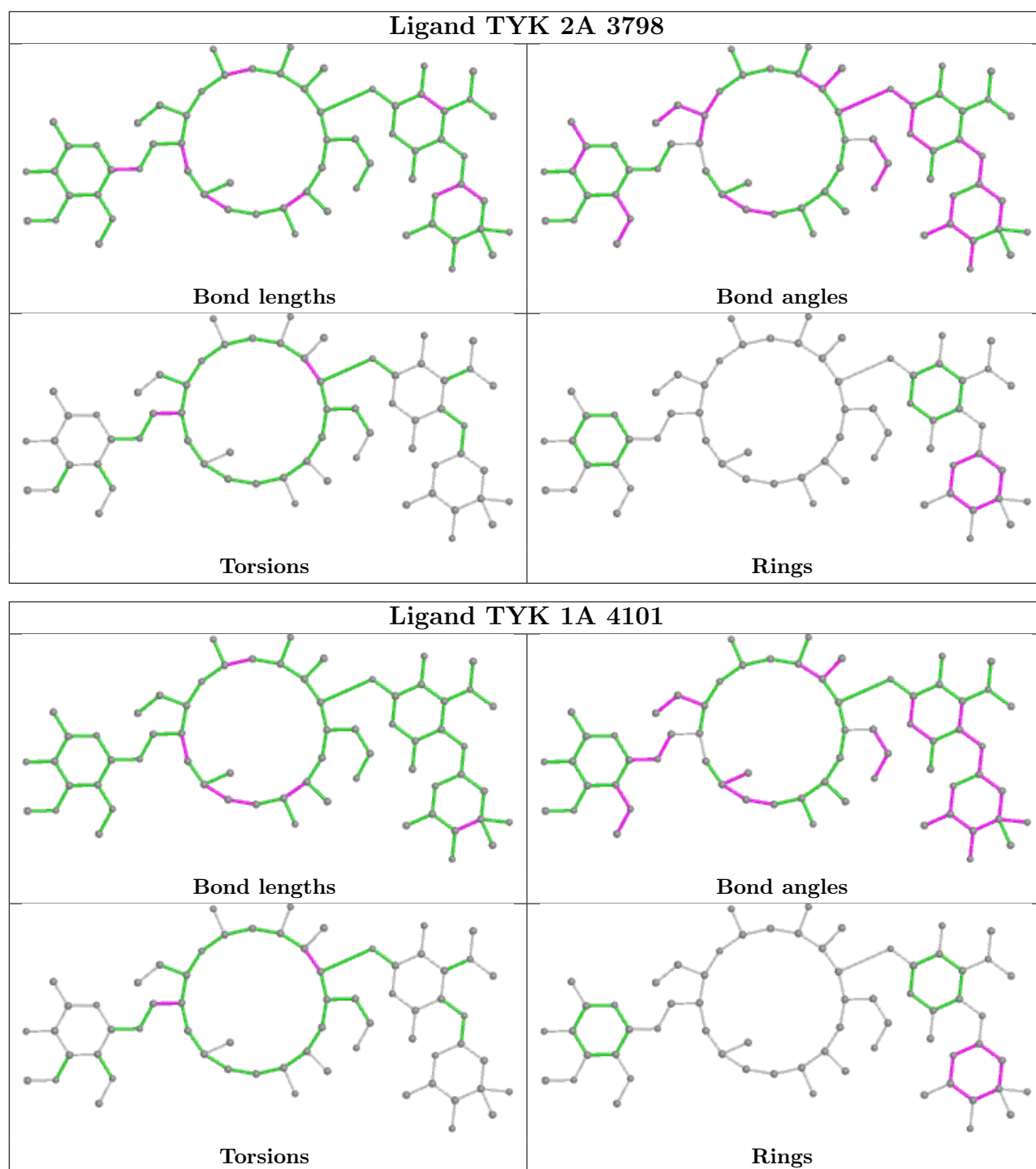
Mol	Chain	Res	Type	Atoms
59	1A	4101	TYK	C15-C14-C23-O1C
59	2A	3798	TYK	C15-C14-C23-O1C
59	1A	4101	TYK	C18-C4-C5-C6
59	2A	3798	TYK	C18-C4-C5-C6
59	2A	3798	TYK	C3-C4-C5-O1A

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	2A	3798	TYK	C1B-C2B-C3B-C4B-C5B-O5B
59	1A	4101	TYK	C1B-C2B-C3B-C4B-C5B-O5B

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	0.11	136 (4%) 30 27	20, 36, 98, 108	0
1	2A	2789/2915 (95%)	0.03	94 (3%) 45 41	33, 57, 95, 107	0
2	1B	120/121 (99%)	-0.45	0 100 100	29, 48, 63, 89	0
2	2B	120/121 (99%)	-0.69	0 100 100	61, 75, 84, 91	0
3	1D	275/276 (99%)	0.39	6 (2%) 62 57	21, 37, 52, 77	0
3	2D	275/276 (99%)	0.49	3 (1%) 80 79	33, 50, 62, 82	0
4	1E	204/206 (99%)	0.11	1 (0%) 91 91	20, 39, 59, 76	0
4	2E	204/206 (99%)	0.13	0 100 100	38, 59, 72, 81	0
5	1F	202/210 (96%)	0.24	1 (0%) 91 91	19, 41, 66, 84	0
5	2F	202/210 (96%)	0.43	4 (1%) 65 60	37, 66, 79, 87	0
6	1G	181/182 (99%)	-0.16	0 100 100	39, 56, 71, 81	0
6	2G	181/182 (99%)	0.74	28 (15%) 2 1	67, 77, 85, 94	0
7	1H	174/180 (96%)	-0.10	1 (0%) 89 89	36, 53, 67, 73	0
7	2H	174/180 (96%)	1.85	74 (42%) 0 0	69, 83, 90, 95	0
8	1I	146/148 (98%)	-0.06	0 100 100	46, 72, 80, 83	0
8	2I	146/148 (98%)	0.44	8 (5%) 25 21	53, 73, 80, 85	0
9	1N	140/140 (100%)	0.14	0 100 100	25, 38, 61, 67	0
9	2N	140/140 (100%)	0.48	4 (2%) 51 48	48, 66, 79, 85	0
10	1O	122/122 (100%)	0.12	0 100 100	28, 39, 57, 61	0
10	2O	122/122 (100%)	0.51	3 (2%) 57 53	47, 58, 70, 76	0
11	1P	149/150 (99%)	0.27	2 (1%) 77 75	23, 45, 68, 73	0
11	2P	149/150 (99%)	1.14	32 (21%) 0 0	40, 65, 80, 89	0
12	1Q	141/141 (100%)	0.03	0 100 100	25, 39, 55, 72	0
12	2Q	141/141 (100%)	0.24	1 (0%) 87 87	48, 66, 77, 81	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.19	0 100 100	25, 34, 46, 56	0
13	2R	118/118 (100%)	0.35	3 (2%) 57 53	44, 53, 63, 70	0
14	1S	110/112 (98%)	-0.12	0 100 100	38, 49, 60, 66	0
14	2S	110/112 (98%)	0.06	2 (1%) 68 65	61, 70, 78, 84	0
15	1T	131/146 (89%)	0.26	1 (0%) 86 85	33, 44, 68, 78	0
15	2T	131/146 (89%)	0.70	9 (6%) 16 13	52, 62, 75, 82	0
16	1U	116/118 (98%)	0.17	0 100 100	22, 30, 44, 64	0
16	2U	116/118 (98%)	0.33	1 (0%) 84 83	44, 62, 72, 77	0
17	1V	101/101 (100%)	0.19	0 100 100	23, 38, 55, 65	0
17	2V	101/101 (100%)	0.36	4 (3%) 38 34	43, 71, 77, 83	0
18	1W	112/113 (99%)	0.03	1 (0%) 84 83	25, 32, 49, 85	0
18	2W	112/113 (99%)	0.14	0 100 100	40, 51, 69, 86	0
19	1X	95/96 (98%)	-0.02	1 (1%) 80 79	26, 38, 62, 77	0
19	2X	95/96 (98%)	0.31	3 (3%) 47 44	45, 58, 75, 82	0
20	1Y	107/110 (97%)	-0.09	0 100 100	36, 50, 67, 80	0
20	2Y	107/110 (97%)	0.34	5 (4%) 31 28	58, 71, 80, 86	0
21	1Z	154/206 (74%)	0.06	4 (2%) 56 52	38, 64, 83, 91	0
21	2Z	160/206 (77%)	0.66	19 (11%) 4 3	64, 81, 88, 92	0
22	10	83/85 (97%)	0.04	0 100 100	29, 37, 50, 67	0
22	20	83/85 (97%)	0.13	0 100 100	47, 61, 73, 78	0
23	11	97/98 (98%)	0.37	2 (2%) 63 59	29, 47, 71, 75	0
23	21	97/98 (98%)	0.57	6 (6%) 20 17	39, 55, 75, 84	0
24	12	70/72 (97%)	0.03	0 100 100	35, 48, 59, 76	0
24	22	70/72 (97%)	-0.06	0 100 100	58, 69, 76, 80	0
25	13	59/60 (98%)	0.24	1 (1%) 70 67	26, 36, 62, 79	0
25	23	59/60 (98%)	0.83	5 (8%) 10 8	57, 66, 79, 87	0
26	14	69/71 (97%)	0.27	6 (8%) 10 8	52, 73, 88, 89	0
26	24	69/71 (97%)	1.27	16 (23%) 0 0	75, 84, 92, 94	0
27	15	59/60 (98%)	0.10	1 (1%) 70 67	20, 32, 51, 54	0
27	25	59/60 (98%)	0.18	3 (5%) 28 25	39, 54, 66, 78	0
28	16	53/54 (98%)	0.11	0 100 100	33, 43, 57, 60	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%)	0.51	3 (5%) 23 20	51, 60, 68, 72	0
29	17	48/49 (97%)	0.26	1 (2%) 63 59	24, 29, 54, 63	0
29	27	48/49 (97%)	0.54	4 (8%) 11 9	35, 42, 64, 74	0
30	18	64/65 (98%)	0.16	0 100 100	29, 34, 42, 56	0
30	28	64/65 (98%)	0.75	3 (4%) 31 28	44, 55, 62, 65	0
31	19	37/37 (100%)	-0.04	0 100 100	30, 38, 54, 61	0
31	29	37/37 (100%)	0.54	4 (10%) 5 4	60, 68, 77, 83	0
32	1a	1488/1521 (97%)	-0.22	27 (1%) 68 65	34, 64, 92, 105	0
32	2a	1491/1521 (98%)	0.02	66 (4%) 34 31	49, 75, 95, 106	0
33	1b	231/256 (90%)	0.73	28 (12%) 4 3	62, 77, 87, 92	0
33	2b	231/256 (90%)	1.77	82 (35%) 0 0	73, 83, 89, 92	0
34	1c	206/239 (86%)	-0.00	1 (0%) 91 91	56, 68, 79, 86	0
34	2c	206/239 (86%)	1.69	78 (37%) 0 0	73, 82, 88, 91	0
35	1d	208/209 (99%)	0.51	11 (5%) 26 23	52, 67, 76, 82	0
35	2d	208/209 (99%)	0.64	12 (5%) 23 19	59, 71, 79, 82	0
36	1e	148/162 (91%)	0.14	0 100 100	48, 62, 72, 80	0
36	2e	148/162 (91%)	0.88	22 (14%) 2 1	65, 75, 81, 86	0
37	1f	100/101 (99%)	0.46	5 (5%) 28 25	52, 65, 72, 77	0
37	2f	100/101 (99%)	0.26	1 (1%) 82 81	49, 67, 75, 82	0
38	1g	155/156 (99%)	0.36	10 (6%) 18 16	59, 70, 84, 88	0
38	2g	155/156 (99%)	1.23	34 (21%) 0 0	68, 78, 87, 92	0
39	1h	137/138 (99%)	0.74	14 (10%) 6 4	52, 65, 72, 76	0
39	2h	137/138 (99%)	0.54	13 (9%) 8 6	65, 74, 80, 83	0
40	1i	127/128 (99%)	0.42	8 (6%) 20 17	50, 74, 83, 87	0
40	2i	127/128 (99%)	2.24	71 (55%) 0 0	71, 83, 88, 92	0
41	1j	97/105 (92%)	0.77	14 (14%) 2 1	53, 76, 84, 91	0
41	2j	96/105 (91%)	2.16	46 (47%) 0 0	74, 84, 90, 92	0
42	1k	114/129 (88%)	0.67	8 (7%) 16 13	41, 66, 76, 80	0
42	2k	114/129 (88%)	0.14	1 (0%) 84 83	52, 72, 79, 82	0
43	1l	121/132 (91%)	0.15	0 100 100	41, 50, 63, 71	0
43	2l	121/132 (91%)	0.30	3 (2%) 57 53	50, 66, 75, 81	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	-0.15	3 (2%) 59 54	53, 67, 76, 88	0
44	2m	122/126 (96%)	1.34	28 (22%) 0 0	67, 80, 85, 88	0
45	1n	60/61 (98%)	0.18	0 100 100	54, 64, 71, 76	0
45	2n	60/61 (98%)	3.66	43 (71%) 0 0	73, 82, 87, 90	0
46	1o	88/89 (98%)	0.70	5 (5%) 23 20	47, 63, 72, 79	0
46	2o	88/89 (98%)	0.23	0 100 100	59, 70, 80, 85	0
47	1p	82/88 (93%)	0.11	0 100 100	58, 69, 77, 86	0
47	2p	82/88 (93%)	0.37	3 (3%) 41 38	59, 69, 77, 81	0
48	1q	99/105 (94%)	1.11	15 (15%) 2 1	48, 66, 75, 76	0
48	2q	99/105 (94%)	0.58	6 (6%) 21 18	62, 72, 80, 81	0
49	1r	68/88 (77%)	1.31	17 (25%) 0 0	53, 64, 76, 77	0
49	2r	68/88 (77%)	0.23	1 (1%) 73 71	59, 69, 78, 83	0
50	1s	83/93 (89%)	0.33	3 (3%) 42 39	59, 69, 79, 84	0
50	2s	83/93 (89%)	2.06	37 (44%) 0 0	78, 83, 89, 95	0
51	1t	96/106 (90%)	1.10	15 (15%) 2 1	61, 68, 78, 82	0
51	2t	96/106 (90%)	1.43	27 (28%) 0 0	60, 70, 81, 87	0
52	1u	23/27 (85%)	0.42	0 100 100	59, 64, 70, 74	0
52	2u	23/27 (85%)	2.83	18 (78%) 0 0	74, 78, 83, 89	0
53	1v	13/24 (54%)	0.62	2 (15%) 2 1	47, 51, 92, 98	0
53	2v	13/24 (54%)	0.44	2 (15%) 2 1	63, 73, 96, 102	0
54	1w	66/76 (86%)	0.22	6 (9%) 9 7	29, 86, 98, 103	0
54	2w	64/76 (84%)	0.12	7 (10%) 5 4	48, 91, 100, 102	0
55	1x	72/77 (93%)	-0.20	1 (1%) 75 73	25, 58, 78, 91	0
55	2x	72/77 (93%)	-0.29	0 100 100	42, 73, 87, 97	0
56	1y	67/76 (88%)	3.40	58 (86%) 0 0	58, 99, 103, 105	0
56	2y	66/76 (86%)	4.24	64 (96%) 0 0	69, 101, 103, 105	0
All	All	20871/21748 (95%)	0.31	1422 (6%) 17 14	19, 63, 89, 108	0

The worst 5 of 1422 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2A	653	A	16.8
1	2A	652(U)	G	14.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	652(V)	C	14.5
1	2A	652(V)	C	14.2
1	2A	652(C)	G	13.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	4SU	2y	8	20/21	0.61	0.30	95,104,112,126	0
56	PSU	1y	55	20/21	0.66	0.49	96,101,106,114	0
56	5MU	1y	54	21/22	0.73	0.50	89,99,104,118	0
56	G7M	2y	46	24/25	0.74	0.41	86,99,105,120	0
56	MIA	2y	37	22/30	0.77	0.41	83,97,109,123	0
56	PSU	2y	55	20/21	0.77	0.33	89,97,106,108	0
56	PSU	2y	32	20/21	0.78	0.42	86,98,107,115	0
54	G7M	2w	46	24/25	0.78	0.18	84,94,109,123	0
56	PSU	1y	39	20/21	0.79	0.30	83,94,107,109	0
56	5MU	2y	54	21/22	0.79	0.44	91,96,106,126	0
56	G7M	1y	46	24/25	0.79	0.36	91,99,104,117	0
56	PSU	2y	39	20/21	0.81	0.35	90,95,104,111	0
54	G7M	1w	46	24/25	0.81	0.15	78,88,100,121	0
56	PSU	1y	32	20/21	0.82	0.36	88,96,106,112	0
54	4SU	2w	8	20/21	0.85	0.14	90,94,105,108	0
54	PSU	2w	55	20/21	0.87	0.12	77,83,94,96	0
56	4SU	1y	8	20/21	0.87	0.25	93,97,105,116	0
54	4SU	1w	8	20/21	0.87	0.16	71,85,92,94	0
56	MIA	1y	37	22/30	0.87	0.24	86,93,100,113	0
32	2MG	2a	1207	24/25	0.90	0.16	76,83,86,90	0
55	4SU	2x	8	20/21	0.91	0.17	64,75,83,83	0
54	MIA	2w	37	25/30	0.91	0.18	68,76,85,103	0
55	PSU	2x	55	20/21	0.92	0.14	69,75,84,86	0
54	PSU	2w	32	20/21	0.92	0.17	76,84,91,92	0
32	G7M	2a	527	24/25	0.93	0.18	61,67,71,76	0
32	5MC	2a	967	21/22	0.93	0.14	62,66,76,82	0
54	5MU	2w	54	21/22	0.93	0.13	74,80,84,89	0
54	PSU	1w	55	20/21	0.93	0.14	61,73,81,81	0
43	0TD	1l	92	10/11	0.93	0.15	41,49,50,61	0
55	5MU	2x	54	21/22	0.93	0.16	72,79,84,96	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	PSU	2a	516	20/21	0.93	0.16	61,71,78,79	0
54	PSU	1w	32	20/21	0.94	0.13	60,65,74,77	0
54	PSU	2w	39	20/21	0.94	0.19	62,78,85,85	0
54	MIA	1w	37	29/30	0.94	0.22	43,53,70,87	0
55	PSU	1x	55	20/21	0.94	0.15	49,56,67,70	0
32	M2G	2a	966	25/26	0.94	0.18	55,65,76,81	0
55	5MC	2x	32	21/22	0.95	0.18	63,69,78,80	0
55	4SU	1x	8	20/21	0.95	0.19	52,60,67,77	0
32	5MC	2a	1400	21/22	0.95	0.19	63,71,76,80	0
32	4OC	2a	1402	22/23	0.95	0.17	55,60,66,71	0
43	0TD	2l	92	10/11	0.95	0.17	61,65,67,78	0
1	5MU	1A	1915	21/22	0.95	0.21	42,51,55,55	0
1	5MU	2A	1915	21/22	0.95	0.18	57,64,73,75	0
32	M2G	1a	966	25/26	0.96	0.15	46,50,57,61	0
32	5MC	2a	1407	21/22	0.96	0.19	50,57,61,65	0
32	MA6	2a	1518	24/25	0.96	0.19	49,60,69,69	0
32	MA6	2a	1519	24/25	0.96	0.18	55,61,67,71	0
55	31H	2x	76	32/33	0.96	0.22	36,46,54,63	0
1	PSU	2A	1911	20/21	0.96	0.18	52,62,67,71	0
55	31H	1x	76	32/33	0.96	0.20	22,26,37,41	10
54	5MU	1w	54	21/22	0.96	0.16	46,62,67,69	0
1	PSU	2A	1917	20/21	0.96	0.18	54,61,69,72	0
1	5MC	2A	1962	21/22	0.96	0.22	39,51,58,67	0
32	5MC	1a	1400	21/22	0.97	0.17	39,47,49,50	0
32	5MC	1a	1404	21/22	0.97	0.18	33,39,42,45	0
32	G7M	1a	527	24/25	0.97	0.15	36,42,50,50	0
32	PSU	1a	516	20/21	0.97	0.16	51,55,58,59	0
32	5MC	2a	1404	21/22	0.97	0.16	53,57,62,66	0
55	5MC	1x	32	21/22	0.97	0.17	51,53,59,70	0
54	F3N	2w	76	33/34	0.97	0.23	38,43,48,51	0
1	PSU	1A	1911	20/21	0.97	0.20	42,46,49,50	0
32	UR3	2a	1498	21/22	0.97	0.21	52,58,61,65	0
55	5MU	1x	54	21/22	0.97	0.15	55,61,65,70	0
32	5MC	1a	967	21/22	0.97	0.14	45,51,59,61	0
1	PSU	1A	1917	20/21	0.97	0.17	39,45,50,52	0
32	2MG	1a	1207	24/25	0.97	0.14	61,67,71,71	0
1	OMC	2A	1920	21/22	0.97	0.18	53,61,63,65	0
1	5MC	2A	1942	21/22	0.97	0.20	43,53,57,62	0
54	PSU	1w	39	20/21	0.97	0.16	53,61,67,76	0
1	2MU	2A	2552	21/23	0.97	0.19	35,41,45,55	0
1	PSU	2A	2605	20/21	0.97	0.19	30,38,42,44	0
32	4OC	1a	1402	22/23	0.98	0.17	38,45,48,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	OMC	1A	1920	21/22	0.98	0.20	35,43,45,52	0
32	5MC	1a	1407	21/22	0.98	0.18	30,39,42,43	0
1	5MU	1A	1939	21/22	0.98	0.19	21,28,30,32	0
1	5MU	2A	1939	21/22	0.98	0.20	32,38,42,45	0
1	5MC	1A	1942	21/22	0.98	0.21	34,39,43,51	0
32	UR3	1a	1498	21/22	0.98	0.17	36,41,45,46	0
1	5MC	1A	1962	21/22	0.98	0.20	24,32,37,42	0
54	F3N	1w	76	33/34	0.98	0.22	22,25,30,32	0
1	OMG	2A	2251	24/25	0.98	0.20	35,43,45,51	0
1	8AH	2A	2503	24/25	0.98	0.22	32,38,44,45	0
1	2MU	1A	2552	21/23	0.98	0.21	23,27,34,36	0
32	MA6	1a	1518	24/25	0.98	0.21	31,39,45,46	0
1	PSU	1A	2605	20/21	0.98	0.20	23,26,31,32	0
32	MA6	1a	1519	24/25	0.98	0.20	35,42,45,47	0
1	8AH	1A	2503	24/25	0.99	0.19	15,21,26,27	0
1	OMG	1A	2251	24/25	0.99	0.18	22,25,28,30	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3735	1/1	0.34	0.10	79,79,79,79	0
57	MG	1a	1792	1/1	0.44	0.21	74,74,74,74	0
57	MG	2A	3516	1/1	0.45	0.20	40,40,40,40	0
57	MG	2a	1808	1/1	0.45	0.11	91,91,91,91	0
57	MG	1a	1796	1/1	0.46	0.27	67,67,67,67	0
57	MG	2A	3271	1/1	0.47	0.26	73,73,73,73	0
57	MG	1A	3395	1/1	0.47	0.28	69,69,69,69	0
57	MG	1a	1704	1/1	0.48	0.38	72,72,72,72	0
57	MG	1A	3979	1/1	0.49	0.16	70,70,70,70	0
57	MG	2A	3216	1/1	0.49	0.25	73,73,73,73	0
57	MG	2A	3001	1/1	0.50	0.33	59,59,59,59	0
57	MG	1a	1673	1/1	0.51	0.20	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	2A	3077	1/1	0.53	0.49	60,60,60,60	0
57	MG	2v	102	1/1	0.53	0.41	80,80,80,80	0
57	MG	1O	201	1/1	0.55	0.33	72,72,72,72	0
57	MG	2A	3143	1/1	0.55	0.26	72,72,72,72	0
57	MG	1A	4076	1/1	0.56	0.16	70,70,70,70	0
57	MG	2A	3282	1/1	0.56	0.16	76,76,76,76	0
57	MG	1A	3375	1/1	0.56	0.21	74,74,74,74	0
57	MG	2A	3547	1/1	0.58	0.30	72,72,72,72	0
57	MG	1A	3970	1/1	0.58	0.26	47,47,47,47	0
57	MG	2a	1650	1/1	0.58	0.16	66,66,66,66	0
57	MG	2A	3159	1/1	0.58	0.17	82,82,82,82	0
57	MG	1A	3491	1/1	0.58	0.35	64,64,64,64	0
57	MG	2a	1628	1/1	0.59	0.17	79,79,79,79	0
57	MG	2A	3235	1/1	0.60	0.32	68,68,68,68	0
57	MG	2a	1696	1/1	0.60	0.19	74,74,74,74	0
57	MG	2y	102	1/1	0.60	0.23	75,75,75,75	0
57	MG	1A	3431	1/1	0.61	0.18	66,66,66,66	0
57	MG	2A	3058	1/1	0.62	0.23	68,68,68,68	0
57	MG	1A	4042	1/1	0.62	0.17	70,70,70,70	0
57	MG	2a	1642	1/1	0.62	0.33	73,73,73,73	0
57	MG	2A	3711	1/1	0.62	0.23	47,47,47,47	0
57	MG	2A	3482	1/1	0.63	0.14	69,69,69,69	0
57	MG	1A	3732	1/1	0.64	0.25	70,70,70,70	0
57	MG	2a	1781	1/1	0.64	0.15	81,81,81,81	0
57	MG	1A	3373	1/1	0.64	0.27	69,69,69,69	0
57	MG	1x	108	1/1	0.64	0.27	67,67,67,67	0
57	MG	1a	1778	1/1	0.64	0.17	78,78,78,78	0
57	MG	1A	4029	1/1	0.65	0.27	27,27,27,27	0
57	MG	1A	3766	1/1	0.65	0.30	51,51,51,51	0
57	MG	2a	1768	1/1	0.65	0.17	69,69,69,69	0
57	MG	1A	3670	1/1	0.65	0.28	62,62,62,62	0
57	MG	2A	3065	1/1	0.65	0.25	64,64,64,64	0
57	MG	1A	3747	1/1	0.65	0.17	82,82,82,82	0
57	MG	1V	205	1/1	0.65	0.39	63,63,63,63	0
57	MG	2A	3019	1/1	0.66	0.12	79,79,79,79	0
57	MG	2A	3690	1/1	0.66	0.15	58,58,58,58	0
57	MG	2A	3347	1/1	0.66	0.19	70,70,70,70	0
57	MG	1A	3794	1/1	0.66	0.18	59,59,59,59	0
57	MG	2B	202	1/1	0.66	0.35	70,70,70,70	0
57	MG	2T	201	1/1	0.66	0.34	70,70,70,70	0
57	MG	2q	202	1/1	0.66	0.09	82,82,82,82	0
57	MG	2a	1619	1/1	0.66	0.26	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1A	3930	1/1	0.66	0.08	62,62,62,62	0
57	MG	2A	3775	1/1	0.67	0.36	73,73,73,73	0
57	MG	1A	3432	1/1	0.67	0.16	64,64,64,64	0
57	MG	2A	3573	1/1	0.67	0.28	68,68,68,68	0
57	MG	2A	3359	1/1	0.67	0.76	73,73,73,73	0
57	MG	1A	3888	1/1	0.67	0.08	70,70,70,70	0
57	MG	1A	3641	1/1	0.67	0.14	43,43,43,43	0
57	MG	2A	3762	1/1	0.67	0.23	53,53,53,53	0
57	MG	2A	3176	1/1	0.68	0.33	63,63,63,63	0
57	MG	2V	202	1/1	0.68	0.27	67,67,67,67	0
57	MG	2W	201	1/1	0.68	0.14	67,67,67,67	0
57	MG	1A	4078	1/1	0.68	0.28	62,62,62,62	0
57	MG	2A	3231	1/1	0.68	0.15	71,71,71,71	0
57	MG	1A	3804	1/1	0.68	0.24	69,69,69,69	0
57	MG	2A	3639	1/1	0.68	0.19	72,72,72,72	0
57	MG	1x	111	1/1	0.68	0.31	70,70,70,70	0
57	MG	2A	3119	1/1	0.68	0.15	69,69,69,69	0
57	MG	2A	3298	1/1	0.68	0.14	76,76,76,76	0
57	MG	1A	3235	1/1	0.68	0.21	71,71,71,71	0
57	MG	1a	1604	1/1	0.68	0.12	58,58,58,58	0
57	MG	2A	3415	1/1	0.68	0.20	71,71,71,71	0
57	MG	2B	204	1/1	0.68	0.11	75,75,75,75	0
57	MG	2A	3156	1/1	0.69	0.19	76,76,76,76	0
57	MG	1A	3876	1/1	0.69	0.14	61,61,61,61	0
57	MG	1a	1647	1/1	0.69	0.21	67,67,67,67	0
57	MG	2A	3606	1/1	0.69	0.14	66,66,66,66	0
57	MG	2A	3181	1/1	0.69	0.26	65,65,65,65	0
57	MG	2A	3675	1/1	0.69	0.40	69,69,69,69	0
57	MG	1U	210	1/1	0.69	0.43	55,55,55,55	0
57	MG	1A	3990	1/1	0.69	0.10	54,54,54,54	0
57	MG	2A	3155	1/1	0.69	0.33	67,67,67,67	0
57	MG	1a	1694	1/1	0.70	0.20	63,63,63,63	0
57	MG	2A	3173	1/1	0.70	0.29	70,70,70,70	0
57	MG	2A	3382	1/1	0.70	0.32	72,72,72,72	0
57	MG	2a	1710	1/1	0.70	0.15	79,79,79,79	0
57	MG	2a	1716	1/1	0.70	0.21	63,63,63,63	0
57	MG	2A	3400	1/1	0.70	0.23	73,73,73,73	0
57	MG	1A	3477	1/1	0.70	0.16	74,74,74,74	0
57	MG	2A	3450	1/1	0.70	0.22	49,49,49,49	0
57	MG	2A	3703	1/1	0.70	0.12	63,63,63,63	0
57	MG	1A	3793	1/1	0.70	0.17	57,57,57,57	0
57	MG	1A	4095	1/1	0.70	0.16	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	2A	3260	1/1	0.71	0.18	67,67,67,67	0
57	MG	1a	1615	1/1	0.71	0.14	56,56,56,56	0
57	MG	1A	3428	1/1	0.71	0.18	57,57,57,57	0
57	MG	1a	1666	1/1	0.71	0.21	72,72,72,72	0
57	MG	2A	3043	1/1	0.71	0.32	70,70,70,70	0
57	MG	2A	3784	1/1	0.71	0.21	70,70,70,70	0
57	MG	2A	3584	1/1	0.71	0.17	69,69,69,69	0
57	MG	1A	3898	1/1	0.71	0.16	35,35,35,35	0
57	MG	2B	214	1/1	0.71	0.24	66,66,66,66	0
57	MG	2P	202	1/1	0.71	0.31	66,66,66,66	0
57	MG	1A	3885	1/1	0.71	0.14	43,43,43,43	0
57	MG	2A	3236	1/1	0.71	0.27	63,63,63,63	0
57	MG	2A	3257	1/1	0.71	0.24	68,68,68,68	0
57	MG	1A	3308	1/1	0.72	0.13	50,50,50,50	0
57	MG	2a	1633	1/1	0.72	0.13	73,73,73,73	0
57	MG	1A	3561	1/1	0.72	0.22	39,39,39,39	0
57	MG	2A	3548	1/1	0.72	0.47	65,65,65,65	0
57	MG	2A	3100	1/1	0.72	0.14	70,70,70,70	0
57	MG	1A	4023	1/1	0.72	0.20	50,50,50,50	0
57	MG	1A	3796	1/1	0.72	0.18	49,49,49,49	0
57	MG	2A	3614	1/1	0.72	0.22	63,63,63,63	0
57	MG	1A	3620	1/1	0.72	0.13	65,65,65,65	0
57	MG	14	101	1/1	0.72	0.13	80,80,80,80	0
57	MG	1a	1755	1/1	0.72	0.13	64,64,64,64	0
57	MG	1A	3427	1/1	0.72	0.52	55,55,55,55	0
57	MG	2A	3509	1/1	0.72	0.13	68,68,68,68	0
57	MG	2A	3086	1/1	0.73	0.26	44,44,44,44	0
57	MG	2A	3395	1/1	0.73	0.48	58,58,58,58	0
57	MG	2A	3580	1/1	0.73	0.21	55,55,55,55	0
57	MG	2A	3399	1/1	0.73	0.20	83,83,83,83	0
57	MG	1A	3795	1/1	0.73	0.28	60,60,60,60	0
57	MG	1A	3909	1/1	0.73	0.50	85,85,85,85	0
57	MG	1A	3126	1/1	0.73	0.30	48,48,48,48	0
57	MG	10	109	1/1	0.73	0.22	69,69,69,69	0
57	MG	2a	1779	1/1	0.73	0.16	71,71,71,71	0
57	MG	1A	3158	1/1	0.73	0.18	62,62,62,62	0
57	MG	1F	315	1/1	0.73	0.49	58,58,58,58	0
57	MG	2A	3360	1/1	0.73	0.26	67,67,67,67	0
57	MG	2a	1604	1/1	0.73	0.10	73,73,73,73	0
57	MG	2A	3717	1/1	0.73	0.12	64,64,64,64	0
57	MG	1A	3371	1/1	0.74	0.19	54,54,54,54	0
57	MG	2A	3091	1/1	0.74	0.22	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3806	1/1	0.74	0.17	58,58,58,58	0
57	MG	1A	3829	1/1	0.74	0.10	37,37,37,37	0
57	MG	1A	3258	1/1	0.74	0.21	55,55,55,55	0
57	MG	1a	1802	1/1	0.74	0.12	84,84,84,84	0
57	MG	1A	3445	1/1	0.74	0.15	58,58,58,58	0
57	MG	1A	3476	1/1	0.74	0.21	49,49,49,49	0
57	MG	1A	3139	1/1	0.74	0.22	47,47,47,47	0
57	MG	2a	1745	1/1	0.74	0.09	75,75,75,75	0
57	MG	2B	208	1/1	0.74	0.19	56,56,56,56	0
57	MG	1A	3904	1/1	0.74	0.08	74,74,74,74	0
57	MG	1A	3689	1/1	0.74	0.12	56,56,56,56	0
57	MG	1B	227	1/1	0.74	0.15	81,81,81,81	0
57	MG	2T	202	1/1	0.74	0.17	64,64,64,64	0
57	MG	1E	307	1/1	0.74	0.13	67,67,67,67	0
57	MG	1A	3724	1/1	0.74	0.19	45,45,45,45	0
60	ZN	24	501	1/1	0.74	0.10	126,126,126,126	0
57	MG	2A	3035	1/1	0.75	0.24	69,69,69,69	0
57	MG	1A	3327	1/1	0.75	0.49	59,59,59,59	0
57	MG	2a	1691	1/1	0.75	0.29	76,76,76,76	0
57	MG	2A	3247	1/1	0.75	0.25	65,65,65,65	0
57	MG	2A	3248	1/1	0.75	0.25	57,57,57,57	0
57	MG	1a	1654	1/1	0.75	0.10	61,61,61,61	0
57	MG	1B	214	1/1	0.75	0.15	59,59,59,59	0
57	MG	1A	3297	1/1	0.75	0.24	58,58,58,58	0
57	MG	1A	3583	1/1	0.75	0.17	58,58,58,58	0
57	MG	1A	3309	1/1	0.75	0.13	58,58,58,58	0
57	MG	2a	1795	1/1	0.75	0.48	72,72,72,72	0
57	MG	2a	1798	1/1	0.75	0.35	73,73,73,73	0
57	MG	2A	3343	1/1	0.75	0.15	64,64,64,64	0
57	MG	2a	1812	1/1	0.75	0.12	65,65,65,65	0
57	MG	2A	3203	1/1	0.75	0.42	54,54,54,54	0
57	MG	1A	4011	1/1	0.75	0.15	51,51,51,51	0
57	MG	2x	105	1/1	0.75	0.21	65,65,65,65	0
57	MG	1a	1777	1/1	0.75	0.09	85,85,85,85	0
57	MG	2a	1637	1/1	0.75	0.14	64,64,64,64	0
57	MG	1b	301	1/1	0.76	0.09	68,68,68,68	0
57	MG	1A	3454	1/1	0.76	0.23	36,36,36,36	0
57	MG	1D	311	1/1	0.76	0.25	55,55,55,55	0
57	MG	2a	1674	1/1	0.76	0.26	59,59,59,59	0
57	MG	2A	3151	1/1	0.76	0.27	45,45,45,45	0
57	MG	1a	1747	1/1	0.76	0.15	59,59,59,59	0
57	MG	1A	3467	1/1	0.76	0.49	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	2A	3518	1/1	0.76	0.15	51,51,51,51	0
57	MG	2a	1722	1/1	0.76	0.08	62,62,62,62	0
57	MG	1a	1764	1/1	0.76	0.18	48,48,48,48	0
57	MG	1A	3374	1/1	0.76	0.34	61,61,61,61	0
57	MG	1A	3277	1/1	0.76	0.15	64,64,64,64	0
57	MG	2A	3177	1/1	0.76	0.75	80,80,80,80	0
57	MG	2A	3344	1/1	0.76	0.20	63,63,63,63	0
57	MG	1T	201	1/1	0.76	0.21	65,65,65,65	0
57	MG	2A	3193	1/1	0.76	0.18	55,55,55,55	0
57	MG	1B	213	1/1	0.76	0.23	73,73,73,73	0
57	MG	2A	3645	1/1	0.76	0.30	48,48,48,48	0
57	MG	2a	1610	1/1	0.76	0.36	78,78,78,78	0
57	MG	2A	3215	1/1	0.76	0.25	77,77,77,77	0
57	MG	1A	3388	1/1	0.76	0.44	70,70,70,70	0
57	MG	1a	1809	1/1	0.76	0.17	69,69,69,69	0
57	MG	2A	3167	1/1	0.77	0.27	57,57,57,57	0
57	MG	1A	3621	1/1	0.77	0.16	38,38,38,38	0
57	MG	1A	3694	1/1	0.77	0.14	57,57,57,57	0
57	MG	2A	3783	1/1	0.77	0.30	75,75,75,75	0
57	MG	2A	3562	1/1	0.77	0.16	68,68,68,68	0
57	MG	1A	3607	1/1	0.77	0.16	68,68,68,68	0
57	MG	2A	3576	1/1	0.77	0.28	42,42,42,42	0
57	MG	2A	3251	1/1	0.77	0.25	62,62,62,62	0
57	MG	1a	1662	1/1	0.77	0.27	71,71,71,71	0
57	MG	2D	303	1/1	0.77	0.27	61,61,61,61	0
57	MG	2D	306	1/1	0.77	0.77	54,54,54,54	0
57	MG	2A	3047	1/1	0.77	0.27	69,69,69,69	0
57	MG	1A	4049	1/1	0.77	0.18	44,44,44,44	0
57	MG	2A	3636	1/1	0.77	0.24	67,67,67,67	0
57	MG	2A	3412	1/1	0.77	0.14	57,57,57,57	0
57	MG	1a	1667	1/1	0.77	0.14	50,50,50,50	0
57	MG	20	102	1/1	0.77	0.28	73,73,73,73	0
57	MG	2a	1819	1/1	0.77	0.09	69,69,69,69	0
57	MG	2A	3290	1/1	0.77	0.16	64,64,64,64	0
57	MG	2A	3074	1/1	0.77	0.17	63,63,63,63	0
57	MG	2A	3483	1/1	0.77	0.16	84,84,84,84	0
57	MG	2A	3299	1/1	0.77	0.21	75,75,75,75	0
57	MG	1A	3378	1/1	0.77	0.30	62,62,62,62	0
57	MG	1T	202	1/1	0.78	0.31	54,54,54,54	0
57	MG	2A	3346	1/1	0.78	0.36	68,68,68,68	0
57	MG	2A	3092	1/1	0.78	0.29	65,65,65,65	0
57	MG	2a	1652	1/1	0.78	0.10	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3792	1/1	0.78	0.06	77,77,77,77	0
57	MG	2A	3793	1/1	0.78	0.07	64,64,64,64	0
57	MG	1A	3256	1/1	0.78	0.14	56,56,56,56	0
57	MG	2a	1707	1/1	0.78	0.10	76,76,76,76	0
57	MG	1A	3988	1/1	0.78	0.17	51,51,51,51	0
57	MG	1A	4045	1/1	0.78	0.10	44,44,44,44	0
57	MG	2A	3238	1/1	0.78	0.29	60,60,60,60	0
57	MG	2a	1726	1/1	0.78	0.13	66,66,66,66	0
57	MG	1A	3333	1/1	0.78	0.16	60,60,60,60	0
57	MG	18	107	1/1	0.78	0.43	70,70,70,70	0
57	MG	1A	4066	1/1	0.78	0.14	52,52,52,52	0
57	MG	1A	3677	1/1	0.78	0.18	42,42,42,42	0
57	MG	2A	3662	1/1	0.78	0.42	60,60,60,60	0
57	MG	1a	1768	1/1	0.78	0.15	53,53,53,53	0
57	MG	2A	3686	1/1	0.78	0.08	55,55,55,55	0
57	MG	1a	1772	1/1	0.78	0.09	77,77,77,77	0
57	MG	1I	201	1/1	0.78	0.14	65,65,65,65	0
57	MG	2f	202	1/1	0.78	0.23	76,76,76,76	0
57	MG	1A	3025	1/1	0.78	0.18	55,55,55,55	0
57	MG	1a	1779	1/1	0.78	0.09	75,75,75,75	0
57	MG	2a	1620	1/1	0.78	0.22	76,76,76,76	0
57	MG	1A	4028	1/1	0.78	0.13	62,62,62,62	0
57	MG	1a	1663	1/1	0.78	0.20	68,68,68,68	0
57	MG	1a	1743	1/1	0.79	0.08	81,81,81,81	0
57	MG	1A	4075	1/1	0.79	0.15	62,62,62,62	0
57	MG	2a	1632	1/1	0.79	0.37	74,74,74,74	0
57	MG	1A	3276	1/1	0.79	0.22	45,45,45,45	0
57	MG	1A	3975	1/1	0.79	0.20	61,61,61,61	0
57	MG	2a	1638	1/1	0.79	0.14	82,82,82,82	0
57	MG	2A	3078	1/1	0.79	0.14	58,58,58,58	0
57	MG	2A	3430	1/1	0.79	0.13	39,39,39,39	0
57	MG	2A	3754	1/1	0.79	0.17	77,77,77,77	0
57	MG	1A	3840	1/1	0.79	0.20	48,48,48,48	0
57	MG	2a	1686	1/1	0.79	0.19	72,72,72,72	0
57	MG	2A	3478	1/1	0.79	0.25	50,50,50,50	0
57	MG	1A	3849	1/1	0.79	0.12	35,35,35,35	0
57	MG	1a	1612	1/1	0.79	0.10	66,66,66,66	0
57	MG	1A	3643	1/1	0.79	0.23	72,72,72,72	0
57	MG	2A	3253	1/1	0.79	0.25	72,72,72,72	0
57	MG	1a	1639	1/1	0.79	0.31	67,67,67,67	0
57	MG	2A	3132	1/1	0.79	0.17	64,64,64,64	0
57	MG	2A	3262	1/1	0.79	0.15	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	2a	1749	1/1	0.79	0.06	78,78,78,78	0
57	MG	2a	1767	1/1	0.79	0.36	69,69,69,69	0
57	MG	2B	209	1/1	0.79	0.19	69,69,69,69	0
57	MG	2a	1777	1/1	0.79	0.12	75,75,75,75	0
57	MG	1A	3526	1/1	0.79	0.31	56,56,56,56	0
57	MG	1A	3243	1/1	0.79	0.36	41,41,41,41	0
57	MG	1A	3246	1/1	0.79	0.29	28,28,28,28	0
57	MG	1A	3305	1/1	0.79	0.18	63,63,63,63	0
57	MG	1A	3908	1/1	0.79	0.08	53,53,53,53	0
57	MG	1A	3222	1/1	0.79	0.25	63,63,63,63	0
57	MG	1A	3239	1/1	0.79	0.20	64,64,64,64	0
57	MG	1A	4063	1/1	0.79	0.19	71,71,71,71	0
57	MG	1a	1697	1/1	0.79	0.15	49,49,49,49	0
57	MG	1A	3943	1/1	0.79	0.23	33,33,33,33	0
57	MG	2w	106	1/1	0.79	0.15	75,75,75,75	0
57	MG	2a	1606	1/1	0.79	0.11	74,74,74,74	0
57	MG	1a	1711	1/1	0.79	0.21	55,55,55,55	0
57	MG	1a	1727	1/1	0.79	0.14	64,64,64,64	0
57	MG	1Y	201	1/1	0.80	0.16	69,69,69,69	0
57	MG	1A	3204	1/1	0.80	0.14	53,53,53,53	0
57	MG	2A	3264	1/1	0.80	0.31	69,69,69,69	0
57	MG	1A	3933	1/1	0.80	0.12	66,66,66,66	0
57	MG	2A	3057	1/1	0.80	0.14	65,65,65,65	0
57	MG	2a	1693	1/1	0.80	0.24	65,65,65,65	0
57	MG	1A	3821	1/1	0.80	0.17	56,56,56,56	0
57	MG	1A	3962	1/1	0.80	0.22	58,58,58,58	0
57	MG	1a	1681	1/1	0.80	0.20	57,57,57,57	0
57	MG	2A	3185	1/1	0.80	0.18	63,63,63,63	0
57	MG	1a	1688	1/1	0.80	0.23	51,51,51,51	0
57	MG	2A	3199	1/1	0.80	0.41	55,55,55,55	0
57	MG	2A	3590	1/1	0.80	0.23	50,50,50,50	0
57	MG	1a	1785	1/1	0.80	0.21	59,59,59,59	0
57	MG	1A	3485	1/1	0.80	0.17	65,65,65,65	0
57	MG	1A	3434	1/1	0.80	0.40	60,60,60,60	0
57	MG	2A	3369	1/1	0.80	0.20	70,70,70,70	0
57	MG	1a	1622	1/1	0.80	0.19	65,65,65,65	0
57	MG	1a	1626	1/1	0.80	0.23	59,59,59,59	0
57	MG	2a	1784	1/1	0.80	0.15	65,65,65,65	0
57	MG	2A	3671	1/1	0.80	0.16	73,73,73,73	0
57	MG	2A	3105	1/1	0.80	0.35	55,55,55,55	0
57	MG	2A	3106	1/1	0.80	0.26	59,59,59,59	0
57	MG	2a	1611	1/1	0.80	0.13	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	2a	1816	1/1	0.80	0.14	81,81,81,81	0
57	MG	2A	3244	1/1	0.80	0.23	63,63,63,63	0
57	MG	1a	1720	1/1	0.80	0.23	44,44,44,44	0
57	MG	1A	4044	1/1	0.80	0.21	59,59,59,59	0
57	MG	1A	3514	1/1	0.80	0.45	48,48,48,48	0
57	MG	2A	3731	1/1	0.80	0.11	59,59,59,59	0
57	MG	2x	102	1/1	0.80	0.34	82,82,82,82	0
57	MG	2A	3470	1/1	0.80	0.15	39,39,39,39	0
57	MG	2x	107	1/1	0.80	0.17	64,64,64,64	0
57	MG	1A	3016	1/1	0.80	0.53	66,66,66,66	0
57	MG	1a	1752	1/1	0.80	0.11	63,63,63,63	0
57	MG	2A	3753	1/1	0.81	0.16	66,66,66,66	0
57	MG	1A	3739	1/1	0.81	0.15	27,27,27,27	0
57	MG	1A	3627	1/1	0.81	0.11	43,43,43,43	0
57	MG	2A	3774	1/1	0.81	0.40	68,68,68,68	0
57	MG	1A	3866	1/1	0.81	0.18	44,44,44,44	0
57	MG	1A	3413	1/1	0.81	0.38	67,67,67,67	0
57	MG	2A	3498	1/1	0.81	0.11	79,79,79,79	0
57	MG	2A	3785	1/1	0.81	0.19	57,57,57,57	0
57	MG	1A	3536	1/1	0.81	0.20	63,63,63,63	0
57	MG	1A	3314	1/1	0.81	0.28	54,54,54,54	0
57	MG	1A	3337	1/1	0.81	0.41	36,36,36,36	0
57	MG	2A	3071	1/1	0.81	0.28	60,60,60,60	0
57	MG	1A	3680	1/1	0.81	0.22	56,56,56,56	0
57	MG	2A	3183	1/1	0.81	0.21	56,56,56,56	0
57	MG	2a	1761	1/1	0.81	0.12	73,73,73,73	0
57	MG	1B	208	1/1	0.81	0.11	65,65,65,65	0
57	MG	2A	3309	1/1	0.81	0.16	66,66,66,66	0
57	MG	2A	3339	1/1	0.81	0.26	58,58,58,58	0
57	MG	2A	3186	1/1	0.81	0.21	57,57,57,57	0
57	MG	2A	3190	1/1	0.81	0.37	60,60,60,60	0
57	MG	11	103	1/1	0.81	0.11	42,42,42,42	0
57	MG	1B	210	1/1	0.81	0.25	51,51,51,51	0
57	MG	2A	3354	1/1	0.81	0.33	65,65,65,65	0
57	MG	1A	3600	1/1	0.81	0.10	66,66,66,66	0
57	MG	2a	1811	1/1	0.81	0.08	70,70,70,70	0
57	MG	1A	3282	1/1	0.81	0.15	46,46,46,46	0
57	MG	1A	3915	1/1	0.81	0.23	62,62,62,62	0
57	MG	1B	229	1/1	0.81	0.11	75,75,75,75	0
57	MG	2A	3392	1/1	0.81	0.09	47,47,47,47	0
57	MG	2A	3232	1/1	0.81	0.22	66,66,66,66	0
57	MG	1x	106	1/1	0.81	0.23	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	3699	1/1	0.81	0.16	59,59,59,59	0
57	MG	1A	3456	1/1	0.81	0.14	58,58,58,58	0
57	MG	2A	3121	1/1	0.81	0.39	42,42,42,42	0
57	MG	1A	3459	1/1	0.81	0.15	52,52,52,52	0
57	MG	2A	3137	1/1	0.81	0.15	58,58,58,58	0
57	MG	1a	1745	1/1	0.81	0.17	74,74,74,74	0
57	MG	1A	4064	1/1	0.82	0.19	64,64,64,64	0
57	MG	1A	3446	1/1	0.82	0.19	65,65,65,65	0
57	MG	1A	3414	1/1	0.82	0.14	51,51,51,51	0
57	MG	2A	3039	1/1	0.82	0.13	56,56,56,56	0
57	MG	2a	1643	1/1	0.82	0.18	73,73,73,73	0
57	MG	1A	3704	1/1	0.82	0.17	61,61,61,61	0
57	MG	1a	1762	1/1	0.82	0.12	64,64,64,64	0
57	MG	1A	3903	1/1	0.82	0.14	61,61,61,61	0
57	MG	1A	3287	1/1	0.82	0.19	30,30,30,30	0
57	MG	1B	206	1/1	0.82	0.14	47,47,47,47	0
57	MG	2A	3472	1/1	0.82	0.21	47,47,47,47	0
57	MG	2a	1695	1/1	0.82	0.26	67,67,67,67	0
57	MG	2A	3769	1/1	0.82	0.09	71,71,71,71	0
57	MG	2a	1700	1/1	0.82	0.12	82,82,82,82	0
57	MG	1A	4012	1/1	0.82	0.14	67,67,67,67	0
57	MG	2a	1708	1/1	0.82	0.15	62,62,62,62	0
57	MG	1A	3808	1/1	0.82	0.20	22,22,22,22	0
57	MG	2A	3266	1/1	0.82	0.18	69,69,69,69	0
57	MG	2a	1717	1/1	0.82	0.12	75,75,75,75	0
57	MG	2a	1720	1/1	0.82	0.17	68,68,68,68	0
57	MG	2A	3487	1/1	0.82	0.21	63,63,63,63	0
57	MG	1a	1682	1/1	0.82	0.35	62,62,62,62	0
57	MG	2A	3788	1/1	0.82	0.23	64,64,64,64	0
57	MG	2a	1748	1/1	0.82	0.17	78,78,78,78	0
57	MG	1a	1687	1/1	0.82	0.29	55,55,55,55	0
57	MG	2A	3283	1/1	0.82	0.15	83,83,83,83	0
57	MG	2A	3797	1/1	0.82	0.15	69,69,69,69	0
57	MG	2A	3517	1/1	0.82	0.20	51,51,51,51	0
57	MG	2a	1773	1/1	0.82	0.09	68,68,68,68	0
57	MG	2A	3289	1/1	0.82	0.18	62,62,62,62	0
57	MG	1A	3381	1/1	0.82	0.17	57,57,57,57	0
57	MG	2A	3294	1/1	0.82	0.23	69,69,69,69	0
57	MG	1A	3196	1/1	0.82	0.18	53,53,53,53	0
57	MG	2a	1793	1/1	0.82	0.27	64,64,64,64	0
57	MG	1A	3663	1/1	0.82	0.18	28,28,28,28	0
57	MG	2A	3196	1/1	0.82	0.24	74,74,74,74	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	3330	1/1	0.82	0.27	56,56,56,56	0
57	MG	1a	1806	1/1	0.82	0.12	60,60,60,60	0
57	MG	1A	3841	1/1	0.82	0.24	24,24,24,24	0
57	MG	2A	3605	1/1	0.82	0.27	67,67,67,67	0
57	MG	2A	3211	1/1	0.82	0.25	49,49,49,49	0
57	MG	2A	3214	1/1	0.82	0.09	77,77,77,77	0
57	MG	2A	3634	1/1	0.82	0.12	45,45,45,45	0
57	MG	1A	3394	1/1	0.82	0.18	69,69,69,69	0
57	MG	2A	3353	1/1	0.82	0.36	81,81,81,81	0
57	MG	1A	3335	1/1	0.82	0.23	56,56,56,56	0
57	MG	2x	104	1/1	0.82	0.60	72,72,72,72	0
57	MG	2A	3223	1/1	0.82	0.27	63,63,63,63	0
57	MG	1a	1623	1/1	0.82	0.22	58,58,58,58	0
57	MG	1A	3315	1/1	0.82	0.18	61,61,61,61	0
57	MG	2A	3134	1/1	0.82	0.27	63,63,63,63	0
57	MG	2A	3055	1/1	0.83	0.23	57,57,57,57	0
57	MG	1A	3924	1/1	0.83	0.58	55,55,55,55	0
57	MG	1F	311	1/1	0.83	0.23	46,46,46,46	0
57	MG	1A	3827	1/1	0.83	0.17	37,37,37,37	0
57	MG	1G	203	1/1	0.83	0.11	68,68,68,68	0
57	MG	1A	3271	1/1	0.83	0.65	40,40,40,40	0
57	MG	1A	3648	1/1	0.83	0.17	20,20,20,20	0
57	MG	2A	3195	1/1	0.83	0.21	56,56,56,56	0
57	MG	1A	3205	1/1	0.83	0.11	48,48,48,48	0
57	MG	1a	1672	1/1	0.83	0.20	70,70,70,70	0
57	MG	1A	3783	1/1	0.83	0.14	49,49,49,49	0
57	MG	2A	3321	1/1	0.83	0.16	64,64,64,64	0
57	MG	2A	3568	1/1	0.83	0.28	60,60,60,60	0
57	MG	1A	3859	1/1	0.83	0.22	50,50,50,50	0
57	MG	2A	3574	1/1	0.83	0.26	71,71,71,71	0
57	MG	2A	3095	1/1	0.83	0.22	75,75,75,75	0
57	MG	1A	3785	1/1	0.83	0.20	55,55,55,55	0
57	MG	2B	213	1/1	0.83	0.17	65,65,65,65	0
57	MG	1A	3786	1/1	0.83	0.23	47,47,47,47	0
57	MG	2A	3217	1/1	0.83	0.14	70,70,70,70	0
57	MG	2a	1766	1/1	0.83	0.22	61,61,61,61	0
57	MG	2A	3593	1/1	0.83	0.35	63,63,63,63	0
57	MG	2F	308	1/1	0.83	0.29	69,69,69,69	0
57	MG	2a	1770	1/1	0.83	0.28	70,70,70,70	0
57	MG	1Z	301	1/1	0.83	0.14	67,67,67,67	0
57	MG	2A	3224	1/1	0.83	0.17	65,65,65,65	0
57	MG	2A	3610	1/1	0.83	0.15	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3225	1/1	0.83	0.21	75,75,75,75	0
57	MG	2A	3230	1/1	0.83	0.15	81,81,81,81	0
57	MG	2a	1788	1/1	0.83	0.16	83,83,83,83	0
57	MG	1B	203	1/1	0.83	0.36	66,66,66,66	0
57	MG	2I	101	1/1	0.83	0.16	54,54,54,54	0
57	MG	1A	3185	1/1	0.83	0.14	57,57,57,57	0
57	MG	1w	104	1/1	0.83	0.37	81,81,81,81	0
57	MG	1A	3247	1/1	0.83	0.26	42,42,42,42	0
57	MG	1A	3096	1/1	0.83	0.12	65,65,65,65	0
57	MG	2A	3673	1/1	0.83	0.11	49,49,49,49	0
57	MG	1a	1717	1/1	0.83	0.14	67,67,67,67	0
57	MG	1B	211	1/1	0.83	0.27	64,64,64,64	0
57	MG	2I	201	1/1	0.83	0.20	78,78,78,78	0
57	MG	1A	3061	1/1	0.83	0.19	59,59,59,59	0
57	MG	2A	3025	1/1	0.83	0.14	63,63,63,63	0
57	MG	2a	1636	1/1	0.83	0.17	69,69,69,69	0
57	MG	1A	3259	1/1	0.83	0.16	40,40,40,40	0
57	MG	1A	3306	1/1	0.83	0.22	58,58,58,58	0
57	MG	2A	3461	1/1	0.83	0.13	57,57,57,57	0
57	MG	1A	3507	1/1	0.83	0.86	53,53,53,53	0
57	MG	2a	1646	1/1	0.83	0.48	61,61,61,61	0
57	MG	1A	3367	1/1	0.83	0.13	47,47,47,47	0
57	MG	2A	3102	1/1	0.84	0.09	66,66,66,66	0
57	MG	1A	4054	1/1	0.84	0.22	64,64,64,64	0
57	MG	1a	1800	1/1	0.84	0.13	76,76,76,76	0
57	MG	1O	204	1/1	0.84	0.20	71,71,71,71	0
57	MG	1Q	204	1/1	0.84	0.15	54,54,54,54	0
57	MG	2a	1626	1/1	0.84	0.27	77,77,77,77	0
57	MG	1A	3823	1/1	0.84	0.19	29,29,29,29	0
57	MG	1a	1812	1/1	0.84	0.18	67,67,67,67	0
57	MG	2A	3582	1/1	0.84	0.13	70,70,70,70	0
57	MG	1a	1813	1/1	0.84	0.10	47,47,47,47	0
57	MG	1A	3481	1/1	0.84	0.33	56,56,56,56	0
57	MG	2A	3144	1/1	0.84	0.53	44,44,44,44	0
57	MG	1A	3401	1/1	0.84	0.30	56,56,56,56	0
57	MG	1x	101	1/1	0.84	0.20	60,60,60,60	0
57	MG	1A	3406	1/1	0.84	0.33	41,41,41,41	0
57	MG	1A	3953	1/1	0.84	0.22	60,60,60,60	0
57	MG	2A	3160	1/1	0.84	0.28	63,63,63,63	0
57	MG	2A	3161	1/1	0.84	0.16	57,57,57,57	0
57	MG	2A	3313	1/1	0.84	0.27	63,63,63,63	0
57	MG	2A	3314	1/1	0.84	0.26	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1A	3632	1/1	0.84	0.17	29,29,29,29	0
57	MG	2A	3664	1/1	0.84	0.28	71,71,71,71	0
57	MG	10	102	1/1	0.84	0.14	66,66,66,66	0
57	MG	2A	3335	1/1	0.84	0.36	62,62,62,62	0
57	MG	2A	3011	1/1	0.84	0.16	46,46,46,46	0
57	MG	1a	1710	1/1	0.84	0.09	57,57,57,57	0
57	MG	2A	3023	1/1	0.84	0.29	71,71,71,71	0
57	MG	2a	1714	1/1	0.84	0.13	74,74,74,74	0
57	MG	2A	3695	1/1	0.84	0.13	70,70,70,70	0
57	MG	1A	3844	1/1	0.84	0.20	30,30,30,30	0
57	MG	2A	3026	1/1	0.84	0.22	43,43,43,43	0
57	MG	2A	3348	1/1	0.84	0.33	58,58,58,58	0
57	MG	2A	3350	1/1	0.84	0.34	59,59,59,59	0
57	MG	2A	3029	1/1	0.84	0.28	48,48,48,48	0
57	MG	2A	3187	1/1	0.84	0.14	63,63,63,63	0
57	MG	1A	3637	1/1	0.84	0.07	45,45,45,45	0
57	MG	1A	3039	1/1	0.84	0.25	63,63,63,63	0
57	MG	2A	3367	1/1	0.84	0.20	74,74,74,74	0
57	MG	1A	3513	1/1	0.84	0.28	50,50,50,50	0
57	MG	1A	3452	1/1	0.84	0.24	65,65,65,65	0
57	MG	2A	3050	1/1	0.84	0.17	65,65,65,65	0
57	MG	1A	3993	1/1	0.84	0.21	50,50,50,50	0
57	MG	1A	3340	1/1	0.84	0.24	49,49,49,49	0
57	MG	1A	3423	1/1	0.84	0.28	65,65,65,65	0
57	MG	2A	3410	1/1	0.84	0.15	76,76,76,76	0
57	MG	1A	4020	1/1	0.84	0.17	47,47,47,47	0
57	MG	2A	3069	1/1	0.84	0.23	52,52,52,52	0
57	MG	1A	3892	1/1	0.84	0.13	62,62,62,62	0
57	MG	2A	3072	1/1	0.84	0.12	57,57,57,57	0
57	MG	1a	1627	1/1	0.84	0.09	63,63,63,63	0
57	MG	2A	3466	1/1	0.84	0.23	40,40,40,40	0
57	MG	1A	3558	1/1	0.84	0.16	55,55,55,55	0
57	MG	1A	3320	1/1	0.84	0.33	56,56,56,56	0
57	MG	2A	3080	1/1	0.84	0.34	66,66,66,66	0
57	MG	2A	3085	1/1	0.84	0.25	47,47,47,47	0
57	MG	2A	3233	1/1	0.84	0.12	69,69,69,69	0
57	MG	2F	302	1/1	0.84	0.21	74,74,74,74	0
57	MG	1a	1648	1/1	0.84	0.26	66,66,66,66	0
57	MG	1A	3201	1/1	0.84	0.24	49,49,49,49	0
57	MG	2A	3501	1/1	0.84	0.26	63,63,63,63	0
57	MG	1A	3060	1/1	0.84	0.20	39,39,39,39	0
57	MG	2A	3514	1/1	0.84	0.09	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	3241	1/1	0.84	0.26	63,63,63,63	0
57	MG	1A	3193	1/1	0.84	0.21	47,47,47,47	0
57	MG	2x	108	1/1	0.84	0.19	56,56,56,56	0
57	MG	2A	3099	1/1	0.84	0.19	77,77,77,77	0
60	ZN	14	102	1/1	0.84	0.05	100,100,100,100	0
57	MG	1A	3709	1/1	0.84	0.16	44,44,44,44	0
57	MG	28	102	1/1	0.85	0.18	69,69,69,69	0
57	MG	1A	3138	1/1	0.85	0.14	57,57,57,57	0
57	MG	2A	3296	1/1	0.85	0.20	75,75,75,75	0
57	MG	2A	3579	1/1	0.85	0.15	58,58,58,58	0
57	MG	1A	3716	1/1	0.85	0.15	44,44,44,44	0
57	MG	1A	4060	1/1	0.85	0.17	53,53,53,53	0
57	MG	1A	3936	1/1	0.85	0.13	68,68,68,68	0
57	MG	2A	3589	1/1	0.85	0.15	54,54,54,54	0
57	MG	1A	3940	1/1	0.85	0.14	51,51,51,51	0
57	MG	1A	3349	1/1	0.85	0.18	40,40,40,40	0
57	MG	1A	4067	1/1	0.85	0.20	59,59,59,59	0
57	MG	1A	3944	1/1	0.85	0.18	27,27,27,27	0
57	MG	2A	3609	1/1	0.85	0.28	40,40,40,40	0
57	MG	1A	3946	1/1	0.85	0.17	28,28,28,28	0
57	MG	2A	3198	1/1	0.85	0.26	69,69,69,69	0
57	MG	2A	3619	1/1	0.85	0.18	40,40,40,40	0
57	MG	2A	3341	1/1	0.85	0.47	71,71,71,71	0
57	MG	1A	3952	1/1	0.85	0.12	48,48,48,48	0
57	MG	2A	3202	1/1	0.85	0.28	50,50,50,50	0
57	MG	2a	1661	1/1	0.85	0.33	59,59,59,59	0
57	MG	1A	3626	1/1	0.85	0.13	32,32,32,32	0
57	MG	2A	3648	1/1	0.85	0.17	46,46,46,46	0
57	MG	2A	3205	1/1	0.85	0.62	47,47,47,47	0
57	MG	2A	3206	1/1	0.85	0.30	45,45,45,45	0
57	MG	1A	3960	1/1	0.85	0.10	65,65,65,65	0
57	MG	1A	3262	1/1	0.85	0.15	51,51,51,51	0
57	MG	1A	3226	1/1	0.85	0.33	31,31,31,31	0
57	MG	2a	1704	1/1	0.85	0.18	69,69,69,69	0
57	MG	1A	3528	1/1	0.85	0.17	57,57,57,57	0
57	MG	1A	3034	1/1	0.85	0.14	46,46,46,46	0
57	MG	2A	3362	1/1	0.85	0.21	50,50,50,50	0
57	MG	2a	1712	1/1	0.85	0.23	51,51,51,51	0
57	MG	2A	3366	1/1	0.85	0.30	46,46,46,46	0
57	MG	1A	3981	1/1	0.85	0.11	69,69,69,69	0
57	MG	1A	3546	1/1	0.85	0.18	44,44,44,44	0
57	MG	1A	3647	1/1	0.85	0.23	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	2A	3227	1/1	0.85	0.23	71,71,71,71	0
57	MG	2A	3229	1/1	0.85	0.22	72,72,72,72	0
57	MG	2a	1728	1/1	0.85	0.17	64,64,64,64	0
57	MG	2A	3749	1/1	0.85	0.09	58,58,58,58	0
57	MG	1A	3992	1/1	0.85	0.15	53,53,53,53	0
57	MG	1A	3556	1/1	0.85	0.24	72,72,72,72	0
57	MG	2a	1754	1/1	0.85	0.25	49,49,49,49	0
57	MG	2A	3402	1/1	0.85	0.12	71,71,71,71	0
57	MG	1A	4006	1/1	0.85	0.11	59,59,59,59	0
57	MG	1A	4007	1/1	0.85	0.26	77,77,77,77	0
57	MG	1t	201	1/1	0.85	0.10	57,57,57,57	0
57	MG	2A	3778	1/1	0.85	0.10	60,60,60,60	0
57	MG	1w	103	1/1	0.85	0.30	73,73,73,73	0
57	MG	2A	3436	1/1	0.85	0.22	66,66,66,66	0
57	MG	1A	3653	1/1	0.85	0.10	37,37,37,37	0
57	MG	1A	3402	1/1	0.85	0.22	61,61,61,61	0
57	MG	2a	1783	1/1	0.85	0.17	66,66,66,66	0
57	MG	1x	103	1/1	0.85	0.27	55,55,55,55	0
57	MG	2A	3245	1/1	0.85	0.60	73,73,73,73	0
57	MG	1A	4018	1/1	0.85	0.21	72,72,72,72	0
57	MG	2B	201	1/1	0.85	0.14	69,69,69,69	0
57	MG	1A	3307	1/1	0.85	0.14	60,60,60,60	0
57	MG	1A	3238	1/1	0.85	0.39	41,41,41,41	0
57	MG	1a	1690	1/1	0.85	0.25	69,69,69,69	0
57	MG	1A	3584	1/1	0.85	0.25	30,30,30,30	0
57	MG	2B	212	1/1	0.85	0.24	65,65,65,65	0
57	MG	2A	3258	1/1	0.85	0.24	51,51,51,51	0
57	MG	2A	3013	1/1	0.85	0.16	78,78,78,78	0
57	MG	2f	203	1/1	0.85	0.13	75,75,75,75	0
57	MG	2k	201	1/1	0.85	0.31	66,66,66,66	0
57	MG	2D	302	1/1	0.85	0.33	66,66,66,66	0
57	MG	2A	3261	1/1	0.85	0.19	56,56,56,56	0
57	MG	1R	205	1/1	0.85	0.28	36,36,36,36	0
57	MG	1A	3089	1/1	0.85	0.10	76,76,76,76	0
57	MG	1A	3494	1/1	0.85	0.35	69,69,69,69	0
57	MG	2A	3267	1/1	0.85	0.22	64,64,64,64	0
57	MG	2A	3165	1/1	0.85	0.17	67,67,67,67	0
57	MG	1U	209	1/1	0.85	0.70	37,37,37,37	0
57	MG	1A	3916	1/1	0.85	0.08	23,23,23,23	0
57	MG	2A	3567	1/1	0.85	0.12	59,59,59,59	0
57	MG	1A	3617	1/1	0.85	0.17	25,25,25,25	0
57	MG	1a	1721	1/1	0.85	0.15	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3515	1/1	0.86	0.16	34,34,34,34	0
57	MG	1a	1814	1/1	0.86	0.18	65,65,65,65	0
57	MG	1A	3867	1/1	0.86	0.19	33,33,33,33	0
57	MG	1A	3379	1/1	0.86	0.51	47,47,47,47	0
57	MG	1a	1651	1/1	0.86	0.11	54,54,54,54	0
57	MG	1A	3495	1/1	0.86	0.29	59,59,59,59	0
57	MG	2A	3557	1/1	0.86	0.16	83,83,83,83	0
57	MG	2A	3560	1/1	0.86	0.07	74,74,74,74	0
57	MG	2A	3278	1/1	0.86	0.23	59,59,59,59	0
57	MG	25	103	1/1	0.86	0.23	63,63,63,63	0
57	MG	2A	3566	1/1	0.86	0.12	33,33,33,33	0
57	MG	1a	1659	1/1	0.86	0.70	61,61,61,61	0
57	MG	1A	3500	1/1	0.86	0.19	59,59,59,59	0
57	MG	1A	3111	1/1	0.86	0.33	39,39,39,39	0
57	MG	2A	3171	1/1	0.86	0.39	70,70,70,70	0
57	MG	1B	219	1/1	0.86	0.20	34,34,34,34	0
57	MG	1A	3001	1/1	0.86	0.09	43,43,43,43	0
57	MG	2A	3297	1/1	0.86	0.33	69,69,69,69	0
57	MG	1A	3996	1/1	0.86	0.11	53,53,53,53	0
57	MG	2a	1630	1/1	0.86	0.17	68,68,68,68	0
57	MG	2A	3180	1/1	0.86	0.11	60,60,60,60	0
57	MG	2A	3307	1/1	0.86	0.42	71,71,71,71	0
57	MG	2A	3003	1/1	0.86	0.51	57,57,57,57	0
57	MG	2A	3182	1/1	0.86	0.12	64,64,64,64	0
57	MG	1B	232	1/1	0.86	0.16	68,68,68,68	0
57	MG	2A	3315	1/1	0.86	0.14	65,65,65,65	0
57	MG	2A	3317	1/1	0.86	0.22	58,58,58,58	0
57	MG	1B	233	1/1	0.86	0.10	61,61,61,61	0
57	MG	2A	3611	1/1	0.86	0.16	55,55,55,55	0
57	MG	2A	3326	1/1	0.86	0.22	63,63,63,63	0
57	MG	2A	3618	1/1	0.86	0.18	47,47,47,47	0
57	MG	2a	1664	1/1	0.86	0.07	64,64,64,64	0
57	MG	2a	1666	1/1	0.86	0.33	68,68,68,68	0
57	MG	1A	3997	1/1	0.86	0.15	53,53,53,53	0
57	MG	2A	3626	1/1	0.86	0.12	62,62,62,62	0
57	MG	2A	3630	1/1	0.86	0.21	65,65,65,65	0
57	MG	1A	4000	1/1	0.86	0.17	33,33,33,33	0
57	MG	1F	308	1/1	0.86	0.11	50,50,50,50	0
57	MG	1A	3902	1/1	0.86	0.13	47,47,47,47	0
57	MG	1A	3441	1/1	0.86	0.15	64,64,64,64	0
57	MG	1A	3163	1/1	0.86	0.25	59,59,59,59	0
57	MG	2A	3656	1/1	0.86	0.16	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	3036	1/1	0.86	0.14	66,66,66,66	0
57	MG	1A	3359	1/1	0.86	0.38	36,36,36,36	0
57	MG	1A	4013	1/1	0.86	0.32	41,41,41,41	0
57	MG	1A	3203	1/1	0.86	0.09	40,40,40,40	0
57	MG	1A	3911	1/1	0.86	0.08	43,43,43,43	0
57	MG	1A	3912	1/1	0.86	0.15	64,64,64,64	0
57	MG	2A	3056	1/1	0.86	0.13	73,73,73,73	0
57	MG	2a	1721	1/1	0.86	0.14	76,76,76,76	0
57	MG	2A	3692	1/1	0.86	0.15	71,71,71,71	0
57	MG	2a	1723	1/1	0.86	0.22	80,80,80,80	0
57	MG	2A	3213	1/1	0.86	0.30	72,72,72,72	0
57	MG	1A	3541	1/1	0.86	0.22	65,65,65,65	0
57	MG	1a	1725	1/1	0.86	0.15	49,49,49,49	0
57	MG	1A	3178	1/1	0.86	0.08	74,74,74,74	0
57	MG	1A	3372	1/1	0.86	0.74	53,53,53,53	0
57	MG	2A	3381	1/1	0.86	0.30	50,50,50,50	0
57	MG	2a	1760	1/1	0.86	0.22	54,54,54,54	0
57	MG	2A	3733	1/1	0.86	0.21	68,68,68,68	0
57	MG	2A	3219	1/1	0.86	0.22	49,49,49,49	0
57	MG	2A	3385	1/1	0.86	0.21	73,73,73,73	0
57	MG	1A	3927	1/1	0.86	0.14	65,65,65,65	0
57	MG	1A	3929	1/1	0.86	0.18	65,65,65,65	0
57	MG	1A	3080	1/1	0.86	0.21	34,34,34,34	0
57	MG	2A	3765	1/1	0.86	0.06	63,63,63,63	0
57	MG	1A	3244	1/1	0.86	0.14	59,59,59,59	0
57	MG	1A	3573	1/1	0.86	0.18	35,35,35,35	0
57	MG	10	105	1/1	0.86	0.56	43,43,43,43	0
57	MG	2A	3776	1/1	0.86	0.16	67,67,67,67	0
57	MG	1a	1767	1/1	0.86	0.07	59,59,59,59	0
57	MG	2a	1790	1/1	0.86	0.25	75,75,75,75	0
57	MG	2A	3413	1/1	0.86	0.21	38,38,38,38	0
57	MG	1A	3419	1/1	0.86	0.17	66,66,66,66	0
57	MG	1A	3701	1/1	0.86	0.15	19,19,19,19	0
57	MG	1A	3334	1/1	0.86	0.14	53,53,53,53	0
57	MG	1A	3376	1/1	0.86	0.16	42,42,42,42	0
57	MG	1A	3275	1/1	0.86	0.16	53,53,53,53	0
57	MG	1A	3723	1/1	0.86	0.21	26,26,26,26	0
57	MG	1A	3488	1/1	0.86	0.27	60,60,60,60	0
57	MG	1a	1795	1/1	0.86	0.10	68,68,68,68	0
57	MG	2A	3477	1/1	0.86	0.28	50,50,50,50	0
57	MG	1A	3861	1/1	0.86	0.23	37,37,37,37	0
57	MG	1a	1799	1/1	0.86	0.13	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2B	211	1/1	0.86	0.26	76,76,76,76	0
57	MG	1A	4098	1/1	0.86	0.14	51,51,51,51	0
57	MG	2w	103	1/1	0.86	0.25	70,70,70,70	0
57	MG	1B	201	1/1	0.86	0.11	51,51,51,51	0
57	MG	1A	3863	1/1	0.86	0.17	44,44,44,44	0
57	MG	1a	1629	1/1	0.86	0.30	69,69,69,69	0
57	MG	1a	1636	1/1	0.86	0.12	57,57,57,57	0
57	MG	1A	3429	1/1	0.86	0.17	50,50,50,50	0
57	MG	2D	307	1/1	0.86	0.16	68,68,68,68	0
57	MG	2D	308	1/1	0.86	0.18	59,59,59,59	0
57	MG	2E	301	1/1	0.86	0.21	68,68,68,68	0
57	MG	2E	305	1/1	0.86	0.15	63,63,63,63	0
57	MG	1A	3399	1/1	0.87	0.34	34,34,34,34	0
57	MG	2A	3293	1/1	0.87	0.24	67,67,67,67	0
57	MG	2A	3094	1/1	0.87	0.13	67,67,67,67	0
57	MG	1A	3763	1/1	0.87	0.14	32,32,32,32	0
57	MG	2A	3096	1/1	0.87	0.09	62,62,62,62	0
57	MG	1x	107	1/1	0.87	0.26	72,72,72,72	0
57	MG	1A	3051	1/1	0.87	0.15	54,54,54,54	0
57	MG	2A	3301	1/1	0.87	0.19	67,67,67,67	0
57	MG	2A	3304	1/1	0.87	0.12	62,62,62,62	0
57	MG	1A	4039	1/1	0.87	0.13	48,48,48,48	0
57	MG	2A	3103	1/1	0.87	0.23	68,68,68,68	0
57	MG	2A	3507	1/1	0.87	0.08	61,61,61,61	0
57	MG	1a	1624	1/1	0.87	0.12	46,46,46,46	0
57	MG	1A	3223	1/1	0.87	0.25	57,57,57,57	0
57	MG	1A	3529	1/1	0.87	0.12	56,56,56,56	0
57	MG	1E	310	1/1	0.87	0.09	39,39,39,39	0
57	MG	1A	3405	1/1	0.87	0.30	62,62,62,62	0
57	MG	2A	3322	1/1	0.87	0.22	57,57,57,57	0
57	MG	2A	3542	1/1	0.87	0.23	72,72,72,72	0
57	MG	2A	3325	1/1	0.87	0.14	67,67,67,67	0
57	MG	2A	3020	1/1	0.87	0.25	49,49,49,49	0
57	MG	2A	3549	1/1	0.87	0.12	53,53,53,53	0
57	MG	1A	3540	1/1	0.87	0.31	59,59,59,59	0
57	MG	2a	1719	1/1	0.87	0.11	69,69,69,69	0
57	MG	1A	3026	1/1	0.87	0.23	65,65,65,65	0
57	MG	1A	3046	1/1	0.87	0.12	35,35,35,35	0
57	MG	2A	3150	1/1	0.87	0.14	63,63,63,63	0
57	MG	1A	3468	1/1	0.87	0.20	54,54,54,54	0
57	MG	2a	1725	1/1	0.87	0.07	84,84,84,84	0
57	MG	2A	3030	1/1	0.87	0.28	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	1727	1/1	0.87	0.14	71,71,71,71	0
57	MG	1A	3146	1/1	0.87	0.40	34,34,34,34	0
57	MG	1O	203	1/1	0.87	0.25	55,55,55,55	0
57	MG	2A	3575	1/1	0.87	0.24	60,60,60,60	0
57	MG	1A	3984	1/1	0.87	0.09	43,43,43,43	0
57	MG	2a	1751	1/1	0.87	0.21	60,60,60,60	0
57	MG	1A	3199	1/1	0.87	0.13	71,71,71,71	0
57	MG	2A	3351	1/1	0.87	0.30	57,57,57,57	0
57	MG	2A	3239	1/1	0.87	0.22	55,55,55,55	0
57	MG	1A	3326	1/1	0.87	0.39	62,62,62,62	0
57	MG	2A	3357	1/1	0.87	0.35	58,58,58,58	0
57	MG	2A	3166	1/1	0.87	0.17	65,65,65,65	0
57	MG	1A	3148	1/1	0.87	0.12	32,32,32,32	0
57	MG	2A	3053	1/1	0.87	0.15	58,58,58,58	0
57	MG	2A	3364	1/1	0.87	0.35	54,54,54,54	0
57	MG	1A	3068	1/1	0.87	0.18	58,58,58,58	0
57	MG	1A	3159	1/1	0.87	0.15	40,40,40,40	0
57	MG	1A	3124	1/1	0.87	0.23	37,37,37,37	0
57	MG	2G	201	1/1	0.87	0.07	77,77,77,77	0
57	MG	2a	1786	1/1	0.87	0.24	68,68,68,68	0
57	MG	2N	201	1/1	0.87	0.32	85,85,85,85	0
57	MG	1A	3384	1/1	0.87	0.17	51,51,51,51	0
57	MG	1A	3299	1/1	0.87	0.45	37,37,37,37	0
57	MG	2A	3259	1/1	0.87	0.20	65,65,65,65	0
57	MG	2A	3391	1/1	0.87	0.13	61,61,61,61	0
57	MG	2a	1804	1/1	0.87	0.26	65,65,65,65	0
57	MG	1B	204	1/1	0.87	0.21	44,44,44,44	0
57	MG	2A	3631	1/1	0.87	0.24	86,86,86,86	0
57	MG	1A	3843	1/1	0.87	0.19	31,31,31,31	0
57	MG	2a	1815	1/1	0.87	0.08	67,67,67,67	0
57	MG	1A	4008	1/1	0.87	0.13	18,18,18,18	0
57	MG	2A	3637	1/1	0.87	0.13	54,54,54,54	0
57	MG	2a	1602	1/1	0.87	0.10	81,81,81,81	0
57	MG	10	106	1/1	0.87	0.28	64,64,64,64	0
57	MG	2A	3643	1/1	0.87	0.12	71,71,71,71	0
57	MG	1A	3251	1/1	0.87	0.22	64,64,64,64	0
57	MG	1A	3511	1/1	0.87	0.29	58,58,58,58	0
57	MG	2a	1616	1/1	0.87	0.14	79,79,79,79	0
57	MG	1v	101	1/1	0.87	0.28	82,82,82,82	0
57	MG	2A	3194	1/1	0.87	0.16	59,59,59,59	0
57	MG	1A	3854	1/1	0.87	0.15	58,58,58,58	0
57	MG	1A	3858	1/1	0.87	0.10	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	3288	1/1	0.87	0.11	57,57,57,57	0
57	MG	2A	3441	1/1	0.87	0.30	59,59,59,59	0
57	MG	2A	3678	1/1	0.87	0.16	68,68,68,68	0
57	MG	2y	101	1/1	0.87	0.14	81,81,81,81	0
57	MG	1A	3216	1/1	0.87	0.15	53,53,53,53	0
57	MG	2A	3688	1/1	0.87	0.15	50,50,50,50	0
57	MG	2A	3451	1/1	0.87	0.15	42,42,42,42	0
57	MG	1a	1741	1/1	0.88	0.17	58,58,58,58	0
57	MG	2A	3494	1/1	0.88	0.22	76,76,76,76	0
57	MG	1A	4040	1/1	0.88	0.12	67,67,67,67	0
57	MG	2A	3249	1/1	0.88	0.18	55,55,55,55	0
57	MG	2A	3087	1/1	0.88	0.28	69,69,69,69	0
57	MG	2A	3088	1/1	0.88	0.12	75,75,75,75	0
57	MG	2F	303	1/1	0.88	0.35	54,54,54,54	0
57	MG	1U	205	1/1	0.88	0.35	36,36,36,36	0
57	MG	1A	3449	1/1	0.88	0.43	48,48,48,48	0
57	MG	1A	3272	1/1	0.88	0.37	46,46,46,46	0
57	MG	1A	3918	1/1	0.88	0.11	65,65,65,65	0
57	MG	1A	3101	1/1	0.88	0.15	31,31,31,31	0
57	MG	1A	4051	1/1	0.88	0.25	57,57,57,57	0
57	MG	2A	3543	1/1	0.88	0.23	35,35,35,35	0
57	MG	1A	3416	1/1	0.88	0.16	67,67,67,67	0
57	MG	2A	3101	1/1	0.88	0.09	50,50,50,50	0
57	MG	10	103	1/1	0.88	0.36	52,52,52,52	0
57	MG	25	101	1/1	0.88	0.30	67,67,67,67	0
57	MG	2A	3552	1/1	0.88	0.22	39,39,39,39	0
57	MG	1A	3088	1/1	0.88	0.26	53,53,53,53	0
57	MG	28	104	1/1	0.88	0.25	58,58,58,58	0
57	MG	1a	1773	1/1	0.88	0.08	63,63,63,63	0
57	MG	2A	3279	1/1	0.88	0.50	60,60,60,60	0
57	MG	2A	3564	1/1	0.88	0.21	75,75,75,75	0
57	MG	2A	3280	1/1	0.88	0.21	47,47,47,47	0
57	MG	1A	3208	1/1	0.88	0.20	50,50,50,50	0
57	MG	2a	1614	1/1	0.88	0.11	63,63,63,63	0
57	MG	2A	3112	1/1	0.88	0.12	75,75,75,75	0
57	MG	1A	3533	1/1	0.88	0.20	38,38,38,38	0
57	MG	11	102	1/1	0.88	0.29	60,60,60,60	0
57	MG	2A	3126	1/1	0.88	0.09	61,61,61,61	0
57	MG	2A	3291	1/1	0.88	0.17	67,67,67,67	0
57	MG	1A	3424	1/1	0.88	0.23	60,60,60,60	0
57	MG	1a	1791	1/1	0.88	0.13	69,69,69,69	0
57	MG	11	105	1/1	0.88	0.18	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	12	102	1/1	0.88	0.14	50,50,50,50	0
57	MG	12	103	1/1	0.88	0.20	43,43,43,43	0
57	MG	2A	3146	1/1	0.88	0.17	66,66,66,66	0
57	MG	2a	1639	1/1	0.88	0.19	71,71,71,71	0
57	MG	2A	3147	1/1	0.88	0.16	56,56,56,56	0
57	MG	2A	3303	1/1	0.88	0.15	72,72,72,72	0
57	MG	1A	3538	1/1	0.88	0.14	68,68,68,68	0
57	MG	15	101	1/1	0.88	0.23	39,39,39,39	0
57	MG	16	101	1/1	0.88	0.41	52,52,52,52	0
57	MG	18	104	1/1	0.88	0.37	41,41,41,41	0
57	MG	1A	4074	1/1	0.88	0.18	62,62,62,62	0
57	MG	1A	3209	1/1	0.88	0.40	44,44,44,44	0
57	MG	1A	3654	1/1	0.88	0.15	27,27,27,27	0
57	MG	2a	1684	1/1	0.88	0.17	67,67,67,67	0
57	MG	1A	3313	1/1	0.88	0.18	53,53,53,53	0
57	MG	1A	4086	1/1	0.88	0.10	40,40,40,40	0
57	MG	2A	3324	1/1	0.88	0.63	55,55,55,55	0
57	MG	1A	3949	1/1	0.88	0.13	57,57,57,57	0
57	MG	1A	4097	1/1	0.88	0.10	46,46,46,46	0
57	MG	1A	3479	1/1	0.88	0.14	67,67,67,67	0
57	MG	2a	1701	1/1	0.88	0.23	51,51,51,51	0
57	MG	2A	3334	1/1	0.88	0.42	54,54,54,54	0
57	MG	1A	3555	1/1	0.88	0.30	54,54,54,54	0
57	MG	1A	3260	1/1	0.88	0.52	47,47,47,47	0
57	MG	1x	102	1/1	0.88	0.21	70,70,70,70	0
57	MG	2A	3652	1/1	0.88	0.08	54,54,54,54	0
57	MG	1A	3557	1/1	0.88	0.45	66,66,66,66	0
57	MG	2A	3658	1/1	0.88	0.17	67,67,67,67	0
57	MG	1A	3294	1/1	0.88	0.20	63,63,63,63	0
57	MG	1a	1640	1/1	0.88	0.22	61,61,61,61	0
57	MG	1A	3855	1/1	0.88	0.28	34,34,34,34	0
57	MG	1A	3234	1/1	0.88	0.34	52,52,52,52	0
57	MG	1y	101	1/1	0.88	0.32	55,55,55,55	0
57	MG	2A	3677	1/1	0.88	0.15	60,60,60,60	0
57	MG	1A	3563	1/1	0.88	0.21	25,25,25,25	0
57	MG	1A	3565	1/1	0.88	0.13	23,23,23,23	0
57	MG	2A	3687	1/1	0.88	0.31	70,70,70,70	0
57	MG	1A	3567	1/1	0.88	0.13	30,30,30,30	0
57	MG	2a	1738	1/1	0.88	0.09	75,75,75,75	0
57	MG	2a	1739	1/1	0.88	0.14	69,69,69,69	0
57	MG	2a	1744	1/1	0.88	0.15	64,64,64,64	0
57	MG	2A	3689	1/1	0.88	0.22	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1A	3720	1/1	0.88	0.16	29,29,29,29	0
57	MG	2A	3358	1/1	0.88	0.35	52,52,52,52	0
57	MG	2A	3694	1/1	0.88	0.15	64,64,64,64	0
57	MG	1A	3722	1/1	0.88	0.20	30,30,30,30	0
57	MG	2A	3197	1/1	0.88	0.40	58,58,58,58	0
57	MG	1a	1665	1/1	0.88	0.11	65,65,65,65	0
57	MG	2A	3707	1/1	0.88	0.17	51,51,51,51	0
57	MG	1A	3871	1/1	0.88	0.20	24,24,24,24	0
57	MG	1A	3994	1/1	0.88	0.13	29,29,29,29	0
57	MG	2A	3730	1/1	0.88	0.08	63,63,63,63	0
57	MG	1A	3873	1/1	0.88	0.26	42,42,42,42	0
57	MG	2A	3027	1/1	0.88	0.16	45,45,45,45	0
57	MG	1A	3571	1/1	0.88	0.12	43,43,43,43	0
57	MG	2A	3745	1/1	0.88	0.15	57,57,57,57	0
57	MG	1a	1679	1/1	0.88	0.38	47,47,47,47	0
57	MG	1A	3298	1/1	0.88	0.31	39,39,39,39	0
57	MG	1A	3439	1/1	0.88	0.38	46,46,46,46	0
57	MG	2A	3757	1/1	0.88	0.09	64,64,64,64	0
57	MG	1a	1684	1/1	0.88	0.06	68,68,68,68	0
57	MG	1a	1686	1/1	0.88	0.19	62,62,62,62	0
57	MG	2A	3768	1/1	0.88	0.12	72,72,72,72	0
57	MG	2A	3046	1/1	0.88	0.18	70,70,70,70	0
57	MG	1F	305	1/1	0.88	0.59	60,60,60,60	0
57	MG	2a	1805	1/1	0.88	0.26	58,58,58,58	0
57	MG	2A	3221	1/1	0.88	0.23	65,65,65,65	0
57	MG	2a	1810	1/1	0.88	0.20	77,77,77,77	0
57	MG	2A	3403	1/1	0.88	0.45	56,56,56,56	0
57	MG	1A	3210	1/1	0.88	0.20	49,49,49,49	0
57	MG	2A	3782	1/1	0.88	0.11	54,54,54,54	0
57	MG	2A	3051	1/1	0.88	0.29	56,56,56,56	0
57	MG	2a	1818	1/1	0.88	0.08	72,72,72,72	0
57	MG	1A	3586	1/1	0.88	0.08	33,33,33,33	0
57	MG	1a	1692	1/1	0.88	0.09	69,69,69,69	0
57	MG	1A	3900	1/1	0.88	0.23	65,65,65,65	0
57	MG	1A	3587	1/1	0.88	0.07	41,41,41,41	0
57	MG	2A	3439	1/1	0.88	0.14	68,68,68,68	0
57	MG	2A	3794	1/1	0.88	0.14	47,47,47,47	0
57	MG	1A	3498	1/1	0.88	0.15	63,63,63,63	0
57	MG	2A	3448	1/1	0.88	0.22	47,47,47,47	0
57	MG	1A	3776	1/1	0.88	0.12	46,46,46,46	0
57	MG	1A	3905	1/1	0.88	0.08	62,62,62,62	0
57	MG	2x	103	1/1	0.88	0.23	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	3328	1/1	0.88	0.17	57,57,57,57	0
57	MG	1A	3332	1/1	0.88	0.24	66,66,66,66	0
57	MG	1A	3509	1/1	0.88	0.24	35,35,35,35	0
57	MG	1R	206	1/1	0.88	0.12	71,71,71,71	0
57	MG	1A	3792	1/1	0.88	0.12	28,28,28,28	0
57	MG	1a	1733	1/1	0.88	0.17	71,71,71,71	0
57	MG	2A	3081	1/1	0.88	0.21	52,52,52,52	0
57	MG	2A	3246	1/1	0.88	0.13	68,68,68,68	0
57	MG	1H	201	1/1	0.89	0.21	48,48,48,48	0
57	MG	2P	201	1/1	0.89	0.29	63,63,63,63	0
57	MG	2A	3168	1/1	0.89	0.23	49,49,49,49	0
57	MG	2Q	201	1/1	0.89	0.07	65,65,65,65	0
57	MG	2R	202	1/1	0.89	0.16	50,50,50,50	0
57	MG	2A	3005	1/1	0.89	0.33	56,56,56,56	0
57	MG	1A	3330	1/1	0.89	0.48	39,39,39,39	0
57	MG	2A	3565	1/1	0.89	0.13	66,66,66,66	0
57	MG	1A	3910	1/1	0.89	0.16	67,67,67,67	0
57	MG	1A	3212	1/1	0.89	0.21	45,45,45,45	0
57	MG	2A	3305	1/1	0.89	0.15	58,58,58,58	0
57	MG	2A	3570	1/1	0.89	0.12	73,73,73,73	0
57	MG	1A	4032	1/1	0.89	0.20	40,40,40,40	0
57	MG	1A	4033	1/1	0.89	0.21	60,60,60,60	0
57	MG	2A	3312	1/1	0.89	0.25	69,69,69,69	0
57	MG	1A	3301	1/1	0.89	0.27	39,39,39,39	0
57	MG	2A	3578	1/1	0.89	0.16	69,69,69,69	0
57	MG	1A	3807	1/1	0.89	0.19	43,43,43,43	0
57	MG	2A	3184	1/1	0.89	0.22	66,66,66,66	0
57	MG	1A	3668	1/1	0.89	0.19	61,61,61,61	0
57	MG	2A	3583	1/1	0.89	0.16	43,43,43,43	0
57	MG	2A	3319	1/1	0.89	0.13	73,73,73,73	0
57	MG	2a	1617	1/1	0.89	0.24	57,57,57,57	0
57	MG	2a	1618	1/1	0.89	0.15	71,71,71,71	0
57	MG	2A	3320	1/1	0.89	0.26	69,69,69,69	0
57	MG	1A	3810	1/1	0.89	0.14	69,69,69,69	0
57	MG	2a	1623	1/1	0.89	0.29	63,63,63,63	0
57	MG	1a	1698	1/1	0.89	0.21	63,63,63,63	0
57	MG	2A	3596	1/1	0.89	0.21	56,56,56,56	0
57	MG	1A	3815	1/1	0.89	0.10	57,57,57,57	0
57	MG	2A	3192	1/1	0.89	0.34	45,45,45,45	0
57	MG	1A	3490	1/1	0.89	0.21	49,49,49,49	0
57	MG	1A	3024	1/1	0.89	0.29	35,35,35,35	0
57	MG	1a	1712	1/1	0.89	0.16	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3157	1/1	0.89	0.12	52,52,52,52	0
57	MG	1W	202	1/1	0.89	0.13	57,57,57,57	0
57	MG	1A	3681	1/1	0.89	0.17	62,62,62,62	0
57	MG	1a	1723	1/1	0.89	0.17	58,58,58,58	0
57	MG	2a	1644	1/1	0.89	0.10	83,83,83,83	0
57	MG	1A	3934	1/1	0.89	0.09	61,61,61,61	0
57	MG	1a	1726	1/1	0.89	0.12	52,52,52,52	0
57	MG	1A	3438	1/1	0.89	0.19	45,45,45,45	0
57	MG	2a	1654	1/1	0.89	0.13	64,64,64,64	0
57	MG	1a	1728	1/1	0.89	0.29	67,67,67,67	0
57	MG	1A	3497	1/1	0.89	0.16	47,47,47,47	0
57	MG	2a	1665	1/1	0.89	0.37	64,64,64,64	0
57	MG	2A	3063	1/1	0.89	0.17	53,53,53,53	0
57	MG	1A	3697	1/1	0.89	0.07	53,53,53,53	0
57	MG	1A	3191	1/1	0.89	0.12	40,40,40,40	0
57	MG	1A	3440	1/1	0.89	0.23	46,46,46,46	0
57	MG	2a	1689	1/1	0.89	0.33	67,67,67,67	0
57	MG	1A	3015	1/1	0.89	0.26	37,37,37,37	0
57	MG	1A	3443	1/1	0.89	0.24	43,43,43,43	0
57	MG	2A	3075	1/1	0.89	0.21	57,57,57,57	0
57	MG	1A	3444	1/1	0.89	0.15	57,57,57,57	0
57	MG	2A	3363	1/1	0.89	0.34	65,65,65,65	0
57	MG	2A	3666	1/1	0.89	0.08	72,72,72,72	0
57	MG	1A	4087	1/1	0.89	0.16	51,51,51,51	0
57	MG	1A	4091	1/1	0.89	0.27	40,40,40,40	0
57	MG	1A	3342	1/1	0.89	0.46	60,60,60,60	0
57	MG	1A	3601	1/1	0.89	0.11	70,70,70,70	0
57	MG	2A	3376	1/1	0.89	0.44	62,62,62,62	0
57	MG	2a	1713	1/1	0.89	0.13	68,68,68,68	0
57	MG	1A	3233	1/1	0.89	0.19	47,47,47,47	0
57	MG	1A	3865	1/1	0.89	0.14	47,47,47,47	0
57	MG	1a	1775	1/1	0.89	0.06	62,62,62,62	0
57	MG	2A	3386	1/1	0.89	0.15	56,56,56,56	0
57	MG	1A	3613	1/1	0.89	0.13	43,43,43,43	0
57	MG	1a	1603	1/1	0.89	0.14	59,59,59,59	0
57	MG	1A	3615	1/1	0.89	0.14	36,36,36,36	0
57	MG	2A	3397	1/1	0.89	0.33	62,62,62,62	0
57	MG	1a	1610	1/1	0.89	0.17	65,65,65,65	0
57	MG	1A	3516	1/1	0.89	0.21	33,33,33,33	0
57	MG	2A	3240	1/1	0.89	0.16	63,63,63,63	0
57	MG	2A	3098	1/1	0.89	0.18	49,49,49,49	0
57	MG	2a	1737	1/1	0.89	0.13	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	2A	3713	1/1	0.89	0.20	50,50,50,50	0
57	MG	2A	3714	1/1	0.89	0.12	52,52,52,52	0
57	MG	2A	3407	1/1	0.89	0.16	66,66,66,66	0
57	MG	2A	3242	1/1	0.89	0.10	66,66,66,66	0
57	MG	1A	3312	1/1	0.89	0.22	49,49,49,49	0
57	MG	1A	3252	1/1	0.89	0.15	46,46,46,46	0
57	MG	1A	3880	1/1	0.89	0.19	51,51,51,51	0
57	MG	2A	3416	1/1	0.89	0.21	35,35,35,35	0
57	MG	2A	3425	1/1	0.89	0.09	73,73,73,73	0
57	MG	1A	3882	1/1	0.89	0.14	43,43,43,43	0
57	MG	1A	3768	1/1	0.89	0.14	45,45,45,45	0
57	MG	1B	217	1/1	0.89	0.08	52,52,52,52	0
57	MG	1A	3409	1/1	0.89	0.46	39,39,39,39	0
57	MG	2A	3447	1/1	0.89	0.23	41,41,41,41	0
57	MG	2A	3252	1/1	0.89	0.40	62,62,62,62	0
57	MG	2A	3108	1/1	0.89	0.19	40,40,40,40	0
57	MG	1a	1633	1/1	0.89	0.18	58,58,58,58	0
57	MG	1a	1811	1/1	0.89	0.35	61,61,61,61	0
57	MG	2A	3463	1/1	0.89	0.32	53,53,53,53	0
57	MG	2A	3777	1/1	0.89	0.12	70,70,70,70	0
57	MG	1B	222	1/1	0.89	0.20	56,56,56,56	0
57	MG	2A	3124	1/1	0.89	0.35	46,46,46,46	0
57	MG	1A	3283	1/1	0.89	0.38	50,50,50,50	0
57	MG	1A	3144	1/1	0.89	0.34	32,32,32,32	0
57	MG	1A	4005	1/1	0.89	0.21	26,26,26,26	0
57	MG	2A	3481	1/1	0.89	0.14	52,52,52,52	0
57	MG	2A	3791	1/1	0.89	0.07	71,71,71,71	0
57	MG	2A	3265	1/1	0.89	0.18	60,60,60,60	0
57	MG	1A	3293	1/1	0.89	0.10	57,57,57,57	0
57	MG	2A	3138	1/1	0.89	0.23	45,45,45,45	0
57	MG	1A	3789	1/1	0.89	0.27	60,60,60,60	0
57	MG	2A	3274	1/1	0.89	0.51	74,74,74,74	0
57	MG	2A	3275	1/1	0.89	0.25	78,78,78,78	0
57	MG	1E	302	1/1	0.89	0.26	36,36,36,36	0
57	MG	2a	1817	1/1	0.89	0.14	54,54,54,54	0
57	MG	1a	1657	1/1	0.89	0.15	65,65,65,65	0
57	MG	2A	3510	1/1	0.89	0.14	51,51,51,51	0
57	MG	1E	305	1/1	0.89	0.19	28,28,28,28	0
57	MG	1A	3321	1/1	0.89	0.27	41,41,41,41	0
57	MG	1A	3197	1/1	0.89	0.18	39,39,39,39	0
57	MG	2A	3286	1/1	0.89	0.21	61,61,61,61	0
57	MG	2B	215	1/1	0.89	0.16	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	2v	101	1/1	0.89	0.19	78,78,78,78	0
57	MG	1A	3237	1/1	0.89	0.09	56,56,56,56	0
57	MG	2A	3526	1/1	0.89	0.16	65,65,65,65	0
57	MG	2A	3529	1/1	0.89	0.08	62,62,62,62	0
57	MG	2A	3534	1/1	0.89	0.26	63,63,63,63	0
57	MG	1F	307	1/1	0.89	0.16	38,38,38,38	0
57	MG	1A	3906	1/1	0.89	0.17	48,48,48,48	0
57	MG	2A	3544	1/1	0.89	0.20	50,50,50,50	0
57	MG	1x	109	1/1	0.89	0.33	71,71,71,71	0
57	MG	1A	4014	1/1	0.89	0.22	29,29,29,29	0
57	MG	2F	304	1/1	0.89	0.17	49,49,49,49	0
57	MG	2F	305	1/1	0.89	0.11	63,63,63,63	0
57	MG	1A	3907	1/1	0.89	0.09	70,70,70,70	0
60	ZN	2Y	202	1/1	0.89	0.12	105,105,105,105	0
57	MG	1A	3133	1/1	0.89	0.18	48,48,48,48	0
57	MG	2A	3561	1/1	0.90	0.27	67,67,67,67	0
57	MG	1A	4055	1/1	0.90	0.13	58,58,58,58	0
57	MG	1A	3598	1/1	0.90	0.14	19,19,19,19	0
57	MG	1A	4062	1/1	0.90	0.11	48,48,48,48	0
57	MG	1A	3346	1/1	0.90	0.30	38,38,38,38	0
57	MG	1A	3099	1/1	0.90	0.36	54,54,54,54	0
57	MG	1A	3422	1/1	0.90	0.24	48,48,48,48	0
57	MG	20	101	1/1	0.90	0.11	63,63,63,63	0
57	MG	2A	3158	1/1	0.90	0.27	70,70,70,70	0
57	MG	17	104	1/1	0.90	0.13	51,51,51,51	0
57	MG	1A	3019	1/1	0.90	0.20	48,48,48,48	0
57	MG	1A	3493	1/1	0.90	0.34	49,49,49,49	0
57	MG	1A	3922	1/1	0.90	0.17	49,49,49,49	0
57	MG	1A	3006	1/1	0.90	0.19	55,55,55,55	0
57	MG	1A	4077	1/1	0.90	0.06	61,61,61,61	0
57	MG	1A	3925	1/1	0.90	0.13	56,56,56,56	0
57	MG	2a	1605	1/1	0.90	0.23	69,69,69,69	0
57	MG	1A	3618	1/1	0.90	0.18	21,21,21,21	0
57	MG	1a	1620	1/1	0.90	0.14	50,50,50,50	0
57	MG	2A	3175	1/1	0.90	0.52	65,65,65,65	0
57	MG	2a	1612	1/1	0.90	0.09	60,60,60,60	0
57	MG	2A	3586	1/1	0.90	0.07	67,67,67,67	0
57	MG	2a	1615	1/1	0.90	0.44	62,62,62,62	0
57	MG	1A	3114	1/1	0.90	0.23	43,43,43,43	0
57	MG	1A	3175	1/1	0.90	0.14	38,38,38,38	0
57	MG	1A	4093	1/1	0.90	0.31	49,49,49,49	0
57	MG	1A	4094	1/1	0.90	0.34	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	3224	1/1	0.90	0.52	50,50,50,50	0
57	MG	1A	3430	1/1	0.90	0.33	69,69,69,69	0
57	MG	1a	1630	1/1	0.90	0.25	71,71,71,71	0
57	MG	1A	3935	1/1	0.90	0.12	39,39,39,39	0
57	MG	1A	3074	1/1	0.90	0.25	42,42,42,42	0
57	MG	2a	1631	1/1	0.90	0.25	66,66,66,66	0
57	MG	2A	3613	1/1	0.90	0.47	56,56,56,56	0
57	MG	1A	3052	1/1	0.90	0.23	51,51,51,51	0
57	MG	1A	3817	1/1	0.90	0.10	61,61,61,61	0
57	MG	2A	3191	1/1	0.90	0.19	56,56,56,56	0
57	MG	1A	3127	1/1	0.90	0.43	41,41,41,41	0
57	MG	1A	3822	1/1	0.90	0.21	61,61,61,61	0
57	MG	1A	3947	1/1	0.90	0.20	50,50,50,50	0
57	MG	2A	3017	1/1	0.90	0.31	61,61,61,61	0
57	MG	1A	3083	1/1	0.90	0.20	39,39,39,39	0
57	MG	1B	212	1/1	0.90	0.21	60,60,60,60	0
57	MG	2A	3638	1/1	0.90	0.07	68,68,68,68	0
57	MG	1A	3646	1/1	0.90	0.22	34,34,34,34	0
57	MG	1A	3134	1/1	0.90	0.26	41,41,41,41	0
57	MG	1A	3830	1/1	0.90	0.44	45,45,45,45	0
57	MG	1A	3085	1/1	0.90	0.17	54,54,54,54	0
57	MG	1A	3086	1/1	0.90	0.17	59,59,59,59	0
57	MG	1B	224	1/1	0.90	0.24	57,57,57,57	0
57	MG	1A	3291	1/1	0.90	0.22	61,61,61,61	0
57	MG	2a	1682	1/1	0.90	0.43	60,60,60,60	0
57	MG	1A	3389	1/1	0.90	0.33	38,38,38,38	0
57	MG	1a	1676	1/1	0.90	0.19	73,73,73,73	0
57	MG	2A	3379	1/1	0.90	0.32	58,58,58,58	0
57	MG	1a	1677	1/1	0.90	0.30	41,41,41,41	0
57	MG	1A	3665	1/1	0.90	0.18	43,43,43,43	0
57	MG	1A	3390	1/1	0.90	0.27	37,37,37,37	0
57	MG	1A	3985	1/1	0.90	0.13	57,57,57,57	0
57	MG	1A	3143	1/1	0.90	0.49	39,39,39,39	0
57	MG	2A	3680	1/1	0.90	0.16	63,63,63,63	0
57	MG	1A	3537	1/1	0.90	0.34	45,45,45,45	0
57	MG	1A	3447	1/1	0.90	0.22	50,50,50,50	0
57	MG	1A	3056	1/1	0.90	0.20	37,37,37,37	0
57	MG	1A	3451	1/1	0.90	0.69	46,46,46,46	0
57	MG	1A	3545	1/1	0.90	0.45	61,61,61,61	0
57	MG	1A	3396	1/1	0.90	0.14	53,53,53,53	0
57	MG	2A	3064	1/1	0.90	0.19	49,49,49,49	0
57	MG	2a	1715	1/1	0.90	0.53	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	3058	1/1	0.90	0.28	54,54,54,54	0
57	MG	1F	312	1/1	0.90	0.11	54,54,54,54	0
57	MG	1F	313	1/1	0.90	0.19	32,32,32,32	0
57	MG	2A	3704	1/1	0.90	0.05	72,72,72,72	0
57	MG	1a	1705	1/1	0.90	0.13	55,55,55,55	0
57	MG	2A	3073	1/1	0.90	0.25	49,49,49,49	0
57	MG	1A	3042	1/1	0.90	0.34	35,35,35,35	0
57	MG	1A	3249	1/1	0.90	0.19	40,40,40,40	0
57	MG	2A	3076	1/1	0.90	0.20	52,52,52,52	0
57	MG	2A	3432	1/1	0.90	0.14	30,30,30,30	0
57	MG	2A	3433	1/1	0.90	0.14	45,45,45,45	0
57	MG	2a	1732	1/1	0.90	0.16	83,83,83,83	0
57	MG	1A	3461	1/1	0.90	0.13	62,62,62,62	0
57	MG	2A	3734	1/1	0.90	0.22	24,24,24,24	0
57	MG	2A	3243	1/1	0.90	0.11	77,77,77,77	0
57	MG	2A	3742	1/1	0.90	0.20	48,48,48,48	0
57	MG	1A	3877	1/1	0.90	0.18	33,33,33,33	0
57	MG	1N	201	1/1	0.90	0.48	45,45,45,45	0
57	MG	1A	3878	1/1	0.90	0.10	48,48,48,48	0
57	MG	1A	3463	1/1	0.90	0.16	55,55,55,55	0
57	MG	2A	3755	1/1	0.90	0.21	62,62,62,62	0
57	MG	1A	3881	1/1	0.90	0.18	26,26,26,26	0
57	MG	2A	3758	1/1	0.90	0.19	50,50,50,50	0
57	MG	1O	205	1/1	0.90	0.14	48,48,48,48	0
57	MG	1P	203	1/1	0.90	0.48	32,32,32,32	0
57	MG	1A	3339	1/1	0.90	0.48	48,48,48,48	0
57	MG	1A	3150	1/1	0.90	0.25	48,48,48,48	0
57	MG	1a	1737	1/1	0.90	0.15	56,56,56,56	0
57	MG	1A	3471	1/1	0.90	0.60	40,40,40,40	0
57	MG	1S	203	1/1	0.90	0.22	67,67,67,67	0
57	MG	1A	3891	1/1	0.90	0.13	33,33,33,33	0
57	MG	1A	4026	1/1	0.90	0.24	46,46,46,46	0
57	MG	1A	3726	1/1	0.90	0.15	31,31,31,31	0
57	MG	2a	1785	1/1	0.90	0.25	66,66,66,66	0
57	MG	2A	3484	1/1	0.90	0.25	32,32,32,32	0
57	MG	2A	3485	1/1	0.90	0.14	67,67,67,67	0
57	MG	1U	207	1/1	0.90	0.47	38,38,38,38	0
57	MG	2a	1791	1/1	0.90	0.15	79,79,79,79	0
57	MG	2A	3489	1/1	0.90	0.27	60,60,60,60	0
57	MG	1A	3895	1/1	0.90	0.09	53,53,53,53	0
57	MG	2a	1797	1/1	0.90	0.18	54,54,54,54	0
57	MG	1A	3568	1/1	0.90	0.14	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1799	1/1	0.90	0.22	60,60,60,60	0
57	MG	1A	3738	1/1	0.90	0.14	48,48,48,48	0
57	MG	1A	4034	1/1	0.90	0.22	48,48,48,48	0
57	MG	2A	3795	1/1	0.90	0.15	71,71,71,71	0
57	MG	1a	1770	1/1	0.90	0.18	53,53,53,53	0
57	MG	1A	4035	1/1	0.90	0.33	58,58,58,58	0
57	MG	2A	3512	1/1	0.90	0.13	53,53,53,53	0
57	MG	2A	3276	1/1	0.90	0.17	52,52,52,52	0
57	MG	2A	3115	1/1	0.90	0.16	61,61,61,61	0
57	MG	1A	3474	1/1	0.90	0.15	54,54,54,54	0
57	MG	2A	3120	1/1	0.90	0.10	53,53,53,53	0
57	MG	1A	3475	1/1	0.90	0.23	60,60,60,60	0
57	MG	2a	1820	1/1	0.90	0.10	69,69,69,69	0
57	MG	2A	3519	1/1	0.90	0.34	50,50,50,50	0
57	MG	2A	3523	1/1	0.90	0.13	59,59,59,59	0
57	MG	1A	3152	1/1	0.90	0.19	42,42,42,42	0
57	MG	2A	3125	1/1	0.90	0.26	44,44,44,44	0
57	MG	1A	3411	1/1	0.90	0.14	58,58,58,58	0
57	MG	2A	3536	1/1	0.90	0.29	46,46,46,46	0
57	MG	2A	3538	1/1	0.90	0.13	41,41,41,41	0
57	MG	2A	3539	1/1	0.90	0.24	47,47,47,47	0
57	MG	2A	3541	1/1	0.90	0.38	63,63,63,63	0
57	MG	2E	302	1/1	0.90	0.11	55,55,55,55	0
57	MG	2A	3131	1/1	0.90	0.35	53,53,53,53	0
57	MG	2E	306	1/1	0.90	0.19	54,54,54,54	0
57	MG	1A	3343	1/1	0.90	0.18	45,45,45,45	0
57	MG	10	107	1/1	0.90	0.17	54,54,54,54	0
57	MG	2A	3292	1/1	0.90	0.21	58,58,58,58	0
57	MG	1a	1786	1/1	0.90	0.11	53,53,53,53	0
57	MG	1A	3773	1/1	0.90	0.07	58,58,58,58	0
57	MG	2A	3140	1/1	0.90	0.06	73,73,73,73	0
57	MG	1A	3344	1/1	0.90	0.44	45,45,45,45	0
57	MG	1A	3596	1/1	0.90	0.18	35,35,35,35	0
57	MG	1a	1708	1/1	0.91	0.15	60,60,60,60	0
57	MG	2F	301	1/1	0.91	0.18	47,47,47,47	0
57	MG	1A	3552	1/1	0.91	0.34	42,42,42,42	0
57	MG	2A	3079	1/1	0.91	0.23	58,58,58,58	0
57	MG	1A	3696	1/1	0.91	0.18	66,66,66,66	0
57	MG	2A	3525	1/1	0.91	0.20	35,35,35,35	0
57	MG	2F	307	1/1	0.91	0.52	51,51,51,51	0
57	MG	1A	3554	1/1	0.91	0.11	63,63,63,63	0
57	MG	1a	1716	1/1	0.91	0.08	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3137	1/1	0.91	0.17	51,51,51,51	0
57	MG	1A	3874	1/1	0.91	0.18	52,52,52,52	0
57	MG	1A	3227	1/1	0.91	0.19	29,29,29,29	0
57	MG	2A	3089	1/1	0.91	0.17	46,46,46,46	0
57	MG	2A	3090	1/1	0.91	0.14	51,51,51,51	0
57	MG	1R	203	1/1	0.91	0.64	38,38,38,38	0
57	MG	2A	3277	1/1	0.91	0.29	72,72,72,72	0
57	MG	1A	3002	1/1	0.91	0.19	60,60,60,60	0
57	MG	2A	3093	1/1	0.91	0.14	28,28,28,28	0
57	MG	1A	3711	1/1	0.91	0.18	27,27,27,27	0
57	MG	1S	202	1/1	0.91	0.13	54,54,54,54	0
57	MG	1A	3712	1/1	0.91	0.23	61,61,61,61	0
57	MG	1A	3267	1/1	0.91	0.26	34,34,34,34	0
57	MG	1A	3348	1/1	0.91	0.17	61,61,61,61	0
57	MG	27	102	1/1	0.91	0.20	57,57,57,57	0
57	MG	28	101	1/1	0.91	0.32	70,70,70,70	0
57	MG	1a	1738	1/1	0.91	0.23	76,76,76,76	0
57	MG	1a	1739	1/1	0.91	0.14	67,67,67,67	0
57	MG	1a	1740	1/1	0.91	0.21	43,43,43,43	0
57	MG	1A	4030	1/1	0.91	0.18	43,43,43,43	0
57	MG	1A	3202	1/1	0.91	0.27	36,36,36,36	0
57	MG	1A	3352	1/1	0.91	0.13	47,47,47,47	0
57	MG	1A	3119	1/1	0.91	0.37	32,32,32,32	0
57	MG	1A	3420	1/1	0.91	0.23	43,43,43,43	0
57	MG	1A	3731	1/1	0.91	0.07	40,40,40,40	0
57	MG	1a	1761	1/1	0.91	0.24	58,58,58,58	0
57	MG	2A	3300	1/1	0.91	0.18	64,64,64,64	0
57	MG	1X	102	1/1	0.91	0.29	37,37,37,37	0
57	MG	2A	3302	1/1	0.91	0.78	57,57,57,57	0
57	MG	1A	3897	1/1	0.91	0.17	18,18,18,18	0
57	MG	1A	3361	1/1	0.91	0.27	33,33,33,33	0
57	MG	1A	3483	1/1	0.91	0.29	35,35,35,35	0
57	MG	1A	3484	1/1	0.91	0.38	44,44,44,44	0
57	MG	1A	3740	1/1	0.91	0.07	71,71,71,71	0
57	MG	2a	1627	1/1	0.91	0.28	45,45,45,45	0
57	MG	1A	3742	1/1	0.91	0.08	35,35,35,35	0
57	MG	2A	3588	1/1	0.91	0.13	60,60,60,60	0
57	MG	2A	3133	1/1	0.91	0.12	60,60,60,60	0
57	MG	1A	3744	1/1	0.91	0.10	42,42,42,42	0
57	MG	10	108	1/1	0.91	0.41	70,70,70,70	0
57	MG	1A	3745	1/1	0.91	0.08	39,39,39,39	0
57	MG	2A	3600	1/1	0.91	0.20	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	2A	3318	1/1	0.91	0.14	61,61,61,61	0
57	MG	1A	3363	1/1	0.91	0.48	41,41,41,41	0
57	MG	1A	3755	1/1	0.91	0.15	42,42,42,42	0
57	MG	1A	3757	1/1	0.91	0.07	61,61,61,61	0
57	MG	1a	1787	1/1	0.91	0.11	52,52,52,52	0
57	MG	2a	1645	1/1	0.91	0.33	70,70,70,70	0
57	MG	12	101	1/1	0.91	0.15	38,38,38,38	0
57	MG	2a	1647	1/1	0.91	0.26	78,78,78,78	0
57	MG	2A	3148	1/1	0.91	0.35	46,46,46,46	0
57	MG	2A	3615	1/1	0.91	0.31	68,68,68,68	0
57	MG	1A	3366	1/1	0.91	0.11	44,44,44,44	0
57	MG	2a	1658	1/1	0.91	0.27	57,57,57,57	0
57	MG	2A	3327	1/1	0.91	0.22	39,39,39,39	0
57	MG	2A	3622	1/1	0.91	0.26	48,48,48,48	0
57	MG	2A	3625	1/1	0.91	0.20	50,50,50,50	0
57	MG	1a	1793	1/1	0.91	0.15	65,65,65,65	0
57	MG	2A	3153	1/1	0.91	0.18	48,48,48,48	0
57	MG	2a	1680	1/1	0.91	0.12	66,66,66,66	0
57	MG	1A	3425	1/1	0.91	0.26	37,37,37,37	0
57	MG	2a	1683	1/1	0.91	0.09	75,75,75,75	0
57	MG	2A	3633	1/1	0.91	0.11	64,64,64,64	0
57	MG	13	103	1/1	0.91	0.12	59,59,59,59	0
57	MG	13	104	1/1	0.91	0.18	55,55,55,55	0
57	MG	1A	3097	1/1	0.91	0.13	37,37,37,37	0
57	MG	1a	1801	1/1	0.91	0.21	56,56,56,56	0
57	MG	2a	1694	1/1	0.91	0.19	63,63,63,63	0
57	MG	1A	3492	1/1	0.91	0.20	24,24,24,24	0
57	MG	2A	3640	1/1	0.91	0.07	68,68,68,68	0
57	MG	2a	1699	1/1	0.91	0.28	57,57,57,57	0
57	MG	15	104	1/1	0.91	0.40	40,40,40,40	0
57	MG	1A	3775	1/1	0.91	0.12	45,45,45,45	0
57	MG	1a	1810	1/1	0.91	0.10	56,56,56,56	0
57	MG	1A	3368	1/1	0.91	0.14	43,43,43,43	0
57	MG	1A	3166	1/1	0.91	0.42	60,60,60,60	0
57	MG	1A	3923	1/1	0.91	0.28	50,50,50,50	0
57	MG	2a	1711	1/1	0.91	0.09	83,83,83,83	0
57	MG	2A	3174	1/1	0.91	0.35	60,60,60,60	0
57	MG	1A	4082	1/1	0.91	0.38	33,33,33,33	0
57	MG	1A	3603	1/1	0.91	0.17	32,32,32,32	0
57	MG	1A	3125	1/1	0.91	0.09	64,64,64,64	0
57	MG	1A	3612	1/1	0.91	0.16	46,46,46,46	0
57	MG	1A	3928	1/1	0.91	0.10	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3496	1/1	0.91	0.33	54,54,54,54	0
57	MG	2A	3365	1/1	0.91	0.26	69,69,69,69	0
57	MG	1A	3318	1/1	0.91	0.39	54,54,54,54	0
57	MG	1A	3280	1/1	0.91	0.17	39,39,39,39	0
57	MG	2A	3368	1/1	0.91	0.62	57,57,57,57	0
57	MG	1A	3240	1/1	0.91	0.18	48,48,48,48	0
57	MG	1x	104	1/1	0.91	0.13	66,66,66,66	0
57	MG	1A	4100	1/1	0.91	0.28	53,53,53,53	0
57	MG	1A	3501	1/1	0.91	0.35	32,32,32,32	0
57	MG	2a	1729	1/1	0.91	0.17	74,74,74,74	0
57	MG	1A	3798	1/1	0.91	0.23	51,51,51,51	0
57	MG	2a	1733	1/1	0.91	0.15	72,72,72,72	0
57	MG	1A	3803	1/1	0.91	0.12	57,57,57,57	0
57	MG	1A	3435	1/1	0.91	0.15	56,56,56,56	0
57	MG	2A	3390	1/1	0.91	0.15	64,64,64,64	0
57	MG	2a	1740	1/1	0.91	0.12	56,56,56,56	0
57	MG	1A	3076	1/1	0.91	0.39	42,42,42,42	0
57	MG	1a	1638	1/1	0.91	0.08	60,60,60,60	0
57	MG	2A	3002	1/1	0.91	0.40	49,49,49,49	0
57	MG	1A	3510	1/1	0.91	0.23	54,54,54,54	0
57	MG	1A	3179	1/1	0.91	0.20	38,38,38,38	0
57	MG	2A	3007	1/1	0.91	0.11	59,59,59,59	0
57	MG	2a	1755	1/1	0.91	0.21	46,46,46,46	0
57	MG	1a	1645	1/1	0.91	0.17	54,54,54,54	0
57	MG	1A	3147	1/1	0.91	0.43	38,38,38,38	0
57	MG	2a	1765	1/1	0.91	0.12	67,67,67,67	0
57	MG	2A	3405	1/1	0.91	0.25	61,61,61,61	0
57	MG	1A	3638	1/1	0.91	0.15	31,31,31,31	0
57	MG	1A	3079	1/1	0.91	0.46	33,33,33,33	0
57	MG	2A	3209	1/1	0.91	0.17	47,47,47,47	0
57	MG	2A	3743	1/1	0.91	0.16	70,70,70,70	0
57	MG	2A	3210	1/1	0.91	0.32	63,63,63,63	0
57	MG	1A	3818	1/1	0.91	0.07	41,41,41,41	0
57	MG	2A	3751	1/1	0.91	0.09	65,65,65,65	0
57	MG	2a	1782	1/1	0.91	0.21	70,70,70,70	0
57	MG	1a	1656	1/1	0.91	0.14	49,49,49,49	0
57	MG	2A	3419	1/1	0.91	0.32	61,61,61,61	0
57	MG	1A	3331	1/1	0.91	0.19	56,56,56,56	0
57	MG	1A	3964	1/1	0.91	0.17	24,24,24,24	0
57	MG	1a	1660	1/1	0.91	0.10	60,60,60,60	0
57	MG	1A	3517	1/1	0.91	0.26	23,23,23,23	0
57	MG	1A	3973	1/1	0.91	0.06	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	3033	1/1	0.91	0.50	55,55,55,55	0
57	MG	2a	1794	1/1	0.91	0.31	67,67,67,67	0
57	MG	2A	3222	1/1	0.91	0.19	62,62,62,62	0
57	MG	1A	3974	1/1	0.91	0.15	62,62,62,62	0
57	MG	1B	231	1/1	0.91	0.19	63,63,63,63	0
57	MG	1A	3218	1/1	0.91	0.41	36,36,36,36	0
57	MG	1A	3219	1/1	0.91	0.52	33,33,33,33	0
57	MG	2A	3452	1/1	0.91	0.14	39,39,39,39	0
57	MG	2a	1806	1/1	0.91	0.20	53,53,53,53	0
57	MG	2A	3460	1/1	0.91	0.26	51,51,51,51	0
57	MG	2A	3044	1/1	0.91	0.23	58,58,58,58	0
57	MG	1A	3103	1/1	0.91	0.49	34,34,34,34	0
57	MG	1A	3983	1/1	0.91	0.16	39,39,39,39	0
57	MG	1A	3091	1/1	0.91	0.12	32,32,32,32	0
57	MG	1A	3656	1/1	0.91	0.10	31,31,31,31	0
57	MG	2A	3052	1/1	0.91	0.21	59,59,59,59	0
57	MG	1A	3336	1/1	0.91	0.15	51,51,51,51	0
57	MG	1A	3664	1/1	0.91	0.22	38,38,38,38	0
57	MG	1A	3991	1/1	0.91	0.08	56,56,56,56	0
57	MG	2d	301	1/1	0.91	0.11	69,69,69,69	0
57	MG	1A	3300	1/1	0.91	0.21	56,56,56,56	0
57	MG	1A	3397	1/1	0.91	0.46	42,42,42,42	0
57	MG	2A	3061	1/1	0.91	0.20	37,37,37,37	0
57	MG	1A	3153	1/1	0.91	0.21	32,32,32,32	0
57	MG	1A	3673	1/1	0.91	0.08	37,37,37,37	0
57	MG	1a	1691	1/1	0.91	0.18	56,56,56,56	0
57	MG	2A	3497	1/1	0.91	0.10	40,40,40,40	0
57	MG	2A	3066	1/1	0.91	0.14	68,68,68,68	0
57	MG	2A	3067	1/1	0.91	0.27	51,51,51,51	0
57	MG	2A	3502	1/1	0.91	0.12	67,67,67,67	0
57	MG	2A	3503	1/1	0.91	0.15	40,40,40,40	0
57	MG	2D	301	1/1	0.91	0.17	42,42,42,42	0
57	MG	1A	3400	1/1	0.91	0.19	46,46,46,46	0
57	MG	2A	3508	1/1	0.91	0.13	76,76,76,76	0
57	MG	1A	3304	1/1	0.91	0.27	45,45,45,45	0
57	MG	1a	1696	1/1	0.91	0.23	57,57,57,57	0
57	MG	1G	205	1/1	0.91	0.17	49,49,49,49	0
57	MG	1A	3341	1/1	0.91	0.23	35,35,35,35	0
57	MG	1A	3547	1/1	0.91	0.14	42,42,42,42	0
57	MG	1A	3690	1/1	0.91	0.17	62,62,62,62	0
57	MG	1A	3480	1/1	0.92	0.12	52,52,52,52	0
57	MG	1A	3171	1/1	0.92	0.19	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	1a	1763	1/1	0.92	0.20	64,64,64,64	0
57	MG	1A	3839	1/1	0.92	0.14	30,30,30,30	0
57	MG	1A	3614	1/1	0.92	0.22	50,50,50,50	0
57	MG	1A	3715	1/1	0.92	0.17	20,20,20,20	0
57	MG	1A	3365	1/1	0.92	0.19	42,42,42,42	0
57	MG	1a	1771	1/1	0.92	0.13	45,45,45,45	0
57	MG	1A	3718	1/1	0.92	0.19	20,20,20,20	0
57	MG	1A	3957	1/1	0.92	0.12	26,26,26,26	0
57	MG	2A	3545	1/1	0.92	0.14	50,50,50,50	0
57	MG	2A	3295	1/1	0.92	0.09	70,70,70,70	0
57	MG	2A	3116	1/1	0.92	0.24	65,65,65,65	0
57	MG	15	106	1/1	0.92	0.09	61,61,61,61	0
57	MG	1A	3719	1/1	0.92	0.16	38,38,38,38	0
57	MG	2A	3554	1/1	0.92	0.33	63,63,63,63	0
57	MG	1A	4099	1/1	0.92	0.34	53,53,53,53	0
57	MG	2A	3559	1/1	0.92	0.12	67,67,67,67	0
57	MG	2A	3122	1/1	0.92	0.18	44,44,44,44	0
57	MG	1A	3084	1/1	0.92	0.54	45,45,45,45	0
57	MG	1a	1780	1/1	0.92	0.19	64,64,64,64	0
57	MG	1a	1782	1/1	0.92	0.14	54,54,54,54	0
57	MG	1a	1784	1/1	0.92	0.11	46,46,46,46	0
57	MG	1A	3721	1/1	0.92	0.15	42,42,42,42	0
57	MG	1a	1602	1/1	0.92	0.11	71,71,71,71	0
57	MG	2A	3308	1/1	0.92	0.17	70,70,70,70	0
57	MG	1A	3968	1/1	0.92	0.10	37,37,37,37	0
57	MG	1A	3230	1/1	0.92	0.40	28,28,28,28	0
57	MG	1a	1605	1/1	0.92	0.09	62,62,62,62	0
57	MG	1A	3198	1/1	0.92	0.14	59,59,59,59	0
57	MG	2a	1608	1/1	0.92	0.14	67,67,67,67	0
57	MG	1A	3542	1/1	0.92	0.26	37,37,37,37	0
57	MG	2A	3316	1/1	0.92	0.12	75,75,75,75	0
57	MG	1A	3623	1/1	0.92	0.26	30,30,30,30	0
57	MG	2a	1613	1/1	0.92	0.16	53,53,53,53	0
57	MG	1a	1797	1/1	0.92	0.09	66,66,66,66	0
57	MG	1A	3727	1/1	0.92	0.15	26,26,26,26	0
57	MG	1a	1621	1/1	0.92	0.09	43,43,43,43	0
57	MG	1A	3370	1/1	0.92	0.18	52,52,52,52	0
57	MG	1A	3255	1/1	0.92	0.32	46,46,46,46	0
57	MG	1a	1803	1/1	0.92	0.10	50,50,50,50	0
57	MG	1A	3736	1/1	0.92	0.15	33,33,33,33	0
57	MG	2a	1622	1/1	0.92	0.19	59,59,59,59	0
57	MG	1a	1808	1/1	0.92	0.14	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	1624	1/1	0.92	0.36	64,64,64,64	0
57	MG	2A	3591	1/1	0.92	0.06	66,66,66,66	0
57	MG	2A	3157	1/1	0.92	0.17	76,76,76,76	0
57	MG	1A	3737	1/1	0.92	0.13	50,50,50,50	0
57	MG	1A	3631	1/1	0.92	0.17	17,17,17,17	0
57	MG	2A	3602	1/1	0.92	0.15	31,31,31,31	0
57	MG	2A	3603	1/1	0.92	0.15	76,76,76,76	0
57	MG	1B	221	1/1	0.92	0.30	56,56,56,56	0
57	MG	2a	1634	1/1	0.92	0.27	62,62,62,62	0
57	MG	1A	3285	1/1	0.92	0.36	52,52,52,52	0
57	MG	2A	3340	1/1	0.92	0.37	56,56,56,56	0
57	MG	2A	3164	1/1	0.92	0.20	66,66,66,66	0
57	MG	1a	1631	1/1	0.92	0.28	59,59,59,59	0
57	MG	1A	3636	1/1	0.92	0.20	56,56,56,56	0
57	MG	1a	1634	1/1	0.92	0.15	74,74,74,74	0
57	MG	1r	101	1/1	0.92	0.18	69,69,69,69	0
57	MG	2A	3617	1/1	0.92	0.23	58,58,58,58	0
57	MG	2A	3169	1/1	0.92	0.18	40,40,40,40	0
57	MG	1B	225	1/1	0.92	0.17	37,37,37,37	0
57	MG	1a	1637	1/1	0.92	0.23	57,57,57,57	0
57	MG	1w	101	1/1	0.92	0.21	43,43,43,43	0
57	MG	2a	1653	1/1	0.92	0.17	47,47,47,47	0
57	MG	1A	3549	1/1	0.92	0.24	59,59,59,59	0
57	MG	2a	1655	1/1	0.92	0.14	68,68,68,68	0
57	MG	2A	3628	1/1	0.92	0.19	76,76,76,76	0
57	MG	2a	1659	1/1	0.92	0.09	64,64,64,64	0
57	MG	2a	1660	1/1	0.92	0.29	42,42,42,42	0
57	MG	2A	3629	1/1	0.92	0.23	61,61,61,61	0
57	MG	2A	3356	1/1	0.92	0.40	53,53,53,53	0
57	MG	1A	3018	1/1	0.92	0.21	50,50,50,50	0
57	MG	1w	105	1/1	0.92	0.08	68,68,68,68	0
57	MG	1A	3288	1/1	0.92	0.24	42,42,42,42	0
57	MG	1a	1641	1/1	0.92	0.08	61,61,61,61	0
57	MG	2A	3361	1/1	0.92	0.22	54,54,54,54	0
57	MG	1a	1642	1/1	0.92	0.21	64,64,64,64	0
57	MG	1A	3415	1/1	0.92	0.57	55,55,55,55	0
57	MG	1A	3645	1/1	0.92	0.17	29,29,29,29	0
57	MG	2a	1688	1/1	0.92	0.10	71,71,71,71	0
57	MG	1D	309	1/1	0.92	0.30	52,52,52,52	0
57	MG	1a	1650	1/1	0.92	0.10	44,44,44,44	0
57	MG	1A	3887	1/1	0.92	0.07	39,39,39,39	0
57	MG	2A	3189	1/1	0.92	0.16	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	1652	1/1	0.92	0.15	45,45,45,45	0
57	MG	2A	3657	1/1	0.92	0.17	49,49,49,49	0
57	MG	2a	1697	1/1	0.92	0.11	81,81,81,81	0
57	MG	2a	1698	1/1	0.92	0.08	74,74,74,74	0
57	MG	2A	3374	1/1	0.92	0.16	40,40,40,40	0
57	MG	2A	3659	1/1	0.92	0.10	69,69,69,69	0
57	MG	2A	3660	1/1	0.92	0.18	42,42,42,42	0
57	MG	1x	112	1/1	0.92	0.11	72,72,72,72	0
57	MG	2A	3378	1/1	0.92	0.15	59,59,59,59	0
57	MG	1A	4001	1/1	0.92	0.17	29,29,29,29	0
57	MG	2A	3668	1/1	0.92	0.10	56,56,56,56	0
57	MG	2A	3669	1/1	0.92	0.06	73,73,73,73	0
57	MG	1A	4003	1/1	0.92	0.17	45,45,45,45	0
57	MG	1A	3214	1/1	0.92	0.20	49,49,49,49	0
57	MG	2A	3383	1/1	0.92	0.23	42,42,42,42	0
57	MG	1A	3417	1/1	0.92	0.28	45,45,45,45	0
57	MG	1A	3453	1/1	0.92	0.43	48,48,48,48	0
57	MG	2A	3388	1/1	0.92	0.18	66,66,66,66	0
57	MG	1A	3292	1/1	0.92	0.32	47,47,47,47	0
57	MG	1A	4009	1/1	0.92	0.27	56,56,56,56	0
57	MG	1a	1664	1/1	0.92	0.20	64,64,64,64	0
57	MG	2A	3014	1/1	0.92	0.24	50,50,50,50	0
57	MG	2A	3015	1/1	0.92	0.20	58,58,58,58	0
57	MG	1A	4010	1/1	0.92	0.11	58,58,58,58	0
57	MG	1A	3896	1/1	0.92	0.11	36,36,36,36	0
57	MG	1A	3772	1/1	0.92	0.12	30,30,30,30	0
57	MG	1A	3316	1/1	0.92	0.11	55,55,55,55	0
57	MG	2A	3404	1/1	0.92	0.11	63,63,63,63	0
57	MG	2a	1730	1/1	0.92	0.12	87,87,87,87	0
57	MG	1A	3503	1/1	0.92	0.19	44,44,44,44	0
57	MG	2A	3706	1/1	0.92	0.14	39,39,39,39	0
57	MG	1a	1674	1/1	0.92	0.18	67,67,67,67	0
57	MG	2A	3409	1/1	0.92	0.17	54,54,54,54	0
57	MG	1A	4016	1/1	0.92	0.10	25,25,25,25	0
57	MG	1A	3661	1/1	0.92	0.16	46,46,46,46	0
57	MG	2a	1741	1/1	0.92	0.10	77,77,77,77	0
57	MG	1A	3782	1/1	0.92	0.11	34,34,34,34	0
57	MG	2A	3719	1/1	0.92	0.12	56,56,56,56	0
57	MG	2A	3720	1/1	0.92	0.15	58,58,58,58	0
57	MG	1A	3215	1/1	0.92	0.17	48,48,48,48	0
57	MG	2A	3218	1/1	0.92	0.14	58,58,58,58	0
57	MG	2a	1753	1/1	0.92	0.33	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1A	3319	1/1	0.92	0.10	67,67,67,67	0
57	MG	1A	3032	1/1	0.92	0.43	27,27,27,27	0
57	MG	2a	1759	1/1	0.92	0.12	81,81,81,81	0
57	MG	2A	3427	1/1	0.92	0.28	74,74,74,74	0
57	MG	2A	3736	1/1	0.92	0.09	56,56,56,56	0
57	MG	2A	3739	1/1	0.92	0.17	52,52,52,52	0
57	MG	2A	3740	1/1	0.92	0.17	62,62,62,62	0
57	MG	1A	3667	1/1	0.92	0.11	57,57,57,57	0
57	MG	1A	3107	1/1	0.92	0.16	33,33,33,33	0
57	MG	1A	3669	1/1	0.92	0.07	61,61,61,61	0
57	MG	2A	3746	1/1	0.92	0.11	55,55,55,55	0
57	MG	2a	1776	1/1	0.92	0.32	75,75,75,75	0
57	MG	1a	1689	1/1	0.92	0.22	53,53,53,53	0
57	MG	1P	205	1/1	0.92	0.38	41,41,41,41	0
57	MG	2A	3752	1/1	0.92	0.07	71,71,71,71	0
57	MG	1A	3576	1/1	0.92	0.14	41,41,41,41	0
57	MG	1A	3187	1/1	0.92	0.55	37,37,37,37	0
57	MG	1A	3674	1/1	0.92	0.19	58,58,58,58	0
57	MG	2A	3449	1/1	0.92	0.13	49,49,49,49	0
57	MG	1A	4037	1/1	0.92	0.14	58,58,58,58	0
57	MG	2A	3760	1/1	0.92	0.23	73,73,73,73	0
57	MG	2A	3761	1/1	0.92	0.09	57,57,57,57	0
57	MG	1A	3675	1/1	0.92	0.27	49,49,49,49	0
57	MG	1A	3801	1/1	0.92	0.07	53,53,53,53	0
57	MG	2A	3459	1/1	0.92	0.26	38,38,38,38	0
57	MG	1a	1699	1/1	0.92	0.23	51,51,51,51	0
57	MG	1A	3110	1/1	0.92	0.24	35,35,35,35	0
57	MG	1A	3354	1/1	0.92	0.35	43,43,43,43	0
57	MG	1U	203	1/1	0.92	0.59	53,53,53,53	0
57	MG	1A	3022	1/1	0.92	0.12	17,17,17,17	0
57	MG	1A	3521	1/1	0.92	0.26	40,40,40,40	0
57	MG	2A	3476	1/1	0.92	0.14	71,71,71,71	0
57	MG	1A	3360	1/1	0.92	0.16	57,57,57,57	0
57	MG	1A	3207	1/1	0.92	0.17	36,36,36,36	0
57	MG	1V	204	1/1	0.92	0.14	49,49,49,49	0
57	MG	2A	3787	1/1	0.92	0.08	58,58,58,58	0
57	MG	1A	3398	1/1	0.92	0.25	45,45,45,45	0
57	MG	1W	201	1/1	0.92	0.34	49,49,49,49	0
57	MG	1A	3531	1/1	0.92	0.27	42,42,42,42	0
57	MG	1a	1724	1/1	0.92	0.19	59,59,59,59	0
57	MG	1W	204	1/1	0.92	0.17	38,38,38,38	0
57	MG	1A	3698	1/1	0.92	0.22	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1821	1/1	0.92	0.05	66,66,66,66	0
57	MG	2A	3493	1/1	0.92	0.06	64,64,64,64	0
57	MG	2f	201	1/1	0.92	0.24	49,49,49,49	0
57	MG	1X	106	1/1	0.92	0.13	34,34,34,34	0
57	MG	1A	3820	1/1	0.92	0.21	56,56,56,56	0
57	MG	1a	1730	1/1	0.92	0.12	54,54,54,54	0
57	MG	1A	3605	1/1	0.92	0.11	27,27,27,27	0
57	MG	1a	1734	1/1	0.92	0.08	76,76,76,76	0
57	MG	2t	201	1/1	0.92	0.07	58,58,58,58	0
57	MG	2A	3082	1/1	0.92	0.07	78,78,78,78	0
57	MG	2A	3505	1/1	0.92	0.18	59,59,59,59	0
57	MG	1a	1736	1/1	0.92	0.19	54,54,54,54	0
57	MG	2w	105	1/1	0.92	0.39	51,51,51,51	0
57	MG	1A	3702	1/1	0.92	0.19	67,67,67,67	0
57	MG	1A	3532	1/1	0.92	0.44	46,46,46,46	0
57	MG	1A	4071	1/1	0.92	0.09	59,59,59,59	0
57	MG	1A	4073	1/1	0.92	0.13	66,66,66,66	0
57	MG	1A	3938	1/1	0.92	0.09	66,66,66,66	0
57	MG	1A	3939	1/1	0.92	0.15	65,65,65,65	0
57	MG	1a	1744	1/1	0.92	0.16	43,43,43,43	0
57	MG	1A	3706	1/1	0.92	0.16	40,40,40,40	0
57	MG	1A	3941	1/1	0.92	0.24	18,18,18,18	0
57	MG	1A	3942	1/1	0.92	0.16	31,31,31,31	0
57	MG	1a	1754	1/1	0.92	0.09	64,64,64,64	0
57	MG	1A	4079	1/1	0.92	0.21	48,48,48,48	0
57	MG	1A	3356	1/1	0.93	0.28	34,34,34,34	0
57	MG	1A	3845	1/1	0.93	0.13	29,29,29,29	0
57	MG	2A	3604	1/1	0.93	0.26	76,76,76,76	0
57	MG	1a	1713	1/1	0.93	0.22	37,37,37,37	0
57	MG	2A	3040	1/1	0.93	0.09	60,60,60,60	0
57	MG	2A	3201	1/1	0.93	0.11	59,59,59,59	0
57	MG	2a	1607	1/1	0.93	0.29	69,69,69,69	0
57	MG	1A	3639	1/1	0.93	0.19	61,61,61,61	0
57	MG	10	104	1/1	0.93	0.27	44,44,44,44	0
57	MG	1a	1718	1/1	0.93	0.12	55,55,55,55	0
57	MG	2A	3375	1/1	0.93	0.14	69,69,69,69	0
57	MG	1A	3852	1/1	0.93	0.16	23,23,23,23	0
57	MG	2A	3208	1/1	0.93	0.14	54,54,54,54	0
57	MG	2A	3048	1/1	0.93	0.11	48,48,48,48	0
57	MG	2A	3049	1/1	0.93	0.08	67,67,67,67	0
57	MG	2A	3620	1/1	0.93	0.24	71,71,71,71	0
57	MG	1A	3082	1/1	0.93	0.07	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	3948	1/1	0.93	0.22	40,40,40,40	0
57	MG	1A	3183	1/1	0.93	0.43	45,45,45,45	0
57	MG	1A	3856	1/1	0.93	0.19	49,49,49,49	0
57	MG	1A	4083	1/1	0.93	0.33	31,31,31,31	0
57	MG	1A	3011	1/1	0.93	0.10	48,48,48,48	0
57	MG	1A	3066	1/1	0.93	0.31	31,31,31,31	0
57	MG	1A	3958	1/1	0.93	0.07	37,37,37,37	0
57	MG	2A	3394	1/1	0.93	0.24	57,57,57,57	0
57	MG	2A	3635	1/1	0.93	0.07	68,68,68,68	0
57	MG	1a	1732	1/1	0.93	0.12	53,53,53,53	0
57	MG	2A	3062	1/1	0.93	0.22	55,55,55,55	0
57	MG	1A	3364	1/1	0.93	0.28	34,34,34,34	0
57	MG	1A	3017	1/1	0.93	0.24	28,28,28,28	0
57	MG	2a	1635	1/1	0.93	0.09	69,69,69,69	0
57	MG	1a	1735	1/1	0.93	0.20	58,58,58,58	0
57	MG	2A	3226	1/1	0.93	0.20	59,59,59,59	0
57	MG	1A	3963	1/1	0.93	0.13	34,34,34,34	0
57	MG	2A	3228	1/1	0.93	0.14	54,54,54,54	0
57	MG	2a	1640	1/1	0.93	0.12	67,67,67,67	0
57	MG	2a	1641	1/1	0.93	0.07	67,67,67,67	0
57	MG	1A	4096	1/1	0.93	0.14	50,50,50,50	0
57	MG	2A	3654	1/1	0.93	0.22	58,58,58,58	0
57	MG	1A	3071	1/1	0.93	0.42	47,47,47,47	0
57	MG	1A	3562	1/1	0.93	0.12	46,46,46,46	0
57	MG	1A	3969	1/1	0.93	0.12	37,37,37,37	0
57	MG	15	105	1/1	0.93	0.18	43,43,43,43	0
57	MG	2a	1648	1/1	0.93	0.08	66,66,66,66	0
57	MG	1a	1742	1/1	0.93	0.11	65,65,65,65	0
57	MG	2A	3661	1/1	0.93	0.18	41,41,41,41	0
57	MG	1A	3407	1/1	0.93	0.31	43,43,43,43	0
57	MG	2A	3663	1/1	0.93	0.10	66,66,66,66	0
57	MG	2A	3418	1/1	0.93	0.22	28,28,28,28	0
57	MG	2a	1656	1/1	0.93	0.26	63,63,63,63	0
57	MG	2A	3665	1/1	0.93	0.06	70,70,70,70	0
57	MG	1A	3749	1/1	0.93	0.20	47,47,47,47	0
57	MG	2A	3423	1/1	0.93	0.14	64,64,64,64	0
57	MG	1A	3658	1/1	0.93	0.24	31,31,31,31	0
57	MG	2a	1662	1/1	0.93	0.07	51,51,51,51	0
57	MG	17	105	1/1	0.93	0.16	50,50,50,50	0
57	MG	18	101	1/1	0.93	0.52	53,53,53,53	0
57	MG	18	102	1/1	0.93	0.19	39,39,39,39	0
57	MG	2a	1668	1/1	0.93	0.09	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1670	1/1	0.93	0.08	74,74,74,74	0
57	MG	1A	3263	1/1	0.93	0.40	39,39,39,39	0
57	MG	18	106	1/1	0.93	0.23	53,53,53,53	0
57	MG	2A	3438	1/1	0.93	0.19	69,69,69,69	0
57	MG	2A	3682	1/1	0.93	0.11	67,67,67,67	0
57	MG	1A	3978	1/1	0.93	0.07	66,66,66,66	0
57	MG	1a	1601	1/1	0.93	0.29	55,55,55,55	0
57	MG	1A	3875	1/1	0.93	0.08	31,31,31,31	0
57	MG	1A	3762	1/1	0.93	0.08	37,37,37,37	0
57	MG	1A	3264	1/1	0.93	0.25	49,49,49,49	0
57	MG	1A	3450	1/1	0.93	0.21	43,43,43,43	0
57	MG	1A	3194	1/1	0.93	0.14	22,22,22,22	0
57	MG	1A	3986	1/1	0.93	0.15	41,41,41,41	0
57	MG	2A	3697	1/1	0.93	0.06	72,72,72,72	0
57	MG	2A	3457	1/1	0.93	0.11	71,71,71,71	0
57	MG	2A	3458	1/1	0.93	0.16	46,46,46,46	0
57	MG	2A	3254	1/1	0.93	0.14	67,67,67,67	0
57	MG	1A	3769	1/1	0.93	0.08	57,57,57,57	0
57	MG	1A	3989	1/1	0.93	0.18	58,58,58,58	0
57	MG	1B	220	1/1	0.93	0.21	57,57,57,57	0
57	MG	2A	3465	1/1	0.93	0.10	60,60,60,60	0
57	MG	1A	3770	1/1	0.93	0.18	68,68,68,68	0
57	MG	1A	3883	1/1	0.93	0.12	45,45,45,45	0
57	MG	2A	3471	1/1	0.93	0.12	45,45,45,45	0
57	MG	1A	3302	1/1	0.93	0.16	54,54,54,54	0
57	MG	2A	3724	1/1	0.93	0.17	56,56,56,56	0
57	MG	2A	3726	1/1	0.93	0.10	61,61,61,61	0
57	MG	2A	3473	1/1	0.93	0.28	54,54,54,54	0
57	MG	2A	3475	1/1	0.93	0.12	46,46,46,46	0
57	MG	1A	3053	1/1	0.93	0.14	33,33,33,33	0
57	MG	1A	3579	1/1	0.93	0.10	34,34,34,34	0
57	MG	1A	3890	1/1	0.93	0.13	31,31,31,31	0
57	MG	2A	3479	1/1	0.93	0.13	39,39,39,39	0
57	MG	1A	3508	1/1	0.93	0.25	36,36,36,36	0
57	MG	2A	3268	1/1	0.93	0.16	44,44,44,44	0
57	MG	1A	3781	1/1	0.93	0.14	31,31,31,31	0
57	MG	1A	3893	1/1	0.93	0.15	43,43,43,43	0
57	MG	1A	3020	1/1	0.93	0.21	26,26,26,26	0
57	MG	2A	3109	1/1	0.93	0.31	45,45,45,45	0
57	MG	1A	3455	1/1	0.93	0.24	28,28,28,28	0
57	MG	2A	3113	1/1	0.93	0.17	52,52,52,52	0
57	MG	1A	3784	1/1	0.93	0.10	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	1A	3273	1/1	0.93	0.29	51,51,51,51	0
57	MG	2a	1734	1/1	0.93	0.43	70,70,70,70	0
57	MG	2a	1735	1/1	0.93	0.15	52,52,52,52	0
57	MG	2a	1736	1/1	0.93	0.19	56,56,56,56	0
57	MG	2A	3117	1/1	0.93	0.11	54,54,54,54	0
57	MG	1A	3899	1/1	0.93	0.22	66,66,66,66	0
57	MG	1E	308	1/1	0.93	0.27	40,40,40,40	0
57	MG	1A	3589	1/1	0.93	0.20	32,32,32,32	0
57	MG	1A	3901	1/1	0.93	0.07	53,53,53,53	0
57	MG	2A	3123	1/1	0.93	0.16	57,57,57,57	0
57	MG	1a	1644	1/1	0.93	0.07	49,49,49,49	0
57	MG	1A	3679	1/1	0.93	0.14	66,66,66,66	0
57	MG	1a	1804	1/1	0.93	0.20	64,64,64,64	0
57	MG	2A	3511	1/1	0.93	0.23	41,41,41,41	0
57	MG	1a	1646	1/1	0.93	0.09	54,54,54,54	0
57	MG	2A	3513	1/1	0.93	0.11	76,76,76,76	0
57	MG	1A	3791	1/1	0.93	0.24	40,40,40,40	0
57	MG	2a	1756	1/1	0.93	0.28	59,59,59,59	0
57	MG	1A	3590	1/1	0.93	0.18	24,24,24,24	0
57	MG	1A	3457	1/1	0.93	0.16	39,39,39,39	0
57	MG	1A	3683	1/1	0.93	0.08	62,62,62,62	0
57	MG	1A	3418	1/1	0.93	0.34	54,54,54,54	0
57	MG	2A	3139	1/1	0.93	0.16	61,61,61,61	0
57	MG	2A	3520	1/1	0.93	0.22	41,41,41,41	0
57	MG	2A	3521	1/1	0.93	0.17	45,45,45,45	0
57	MG	2a	1769	1/1	0.93	0.09	64,64,64,64	0
57	MG	1G	202	1/1	0.93	0.24	67,67,67,67	0
57	MG	2a	1772	1/1	0.93	0.17	62,62,62,62	0
57	MG	1A	3241	1/1	0.93	0.15	49,49,49,49	0
57	MG	1A	3242	1/1	0.93	0.66	57,57,57,57	0
57	MG	2A	3527	1/1	0.93	0.25	59,59,59,59	0
57	MG	1a	1658	1/1	0.93	0.20	65,65,65,65	0
57	MG	2A	3530	1/1	0.93	0.30	39,39,39,39	0
57	MG	1A	4024	1/1	0.93	0.14	22,22,22,22	0
57	MG	1A	3465	1/1	0.93	0.16	52,52,52,52	0
57	MG	1A	3522	1/1	0.93	0.61	38,38,38,38	0
57	MG	1A	3466	1/1	0.93	0.37	56,56,56,56	0
57	MG	2B	206	1/1	0.93	0.21	73,73,73,73	0
57	MG	1A	3914	1/1	0.93	0.14	32,32,32,32	0
57	MG	2A	3154	1/1	0.93	0.10	60,60,60,60	0
57	MG	1A	3608	1/1	0.93	0.14	44,44,44,44	0
57	MG	1A	3611	1/1	0.93	0.18	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1P	201	1/1	0.93	0.54	32,32,32,32	0
57	MG	1a	1668	1/1	0.93	0.23	56,56,56,56	0
57	MG	1a	1670	1/1	0.93	0.16	75,75,75,75	0
57	MG	1x	105	1/1	0.93	0.20	63,63,63,63	0
57	MG	1A	3161	1/1	0.93	0.14	38,38,38,38	0
57	MG	2A	3553	1/1	0.93	0.15	61,61,61,61	0
57	MG	2D	304	1/1	0.93	0.19	27,27,27,27	0
57	MG	1A	3920	1/1	0.93	0.26	52,52,52,52	0
57	MG	1Q	202	1/1	0.93	0.17	35,35,35,35	0
57	MG	1A	4036	1/1	0.93	0.14	50,50,50,50	0
57	MG	1A	3921	1/1	0.93	0.12	27,27,27,27	0
57	MG	1A	3311	1/1	0.93	0.09	54,54,54,54	0
57	MG	2a	1813	1/1	0.93	0.22	45,45,45,45	0
57	MG	2E	304	1/1	0.93	0.22	34,34,34,34	0
57	MG	1A	3278	1/1	0.93	0.26	53,53,53,53	0
57	MG	1A	3472	1/1	0.93	0.37	35,35,35,35	0
57	MG	2E	307	1/1	0.93	0.20	45,45,45,45	0
57	MG	2E	309	1/1	0.93	0.11	67,67,67,67	0
57	MG	1A	3115	1/1	0.93	0.24	38,38,38,38	0
57	MG	1A	3534	1/1	0.93	0.15	40,40,40,40	0
57	MG	1A	3387	1/1	0.93	0.25	51,51,51,51	0
57	MG	1A	4050	1/1	0.93	0.11	61,61,61,61	0
57	MG	1A	3220	1/1	0.93	0.19	51,51,51,51	0
57	MG	2F	306	1/1	0.93	0.41	48,48,48,48	0
57	MG	2A	3012	1/1	0.93	0.21	48,48,48,48	0
57	MG	1A	3078	1/1	0.93	0.22	34,34,34,34	0
57	MG	2q	201	1/1	0.93	0.08	77,77,77,77	0
57	MG	1A	3478	1/1	0.93	0.08	74,74,74,74	0
57	MG	1A	4056	1/1	0.93	0.08	50,50,50,50	0
57	MG	1A	3828	1/1	0.93	0.42	38,38,38,38	0
57	MG	2A	3349	1/1	0.93	0.39	54,54,54,54	0
57	MG	2v	104	1/1	0.93	0.31	62,62,62,62	0
57	MG	1A	3145	1/1	0.93	0.57	39,39,39,39	0
57	MG	1A	3629	1/1	0.93	0.14	21,21,21,21	0
57	MG	1A	3351	1/1	0.93	0.57	47,47,47,47	0
57	MG	2w	107	1/1	0.93	0.17	70,70,70,70	0
57	MG	2x	101	1/1	0.93	0.27	68,68,68,68	0
57	MG	2A	3188	1/1	0.93	0.30	51,51,51,51	0
57	MG	2A	3355	1/1	0.93	0.20	42,42,42,42	0
57	MG	1A	3047	1/1	0.93	0.30	34,34,34,34	0
57	MG	1a	1702	1/1	0.93	0.23	38,38,38,38	0
57	MG	2x	106	1/1	0.93	0.09	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3433	1/1	0.93	0.21	47,47,47,47	0
57	MG	1A	3048	1/1	0.93	0.16	27,27,27,27	0
57	MG	1A	4072	1/1	0.93	0.14	57,57,57,57	0
57	MG	2A	3595	1/1	0.93	0.32	56,56,56,56	0
58	K	1A	3512	1/1	0.93	0.12	54,54,54,54	0
59	TYK	2A	3798	64/64	0.93	0.26	32,46,61,66	0
57	MG	25	104	1/1	0.93	0.16	57,57,57,57	0
57	MG	1Y	202	1/1	0.93	0.54	46,46,46,46	0
57	MG	2A	3034	1/1	0.93	0.25	60,60,60,60	0
60	ZN	29	102	1/1	0.93	0.09	78,78,78,78	0
57	MG	1S	201	1/1	0.94	0.35	44,44,44,44	0
57	MG	28	103	1/1	0.94	0.36	57,57,57,57	0
57	MG	1A	4046	1/1	0.94	0.16	43,43,43,43	0
57	MG	28	105	1/1	0.94	0.12	63,63,63,63	0
57	MG	29	101	1/1	0.94	0.30	69,69,69,69	0
57	MG	2a	1601	1/1	0.94	0.22	81,81,81,81	0
57	MG	1A	3059	1/1	0.94	0.25	44,44,44,44	0
57	MG	2a	1603	1/1	0.94	0.12	58,58,58,58	0
57	MG	1a	1683	1/1	0.94	0.12	55,55,55,55	0
57	MG	1A	3606	1/1	0.94	0.10	31,31,31,31	0
57	MG	2A	3607	1/1	0.94	0.14	50,50,50,50	0
57	MG	1A	3250	1/1	0.94	0.13	51,51,51,51	0
57	MG	2A	3372	1/1	0.94	0.12	59,59,59,59	0
57	MG	2a	1609	1/1	0.94	0.06	71,71,71,71	0
57	MG	1U	202	1/1	0.94	0.29	36,36,36,36	0
57	MG	1A	4052	1/1	0.94	0.13	50,50,50,50	0
57	MG	1A	4053	1/1	0.94	0.17	24,24,24,24	0
57	MG	1U	206	1/1	0.94	0.22	33,33,33,33	0
57	MG	1A	3825	1/1	0.94	0.13	38,38,38,38	0
57	MG	2A	3380	1/1	0.94	0.23	58,58,58,58	0
57	MG	1A	3195	1/1	0.94	0.15	34,34,34,34	0
57	MG	2A	3028	1/1	0.94	0.29	50,50,50,50	0
57	MG	1A	3098	1/1	0.94	0.27	35,35,35,35	0
57	MG	2A	3384	1/1	0.94	0.15	63,63,63,63	0
57	MG	2A	3200	1/1	0.94	0.34	60,60,60,60	0
57	MG	2a	1621	1/1	0.94	0.20	61,61,61,61	0
57	MG	1A	3253	1/1	0.94	0.15	60,60,60,60	0
57	MG	1A	3518	1/1	0.94	0.40	54,54,54,54	0
57	MG	1A	3834	1/1	0.94	0.26	49,49,49,49	0
57	MG	1A	3013	1/1	0.94	0.24	29,29,29,29	0
57	MG	1A	3347	1/1	0.94	0.21	47,47,47,47	0
57	MG	2A	3393	1/1	0.94	0.22	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	2A	3038	1/1	0.94	0.10	70,70,70,70	0
57	MG	1W	205	1/1	0.94	0.09	35,35,35,35	0
57	MG	1W	206	1/1	0.94	0.17	28,28,28,28	0
57	MG	1a	1706	1/1	0.94	0.25	63,63,63,63	0
57	MG	1A	3004	1/1	0.94	0.12	25,25,25,25	0
57	MG	1X	104	1/1	0.94	0.21	40,40,40,40	0
57	MG	1A	3842	1/1	0.94	0.14	23,23,23,23	0
57	MG	1A	3257	1/1	0.94	0.34	58,58,58,58	0
57	MG	1A	3458	1/1	0.94	0.19	55,55,55,55	0
57	MG	2A	3650	1/1	0.94	0.37	47,47,47,47	0
57	MG	1A	3530	1/1	0.94	0.14	41,41,41,41	0
57	MG	2A	3408	1/1	0.94	0.10	65,65,65,65	0
57	MG	2A	3655	1/1	0.94	0.12	70,70,70,70	0
57	MG	1A	3847	1/1	0.94	0.14	42,42,42,42	0
57	MG	1A	3950	1/1	0.94	0.08	58,58,58,58	0
57	MG	1a	1719	1/1	0.94	0.06	82,82,82,82	0
57	MG	1A	3951	1/1	0.94	0.22	52,52,52,52	0
57	MG	1A	3033	1/1	0.94	0.71	39,39,39,39	0
57	MG	1A	3460	1/1	0.94	0.09	51,51,51,51	0
57	MG	2A	3417	1/1	0.94	0.22	63,63,63,63	0
57	MG	1A	4081	1/1	0.94	0.07	57,57,57,57	0
57	MG	2A	3059	1/1	0.94	0.36	55,55,55,55	0
57	MG	1A	3954	1/1	0.94	0.25	31,31,31,31	0
57	MG	1A	3733	1/1	0.94	0.11	36,36,36,36	0
57	MG	2A	3426	1/1	0.94	0.11	44,44,44,44	0
57	MG	2a	1657	1/1	0.94	0.07	62,62,62,62	0
57	MG	11	101	1/1	0.94	1.08	39,39,39,39	0
57	MG	2A	3429	1/1	0.94	0.25	67,67,67,67	0
57	MG	2A	3672	1/1	0.94	0.07	65,65,65,65	0
57	MG	1A	3734	1/1	0.94	0.14	27,27,27,27	0
57	MG	1A	3225	1/1	0.94	0.22	61,61,61,61	0
57	MG	11	104	1/1	0.94	0.14	78,78,78,78	0
57	MG	2A	3434	1/1	0.94	0.20	38,38,38,38	0
57	MG	2A	3679	1/1	0.94	0.10	71,71,71,71	0
57	MG	2A	3234	1/1	0.94	0.28	62,62,62,62	0
57	MG	2a	1669	1/1	0.94	0.24	72,72,72,72	0
57	MG	1A	4089	1/1	0.94	0.30	58,58,58,58	0
57	MG	2a	1673	1/1	0.94	0.12	64,64,64,64	0
57	MG	2A	3683	1/1	0.94	0.13	72,72,72,72	0
57	MG	2a	1679	1/1	0.94	0.27	69,69,69,69	0
57	MG	2A	3684	1/1	0.94	0.17	50,50,50,50	0
57	MG	2A	3068	1/1	0.94	0.34	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	3961	1/1	0.94	0.19	64,64,64,64	0
57	MG	2A	3442	1/1	0.94	0.18	41,41,41,41	0
57	MG	1A	3106	1/1	0.94	0.35	40,40,40,40	0
57	MG	1A	3050	1/1	0.94	0.11	45,45,45,45	0
57	MG	2A	3691	1/1	0.94	0.10	57,57,57,57	0
57	MG	1A	3410	1/1	0.94	0.17	31,31,31,31	0
57	MG	2A	3693	1/1	0.94	0.17	71,71,71,71	0
57	MG	1A	3966	1/1	0.94	0.20	40,40,40,40	0
57	MG	1A	3228	1/1	0.94	0.17	24,24,24,24	0
57	MG	1A	3539	1/1	0.94	0.18	49,49,49,49	0
57	MG	2A	3453	1/1	0.94	0.16	38,38,38,38	0
57	MG	2A	3702	1/1	0.94	0.15	69,69,69,69	0
57	MG	1A	3229	1/1	0.94	0.17	45,45,45,45	0
57	MG	1A	3470	1/1	0.94	0.59	35,35,35,35	0
57	MG	1A	3108	1/1	0.94	0.29	37,37,37,37	0
57	MG	2a	1702	1/1	0.94	0.27	64,64,64,64	0
57	MG	1A	3872	1/1	0.94	0.16	41,41,41,41	0
57	MG	17	101	1/1	0.94	0.11	32,32,32,32	0
57	MG	2A	3250	1/1	0.94	0.25	57,57,57,57	0
57	MG	2a	1709	1/1	0.94	0.21	72,72,72,72	0
57	MG	1a	1746	1/1	0.94	0.14	58,58,58,58	0
57	MG	2A	3083	1/1	0.94	0.12	75,75,75,75	0
57	MG	1A	3231	1/1	0.94	0.58	42,42,42,42	0
57	MG	1B	205	1/1	0.94	0.29	58,58,58,58	0
57	MG	2A	3723	1/1	0.94	0.26	43,43,43,43	0
57	MG	2A	3256	1/1	0.94	0.11	73,73,73,73	0
57	MG	1A	3750	1/1	0.94	0.19	53,53,53,53	0
57	MG	2A	3727	1/1	0.94	0.26	50,50,50,50	0
57	MG	2a	1718	1/1	0.94	0.22	82,82,82,82	0
57	MG	2A	3729	1/1	0.94	0.10	74,74,74,74	0
57	MG	2A	3474	1/1	0.94	0.18	78,78,78,78	0
57	MG	1A	3754	1/1	0.94	0.16	19,19,19,19	0
57	MG	1a	1758	1/1	0.94	0.06	63,63,63,63	0
57	MG	1A	3232	1/1	0.94	0.10	46,46,46,46	0
57	MG	18	105	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	3756	1/1	0.94	0.06	39,39,39,39	0
57	MG	1A	3142	1/1	0.94	0.16	32,32,32,32	0
57	MG	1a	1765	1/1	0.94	0.14	57,57,57,57	0
57	MG	1a	1766	1/1	0.94	0.15	64,64,64,64	0
57	MG	19	101	1/1	0.94	0.21	52,52,52,52	0
57	MG	2A	3744	1/1	0.94	0.16	43,43,43,43	0
57	MG	2A	3097	1/1	0.94	0.46	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3269	1/1	0.94	0.24	66,66,66,66	0
57	MG	2A	3747	1/1	0.94	0.15	58,58,58,58	0
57	MG	1A	3317	1/1	0.94	0.43	41,41,41,41	0
57	MG	1A	3551	1/1	0.94	0.14	33,33,33,33	0
57	MG	1A	3274	1/1	0.94	0.07	37,37,37,37	0
57	MG	2A	3495	1/1	0.94	0.17	63,63,63,63	0
57	MG	1A	3007	1/1	0.94	0.17	35,35,35,35	0
57	MG	1A	3369	1/1	0.94	0.12	55,55,55,55	0
57	MG	1a	1606	1/1	0.94	0.26	60,60,60,60	0
57	MG	2A	3104	1/1	0.94	0.23	55,55,55,55	0
57	MG	2a	1747	1/1	0.94	0.12	72,72,72,72	0
57	MG	1a	1609	1/1	0.94	0.36	56,56,56,56	0
57	MG	2A	3504	1/1	0.94	0.24	72,72,72,72	0
57	MG	2A	3281	1/1	0.94	0.24	67,67,67,67	0
57	MG	2A	3763	1/1	0.94	0.22	60,60,60,60	0
57	MG	1A	3206	1/1	0.94	0.11	39,39,39,39	0
57	MG	1A	3236	1/1	0.94	0.30	36,36,36,36	0
57	MG	1a	1614	1/1	0.94	0.24	56,56,56,56	0
57	MG	2a	1757	1/1	0.94	0.23	69,69,69,69	0
57	MG	2A	3111	1/1	0.94	0.33	57,57,57,57	0
57	MG	1A	3325	1/1	0.94	0.27	39,39,39,39	0
57	MG	1a	1616	1/1	0.94	0.13	61,61,61,61	0
57	MG	1A	3559	1/1	0.94	0.28	44,44,44,44	0
57	MG	1A	3560	1/1	0.94	0.17	21,21,21,21	0
57	MG	1A	3999	1/1	0.94	0.26	34,34,34,34	0
57	MG	1A	3780	1/1	0.94	0.11	37,37,37,37	0
57	MG	1A	3666	1/1	0.94	0.12	43,43,43,43	0
57	MG	1A	4002	1/1	0.94	0.11	34,34,34,34	0
57	MG	2a	1771	1/1	0.94	0.19	76,76,76,76	0
57	MG	1A	3087	1/1	0.94	0.20	27,27,27,27	0
57	MG	1A	3113	1/1	0.94	0.18	34,34,34,34	0
57	MG	2A	3789	1/1	0.94	0.31	55,55,55,55	0
57	MG	1A	3281	1/1	0.94	0.13	58,58,58,58	0
57	MG	1a	1798	1/1	0.94	0.15	70,70,70,70	0
57	MG	1E	303	1/1	0.94	0.22	36,36,36,36	0
57	MG	2A	3130	1/1	0.94	0.24	43,43,43,43	0
57	MG	1A	3010	1/1	0.94	0.16	31,31,31,31	0
57	MG	1A	3184	1/1	0.94	0.15	30,30,30,30	0
57	MG	1a	1635	1/1	0.94	0.10	49,49,49,49	0
57	MG	2A	3533	1/1	0.94	0.12	60,60,60,60	0
57	MG	2a	1787	1/1	0.94	0.20	67,67,67,67	0
57	MG	1A	3787	1/1	0.94	0.28	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	1789	1/1	0.94	0.20	60,60,60,60	0
57	MG	2A	3135	1/1	0.94	0.34	44,44,44,44	0
57	MG	1A	3788	1/1	0.94	0.20	59,59,59,59	0
57	MG	2a	1792	1/1	0.94	0.15	76,76,76,76	0
57	MG	1F	301	1/1	0.94	0.23	34,34,34,34	0
57	MG	1A	3005	1/1	0.94	0.23	45,45,45,45	0
57	MG	1A	3790	1/1	0.94	0.16	70,70,70,70	0
57	MG	2A	3141	1/1	0.94	0.16	50,50,50,50	0
57	MG	2A	3142	1/1	0.94	0.16	62,62,62,62	0
57	MG	1A	3380	1/1	0.94	0.10	68,68,68,68	0
57	MG	2a	1801	1/1	0.94	0.09	83,83,83,83	0
57	MG	2B	216	1/1	0.94	0.14	68,68,68,68	0
57	MG	2A	3546	1/1	0.94	0.15	46,46,46,46	0
57	MG	1A	3676	1/1	0.94	0.15	45,45,45,45	0
57	MG	1a	1643	1/1	0.94	0.17	67,67,67,67	0
57	MG	1A	3572	1/1	0.94	0.13	21,21,21,21	0
57	MG	1A	3213	1/1	0.94	0.50	45,45,45,45	0
57	MG	2A	3149	1/1	0.94	0.43	72,72,72,72	0
57	MG	1A	3382	1/1	0.94	0.12	59,59,59,59	0
57	MG	1e	201	1/1	0.94	0.12	72,72,72,72	0
57	MG	1f	201	1/1	0.94	0.16	41,41,41,41	0
57	MG	1m	3001	1/1	0.94	0.11	58,58,58,58	0
57	MG	2A	3329	1/1	0.94	0.27	43,43,43,43	0
57	MG	1A	4021	1/1	0.94	0.21	19,19,19,19	0
57	MG	1A	3437	1/1	0.94	0.11	45,45,45,45	0
57	MG	2E	308	1/1	0.94	0.08	61,61,61,61	0
57	MG	1A	3383	1/1	0.94	0.22	54,54,54,54	0
57	MG	2A	3336	1/1	0.94	0.28	47,47,47,47	0
57	MG	1A	3044	1/1	0.94	0.16	35,35,35,35	0
57	MG	1A	3913	1/1	0.94	0.06	43,43,43,43	0
57	MG	1A	3499	1/1	0.94	0.07	58,58,58,58	0
57	MG	2A	3572	1/1	0.94	0.10	56,56,56,56	0
57	MG	1N	203	1/1	0.94	0.12	44,44,44,44	0
57	MG	1A	3385	1/1	0.94	0.35	63,63,63,63	0
57	MG	1O	202	1/1	0.94	0.30	50,50,50,50	0
57	MG	1A	3386	1/1	0.94	0.20	48,48,48,48	0
57	MG	1A	3045	1/1	0.94	0.15	39,39,39,39	0
57	MG	1A	3919	1/1	0.94	0.22	51,51,51,51	0
57	MG	2w	101	1/1	0.94	0.38	66,66,66,66	0
57	MG	1O	206	1/1	0.94	0.24	65,65,65,65	0
57	MG	2A	3581	1/1	0.94	0.20	64,64,64,64	0
57	MG	2Q	204	1/1	0.94	0.18	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	2R	201	1/1	0.94	0.34	50,50,50,50	0
57	MG	1A	3594	1/1	0.94	0.08	58,58,58,58	0
57	MG	1A	3504	1/1	0.94	0.37	37,37,37,37	0
57	MG	1P	204	1/1	0.94	0.72	28,28,28,28	0
57	MG	2A	3585	1/1	0.94	0.28	57,57,57,57	0
57	MG	1A	3811	1/1	0.94	0.07	64,64,64,64	0
57	MG	1A	3245	1/1	0.94	0.14	77,77,77,77	0
57	MG	1A	3816	1/1	0.94	0.65	41,41,41,41	0
57	MG	1R	202	1/1	0.94	0.30	37,37,37,37	0
57	MG	2I	102	1/1	0.94	0.14	68,68,68,68	0
57	MG	23	102	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3151	1/1	0.94	0.54	39,39,39,39	0
57	MG	1R	204	1/1	0.94	0.21	30,30,30,30	0
60	ZN	1Y	203	1/1	0.94	0.12	68,68,68,68	0
57	MG	1A	3217	1/1	0.94	0.12	22,22,22,22	0
57	MG	27	101	1/1	0.94	0.27	59,59,59,59	0
57	MG	1A	3391	1/1	0.94	0.20	36,36,36,36	0
57	MG	2A	3008	1/1	0.94	0.20	49,49,49,49	0
60	ZN	2n	501	1/1	0.94	0.07	86,86,86,86	0
57	MG	2A	3454	1/1	0.95	0.17	35,35,35,35	0
57	MG	2A	3118	1/1	0.95	0.18	49,49,49,49	0
57	MG	1A	4068	1/1	0.95	0.29	36,36,36,36	0
57	MG	2a	1629	1/1	0.95	0.31	73,73,73,73	0
57	MG	2A	3272	1/1	0.95	0.30	52,52,52,52	0
57	MG	2A	3676	1/1	0.95	0.07	61,61,61,61	0
57	MG	1A	4069	1/1	0.95	0.09	63,63,63,63	0
57	MG	1A	4070	1/1	0.95	0.15	45,45,45,45	0
57	MG	2A	3462	1/1	0.95	0.23	31,31,31,31	0
57	MG	1A	3771	1/1	0.95	0.14	73,73,73,73	0
57	MG	2A	3681	1/1	0.95	0.11	40,40,40,40	0
57	MG	2A	3464	1/1	0.95	0.24	59,59,59,59	0
57	MG	1A	3591	1/1	0.95	0.22	54,54,54,54	0
57	MG	1A	3965	1/1	0.95	0.11	32,32,32,32	0
57	MG	2A	3469	1/1	0.95	0.15	39,39,39,39	0
57	MG	1A	3592	1/1	0.95	0.12	27,27,27,27	0
57	MG	1A	3593	1/1	0.95	0.09	22,22,22,22	0
57	MG	2A	3128	1/1	0.95	0.25	56,56,56,56	0
57	MG	2A	3129	1/1	0.95	0.29	41,41,41,41	0
57	MG	1A	3473	1/1	0.95	0.60	38,38,38,38	0
57	MG	1e	202	1/1	0.95	0.40	58,58,58,58	0
57	MG	1A	3779	1/1	0.95	0.10	30,30,30,30	0
57	MG	1h	201	1/1	0.95	0.29	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1T	203	1/1	0.95	0.20	62,62,62,62	0
57	MG	1A	3972	1/1	0.95	0.12	46,46,46,46	0
57	MG	1A	3595	1/1	0.95	0.15	36,36,36,36	0
57	MG	1a	1669	1/1	0.95	0.18	64,64,64,64	0
57	MG	1U	204	1/1	0.95	0.18	35,35,35,35	0
57	MG	1A	3248	1/1	0.95	0.19	32,32,32,32	0
57	MG	1A	3064	1/1	0.95	0.37	48,48,48,48	0
57	MG	1A	3976	1/1	0.95	0.12	57,57,57,57	0
57	MG	1a	1675	1/1	0.95	0.28	58,58,58,58	0
57	MG	1A	4084	1/1	0.95	0.22	73,73,73,73	0
57	MG	1A	3172	1/1	0.95	0.12	35,35,35,35	0
57	MG	1V	201	1/1	0.95	0.27	28,28,28,28	0
57	MG	1A	3065	1/1	0.95	0.19	14,14,14,14	0
57	MG	1A	4088	1/1	0.95	0.19	75,75,75,75	0
57	MG	1A	3980	1/1	0.95	0.05	54,54,54,54	0
57	MG	1A	3284	1/1	0.95	0.27	41,41,41,41	0
57	MG	1A	4092	1/1	0.95	0.10	72,72,72,72	0
57	MG	1A	3353	1/1	0.95	0.20	55,55,55,55	0
57	MG	1A	3692	1/1	0.95	0.10	46,46,46,46	0
57	MG	2A	3310	1/1	0.95	0.17	64,64,64,64	0
57	MG	1A	3392	1/1	0.95	0.24	49,49,49,49	0
57	MG	2A	3732	1/1	0.95	0.11	64,64,64,64	0
57	MG	2a	1681	1/1	0.95	0.33	35,35,35,35	0
57	MG	1A	3393	1/1	0.95	0.38	47,47,47,47	0
57	MG	1A	3436	1/1	0.95	0.18	46,46,46,46	0
57	MG	1A	3609	1/1	0.95	0.22	39,39,39,39	0
57	MG	2a	1685	1/1	0.95	0.17	65,65,65,65	0
57	MG	2A	3004	1/1	0.95	0.10	50,50,50,50	0
57	MG	2A	3737	1/1	0.95	0.18	48,48,48,48	0
57	MG	2A	3738	1/1	0.95	0.10	58,58,58,58	0
57	MG	2a	1690	1/1	0.95	0.08	66,66,66,66	0
57	MG	1A	3700	1/1	0.95	0.18	24,24,24,24	0
57	MG	2a	1692	1/1	0.95	0.12	73,73,73,73	0
57	MG	2A	3163	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3176	1/1	0.95	0.20	48,48,48,48	0
57	MG	10	101	1/1	0.95	0.30	43,43,43,43	0
57	MG	1A	3043	1/1	0.95	0.22	42,42,42,42	0
57	MG	1A	3081	1/1	0.95	0.27	37,37,37,37	0
57	MG	2A	3323	1/1	0.95	0.07	67,67,67,67	0
57	MG	1A	3544	1/1	0.95	0.25	27,27,27,27	0
57	MG	2A	3748	1/1	0.95	0.20	68,68,68,68	0
57	MG	1a	1703	1/1	0.95	0.26	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3995	1/1	0.95	0.14	37,37,37,37	0
57	MG	2A	3172	1/1	0.95	0.13	56,56,56,56	0
57	MG	1A	3797	1/1	0.95	0.10	36,36,36,36	0
57	MG	1A	3707	1/1	0.95	0.14	67,67,67,67	0
57	MG	2A	3331	1/1	0.95	0.37	48,48,48,48	0
57	MG	2A	3333	1/1	0.95	0.26	61,61,61,61	0
57	MG	1B	209	1/1	0.95	0.25	57,57,57,57	0
57	MG	2A	3759	1/1	0.95	0.18	64,64,64,64	0
57	MG	1A	3489	1/1	0.95	0.27	38,38,38,38	0
57	MG	2A	3024	1/1	0.95	0.12	39,39,39,39	0
57	MG	2A	3338	1/1	0.95	0.18	39,39,39,39	0
57	MG	2A	3179	1/1	0.95	0.68	65,65,65,65	0
57	MG	10	110	1/1	0.95	0.07	42,42,42,42	0
57	MG	2A	3767	1/1	0.95	0.28	66,66,66,66	0
57	MG	1A	3802	1/1	0.95	0.25	50,50,50,50	0
57	MG	2A	3342	1/1	0.95	0.42	54,54,54,54	0
57	MG	2A	3772	1/1	0.95	0.14	49,49,49,49	0
57	MG	1A	3289	1/1	0.95	0.47	56,56,56,56	0
57	MG	1A	3290	1/1	0.95	0.15	35,35,35,35	0
57	MG	2a	1724	1/1	0.95	0.12	69,69,69,69	0
57	MG	2A	3345	1/1	0.95	0.17	56,56,56,56	0
57	MG	1A	3713	1/1	0.95	0.17	51,51,51,51	0
57	MG	1A	3548	1/1	0.95	0.16	36,36,36,36	0
57	MG	2A	3779	1/1	0.95	0.20	82,82,82,82	0
57	MG	2A	3031	1/1	0.95	0.12	47,47,47,47	0
57	MG	1A	3323	1/1	0.95	0.18	35,35,35,35	0
57	MG	1A	3622	1/1	0.95	0.11	39,39,39,39	0
57	MG	1A	3182	1/1	0.95	0.11	51,51,51,51	0
57	MG	1A	3624	1/1	0.95	0.12	29,29,29,29	0
57	MG	1B	223	1/1	0.95	0.11	58,58,58,58	0
57	MG	1A	3129	1/1	0.95	0.16	39,39,39,39	0
57	MG	2A	3790	1/1	0.95	0.17	60,60,60,60	0
57	MG	1A	3132	1/1	0.95	0.12	29,29,29,29	0
57	MG	2A	3041	1/1	0.95	0.08	62,62,62,62	0
57	MG	1A	3917	1/1	0.95	0.22	52,52,52,52	0
57	MG	1B	228	1/1	0.95	0.30	77,77,77,77	0
57	MG	2a	1742	1/1	0.95	0.24	47,47,47,47	0
57	MG	2a	1743	1/1	0.95	0.15	69,69,69,69	0
57	MG	1A	3404	1/1	0.95	0.29	37,37,37,37	0
57	MG	2A	3796	1/1	0.95	0.40	77,77,77,77	0
57	MG	1B	230	1/1	0.95	0.14	49,49,49,49	0
57	MG	1A	3094	1/1	0.95	0.13	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	3295	1/1	0.95	0.37	63,63,63,63	0
57	MG	2B	203	1/1	0.95	0.15	73,73,73,73	0
57	MG	2a	1752	1/1	0.95	0.11	53,53,53,53	0
57	MG	2A	3571	1/1	0.95	0.17	46,46,46,46	0
57	MG	2B	205	1/1	0.95	0.17	57,57,57,57	0
57	MG	1A	3211	1/1	0.95	0.20	45,45,45,45	0
57	MG	1D	301	1/1	0.95	0.27	36,36,36,36	0
57	MG	1A	3408	1/1	0.95	0.55	46,46,46,46	0
57	MG	2A	3204	1/1	0.95	0.40	48,48,48,48	0
57	MG	1A	3038	1/1	0.95	0.39	36,36,36,36	0
57	MG	1D	312	1/1	0.95	0.27	39,39,39,39	0
57	MG	2a	1762	1/1	0.95	0.22	63,63,63,63	0
57	MG	2A	3370	1/1	0.95	0.41	51,51,51,51	0
57	MG	2A	3207	1/1	0.95	0.30	56,56,56,56	0
57	MG	1E	301	1/1	0.95	0.36	36,36,36,36	0
57	MG	2B	218	1/1	0.95	0.20	78,78,78,78	0
57	MG	1A	3826	1/1	0.95	0.26	41,41,41,41	0
57	MG	1A	3189	1/1	0.95	0.50	38,38,38,38	0
57	MG	1E	304	1/1	0.95	0.22	29,29,29,29	0
57	MG	2A	3212	1/1	0.95	0.20	58,58,58,58	0
57	MG	1A	3640	1/1	0.95	0.20	22,22,22,22	0
57	MG	2A	3587	1/1	0.95	0.14	68,68,68,68	0
57	MG	1A	3735	1/1	0.95	0.20	25,25,25,25	0
57	MG	1A	3190	1/1	0.95	0.17	46,46,46,46	0
57	MG	1A	3412	1/1	0.95	0.21	48,48,48,48	0
57	MG	1a	1748	1/1	0.95	0.14	71,71,71,71	0
57	MG	2A	3592	1/1	0.95	0.28	36,36,36,36	0
57	MG	1a	1749	1/1	0.95	0.06	73,73,73,73	0
57	MG	1a	1750	1/1	0.95	0.07	64,64,64,64	0
57	MG	2A	3387	1/1	0.95	0.11	53,53,53,53	0
57	MG	2A	3597	1/1	0.95	0.13	74,74,74,74	0
57	MG	2A	3598	1/1	0.95	0.17	61,61,61,61	0
57	MG	2A	3599	1/1	0.95	0.20	67,67,67,67	0
57	MG	1a	1751	1/1	0.95	0.17	64,64,64,64	0
57	MG	2A	3601	1/1	0.95	0.08	68,68,68,68	0
57	MG	1A	3644	1/1	0.95	0.17	26,26,26,26	0
57	MG	1a	1753	1/1	0.95	0.10	66,66,66,66	0
57	MG	1F	302	1/1	0.95	0.22	33,33,33,33	0
57	MG	1F	304	1/1	0.95	0.09	69,69,69,69	0
57	MG	1a	1757	1/1	0.95	0.17	45,45,45,45	0
57	MG	1A	3021	1/1	0.95	0.26	47,47,47,47	0
57	MG	2A	3396	1/1	0.95	0.42	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	1613	1/1	0.95	0.06	62,62,62,62	0
57	MG	2a	1802	1/1	0.95	0.38	55,55,55,55	0
57	MG	1A	3073	1/1	0.95	0.17	31,31,31,31	0
57	MG	1A	3303	1/1	0.95	0.19	56,56,56,56	0
57	MG	1F	310	1/1	0.95	0.17	29,29,29,29	0
57	MG	2a	1807	1/1	0.95	0.04	69,69,69,69	0
57	MG	1a	1619	1/1	0.95	0.14	51,51,51,51	0
57	MG	2A	3616	1/1	0.95	0.15	49,49,49,49	0
57	MG	1A	3569	1/1	0.95	0.13	39,39,39,39	0
57	MG	2V	201	1/1	0.95	0.87	51,51,51,51	0
57	MG	1A	3650	1/1	0.95	0.11	61,61,61,61	0
57	MG	1A	3338	1/1	0.95	0.62	48,48,48,48	0
57	MG	2X	101	1/1	0.95	0.20	65,65,65,65	0
57	MG	1A	3748	1/1	0.95	0.19	51,51,51,51	0
57	MG	1G	201	1/1	0.95	0.17	39,39,39,39	0
57	MG	2A	3624	1/1	0.95	0.13	33,33,33,33	0
57	MG	1A	3377	1/1	0.95	0.17	37,37,37,37	0
57	MG	1A	3040	1/1	0.95	0.11	35,35,35,35	0
57	MG	2A	3627	1/1	0.95	0.21	61,61,61,61	0
57	MG	1a	1628	1/1	0.95	0.14	43,43,43,43	0
57	MG	2A	3414	1/1	0.95	0.26	62,62,62,62	0
57	MG	1G	204	1/1	0.95	0.13	62,62,62,62	0
57	MG	2j	201	1/1	0.95	0.07	74,74,74,74	0
57	MG	1A	3752	1/1	0.95	0.17	20,20,20,20	0
57	MG	1A	3945	1/1	0.95	0.18	26,26,26,26	0
57	MG	1A	3116	1/1	0.95	0.54	45,45,45,45	0
57	MG	1A	3577	1/1	0.95	0.06	56,56,56,56	0
57	MG	2A	3421	1/1	0.95	0.19	39,39,39,39	0
57	MG	1a	1783	1/1	0.95	0.13	64,64,64,64	0
57	MG	1A	3578	1/1	0.95	0.25	35,35,35,35	0
57	MG	1N	205	1/1	0.95	0.19	44,44,44,44	0
57	MG	1A	3162	1/1	0.95	0.27	42,42,42,42	0
57	MG	1A	3758	1/1	0.95	0.10	49,49,49,49	0
57	MG	1A	3862	1/1	0.95	0.17	47,47,47,47	0
57	MG	2A	3431	1/1	0.95	0.23	53,53,53,53	0
57	MG	1A	3036	1/1	0.95	0.19	28,28,28,28	0
57	MG	1A	3520	1/1	0.95	0.40	40,40,40,40	0
57	MG	2A	3653	1/1	0.95	0.26	64,64,64,64	0
57	MG	1a	1794	1/1	0.95	0.15	57,57,57,57	0
57	MG	1A	4059	1/1	0.95	0.20	61,61,61,61	0
57	MG	1A	3765	1/1	0.95	0.22	54,54,54,54	0
57	MG	1A	3123	1/1	0.95	0.30	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1A	3767	1/1	0.95	0.14	38,38,38,38	0
57	MG	1A	3168	1/1	0.95	0.24	37,37,37,37	0
57	MG	2A	3443	1/1	0.95	0.12	44,44,44,44	0
57	MG	2A	3445	1/1	0.95	0.25	36,36,36,36	0
57	MG	1A	3345	1/1	0.95	0.10	43,43,43,43	0
59	TYK	1A	4101	64/64	0.95	0.23	16,30,46,51	0
57	MG	2A	3263	1/1	0.95	0.12	73,73,73,73	0
57	MG	1Q	203	1/1	0.95	0.22	52,52,52,52	0
57	MG	1a	1649	1/1	0.95	0.23	46,46,46,46	0
57	MG	1A	3200	1/1	0.95	0.26	36,36,36,36	0
57	MG	1Q	205	1/1	0.95	0.18	46,46,46,46	0
57	MG	1Q	206	1/1	0.95	0.18	43,43,43,43	0
57	MG	2A	3670	1/1	0.95	0.21	48,48,48,48	0
57	MG	2a	1649	1/1	0.96	0.27	67,67,67,67	0
57	MG	1A	3009	1/1	0.96	0.12	22,22,22,22	0
57	MG	2A	3110	1/1	0.96	0.10	76,76,76,76	0
57	MG	1D	310	1/1	0.96	0.27	26,26,26,26	0
57	MG	1A	3426	1/1	0.96	0.12	43,43,43,43	0
57	MG	1l	3200	1/1	0.96	0.12	71,71,71,71	0
57	MG	2A	3550	1/1	0.96	0.12	68,68,68,68	0
57	MG	2A	3551	1/1	0.96	0.22	40,40,40,40	0
57	MG	1A	3104	1/1	0.96	0.50	29,29,29,29	0
57	MG	1A	4041	1/1	0.96	0.06	53,53,53,53	0
57	MG	1A	3177	1/1	0.96	0.18	54,54,54,54	0
57	MG	1A	3649	1/1	0.96	0.15	28,28,28,28	0
57	MG	2A	3558	1/1	0.96	0.09	46,46,46,46	0
57	MG	1a	1695	1/1	0.96	0.14	43,43,43,43	0
57	MG	2A	3389	1/1	0.96	0.15	54,54,54,54	0
57	MG	1w	102	1/1	0.96	0.16	49,49,49,49	0
57	MG	1A	3008	1/1	0.96	0.15	26,26,26,26	0
57	MG	1A	3652	1/1	0.96	0.14	40,40,40,40	0
57	MG	1E	306	1/1	0.96	0.21	23,23,23,23	0
57	MG	2a	1672	1/1	0.96	0.12	56,56,56,56	0
57	MG	2A	3255	1/1	0.96	0.26	65,65,65,65	0
57	MG	1A	4047	1/1	0.96	0.16	55,55,55,55	0
57	MG	2a	1676	1/1	0.96	0.31	61,61,61,61	0
57	MG	13	105	1/1	0.96	0.17	52,52,52,52	0
57	MG	2A	3756	1/1	0.96	0.28	48,48,48,48	0
57	MG	1A	3955	1/1	0.96	0.16	16,16,16,16	0
57	MG	2A	3398	1/1	0.96	0.37	62,62,62,62	0
57	MG	1E	309	1/1	0.96	0.14	51,51,51,51	0
57	MG	1A	3023	1/1	0.96	0.23	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3401	1/1	0.96	0.07	42,42,42,42	0
57	MG	1A	3725	1/1	0.96	0.16	27,27,27,27	0
57	MG	2a	1687	1/1	0.96	0.11	57,57,57,57	0
57	MG	1A	3180	1/1	0.96	0.31	50,50,50,50	0
57	MG	2A	3764	1/1	0.96	0.16	73,73,73,73	0
57	MG	2A	3577	1/1	0.96	0.20	53,53,53,53	0
57	MG	1a	1709	1/1	0.96	0.14	41,41,41,41	0
57	MG	1F	303	1/1	0.96	0.19	31,31,31,31	0
57	MG	2A	3406	1/1	0.96	0.18	65,65,65,65	0
57	MG	2A	3770	1/1	0.96	0.10	58,58,58,58	0
57	MG	2A	3771	1/1	0.96	0.12	61,61,61,61	0
57	MG	1A	3310	1/1	0.96	0.20	51,51,51,51	0
57	MG	2A	3773	1/1	0.96	0.14	70,70,70,70	0
57	MG	17	102	1/1	0.96	0.17	33,33,33,33	0
57	MG	1A	3729	1/1	0.96	0.17	18,18,18,18	0
57	MG	1a	1715	1/1	0.96	0.09	57,57,57,57	0
57	MG	1A	3730	1/1	0.96	0.14	22,22,22,22	0
57	MG	2A	3270	1/1	0.96	0.10	51,51,51,51	0
57	MG	2a	1703	1/1	0.96	0.27	64,64,64,64	0
57	MG	1A	3884	1/1	0.96	0.08	45,45,45,45	0
57	MG	2a	1705	1/1	0.96	0.24	44,44,44,44	0
57	MG	2A	3780	1/1	0.96	0.18	67,67,67,67	0
57	MG	1A	4057	1/1	0.96	0.13	51,51,51,51	0
57	MG	2A	3273	1/1	0.96	0.15	70,70,70,70	0
57	MG	1A	3597	1/1	0.96	0.28	63,63,63,63	0
57	MG	1A	3800	1/1	0.96	0.13	69,69,69,69	0
57	MG	1A	3967	1/1	0.96	0.15	28,28,28,28	0
57	MG	1F	314	1/1	0.96	0.12	55,55,55,55	0
57	MG	1A	3181	1/1	0.96	0.43	39,39,39,39	0
57	MG	2A	3424	1/1	0.96	0.10	65,65,65,65	0
57	MG	1A	3063	1/1	0.96	0.14	31,31,31,31	0
57	MG	1A	3505	1/1	0.96	0.20	33,33,33,33	0
57	MG	1A	3971	1/1	0.96	0.14	38,38,38,38	0
57	MG	2A	3428	1/1	0.96	0.14	45,45,45,45	0
57	MG	2A	3016	1/1	0.96	0.38	39,39,39,39	0
57	MG	1A	3469	1/1	0.96	0.28	29,29,29,29	0
57	MG	2A	3284	1/1	0.96	0.21	66,66,66,66	0
57	MG	1A	3805	1/1	0.96	0.12	51,51,51,51	0
57	MG	2A	3287	1/1	0.96	0.42	58,58,58,58	0
57	MG	1a	1731	1/1	0.96	0.13	57,57,57,57	0
57	MG	2A	3435	1/1	0.96	0.26	69,69,69,69	0
57	MG	1A	3035	1/1	0.96	0.22	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	1608	1/1	0.96	0.11	52,52,52,52	0
57	MG	1A	3054	1/1	0.96	0.14	28,28,28,28	0
57	MG	2A	3612	1/1	0.96	0.29	68,68,68,68	0
57	MG	2B	210	1/1	0.96	0.06	78,78,78,78	0
57	MG	1A	3112	1/1	0.96	0.32	30,30,30,30	0
57	MG	1N	202	1/1	0.96	0.22	45,45,45,45	0
57	MG	1A	3809	1/1	0.96	0.25	45,45,45,45	0
57	MG	2A	3444	1/1	0.96	0.16	70,70,70,70	0
57	MG	1A	3186	1/1	0.96	0.43	33,33,33,33	0
57	MG	2A	3446	1/1	0.96	0.17	45,45,45,45	0
57	MG	1A	3028	1/1	0.96	0.17	41,41,41,41	0
57	MG	2B	219	1/1	0.96	0.17	62,62,62,62	0
57	MG	1A	3812	1/1	0.96	0.22	18,18,18,18	0
57	MG	2A	3621	1/1	0.96	0.12	34,34,34,34	0
57	MG	1A	3813	1/1	0.96	0.20	32,32,32,32	0
57	MG	2A	3623	1/1	0.96	0.11	69,69,69,69	0
57	MG	2D	305	1/1	0.96	0.84	52,52,52,52	0
57	MG	1A	3057	1/1	0.96	0.08	63,63,63,63	0
57	MG	1A	3743	1/1	0.96	0.11	38,38,38,38	0
57	MG	1A	3261	1/1	0.96	0.22	33,33,33,33	0
57	MG	2A	3170	1/1	0.96	0.08	62,62,62,62	0
57	MG	1A	3987	1/1	0.96	0.15	21,21,21,21	0
57	MG	2E	303	1/1	0.96	0.13	43,43,43,43	0
57	MG	1P	202	1/1	0.96	0.47	26,26,26,26	0
57	MG	1a	1625	1/1	0.96	0.24	52,52,52,52	0
57	MG	1A	3442	1/1	0.96	0.17	57,57,57,57	0
57	MG	2A	3632	1/1	0.96	0.10	61,61,61,61	0
57	MG	1A	3746	1/1	0.96	0.21	16,16,16,16	0
57	MG	1A	3069	1/1	0.96	0.14	27,27,27,27	0
57	MG	1A	3070	1/1	0.96	0.14	33,33,33,33	0
57	MG	2A	3311	1/1	0.96	0.07	65,65,65,65	0
57	MG	2a	1763	1/1	0.96	0.13	67,67,67,67	0
57	MG	2a	1764	1/1	0.96	0.16	66,66,66,66	0
57	MG	1A	3564	1/1	0.96	0.12	53,53,53,53	0
57	MG	1A	3322	1/1	0.96	0.59	39,39,39,39	0
57	MG	1A	4090	1/1	0.96	0.34	31,31,31,31	0
57	MG	2A	3467	1/1	0.96	0.21	63,63,63,63	0
57	MG	2A	3641	1/1	0.96	0.34	41,41,41,41	0
57	MG	2A	3642	1/1	0.96	0.14	69,69,69,69	0
57	MG	2A	3468	1/1	0.96	0.19	39,39,39,39	0
57	MG	1A	3566	1/1	0.96	0.07	52,52,52,52	0
57	MG	2A	3646	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	1774	1/1	0.96	0.30	68,68,68,68	0
57	MG	2A	3647	1/1	0.96	0.19	54,54,54,54	0
57	MG	1a	1756	1/1	0.96	0.11	64,64,64,64	0
57	MG	2a	1778	1/1	0.96	0.23	56,56,56,56	0
57	MG	2A	3649	1/1	0.96	0.13	51,51,51,51	0
57	MG	1R	201	1/1	0.96	0.18	43,43,43,43	0
57	MG	1A	3192	1/1	0.96	0.16	29,29,29,29	0
57	MG	1A	3524	1/1	0.96	0.17	37,37,37,37	0
57	MG	1A	3525	1/1	0.96	0.20	39,39,39,39	0
57	MG	2U	201	1/1	0.96	0.42	54,54,54,54	0
57	MG	1A	3691	1/1	0.96	0.16	45,45,45,45	0
57	MG	1A	3833	1/1	0.96	0.24	32,32,32,32	0
57	MG	1A	3570	1/1	0.96	0.25	50,50,50,50	0
57	MG	2A	3060	1/1	0.96	0.19	50,50,50,50	0
57	MG	2Y	201	1/1	0.96	0.17	60,60,60,60	0
57	MG	1A	3760	1/1	0.96	0.16	24,24,24,24	0
57	MG	1A	3296	1/1	0.96	0.17	56,56,56,56	0
57	MG	1A	3695	1/1	0.96	0.12	44,44,44,44	0
57	MG	1A	3266	1/1	0.96	0.18	28,28,28,28	0
57	MG	1A	3628	1/1	0.96	0.15	36,36,36,36	0
57	MG	1A	3165	1/1	0.96	0.49	45,45,45,45	0
57	MG	2A	3486	1/1	0.96	0.20	60,60,60,60	0
57	MG	1A	3699	1/1	0.96	0.13	29,29,29,29	0
57	MG	2a	1800	1/1	0.96	0.12	56,56,56,56	0
57	MG	2A	3667	1/1	0.96	0.14	50,50,50,50	0
57	MG	2A	3488	1/1	0.96	0.21	52,52,52,52	0
57	MG	1a	1774	1/1	0.96	0.10	44,44,44,44	0
57	MG	2A	3491	1/1	0.96	0.06	73,73,73,73	0
57	MG	1A	3926	1/1	0.96	0.08	61,61,61,61	0
57	MG	1A	3486	1/1	0.96	0.30	43,43,43,43	0
57	MG	1A	3848	1/1	0.96	0.16	22,22,22,22	0
57	MG	1A	3487	1/1	0.96	0.21	41,41,41,41	0
57	MG	1a	1653	1/1	0.96	0.27	50,50,50,50	0
57	MG	2A	3499	1/1	0.96	0.18	54,54,54,54	0
57	MG	1A	3851	1/1	0.96	0.12	24,24,24,24	0
57	MG	1a	1655	1/1	0.96	0.18	51,51,51,51	0
57	MG	1A	3118	1/1	0.96	0.24	52,52,52,52	0
57	MG	1A	3853	1/1	0.96	0.23	77,77,77,77	0
57	MG	1V	202	1/1	0.96	0.38	36,36,36,36	0
57	MG	2A	3506	1/1	0.96	0.21	62,62,62,62	0
57	MG	1A	4019	1/1	0.96	0.12	41,41,41,41	0
57	MG	2A	3685	1/1	0.96	0.12	88,88,88,88	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	1789	1/1	0.96	0.28	60,60,60,60	0
57	MG	1a	1790	1/1	0.96	0.05	74,74,74,74	0
57	MG	1A	3049	1/1	0.96	0.31	32,32,32,32	0
57	MG	2A	3084	1/1	0.96	0.35	41,41,41,41	0
57	MG	1a	1661	1/1	0.96	0.07	65,65,65,65	0
57	MG	2A	3352	1/1	0.96	0.26	63,63,63,63	0
57	MG	1B	218	1/1	0.96	0.33	46,46,46,46	0
57	MG	1A	3705	1/1	0.96	0.20	36,36,36,36	0
57	MG	1A	3937	1/1	0.96	0.14	53,53,53,53	0
57	MG	1A	3580	1/1	0.96	0.17	27,27,27,27	0
57	MG	1A	4025	1/1	0.96	0.17	53,53,53,53	0
57	MG	2A	3698	1/1	0.96	0.25	54,54,54,54	0
57	MG	2v	103	1/1	0.96	0.27	60,60,60,60	0
57	MG	1X	101	1/1	0.96	0.35	40,40,40,40	0
57	MG	2A	3700	1/1	0.96	0.08	47,47,47,47	0
57	MG	1A	3857	1/1	0.96	0.13	34,34,34,34	0
57	MG	1A	4027	1/1	0.96	0.11	49,49,49,49	0
57	MG	1A	3581	1/1	0.96	0.10	39,39,39,39	0
57	MG	2A	3705	1/1	0.96	0.20	51,51,51,51	0
57	MG	1A	3421	1/1	0.96	0.13	52,52,52,52	0
57	MG	1A	3120	1/1	0.96	0.47	35,35,35,35	0
57	MG	2A	3709	1/1	0.96	0.21	36,36,36,36	0
57	MG	1A	4031	1/1	0.96	0.23	40,40,40,40	0
57	MG	2A	3528	1/1	0.96	0.10	36,36,36,36	0
57	MG	1A	3642	1/1	0.96	0.18	29,29,29,29	0
57	MG	1A	3102	1/1	0.96	0.29	40,40,40,40	0
57	MG	2A	3718	1/1	0.96	0.10	51,51,51,51	0
57	MG	1A	3864	1/1	0.96	0.12	38,38,38,38	0
57	MG	1a	1678	1/1	0.96	0.28	54,54,54,54	0
57	MG	1A	3714	1/1	0.96	0.18	51,51,51,51	0
57	MG	1B	234	1/1	0.96	0.11	37,37,37,37	0
57	MG	1A	3174	1/1	0.96	0.19	32,32,32,32	0
57	MG	2A	3540	1/1	0.96	0.10	48,48,48,48	0
57	MG	2A	3728	1/1	0.96	0.22	36,36,36,36	0
57	MG	1D	303	1/1	0.96	0.29	39,39,39,39	0
57	MG	1D	305	1/1	0.96	0.21	41,41,41,41	0
57	MG	2A	3107	1/1	0.96	0.12	70,70,70,70	0
57	MG	1D	307	1/1	0.96	0.39	36,36,36,36	0
57	MG	2A	3045	1/1	0.97	0.13	55,55,55,55	0
57	MG	1A	3932	1/1	0.97	0.12	43,43,43,43	0
57	MG	2A	3178	1/1	0.97	0.15	67,67,67,67	0
57	MG	2a	1675	1/1	0.97	0.32	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4017	1/1	0.97	0.08	43,43,43,43	0
57	MG	2a	1677	1/1	0.97	0.21	68,68,68,68	0
57	MG	2a	1678	1/1	0.97	0.24	55,55,55,55	0
57	MG	1U	201	1/1	0.97	0.31	30,30,30,30	0
57	MG	2A	3455	1/1	0.97	0.26	35,35,35,35	0
57	MG	2A	3456	1/1	0.97	0.28	51,51,51,51	0
57	MG	1A	3155	1/1	0.97	0.25	27,27,27,27	0
57	MG	1A	3777	1/1	0.97	0.11	26,26,26,26	0
57	MG	1B	215	1/1	0.97	0.12	55,55,55,55	0
57	MG	2A	3786	1/1	0.97	0.09	64,64,64,64	0
57	MG	1A	3778	1/1	0.97	0.13	28,28,28,28	0
57	MG	1A	3221	1/1	0.97	0.12	42,42,42,42	0
57	MG	1A	3350	1/1	0.97	0.21	24,24,24,24	0
57	MG	1A	3269	1/1	0.97	0.13	30,30,30,30	0
57	MG	1a	1769	1/1	0.97	0.17	58,58,58,58	0
57	MG	1A	3717	1/1	0.97	0.18	41,41,41,41	0
57	MG	1A	3270	1/1	0.97	0.26	33,33,33,33	0
57	MG	1A	3657	1/1	0.97	0.13	55,55,55,55	0
57	MG	1V	203	1/1	0.97	0.29	27,27,27,27	0
57	MG	1A	3324	1/1	0.97	0.27	30,30,30,30	0
57	MG	1A	3659	1/1	0.97	0.10	23,23,23,23	0
57	MG	1B	226	1/1	0.97	0.11	45,45,45,45	0
57	MG	2A	3328	1/1	0.97	0.20	61,61,61,61	0
57	MG	1A	3660	1/1	0.97	0.14	16,16,16,16	0
57	MG	1A	3156	1/1	0.97	0.62	35,35,35,35	0
57	MG	1A	3448	1/1	0.97	0.22	37,37,37,37	0
57	MG	1A	3014	1/1	0.97	0.17	28,28,28,28	0
57	MG	2B	207	1/1	0.97	0.13	65,65,65,65	0
57	MG	1A	3869	1/1	0.97	0.14	25,25,25,25	0
57	MG	1A	3870	1/1	0.97	0.13	26,26,26,26	0
57	MG	2a	1706	1/1	0.97	0.22	61,61,61,61	0
57	MG	1A	3610	1/1	0.97	0.08	41,41,41,41	0
57	MG	2A	3480	1/1	0.97	0.15	31,31,31,31	0
57	MG	1A	3357	1/1	0.97	0.19	27,27,27,27	0
57	MG	1A	3728	1/1	0.97	0.10	54,54,54,54	0
57	MG	1a	1788	1/1	0.97	0.18	50,50,50,50	0
57	MG	1D	302	1/1	0.97	0.64	40,40,40,40	0
57	MG	1A	3523	1/1	0.97	0.74	42,42,42,42	0
57	MG	1D	304	1/1	0.97	0.21	22,22,22,22	0
57	MG	1A	3029	1/1	0.97	0.38	31,31,31,31	0
57	MG	1a	1671	1/1	0.97	0.28	65,65,65,65	0
57	MG	1D	306	1/1	0.97	0.15	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	2A	3490	1/1	0.97	0.20	35,35,35,35	0
57	MG	1A	3109	1/1	0.97	0.09	33,33,33,33	0
57	MG	2A	3492	1/1	0.97	0.10	59,59,59,59	0
57	MG	2A	3651	1/1	0.97	0.23	51,51,51,51	0
57	MG	1A	4043	1/1	0.97	0.19	55,55,55,55	0
57	MG	1A	3956	1/1	0.97	0.27	38,38,38,38	0
57	MG	1A	3160	1/1	0.97	0.26	35,35,35,35	0
57	MG	1A	3672	1/1	0.97	0.13	63,63,63,63	0
57	MG	1A	3959	1/1	0.97	0.07	53,53,53,53	0
57	MG	1A	3799	1/1	0.97	0.13	32,32,32,32	0
57	MG	2A	3500	1/1	0.97	0.20	59,59,59,59	0
57	MG	1a	1680	1/1	0.97	0.29	40,40,40,40	0
57	MG	2A	3220	1/1	0.97	0.11	63,63,63,63	0
57	MG	2a	1731	1/1	0.97	0.06	70,70,70,70	0
57	MG	1A	3616	1/1	0.97	0.12	25,25,25,25	0
57	MG	1A	3527	1/1	0.97	0.30	34,34,34,34	0
57	MG	1A	3362	1/1	0.97	0.10	29,29,29,29	0
57	MG	1a	1807	1/1	0.97	0.10	70,70,70,70	0
57	MG	1A	3067	1/1	0.97	0.13	16,16,16,16	0
57	MG	1a	1685	1/1	0.97	0.22	61,61,61,61	0
57	MG	1A	3041	1/1	0.97	0.32	30,30,30,30	0
57	MG	1A	3886	1/1	0.97	0.12	12,12,12,12	0
57	MG	1A	3075	1/1	0.97	0.18	33,33,33,33	0
57	MG	1A	3279	1/1	0.97	0.29	30,30,30,30	0
57	MG	13	102	1/1	0.97	0.39	39,39,39,39	0
57	MG	1A	3164	1/1	0.97	0.22	17,17,17,17	0
57	MG	2O	201	1/1	0.97	0.18	51,51,51,51	0
57	MG	1A	3682	1/1	0.97	0.11	57,57,57,57	0
57	MG	2a	1746	1/1	0.97	0.09	64,64,64,64	0
57	MG	2A	3674	1/1	0.97	0.07	52,52,52,52	0
57	MG	1A	3188	1/1	0.97	0.41	31,31,31,31	0
57	MG	2Q	202	1/1	0.97	0.34	47,47,47,47	0
57	MG	2Q	203	1/1	0.97	0.10	48,48,48,48	0
57	MG	1A	3684	1/1	0.97	0.21	50,50,50,50	0
57	MG	2A	3371	1/1	0.97	0.19	24,24,24,24	0
57	MG	1A	3894	1/1	0.97	0.06	54,54,54,54	0
57	MG	2A	3373	1/1	0.97	0.62	42,42,42,42	0
57	MG	2A	3237	1/1	0.97	0.33	53,53,53,53	0
57	MG	2A	3522	1/1	0.97	0.08	69,69,69,69	0
57	MG	2a	1758	1/1	0.97	0.12	67,67,67,67	0
57	MG	1F	306	1/1	0.97	0.46	36,36,36,36	0
57	MG	2A	3524	1/1	0.97	0.23	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1l	3201	1/1	0.97	0.21	60,60,60,60	0
57	MG	2W	202	1/1	0.97	0.16	47,47,47,47	0
57	MG	2A	3377	1/1	0.97	0.18	37,37,37,37	0
57	MG	2X	102	1/1	0.97	0.15	48,48,48,48	0
57	MG	1A	4065	1/1	0.97	0.10	51,51,51,51	0
57	MG	1p	101	1/1	0.97	0.06	63,63,63,63	0
57	MG	1A	3685	1/1	0.97	0.17	44,44,44,44	0
57	MG	1a	1700	1/1	0.97	0.21	50,50,50,50	0
57	MG	2A	3531	1/1	0.97	0.07	64,64,64,64	0
57	MG	23	101	1/1	0.97	0.12	58,58,58,58	0
57	MG	2A	3532	1/1	0.97	0.21	38,38,38,38	0
57	MG	1a	1701	1/1	0.97	0.28	38,38,38,38	0
57	MG	25	102	1/1	0.97	0.30	45,45,45,45	0
57	MG	1F	309	1/1	0.97	0.38	29,29,29,29	0
57	MG	2a	1775	1/1	0.97	0.08	78,78,78,78	0
57	MG	1A	3686	1/1	0.97	0.10	48,48,48,48	0
57	MG	1A	3254	1/1	0.97	0.17	34,34,34,34	0
57	MG	2A	3696	1/1	0.97	0.12	73,73,73,73	0
57	MG	1A	3977	1/1	0.97	0.15	56,56,56,56	0
57	MG	2a	1780	1/1	0.97	0.25	62,62,62,62	0
57	MG	1A	3814	1/1	0.97	0.09	41,41,41,41	0
57	MG	1A	3462	1/1	0.97	0.27	39,39,39,39	0
57	MG	1A	3090	1/1	0.97	0.29	37,37,37,37	0
57	MG	18	103	1/1	0.97	0.34	33,33,33,33	0
57	MG	1A	3751	1/1	0.97	0.14	23,23,23,23	0
57	MG	1A	3982	1/1	0.97	0.16	55,55,55,55	0
57	MG	1A	3630	1/1	0.97	0.20	26,26,26,26	0
57	MG	1A	3819	1/1	0.97	0.13	43,43,43,43	0
57	MG	1A	3753	1/1	0.97	0.16	22,22,22,22	0
57	MG	1A	3464	1/1	0.97	0.19	29,29,29,29	0
57	MG	2A	3710	1/1	0.97	0.16	58,58,58,58	0
57	MG	1x	110	1/1	0.97	0.18	22,22,22,22	0
57	MG	2A	3712	1/1	0.97	0.18	40,40,40,40	0
57	MG	1A	3582	1/1	0.97	0.10	51,51,51,51	0
57	MG	1A	3031	1/1	0.97	0.23	23,23,23,23	0
57	MG	2a	1796	1/1	0.97	0.21	63,63,63,63	0
57	MG	2A	3716	1/1	0.97	0.19	37,37,37,37	0
57	MG	1x	113	1/1	0.97	0.30	62,62,62,62	0
57	MG	1A	3824	1/1	0.97	0.11	42,42,42,42	0
57	MG	2A	3555	1/1	0.97	0.24	50,50,50,50	0
57	MG	2A	3556	1/1	0.97	0.16	62,62,62,62	0
57	MG	1A	3093	1/1	0.97	0.23	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1722	1/1	0.97	0.14	35,35,35,35	0
57	MG	2A	3725	1/1	0.97	0.17	42,42,42,42	0
57	MG	2A	3136	1/1	0.97	0.24	32,32,32,32	0
57	MG	1N	204	1/1	0.97	0.69	44,44,44,44	0
57	MG	1A	3149	1/1	0.97	0.27	37,37,37,37	0
57	MG	2a	1809	1/1	0.97	0.31	78,78,78,78	0
57	MG	1A	4085	1/1	0.97	0.07	62,62,62,62	0
57	MG	1A	3759	1/1	0.97	0.09	55,55,55,55	0
57	MG	1a	1611	1/1	0.97	0.14	29,29,29,29	0
57	MG	2a	1625	1/1	0.97	0.16	86,86,86,86	0
57	MG	1A	3543	1/1	0.97	0.25	55,55,55,55	0
57	MG	1A	3761	1/1	0.97	0.20	20,20,20,20	0
57	MG	1A	3588	1/1	0.97	0.13	18,18,18,18	0
57	MG	2A	3569	1/1	0.97	0.20	61,61,61,61	0
57	MG	2A	3145	1/1	0.97	0.20	55,55,55,55	0
57	MG	1A	3832	1/1	0.97	0.20	37,37,37,37	0
57	MG	1A	3502	1/1	0.97	0.14	28,28,28,28	0
57	MG	1a	1618	1/1	0.97	0.14	36,36,36,36	0
57	MG	2d	302	1/1	0.97	0.24	56,56,56,56	0
57	MG	1A	3998	1/1	0.97	0.18	34,34,34,34	0
57	MG	2A	3741	1/1	0.97	0.19	48,48,48,48	0
57	MG	2A	3018	1/1	0.97	0.23	33,33,33,33	0
57	MG	2A	3420	1/1	0.97	0.26	48,48,48,48	0
57	MG	1A	3764	1/1	0.97	0.54	30,30,30,30	0
57	MG	2A	3422	1/1	0.97	0.11	59,59,59,59	0
57	MG	2A	3152	1/1	0.97	0.12	58,58,58,58	0
57	MG	1A	3836	1/1	0.97	0.40	40,40,40,40	0
57	MG	2A	3021	1/1	0.97	0.11	44,44,44,44	0
57	MG	2A	3285	1/1	0.97	0.16	58,58,58,58	0
57	MG	2A	3750	1/1	0.97	0.08	59,59,59,59	0
57	MG	1A	3105	1/1	0.97	0.11	40,40,40,40	0
57	MG	1Q	201	1/1	0.97	0.14	35,35,35,35	0
57	MG	1A	3703	1/1	0.97	0.13	46,46,46,46	0
57	MG	2w	102	1/1	0.97	0.23	84,84,84,84	0
57	MG	1A	3173	1/1	0.97	0.18	20,20,20,20	0
57	MG	2w	104	1/1	0.97	0.13	87,87,87,87	0
57	MG	1A	3117	1/1	0.97	0.45	37,37,37,37	0
57	MG	1A	3506	1/1	0.97	0.47	34,34,34,34	0
57	MG	2a	1651	1/1	0.97	0.15	67,67,67,67	0
57	MG	1A	3135	1/1	0.97	0.18	33,33,33,33	0
57	MG	2A	3162	1/1	0.97	0.22	34,34,34,34	0
57	MG	1Q	207	1/1	0.97	0.20	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3708	1/1	0.97	0.13	42,42,42,42	0
57	MG	2A	3437	1/1	0.97	0.10	33,33,33,33	0
57	MG	2A	3594	1/1	0.97	0.09	65,65,65,65	0
57	MG	2A	3032	1/1	0.97	0.15	25,25,25,25	0
57	MG	1B	202	1/1	0.97	0.20	49,49,49,49	0
57	MG	2x	109	1/1	0.97	0.12	70,70,70,70	0
57	MG	1a	1632	1/1	0.97	0.24	23,23,23,23	0
57	MG	1A	3846	1/1	0.97	0.17	46,46,46,46	0
57	MG	1A	3550	1/1	0.97	0.19	52,52,52,52	0
57	MG	1A	3077	1/1	0.97	0.18	36,36,36,36	0
57	MG	1A	3774	1/1	0.97	0.25	32,32,32,32	0
57	MG	1B	207	1/1	0.97	0.13	42,42,42,42	0
57	MG	2a	1667	1/1	0.97	0.11	66,66,66,66	0
57	MG	1A	3154	1/1	0.97	0.20	30,30,30,30	0
57	MG	1A	3931	1/1	0.97	0.12	72,72,72,72	0
60	ZN	26	501	1/1	0.97	0.12	61,61,61,61	0
57	MG	1A	4015	1/1	0.97	0.07	37,37,37,37	0
57	MG	2a	1671	1/1	0.97	0.23	65,65,65,65	0
57	MG	2A	3537	1/1	0.98	0.29	52,52,52,52	0
57	MG	1A	3167	1/1	0.98	0.28	45,45,45,45	0
57	MG	1A	3837	1/1	0.98	0.07	63,63,63,63	0
57	MG	2A	3701	1/1	0.98	0.09	46,46,46,46	0
57	MG	1A	3838	1/1	0.98	0.13	36,36,36,36	0
57	MG	1W	203	1/1	0.98	0.26	33,33,33,33	0
57	MG	1A	3141	1/1	0.98	0.23	32,32,32,32	0
57	MG	1A	4022	1/1	0.98	0.16	22,22,22,22	0
57	MG	1a	1607	1/1	0.98	0.28	60,60,60,60	0
57	MG	1a	1729	1/1	0.98	0.28	45,45,45,45	0
57	MG	2A	3708	1/1	0.98	0.26	39,39,39,39	0
57	MG	1A	3535	1/1	0.98	0.45	28,28,28,28	0
57	MG	1A	3169	1/1	0.98	0.36	29,29,29,29	0
57	MG	1A	3678	1/1	0.98	0.20	16,16,16,16	0
57	MG	1X	103	1/1	0.98	0.22	44,44,44,44	0
57	MG	1A	3889	1/1	0.98	0.14	23,23,23,23	0
57	MG	1X	105	1/1	0.98	0.16	51,51,51,51	0
57	MG	2A	3715	1/1	0.98	0.15	38,38,38,38	0
57	MG	1A	3515	1/1	0.98	0.28	31,31,31,31	0
57	MG	1A	3585	1/1	0.98	0.12	56,56,56,56	0
57	MG	1a	1805	1/1	0.98	0.20	53,53,53,53	0
57	MG	1A	4080	1/1	0.98	0.33	43,43,43,43	0
57	MG	1a	1617	1/1	0.98	0.18	45,45,45,45	0
57	MG	2A	3721	1/1	0.98	0.08	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	2A	3722	1/1	0.98	0.18	61,61,61,61	0
57	MG	1A	3037	1/1	0.98	0.19	32,32,32,32	0
57	MG	1Z	302	1/1	0.98	0.27	47,47,47,47	0
57	MG	1A	3130	1/1	0.98	0.13	42,42,42,42	0
57	MG	2B	217	1/1	0.98	0.25	71,71,71,71	0
57	MG	1A	3329	1/1	0.98	0.13	54,54,54,54	0
57	MG	2a	1803	1/1	0.98	0.13	61,61,61,61	0
57	MG	1A	3519	1/1	0.98	0.22	35,35,35,35	0
57	MG	2A	3332	1/1	0.98	0.30	39,39,39,39	0
57	MG	2A	3563	1/1	0.98	0.07	71,71,71,71	0
57	MG	2A	3644	1/1	0.98	0.21	68,68,68,68	0
57	MG	1A	3131	1/1	0.98	0.18	28,28,28,28	0
57	MG	1A	3850	1/1	0.98	0.18	21,21,21,21	0
57	MG	2A	3114	1/1	0.98	0.05	62,62,62,62	0
57	MG	2A	3411	1/1	0.98	0.12	52,52,52,52	0
57	MG	2A	3042	1/1	0.98	0.30	36,36,36,36	0
57	MG	1A	3403	1/1	0.98	0.44	42,42,42,42	0
57	MG	2a	1814	1/1	0.98	0.08	60,60,60,60	0
57	MG	1A	3687	1/1	0.98	0.16	21,21,21,21	0
57	MG	1A	3651	1/1	0.98	0.21	28,28,28,28	0
57	MG	1A	4038	1/1	0.98	0.16	62,62,62,62	0
57	MG	1A	3619	1/1	0.98	0.18	19,19,19,19	0
57	MG	1A	3092	1/1	0.98	0.20	24,24,24,24	0
57	MG	1A	3265	1/1	0.98	0.52	40,40,40,40	0
57	MG	1A	3693	1/1	0.98	0.11	52,52,52,52	0
57	MG	1n	101	1/1	0.98	0.14	46,46,46,46	0
57	MG	1A	3655	1/1	0.98	0.16	28,28,28,28	0
57	MG	2e	201	1/1	0.98	0.04	73,73,73,73	0
57	MG	1a	1693	1/1	0.98	0.06	61,61,61,61	0
57	MG	2A	3127	1/1	0.98	0.32	44,44,44,44	0
57	MG	2A	3054	1/1	0.98	0.12	45,45,45,45	0
57	MG	1A	3121	1/1	0.98	0.36	33,33,33,33	0
57	MG	1A	3100	1/1	0.98	0.25	41,41,41,41	0
57	MG	1a	1760	1/1	0.98	0.15	49,49,49,49	0
57	MG	1A	3072	1/1	0.98	0.13	39,39,39,39	0
57	MG	1A	3625	1/1	0.98	0.10	21,21,21,21	0
57	MG	1A	4048	1/1	0.98	0.07	61,61,61,61	0
57	MG	1A	3136	1/1	0.98	0.17	16,16,16,16	0
57	MG	1A	3030	1/1	0.98	0.11	22,22,22,22	0
57	MG	1A	3662	1/1	0.98	0.16	27,27,27,27	0
57	MG	1A	3741	1/1	0.98	0.24	47,47,47,47	0
57	MG	1A	4004	1/1	0.98	0.10	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1A	3868	1/1	0.98	0.46	33,33,33,33	0
57	MG	1A	3599	1/1	0.98	0.11	16,16,16,16	0
57	MG	1A	3575	1/1	0.98	0.15	29,29,29,29	0
57	MG	2A	3440	1/1	0.98	0.26	55,55,55,55	0
57	MG	2a	1750	1/1	0.98	0.24	63,63,63,63	0
57	MG	1a	1707	1/1	0.98	0.17	65,65,65,65	0
57	MG	1A	3055	1/1	0.98	0.28	49,49,49,49	0
57	MG	2a	1663	1/1	0.98	0.12	67,67,67,67	0
57	MG	2A	3766	1/1	0.98	0.07	54,54,54,54	0
57	MG	1A	4058	1/1	0.98	0.09	35,35,35,35	0
57	MG	1A	3602	1/1	0.98	0.19	24,24,24,24	0
57	MG	1a	1776	1/1	0.98	0.10	49,49,49,49	0
57	MG	1A	3062	1/1	0.98	0.19	30,30,30,30	0
57	MG	1A	4061	1/1	0.98	0.16	40,40,40,40	0
57	MG	1A	3634	1/1	0.98	0.16	20,20,20,20	0
57	MG	1a	1714	1/1	0.98	0.16	45,45,45,45	0
57	MG	1a	1781	1/1	0.98	0.13	53,53,53,53	0
57	MG	1U	208	1/1	0.98	0.48	37,37,37,37	0
57	MG	2A	3608	1/1	0.98	0.17	32,32,32,32	0
57	MG	1A	3635	1/1	0.98	0.12	26,26,26,26	0
57	MG	1A	3604	1/1	0.98	0.15	29,29,29,29	0
57	MG	1A	3710	1/1	0.98	0.17	19,19,19,19	0
60	ZN	15	107	1/1	0.98	0.16	43,43,43,43	0
60	ZN	1n	102	1/1	0.98	0.15	57,57,57,57	0
57	MG	2A	3009	1/1	0.98	0.10	40,40,40,40	0
57	MG	1A	3671	1/1	0.98	0.08	21,21,21,21	0
60	ZN	25	105	1/1	0.98	0.19	57,57,57,57	0
57	MG	1A	3358	1/1	0.98	0.07	38,38,38,38	0
57	MG	2A	3535	1/1	0.98	0.17	38,38,38,38	0
57	MG	1A	3140	1/1	0.98	0.22	32,32,32,32	0
57	MG	15	102	1/1	0.99	0.18	36,36,36,36	0
57	MG	15	103	1/1	0.99	0.51	28,28,28,28	0
57	MG	1a	1759	1/1	0.99	0.09	67,67,67,67	0
57	MG	1A	3355	1/1	0.99	0.49	27,27,27,27	0
57	MG	2A	3496	1/1	0.99	0.16	33,33,33,33	0
57	MG	1A	3688	1/1	0.99	0.15	21,21,21,21	0
57	MG	2A	3022	1/1	0.99	0.56	47,47,47,47	0
57	MG	1A	3122	1/1	0.99	0.19	32,32,32,32	0
57	MG	1A	3633	1/1	0.99	0.16	27,27,27,27	0
57	MG	1A	3860	1/1	0.99	0.09	36,36,36,36	0
57	MG	1A	3879	1/1	0.99	0.12	68,68,68,68	0
57	MG	2A	3337	1/1	0.99	0.18	32,32,32,32	0

Continued on next page...

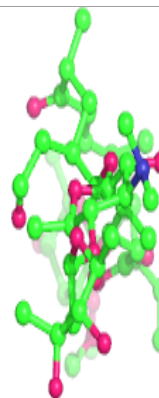
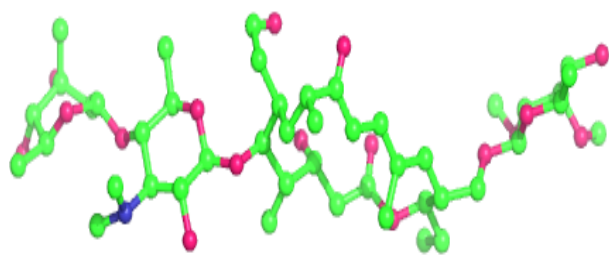
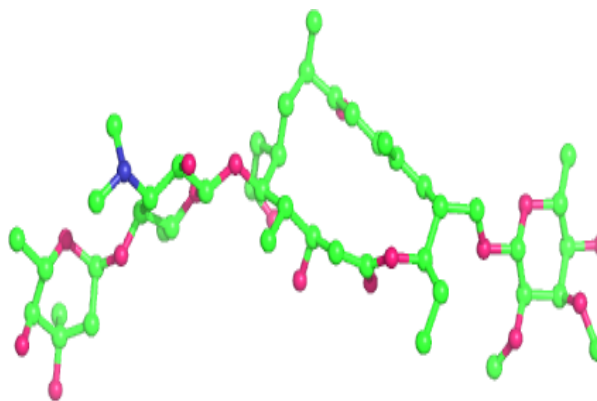
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	17	103	1/1	0.99	0.14	29,29,29,29	0
57	MG	2A	3306	1/1	0.99	0.14	43,43,43,43	0
57	MG	1A	3268	1/1	0.99	0.24	33,33,33,33	0
57	MG	1A	3170	1/1	0.99	0.19	27,27,27,27	0
57	MG	1A	3286	1/1	0.99	0.19	31,31,31,31	0
57	MG	2A	3781	1/1	0.99	0.15	52,52,52,52	0
57	MG	1A	3128	1/1	0.99	0.17	36,36,36,36	0
57	MG	1A	3003	1/1	0.99	0.13	22,22,22,22	0
57	MG	1A	3831	1/1	0.99	0.20	41,41,41,41	0
57	MG	1A	3482	1/1	0.99	0.37	37,37,37,37	0
57	MG	2A	3006	1/1	0.99	0.17	40,40,40,40	0
57	MG	1A	3574	1/1	0.99	0.20	13,13,13,13	0
57	MG	2A	3037	1/1	0.99	0.15	52,52,52,52	0
57	MG	1B	216	1/1	0.99	0.21	38,38,38,38	0
57	MG	13	101	1/1	0.99	0.15	36,36,36,36	0
57	MG	2A	3070	1/1	0.99	0.20	28,28,28,28	0
60	ZN	19	102	1/1	0.99	0.19	42,42,42,42	0
57	MG	2A	3010	1/1	0.99	0.14	47,47,47,47	0
57	MG	1A	3095	1/1	0.99	0.21	42,42,42,42	0
57	MG	1A	3835	1/1	0.99	0.16	25,25,25,25	0
57	MG	1A	3012	1/1	0.99	0.11	23,23,23,23	0
57	MG	1A	3027	1/1	0.99	0.45	32,32,32,32	0
57	MG	1A	3553	1/1	0.99	0.43	31,31,31,31	0
57	MG	1D	308	1/1	0.99	0.39	47,47,47,47	0
61	SF4	1d	501	8/8	0.99	0.18	56,62,68,68	0
61	SF4	2d	303	8/8	0.99	0.13	67,73,84,84	0
60	ZN	16	102	1/1	1.00	0.16	44,44,44,44	0

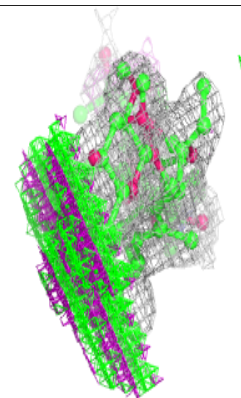
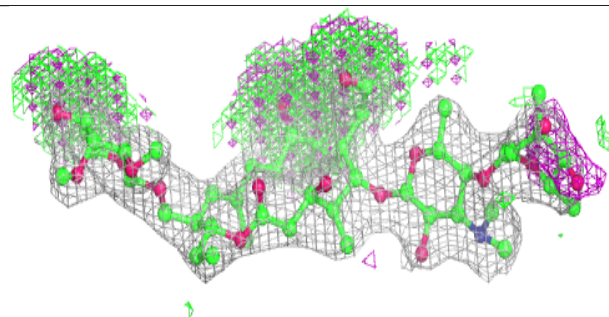
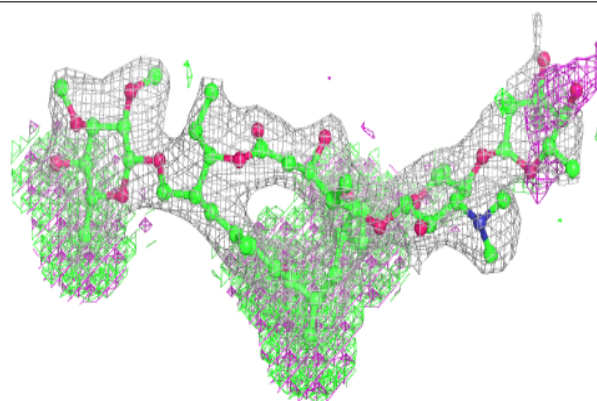
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TYK 2A 3798:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around TYK 1A 4101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.