



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 06:54 AM EDT

PDB ID : 8G2C / pdb_00008g2c
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12

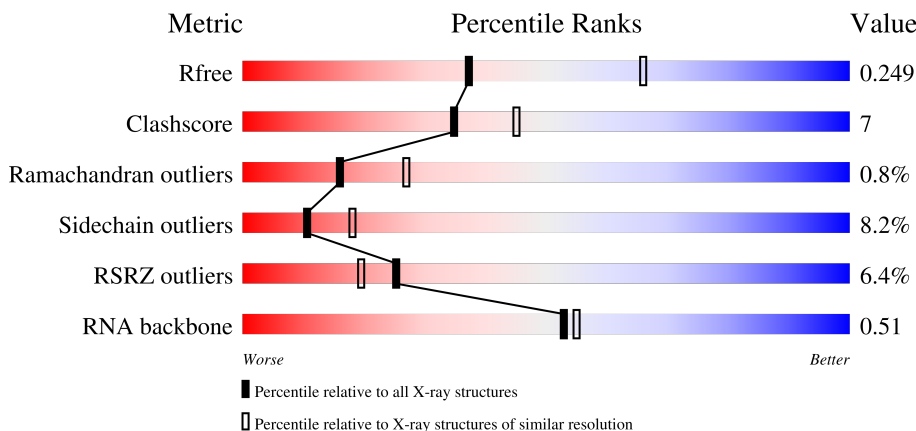
1 Overall quality at a glance

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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)
RNA backbone	3983	1090 (2.90-2.42)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	

Continued on next page...

Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.50

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	PSU	2y	55	-	-	X	-
57	MG	2A	3177	-	-	-	X
57	MG	2A	3252	-	-	-	X
57	MG	2A	3775	-	-	-	X
57	MG	2a	1610	-	-	-	X
57	MG	2a	1629	-	-	-	X
57	MG	2v	102	-	-	-	X

2 Entry composition

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
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
2	1B	120	Total	C	N	O	P	0	0	0
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	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
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called 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 (CCD ID: 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 5	Mg 5	0	0
57	1H	1	Total 1	Mg 1	0	0
57	1I	1	Total 1	Mg 1	0	0
57	1N	5	Total 5	Mg 5	0	0
57	1O	6	Total 6	Mg 6	0	0
57	1P	5	Total 5	Mg 5	0	0
57	1Q	7	Total 7	Mg 7	0	0
57	1R	6	Total 6	Mg 6	0	0
57	1S	3	Total 3	Mg 3	0	0
57	1T	3	Total 3	Mg 3	0	0
57	1U	10	Total 10	Mg 10	0	0
57	1V	5	Total 5	Mg 5	0	0
57	1W	6	Total 6	Mg 6	0	0
57	1X	6	Total 6	Mg 6	0	0
57	1Y	2	Total 2	Mg 2	0	0
57	1Z	2	Total 2	Mg 2	0	0
57	10	10	Total 10	Mg 10	0	0
57	11	5	Total 5	Mg 5	0	0
57	12	3	Total 3	Mg 3	0	0
57	13	5	Total 5	Mg 5	0	0
57	14	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

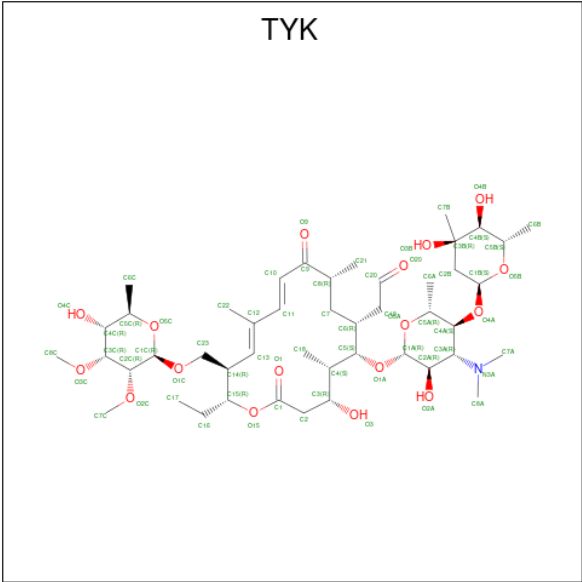
Continued from previous page...

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

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

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

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

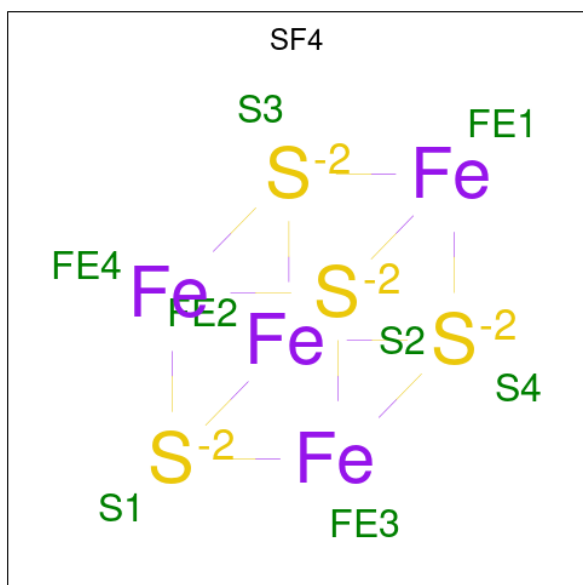
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1Y	1	Total	Zn	0	0
			1	1		
60	14	1	Total	Zn	0	0
			1	1		
60	15	1	Total	Zn	0	0
			1	1		
60	16	1	Total	Zn	0	0
			1	1		
60	19	1	Total	Zn	0	0
			1	1		
60	1n	1	Total	Zn	0	0
			1	1		
60	2Y	1	Total	Zn	0	0
			1	1		
60	24	1	Total	Zn	0	0
			1	1		
60	25	1	Total	Zn	0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

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



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

- Molecule 62 is water.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

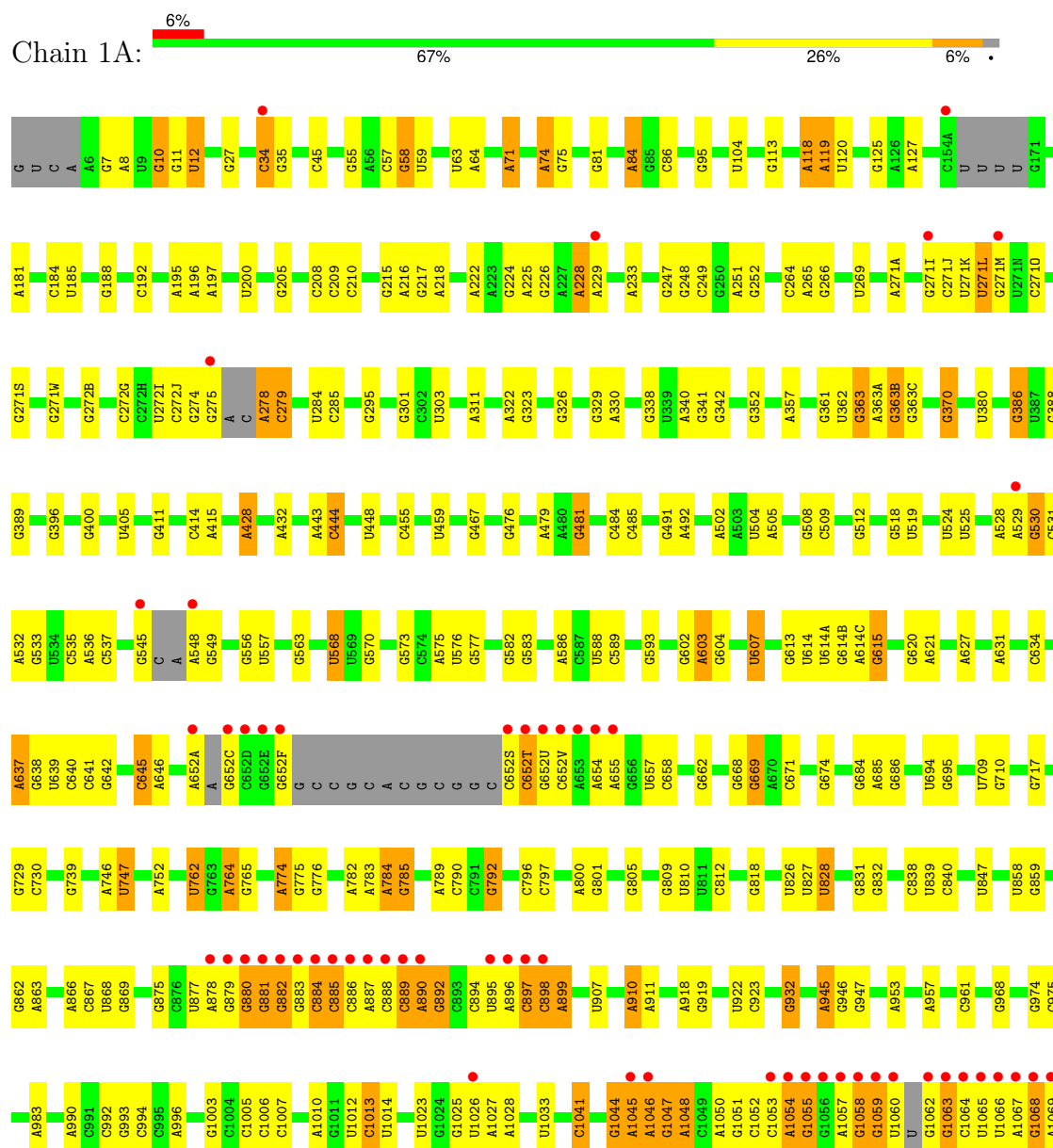
Continued from previous page...

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

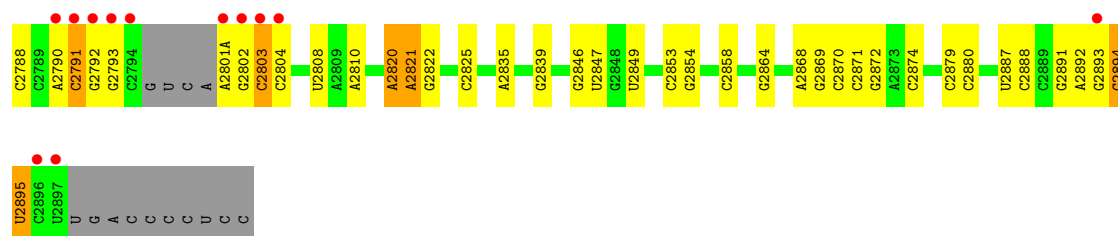
3 Residue-property plots [i](#)

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.

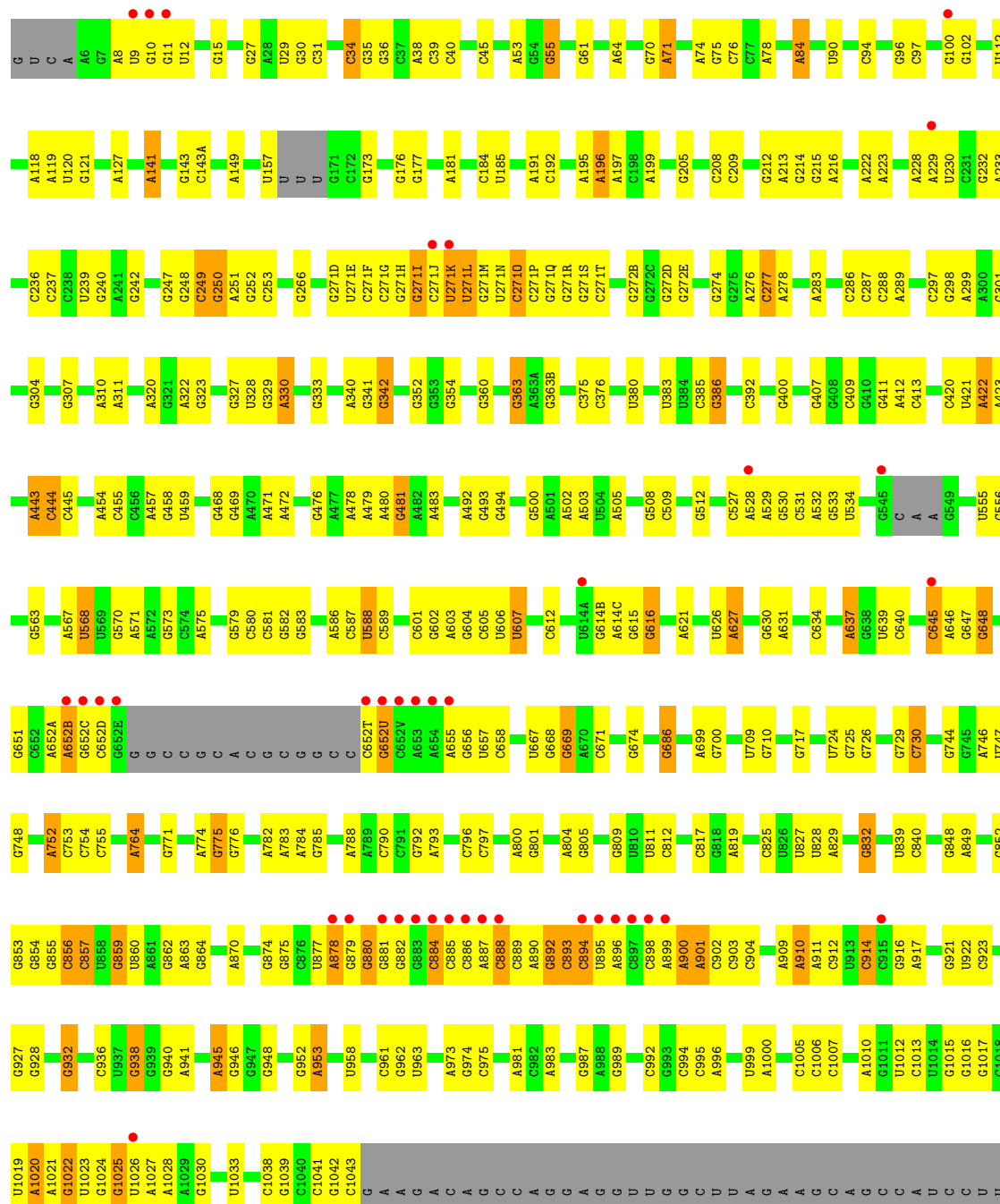
• Molecule 1: 23S Ribosomal RNA



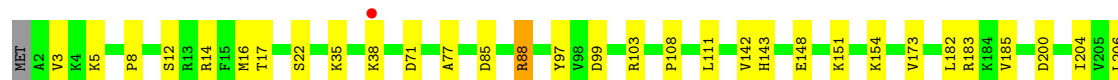
C2667	G2668	U2537	C2538	G2410	C2306	G2181	U2121	A2020	C1882	U1739	C1584	A1445	A1301	A1424A	A1070
G2669	C2670	C2539	G2540	A2422	G2307	G2182	U2122	C2021	G1883	G1740	A1586	G1448	A1302	A1143	G1071
C2683	U2684	G2541	C2542	A2423	G2308	G2183	G2123	C2022	A1587	A1741	C1587	G1449	G1303	G1144	A1072
G2685	U2686	G2543	C2544	A2425	U2312	G2185	G2124	G2023	C1588	G1745	C1589	G1450	U1313	C1163	G1074
U2689	C2690	U2552	A2426	A2426	C2316	G2187	A2126	G2029	G1899	G1756	G1593	U1453	G1314	G1164	G1075
C2691	U2692	U2553	C2427	A2427	G2319	G2188	G2127	A2030	A1900	A1762	G1594	G1455	C1315	A1165	G1076
U2693	C2694	U2554	G2428	A2428	A2320	U2189	C2128	A2031	G1903	G1763	G1595	G1456	U1316	A1166	A1077
A2693	U2694	U2563	A2430	A2430	G2325	G2191	G2130	A2033	G1602	G1764	U1602	G1461	G1324	U1165	C1079
G2694	U2695	U2564	U2431	U2431	C2326	G2192	G2132	G2038	A1603	A1773	A1603	C1467	G1332	G1171	U1081
C2699	U2700	A2566	A2435	A2435	A2327	G2193	G2134	C2039	C1607	U1907	C1607	C1467	G1332	G1172	U1082
C2701	U2702	U2572	A2439	A2439	G2329	U2198	A2135	C2040	A1608	U1779	A1608	G1460	G1338	G1173	U1083
C2703	U2704	G2573	C2440	C2440	G2330	G2199	C2136	U2041	A1609	A1780	A1609	U1481	U1352	A1174	A1085
U2712	A2713	G2574	C2441	C2441	G2331	G2205	C2137	A2042	A1510	G1781	A1510	G1482	U1352	G1176	A1086
A2714	U2715	U2582	G2445	G2445	G2334	G2206	C2138	C2043	G1622	C1782	G1622	C1493	A1359	A1177	G1087
C2716	U2717	U2583	A2448	A2448	A2335	A2207	G2140	G2053	G1623	A1786	G1623	A1494	A1360	C1178	A1088
U2585	U2586	U2584	U2449	U2449	G2337	A2208	G2141	A2054	G1628	U1790	G1628	A1495	A1364	C1179	A1089
U2587	U2588	U2589	G2458	G2458	U2344	G2218	C2142	G2056	U1629	C1791	U1629	A1496	A1365	U1187	G1091
C2589	U2590	U2591	C2464	C2464	G2345	G2219	C2143	G2056	A1791	A1791	A1632	C1498	U1372	G1191	G1092
C2592	U2593	U2594	A2469	A2469	G2346	A2225	C2144	A2060	U1931	U1794	A1632	U1503	U1372	G1191	G1093
U2602	U2603	U2604	C2474	C2474	C2347	G2235	C2145	C2061	U1503	C1795	U1639	U1504	A1379	C1201	A1095
U2605	U2606	U2607	C2475	C2475	U2348	G2236	C2146	A2062	C1504	U1796	C1640	C1505	A1380	C1201	A1096
U2608	U2609	U2610	C2476	C2476	G2349	G2238	G2147	C2065	C1506	C1797	C1640	C1506	A1220	A1220	A1097
U2611	U2612	U2613	C2477	C2477	C2350	G2239	G2148	C2069	A1507	U1798	G1642	A1507	A1384	A1226	A1098
U2615	U2616	U2617	C2478	C2478	C2351	U2243	C2149	G2074	C1508	U1799	G1643	C1508	A1385	A1226	A1099
U2618	U2619	U2620	C2483	C2483	G2352	U2244	G2150	U2075	C1509	C1800	A1664	C1509	A1393	G1236	U1101
U2621	U2622	U2623	U2491	U2491	C2353	U2245	G2151	A1952	U1963	G1801	A1664	C1509	A1393	G1236	U1102
U2625	U2626	U2627	U2498	U2498	G2354	G2251	C2152	A1953	U1963	A1803	A1668	U1518	U1396	G1243	A1103
U2629	U2630	U2631	C2499	C2499	C2355	A2268	G2153	G1954	C1962	A1810	A1669	G1519	U1396	G1243	U1105
U2633	U2634	U2635	U2502	U2502	G2356	A2269	G2154	U1955	U1963	G1811	A1670	G1519	U1396	G1244	G1106
U2636	U2637	U2638	U2504	U2504	C2357	G2270	G2155	U1963	U1963	G1812	C1670	G1519	U1396	G1244	G1107
U2640	U2641	U2642	U2505	U2505	C2358	G2271	C2156	U1963	U1963	A1815	G1674	G1519	U1396	G1244	G1108
U2643	U2644	U2645	U2506	U2506	C2359	G2272	G2157	U1963	U1963	G1816	G1674	G1519	U1396	G1244	G1109
U2646	U2647	U2648	U2507	U2507	C2360	G2273	C2158	U1963	U1963	G1817	G1683	G1519	U1396	G1244	G1110
U2649	U2650	U2651	U2508	U2508	C2361	G2274	G2159	U1963	U1963	G1818	C1684	G1519	U1396	G1244	G1111
U2652	U2653	U2654	U2509	U2509	C2362	G2275	G2160	U1963	U1963	G1819	C1684	G1519	U1396	G1244	G1112
U2655	U2656	U2657	U2510	U2510	C2363	G2276	G2161	U1963	U1963	G1820	C1684	G1519	U1396	G1244	G1113
U2658	U2659	U2660	U2511	U2511	C2364	G2277	G2162	U1963	U1963	G1821	C1684	G1519	U1396	G1244	G1114
U2661	U2662	U2663	U2512	U2512	C2365	G2278	G2163	U1963	U1963	G1822	C1684	G1519	U1396	G1244	G1115
U2664	U2665	U2666	U2513	U2513	C2366	G2279	G2164	U1963	U1963	G1823	C1684	G1519	U1396	G1244	G1116
U2667	U2668	U2669	U2514	U2514	C2367	G2280	G2165	U1963	U1963	G1824	C1684	G1519	U1396	G1244	G1117
U2670	U2671	U2672	U2515	U2515	C2368	G2281	G2166	U1963	U1963	G1825	C1684	G1519	U1396	G1244	G1118
U2673	U2674	U2675	U2516	U2516	C2369	G2282	G2167	U1963	U1963	G1826	C1684	G1519	U1396	G1244	G1119
U2676	U2677	U2678	U2517	U2517	C2370	G2283	G2168	U1963	U1963	G1827	C1684	G1519	U1396	G1244	G1120
U2679	U2680	U2681	U2518	U2518	C2371	G2284	G2169	U1963	U1963	G1828	C1684	G1519	U1396	G1244	G1121
U2682	U2683	U2684	U2519	U2519	C2372	G2285	G2170	U1963	U1963	G1829	C1684	G1519	U1396	G1244	G1122
U2685	U2686	U2687	U2520	U2520	C2373	G2286	G2171	U1963	U1963	G1830	C1684	G1519	U1396	G1244	G1123
U2688	U2689	U2690	U2521	U2521	C2374	G2287	G2172	U1963	U1963	G1831	C1684	G1519	U1396	G1244	G1124
U2691	U2692	U2693	U2522	U2522	C2375	G2288	G2173	U1963	U1963	G1832	C1684	G1519	U1396	G1244	G1125
U2694	U2695	U2696	U2523	U2523	C2376	G2289	G2174	U1963	U1963	G1833	C1684	G1519	U1396	G1244	G1126
U2697	U2698	U2699	U2524	U2524	C2377	G2290	G2175	U1963	U1963	G1834	C1684	G1519	U1396	G1244	G1127
U2700	U2701	U2702	U2525	U2525	C2378	G2291	G2176	U1963	U1963	G1835	C1684	G1519	U1396	G1244	G1128
U2703	U2704	U2705	U2526	U2526	C2379	G2292	G2177	U1963	U1963	G1836	C1684	G1519	U1396	G1244	G1129
U2706	U2707	U2708	U2527	U2527	C2380	G2293	G2178	U1963	U1963	G1837	C1684	G1519	U1396	G1244	G1130
U2709	U2710	U2711	U2528	U2528	C2381	G2294	G2179	U1963	U1963	G1838	C1684	G1519	U1396	G1244	G1131
U2712	U2713	U2714	U2529	U2529	C2382	G2295	G2180	U1963	U1963	G1839	C1684	G1519	U1396	G1244	G1132
U2715	U2716	U2717	U2530	U2530	C2383	G2296	G2181	U1963	U1963	G1840	C1684	G1519	U1396	G1244	G1133
U2718	U2719	U2720	U2531	U2531	C2384	G2297	G2182	U1963	U1963	G1841	C1684	G1519	U1396	G1244	G1134
U2721	U2722	U2723	U2532	U2532	C2385	G2298	G2183	U1963	U1963	G1842	C1684	G1519	U1396	G1244	G1135
U2724	U2725	U2726	U2533	U2533	C2386	G2299	G2184	U1963	U1963	G1843	C1684	G1519	U1396	G1244	G1136
U2727	U2728	U2729	U2534	U2534	C2387	G2300	G2185	U1963	U1963	G1844	C1684	G1519	U1396	G1244	G1137
U2730	U2731	U2732	U2535	U2535	C2388	G2301	G2186	U1963	U1963	G1845	C1684	G1519	U1396	G1244	G1138
U2733	U2734	U2735	U2536	U2536	C2389	G2302	G2187	U1963	U1963	G1846	C1684	G1519	U1396	G1244	G1139
U2736	U2737	U2738	U2537	U2537	C2390	G2303	G2188	U1963	U1963	G1847	C1684	G1519	U1396	G1244	G1140
U2739	U2740	U2741	U2538	U2538	C2391	G2304	G2189	U1963	U1963	G1848	C1684	G1519	U1396	G1244	G1141
U2742	U2743	U2744	U2539	U2539	C2392	G2305	G2190	U1963	U1963	G1849	C1684	G1519	U1396	G1244	G1142
U2745	U2746	U2747	U2540	U2540	C2393	G2306	G2191	U1963	U1963	G1850	C1684	G1519	U1396	G1244	G1143
U2748	U2749	U2750	U2541	U2541	C2394	G2307	G2192	U1963	U1963	G1851	C1684	G1519	U1396	G1244	G1144
U2751	U2752	U2753	U2542	U2542	C2395	G2308	G2193	U1963	U1963	G1852	C1684	G1519	U1396	G1244	G1145
U2754	U2755	U2756	U2543	U2543	C2396	G2309	G2194	U1963	U1963	G1853	C1684	G1519	U1396	G1244	G1146
U2757	U2758	U2759	U2544	U2544	C2397	G2310	G2195	U1963	U1963	G1854	C1684	G1519	U1396	G1244	G1147
U2760	U2761	U2762	U2545	U2545	C2398	G2311	G2196	U1963	U1963	G1855	C1684	G1519	U1396	G1244	G1148
U2763	U2764	U2765	U2546	U2546	C2399	G2312	G2197	U1963	U1963	G1856	C1684	G1519	U1396	G1244	G1149
U2766	U2767	U2768	U2547	U2547	C2400	G2313	G2198	U1963	U1963	G1857	C1684	G1519	U1396	G1244	G1150
U2769	U2770	U2771	U2548	U2548	C2401	G2314	G2199	U1963	U1963	G1858	C1684	G1519	U1396	G1244	G1151
U2772	U2773	U2774	U2549	U2549	C2402	G2315	G2200	U1963	U1963	G1859	C1684	G1519	U1396	G1244	G1152
U2775	U2776	U2777	U2550	U2550	C2403	G2316	G2201	U1963	U1963	G1860	C1684	G1519	U1396	G1244	G1153
U2778	U2779	U2780	U2551	U2551	C2404	G2317	G2202	U1963	U1963	G1861	C1684	G1519	U1396	G1244	G1154
U2781	U2782	U2783	U2552	U2552	C2405	G2318	G2203	U1963	U1963	G1862	C1684	G1519	U1396	G1244	G1155
U2784	U2785	U2786	U2553	U2553	C2406	G2319	G2204	U1963	U1963	G1863	C1684	G1519	U1396	G1244	G1156
U2787	U2788	U2789	U255												



• Molecule 1: 23S Ribosomal RNA



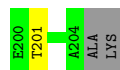






- Molecule 4: 50S ribosomal protein L3

Chain 1E: 82% 16% ..



- Molecule 4: 50S ribosomal protein L3

Chain 2E: 75% 21% ..



- Molecule 5: 50S ribosomal protein L4

Chain 1F: 69% 23% ..



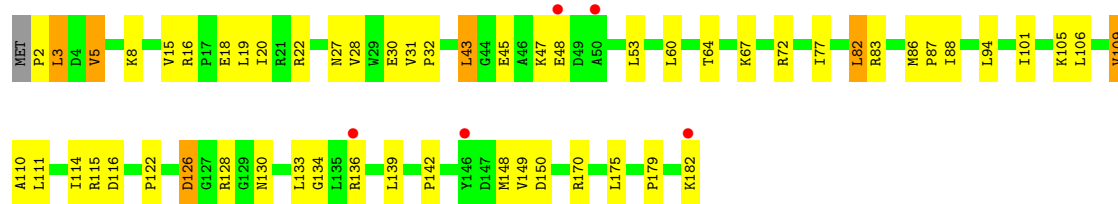
- Molecule 5: 50S ribosomal protein L4

Chain 2F: 68% 27% ..

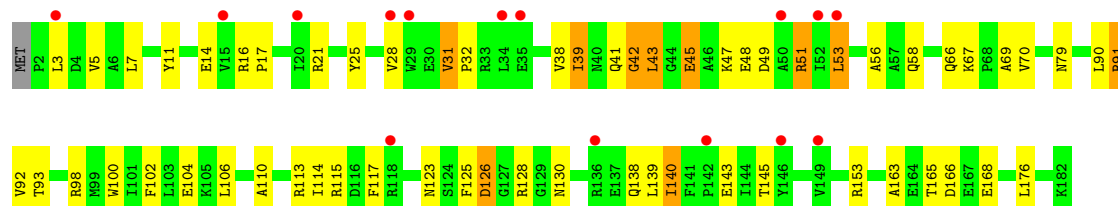


- Molecule 6: 50S ribosomal protein L5

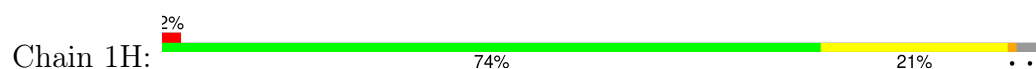
Chain 1G: 69% 27% ..



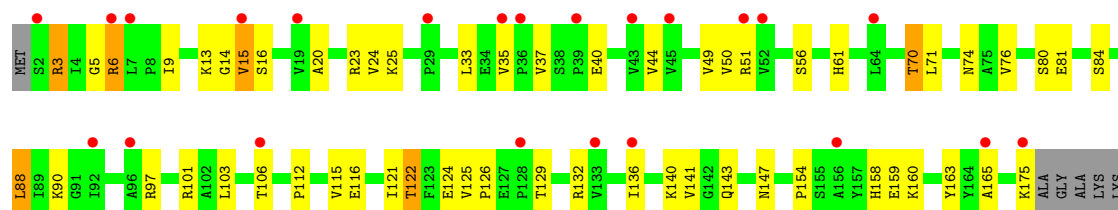
• Molecule 6: 50S ribosomal protein L5



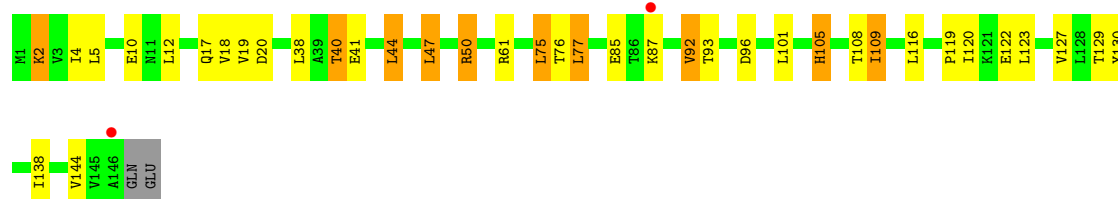
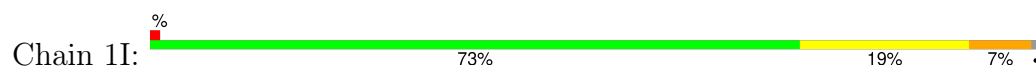
• Molecule 7: 50S ribosomal protein L6



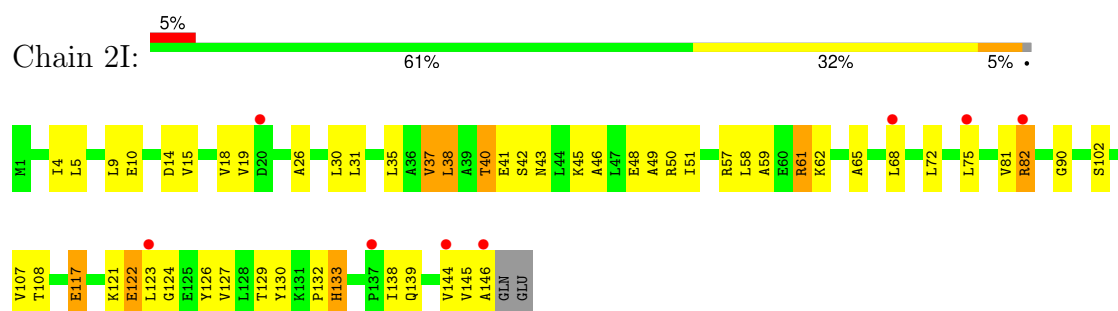
• Molecule 7: 50S ribosomal protein L6



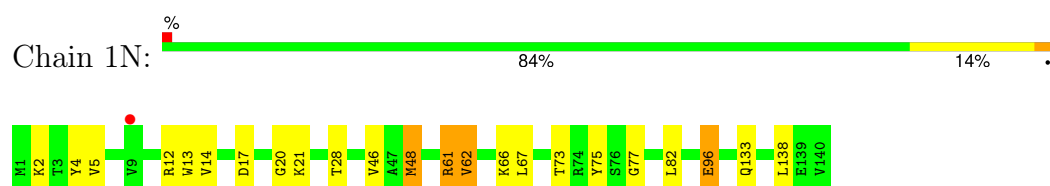
• Molecule 8: 50S ribosomal protein L9



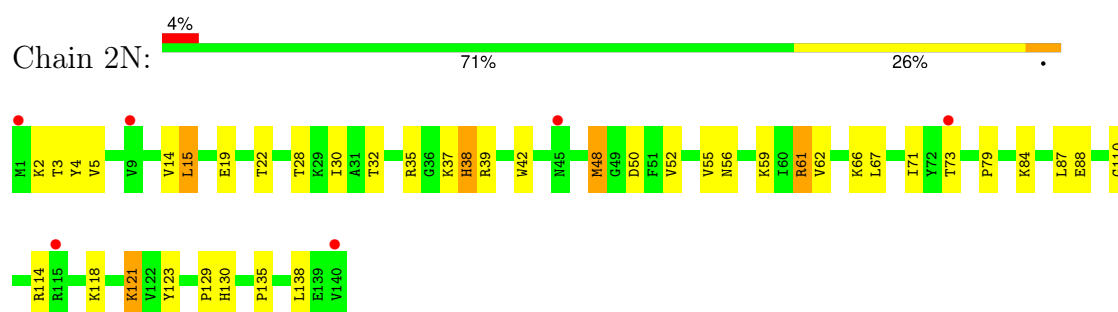
- Molecule 8: 50S ribosomal protein L9



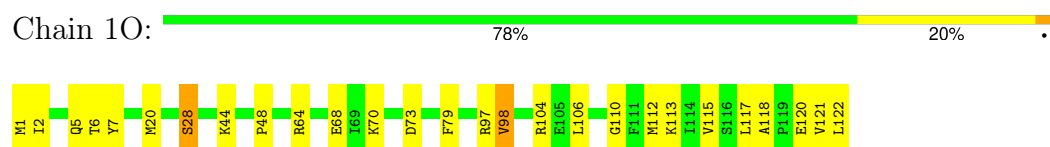
- Molecule 9: 50S ribosomal protein L13



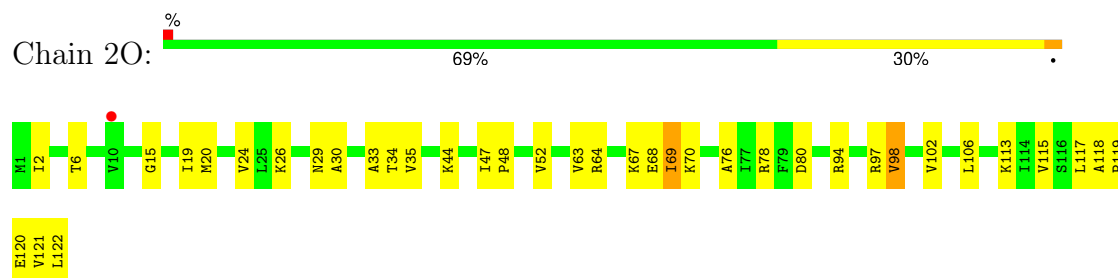
- Molecule 9: 50S ribosomal protein L13



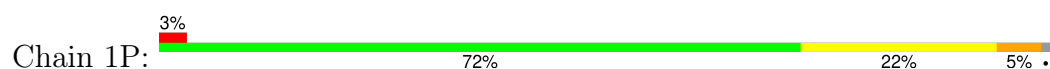
- Molecule 10: 50S ribosomal protein L14

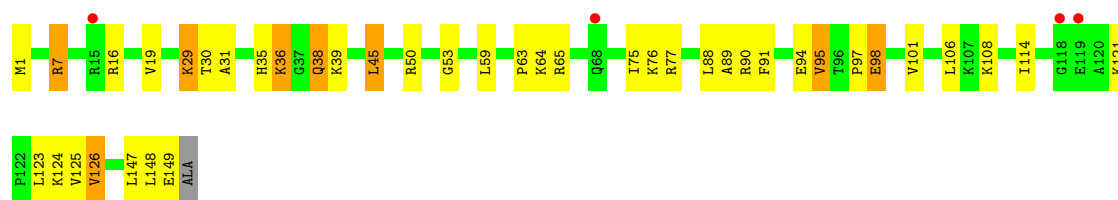


- Molecule 10: 50S ribosomal protein L14

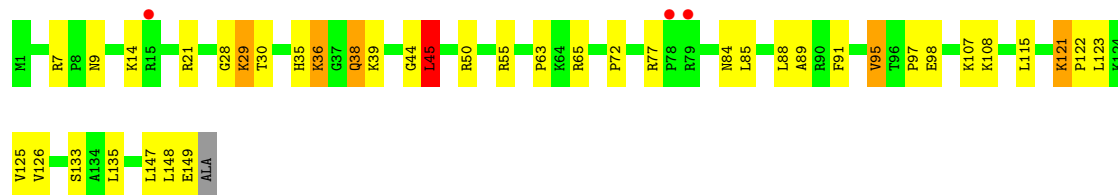
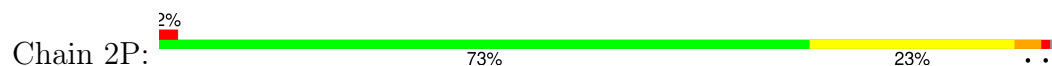


- Molecule 11: 50S ribosomal protein L15

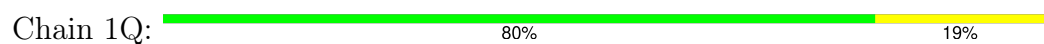




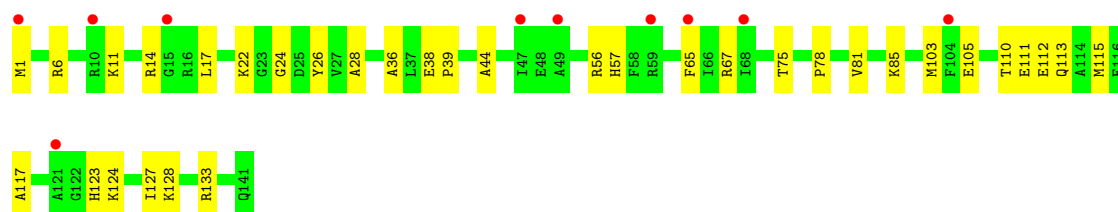
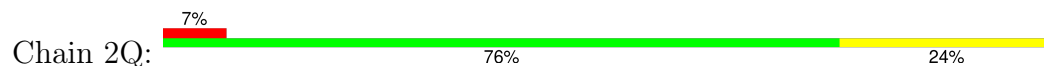
- Molecule 11: 50S ribosomal protein L15



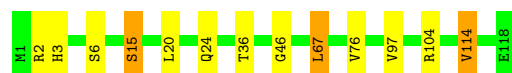
- Molecule 12: 50S ribosomal protein L16



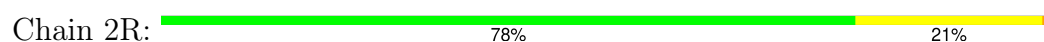
- Molecule 12: 50S ribosomal protein L16



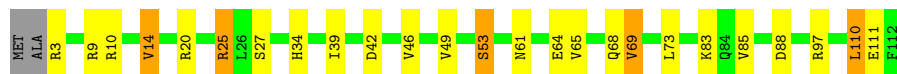
- Molecule 13: 50S ribosomal protein L17



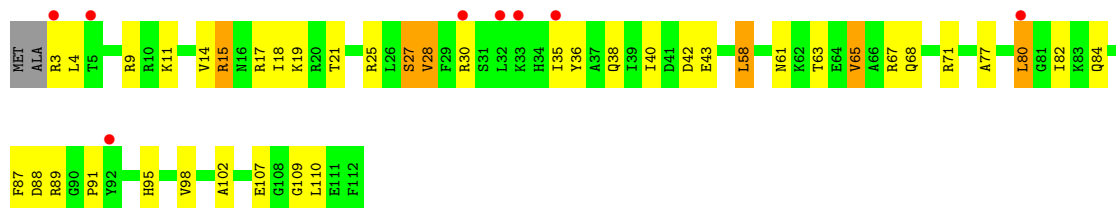
- Molecule 13: 50S ribosomal protein L17



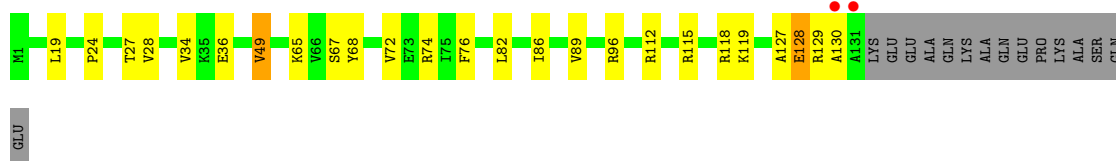
• Molecule 14: 50S ribosomal protein L18

Chain 1S:  76% 18% . .

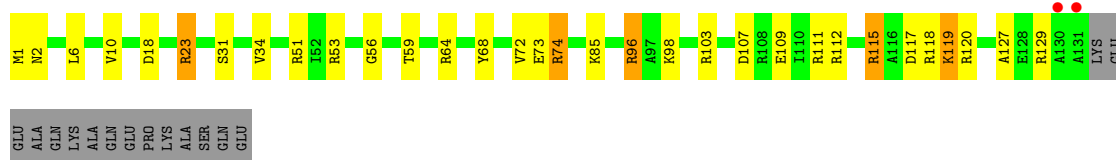
• Molecule 14: 50S ribosomal protein L18

Chain 2S:  7% 62% 31% 5% .

• Molecule 15: 50S ribosomal protein L19

Chain 1T:  % 73% 16% . 10%

• Molecule 15: 50S ribosomal protein L19

Chain 2T:  % 68% 18% . 10%

• Molecule 16: 50S ribosomal protein L20

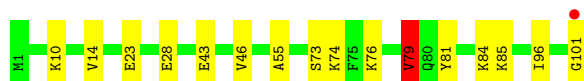
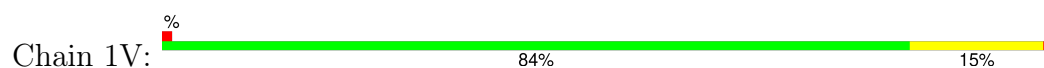
Chain 1U:  81% 16% . .

• Molecule 16: 50S ribosomal protein L20

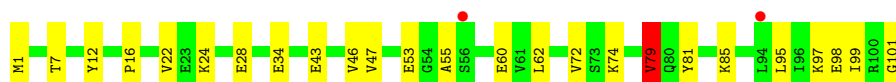
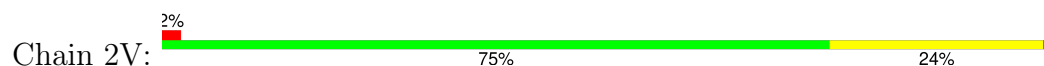
Chain 2U:  % 79% 18% . .



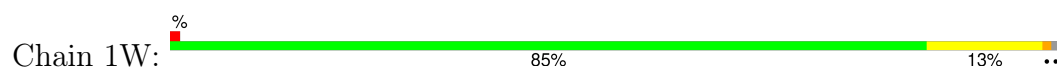
- Molecule 17: 50S ribosomal protein L21



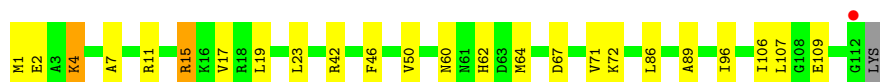
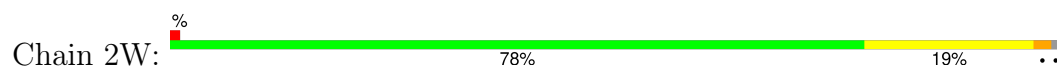
- Molecule 17: 50S ribosomal protein L21



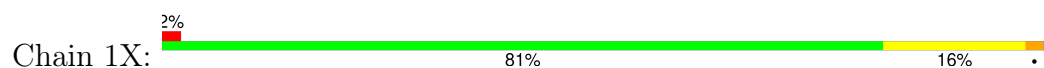
- Molecule 18: 50S ribosomal protein L22



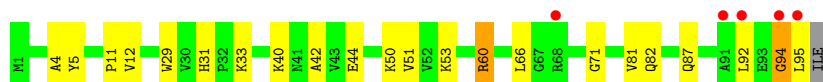
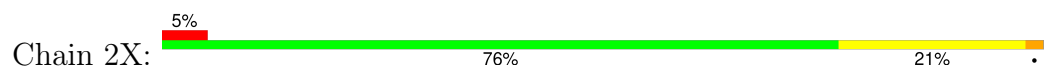
- Molecule 18: 50S ribosomal protein L22



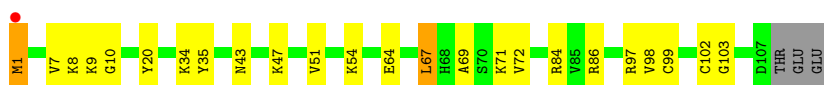
- Molecule 19: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24



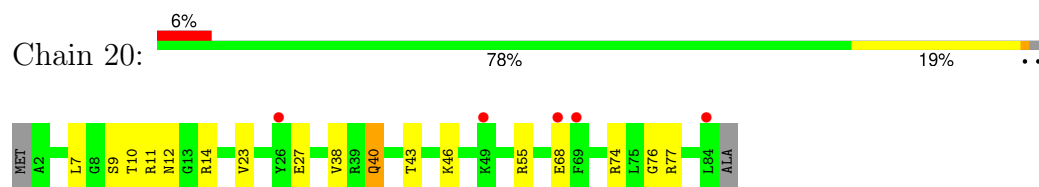
-

- | | | |
|-----|------|------|
| GLU | P130 | M1 |
| PRO | R131 | E2 |
| GLU | M132 | |
| GLU | I133 | A7 |
| ILE | P134 | Y8 |
| LYS | E135 | |
| LYS | F136 | E11 |
| GLY | I137 | |
| GLY | E138 | R31 |
| LYS | E139 | |
| GLU | V139 | |
| GLU | D140 | K36 |
| GLU | V141 | V37 |
| GLU | SER | Y38 |
| GLU | GLY | |
| GLU | LEU | V42 |
| GLU | GLU | |
| | I146 | R49 |
| | G147 | |
| | D148 | S52 |
| | S149 | I53 |
| | L150 | H54 |
| | H151 | |
| | A152 | L61 |
| | S153 | |
| | D154 | R72 |
| | L155 | Q73 |
| | K156 | |
| | L157 | D77 |
| | P158 | |
| | P159 | S92 |
| | | D93 |
| | A164 | |
| | V165 | E97 |
| | S166 | |
| LYS | P167 | L102 |
| | E168 | R103 |
| | E169 | F104 |
| | T170 | V105 |
| | I171 | GLY |
| ALA | ALA | THR |
| ALA | ALA | PRO |
| VAL | VAL | ALA |
| VAL | VAL | GLY |
| PRO | PRO | VAL |
| PRO | PRO | ARG |
| GLU | GLU | ALA |
| ASP | ASP | GLY |
| VAL | VAL | GLY |
| GLU | GLU | VAL |
| LYS | LYS | LEU |
| LEU | LEU | GLN |
| ALA | ALA | E119 |
| GLU | GLU | I120 |
| GLU | GLU | |
| ALA | ALA | D123 |
| ALA | ALA | I124 |
| ALA | ALA | L125 |
| GLU | GLU | V126 |
| VAL | VAL | |
| ALA | ALA | S129 |

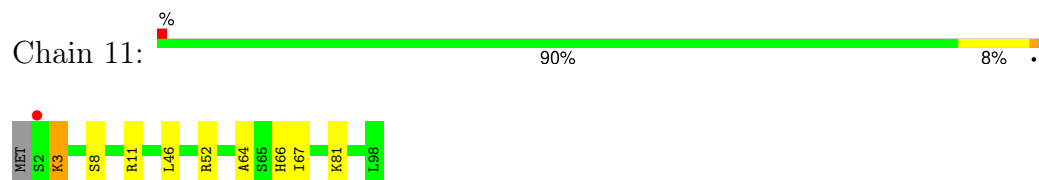
- [illegible]

-
- Sequence logo for the 12-mer motif. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows positions 1 to 12. The sequence is MET A2 T10 R11 N12 A18 T43 V51 Q70 H80 L84 ALA. MET and ALA are in grey boxes, while the others are in yellow boxes.

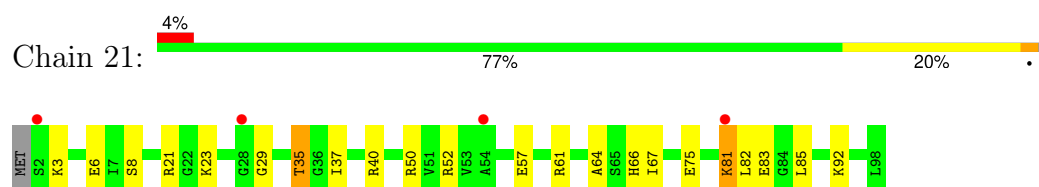
- Molecule 22: 50S ribosomal protein L27



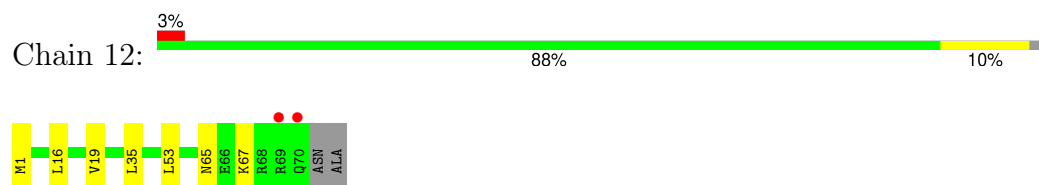
- Molecule 23: 50S ribosomal protein L28



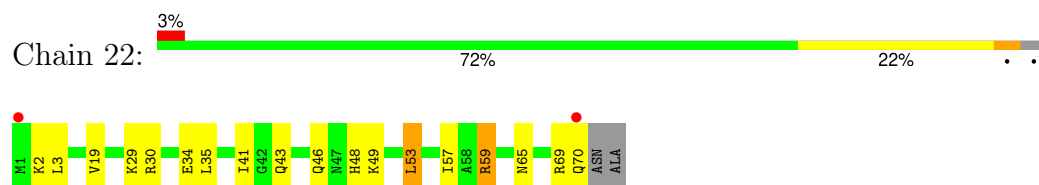
- Molecule 23: 50S ribosomal protein L28



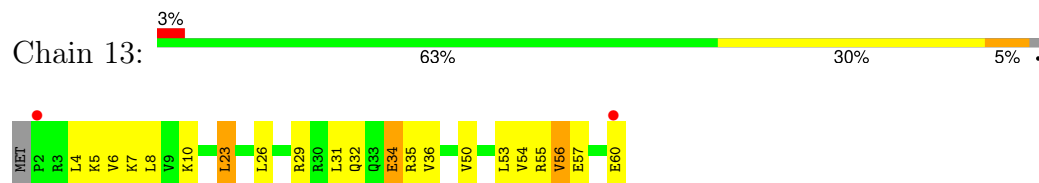
- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30

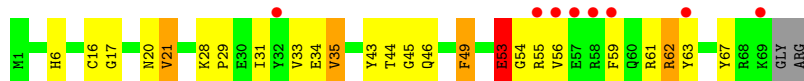


- Molecule 25: 50S ribosomal protein L30





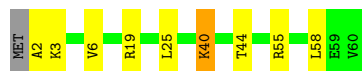
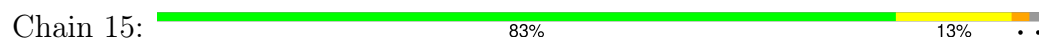
- Molecule 26: 50S ribosomal protein L31



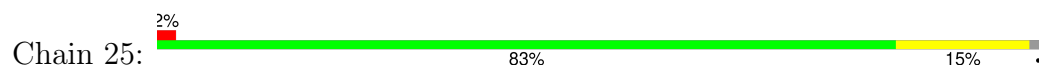
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



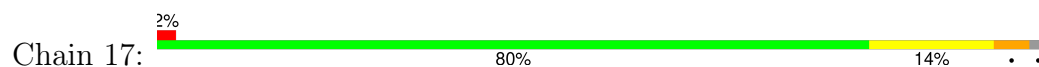
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33

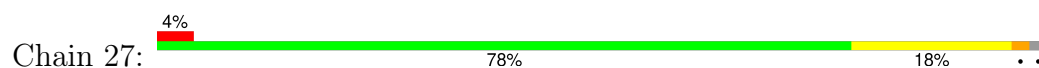


- Molecule 29: 50S ribosomal protein L34

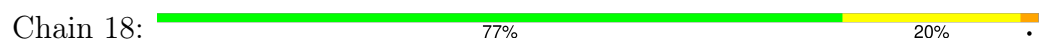




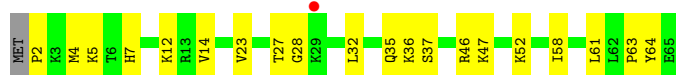
- Molecule 29: 50S ribosomal protein L34



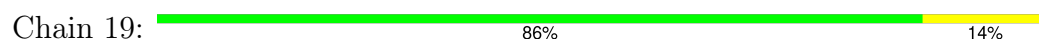
- Molecule 30: 50S ribosomal protein L35



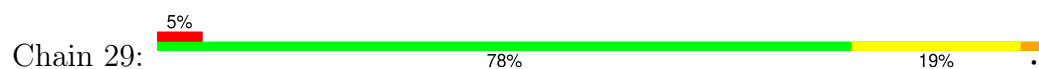
- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36

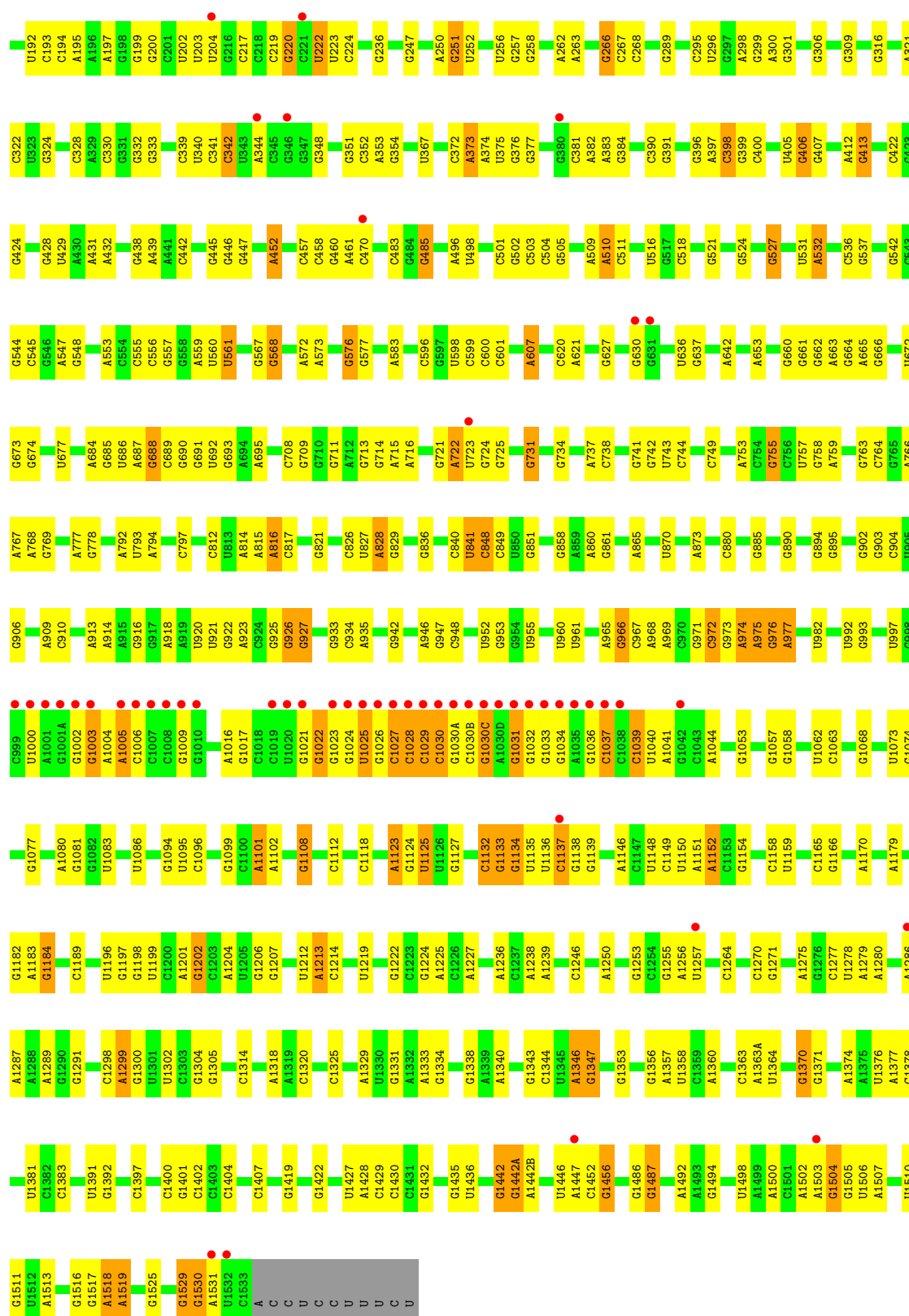


- Molecule 31: 50S ribosomal protein L36

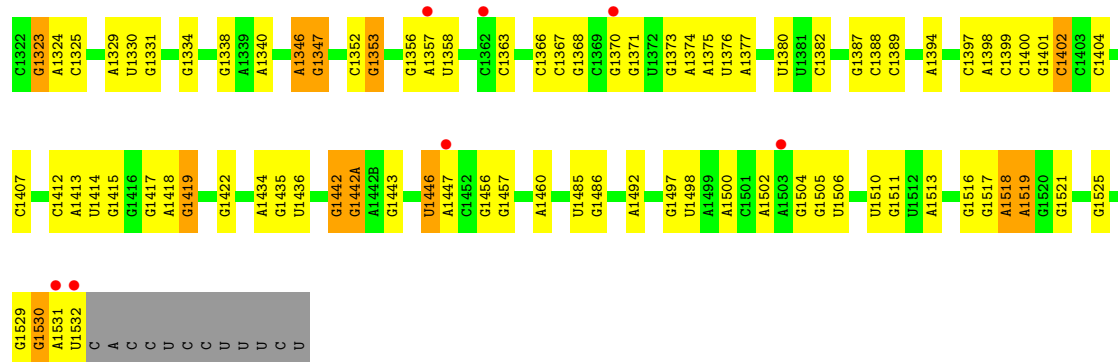


- Molecule 32: 16S Ribosomal RNA

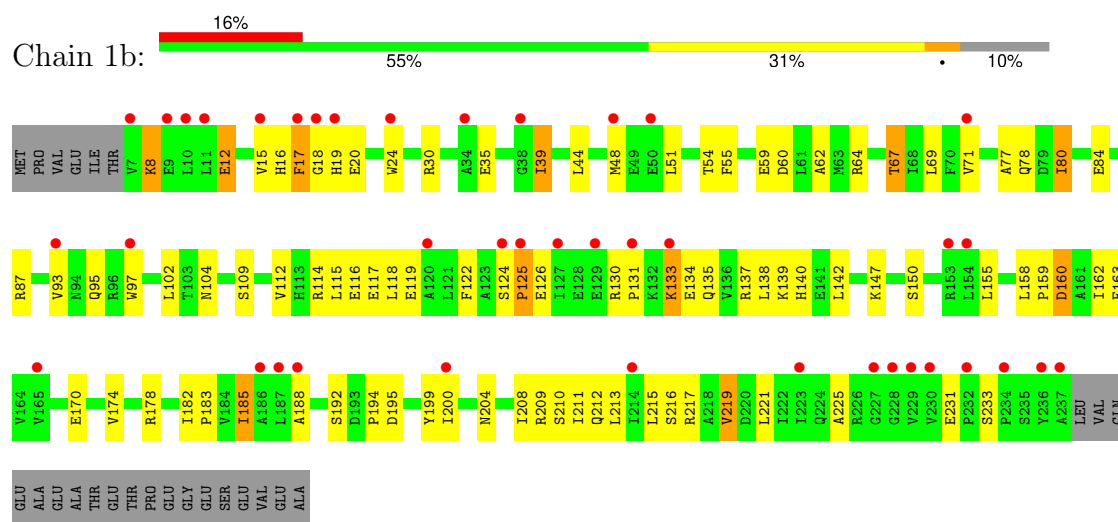




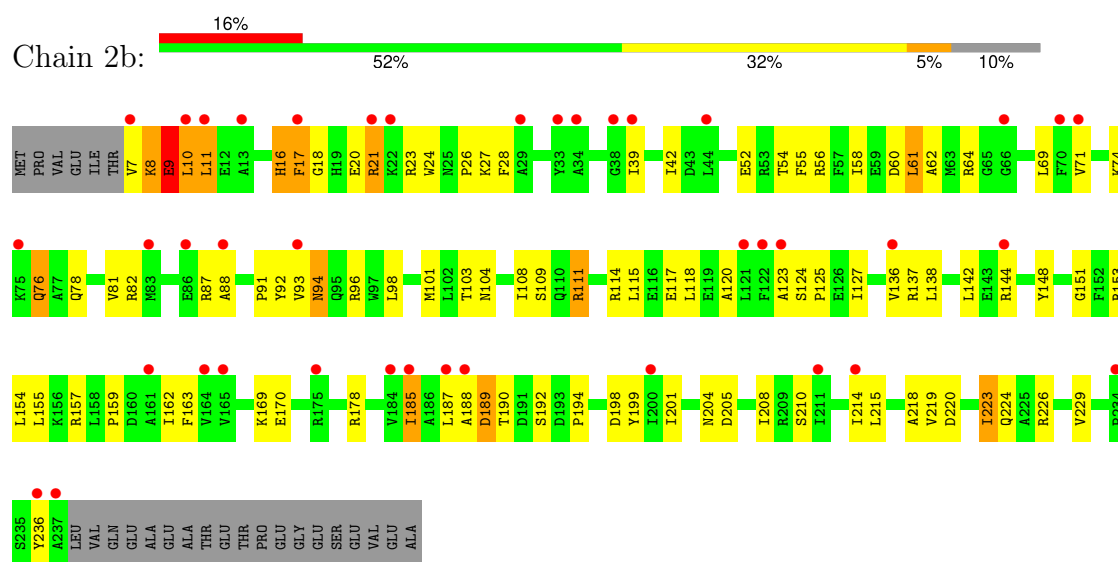




• Molecule 33: 30S ribosomal protein S2

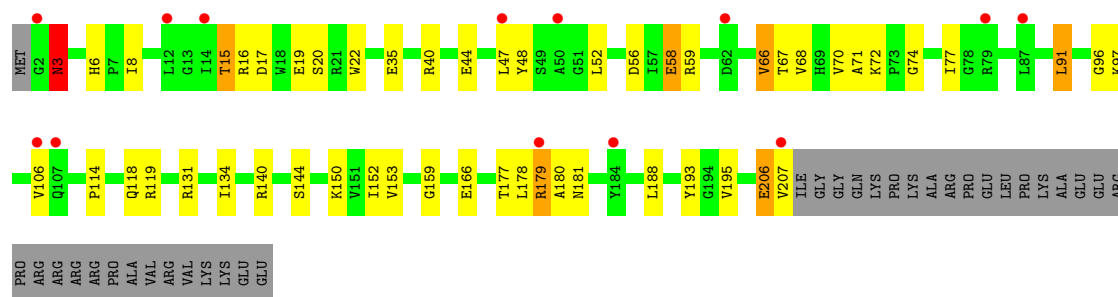


• Molecule 33: 30S ribosomal protein S2

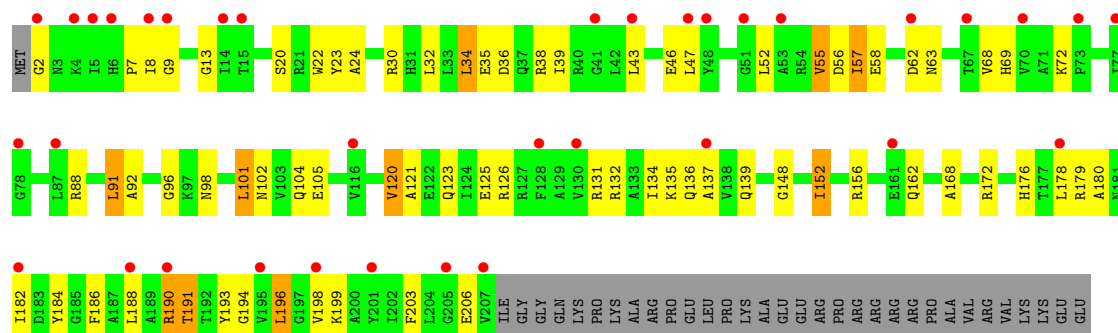


• Molecule 34: 30S ribosomal protein S3

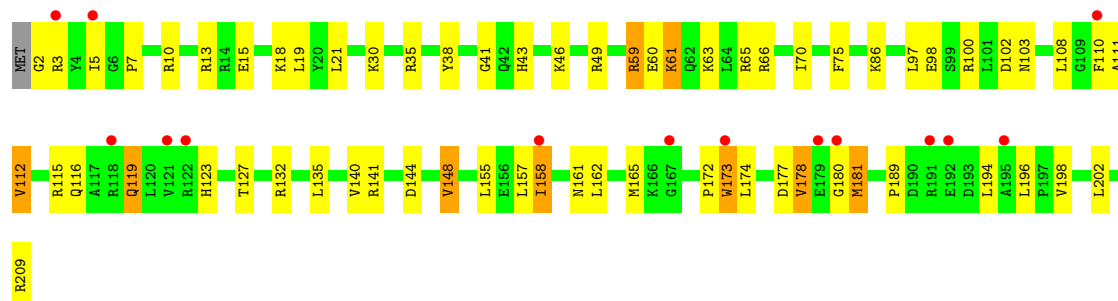




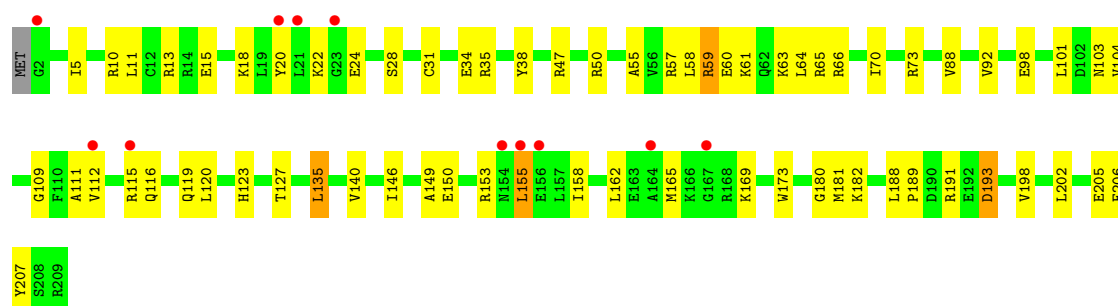
• Molecule 34: 30S ribosomal protein S3



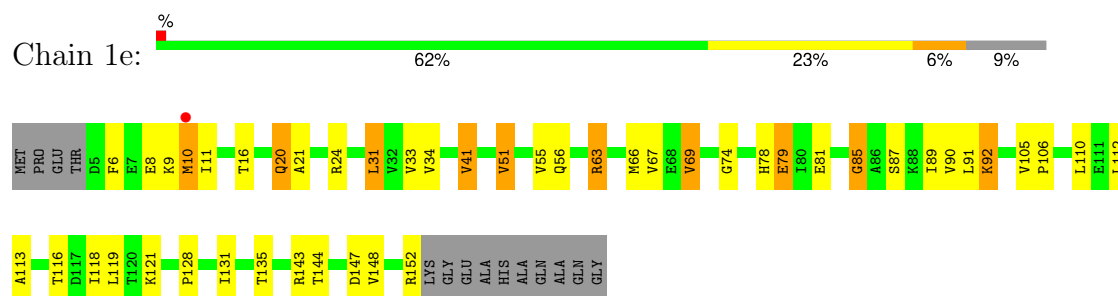
• Molecule 35: 30S ribosomal protein S4



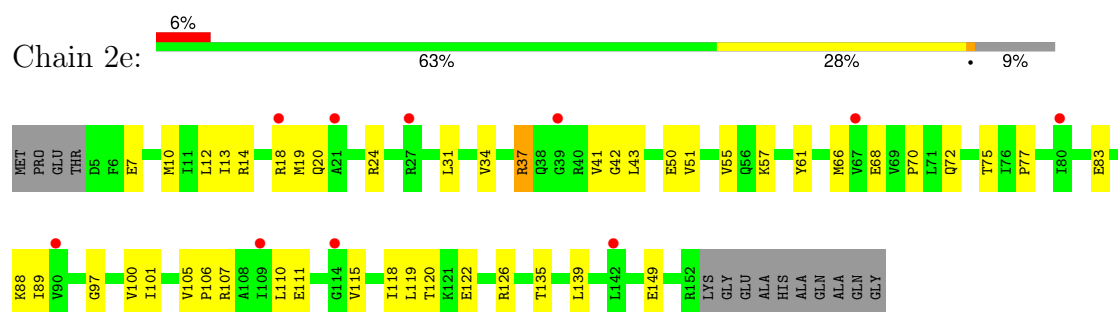
• Molecule 35: 30S ribosomal protein S4



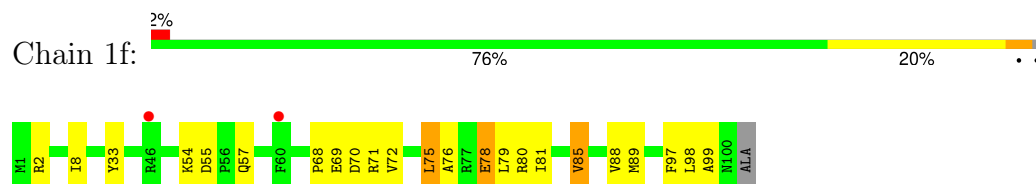
- Molecule 36: 30S ribosomal protein S5



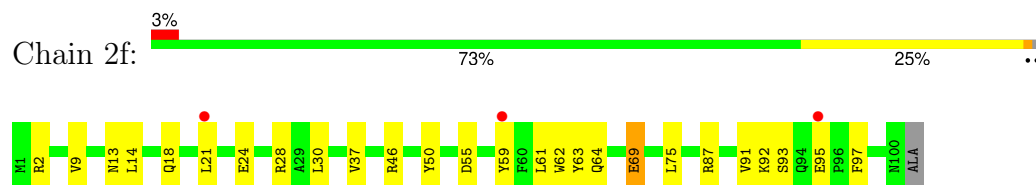
- Molecule 36: 30S ribosomal protein S5



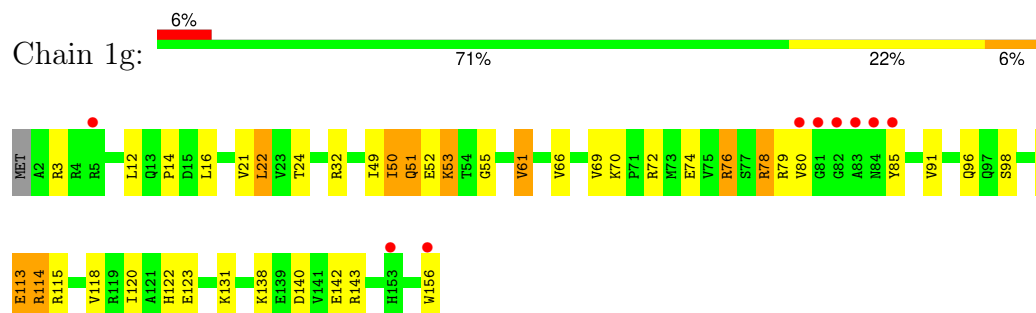
- Molecule 37: 30S ribosomal protein S6



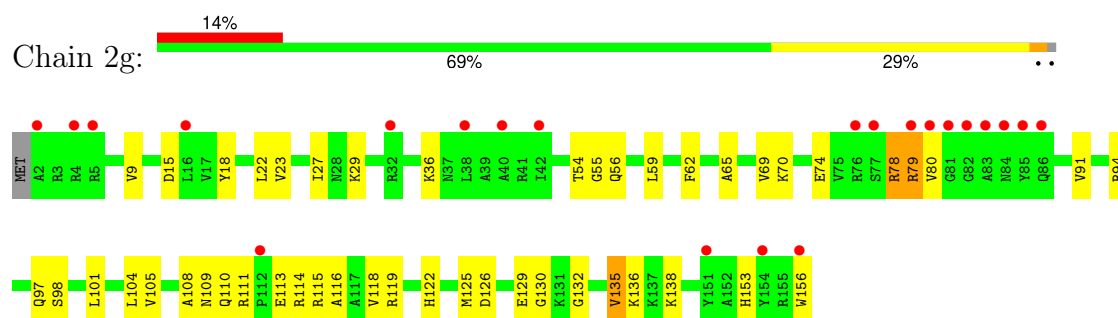
- Molecule 37: 30S ribosomal protein S6



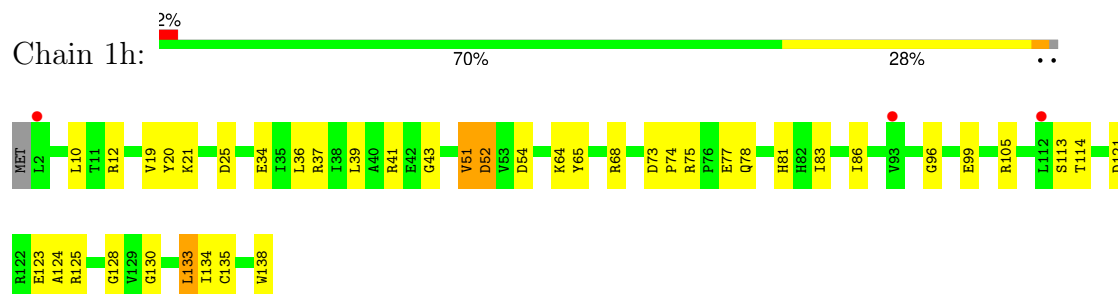
- Molecule 38: 30S ribosomal protein S7



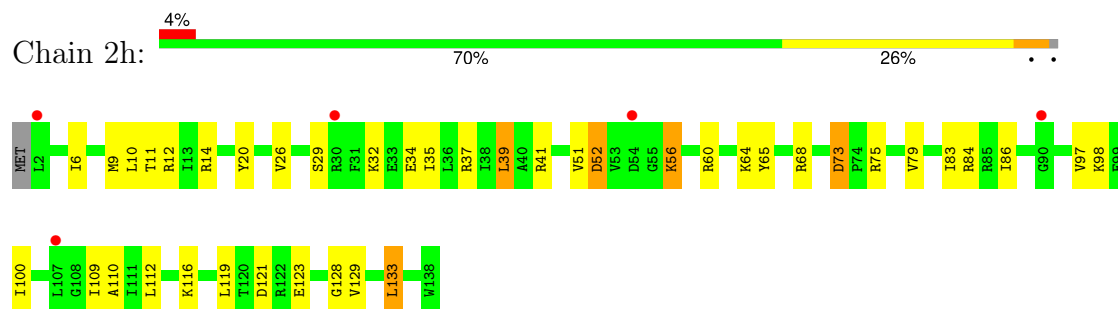
- Molecule 38: 30S ribosomal protein S7



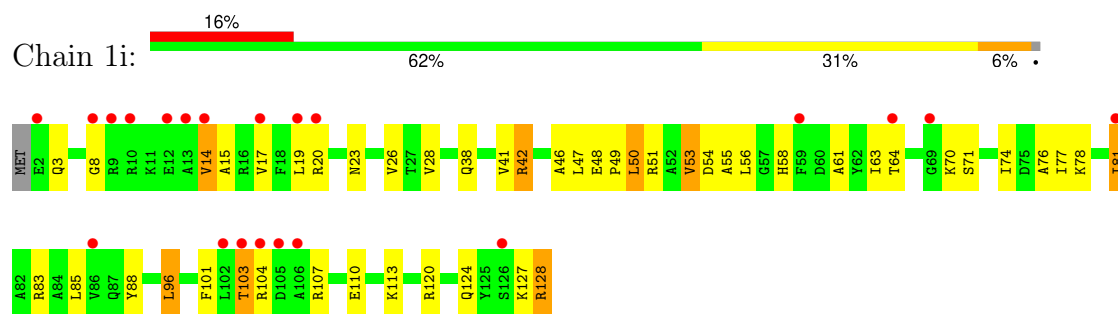
• Molecule 39: 30S ribosomal protein S8



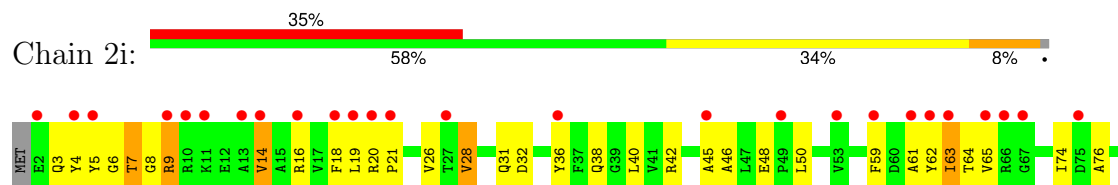
• Molecule 39: 30S ribosomal protein S8

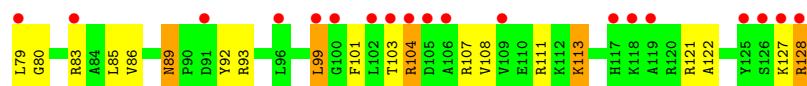


• Molecule 40: 30S ribosomal protein S9

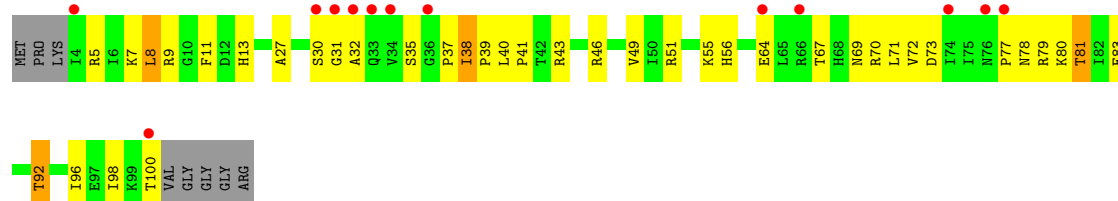


• Molecule 40: 30S ribosomal protein S9

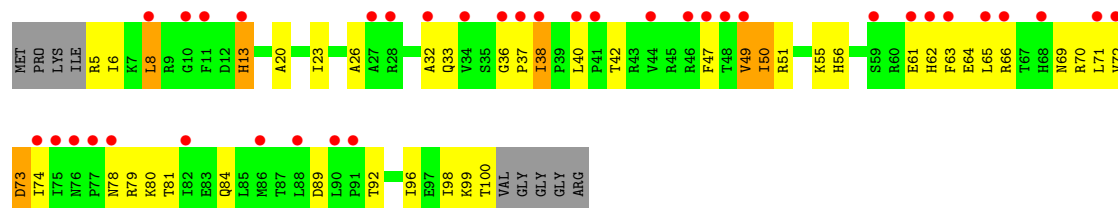




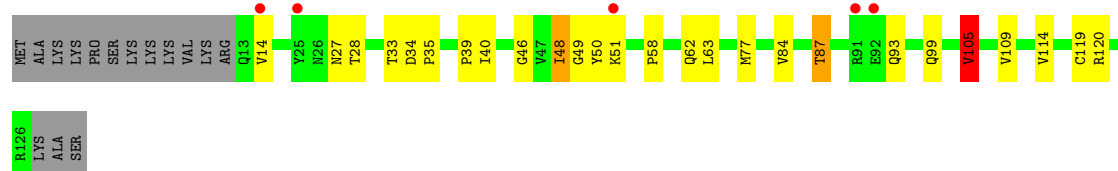
- Molecule 41: 30S ribosomal protein S10



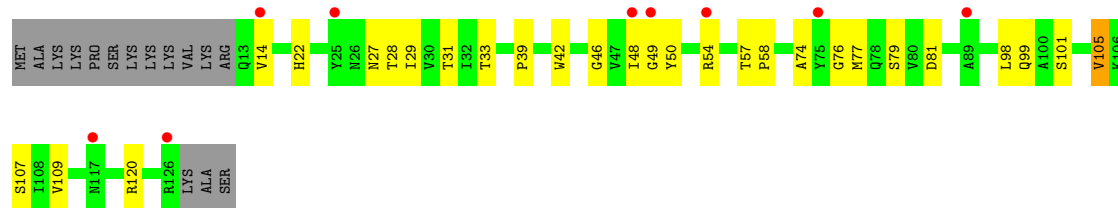
- Molecule 41: 30S ribosomal protein S10



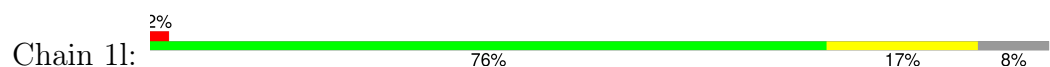
- Molecule 42: 30S ribosomal protein S11

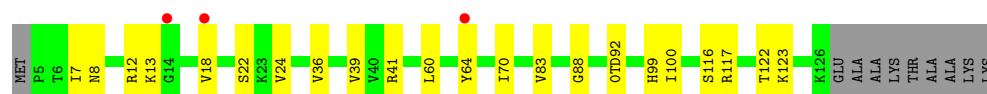


- Molecule 42: 30S ribosomal protein S11

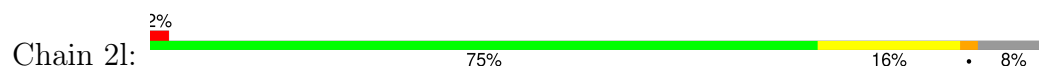


- Molecule 43: 30S ribosomal protein S12

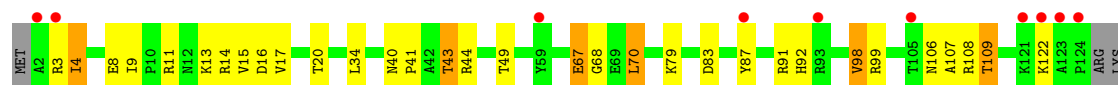




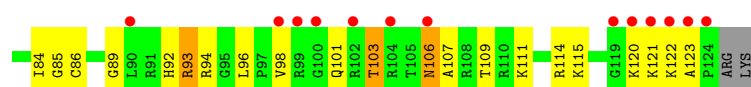
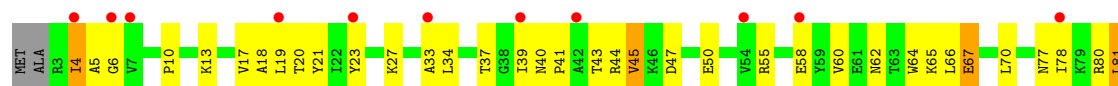
- Molecule 43: 30S ribosomal protein S12



- Molecule 44: 30S ribosomal protein S13



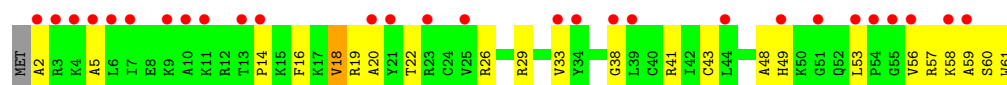
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z

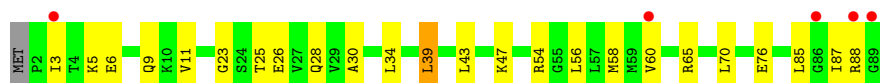
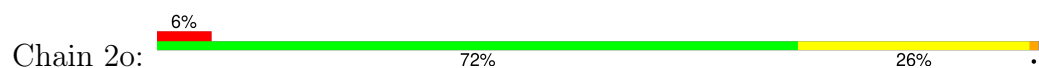


- Molecule 46: 30S ribosomal protein S15





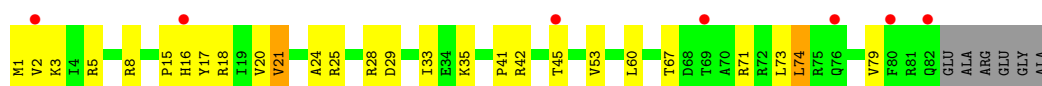
- Molecule 46: 30S ribosomal protein S15



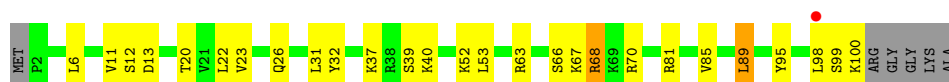
- Molecule 47: 30S ribosomal protein S16



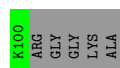
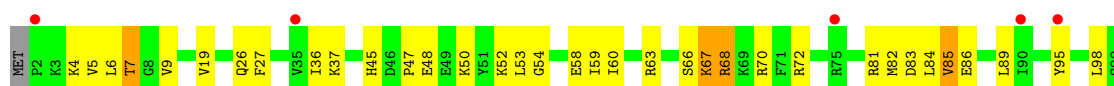
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17

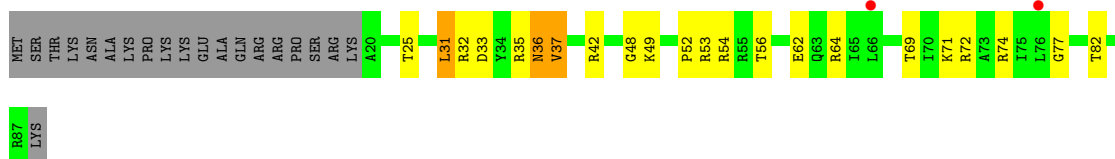


- Molecule 49: 30S ribosomal protein S18





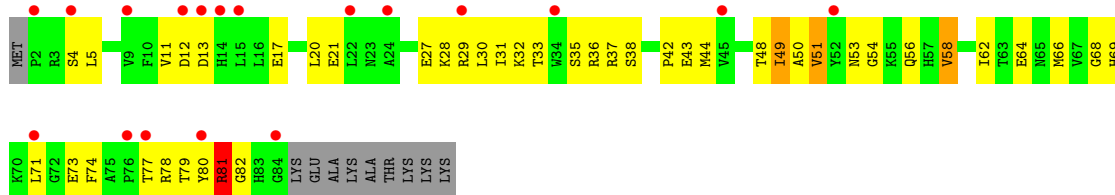
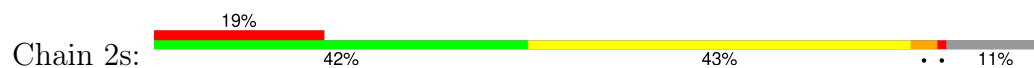
- Molecule 49: 30S ribosomal protein S18



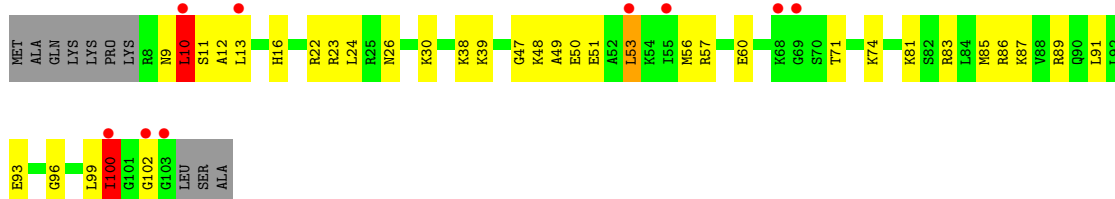
- Molecule 50: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S19

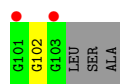


- Molecule 51: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S20

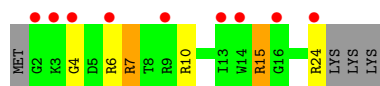




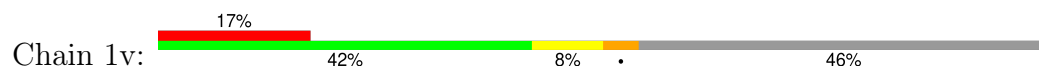
- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



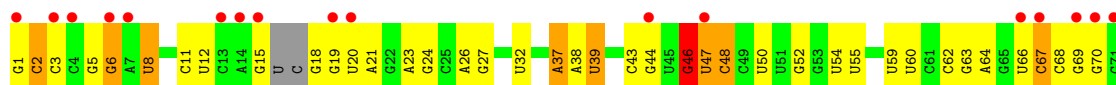
- Molecule 53: MF-mRNA



- Molecule 53: MF-mRNA

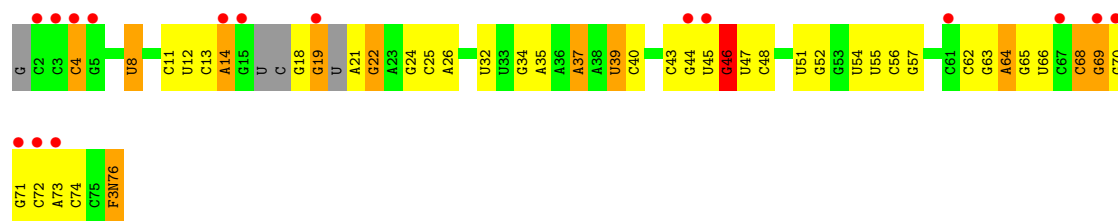


- Molecule 54: A-site Aminoacylated Phe-tRNAphe

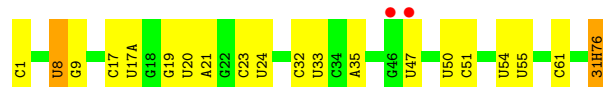
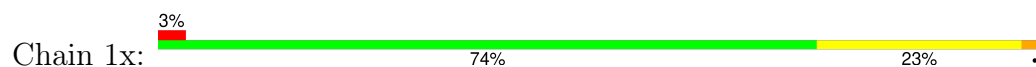


- Molecule 54: A-site Aminoacylated Phe-tRNAphe





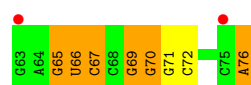
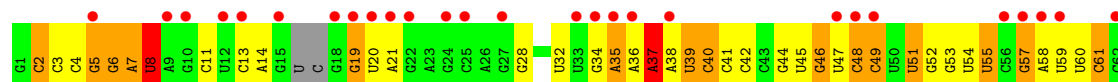
- Molecule 55: P-site Aminoacylated fMet-tRNA^{Met}



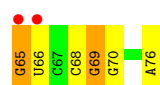
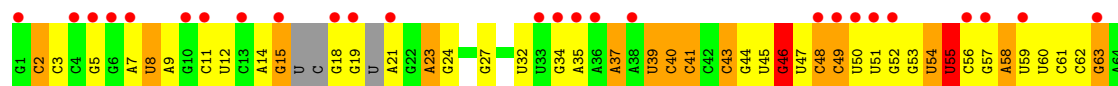
- Molecule 55: P-site Aminoacylated fMet-tRNA^{Met}



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.207 , 0.249 0.209 , 0.249	Depositor DCC
R_{free} test set	82773 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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: OMC, MG, MIA, UR3, 2MG, 5MU, 31H, PSU, 0TD, ZN, M2G, 5MC, TYK, OMG, 2MU, MA6, 8AH, SF4, 4SU, 4OC, F3N, K, G7M

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	0.28	0/69010	0.46	3/107716 (0.0%)
1	2A	0.21	0/67294	0.39	1/105038 (0.0%)
2	1B	0.21	0/2882	0.40	0/4494
2	2B	0.18	0/2879	0.34	0/4487
3	1D	0.27	0/2186	0.51	0/2944
3	2D	0.23	0/2186	0.47	0/2944
4	1E	0.27	0/1592	0.50	0/2149
4	2E	0.20	0/1592	0.43	0/2149
5	1F	0.25	0/1618	0.47	0/2191
5	2F	0.21	0/1614	0.48	3/2186 (0.1%)
6	1G	0.24	0/1448	0.50	1/1957 (0.1%)
6	2G	0.19	0/1453	0.43	0/1963
7	1H	0.22	0/1356	0.42	0/1834
7	2H	0.19	0/1356	0.37	0/1834
8	1I	0.21	0/1112	0.50	1/1514 (0.1%)
8	2I	0.21	0/1079	0.45	0/1475
9	1N	0.25	0/1144	0.49	0/1543
9	2N	0.18	0/1144	0.39	0/1543
10	1O	0.25	0/943	0.46	0/1269
10	2O	0.21	0/943	0.45	0/1269
11	1P	0.25	0/1152	0.61	0/1533
11	2P	0.20	0/1152	0.49	0/1533
12	1Q	0.28	0/1143	0.47	0/1527
12	2Q	0.21	0/1143	0.44	0/1527
13	1R	0.28	0/982	0.47	0/1312
13	2R	0.21	0/982	0.50	0/1312
14	1S	0.23	0/883	0.46	0/1176
14	2S	0.20	0/880	0.41	0/1172
15	1T	0.24	0/1105	0.46	0/1477
15	2T	0.20	0/1097	0.41	0/1468
16	1U	0.28	0/977	0.45	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.19	0/977	0.39	0/1301
17	1V	0.25	0/782	0.47	0/1049
17	2V	0.19	0/782	0.42	0/1049
18	1W	0.28	0/897	0.46	0/1205
18	2W	0.20	0/897	0.39	0/1205
19	1X	0.27	0/764	0.55	2/1025 (0.2%)
19	2X	0.20	0/764	0.48	2/1025 (0.2%)
20	1Y	0.22	0/819	0.48	0/1095
20	2Y	0.19	0/819	0.43	0/1095
21	1Z	0.21	0/1267	0.44	0/1717
21	2Z	0.20	0/1299	0.44	0/1763
22	10	0.28	0/662	0.51	0/881
22	20	0.20	0/662	0.45	0/881
23	11	0.23	0/762	0.44	0/1014
23	21	0.22	0/762	0.39	0/1014
24	12	0.24	0/590	0.41	0/781
24	22	0.18	0/590	0.37	0/781
25	13	0.24	0/474	0.44	0/635
25	23	0.20	0/469	0.45	0/630
26	14	0.24	0/565	0.61	0/761
26	24	0.26	0/545	0.44	0/737
27	15	0.27	0/469	0.50	0/635
27	25	0.22	0/469	0.44	0/635
28	16	0.27	0/460	0.48	0/613
28	26	0.23	0/456	0.44	0/608
29	17	0.29	0/426	0.53	0/561
29	27	0.25	0/426	0.50	0/561
30	18	0.28	0/525	0.47	0/691
30	28	0.21	0/525	0.40	0/691
31	19	0.26	0/310	0.51	0/407
31	29	0.20	0/310	0.55	1/407 (0.2%)
32	1a	0.20	0/35795	0.38	0/55864
32	2a	0.19	0/35886	0.37	3/56005 (0.0%)
33	1b	0.22	0/1881	0.47	0/2542
33	2b	0.23	0/1860	0.46	0/2518
34	1c	0.20	0/1572	0.40	1/2126 (0.0%)
34	2c	0.25	0/1566	0.44	0/2119
35	1d	0.19	0/1685	0.42	0/2262
35	2d	0.19	0/1704	0.44	0/2284
36	1e	0.20	0/1145	0.44	0/1543
36	2e	0.22	0/1149	0.45	0/1548
37	1f	0.19	0/823	0.40	0/1115
37	2f	0.19	0/829	0.40	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1250	0.39	0/1679
38	2g	0.22	0/1254	0.43	0/1683
39	1h	0.19	0/1108	0.41	0/1494
39	2h	0.23	0/1108	0.42	0/1494
40	1i	0.22	0/1002	0.47	0/1346
40	2i	0.21	0/997	0.44	0/1343
41	1j	0.22	0/722	0.45	0/982
41	2j	0.22	0/727	0.50	0/988
42	1k	0.25	0/844	0.38	0/1145
42	2k	0.20	0/848	0.41	0/1149
43	1l	0.25	0/937	0.45	0/1260
43	2l	0.18	0/937	0.40	0/1260
44	1m	0.19	0/969	0.50	0/1302
44	2m	0.23	0/961	0.58	2/1291 (0.2%)
45	1n	0.21	0/501	0.45	0/664
45	2n	0.20	0/501	0.46	0/664
46	1o	0.19	0/739	0.37	0/985
46	2o	0.18	0/739	0.39	0/985
47	1p	0.19	0/697	0.44	0/939
47	2p	0.19	0/693	0.44	0/935
48	1q	0.19	0/836	0.45	0/1117
48	2q	0.17	0/836	0.43	0/1117
49	1r	0.19	0/560	0.41	0/746
49	2r	0.19	0/560	0.41	0/746
50	1s	0.22	0/667	0.45	0/900
50	2s	0.30	0/661	0.58	0/893
51	1t	0.21	0/730	0.48	0/965
51	2t	0.20	0/729	0.42	0/965
52	1u	0.18	0/203	0.42	0/266
52	2u	0.23	0/203	0.45	0/266
53	1v	0.23	0/310	0.37	0/480
53	2v	0.20	0/310	0.33	0/480
54	1w	0.30	1/1581 (0.1%)	0.40	0/2458
54	2w	0.29	1/1531 (0.1%)	0.40	0/2379
55	1x	0.27	0/1723	0.40	0/2684
55	2x	0.25	0/1723	0.37	0/2684
56	1y	0.31	2/1606 (0.1%)	0.40	0/2497
56	2y	0.30	2/1583 (0.1%)	0.40	0/2459
All	All	0.23	6/316632 (0.0%)	0.42	20/474029 (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 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	46	G7M	O3'-P	5.75	1.61	1.56
54	2w	46	G7M	O3'-P	5.52	1.61	1.56
56	2y	46	G7M	O3'-P	5.44	1.61	1.56
56	1y	46	G7M	O3'-P	5.43	1.61	1.56
56	1y	8	4SU	O3'-P	5.30	1.61	1.56

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1G	150	ASP	N-CA-C	-9.76	103.50	114.62
8	1I	50	ARG	N-CA-C	-9.26	104.07	114.62
1	1A	1992	G	C2'-C3'-O3'	7.09	120.14	109.50
44	2m	107	ALA	N-CA-C	-7.07	104.59	112.57
19	1X	94	GLY	CA-C-N	5.73	132.02	121.70

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](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61853	0	31182	521	0
1	2A	60323	0	30412	600	0
2	1B	2577	0	1305	19	0
2	2B	2575	0	1303	34	0
3	1D	2136	0	2218	48	0
3	2D	2136	0	2218	32	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1E	1559	0	1618	19	0
4	2E	1559	0	1618	31	0
5	1F	1583	0	1625	33	0
5	2F	1579	0	1619	37	0
6	1G	1423	0	1436	35	0
6	2G	1428	0	1438	42	0
7	1H	1330	0	1407	25	0
7	2H	1330	0	1407	28	0
8	1I	1097	0	1140	23	0
8	2I	1064	0	1082	36	0
9	1N	1117	0	1184	10	0
9	2N	1117	0	1184	26	0
10	1O	933	0	996	21	0
10	2O	933	0	996	25	0
11	1P	1135	0	1212	32	0
11	2P	1135	0	1212	32	0
12	1Q	1122	0	1179	18	0
12	2Q	1122	0	1179	22	0
13	1R	968	0	1033	7	0
13	2R	968	0	1033	18	0
14	1S	873	0	927	17	0
14	2S	870	0	923	31	0
15	1T	1091	0	1151	16	0
15	2T	1083	0	1136	26	0
16	1U	959	0	1019	17	0
16	2U	959	0	1019	17	0
17	1V	771	0	830	9	0
17	2V	771	0	830	13	0
18	1W	886	0	940	8	0
18	2W	886	0	940	12	0
19	1X	750	0	814	13	0
19	2X	750	0	814	15	0
20	1Y	806	0	881	14	0
20	2Y	806	0	881	13	0
21	1Z	1240	0	1240	24	0
21	2Z	1271	0	1273	34	0
22	10	653	0	674	8	0
22	20	653	0	674	16	0
23	11	755	0	826	5	0
23	21	755	0	826	15	0
24	12	588	0	643	4	0
24	22	588	0	643	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	13	469	0	518	12	0
25	23	464	0	514	14	0
26	14	552	0	533	19	0
26	24	532	0	503	26	0
27	15	455	0	465	5	0
27	25	455	0	465	6	0
28	16	453	0	473	9	0
28	26	449	0	469	10	0
29	17	418	0	467	5	0
29	27	418	0	467	7	0
30	18	517	0	582	12	0
30	28	517	0	582	15	0
31	19	307	0	335	3	0
31	29	307	0	335	4	0
32	1a	32246	0	16295	315	0
32	2a	32327	0	16338	443	0
33	1b	1846	0	1867	58	0
33	2b	1825	0	1828	62	0
34	1c	1548	0	1535	33	0
34	2c	1542	0	1517	48	0
35	1d	1655	0	1672	48	0
35	2d	1674	0	1714	53	0
36	1e	1129	0	1185	26	0
36	2e	1133	0	1191	31	0
37	1f	810	0	804	12	0
37	2f	816	0	808	17	0
38	1g	1231	0	1238	24	0
38	2g	1235	0	1249	33	0
39	1h	1088	0	1126	26	0
39	2h	1088	0	1126	26	0
40	1i	983	0	986	31	0
40	2i	978	0	966	38	0
41	1j	709	0	650	28	0
41	2j	714	0	672	35	0
42	1k	829	0	825	15	0
42	2k	833	0	836	18	0
43	1l	932	0	981	10	0
43	2l	932	0	981	13	0
44	1m	958	0	1002	19	0
44	2m	950	0	988	38	0
45	1n	492	0	529	11	0
45	2n	492	0	529	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	1o	728	0	760	16	0
46	2o	728	0	760	15	0
47	1p	681	0	697	15	0
47	2p	677	0	686	16	0
48	1q	823	0	891	15	0
48	2q	823	0	891	19	0
49	1r	555	0	618	10	0
49	2r	555	0	618	18	0
50	1s	652	0	662	17	0
50	2s	646	0	644	34	0
51	1t	728	0	798	22	0
51	2t	727	0	796	14	0
52	1u	199	0	208	4	0
52	2u	199	0	208	6	0
53	1v	277	0	140	2	0
53	2v	277	0	140	1	0
54	1w	1603	0	828	18	0
54	2w	1555	0	797	28	0
55	1x	1656	0	849	11	0
55	2x	1656	0	850	19	0
56	1y	1585	0	803	26	0
56	2y	1565	0	794	33	0
57	10	10	0	0	0	0
57	11	5	0	0	0	0
57	12	3	0	0	0	0
57	13	5	0	0	0	0
57	14	1	0	0	0	0
57	15	6	0	0	0	0
57	16	1	0	0	0	0
57	17	5	0	0	0	0
57	18	7	0	0	0	0
57	19	1	0	0	0	0
57	1A	1099	0	0	0	0
57	1B	34	0	0	0	0
57	1D	12	0	0	0	0
57	1E	10	0	0	0	0
57	1F	15	0	0	0	0
57	1G	5	0	0	0	0
57	1H	1	0	0	0	0
57	1I	1	0	0	0	0
57	1N	5	0	0	0	0
57	1O	6	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1P	5	0	0	0	0
57	1Q	7	0	0	0	0
57	1R	6	0	0	0	0
57	1S	3	0	0	0	0
57	1T	3	0	0	0	0
57	1U	10	0	0	0	0
57	1V	5	0	0	0	0
57	1W	6	0	0	0	0
57	1X	6	0	0	0	0
57	1Y	2	0	0	0	0
57	1Z	2	0	0	0	0
57	1a	214	0	0	0	0
57	1b	1	0	0	0	0
57	1e	2	0	0	0	0
57	1f	1	0	0	0	0
57	1h	1	0	0	0	0
57	1l	2	0	0	0	0
57	1m	1	0	0	0	0
57	1n	1	0	0	0	0
57	1p	1	0	0	0	0
57	1r	1	0	0	0	0
57	1t	1	0	0	0	0
57	1v	1	0	0	0	0
57	1w	5	0	0	0	0
57	1x	13	0	0	0	0
57	1y	1	0	0	0	0
57	20	2	0	0	0	0
57	21	2	0	0	0	0
57	23	2	0	0	0	0
57	25	4	0	0	0	0
57	27	2	0	0	0	0
57	28	5	0	0	0	0
57	29	1	0	0	0	0
57	2A	797	0	0	0	0
57	2B	19	0	0	0	0
57	2D	8	0	0	0	0
57	2E	9	0	0	0	0
57	2F	8	0	0	0	0
57	2G	1	0	0	0	0
57	2N	1	0	0	0	0
57	2O	1	0	0	0	0
57	2P	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2Q	4	0	0	0	0
57	2R	2	0	0	0	0
57	2T	2	0	0	0	0
57	2U	1	0	0	0	0
57	2V	2	0	0	0	0
57	2W	2	0	0	0	0
57	2X	2	0	0	0	0
57	2Y	1	0	0	0	0
57	2a	221	0	0	0	0
57	2d	2	0	0	0	0
57	2e	1	0	0	0	0
57	2f	3	0	0	0	0
57	2j	1	0	0	0	0
57	2k	1	0	0	0	0
57	2l	1	0	0	0	0
57	2q	2	0	0	0	0
57	2t	1	0	0	0	0
57	2v	4	0	0	0	0
57	2w	7	0	0	0	0
57	2x	9	0	0	0	0
57	2y	2	0	0	0	0
58	1A	1	0	0	0	0
59	1A	64	0	76	1	0
59	2A	64	0	76	1	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	1	0
61	2d	8	0	0	1	0
62	10	10	0	0	0	0
62	11	6	0	0	0	0
62	12	3	0	0	0	0
62	13	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	14	1	0	0	0	0
62	15	6	0	0	0	0
62	16	2	0	0	0	0
62	17	10	0	0	0	0
62	18	12	0	0	1	0
62	1A	1975	0	0	69	0
62	1B	59	0	0	0	0
62	1D	25	0	0	1	0
62	1E	25	0	0	1	0
62	1F	13	0	0	0	0
62	1G	2	0	0	0	0
62	1H	2	0	0	0	0
62	1N	5	0	0	0	0
62	1O	4	0	0	0	0
62	1P	23	0	0	1	0
62	1Q	6	0	0	0	0
62	1R	9	0	0	0	0
62	1S	2	0	0	0	0
62	1T	7	0	0	0	0
62	1U	11	0	0	0	0
62	1V	8	0	0	0	0
62	1W	7	0	0	1	0
62	1X	6	0	0	0	0
62	1Y	3	0	0	1	0
62	1Z	1	0	0	0	0
62	1a	377	0	0	24	0
62	1b	1	0	0	0	0
62	1e	2	0	0	0	0
62	1f	2	0	0	0	0
62	1l	6	0	0	0	0
62	1m	1	0	0	0	0
62	1o	1	0	0	0	0
62	1p	1	0	0	0	0
62	1q	2	0	0	0	0
62	1u	1	0	0	1	0
62	1v	5	0	0	0	0
62	1w	12	0	0	1	0
62	1x	15	0	0	0	0
62	1y	1	0	0	0	0
62	20	4	0	0	0	0
62	21	7	0	0	0	0
62	23	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	25	1	0	0	0	0
62	26	2	0	0	1	0
62	27	4	0	0	0	0
62	28	4	0	0	0	0
62	29	1	0	0	0	0
62	2A	1136	0	0	67	0
62	2B	22	0	0	0	0
62	2D	21	0	0	1	0
62	2E	16	0	0	0	0
62	2F	13	0	0	0	0
62	2O	2	0	0	0	0
62	2P	5	0	0	2	0
62	2Q	1	0	0	0	0
62	2R	2	0	0	0	0
62	2T	7	0	0	0	0
62	2U	4	0	0	0	0
62	2W	3	0	0	0	0
62	2X	2	0	0	1	0
62	2Z	1	0	0	0	0
62	2a	254	0	0	29	0
62	2c	1	0	0	0	0
62	2d	1	0	0	0	0
62	2e	1	0	0	0	0
62	2j	4	0	0	1	0
62	2l	4	0	0	1	0
62	2n	1	0	0	0	0
62	2o	1	0	0	0	0
62	2p	1	0	0	0	0
62	2q	2	0	0	0	0
62	2t	2	0	0	0	0
62	2v	2	0	0	0	0
62	2w	3	0	0	0	0
62	2x	10	0	0	1	0
62	2y	1	0	0	0	0
All	All	300115	0	196876	3588	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 3588 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.47	1.13
33:2b:185:ILE:HG22	33:2b:199:TYR:HB2	1.47	0.96
10:2O:48:PRO:HB3	32:2a:1422:G:H5"	1.48	0.95
1:1A:1082:U:O4	1:1A:1086:A:N1	2.01	0.94
22:20:10:THR:HG22	22:20:12:ASN:H	1.33	0.94

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	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%)	24	39
4	2E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	24	39
5	1F	200/210 (95%)	195 (98%)	4 (2%)	1 (0%)	24	39
5	2F	200/210 (95%)	194 (97%)	4 (2%)	2 (1%)	12	20
6	1G	179/182 (98%)	168 (94%)	11 (6%)	0	100	100
6	2G	179/182 (98%)	159 (89%)	17 (10%)	3 (2%)	7	12
7	1H	172/180 (96%)	165 (96%)	7 (4%)	0	100	100
7	2H	172/180 (96%)	156 (91%)	15 (9%)	1 (1%)	21	34
8	1I	144/148 (97%)	124 (86%)	20 (14%)	0	100	100
8	2I	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	9	14
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	18	30
10	1O	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	16	27
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	1P	147/150 (98%)	133 (90%)	11 (8%)	3 (2%)	6	10
11	2P	147/150 (98%)	130 (88%)	11 (8%)	6 (4%)	2	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%)	6	10
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%)	12	20
17	2V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	20
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	2 (2%)	1 (1%)	14	24
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%)	12	20
20	2Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
21	1Z	148/206 (72%)	135 (91%)	12 (8%)	1 (1%)	18	30
21	2Z	156/206 (76%)	130 (83%)	22 (14%)	4 (3%)	4	6
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%)	11	19
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%)	6	11
26	14	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	5	9
33	2b	229/256 (90%)	194 (85%)	28 (12%)	7 (3%)	3	5
34	1c	204/239 (85%)	186 (91%)	17 (8%)	1 (0%)	24	39
34	2c	204/239 (85%)	180 (88%)	24 (12%)	0	100	100
35	1d	206/209 (99%)	191 (93%)	14 (7%)	1 (0%)	24	39
35	2d	206/209 (99%)	193 (94%)	13 (6%)	0	100	100
36	1e	146/162 (90%)	133 (91%)	11 (8%)	2 (1%)	9	14
36	2e	146/162 (90%)	137 (94%)	7 (5%)	2 (1%)	9	14
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%)	18	30
38	2g	153/156 (98%)	133 (87%)	18 (12%)	2 (1%)	9	16
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	121 (90%)	13 (10%)	1 (1%)	18	30
40	1i	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	16	27
40	2i	125/128 (98%)	104 (83%)	21 (17%)	0	100	100
41	1j	95/105 (90%)	84 (88%)	9 (10%)	2 (2%)	5	9
41	2j	94/105 (90%)	82 (87%)	10 (11%)	2 (2%)	5	9
42	1k	112/129 (87%)	101 (90%)	8 (7%)	3 (3%)	4	6
42	2k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	14	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	111 (93%)	7 (6%)	1 (1%)	16	27
44	1m	121/126 (96%)	107 (88%)	12 (10%)	2 (2%)	7	12
44	2m	120/126 (95%)	103 (86%)	15 (12%)	2 (2%)	7	12
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	7	12
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%)	12	20
48	2q	97/105 (92%)	90 (93%)	5 (5%)	2 (2%)	5	9
49	1r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
49	2r	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	8	13
50	1s	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
50	2s	81/93 (87%)	66 (82%)	14 (17%)	1 (1%)	10	17
51	1t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2	2
51	2t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	5	9
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%)	16	27

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 ⓘ

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%)	204 (95%)	11 (5%)	21	36
3	2D	215/218 (99%)	200 (93%)	15 (7%)	14	24
4	1E	164/166 (99%)	157 (96%)	7 (4%)	26	44
4	2E	164/166 (99%)	156 (95%)	8 (5%)	22	38
5	1F	160/166 (96%)	142 (89%)	18 (11%)	5	8
5	2F	159/166 (96%)	151 (95%)	8 (5%)	22	37
6	1G	143/156 (92%)	131 (92%)	12 (8%)	10	17
6	2G	143/156 (92%)	126 (88%)	17 (12%)	5	7
7	1H	144/148 (97%)	138 (96%)	6 (4%)	26	45
7	2H	144/148 (97%)	127 (88%)	17 (12%)	5	7
8	1I	113/124 (91%)	91 (80%)	22 (20%)	1	2
8	2I	105/124 (85%)	90 (86%)	15 (14%)	3	4
9	1N	118/119 (99%)	107 (91%)	11 (9%)	8	13
9	2N	118/119 (99%)	107 (91%)	11 (9%)	8	13
10	1O	100/100 (100%)	97 (97%)	3 (3%)	36	57
10	2O	100/100 (100%)	96 (96%)	4 (4%)	28	47
11	1P	115/116 (99%)	105 (91%)	10 (9%)	9	16
11	2P	115/116 (99%)	105 (91%)	10 (9%)	9	16
12	1Q	111/111 (100%)	107 (96%)	4 (4%)	31	51
12	2Q	111/111 (100%)	107 (96%)	4 (4%)	31	51
13	1R	101/101 (100%)	95 (94%)	6 (6%)	18	30
13	2R	101/101 (100%)	97 (96%)	4 (4%)	28	47
14	1S	86/88 (98%)	77 (90%)	9 (10%)	6	10
14	2S	85/88 (97%)	72 (85%)	13 (15%)	3	4
15	1T	115/127 (91%)	110 (96%)	5 (4%)	26	44
15	2T	113/127 (89%)	106 (94%)	7 (6%)	16	29
16	1U	93/94 (99%)	90 (97%)	3 (3%)	34	55
16	2U	93/94 (99%)	88 (95%)	5 (5%)	20	35
17	1V	80/82 (98%)	75 (94%)	5 (6%)	16	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	11
18	1W	90/92 (98%)	84 (93%)	6 (7%)	15	25
18	2W	90/92 (98%)	84 (93%)	6 (7%)	15	25
19	1X	77/78 (99%)	75 (97%)	2 (3%)	40	63
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28	48
20	1Y	85/91 (93%)	79 (93%)	6 (7%)	13	23
20	2Y	85/91 (93%)	74 (87%)	11 (13%)	4	6
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	11	18
21	2Z	137/179 (76%)	123 (90%)	14 (10%)	7	10
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	61 (94%)	4 (6%)	16	29
23	11	80/83 (96%)	78 (98%)	2 (2%)	42	64
23	21	80/83 (96%)	73 (91%)	7 (9%)	9	15
24	12	65/67 (97%)	63 (97%)	2 (3%)	35	56
24	22	65/67 (97%)	59 (91%)	6 (9%)	8	14
25	13	51/52 (98%)	46 (90%)	5 (10%)	7	11
25	23	50/52 (96%)	45 (90%)	5 (10%)	7	11
26	14	59/63 (94%)	54 (92%)	5 (8%)	10	17
26	24	53/63 (84%)	49 (92%)	4 (8%)	12	21
27	15	50/52 (96%)	46 (92%)	4 (8%)	11	19
27	25	50/52 (96%)	48 (96%)	2 (4%)	28	47
28	16	51/52 (98%)	45 (88%)	6 (12%)	5	7
28	26	50/52 (96%)	41 (82%)	9 (18%)	2	2
29	17	41/42 (98%)	36 (88%)	5 (12%)	5	7
29	27	41/42 (98%)	38 (93%)	3 (7%)	13	22
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	32
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	32
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	32 (94%)	2 (6%)	18	30
33	1b	192/220 (87%)	174 (91%)	18 (9%)	8	13
33	2b	187/220 (85%)	163 (87%)	24 (13%)	4	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	1c	142/188 (76%)	127 (89%)	15 (11%)	6	10
34	2c	140/188 (74%)	126 (90%)	14 (10%)	7	11
35	1d	169/181 (93%)	152 (90%)	17 (10%)	7	11
35	2d	173/181 (96%)	162 (94%)	11 (6%)	16	28
36	1e	113/123 (92%)	100 (88%)	13 (12%)	5	8
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8	12
37	1f	84/90 (93%)	75 (89%)	9 (11%)	6	9
37	2f	85/90 (94%)	80 (94%)	5 (6%)	18	30
38	1g	119/127 (94%)	100 (84%)	19 (16%)	2	3
38	2g	120/127 (94%)	114 (95%)	6 (5%)	22	37
39	1h	114/119 (96%)	108 (95%)	6 (5%)	20	35
39	2h	114/119 (96%)	107 (94%)	7 (6%)	17	30
40	1i	90/99 (91%)	76 (84%)	14 (16%)	2	3
40	2i	89/99 (90%)	72 (81%)	17 (19%)	1	2
41	1j	66/92 (72%)	58 (88%)	8 (12%)	5	7
41	2j	69/92 (75%)	59 (86%)	10 (14%)	3	4
42	1k	82/99 (83%)	74 (90%)	8 (10%)	7	11
42	2k	83/99 (84%)	79 (95%)	4 (5%)	23	39
43	1l	96/108 (89%)	90 (94%)	6 (6%)	16	29
43	2l	96/108 (89%)	91 (95%)	5 (5%)	21	36
44	1m	93/101 (92%)	84 (90%)	9 (10%)	8	12
44	2m	92/101 (91%)	80 (87%)	12 (13%)	4	6
45	1n	49/50 (98%)	45 (92%)	4 (8%)	10	18
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	10
46	1o	78/80 (98%)	75 (96%)	3 (4%)	29	49
46	2o	78/80 (98%)	73 (94%)	5 (6%)	16	28
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7	11
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5	7
48	1q	94/97 (97%)	90 (96%)	4 (4%)	26	44
48	2q	94/97 (97%)	85 (90%)	9 (10%)	8	12
49	1r	59/77 (77%)	57 (97%)	2 (3%)	32	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	2r	59/77 (77%)	56 (95%)	3 (5%)	21	36
50	1s	69/80 (86%)	67 (97%)	2 (3%)	37	58
50	2s	67/80 (84%)	58 (87%)	9 (13%)	4	5
51	1t	70/82 (85%)	63 (90%)	7 (10%)	7	11
51	2t	70/82 (85%)	64 (91%)	6 (9%)	10	16
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	32
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	9
All	All	9303/10064 (92%)	8544 (92%)	759 (8%)	10	18

5 of 759 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	2P	147	LEU
28	26	23	THR
14	2S	27	SER
11	2P	135	LEU
20	2Y	14	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 148 such sidechains are listed below:

Mol	Chain	Res	Type
34	2c	98	ASN
49	2r	63	GLN
35	2d	77	ASN
40	2i	58	HIS
36	1e	78	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	435 (15%)	30 (1%)
1	2A	2791/2915 (95%)	463 (16%)	26 (0%)
2	1B	119/121 (98%)	7 (5%)	0
2	2B	118/121 (97%)	31 (26%)	0
32	1a	1497/1521 (98%)	242 (16%)	0
32	2a	1501/1521 (98%)	272 (18%)	0
53	1v	12/24 (50%)	2 (16%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	2v	12/24 (50%)	1 (8%)	0
54	1w	71/76 (93%)	23 (32%)	0
54	2w	68/76 (89%)	20 (29%)	0
55	1x	75/77 (97%)	5 (6%)	0
55	2x	75/77 (97%)	8 (10%)	0
56	1y	72/76 (94%)	35 (48%)	0
56	2y	70/76 (92%)	25 (35%)	0
All	All	9345/9620 (97%)	1569 (16%)	56 (0%)

5 of 1569 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
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	1A	1962	57,1	19,22,23	1.69	3 (15%)	26,32,35	1.17	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MU	2A	2552	57,1	19,22,24	1.31	3 (15%)	25,31,36	1.86	6 (24%)
56	G7M	2y	46	56	23,26,27	1.66	4 (17%)	34,39,42	1.96	4 (11%)
56	MIA	2y	37	56	21,24,32	1.66	4 (19%)	30,35,47	1.99	7 (23%)
56	PSU	2y	39	56	18,21,22	1.41	2 (11%)	21,30,33	1.76	3 (14%)
32	5MC	1a	1407	32	19,22,23	1.63	3 (15%)	26,32,35	1.07	3 (11%)
56	4SU	1y	8	56	18,21,22	1.77	4 (22%)	25,30,33	2.10	5 (20%)
55	5MC	1x	32	55,57	19,22,23	1.68	3 (15%)	26,32,35	1.25	3 (11%)
1	5MC	2A	1942	1	19,22,23	1.70	3 (15%)	26,32,35	1.11	3 (11%)
54	MIA	1w	37	54	28,31,32	2.35	6 (21%)	38,44,47	2.59	12 (31%)
32	5MC	2a	1404	32	19,22,23	1.75	3 (15%)	26,32,35	1.16	3 (11%)
32	5MC	2a	1407	32	19,22,23	1.49	3 (15%)	26,32,35	1.11	2 (7%)
1	OMC	2A	1920	1	19,22,23	0.79	0	25,31,34	0.93	1 (4%)
54	PSU	1w	39	54	18,21,22	1.40	3 (16%)	21,30,33	1.82	3 (14%)
1	5MU	1A	1939	57,1	19,22,23	1.35	5 (26%)	27,32,35	2.19	6 (22%)
32	5MC	1a	967	32	19,22,23	1.60	3 (15%)	26,32,35	1.14	2 (7%)
54	PSU	2w	32	54	18,21,22	1.37	2 (11%)	21,30,33	1.96	4 (19%)
55	4SU	2x	8	55	18,21,22	2.15	5 (27%)	25,30,33	1.44	5 (20%)
56	PSU	1y	39	56	18,21,22	1.44	2 (11%)	21,30,33	1.81	4 (19%)
1	8AH	1A	2503	57,1	22,26,27	1.61	5 (22%)	29,39,42	2.24	5 (17%)
1	PSU	1A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	2.04	3 (14%)
55	PSU	1x	55	55	18,21,22	1.33	2 (11%)	21,30,33	2.03	4 (19%)
54	PSU	1w	55	54	18,21,22	1.38	2 (11%)	21,30,33	2.01	3 (14%)
54	PSU	2w	39	54	18,21,22	1.40	2 (11%)	21,30,33	1.70	4 (19%)
1	PSU	1A	2605	57,1	18,21,22	1.32	3 (16%)	21,30,33	2.03	4 (19%)
1	OMG	2A	2251	55,1	23,26,27	1.23	3 (13%)	32,38,41	1.96	6 (18%)
54	G7M	2w	46	54	23,26,27	1.51	3 (13%)	34,39,42	1.74	4 (11%)
54	4SU	1w	8	54	18,21,22	1.75	4 (22%)	25,30,33	1.89	4 (16%)
55	5MU	1x	54	55,57	19,22,23	1.39	5 (26%)	27,32,35	2.02	6 (22%)
54	G7M	1w	46	54	23,26,27	1.56	3 (13%)	34,39,42	1.68	4 (11%)
54	F3N	1w	76	54,1	33,36,37	1.56	5 (15%)	41,51,54	1.82	10 (24%)
54	5MU	1w	54	54	19,22,23	1.36	4 (21%)	27,32,35	1.94	6 (22%)
54	MIA	2w	37	54	24,27,32	2.15	5 (20%)	32,39,47	2.62	11 (34%)
1	5MU	2A	1915	1	19,22,23	1.46	6 (31%)	27,32,35	2.18	6 (22%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	2.04	5 (23%)
43	0TD	2l	92	43	8,9,10	4.52	1 (12%)	6,11,13	1.91	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	4OC	1a	1402	32	20,23,24	0.72	0	25,32,35	0.97	1 (4%)
32	2MG	2a	1207	32	23,26,27	1.24	2 (8%)	33,38,41	2.15	7 (21%)
1	5MU	2A	1939	57,1	19,22,23	1.40	5 (26%)	27,32,35	2.29	6 (22%)
55	31H	2x	76	55,57	31,34,35	1.20	3 (9%)	35,47,50	2.16	13 (37%)
56	5MU	1y	54	56	19,22,23	1.40	5 (26%)	27,32,35	2.16	7 (25%)
32	UR3	2a	1498	32	19,22,23	1.07	1 (5%)	26,32,35	1.75	2 (7%)
32	4OC	2a	1402	32	20,23,24	0.78	0	25,32,35	1.07	3 (12%)
32	PSU	1a	516	32	18,21,22	1.36	2 (11%)	21,30,33	1.96	6 (28%)
1	5MC	1A	1942	1	19,22,23	1.62	3 (15%)	26,32,35	1.19	4 (15%)
54	4SU	2w	8	54	18,21,22	1.72	4 (22%)	25,30,33	2.81	5 (20%)
1	OMG	1A	2251	55,57,1	23,26,27	1.27	3 (13%)	32,38,41	1.94	6 (18%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	0.86	0
1	8AH	2A	2503	57,1	22,26,27	1.66	5 (22%)	29,39,42	2.09	5 (17%)
55	PSU	2x	55	55	18,21,22	1.39	2 (11%)	21,30,33	2.07	4 (19%)
54	PSU	2w	55	54	18,21,22	1.37	2 (11%)	21,30,33	1.97	3 (14%)
1	PSU	1A	1911	1	18,21,22	1.43	2 (11%)	21,30,33	2.06	3 (14%)
56	PSU	1y	32	56	18,21,22	1.35	2 (11%)	21,30,33	1.95	3 (14%)
56	MIA	1y	37	56	21,24,32	1.65	4 (19%)	30,35,47	1.98	6 (20%)
32	PSU	2a	516	32	18,21,22	1.33	2 (11%)	21,30,33	1.98	4 (19%)
32	2MG	1a	1207	32	23,26,27	1.23	3 (13%)	33,38,41	2.27	8 (24%)
54	F3N	2w	76	54,1	33,36,37	1.49	4 (12%)	41,51,54	1.76	8 (19%)
55	5MU	2x	54	55	19,22,23	1.41	6 (31%)	27,32,35	2.15	6 (22%)
32	MA6	1a	1519	32	23,26,27	0.46	0	33,38,41	2.13	8 (24%)
54	5MU	2w	54	54	19,22,23	1.36	4 (21%)	27,32,35	1.92	6 (22%)
1	PSU	2A	1917	1	18,21,22	1.38	2 (11%)	21,30,33	1.96	3 (14%)
1	5MU	1A	1915	1	19,22,23	1.38	5 (26%)	27,32,35	2.21	7 (25%)
32	M2G	1a	966	32	24,27,28	1.29	3 (12%)	33,40,43	1.81	6 (18%)
32	5MC	1a	1404	32	19,22,23	1.76	3 (15%)	26,32,35	1.19	4 (15%)
1	PSU	2A	2605	1	18,21,22	1.42	3 (16%)	21,30,33	2.08	4 (19%)
1	5MC	2A	1962	57,1	19,22,23	1.67	3 (15%)	26,32,35	1.17	2 (7%)
43	0TD	1l	92	43	8,9,10	4.54	2 (25%)	6,11,13	7.49	2 (33%)
55	4SU	1x	8	55	18,21,22	2.32	5 (27%)	25,30,33	1.74	6 (24%)
32	5MC	2a	967	32	19,22,23	1.69	3 (15%)	26,32,35	1.18	3 (11%)
32	5MC	2a	1400	32	19,22,23	1.69	3 (15%)	26,32,35	1.23	4 (15%)
56	5MU	2y	54	56	19,22,23	1.48	4 (21%)	27,32,35	2.00	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PSU	2y	55	56	18,21,22	1.32	3 (16%)	21,30,33	1.99	4 (19%)
32	G7M	2a	527	57,32	23,26,27	1.53	3 (13%)	34,39,42	1.67	5 (14%)
32	UR3	1a	1498	32	19,22,23	1.06	2 (10%)	26,32,35	1.78	4 (15%)
56	4SU	2y	8	56	18,21,22	1.72	4 (22%)	25,30,33	2.41	6 (24%)
56	PSU	2y	32	56	18,21,22	1.32	2 (11%)	21,30,33	1.95	3 (14%)
56	G7M	1y	46	56	23,26,27	1.63	3 (13%)	34,39,42	1.87	4 (11%)
32	G7M	1a	527	57,32	23,26,27	1.51	3 (13%)	34,39,42	1.73	5 (14%)
32	MA6	2a	1519	32	23,26,27	0.46	0	33,38,41	2.16	8 (24%)
32	M2G	2a	966	32	24,27,28	1.28	4 (16%)	33,40,43	1.84	6 (18%)
1	2MU	1A	2552	57,1	19,22,24	1.19	2 (10%)	25,31,36	1.99	6 (24%)
55	5MC	2x	32	55	19,22,23	1.77	3 (15%)	26,32,35	1.23	3 (11%)
32	5MC	1a	1400	32	19,22,23	1.58	3 (15%)	26,32,35	1.14	3 (11%)
54	PSU	1w	32	57,54	18,21,22	1.31	2 (11%)	21,30,33	1.95	3 (14%)
56	PSU	1y	55	56	18,21,22	1.41	2 (11%)	21,30,33	2.09	4 (19%)
32	MA6	1a	1518	32	23,26,27	0.43	0	33,38,41	2.06	9 (27%)
55	31H	1x	76	55,57	31,34,35	1.23	3 (9%)	35,47,50	2.08	11 (31%)
32	MA6	2a	1518	32	23,26,27	0.43	0	33,38,41	2.07	9 (27%)

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	1A	1962	57,1	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	57,1	-	0/9/27/28	0/2/2/2
56	G7M	2y	46	56	-	2/7/25/26	0/3/3/3
56	MIA	2y	37	56	-	3/7/25/34	0/3/3/3
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
56	4SU	1y	8	56	-	2/7/25/26	0/2/2/2
55	5MC	1x	32	55,57	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	4/15/33/34	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
54	PSU	1w	39	54	-	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	5MU	1A	1939	57,1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
1	8AH	1A	2503	57,1	-	1/7/25/26	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	57,1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/9/27/28	0/3/3/3
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55,57	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
54	F3N	1w	76	54,1	-	2/19/37/38	0/4/4/4
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
32	2MG	2a	1207	32	-	1/9/27/28	0/3/3/3
1	5MU	2A	1939	57,1	-	0/7/25/26	0/2/2/2
55	31H	2x	76	55,57	-	3/22/40/41	0/3/3/3
56	5MU	1y	54	56	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	55,57,1	-	0/9/27/28	0/3/3/3
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
1	8AH	2A	2503	57,1	-	0/7/25/26	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
56	MIA	1y	37	56	-	2/7/25/34	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
54	F3N	2w	76	54,1	-	1/19/37/38	0/4/4/4
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	1/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	57,1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
56	5MU	2y	54	56	-	2/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	6/7/25/26	0/2/2/2
32	G7M	2a	527	57,32	-	3/7/25/26	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
56	4SU	2y	8	56	-	1/7/25/26	0/2/2/2
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
56	G7M	1y	46	56	-	2/7/25/26	0/3/3/3
32	G7M	1a	527	57,32	-	3/7/25/26	0/3/3/3
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	2MU	1A	2552	57,1	-	0/9/27/28	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	57,54	-	0/7/25/26	0/2/2/2
56	PSU	1y	55	56	-	1/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
55	31H	1x	76	55,57	-	3/22/40/41	0/3/3/3
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3

The worst 5 of 257 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.45	1.69	1.82
43	1l	92	0TD	CB-SB	-12.32	1.69	1.82
54	1w	37	MIA	C13-C14	7.03	1.53	1.32
54	2w	37	MIA	C2-S10	-6.98	1.70	1.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C2-S10	-6.77	1.70	1.75

The worst 5 of 429 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-17.81	70.35	102.36
54	2w	37	MIA	C5-C4-N3	-9.04	117.66	127.18
54	2w	8	4SU	C4-N3-C2	-8.98	118.71	127.31
1	1A	2503	8AH	C5-C4-N3	-8.24	118.50	127.18
1	2A	2503	8AH	C5-C4-N3	-8.22	118.52	127.18

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	1w	37	MIA	C12-C13-C14-C15
55	1x	76	31H	C3'-C4'-C5'-O5'
56	1y	8	4SU	O4'-C4'-C5'-O5'
56	1y	46	G7M	C4'-C5'-O5'-P
32	2a	1207	2MG	N3-C2-N2-CM2

There are no ring outliers.

36 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	2552	2MU	1	0
56	2y	46	G7M	1	0
56	2y	39	PSU	1	0
56	1y	8	4SU	1	0
54	1w	37	MIA	1	0
54	1w	39	PSU	1	0
1	1A	1939	5MU	2	0
55	2x	8	4SU	1	0
56	1y	39	PSU	1	0
1	1A	1917	PSU	1	0
54	2w	39	PSU	2	0
54	2w	46	G7M	1	0
54	1w	46	G7M	1	0
54	2w	37	MIA	1	0
1	2A	1915	5MU	1	0
32	2a	1207	2MG	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1939	5MU	1	0
55	2x	76	31H	2	0
32	2a	1402	4OC	1	0
54	2w	8	4SU	2	0
1	1A	2251	OMG	1	0
1	2A	2503	8AH	2	0
55	2x	55	PSU	1	0
56	1y	37	MIA	2	0
54	2w	76	F3N	3	0
32	1a	1519	MA6	2	0
32	1a	966	M2G	1	0
55	1x	8	4SU	2	0
56	2y	55	PSU	7	0
56	2y	8	4SU	2	0
32	2a	1519	MA6	3	0
1	1A	2552	2MU	1	0
56	1y	55	PSU	1	0
32	1a	1518	MA6	3	0
55	1x	76	31H	1	0
32	2a	1518	MA6	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	1.82	8 (11%)	87,97,97	1.52	16 (18%)
61	SF4	1d	501	35	0,12,12	-	-	-		
61	SF4	2d	303	35	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	TYK	1A	4101	1	67,67,67	1.77	7 (10%)	87,97,97	1.35	15 (17%)

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
61	SF4	1d	501	35	-	-	0/6/5/5
61	SF4	2d	303	35	-	-	0/6/5/5
59	TYK	1A	4101	1	-	3/67/126/126	1/3/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1A	4101	TYK	C8-C9	-8.59	1.38	1.51
59	2A	3798	TYK	C8-C9	-8.57	1.38	1.51
59	2A	3798	TYK	C14-C13	-7.21	1.37	1.50
59	1A	4101	TYK	C14-C13	-6.61	1.39	1.50
59	2A	3798	TYK	C2-C1	-4.91	1.41	1.50

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	2A	3798	TYK	C10-C11-C12	-4.40	119.72	126.23
59	1A	4101	TYK	C3B-C2B-C1B	-4.35	106.69	114.77
59	2A	3798	TYK	C1B-O4A-C4A	3.84	122.36	114.72
59	2A	3798	TYK	O4B-C4B-C5B	-3.73	103.04	109.46
59	2A	3798	TYK	C3B-C2B-C1B	-3.72	107.85	114.77

There are no chirality outliers.

5 of 7 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

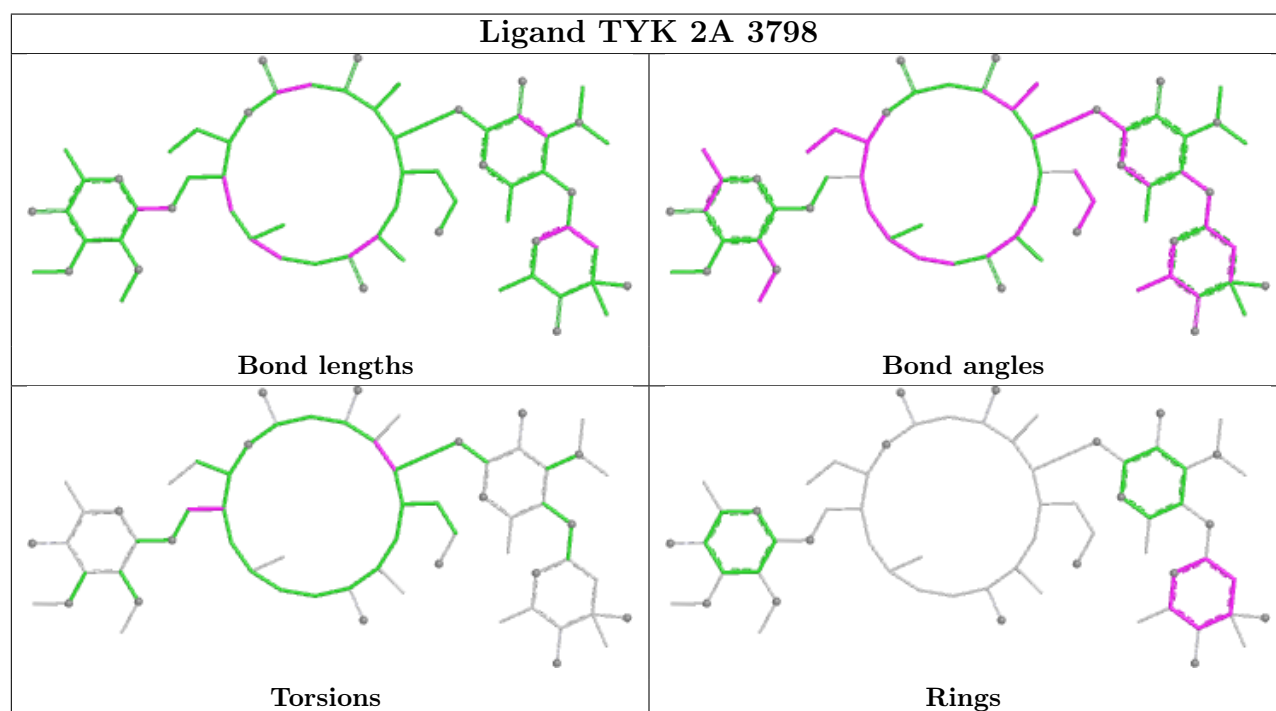
All (2) ring outliers are listed below:

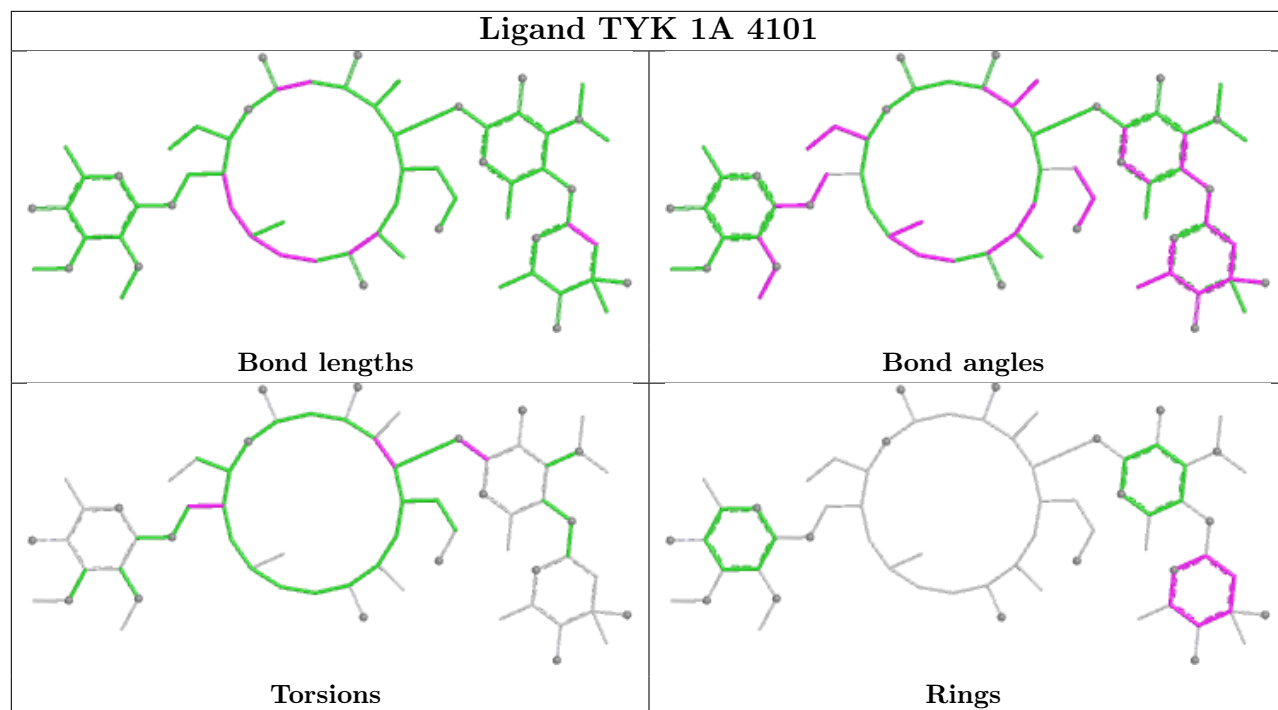
Mol	Chain	Res	Type	Atoms
59	2A	3798	TYK	C1B-C2B-C3B-C4B-C5B-O5B
59	1A	4101	TYK	C1B-C2B-C3B-C4B-C5B-O5B

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	2A	3798	TYK	1	0
61	1d	501	SF4	1	0
61	2d	303	SF4	1	0
59	1A	4101	TYK	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	-0.42	186 (6%) 25 19	20, 36, 98, 108	0
1	2A	2789/2915 (95%)	0.07	147 (5%) 32 25	33, 57, 95, 107	0
2	1B	120/121 (99%)	-0.34	1 (0%) 82 79	29, 48, 63, 89	0
2	2B	120/121 (99%)	0.78	2 (1%) 69 64	61, 75, 84, 91	0
3	1D	275/276 (99%)	-0.26	3 (1%) 78 75	21, 37, 52, 77	0
3	2D	275/276 (99%)	0.13	2 (0%) 84 82	33, 50, 62, 82	0
4	1E	204/206 (99%)	-0.20	1 (0%) 87 85	20, 39, 59, 76	0
4	2E	204/206 (99%)	0.41	4 (1%) 65 59	38, 59, 72, 81	0
5	1F	202/210 (96%)	-0.15	1 (0%) 87 85	19, 41, 66, 84	0
5	2F	202/210 (96%)	0.45	1 (0%) 87 85	37, 66, 79, 87	0
6	1G	181/182 (99%)	0.39	5 (2%) 55 48	39, 56, 71, 81	0
6	2G	181/182 (99%)	1.03	15 (8%) 17 12	67, 77, 85, 94	0
7	1H	174/180 (96%)	0.27	4 (2%) 61 54	36, 53, 67, 73	0
7	2H	174/180 (96%)	1.25	23 (13%) 7 6	69, 83, 90, 95	0
8	1I	146/148 (98%)	0.71	2 (1%) 73 69	46, 72, 80, 83	0
8	2I	146/148 (98%)	0.87	8 (5%) 30 24	53, 73, 80, 85	0
9	1N	140/140 (100%)	-0.21	1 (0%) 84 82	25, 38, 61, 67	0
9	2N	140/140 (100%)	0.62	6 (4%) 40 32	48, 66, 79, 85	0
10	1O	122/122 (100%)	-0.28	0 100 100	28, 39, 57, 61	0
10	2O	122/122 (100%)	0.28	1 (0%) 82 79	47, 58, 70, 76	0
11	1P	149/150 (99%)	0.03	4 (2%) 56 49	23, 45, 68, 73	0
11	2P	149/150 (99%)	0.53	3 (2%) 65 59	40, 65, 80, 89	0
12	1Q	141/141 (100%)	-0.11	0 100 100	25, 39, 55, 72	0
12	2Q	141/141 (100%)	0.99	10 (7%) 22 16	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%)	-0.40	0 100 100	25, 34, 46, 56	0
13	2R	118/118 (100%)	0.23	0 100 100	44, 53, 63, 70	0
14	1S	110/112 (98%)	0.17	0 100 100	38, 49, 60, 66	0
14	2S	110/112 (98%)	1.02	8 (7%) 21 15	61, 70, 78, 84	0
15	1T	131/146 (89%)	0.01	2 (1%) 72 67	33, 44, 68, 78	0
15	2T	131/146 (89%)	0.53	2 (1%) 72 67	52, 62, 75, 82	0
16	1U	116/118 (98%)	-0.43	0 100 100	22, 30, 44, 64	0
16	2U	116/118 (98%)	0.49	1 (0%) 81 78	44, 62, 72, 77	0
17	1V	101/101 (100%)	-0.43	1 (0%) 79 76	23, 38, 55, 65	0
17	2V	101/101 (100%)	0.79	2 (1%) 65 59	43, 71, 77, 83	0
18	1W	112/113 (99%)	-0.35	1 (0%) 81 78	25, 32, 49, 85	0
18	2W	112/113 (99%)	0.29	1 (0%) 81 78	40, 51, 69, 86	0
19	1X	95/96 (98%)	-0.17	2 (2%) 63 57	26, 38, 62, 77	0
19	2X	95/96 (98%)	0.51	5 (5%) 32 25	45, 58, 75, 82	0
20	1Y	107/110 (97%)	0.22	1 (0%) 81 78	36, 50, 67, 80	0
20	2Y	107/110 (97%)	1.07	12 (11%) 10 8	58, 71, 80, 86	0
21	1Z	154/206 (74%)	0.84	21 (13%) 7 5	38, 64, 83, 91	0
21	2Z	160/206 (77%)	1.65	47 (29%) 1 1	64, 81, 88, 92	0
22	10	83/85 (97%)	-0.14	0 100 100	29, 37, 50, 67	0
22	20	83/85 (97%)	0.88	5 (6%) 27 21	47, 61, 73, 78	0
23	11	97/98 (98%)	0.12	1 (1%) 79 76	29, 47, 71, 75	0
23	21	97/98 (98%)	0.35	4 (4%) 41 33	39, 55, 75, 84	0
24	12	70/72 (97%)	0.25	2 (2%) 53 46	35, 48, 59, 76	0
24	22	70/72 (97%)	0.78	2 (2%) 53 46	58, 69, 76, 80	0
25	13	59/60 (98%)	-0.22	2 (3%) 48 40	26, 36, 62, 79	0
25	23	59/60 (98%)	0.50	1 (1%) 69 64	57, 66, 79, 87	0
26	14	69/71 (97%)	0.92	8 (11%) 9 8	52, 73, 88, 89	0
26	24	69/71 (97%)	1.47	18 (26%) 1 1	75, 84, 92, 94	0
27	15	59/60 (98%)	-0.45	0 100 100	20, 32, 51, 54	0
27	25	59/60 (98%)	0.33	1 (1%) 69 64	39, 54, 66, 78	0
28	16	53/54 (98%)	-0.16	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%)	0.57	0 100 100	51, 60, 68, 72	0
29	17	48/49 (97%)	-0.27	1 (2%) 63 57	24, 29, 54, 63	0
29	27	48/49 (97%)	0.14	2 (4%) 40 32	35, 42, 64, 74	0
30	18	64/65 (98%)	-0.28	0 100 100	29, 34, 42, 56	0
30	28	64/65 (98%)	0.38	1 (1%) 70 66	44, 55, 62, 65	0
31	19	37/37 (100%)	-0.25	0 100 100	30, 38, 54, 61	0
31	29	37/37 (100%)	1.01	2 (5%) 31 25	60, 68, 77, 83	0
32	1a	1488/1521 (97%)	0.26	62 (4%) 40 32	34, 64, 92, 105	0
32	2a	1491/1521 (98%)	0.62	96 (6%) 25 19	49, 75, 95, 106	0
33	1b	231/256 (90%)	1.22	40 (17%) 4 3	62, 77, 87, 92	0
33	2b	231/256 (90%)	1.34	40 (17%) 4 3	73, 83, 89, 92	0
34	1c	206/239 (86%)	0.75	13 (6%) 26 19	56, 68, 79, 86	0
34	2c	206/239 (86%)	1.27	35 (16%) 4 3	73, 82, 88, 92	0
35	1d	208/209 (99%)	0.74	14 (6%) 24 18	52, 67, 76, 82	0
35	2d	208/209 (99%)	0.84	11 (5%) 32 25	59, 71, 79, 82	0
36	1e	148/162 (91%)	0.34	1 (0%) 84 82	48, 62, 72, 80	0
36	2e	148/162 (91%)	1.04	10 (6%) 23 17	65, 75, 81, 86	0
37	1f	100/101 (99%)	0.46	2 (2%) 65 59	52, 65, 72, 77	0
37	2f	100/101 (99%)	0.52	3 (3%) 52 45	49, 67, 75, 82	0
38	1g	155/156 (99%)	0.73	9 (5%) 29 22	59, 70, 84, 88	0
38	2g	155/156 (99%)	1.17	22 (14%) 6 5	68, 78, 87, 92	0
39	1h	137/138 (99%)	0.50	3 (2%) 62 56	52, 65, 72, 76	0
39	2h	137/138 (99%)	0.85	5 (3%) 46 38	65, 74, 80, 83	0
40	1i	127/128 (99%)	1.20	21 (16%) 4 3	50, 74, 83, 87	0
40	2i	127/128 (99%)	1.78	45 (35%) 1 0	71, 83, 88, 92	0
41	1j	97/105 (92%)	1.16	13 (13%) 7 6	53, 76, 84, 91	0
41	2j	96/105 (91%)	1.82	37 (38%) 1 0	74, 84, 90, 92	0
42	1k	114/129 (88%)	0.61	5 (4%) 39 31	41, 66, 76, 80	0
42	2k	114/129 (88%)	0.88	9 (7%) 18 14	52, 72, 79, 82	0
43	1l	121/132 (91%)	0.26	3 (2%) 58 52	41, 50, 63, 71	0
43	2l	121/132 (91%)	0.63	3 (2%) 58 52	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%)	0.83	10 (8%)	18 13	53, 67, 76, 88	0
44	2m	122/126 (96%)	1.52	24 (19%)	3 2	67, 80, 85, 88	0
45	1n	60/61 (98%)	0.96	5 (8%)	17 12	54, 64, 71, 76	0
45	2n	60/61 (98%)	2.21	28 (46%)	0 0	73, 82, 87, 90	0
46	1o	88/89 (98%)	0.60	4 (4%)	38 31	47, 63, 72, 79	0
46	2o	88/89 (98%)	0.69	5 (5%)	29 23	59, 70, 80, 85	0
47	1p	82/88 (93%)	1.27	10 (12%)	8 7	58, 69, 77, 86	0
47	2p	82/88 (93%)	0.98	7 (8%)	16 12	59, 69, 77, 81	0
48	1q	99/105 (94%)	0.64	1 (1%)	79 76	48, 66, 75, 76	0
48	2q	99/105 (94%)	0.68	5 (5%)	33 26	62, 72, 80, 81	0
49	1r	68/88 (77%)	0.47	1 (1%)	72 67	53, 64, 76, 77	0
49	2r	68/88 (77%)	0.66	2 (2%)	53 46	59, 69, 78, 83	0
50	1s	83/93 (89%)	0.78	4 (4%)	35 28	59, 69, 79, 84	0
50	2s	83/93 (89%)	1.56	18 (21%)	2 1	78, 83, 89, 95	0
51	1t	96/106 (90%)	0.97	9 (9%)	14 11	61, 68, 78, 82	0
51	2t	96/106 (90%)	0.84	8 (8%)	17 12	60, 70, 81, 87	0
52	1u	23/27 (85%)	0.88	2 (8%)	16 12	59, 64, 70, 74	0
52	2u	23/27 (85%)	1.74	9 (39%)	1 0	74, 78, 83, 89	0
53	1v	13/24 (54%)	0.92	4 (30%)	1 0	47, 51, 92, 98	0
53	2v	13/24 (54%)	1.30	4 (30%)	1 0	63, 73, 96, 102	0
54	1w	66/76 (86%)	1.32	19 (28%)	1 1	29, 86, 98, 103	0
54	2w	64/76 (84%)	1.53	16 (25%)	2 1	48, 91, 100, 102	0
55	1x	72/77 (93%)	0.12	2 (2%)	55 48	25, 58, 78, 91	0
55	2x	72/77 (93%)	0.53	1 (1%)	73 69	42, 73, 87, 97	0
56	1y	67/76 (88%)	2.02	29 (43%)	0 0	58, 99, 103, 105	0
56	2y	66/76 (86%)	2.00	28 (42%)	0 0	69, 101, 103, 105	0
All	All	20871/21748 (95%)	0.37	1343 (6%)	25 19	19, 63, 89, 108	0

The worst 5 of 1343 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	10.0
1	2A	652(U)	G	8.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	653	A	8.2
1	2A	652(V)	C	8.1
1	1A	653	A	7.7

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($\text{\AA}^2$)	Q<0.9
56	4SU	2y	8	20/21	0.43	0.19	95,104,112,126	0
56	G7M	2y	46	24/25	0.46	0.16	86,99,105,120	0
56	MIA	2y	37	22/30	0.52	0.16	83,97,109,123	0
56	PSU	1y	55	20/21	0.52	0.17	96,101,106,114	0
56	5MU	2y	54	21/22	0.54	0.18	91,96,106,126	0
56	G7M	1y	46	24/25	0.55	0.18	91,99,104,117	0
56	5MU	1y	54	21/22	0.59	0.15	89,99,104,118	0
56	PSU	2y	55	20/21	0.59	0.15	89,97,106,108	0
56	PSU	2y	39	20/21	0.61	0.16	90,95,104,111	0
56	MIA	1y	37	22/30	0.61	0.16	86,93,100,113	0
56	4SU	1y	8	20/21	0.63	0.14	93,97,105,116	0
56	PSU	2y	32	20/21	0.64	0.16	86,98,107,115	0
54	G7M	2w	46	24/25	0.66	0.17	84,94,109,123	0
56	PSU	1y	39	20/21	0.70	0.16	83,94,107,109	0
56	PSU	1y	32	20/21	0.70	0.14	88,96,106,112	0
54	G7M	1w	46	24/25	0.71	0.18	78,88,100,121	0
54	PSU	2w	55	20/21	0.82	0.12	77,83,94,96	0
54	4SU	2w	8	20/21	0.85	0.13	90,94,105,108	0
54	4SU	1w	8	20/21	0.85	0.14	71,85,92,94	0
54	5MU	2w	54	21/22	0.87	0.12	74,80,84,89	0
55	PSU	2x	55	20/21	0.88	0.10	69,75,84,86	0
55	5MU	2x	54	21/22	0.89	0.12	72,79,84,96	0
54	PSU	1w	55	20/21	0.89	0.10	61,73,81,81	0
32	2MG	2a	1207	24/25	0.89	0.12	76,83,86,90	0
54	PSU	2w	32	20/21	0.90	0.13	76,84,91,92	0
54	MIA	2w	37	25/30	0.90	0.12	68,76,85,103	0
55	4SU	2x	8	20/21	0.90	0.11	64,75,83,83	0
32	G7M	2a	527	24/25	0.90	0.13	61,67,71,76	0
32	M2G	2a	966	25/26	0.91	0.15	55,65,76,81	0
43	0TD	1l	92	10/11	0.91	0.11	41,49,50,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	5MC	2a	967	21/22	0.92	0.12	62,66,76,82	0
54	PSU	1w	32	20/21	0.92	0.12	60,65,74,77	0
1	5MU	2A	1915	21/22	0.92	0.10	57,64,73,75	0
32	5MC	2a	1400	21/22	0.93	0.17	63,71,76,80	0
32	4OC	2a	1402	22/23	0.93	0.11	55,60,66,71	0
54	MIA	1w	37	29/30	0.93	0.14	43,53,70,87	0
55	5MC	2x	32	21/22	0.93	0.12	63,69,78,80	0
55	PSU	1x	55	20/21	0.93	0.10	49,56,67,70	0
32	2MG	1a	1207	24/25	0.93	0.11	61,67,71,71	0
32	PSU	2a	516	20/21	0.93	0.11	61,71,78,79	0
54	PSU	2w	39	20/21	0.94	0.10	62,78,85,85	0
55	4SU	1x	8	20/21	0.94	0.10	52,60,67,77	0
32	5MC	2a	1407	21/22	0.94	0.10	50,57,61,65	0
43	0TD	2l	92	10/11	0.94	0.09	61,65,67,78	0
1	PSU	2A	1917	20/21	0.94	0.09	54,61,69,72	0
1	OMC	2A	1920	21/22	0.94	0.09	53,61,63,65	0
55	5MU	1x	54	21/22	0.95	0.08	55,61,65,70	0
1	PSU	2A	1911	20/21	0.95	0.09	52,62,67,71	0
32	UR3	2a	1498	21/22	0.95	0.11	52,58,61,65	0
55	5MC	1x	32	21/22	0.95	0.11	51,53,59,70	0
32	5MC	2a	1404	21/22	0.95	0.09	53,57,62,66	0
1	5MC	2A	1962	21/22	0.95	0.10	39,51,58,67	0
55	31H	2x	76	32/33	0.96	0.10	36,46,54,63	0
32	PSU	1a	516	20/21	0.96	0.08	51,55,58,59	0
32	5MC	1a	1400	21/22	0.96	0.09	39,47,49,50	0
54	5MU	1w	54	21/22	0.96	0.07	46,62,67,69	0
32	5MC	1a	1404	21/22	0.96	0.08	33,39,42,45	0
32	5MC	1a	1407	21/22	0.96	0.10	30,39,42,43	0
32	G7M	1a	527	24/25	0.96	0.09	36,42,50,50	0
32	M2G	1a	966	25/26	0.96	0.10	46,50,57,61	0
54	F3N	2w	76	33/34	0.96	0.10	38,43,48,51	0
1	5MU	1A	1915	21/22	0.96	0.09	42,51,55,55	0
32	5MC	1a	967	21/22	0.96	0.09	45,51,59,61	0
32	MA6	2a	1518	24/25	0.96	0.10	49,60,69,69	0
32	MA6	2a	1519	24/25	0.96	0.11	55,61,67,71	0
1	5MC	1A	1942	21/22	0.96	0.08	34,39,43,51	0
55	31H	1x	76	32/33	0.96	0.09	22,26,37,41	10
54	F3N	1w	76	33/34	0.97	0.07	22,25,30,32	0
1	PSU	1A	1917	20/21	0.97	0.07	39,45,50,52	0
32	4OC	1a	1402	22/23	0.97	0.08	38,45,48,49	0
1	OMC	1A	1920	21/22	0.97	0.08	35,43,45,52	0
1	PSU	1A	1911	20/21	0.97	0.07	42,46,49,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MU	2A	1939	21/22	0.97	0.08	32,38,42,45	0
32	MA6	1a	1519	24/25	0.97	0.09	35,42,45,47	0
1	5MC	2A	1942	21/22	0.97	0.08	43,53,57,62	0
1	5MC	1A	1962	21/22	0.97	0.06	24,32,37,42	0
54	PSU	1w	39	20/21	0.97	0.08	53,61,67,76	0
1	OMG	2A	2251	24/25	0.97	0.08	35,43,45,51	0
1	8AH	2A	2503	24/25	0.97	0.09	32,38,44,45	0
1	2MU	2A	2552	21/23	0.97	0.08	35,41,45,55	0
1	PSU	2A	2605	20/21	0.97	0.07	30,38,42,44	0
1	5MU	1A	1939	21/22	0.98	0.06	21,28,30,32	0
1	8AH	1A	2503	24/25	0.98	0.06	15,21,26,27	0
32	MA6	1a	1518	24/25	0.98	0.08	31,39,45,46	0
1	2MU	1A	2552	21/23	0.98	0.07	23,27,34,36	0
32	UR3	1a	1498	21/22	0.98	0.07	36,41,45,46	0
1	PSU	1A	2605	20/21	0.98	0.07	23,26,31,32	0
1	OMG	1A	2251	24/25	0.98	0.06	22,25,28,30	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1808	1/1	0.33	0.20	91,91,91,91	0
57	MG	1a	1792	1/1	0.42	0.40	74,74,74,74	0
57	MG	2v	102	1/1	0.53	0.42	80,80,80,80	0
57	MG	1A	4078	1/1	0.57	0.25	62,62,62,62	0
57	MG	2A	3557	1/1	0.64	0.20	83,83,83,83	0
57	MG	1A	4042	1/1	0.65	0.26	70,70,70,70	0
57	MG	2A	3762	1/1	0.66	0.14	53,53,53,53	0
57	MG	1A	3909	1/1	0.67	0.24	85,85,85,85	0
57	MG	2A	3547	1/1	0.67	0.20	72,72,72,72	0
57	MG	2l	201	1/1	0.67	0.20	78,78,78,78	0
57	MG	1A	3979	1/1	0.67	0.14	70,70,70,70	0
57	MG	1B	213	1/1	0.68	0.26	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1B	228	1/1	0.68	0.27	77,77,77,77	0
57	MG	1A	3178	1/1	0.68	0.18	74,74,74,74	0
57	MG	1a	1673	1/1	0.69	0.26	77,77,77,77	0
57	MG	1w	104	1/1	0.69	0.28	81,81,81,81	0
57	MG	2A	3482	1/1	0.69	0.19	69,69,69,69	0
57	MG	1a	1743	1/1	0.70	0.36	81,81,81,81	0
57	MG	2A	3603	1/1	0.70	0.18	76,76,76,76	0
57	MG	2A	3690	1/1	0.70	0.19	58,58,58,58	0
57	MG	2A	3074	1/1	0.70	0.19	63,63,63,63	0
57	MG	2a	1781	1/1	0.70	0.23	81,81,81,81	0
57	MG	2A	3215	1/1	0.70	0.32	77,77,77,77	0
57	MG	1A	3841	1/1	0.70	0.18	24,24,24,24	0
57	MG	1a	1796	1/1	0.70	0.31	67,67,67,67	0
57	MG	2a	1643	1/1	0.71	0.25	73,73,73,73	0
57	MG	2a	1700	1/1	0.71	0.33	82,82,82,82	0
57	MG	2a	1770	1/1	0.71	0.21	70,70,70,70	0
57	MG	1a	1801	1/1	0.71	0.19	56,56,56,56	0
57	MG	2A	3645	1/1	0.71	0.23	48,48,48,48	0
57	MG	2a	1628	1/1	0.71	0.32	79,79,79,79	0
57	MG	2a	1632	1/1	0.71	0.37	74,74,74,74	0
57	MG	2A	3483	1/1	0.72	0.35	84,84,84,84	0
57	MG	2A	3573	1/1	0.72	0.30	68,68,68,68	0
57	MG	1A	4064	1/1	0.72	0.18	64,64,64,64	0
57	MG	1V	205	1/1	0.73	0.15	63,63,63,63	0
57	MG	2A	3516	1/1	0.73	0.14	40,40,40,40	0
57	MG	2A	3019	1/1	0.73	0.34	79,79,79,79	0
57	MG	1A	4023	1/1	0.73	0.18	50,50,50,50	0
57	MG	1A	3375	1/1	0.73	0.33	74,74,74,74	0
57	MG	1a	1812	1/1	0.73	0.19	67,67,67,67	0
57	MG	2Q	204	1/1	0.74	0.17	77,77,77,77	0
57	MG	1A	3766	1/1	0.74	0.30	51,51,51,51	0
57	MG	2A	3590	1/1	0.74	0.23	50,50,50,50	0
57	MG	1A	3394	1/1	0.74	0.34	69,69,69,69	0
57	MG	2A	3604	1/1	0.74	0.22	76,76,76,76	0
57	MG	1A	3747	1/1	0.74	0.25	82,82,82,82	0
57	MG	2A	3293	1/1	0.74	0.26	67,67,67,67	0
57	MG	2A	3436	1/1	0.74	0.20	66,66,66,66	0
57	MG	2A	3784	1/1	0.74	0.21	70,70,70,70	0
57	MG	2v	101	1/1	0.74	0.24	78,78,78,78	0
57	MG	2B	211	1/1	0.74	0.34	76,76,76,76	0
57	MG	2y	101	1/1	0.74	0.20	81,81,81,81	0
57	MG	2A	3580	1/1	0.75	0.17	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1756	1/1	0.75	0.29	59,59,59,59	0
57	MG	1B	227	1/1	0.75	0.12	81,81,81,81	0
57	MG	2A	3057	1/1	0.75	0.15	65,65,65,65	0
57	MG	2a	1790	1/1	0.75	0.26	75,75,75,75	0
57	MG	11	104	1/1	0.75	0.24	78,78,78,78	0
57	MG	20	102	1/1	0.75	0.31	73,73,73,73	0
57	MG	2A	3606	1/1	0.75	0.19	66,66,66,66	0
57	MG	2A	3564	1/1	0.75	0.15	75,75,75,75	0
57	MG	1A	3898	1/1	0.75	0.16	35,35,35,35	0
57	MG	1a	1738	1/1	0.76	0.36	76,76,76,76	0
57	MG	2A	3775	1/1	0.76	0.48	73,73,73,73	0
57	MG	2A	3779	1/1	0.76	0.29	82,82,82,82	0
57	MG	1v	101	1/1	0.76	0.35	82,82,82,82	0
57	MG	2a	1698	1/1	0.76	0.35	74,74,74,74	0
57	MG	2A	3662	1/1	0.76	0.29	60,60,60,60	0
57	MG	2a	1730	1/1	0.76	0.18	87,87,87,87	0
57	MG	2A	3419	1/1	0.76	0.32	61,61,61,61	0
57	MG	2y	102	1/1	0.76	0.33	75,75,75,75	0
57	MG	2A	3584	1/1	0.77	0.18	69,69,69,69	0
57	MG	2W	201	1/1	0.77	0.13	67,67,67,67	0
57	MG	1A	3863	1/1	0.77	0.13	44,44,44,44	0
57	MG	2A	3415	1/1	0.77	0.27	71,71,71,71	0
57	MG	2a	1629	1/1	0.77	0.44	73,73,73,73	0
57	MG	1A	3732	1/1	0.77	0.13	70,70,70,70	0
57	MG	1a	1662	1/1	0.77	0.32	71,71,71,71	0
57	MG	2a	1665	1/1	0.77	0.28	64,64,64,64	0
57	MG	2a	1670	1/1	0.77	0.33	74,74,74,74	0
57	MG	1A	3785	1/1	0.77	0.20	55,55,55,55	0
57	MG	2A	3658	1/1	0.77	0.22	67,67,67,67	0
57	MG	1A	3804	1/1	0.77	0.17	69,69,69,69	0
57	MG	2A	3675	1/1	0.77	0.29	69,69,69,69	0
57	MG	2a	1759	1/1	0.77	0.25	81,81,81,81	0
57	MG	1B	217	1/1	0.77	0.17	52,52,52,52	0
57	MG	2a	1777	1/1	0.77	0.17	75,75,75,75	0
57	MG	2A	3711	1/1	0.77	0.14	47,47,47,47	0
57	MG	1A	3491	1/1	0.77	0.23	64,64,64,64	0
57	MG	2A	3213	1/1	0.77	0.33	72,72,72,72	0
57	MG	1A	4039	1/1	0.77	0.14	48,48,48,48	0
57	MG	2A	3274	1/1	0.77	0.15	74,74,74,74	0
57	MG	2A	3289	1/1	0.77	0.17	62,62,62,62	0
57	MG	2B	214	1/1	0.77	0.29	66,66,66,66	0
57	MG	2N	201	1/1	0.77	0.25	85,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3176	1/1	0.78	0.14	63,63,63,63	0
57	MG	1a	1719	1/1	0.78	0.20	82,82,82,82	0
57	MG	2A	3749	1/1	0.78	0.14	58,58,58,58	0
57	MG	2a	1686	1/1	0.78	0.30	72,72,72,72	0
57	MG	1O	204	1/1	0.78	0.18	71,71,71,71	0
57	MG	2A	3227	1/1	0.78	0.28	71,71,71,71	0
57	MG	2A	3248	1/1	0.78	0.13	57,57,57,57	0
57	MG	2a	1732	1/1	0.78	0.35	83,83,83,83	0
57	MG	1A	3970	1/1	0.78	0.17	47,47,47,47	0
57	MG	1A	3600	1/1	0.78	0.18	66,66,66,66	0
57	MG	2A	3023	1/1	0.78	0.22	71,71,71,71	0
57	MG	1A	3810	1/1	0.78	0.20	69,69,69,69	0
57	MG	1A	4029	1/1	0.78	0.16	27,27,27,27	0
57	MG	2a	1783	1/1	0.78	0.34	66,66,66,66	0
57	MG	2V	202	1/1	0.78	0.24	67,67,67,67	0
57	MG	2A	3080	1/1	0.78	0.21	66,66,66,66	0
57	MG	2A	3450	1/1	0.78	0.18	49,49,49,49	0
57	MG	2q	202	1/1	0.78	0.18	82,82,82,82	0
57	MG	2A	3460	1/1	0.78	0.19	51,51,51,51	0
57	MG	2A	3102	1/1	0.78	0.24	66,66,66,66	0
57	MG	2A	3112	1/1	0.78	0.27	75,75,75,75	0
57	MG	2a	1633	1/1	0.78	0.36	73,73,73,73	0
57	MG	1a	1684	1/1	0.79	0.15	68,68,68,68	0
57	MG	1A	3690	1/1	0.79	0.19	62,62,62,62	0
57	MG	2A	3225	1/1	0.79	0.34	75,75,75,75	0
57	MG	2a	1696	1/1	0.79	0.39	74,74,74,74	0
57	MG	2a	1697	1/1	0.79	0.27	81,81,81,81	0
57	MG	1A	4040	1/1	0.79	0.19	67,67,67,67	0
57	MG	2A	3233	1/1	0.79	0.14	69,69,69,69	0
57	MG	2a	1711	1/1	0.79	0.26	83,83,83,83	0
57	MG	2A	3236	1/1	0.79	0.19	63,63,63,63	0
57	MG	2A	3055	1/1	0.79	0.18	57,57,57,57	0
57	MG	2A	3252	1/1	0.79	0.50	62,62,62,62	0
57	MG	2D	306	1/1	0.79	0.39	54,54,54,54	0
57	MG	2F	302	1/1	0.79	0.30	74,74,74,74	0
57	MG	1A	3446	1/1	0.79	0.16	65,65,65,65	0
57	MG	1A	3528	1/1	0.79	0.17	57,57,57,57	0
57	MG	1A	3989	1/1	0.79	0.14	58,58,58,58	0
57	MG	2A	3399	1/1	0.79	0.24	83,83,83,83	0
57	MG	1a	1657	1/1	0.79	0.16	65,65,65,65	0
57	MG	1A	3467	1/1	0.79	0.21	60,60,60,60	0
57	MG	2A	3156	1/1	0.79	0.18	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3643	1/1	0.79	0.23	72,72,72,72	0
57	MG	2A	3177	1/1	0.79	0.51	80,80,80,80	0
57	MG	2a	1642	1/1	0.79	0.33	73,73,73,73	0
57	MG	2A	3474	1/1	0.79	0.30	78,78,78,78	0
57	MG	2A	3001	1/1	0.80	0.26	59,59,59,59	0
57	MG	14	101	1/1	0.80	0.20	80,80,80,80	0
57	MG	1A	3488	1/1	0.80	0.36	60,60,60,60	0
57	MG	2A	3044	1/1	0.80	0.22	58,58,58,58	0
57	MG	1A	3704	1/1	0.80	0.20	61,61,61,61	0
57	MG	2A	3294	1/1	0.80	0.26	69,69,69,69	0
57	MG	2A	3639	1/1	0.80	0.15	72,72,72,72	0
57	MG	2a	1666	1/1	0.80	0.35	68,68,68,68	0
57	MG	2A	3320	1/1	0.80	0.10	69,69,69,69	0
57	MG	2A	3354	1/1	0.80	0.29	65,65,65,65	0
57	MG	1A	3854	1/1	0.80	0.16	58,58,58,58	0
57	MG	1A	3727	1/1	0.80	0.12	26,26,26,26	0
57	MG	1A	3039	1/1	0.80	0.29	63,63,63,63	0
57	MG	2A	3427	1/1	0.80	0.23	74,74,74,74	0
57	MG	2a	1710	1/1	0.80	0.29	79,79,79,79	0
57	MG	1a	1728	1/1	0.80	0.25	67,67,67,67	0
57	MG	2A	3760	1/1	0.80	0.17	73,73,73,73	0
57	MG	2A	3448	1/1	0.80	0.14	47,47,47,47	0
57	MG	1A	3314	1/1	0.80	0.18	54,54,54,54	0
57	MG	1A	3954	1/1	0.80	0.16	31,31,31,31	0
57	MG	2a	1768	1/1	0.80	0.14	69,69,69,69	0
57	MG	1A	3356	1/1	0.80	0.33	34,34,34,34	0
57	MG	1A	3607	1/1	0.80	0.18	68,68,68,68	0
57	MG	1O	201	1/1	0.80	0.13	72,72,72,72	0
57	MG	1a	1802	1/1	0.80	0.15	84,84,84,84	0
57	MG	2E	301	1/1	0.80	0.19	68,68,68,68	0
57	MG	2a	1793	1/1	0.80	0.23	64,64,64,64	0
57	MG	1a	1809	1/1	0.80	0.27	69,69,69,69	0
57	MG	2A	3548	1/1	0.80	0.20	65,65,65,65	0
57	MG	1A	3795	1/1	0.80	0.19	60,60,60,60	0
57	MG	2A	3560	1/1	0.80	0.16	74,74,74,74	0
57	MG	1A	3796	1/1	0.80	0.17	49,49,49,49	0
57	MG	1A	3374	1/1	0.80	0.22	61,61,61,61	0
57	MG	2a	1610	1/1	0.80	0.48	78,78,78,78	0
57	MG	2B	206	1/1	0.81	0.33	73,73,73,73	0
57	MG	2A	3582	1/1	0.81	0.15	70,70,70,70	0
57	MG	1A	3907	1/1	0.81	0.11	70,70,70,70	0
57	MG	2A	3223	1/1	0.81	0.19	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1708	1/1	0.81	0.15	62,62,62,62	0
57	MG	1A	3514	1/1	0.81	0.26	48,48,48,48	0
57	MG	1A	3915	1/1	0.81	0.15	62,62,62,62	0
57	MG	2a	1714	1/1	0.81	0.23	74,74,74,74	0
57	MG	2a	1723	1/1	0.81	0.33	80,80,80,80	0
57	MG	2G	201	1/1	0.81	0.14	77,77,77,77	0
57	MG	1A	3620	1/1	0.81	0.14	65,65,65,65	0
57	MG	1l	103	1/1	0.81	0.10	42,42,42,42	0
57	MG	1A	4060	1/1	0.81	0.15	53,53,53,53	0
57	MG	1A	3962	1/1	0.81	0.15	58,58,58,58	0
57	MG	1A	3526	1/1	0.81	0.39	56,56,56,56	0
57	MG	2A	3281	1/1	0.81	0.26	67,67,67,67	0
57	MG	2a	1626	1/1	0.81	0.40	77,77,77,77	0
57	MG	1A	3395	1/1	0.81	0.23	69,69,69,69	0
57	MG	2a	1788	1/1	0.81	0.42	83,83,83,83	0
57	MG	1a	1670	1/1	0.81	0.32	75,75,75,75	0
57	MG	1A	3533	1/1	0.81	0.12	38,38,38,38	0
57	MG	2a	1798	1/1	0.81	0.26	73,73,73,73	0
57	MG	2A	3754	1/1	0.81	0.24	77,77,77,77	0
57	MG	2A	3559	1/1	0.81	0.17	67,67,67,67	0
57	MG	2A	3171	1/1	0.81	0.32	70,70,70,70	0
57	MG	1A	3432	1/1	0.81	0.16	64,64,64,64	0
57	MG	2A	3776	1/1	0.81	0.25	67,67,67,67	0
57	MG	1x	107	1/1	0.81	0.23	72,72,72,72	0
57	MG	1x	111	1/1	0.81	0.23	70,70,70,70	0
57	MG	2A	3441	1/1	0.82	0.23	59,59,59,59	0
57	MG	2a	1638	1/1	0.82	0.22	82,82,82,82	0
57	MG	2A	3680	1/1	0.82	0.11	63,63,63,63	0
57	MG	1A	3680	1/1	0.82	0.21	56,56,56,56	0
57	MG	2A	3695	1/1	0.82	0.13	70,70,70,70	0
57	MG	1A	3222	1/1	0.82	0.16	63,63,63,63	0
57	MG	1A	3802	1/1	0.82	0.17	50,50,50,50	0
57	MG	2a	1671	1/1	0.82	0.24	65,65,65,65	0
57	MG	1a	1704	1/1	0.82	0.36	72,72,72,72	0
57	MG	2A	3235	1/1	0.82	0.27	68,68,68,68	0
57	MG	2A	3035	1/1	0.82	0.34	69,69,69,69	0
57	MG	2A	3774	1/1	0.82	0.18	68,68,68,68	0
57	MG	1A	3558	1/1	0.82	0.15	55,55,55,55	0
57	MG	1A	3500	1/1	0.82	0.18	59,59,59,59	0
57	MG	2A	3255	1/1	0.82	0.14	65,65,65,65	0
57	MG	1A	3239	1/1	0.82	0.12	64,64,64,64	0
57	MG	2B	202	1/1	0.82	0.11	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3277	1/1	0.82	0.12	72,72,72,72	0
57	MG	2B	210	1/1	0.82	0.16	78,78,78,78	0
57	MG	1A	3844	1/1	0.82	0.15	30,30,30,30	0
57	MG	1A	3485	1/1	0.82	0.18	65,65,65,65	0
57	MG	10	108	1/1	0.82	0.23	70,70,70,70	0
57	MG	1A	3855	1/1	0.82	0.15	34,34,34,34	0
57	MG	2A	3305	1/1	0.82	0.26	58,58,58,58	0
57	MG	2F	308	1/1	0.82	0.16	69,69,69,69	0
57	MG	2A	3309	1/1	0.82	0.19	66,66,66,66	0
57	MG	1A	3057	1/1	0.82	0.15	63,63,63,63	0
57	MG	2A	3353	1/1	0.82	0.17	81,81,81,81	0
57	MG	2A	3158	1/1	0.82	0.14	70,70,70,70	0
57	MG	2a	1792	1/1	0.82	0.28	76,76,76,76	0
57	MG	1A	3783	1/1	0.82	0.14	49,49,49,49	0
57	MG	2A	3615	1/1	0.82	0.37	68,68,68,68	0
57	MG	2I	101	1/1	0.82	0.17	54,54,54,54	0
57	MG	2a	1811	1/1	0.82	0.17	70,70,70,70	0
57	MG	2A	3633	1/1	0.82	0.12	64,64,64,64	0
57	MG	1a	1622	1/1	0.82	0.27	65,65,65,65	0
57	MG	1a	1639	1/1	0.82	0.35	67,67,67,67	0
57	MG	1A	3670	1/1	0.82	0.24	62,62,62,62	0
57	MG	2a	1631	1/1	0.82	0.25	66,66,66,66	0
57	MG	1A	3794	1/1	0.82	0.16	59,59,59,59	0
57	MG	2a	1608	1/1	0.83	0.22	67,67,67,67	0
57	MG	2A	3613	1/1	0.83	0.28	56,56,56,56	0
57	MG	1A	3765	1/1	0.83	0.19	54,54,54,54	0
57	MG	2A	3617	1/1	0.83	0.14	58,58,58,58	0
57	MG	2A	3631	1/1	0.83	0.22	86,86,86,86	0
57	MG	2A	3181	1/1	0.83	0.28	65,65,65,65	0
57	MG	2A	3634	1/1	0.83	0.15	45,45,45,45	0
57	MG	2A	3636	1/1	0.83	0.17	67,67,67,67	0
57	MG	2A	3367	1/1	0.83	0.28	74,74,74,74	0
57	MG	2A	3199	1/1	0.83	0.18	55,55,55,55	0
57	MG	2A	3405	1/1	0.83	0.26	61,61,61,61	0
57	MG	1B	220	1/1	0.83	0.18	57,57,57,57	0
57	MG	1a	1661	1/1	0.83	0.27	65,65,65,65	0
57	MG	2A	3678	1/1	0.83	0.17	68,68,68,68	0
57	MG	1B	221	1/1	0.83	0.24	56,56,56,56	0
57	MG	1A	3536	1/1	0.83	0.21	63,63,63,63	0
57	MG	1A	4028	1/1	0.83	0.11	62,62,62,62	0
57	MG	2A	3230	1/1	0.83	0.12	81,81,81,81	0
57	MG	1A	3372	1/1	0.83	0.33	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3822	1/1	0.83	0.18	61,61,61,61	0
57	MG	1R	206	1/1	0.83	0.14	71,71,71,71	0
57	MG	1A	3583	1/1	0.83	0.18	58,58,58,58	0
57	MG	10	102	1/1	0.83	0.23	66,66,66,66	0
57	MG	2A	3509	1/1	0.83	0.17	68,68,68,68	0
57	MG	1A	3949	1/1	0.83	0.12	57,57,57,57	0
57	MG	2A	3777	1/1	0.83	0.20	70,70,70,70	0
57	MG	2A	3523	1/1	0.83	0.15	59,59,59,59	0
57	MG	2A	3256	1/1	0.83	0.16	73,73,73,73	0
57	MG	10	109	1/1	0.83	0.21	69,69,69,69	0
57	MG	2a	1763	1/1	0.83	0.27	67,67,67,67	0
57	MG	2A	3275	1/1	0.83	0.45	78,78,78,78	0
57	MG	2A	3083	1/1	0.83	0.21	75,75,75,75	0
57	MG	1A	3445	1/1	0.83	0.17	58,58,58,58	0
57	MG	2B	213	1/1	0.83	0.11	65,65,65,65	0
57	MG	2A	3562	1/1	0.83	0.19	68,68,68,68	0
57	MG	1a	1800	1/1	0.83	0.30	76,76,76,76	0
57	MG	1A	3674	1/1	0.83	0.14	58,58,58,58	0
57	MG	2A	3574	1/1	0.83	0.15	71,71,71,71	0
57	MG	1A	3677	1/1	0.83	0.13	42,42,42,42	0
57	MG	2A	3159	1/1	0.83	0.26	82,82,82,82	0
57	MG	1A	3858	1/1	0.83	0.12	56,56,56,56	0
57	MG	2a	1810	1/1	0.83	0.09	77,77,77,77	0
57	MG	1a	1637	1/1	0.83	0.34	57,57,57,57	0
57	MG	2a	1816	1/1	0.83	0.19	81,81,81,81	0
57	MG	2A	3325	1/1	0.83	0.19	67,67,67,67	0
57	MG	2A	3333	1/1	0.83	0.22	61,61,61,61	0
57	MG	2A	3350	1/1	0.83	0.22	59,59,59,59	0
57	MG	2A	3612	1/1	0.83	0.27	68,68,68,68	0
57	MG	28	102	1/1	0.83	0.34	69,69,69,69	0
57	MG	2a	1602	1/1	0.83	0.21	81,81,81,81	0
57	MG	1A	3936	1/1	0.84	0.10	68,68,68,68	0
57	MG	2A	3278	1/1	0.84	0.22	59,59,59,59	0
57	MG	1A	3701	1/1	0.84	0.09	19,19,19,19	0
57	MG	2A	3283	1/1	0.84	0.34	83,83,83,83	0
57	MG	1A	3636	1/1	0.84	0.16	56,56,56,56	0
57	MG	1A	3722	1/1	0.84	0.14	30,30,30,30	0
57	MG	2A	3586	1/1	0.84	0.15	67,67,67,67	0
57	MG	1F	304	1/1	0.84	0.26	69,69,69,69	0
57	MG	2A	3298	1/1	0.84	0.38	76,76,76,76	0
57	MG	1A	3641	1/1	0.84	0.12	43,43,43,43	0
57	MG	1A	3821	1/1	0.84	0.15	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3119	1/1	0.84	0.18	69,69,69,69	0
57	MG	2a	1619	1/1	0.84	0.13	71,71,71,71	0
57	MG	1A	3556	1/1	0.84	0.31	72,72,72,72	0
57	MG	1a	1755	1/1	0.84	0.14	64,64,64,64	0
57	MG	1a	1779	1/1	0.84	0.13	75,75,75,75	0
57	MG	2A	3628	1/1	0.84	0.19	76,76,76,76	0
57	MG	2A	3165	1/1	0.84	0.13	67,67,67,67	0
57	MG	1A	3477	1/1	0.84	0.14	74,74,74,74	0
57	MG	2A	3359	1/1	0.84	0.41	73,73,73,73	0
57	MG	2A	3360	1/1	0.84	0.33	67,67,67,67	0
57	MG	2A	3363	1/1	0.84	0.26	65,65,65,65	0
57	MG	2a	1652	1/1	0.84	0.24	73,73,73,73	0
57	MG	1a	1795	1/1	0.84	0.14	68,68,68,68	0
57	MG	2A	3655	1/1	0.84	0.23	70,70,70,70	0
57	MG	1A	3757	1/1	0.84	0.13	61,61,61,61	0
57	MG	2A	3400	1/1	0.84	0.14	73,73,73,73	0
57	MG	2a	1673	1/1	0.84	0.15	64,64,64,64	0
57	MG	1A	3307	1/1	0.84	0.35	60,60,60,60	0
57	MG	2a	1688	1/1	0.84	0.22	71,71,71,71	0
57	MG	2A	3185	1/1	0.84	0.14	63,63,63,63	0
57	MG	1A	3139	1/1	0.84	0.13	47,47,47,47	0
57	MG	2A	3425	1/1	0.84	0.25	73,73,73,73	0
57	MG	2A	3692	1/1	0.84	0.13	71,71,71,71	0
57	MG	2a	1707	1/1	0.84	0.19	76,76,76,76	0
57	MG	1A	3773	1/1	0.84	0.15	58,58,58,58	0
57	MG	1a	1806	1/1	0.84	0.13	60,60,60,60	0
57	MG	2A	3733	1/1	0.84	0.13	68,68,68,68	0
57	MG	2A	3738	1/1	0.84	0.15	58,58,58,58	0
57	MG	2a	1722	1/1	0.84	0.12	62,62,62,62	0
57	MG	2A	3216	1/1	0.84	0.22	73,73,73,73	0
57	MG	1A	3237	1/1	0.84	0.14	56,56,56,56	0
57	MG	1A	4044	1/1	0.84	0.16	59,59,59,59	0
57	MG	1a	1814	1/1	0.84	0.28	65,65,65,65	0
57	MG	2A	3767	1/1	0.84	0.32	66,66,66,66	0
57	MG	1t	201	1/1	0.84	0.22	57,57,57,57	0
57	MG	2A	3478	1/1	0.84	0.15	50,50,50,50	0
57	MG	18	107	1/1	0.84	0.25	70,70,70,70	0
57	MG	2a	1776	1/1	0.84	0.33	75,75,75,75	0
57	MG	1A	3683	1/1	0.84	0.13	62,62,62,62	0
57	MG	2A	3485	1/1	0.84	0.11	67,67,67,67	0
57	MG	1A	3793	1/1	0.84	0.14	57,57,57,57	0
57	MG	2A	3795	1/1	0.84	0.15	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3796	1/1	0.84	0.35	77,77,77,77	0
57	MG	2A	3797	1/1	0.84	0.15	69,69,69,69	0
57	MG	2A	3244	1/1	0.84	0.09	63,63,63,63	0
57	MG	2A	3246	1/1	0.84	0.09	68,68,68,68	0
57	MG	2B	209	1/1	0.84	0.32	69,69,69,69	0
57	MG	1A	3185	1/1	0.84	0.15	57,57,57,57	0
57	MG	1A	4085	1/1	0.84	0.14	62,62,62,62	0
57	MG	1a	1659	1/1	0.84	0.18	61,61,61,61	0
57	MG	1A	3694	1/1	0.84	0.10	57,57,57,57	0
57	MG	2B	216	1/1	0.84	0.14	68,68,68,68	0
57	MG	1A	3930	1/1	0.84	0.12	62,62,62,62	0
57	MG	2A	3561	1/1	0.84	0.26	67,67,67,67	0
57	MG	2x	105	1/1	0.84	0.18	65,65,65,65	0
57	MG	2x	108	1/1	0.84	0.10	56,56,56,56	0
57	MG	2E	309	1/1	0.84	0.21	67,67,67,67	0
57	MG	1a	1666	1/1	0.84	0.27	72,72,72,72	0
57	MG	2A	3498	1/1	0.85	0.12	79,79,79,79	0
57	MG	2A	3702	1/1	0.85	0.13	69,69,69,69	0
57	MG	1A	3696	1/1	0.85	0.11	66,66,66,66	0
57	MG	1A	3997	1/1	0.85	0.11	53,53,53,53	0
57	MG	1A	4018	1/1	0.85	0.19	72,72,72,72	0
57	MG	2A	3741	1/1	0.85	0.12	48,48,48,48	0
57	MG	2A	3529	1/1	0.85	0.21	62,62,62,62	0
57	MG	2A	3196	1/1	0.85	0.38	74,74,74,74	0
57	MG	2A	3757	1/1	0.85	0.11	64,64,64,64	0
57	MG	2A	3310	1/1	0.85	0.16	64,64,64,64	0
57	MG	2a	1669	1/1	0.85	0.27	72,72,72,72	0
57	MG	2A	3552	1/1	0.85	0.11	39,39,39,39	0
57	MG	1A	3789	1/1	0.85	0.14	60,60,60,60	0
57	MG	1A	3623	1/1	0.85	0.15	30,30,30,30	0
57	MG	1a	1711	1/1	0.85	0.13	55,55,55,55	0
57	MG	2A	3347	1/1	0.85	0.23	70,70,70,70	0
57	MG	2a	1695	1/1	0.85	0.09	67,67,67,67	0
57	MG	1A	3144	1/1	0.85	0.23	32,32,32,32	0
57	MG	1A	3034	1/1	0.85	0.12	46,46,46,46	0
57	MG	1A	3541	1/1	0.85	0.17	65,65,65,65	0
57	MG	2A	3356	1/1	0.85	0.25	53,53,53,53	0
57	MG	2a	1704	1/1	0.85	0.20	69,69,69,69	0
57	MG	2A	3576	1/1	0.85	0.20	42,42,42,42	0
57	MG	1a	1740	1/1	0.85	0.17	43,43,43,43	0
57	MG	2A	3047	1/1	0.85	0.20	69,69,69,69	0
57	MG	1A	3546	1/1	0.85	0.15	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2B	208	1/1	0.85	0.17	56,56,56,56	0
57	MG	2a	1720	1/1	0.85	0.23	68,68,68,68	0
57	MG	1A	3419	1/1	0.85	0.20	66,66,66,66	0
57	MG	2A	3390	1/1	0.85	0.22	64,64,64,64	0
57	MG	1A	3807	1/1	0.85	0.23	43,43,43,43	0
57	MG	2A	3078	1/1	0.85	0.14	58,58,58,58	0
57	MG	1A	3428	1/1	0.85	0.16	57,57,57,57	0
57	MG	2A	3407	1/1	0.85	0.17	66,66,66,66	0
57	MG	2a	1762	1/1	0.85	0.15	63,63,63,63	0
57	MG	2D	303	1/1	0.85	0.12	61,61,61,61	0
57	MG	1A	4067	1/1	0.85	0.17	59,59,59,59	0
57	MG	1a	1615	1/1	0.85	0.11	56,56,56,56	0
57	MG	2a	1771	1/1	0.85	0.20	76,76,76,76	0
57	MG	2A	3423	1/1	0.85	0.14	64,64,64,64	0
57	MG	2A	3254	1/1	0.85	0.15	67,67,67,67	0
57	MG	1A	3939	1/1	0.85	0.13	65,65,65,65	0
57	MG	1A	3258	1/1	0.85	0.20	55,55,55,55	0
57	MG	2A	3260	1/1	0.85	0.26	67,67,67,67	0
57	MG	2P	202	1/1	0.85	0.22	66,66,66,66	0
57	MG	2A	3143	1/1	0.85	0.34	72,72,72,72	0
57	MG	2R	202	1/1	0.85	0.14	50,50,50,50	0
57	MG	2U	201	1/1	0.85	0.19	54,54,54,54	0
57	MG	2A	3151	1/1	0.85	0.13	45,45,45,45	0
57	MG	1A	3262	1/1	0.85	0.14	51,51,51,51	0
57	MG	1A	3837	1/1	0.85	0.20	63,63,63,63	0
57	MG	2A	3477	1/1	0.85	0.17	50,50,50,50	0
57	MG	2f	202	1/1	0.85	0.23	76,76,76,76	0
57	MG	1A	3287	1/1	0.85	0.09	30,30,30,30	0
57	MG	1A	3299	1/1	0.85	0.24	37,37,37,37	0
57	MG	1A	3981	1/1	0.85	0.11	69,69,69,69	0
57	MG	1b	301	1/1	0.85	0.17	68,68,68,68	0
57	MG	2a	1614	1/1	0.85	0.26	63,63,63,63	0
57	MG	2A	3687	1/1	0.85	0.25	70,70,70,70	0
57	MG	2A	3491	1/1	0.85	0.17	73,73,73,73	0
57	MG	2A	3494	1/1	0.85	0.17	76,76,76,76	0
57	MG	1A	3320	1/1	0.86	0.22	56,56,56,56	0
57	MG	2A	3382	1/1	0.86	0.10	72,72,72,72	0
57	MG	1A	3993	1/1	0.86	0.14	50,50,50,50	0
57	MG	2A	3392	1/1	0.86	0.17	47,47,47,47	0
57	MG	1A	3709	1/1	0.86	0.09	44,44,44,44	0
57	MG	2a	1611	1/1	0.86	0.39	75,75,75,75	0
57	MG	2A	3229	1/1	0.86	0.34	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3538	1/1	0.86	0.28	68,68,68,68	0
57	MG	2a	1620	1/1	0.86	0.25	76,76,76,76	0
57	MG	2A	3644	1/1	0.86	0.31	68,68,68,68	0
57	MG	1a	1717	1/1	0.86	0.18	67,67,67,67	0
57	MG	2A	3046	1/1	0.86	0.21	70,70,70,70	0
57	MG	1A	3881	1/1	0.86	0.10	26,26,26,26	0
57	MG	1A	3887	1/1	0.86	0.10	39,39,39,39	0
57	MG	1A	3479	1/1	0.86	0.26	67,67,67,67	0
57	MG	2A	3247	1/1	0.86	0.28	65,65,65,65	0
57	MG	2a	1640	1/1	0.86	0.13	67,67,67,67	0
57	MG	1A	3800	1/1	0.86	0.12	69,69,69,69	0
57	MG	2A	3077	1/1	0.86	0.15	60,60,60,60	0
57	MG	1a	1742	1/1	0.86	0.15	65,65,65,65	0
57	MG	1A	3328	1/1	0.86	0.10	57,57,57,57	0
57	MG	2A	3457	1/1	0.86	0.12	71,71,71,71	0
57	MG	1A	3335	1/1	0.86	0.16	56,56,56,56	0
57	MG	2A	3085	1/1	0.86	0.16	47,47,47,47	0
57	MG	2A	3723	1/1	0.86	0.18	43,43,43,43	0
57	MG	2A	3730	1/1	0.86	0.12	63,63,63,63	0
57	MG	2a	1677	1/1	0.86	0.20	68,68,68,68	0
57	MG	2A	3262	1/1	0.86	0.19	71,71,71,71	0
57	MG	2A	3263	1/1	0.86	0.14	73,73,73,73	0
57	MG	2A	3270	1/1	0.86	0.12	51,51,51,51	0
57	MG	2A	3271	1/1	0.86	0.18	73,73,73,73	0
57	MG	2A	3753	1/1	0.86	0.15	66,66,66,66	0
57	MG	2A	3095	1/1	0.86	0.21	75,75,75,75	0
57	MG	1A	3928	1/1	0.86	0.14	59,59,59,59	0
57	MG	1A	3755	1/1	0.86	0.12	42,42,42,42	0
57	MG	1A	3423	1/1	0.86	0.28	65,65,65,65	0
57	MG	2A	3279	1/1	0.86	0.18	60,60,60,60	0
57	MG	2A	3768	1/1	0.86	0.17	72,72,72,72	0
57	MG	2A	3123	1/1	0.86	0.14	57,57,57,57	0
57	MG	2A	3518	1/1	0.86	0.10	51,51,51,51	0
57	MG	2a	1718	1/1	0.86	0.11	82,82,82,82	0
57	MG	1a	1610	1/1	0.86	0.24	65,65,65,65	0
57	MG	2a	1721	1/1	0.86	0.23	76,76,76,76	0
57	MG	2A	3149	1/1	0.86	0.38	72,72,72,72	0
57	MG	2A	3542	1/1	0.86	0.19	72,72,72,72	0
57	MG	2a	1724	1/1	0.86	0.14	69,69,69,69	0
57	MG	2A	3783	1/1	0.86	0.29	75,75,75,75	0
57	MG	2A	3543	1/1	0.86	0.14	35,35,35,35	0
57	MG	2a	1751	1/1	0.86	0.15	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1754	1/1	0.86	0.13	49,49,49,49	0
57	MG	2A	3291	1/1	0.86	0.13	67,67,67,67	0
57	MG	1a	1798	1/1	0.86	0.17	70,70,70,70	0
57	MG	2a	1761	1/1	0.86	0.20	73,73,73,73	0
57	MG	1A	3068	1/1	0.86	0.25	58,58,58,58	0
57	MG	1A	3597	1/1	0.86	0.23	63,63,63,63	0
57	MG	2B	204	1/1	0.86	0.20	75,75,75,75	0
57	MG	2A	3299	1/1	0.86	0.28	75,75,75,75	0
57	MG	2A	3301	1/1	0.86	0.17	67,67,67,67	0
57	MG	2A	3303	1/1	0.86	0.13	72,72,72,72	0
57	MG	1a	1629	1/1	0.86	0.40	69,69,69,69	0
57	MG	1A	3823	1/1	0.86	0.12	29,29,29,29	0
57	MG	2A	3568	1/1	0.86	0.14	60,60,60,60	0
57	MG	1a	1638	1/1	0.86	0.20	60,60,60,60	0
57	MG	2B	215	1/1	0.86	0.17	66,66,66,66	0
57	MG	2A	3315	1/1	0.86	0.09	65,65,65,65	0
57	MG	1A	4095	1/1	0.86	0.15	47,47,47,47	0
57	MG	1A	3961	1/1	0.86	0.18	64,64,64,64	0
57	MG	2A	3330	1/1	0.86	0.31	56,56,56,56	0
57	MG	1B	214	1/1	0.86	0.12	59,59,59,59	0
57	MG	1A	3096	1/1	0.86	0.24	65,65,65,65	0
57	MG	2a	1812	1/1	0.86	0.10	65,65,65,65	0
57	MG	2A	3195	1/1	0.86	0.14	56,56,56,56	0
57	MG	2A	3593	1/1	0.86	0.17	63,63,63,63	0
57	MG	2k	201	1/1	0.86	0.24	66,66,66,66	0
57	MG	2A	3597	1/1	0.86	0.21	74,74,74,74	0
57	MG	1A	3099	1/1	0.86	0.17	54,54,54,54	0
57	MG	1A	3277	1/1	0.86	0.23	64,64,64,64	0
57	MG	2A	3605	1/1	0.86	0.34	67,67,67,67	0
57	MG	2w	106	1/1	0.86	0.17	75,75,75,75	0
57	MG	2x	104	1/1	0.86	0.36	72,72,72,72	0
57	MG	1x	101	1/1	0.86	0.17	60,60,60,60	0
57	MG	1A	3378	1/1	0.86	0.26	62,62,62,62	0
57	MG	1a	1671	1/1	0.86	0.34	65,65,65,65	0
57	MG	2A	3217	1/1	0.86	0.15	70,70,70,70	0
57	MG	25	101	1/1	0.87	0.31	67,67,67,67	0
57	MG	1a	1761	1/1	0.87	0.13	58,58,58,58	0
57	MG	2a	1601	1/1	0.87	0.10	81,81,81,81	0
57	MG	1a	1764	1/1	0.87	0.15	48,48,48,48	0
57	MG	1a	1765	1/1	0.87	0.15	57,57,57,57	0
57	MG	2A	3339	1/1	0.87	0.16	58,58,58,58	0
57	MG	2A	3341	1/1	0.87	0.40	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3343	1/1	0.87	0.36	64,64,64,64	0
57	MG	2a	1617	1/1	0.87	0.18	57,57,57,57	0
57	MG	2A	3346	1/1	0.87	0.34	68,68,68,68	0
57	MG	1A	3559	1/1	0.87	0.20	44,44,44,44	0
57	MG	2A	3164	1/1	0.87	0.21	66,66,66,66	0
57	MG	1a	1791	1/1	0.87	0.12	69,69,69,69	0
57	MG	2A	3166	1/1	0.87	0.16	65,65,65,65	0
57	MG	2A	3167	1/1	0.87	0.21	57,57,57,57	0
57	MG	1A	3427	1/1	0.87	0.20	55,55,55,55	0
57	MG	1A	3045	1/1	0.87	0.12	39,39,39,39	0
57	MG	2A	3653	1/1	0.87	0.12	64,64,64,64	0
57	MG	2a	1639	1/1	0.87	0.27	71,71,71,71	0
57	MG	1A	3308	1/1	0.87	0.14	50,50,50,50	0
57	MG	1A	4030	1/1	0.87	0.13	43,43,43,43	0
57	MG	2A	3182	1/1	0.87	0.18	64,64,64,64	0
57	MG	2A	3664	1/1	0.87	0.13	71,71,71,71	0
57	MG	2a	1659	1/1	0.87	0.13	64,64,64,64	0
57	MG	12	101	1/1	0.87	0.13	38,38,38,38	0
57	MG	12	102	1/1	0.87	0.11	50,50,50,50	0
57	MG	13	104	1/1	0.87	0.10	55,55,55,55	0
57	MG	1A	3434	1/1	0.87	0.22	60,60,60,60	0
57	MG	1a	1807	1/1	0.87	0.23	70,70,70,70	0
57	MG	1A	3618	1/1	0.87	0.09	21,21,21,21	0
57	MG	2A	3412	1/1	0.87	0.14	57,57,57,57	0
57	MG	2a	1684	1/1	0.87	0.21	67,67,67,67	0
57	MG	2a	1685	1/1	0.87	0.18	65,65,65,65	0
57	MG	1a	1810	1/1	0.87	0.13	56,56,56,56	0
57	MG	1A	3922	1/1	0.87	0.13	49,49,49,49	0
57	MG	2a	1689	1/1	0.87	0.23	67,67,67,67	0
57	MG	2A	3221	1/1	0.87	0.22	65,65,65,65	0
57	MG	2A	3729	1/1	0.87	0.19	74,74,74,74	0
57	MG	1A	3924	1/1	0.87	0.20	55,55,55,55	0
57	MG	1A	3927	1/1	0.87	0.18	65,65,65,65	0
57	MG	1A	3803	1/1	0.87	0.10	57,57,57,57	0
57	MG	1A	3313	1/1	0.87	0.19	53,53,53,53	0
57	MG	1w	103	1/1	0.87	0.21	73,73,73,73	0
57	MG	1A	3214	1/1	0.87	0.20	49,49,49,49	0
57	MG	2a	1709	1/1	0.87	0.31	72,72,72,72	0
57	MG	1w	105	1/1	0.87	0.10	68,68,68,68	0
57	MG	1A	3449	1/1	0.87	0.15	48,48,48,48	0
57	MG	2A	3467	1/1	0.87	0.13	63,63,63,63	0
57	MG	2A	3238	1/1	0.87	0.24	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1x	104	1/1	0.87	0.18	66,66,66,66	0
57	MG	1a	1647	1/1	0.87	0.13	67,67,67,67	0
57	MG	2A	3769	1/1	0.87	0.20	71,71,71,71	0
57	MG	1a	1648	1/1	0.87	0.33	66,66,66,66	0
57	MG	1A	3944	1/1	0.87	0.11	27,27,27,27	0
57	MG	1A	3456	1/1	0.87	0.12	58,58,58,58	0
57	MG	1A	3466	1/1	0.87	0.19	56,56,56,56	0
57	MG	2a	1749	1/1	0.87	0.14	78,78,78,78	0
57	MG	2A	3030	1/1	0.87	0.19	63,63,63,63	0
57	MG	1A	3758	1/1	0.87	0.08	49,49,49,49	0
57	MG	1A	3540	1/1	0.87	0.29	59,59,59,59	0
57	MG	2A	3785	1/1	0.87	0.13	57,57,57,57	0
57	MG	2A	3794	1/1	0.87	0.10	47,47,47,47	0
57	MG	1a	1668	1/1	0.87	0.16	56,56,56,56	0
57	MG	1A	3281	1/1	0.87	0.12	58,58,58,58	0
57	MG	2A	3519	1/1	0.87	0.22	50,50,50,50	0
57	MG	2A	3264	1/1	0.87	0.30	69,69,69,69	0
57	MG	2B	203	1/1	0.87	0.23	73,73,73,73	0
57	MG	1B	224	1/1	0.87	0.19	57,57,57,57	0
57	MG	1A	3975	1/1	0.87	0.08	61,61,61,61	0
57	MG	2a	1779	1/1	0.87	0.40	71,71,71,71	0
57	MG	2A	3069	1/1	0.87	0.09	52,52,52,52	0
57	MG	1A	3252	1/1	0.87	0.09	46,46,46,46	0
57	MG	1a	1696	1/1	0.87	0.16	57,57,57,57	0
57	MG	1D	311	1/1	0.87	0.13	55,55,55,55	0
57	MG	2a	1791	1/1	0.87	0.26	79,79,79,79	0
57	MG	1E	310	1/1	0.87	0.08	39,39,39,39	0
57	MG	1A	3033	1/1	0.87	0.39	39,39,39,39	0
57	MG	2A	3282	1/1	0.87	0.25	76,76,76,76	0
57	MG	2a	1805	1/1	0.87	0.22	58,58,58,58	0
57	MG	1A	3784	1/1	0.87	0.18	54,54,54,54	0
57	MG	2A	3088	1/1	0.87	0.12	75,75,75,75	0
57	MG	2A	3092	1/1	0.87	0.27	65,65,65,65	0
57	MG	2A	3094	1/1	0.87	0.12	67,67,67,67	0
57	MG	1a	1727	1/1	0.87	0.11	64,64,64,64	0
57	MG	2a	1820	1/1	0.87	0.16	69,69,69,69	0
57	MG	2A	3099	1/1	0.87	0.23	77,77,77,77	0
57	MG	2f	203	1/1	0.87	0.18	75,75,75,75	0
57	MG	1A	3557	1/1	0.87	0.38	66,66,66,66	0
57	MG	2A	3106	1/1	0.87	0.24	59,59,59,59	0
57	MG	1O	206	1/1	0.87	0.24	65,65,65,65	0
57	MG	1R	205	1/1	0.87	0.13	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3307	1/1	0.87	0.34	71,71,71,71	0
57	MG	2A	3121	1/1	0.87	0.25	42,42,42,42	0
57	MG	2x	102	1/1	0.87	0.39	82,82,82,82	0
57	MG	1A	3305	1/1	0.87	0.19	63,63,63,63	0
57	MG	1U	209	1/1	0.87	0.39	37,37,37,37	0
57	MG	2A	3599	1/1	0.87	0.22	67,67,67,67	0
57	MG	1A	4012	1/1	0.87	0.16	67,67,67,67	0
57	MG	2A	3321	1/1	0.87	0.16	64,64,64,64	0
57	MG	1a	1804	1/1	0.88	0.22	64,64,64,64	0
57	MG	1A	3770	1/1	0.88	0.20	68,68,68,68	0
57	MG	1A	3654	1/1	0.88	0.09	27,27,27,27	0
57	MG	1A	3906	1/1	0.88	0.18	48,48,48,48	0
57	MG	1A	3657	1/1	0.88	0.20	55,55,55,55	0
57	MG	15	106	1/1	0.88	0.13	61,61,61,61	0
57	MG	1A	3410	1/1	0.88	0.14	31,31,31,31	0
57	MG	1a	1605	1/1	0.88	0.12	62,62,62,62	0
57	MG	2a	1637	1/1	0.88	0.12	64,64,64,64	0
57	MG	2A	3205	1/1	0.88	0.38	47,47,47,47	0
57	MG	1l	3200	1/1	0.88	0.10	71,71,71,71	0
57	MG	2A	3214	1/1	0.88	0.17	77,77,77,77	0
57	MG	1A	3412	1/1	0.88	0.12	48,48,48,48	0
57	MG	1A	3413	1/1	0.88	0.13	67,67,67,67	0
57	MG	2a	1647	1/1	0.88	0.23	78,78,78,78	0
57	MG	2a	1650	1/1	0.88	0.28	66,66,66,66	0
57	MG	1A	3923	1/1	0.88	0.12	50,50,50,50	0
57	MG	2a	1654	1/1	0.88	0.19	64,64,64,64	0
57	MG	1A	4075	1/1	0.88	0.15	62,62,62,62	0
57	MG	2a	1661	1/1	0.88	0.19	59,59,59,59	0
57	MG	1A	4076	1/1	0.88	0.11	70,70,70,70	0
57	MG	1A	3547	1/1	0.88	0.09	42,42,42,42	0
57	MG	2A	3699	1/1	0.88	0.11	59,59,59,59	0
57	MG	1A	3475	1/1	0.88	0.12	60,60,60,60	0
57	MG	1A	4086	1/1	0.88	0.09	40,40,40,40	0
57	MG	2A	3720	1/1	0.88	0.10	58,58,58,58	0
57	MG	1x	108	1/1	0.88	0.21	67,67,67,67	0
57	MG	2a	1679	1/1	0.88	0.34	69,69,69,69	0
57	MG	2A	3231	1/1	0.88	0.13	71,71,71,71	0
57	MG	1A	4093	1/1	0.88	0.25	49,49,49,49	0
57	MG	1A	3414	1/1	0.88	0.10	51,51,51,51	0
57	MG	2A	3735	1/1	0.88	0.10	79,79,79,79	0
57	MG	1B	208	1/1	0.88	0.10	65,65,65,65	0
57	MG	2a	1691	1/1	0.88	0.38	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3418	1/1	0.88	0.22	54,54,54,54	0
57	MG	2A	3025	1/1	0.88	0.15	63,63,63,63	0
57	MG	2A	3245	1/1	0.88	0.29	73,73,73,73	0
57	MG	1A	3363	1/1	0.88	0.29	41,41,41,41	0
57	MG	1a	1665	1/1	0.88	0.17	65,65,65,65	0
57	MG	2A	3043	1/1	0.88	0.28	70,70,70,70	0
57	MG	1A	3199	1/1	0.88	0.15	71,71,71,71	0
57	MG	2A	3253	1/1	0.88	0.13	72,72,72,72	0
57	MG	1A	3702	1/1	0.88	0.32	67,67,67,67	0
57	MG	1A	3373	1/1	0.88	0.28	69,69,69,69	0
57	MG	2A	3487	1/1	0.88	0.19	63,63,63,63	0
57	MG	1A	3950	1/1	0.88	0.10	58,58,58,58	0
57	MG	1A	3707	1/1	0.88	0.11	67,67,67,67	0
57	MG	2A	3065	1/1	0.88	0.10	64,64,64,64	0
57	MG	2A	3508	1/1	0.88	0.19	76,76,76,76	0
57	MG	1A	3498	1/1	0.88	0.12	63,63,63,63	0
57	MG	2A	3071	1/1	0.88	0.22	60,60,60,60	0
57	MG	2A	3073	1/1	0.88	0.19	49,49,49,49	0
57	MG	2a	1726	1/1	0.88	0.12	66,66,66,66	0
57	MG	2A	3787	1/1	0.88	0.12	58,58,58,58	0
57	MG	2A	3791	1/1	0.88	0.27	71,71,71,71	0
57	MG	2a	1734	1/1	0.88	0.12	70,70,70,70	0
57	MG	1a	1692	1/1	0.88	0.23	69,69,69,69	0
57	MG	2A	3521	1/1	0.88	0.13	45,45,45,45	0
57	MG	2A	3522	1/1	0.88	0.21	69,69,69,69	0
57	MG	1B	231	1/1	0.88	0.22	63,63,63,63	0
57	MG	2A	3526	1/1	0.88	0.21	65,65,65,65	0
57	MG	1a	1697	1/1	0.88	0.11	49,49,49,49	0
57	MG	2A	3536	1/1	0.88	0.19	46,46,46,46	0
57	MG	1A	3259	1/1	0.88	0.09	40,40,40,40	0
57	MG	1E	305	1/1	0.88	0.11	28,28,28,28	0
57	MG	1E	307	1/1	0.88	0.14	67,67,67,67	0
57	MG	1A	3724	1/1	0.88	0.15	45,45,45,45	0
57	MG	1a	1720	1/1	0.88	0.15	44,44,44,44	0
57	MG	1a	1724	1/1	0.88	0.21	59,59,59,59	0
57	MG	2A	3286	1/1	0.88	0.17	61,61,61,61	0
57	MG	2A	3288	1/1	0.88	0.13	57,57,57,57	0
57	MG	2a	1782	1/1	0.88	0.22	70,70,70,70	0
57	MG	1A	3431	1/1	0.88	0.16	66,66,66,66	0
57	MG	1F	315	1/1	0.88	0.17	58,58,58,58	0
57	MG	2A	3101	1/1	0.88	0.18	50,50,50,50	0
57	MG	1A	3827	1/1	0.88	0.12	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3297	1/1	0.88	0.18	69,69,69,69	0
57	MG	1A	3282	1/1	0.88	0.17	46,46,46,46	0
57	MG	2A	3110	1/1	0.88	0.13	76,76,76,76	0
57	MG	1A	3742	1/1	0.88	0.09	35,35,35,35	0
57	MG	1A	3990	1/1	0.88	0.12	54,54,54,54	0
57	MG	2A	3304	1/1	0.88	0.27	62,62,62,62	0
57	MG	1A	3061	1/1	0.88	0.27	59,59,59,59	0
57	MG	1T	201	1/1	0.88	0.28	65,65,65,65	0
57	MG	2A	3140	1/1	0.88	0.17	73,73,73,73	0
57	MG	1T	202	1/1	0.88	0.17	54,54,54,54	0
57	MG	1A	3849	1/1	0.88	0.08	35,35,35,35	0
57	MG	2A	3317	1/1	0.88	0.07	58,58,58,58	0
57	MG	1U	210	1/1	0.88	0.12	55,55,55,55	0
57	MG	1A	3999	1/1	0.88	0.14	34,34,34,34	0
57	MG	25	103	1/1	0.88	0.18	63,63,63,63	0
57	MG	1A	3348	1/1	0.88	0.24	61,61,61,61	0
57	MG	28	104	1/1	0.88	0.31	58,58,58,58	0
57	MG	2w	103	1/1	0.88	0.15	70,70,70,70	0
57	MG	10	103	1/1	0.88	0.14	52,52,52,52	0
57	MG	2A	3161	1/1	0.88	0.10	57,57,57,57	0
57	MG	10	105	1/1	0.88	0.27	43,43,43,43	0
57	MG	1A	3294	1/1	0.88	0.13	63,63,63,63	0
57	MG	1A	3401	1/1	0.88	0.23	56,56,56,56	0
57	MG	1A	3647	1/1	0.88	0.14	24,24,24,24	0
57	MG	1A	3653	1/1	0.88	0.10	37,37,37,37	0
57	MG	2A	3058	1/1	0.89	0.34	68,68,68,68	0
57	MG	1B	201	1/1	0.89	0.15	51,51,51,51	0
57	MG	2A	3267	1/1	0.89	0.20	64,64,64,64	0
57	MG	2A	3067	1/1	0.89	0.14	51,51,51,51	0
57	MG	1B	204	1/1	0.89	0.09	44,44,44,44	0
57	MG	1A	3203	1/1	0.89	0.06	40,40,40,40	0
57	MG	2V	201	1/1	0.89	0.34	51,51,51,51	0
57	MG	1A	3082	1/1	0.89	0.09	52,52,52,52	0
57	MG	1a	1679	1/1	0.89	0.32	47,47,47,47	0
57	MG	2A	3553	1/1	0.89	0.17	61,61,61,61	0
57	MG	1a	1682	1/1	0.89	0.27	62,62,62,62	0
57	MG	1A	3219	1/1	0.89	0.28	33,33,33,33	0
57	MG	1a	1688	1/1	0.89	0.11	51,51,51,51	0
57	MG	2A	3082	1/1	0.89	0.14	78,78,78,78	0
57	MG	1A	3679	1/1	0.89	0.15	66,66,66,66	0
57	MG	1a	1694	1/1	0.89	0.36	63,63,63,63	0
57	MG	2A	3565	1/1	0.89	0.15	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1606	1/1	0.89	0.23	74,74,74,74	0
57	MG	1A	3023	1/1	0.89	0.26	55,55,55,55	0
57	MG	2A	3570	1/1	0.89	0.22	73,73,73,73	0
57	MG	1A	3934	1/1	0.89	0.09	61,61,61,61	0
57	MG	1A	3296	1/1	0.89	0.23	56,56,56,56	0
57	MG	1A	3223	1/1	0.89	0.11	57,57,57,57	0
57	MG	2A	3578	1/1	0.89	0.12	69,69,69,69	0
57	MG	2A	3579	1/1	0.89	0.16	58,58,58,58	0
57	MG	2a	1624	1/1	0.89	0.38	64,64,64,64	0
57	MG	1A	3388	1/1	0.89	0.48	70,70,70,70	0
57	MG	1A	3947	1/1	0.89	0.13	50,50,50,50	0
57	MG	1A	3151	1/1	0.89	0.23	39,39,39,39	0
57	MG	1A	3159	1/1	0.89	0.10	40,40,40,40	0
57	MG	1A	3805	1/1	0.89	0.10	51,51,51,51	0
57	MG	2A	3302	1/1	0.89	0.26	57,57,57,57	0
57	MG	2a	1634	1/1	0.89	0.19	62,62,62,62	0
57	MG	2a	1636	1/1	0.89	0.32	69,69,69,69	0
57	MG	1A	3960	1/1	0.89	0.11	65,65,65,65	0
57	MG	1a	1734	1/1	0.89	0.14	76,76,76,76	0
57	MG	1A	3468	1/1	0.89	0.17	54,54,54,54	0
57	MG	1A	3576	1/1	0.89	0.11	41,41,41,41	0
57	MG	2A	3134	1/1	0.89	0.35	63,63,63,63	0
57	MG	2A	3135	1/1	0.89	0.23	44,44,44,44	0
57	MG	2a	1644	1/1	0.89	0.27	83,83,83,83	0
57	MG	2A	3609	1/1	0.89	0.16	40,40,40,40	0
57	MG	1A	3247	1/1	0.89	0.11	42,42,42,42	0
57	MG	2A	3316	1/1	0.89	0.24	75,75,75,75	0
57	MG	1A	3584	1/1	0.89	0.18	30,30,30,30	0
57	MG	2A	3144	1/1	0.89	0.30	44,44,44,44	0
57	MG	1A	3405	1/1	0.89	0.15	62,62,62,62	0
57	MG	2A	3630	1/1	0.89	0.13	65,65,65,65	0
57	MG	1a	1760	1/1	0.89	0.13	49,49,49,49	0
57	MG	2A	3329	1/1	0.89	0.19	43,43,43,43	0
57	MG	2A	3153	1/1	0.89	0.14	48,48,48,48	0
57	MG	2A	3635	1/1	0.89	0.15	68,68,68,68	0
57	MG	1A	3723	1/1	0.89	0.13	26,26,26,26	0
57	MG	2a	1675	1/1	0.89	0.22	53,53,53,53	0
57	MG	1A	3982	1/1	0.89	0.10	55,55,55,55	0
57	MG	1S	201	1/1	0.89	0.18	44,44,44,44	0
57	MG	2a	1683	1/1	0.89	0.14	75,75,75,75	0
57	MG	1A	3985	1/1	0.89	0.17	57,57,57,57	0
57	MG	2A	3648	1/1	0.89	0.10	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3652	1/1	0.89	0.18	54,54,54,54	0
57	MG	2A	3345	1/1	0.89	0.26	56,56,56,56	0
57	MG	1A	3829	1/1	0.89	0.08	37,37,37,37	0
57	MG	1A	3478	1/1	0.89	0.20	74,74,74,74	0
57	MG	1A	3601	1/1	0.89	0.14	70,70,70,70	0
57	MG	2A	3352	1/1	0.89	0.25	63,63,63,63	0
57	MG	1A	3996	1/1	0.89	0.09	53,53,53,53	0
57	MG	1A	3248	1/1	0.89	0.08	32,32,32,32	0
57	MG	2A	3173	1/1	0.89	0.10	70,70,70,70	0
57	MG	1A	3484	1/1	0.89	0.30	44,44,44,44	0
57	MG	1A	4011	1/1	0.89	0.12	51,51,51,51	0
57	MG	10	107	1/1	0.89	0.12	54,54,54,54	0
57	MG	2A	3364	1/1	0.89	0.15	54,54,54,54	0
57	MG	1A	3852	1/1	0.89	0.11	23,23,23,23	0
57	MG	2A	3380	1/1	0.89	0.20	58,58,58,58	0
57	MG	1A	3853	1/1	0.89	0.12	77,77,77,77	0
57	MG	2a	1716	1/1	0.89	0.27	63,63,63,63	0
57	MG	2A	3713	1/1	0.89	0.11	50,50,50,50	0
57	MG	2A	3385	1/1	0.89	0.30	73,73,73,73	0
57	MG	2A	3193	1/1	0.89	0.23	55,55,55,55	0
57	MG	11	102	1/1	0.89	0.17	60,60,60,60	0
57	MG	1A	3097	1/1	0.89	0.10	37,37,37,37	0
57	MG	2A	3198	1/1	0.89	0.14	69,69,69,69	0
57	MG	2A	3403	1/1	0.89	0.24	56,56,56,56	0
57	MG	1A	3257	1/1	0.89	0.26	58,58,58,58	0
57	MG	1A	3058	1/1	0.89	0.26	54,54,54,54	0
57	MG	2A	3209	1/1	0.89	0.16	47,47,47,47	0
57	MG	2a	1739	1/1	0.89	0.11	69,69,69,69	0
57	MG	2a	1748	1/1	0.89	0.14	78,78,78,78	0
57	MG	2A	3414	1/1	0.89	0.22	62,62,62,62	0
57	MG	1A	3861	1/1	0.89	0.21	37,37,37,37	0
57	MG	2A	3418	1/1	0.89	0.13	28,28,28,28	0
57	MG	2A	3759	1/1	0.89	0.16	64,64,64,64	0
57	MG	1A	4037	1/1	0.89	0.14	58,58,58,58	0
57	MG	1A	4038	1/1	0.89	0.12	62,62,62,62	0
57	MG	1A	3196	1/1	0.89	0.19	53,53,53,53	0
57	MG	1A	3872	1/1	0.89	0.11	41,41,41,41	0
57	MG	2a	1764	1/1	0.89	0.21	66,66,66,66	0
57	MG	2a	1765	1/1	0.89	0.13	67,67,67,67	0
57	MG	2A	3428	1/1	0.89	0.10	45,45,45,45	0
57	MG	2A	3430	1/1	0.89	0.09	39,39,39,39	0
57	MG	1a	1604	1/1	0.89	0.15	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1775	1/1	0.89	0.26	78,78,78,78	0
57	MG	1A	3879	1/1	0.89	0.10	68,68,68,68	0
57	MG	1A	3759	1/1	0.89	0.10	55,55,55,55	0
57	MG	2A	3449	1/1	0.89	0.10	49,49,49,49	0
57	MG	1A	4047	1/1	0.89	0.18	55,55,55,55	0
57	MG	1A	4051	1/1	0.89	0.23	57,57,57,57	0
57	MG	1a	1626	1/1	0.89	0.31	59,59,59,59	0
57	MG	1A	3885	1/1	0.89	0.09	43,43,43,43	0
57	MG	2A	3470	1/1	0.89	0.10	39,39,39,39	0
57	MG	1a	1634	1/1	0.89	0.25	74,74,74,74	0
57	MG	1x	113	1/1	0.89	0.24	62,62,62,62	0
57	MG	1A	3338	1/1	0.89	0.32	48,48,48,48	0
57	MG	1A	3897	1/1	0.89	0.09	18,18,18,18	0
57	MG	1A	3347	1/1	0.89	0.10	47,47,47,47	0
57	MG	1A	3424	1/1	0.89	0.23	60,60,60,60	0
57	MG	2A	3026	1/1	0.89	0.14	43,43,43,43	0
57	MG	1A	3198	1/1	0.89	0.19	59,59,59,59	0
57	MG	1a	1651	1/1	0.89	0.16	54,54,54,54	0
57	MG	2A	3495	1/1	0.89	0.23	63,63,63,63	0
57	MG	1A	4084	1/1	0.89	0.18	73,73,73,73	0
57	MG	2A	3502	1/1	0.89	0.13	67,67,67,67	0
57	MG	2A	3503	1/1	0.89	0.08	40,40,40,40	0
57	MG	2j	201	1/1	0.89	0.14	74,74,74,74	0
57	MG	1A	3774	1/1	0.89	0.23	32,32,32,32	0
57	MG	1A	3124	1/1	0.89	0.14	37,37,37,37	0
57	MG	2A	3514	1/1	0.89	0.12	65,65,65,65	0
57	MG	2B	218	1/1	0.89	0.33	78,78,78,78	0
57	MG	1A	4088	1/1	0.89	0.22	75,75,75,75	0
57	MG	2w	102	1/1	0.89	0.15	84,84,84,84	0
57	MG	2A	3050	1/1	0.89	0.28	65,65,65,65	0
57	MG	2w	104	1/1	0.89	0.11	87,87,87,87	0
57	MG	2D	308	1/1	0.89	0.16	59,59,59,59	0
57	MG	2A	3257	1/1	0.89	0.10	68,68,68,68	0
57	MG	2E	304	1/1	0.89	0.13	34,34,34,34	0
57	MG	2E	306	1/1	0.89	0.14	54,54,54,54	0
57	MG	2x	107	1/1	0.89	0.18	64,64,64,64	0
57	MG	2A	3259	1/1	0.89	0.17	65,65,65,65	0
57	MG	1A	3916	1/1	0.89	0.07	23,23,23,23	0
57	MG	1A	3666	1/1	0.89	0.12	43,43,43,43	0
57	MG	1A	3179	1/1	0.90	0.15	38,38,38,38	0
57	MG	1A	3656	1/1	0.90	0.08	31,31,31,31	0
57	MG	29	101	1/1	0.90	0.13	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3523	1/1	0.90	0.34	42,42,42,42	0
57	MG	1Q	207	1/1	0.90	0.11	49,49,49,49	0
57	MG	2a	1605	1/1	0.90	0.23	69,69,69,69	0
57	MG	2A	3358	1/1	0.90	0.22	52,52,52,52	0
57	MG	1A	3786	1/1	0.90	0.21	47,47,47,47	0
57	MG	1a	1690	1/1	0.90	0.23	69,69,69,69	0
57	MG	2A	3222	1/1	0.90	0.12	62,62,62,62	0
57	MG	2a	1612	1/1	0.90	0.17	60,60,60,60	0
57	MG	1A	4033	1/1	0.90	0.22	60,60,60,60	0
57	MG	1A	3293	1/1	0.90	0.19	57,57,57,57	0
57	MG	2a	1618	1/1	0.90	0.29	71,71,71,71	0
57	MG	2A	3368	1/1	0.90	0.33	57,57,57,57	0
57	MG	2A	3374	1/1	0.90	0.10	40,40,40,40	0
57	MG	2A	3379	1/1	0.90	0.29	58,58,58,58	0
57	MG	2A	3226	1/1	0.90	0.19	59,59,59,59	0
57	MG	1S	203	1/1	0.90	0.22	67,67,67,67	0
57	MG	1A	3668	1/1	0.90	0.15	61,61,61,61	0
57	MG	2a	1630	1/1	0.90	0.19	68,68,68,68	0
57	MG	1A	3914	1/1	0.90	0.10	32,32,32,32	0
57	MG	1A	3368	1/1	0.90	0.10	43,43,43,43	0
57	MG	2A	3398	1/1	0.90	0.39	62,62,62,62	0
57	MG	1A	3430	1/1	0.90	0.14	69,69,69,69	0
57	MG	2A	3059	1/1	0.90	0.22	55,55,55,55	0
57	MG	2A	3640	1/1	0.90	0.16	68,68,68,68	0
57	MG	2A	3642	1/1	0.90	0.09	69,69,69,69	0
57	MG	1A	3018	1/1	0.90	0.31	50,50,50,50	0
57	MG	1A	3295	1/1	0.90	0.33	63,63,63,63	0
57	MG	2A	3647	1/1	0.90	0.12	54,54,54,54	0
57	MG	2A	3239	1/1	0.90	0.16	55,55,55,55	0
57	MG	2A	3408	1/1	0.90	0.12	65,65,65,65	0
57	MG	2A	3410	1/1	0.90	0.10	76,76,76,76	0
57	MG	2a	1648	1/1	0.90	0.09	66,66,66,66	0
57	MG	2a	1649	1/1	0.90	0.32	67,67,67,67	0
57	MG	2A	3242	1/1	0.90	0.16	66,66,66,66	0
57	MG	2A	3413	1/1	0.90	0.12	38,38,38,38	0
57	MG	2A	3659	1/1	0.90	0.16	69,69,69,69	0
57	MG	1A	4050	1/1	0.90	0.12	61,61,61,61	0
57	MG	1A	3433	1/1	0.90	0.16	47,47,47,47	0
57	MG	1A	4059	1/1	0.90	0.18	61,61,61,61	0
57	MG	1a	1732	1/1	0.90	0.08	53,53,53,53	0
57	MG	1A	3242	1/1	0.90	0.22	57,57,57,57	0
57	MG	2A	3424	1/1	0.90	0.14	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1737	1/1	0.90	0.11	56,56,56,56	0
57	MG	1A	3243	1/1	0.90	0.17	41,41,41,41	0
57	MG	1A	3193	1/1	0.90	0.09	47,47,47,47	0
57	MG	1A	3550	1/1	0.90	0.12	52,52,52,52	0
57	MG	1A	3381	1/1	0.90	0.12	57,57,57,57	0
57	MG	2a	1680	1/1	0.90	0.21	66,66,66,66	0
57	MG	2A	3709	1/1	0.90	0.10	36,36,36,36	0
57	MG	2A	3439	1/1	0.90	0.27	68,68,68,68	0
57	MG	2A	3086	1/1	0.90	0.12	44,44,44,44	0
57	MG	2A	3717	1/1	0.90	0.12	64,64,64,64	0
57	MG	1a	1745	1/1	0.90	0.20	74,74,74,74	0
57	MG	2A	3091	1/1	0.90	0.30	70,70,70,70	0
57	MG	2A	3261	1/1	0.90	0.13	56,56,56,56	0
57	MG	1a	1748	1/1	0.90	0.14	71,71,71,71	0
57	MG	2A	3731	1/1	0.90	0.10	59,59,59,59	0
57	MG	1a	1752	1/1	0.90	0.09	63,63,63,63	0
57	MG	2A	3463	1/1	0.90	0.20	53,53,53,53	0
57	MG	2A	3737	1/1	0.90	0.14	48,48,48,48	0
57	MG	1A	3815	1/1	0.90	0.13	57,57,57,57	0
57	MG	2A	3739	1/1	0.90	0.10	52,52,52,52	0
57	MG	2A	3266	1/1	0.90	0.14	69,69,69,69	0
57	MG	2A	3743	1/1	0.90	0.21	70,70,70,70	0
57	MG	2A	3748	1/1	0.90	0.19	68,68,68,68	0
57	MG	2A	3473	1/1	0.90	0.22	54,54,54,54	0
57	MG	1A	3088	1/1	0.90	0.22	53,53,53,53	0
57	MG	2A	3100	1/1	0.90	0.23	70,70,70,70	0
57	MG	1A	3459	1/1	0.90	0.08	52,52,52,52	0
57	MG	1A	3461	1/1	0.90	0.12	62,62,62,62	0
57	MG	15	104	1/1	0.90	0.25	40,40,40,40	0
57	MG	1A	3089	1/1	0.90	0.08	76,76,76,76	0
57	MG	2A	3764	1/1	0.90	0.11	73,73,73,73	0
57	MG	2A	3765	1/1	0.90	0.09	63,63,63,63	0
57	MG	17	104	1/1	0.90	0.10	51,51,51,51	0
57	MG	1A	4089	1/1	0.90	0.13	58,58,58,58	0
57	MG	1a	1603	1/1	0.90	0.20	59,59,59,59	0
57	MG	2A	3771	1/1	0.90	0.28	61,61,61,61	0
57	MG	1A	4092	1/1	0.90	0.10	72,72,72,72	0
57	MG	1A	3309	1/1	0.90	0.18	58,58,58,58	0
57	MG	2A	3501	1/1	0.90	0.20	63,63,63,63	0
57	MG	1A	3830	1/1	0.90	0.18	45,45,45,45	0
57	MG	1A	3400	1/1	0.90	0.14	46,46,46,46	0
57	MG	2A	3506	1/1	0.90	0.19	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3840	1/1	0.90	0.09	48,48,48,48	0
57	MG	1a	1623	1/1	0.90	0.28	58,58,58,58	0
57	MG	2A	3513	1/1	0.90	0.19	76,76,76,76	0
57	MG	2A	3292	1/1	0.90	0.12	58,58,58,58	0
57	MG	2A	3792	1/1	0.90	0.09	77,77,77,77	0
57	MG	2A	3515	1/1	0.90	0.09	34,34,34,34	0
57	MG	1a	1625	1/1	0.90	0.27	52,52,52,52	0
57	MG	2a	1769	1/1	0.90	0.21	64,64,64,64	0
57	MG	1A	3966	1/1	0.90	0.13	40,40,40,40	0
57	MG	2A	3296	1/1	0.90	0.25	75,75,75,75	0
57	MG	2a	1772	1/1	0.90	0.20	62,62,62,62	0
57	MG	1A	3591	1/1	0.90	0.17	54,54,54,54	0
57	MG	1A	3025	1/1	0.90	0.15	55,55,55,55	0
57	MG	1A	3152	1/1	0.90	0.12	42,42,42,42	0
57	MG	1A	3319	1/1	0.90	0.23	67,67,67,67	0
57	MG	1A	3213	1/1	0.90	0.29	45,45,45,45	0
57	MG	2A	3530	1/1	0.90	0.16	39,39,39,39	0
57	MG	2A	3531	1/1	0.90	0.12	64,64,64,64	0
57	MG	1a	1642	1/1	0.90	0.31	64,64,64,64	0
57	MG	2A	3538	1/1	0.90	0.08	41,41,41,41	0
57	MG	1p	101	1/1	0.90	0.13	63,63,63,63	0
57	MG	1A	3158	1/1	0.90	0.23	62,62,62,62	0
57	MG	1A	3049	1/1	0.90	0.17	32,32,32,32	0
57	MG	1A	3278	1/1	0.90	0.09	53,53,53,53	0
57	MG	2a	1804	1/1	0.90	0.25	65,65,65,65	0
57	MG	2D	302	1/1	0.90	0.23	66,66,66,66	0
57	MG	2a	1807	1/1	0.90	0.17	69,69,69,69	0
57	MG	2A	3549	1/1	0.90	0.11	53,53,53,53	0
57	MG	1B	229	1/1	0.90	0.10	75,75,75,75	0
57	MG	2A	3174	1/1	0.90	0.21	60,60,60,60	0
57	MG	2A	3554	1/1	0.90	0.21	63,63,63,63	0
57	MG	1a	1658	1/1	0.90	0.23	65,65,65,65	0
57	MG	2a	1818	1/1	0.90	0.11	72,72,72,72	0
57	MG	1A	3859	1/1	0.90	0.14	50,50,50,50	0
57	MG	2A	3319	1/1	0.90	0.10	73,73,73,73	0
57	MG	2A	3180	1/1	0.90	0.15	60,60,60,60	0
57	MG	2F	305	1/1	0.90	0.10	63,63,63,63	0
57	MG	1A	3165	1/1	0.90	0.29	45,45,45,45	0
57	MG	2A	3322	1/1	0.90	0.09	57,57,57,57	0
57	MG	1A	3494	1/1	0.90	0.32	69,69,69,69	0
57	MG	1A	3422	1/1	0.90	0.17	48,48,48,48	0
57	MG	2A	3190	1/1	0.90	0.16	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1E	309	1/1	0.90	0.10	51,51,51,51	0
57	MG	1x	112	1/1	0.90	0.14	72,72,72,72	0
57	MG	1A	3646	1/1	0.90	0.14	34,34,34,34	0
57	MG	1A	3056	1/1	0.90	0.11	37,37,37,37	0
57	MG	2A	3013	1/1	0.90	0.43	78,78,78,78	0
57	MG	2A	3200	1/1	0.90	0.26	60,60,60,60	0
57	MG	2A	3017	1/1	0.90	0.16	61,61,61,61	0
57	MG	2I	102	1/1	0.90	0.21	68,68,68,68	0
57	MG	2A	3349	1/1	0.90	0.21	54,54,54,54	0
57	MG	1A	3511	1/1	0.90	0.36	58,58,58,58	0
57	MG	25	104	1/1	0.90	0.13	57,57,57,57	0
57	MG	1A	3825	1/1	0.91	0.09	38,38,38,38	0
57	MG	1A	4008	1/1	0.91	0.07	18,18,18,18	0
57	MG	2D	305	1/1	0.91	0.30	52,52,52,52	0
57	MG	1A	4009	1/1	0.91	0.19	56,56,56,56	0
57	MG	2A	3240	1/1	0.91	0.13	63,63,63,63	0
57	MG	2A	3504	1/1	0.91	0.29	72,72,72,72	0
57	MG	1A	4010	1/1	0.91	0.10	58,58,58,58	0
57	MG	2A	3507	1/1	0.91	0.09	61,61,61,61	0
57	MG	2E	307	1/1	0.91	0.12	45,45,45,45	0
57	MG	2A	3243	1/1	0.91	0.15	77,77,77,77	0
57	MG	1A	3283	1/1	0.91	0.08	50,50,50,50	0
57	MG	1A	3675	1/1	0.91	0.23	49,49,49,49	0
57	MG	1A	3364	1/1	0.91	0.19	34,34,34,34	0
57	MG	1A	3529	1/1	0.91	0.17	56,56,56,56	0
57	MG	1A	4024	1/1	0.91	0.10	22,22,22,22	0
57	MG	2A	3517	1/1	0.91	0.15	51,51,51,51	0
57	MG	1A	3367	1/1	0.91	0.08	47,47,47,47	0
57	MG	1A	3238	1/1	0.91	0.17	41,41,41,41	0
57	MG	2T	201	1/1	0.91	0.14	70,70,70,70	0
57	MG	2T	202	1/1	0.91	0.26	64,64,64,64	0
57	MG	1x	103	1/1	0.91	0.19	55,55,55,55	0
57	MG	15	101	1/1	0.91	0.18	39,39,39,39	0
57	MG	1x	106	1/1	0.91	0.27	61,61,61,61	0
57	MG	1A	3371	1/1	0.91	0.11	54,54,54,54	0
57	MG	2A	3258	1/1	0.91	0.10	51,51,51,51	0
57	MG	1A	3848	1/1	0.91	0.07	22,22,22,22	0
57	MG	1A	4035	1/1	0.91	0.27	58,58,58,58	0
57	MG	1A	3439	1/1	0.91	0.14	46,46,46,46	0
57	MG	1a	1601	1/1	0.91	0.24	55,55,55,55	0
57	MG	2A	3539	1/1	0.91	0.15	47,47,47,47	0
57	MG	28	101	1/1	0.91	0.23	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1602	1/1	0.91	0.25	71,71,71,71	0
57	MG	2A	3007	1/1	0.91	0.13	59,59,59,59	0
57	MG	1A	3442	1/1	0.91	0.10	57,57,57,57	0
57	MG	1A	3545	1/1	0.91	0.41	61,61,61,61	0
57	MG	2A	3268	1/1	0.91	0.08	44,44,44,44	0
57	MG	1A	3444	1/1	0.91	0.10	57,57,57,57	0
57	MG	1A	3019	1/1	0.91	0.22	48,48,48,48	0
57	MG	1a	1614	1/1	0.91	0.30	56,56,56,56	0
57	MG	2a	1609	1/1	0.91	0.22	71,71,71,71	0
57	MG	1A	3084	1/1	0.91	0.25	45,45,45,45	0
57	MG	1A	3552	1/1	0.91	0.14	42,42,42,42	0
57	MG	1A	3711	1/1	0.91	0.07	27,27,27,27	0
57	MG	2A	3039	1/1	0.91	0.13	56,56,56,56	0
57	MG	1a	1624	1/1	0.91	0.07	46,46,46,46	0
57	MG	1A	3718	1/1	0.91	0.09	20,20,20,20	0
57	MG	1A	3868	1/1	0.91	0.28	33,33,33,33	0
57	MG	2A	3567	1/1	0.91	0.10	59,59,59,59	0
57	MG	1A	3106	1/1	0.91	0.21	40,40,40,40	0
57	MG	1A	3876	1/1	0.91	0.10	61,61,61,61	0
57	MG	1a	1636	1/1	0.91	0.29	57,57,57,57	0
57	MG	1A	4066	1/1	0.91	0.11	52,52,52,52	0
57	MG	1A	3454	1/1	0.91	0.16	36,36,36,36	0
57	MG	1A	4072	1/1	0.91	0.15	57,57,57,57	0
57	MG	2A	3062	1/1	0.91	0.13	55,55,55,55	0
57	MG	2A	3295	1/1	0.91	0.23	70,70,70,70	0
57	MG	1A	4073	1/1	0.91	0.12	66,66,66,66	0
57	MG	2A	3066	1/1	0.91	0.19	68,68,68,68	0
57	MG	1a	1646	1/1	0.91	0.09	54,54,54,54	0
57	MG	1A	3245	1/1	0.91	0.17	77,77,77,77	0
57	MG	1A	3246	1/1	0.91	0.20	28,28,28,28	0
57	MG	1A	3561	1/1	0.91	0.12	39,39,39,39	0
57	MG	1a	1652	1/1	0.91	0.08	45,45,45,45	0
57	MG	1A	3565	1/1	0.91	0.08	23,23,23,23	0
57	MG	1A	3568	1/1	0.91	0.11	50,50,50,50	0
57	MG	1A	3899	1/1	0.91	0.12	66,66,66,66	0
57	MG	1a	1660	1/1	0.91	0.15	60,60,60,60	0
57	MG	1A	3900	1/1	0.91	0.14	65,65,65,65	0
57	MG	1A	3748	1/1	0.91	0.14	51,51,51,51	0
57	MG	1a	1663	1/1	0.91	0.22	68,68,68,68	0
57	MG	2A	3614	1/1	0.91	0.13	63,63,63,63	0
57	MG	1A	3570	1/1	0.91	0.18	50,50,50,50	0
57	MG	1A	3908	1/1	0.91	0.10	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1663	1/1	0.91	0.19	67,67,67,67	0
57	MG	2A	3620	1/1	0.91	0.24	71,71,71,71	0
57	MG	2A	3626	1/1	0.91	0.15	62,62,62,62	0
57	MG	1A	3162	1/1	0.91	0.17	42,42,42,42	0
57	MG	1A	4099	1/1	0.91	0.26	53,53,53,53	0
57	MG	1A	3463	1/1	0.91	0.14	55,55,55,55	0
57	MG	1B	203	1/1	0.91	0.34	66,66,66,66	0
57	MG	2A	3326	1/1	0.91	0.18	63,63,63,63	0
57	MG	2A	3328	1/1	0.91	0.20	61,61,61,61	0
57	MG	1a	1678	1/1	0.91	0.32	54,54,54,54	0
57	MG	1A	3204	1/1	0.91	0.14	53,53,53,53	0
57	MG	1A	3589	1/1	0.91	0.10	32,32,32,32	0
57	MG	1A	3251	1/1	0.91	0.20	64,64,64,64	0
57	MG	2A	3643	1/1	0.91	0.10	71,71,71,71	0
57	MG	1a	1686	1/1	0.91	0.29	62,62,62,62	0
57	MG	1A	3769	1/1	0.91	0.08	57,57,57,57	0
57	MG	2A	3114	1/1	0.91	0.07	62,62,62,62	0
57	MG	1A	3210	1/1	0.91	0.11	49,49,49,49	0
57	MG	2a	1692	1/1	0.91	0.13	73,73,73,73	0
57	MG	1B	218	1/1	0.91	0.16	46,46,46,46	0
57	MG	1A	3472	1/1	0.91	0.31	35,35,35,35	0
57	MG	2A	3128	1/1	0.91	0.20	56,56,56,56	0
57	MG	2A	3131	1/1	0.91	0.18	53,53,53,53	0
57	MG	2a	1699	1/1	0.91	0.16	57,57,57,57	0
57	MG	1A	3474	1/1	0.91	0.12	54,54,54,54	0
57	MG	1A	3776	1/1	0.91	0.08	46,46,46,46	0
57	MG	1a	1698	1/1	0.91	0.29	63,63,63,63	0
57	MG	2A	3671	1/1	0.91	0.09	73,73,73,73	0
57	MG	2A	3357	1/1	0.91	0.15	58,58,58,58	0
57	MG	2A	3676	1/1	0.91	0.09	61,61,61,61	0
57	MG	1A	3933	1/1	0.91	0.09	66,66,66,66	0
57	MG	2a	1713	1/1	0.91	0.33	68,68,68,68	0
57	MG	2A	3679	1/1	0.91	0.09	71,71,71,71	0
57	MG	1A	3163	1/1	0.91	0.25	59,59,59,59	0
57	MG	2a	1717	1/1	0.91	0.30	75,75,75,75	0
57	MG	2A	3146	1/1	0.91	0.16	66,66,66,66	0
57	MG	2a	1719	1/1	0.91	0.15	69,69,69,69	0
57	MG	1A	3617	1/1	0.91	0.09	25,25,25,25	0
57	MG	1a	1718	1/1	0.91	0.08	55,55,55,55	0
57	MG	2A	3365	1/1	0.91	0.12	69,69,69,69	0
57	MG	2A	3697	1/1	0.91	0.08	72,72,72,72	0
57	MG	1A	3085	1/1	0.91	0.17	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3155	1/1	0.91	0.10	67,67,67,67	0
57	MG	2a	1728	1/1	0.91	0.12	64,64,64,64	0
57	MG	2A	3707	1/1	0.91	0.11	51,51,51,51	0
57	MG	2A	3369	1/1	0.91	0.15	70,70,70,70	0
57	MG	1B	232	1/1	0.91	0.18	68,68,68,68	0
57	MG	2A	3157	1/1	0.91	0.15	76,76,76,76	0
57	MG	2a	1740	1/1	0.91	0.11	56,56,56,56	0
57	MG	2a	1747	1/1	0.91	0.12	72,72,72,72	0
57	MG	1B	233	1/1	0.91	0.15	61,61,61,61	0
57	MG	1A	3125	1/1	0.91	0.09	64,64,64,64	0
57	MG	2A	3722	1/1	0.91	0.20	61,61,61,61	0
57	MG	2A	3160	1/1	0.91	0.14	63,63,63,63	0
57	MG	2A	3386	1/1	0.91	0.16	56,56,56,56	0
57	MG	2a	1757	1/1	0.91	0.27	69,69,69,69	0
57	MG	2a	1758	1/1	0.91	0.12	67,67,67,67	0
57	MG	1E	302	1/1	0.91	0.19	36,36,36,36	0
57	MG	2A	3163	1/1	0.91	0.09	47,47,47,47	0
57	MG	2A	3394	1/1	0.91	0.19	57,57,57,57	0
57	MG	1A	3621	1/1	0.91	0.09	38,38,38,38	0
57	MG	1A	3220	1/1	0.91	0.12	51,51,51,51	0
57	MG	1A	3481	1/1	0.91	0.21	56,56,56,56	0
57	MG	1A	3326	1/1	0.91	0.29	62,62,62,62	0
57	MG	2A	3168	1/1	0.91	0.11	49,49,49,49	0
57	MG	1a	1739	1/1	0.91	0.15	67,67,67,67	0
57	MG	1A	3271	1/1	0.91	0.41	40,40,40,40	0
57	MG	1F	314	1/1	0.91	0.13	55,55,55,55	0
57	MG	2a	1773	1/1	0.91	0.14	68,68,68,68	0
57	MG	1A	3798	1/1	0.91	0.20	51,51,51,51	0
57	MG	1G	203	1/1	0.91	0.16	68,68,68,68	0
57	MG	2A	3756	1/1	0.91	0.19	48,48,48,48	0
57	MG	1a	1747	1/1	0.91	0.10	59,59,59,59	0
57	MG	1I	201	1/1	0.91	0.10	65,65,65,65	0
57	MG	2A	3417	1/1	0.91	0.17	63,63,63,63	0
57	MG	1A	3331	1/1	0.91	0.12	56,56,56,56	0
57	MG	2a	1785	1/1	0.91	0.28	66,66,66,66	0
57	MG	2a	1787	1/1	0.91	0.12	67,67,67,67	0
57	MG	2A	3184	1/1	0.91	0.27	66,66,66,66	0
57	MG	1A	3276	1/1	0.91	0.15	45,45,45,45	0
57	MG	1A	3026	1/1	0.91	0.34	65,65,65,65	0
57	MG	1P	205	1/1	0.91	0.14	41,41,41,41	0
57	MG	2A	3194	1/1	0.91	0.13	59,59,59,59	0
57	MG	2a	1794	1/1	0.91	0.19	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1795	1/1	0.91	0.31	72,72,72,72	0
57	MG	1a	1763	1/1	0.91	0.16	64,64,64,64	0
57	MG	2a	1800	1/1	0.91	0.17	56,56,56,56	0
57	MG	2a	1801	1/1	0.91	0.13	83,83,83,83	0
57	MG	1A	3495	1/1	0.91	0.10	59,59,59,59	0
57	MG	1A	3977	1/1	0.91	0.14	56,56,56,56	0
57	MG	1a	1772	1/1	0.91	0.09	77,77,77,77	0
57	MG	1a	1778	1/1	0.91	0.09	78,78,78,78	0
57	MG	2A	3444	1/1	0.91	0.25	70,70,70,70	0
57	MG	1A	3340	1/1	0.91	0.13	49,49,49,49	0
57	MG	2A	3207	1/1	0.91	0.32	56,56,56,56	0
57	MG	2a	1814	1/1	0.91	0.11	60,60,60,60	0
57	MG	1a	1780	1/1	0.91	0.09	64,64,64,64	0
57	MG	1a	1789	1/1	0.91	0.30	60,60,60,60	0
57	MG	2A	3788	1/1	0.91	0.12	64,64,64,64	0
57	MG	2e	201	1/1	0.91	0.07	73,73,73,73	0
57	MG	2f	201	1/1	0.91	0.14	49,49,49,49	0
57	MG	1A	3345	1/1	0.91	0.10	43,43,43,43	0
57	MG	1A	3808	1/1	0.91	0.09	22,22,22,22	0
57	MG	2A	3464	1/1	0.91	0.16	59,59,59,59	0
57	MG	1A	3663	1/1	0.91	0.11	28,28,28,28	0
57	MG	1A	3814	1/1	0.91	0.09	41,41,41,41	0
57	MG	1T	203	1/1	0.91	0.14	62,62,62,62	0
57	MG	1a	1799	1/1	0.91	0.13	73,73,73,73	0
57	MG	1U	202	1/1	0.91	0.12	36,36,36,36	0
57	MG	2v	103	1/1	0.91	0.20	60,60,60,60	0
57	MG	2v	104	1/1	0.91	0.20	62,62,62,62	0
57	MG	1U	205	1/1	0.91	0.14	36,36,36,36	0
57	MG	2A	3481	1/1	0.91	0.14	52,52,52,52	0
57	MG	1A	3064	1/1	0.91	0.15	48,48,48,48	0
57	MG	1A	3992	1/1	0.91	0.13	53,53,53,53	0
57	MG	2x	101	1/1	0.91	0.18	68,68,68,68	0
57	MG	2A	3484	1/1	0.91	0.10	32,32,32,32	0
57	MG	2x	103	1/1	0.91	0.13	65,65,65,65	0
57	MG	1A	3667	1/1	0.91	0.14	57,57,57,57	0
57	MG	2A	3486	1/1	0.91	0.18	60,60,60,60	0
57	MG	1W	201	1/1	0.91	0.24	49,49,49,49	0
57	MG	1A	3235	1/1	0.91	0.24	71,71,71,71	0
57	MG	1A	3001	1/1	0.91	0.07	43,43,43,43	0
57	MG	1a	1811	1/1	0.91	0.18	61,61,61,61	0
57	MG	2A	3064	1/1	0.92	0.09	49,49,49,49	0
57	MG	2A	3276	1/1	0.92	0.09	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3118	1/1	0.92	0.23	52,52,52,52	0
57	MG	1A	3184	1/1	0.92	0.13	30,30,30,30	0
57	MG	1A	3493	1/1	0.92	0.25	49,49,49,49	0
57	MG	2P	201	1/1	0.92	0.08	63,63,63,63	0
57	MG	1A	3832	1/1	0.92	0.12	37,37,37,37	0
57	MG	1A	3321	1/1	0.92	0.12	41,41,41,41	0
57	MG	1A	3218	1/1	0.92	0.20	36,36,36,36	0
57	MG	2A	3537	1/1	0.92	0.20	52,52,52,52	0
57	MG	2A	3284	1/1	0.92	0.11	66,66,66,66	0
57	MG	1F	305	1/1	0.92	0.10	60,60,60,60	0
57	MG	2A	3541	1/1	0.92	0.22	63,63,63,63	0
57	MG	1a	1691	1/1	0.92	0.18	56,56,56,56	0
57	MG	1A	3991	1/1	0.92	0.07	56,56,56,56	0
57	MG	2A	3290	1/1	0.92	0.07	64,64,64,64	0
57	MG	1A	3598	1/1	0.92	0.07	19,19,19,19	0
57	MG	1G	202	1/1	0.92	0.32	67,67,67,67	0
57	MG	2A	3550	1/1	0.92	0.15	68,68,68,68	0
57	MG	25	102	1/1	0.92	0.20	45,45,45,45	0
57	MG	2A	3551	1/1	0.92	0.13	40,40,40,40	0
57	MG	1A	3123	1/1	0.92	0.22	52,52,52,52	0
57	MG	1H	201	1/1	0.92	0.18	48,48,48,48	0
57	MG	1a	1700	1/1	0.92	0.19	50,50,50,50	0
57	MG	28	103	1/1	0.92	0.10	57,57,57,57	0
57	MG	2A	3087	1/1	0.92	0.24	69,69,69,69	0
57	MG	2A	3558	1/1	0.92	0.12	46,46,46,46	0
57	MG	1a	1703	1/1	0.92	0.32	53,53,53,53	0
57	MG	1A	3380	1/1	0.92	0.14	68,68,68,68	0
57	MG	2a	1603	1/1	0.92	0.21	58,58,58,58	0
57	MG	1a	1710	1/1	0.92	0.10	57,57,57,57	0
57	MG	1N	204	1/1	0.92	0.19	44,44,44,44	0
57	MG	1A	3736	1/1	0.92	0.11	33,33,33,33	0
57	MG	2A	3097	1/1	0.92	0.31	50,50,50,50	0
57	MG	2A	3566	1/1	0.92	0.08	33,33,33,33	0
57	MG	1A	3739	1/1	0.92	0.09	27,27,27,27	0
57	MG	1O	205	1/1	0.92	0.09	48,48,48,48	0
57	MG	2a	1613	1/1	0.92	0.20	53,53,53,53	0
57	MG	1A	4007	1/1	0.92	0.17	77,77,77,77	0
57	MG	2a	1616	1/1	0.92	0.19	79,79,79,79	0
57	MG	1a	1723	1/1	0.92	0.14	58,58,58,58	0
57	MG	1A	3740	1/1	0.92	0.06	71,71,71,71	0
57	MG	2A	3313	1/1	0.92	0.10	63,63,63,63	0
57	MG	2A	3314	1/1	0.92	0.43	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1623	1/1	0.92	0.09	63,63,63,63	0
57	MG	1Q	204	1/1	0.92	0.13	54,54,54,54	0
57	MG	1A	3507	1/1	0.92	0.32	53,53,53,53	0
57	MG	1a	1731	1/1	0.92	0.15	57,57,57,57	0
57	MG	2A	3318	1/1	0.92	0.12	61,61,61,61	0
57	MG	2A	3116	1/1	0.92	0.17	65,65,65,65	0
57	MG	1A	3746	1/1	0.92	0.08	16,16,16,16	0
57	MG	2A	3591	1/1	0.92	0.08	66,66,66,66	0
57	MG	1A	3608	1/1	0.92	0.10	44,44,44,44	0
57	MG	2A	3596	1/1	0.92	0.13	56,56,56,56	0
57	MG	2a	1635	1/1	0.92	0.21	69,69,69,69	0
57	MG	1A	3509	1/1	0.92	0.17	35,35,35,35	0
57	MG	2A	3598	1/1	0.92	0.12	61,61,61,61	0
57	MG	2A	3323	1/1	0.92	0.11	67,67,67,67	0
57	MG	2A	3324	1/1	0.92	0.28	55,55,55,55	0
57	MG	1A	4013	1/1	0.92	0.18	41,41,41,41	0
57	MG	1A	3754	1/1	0.92	0.08	19,19,19,19	0
57	MG	1A	4020	1/1	0.92	0.10	47,47,47,47	0
57	MG	1A	3510	1/1	0.92	0.20	54,54,54,54	0
57	MG	2A	3137	1/1	0.92	0.18	58,58,58,58	0
57	MG	2A	3138	1/1	0.92	0.13	45,45,45,45	0
57	MG	2A	3334	1/1	0.92	0.36	54,54,54,54	0
57	MG	2A	3139	1/1	0.92	0.24	61,61,61,61	0
57	MG	2A	3340	1/1	0.92	0.36	56,56,56,56	0
57	MG	1A	3865	1/1	0.92	0.10	47,47,47,47	0
57	MG	2a	1655	1/1	0.92	0.09	68,68,68,68	0
57	MG	2a	1657	1/1	0.92	0.15	62,62,62,62	0
57	MG	1A	3866	1/1	0.92	0.12	44,44,44,44	0
57	MG	2A	3627	1/1	0.92	0.16	61,61,61,61	0
57	MG	2A	3344	1/1	0.92	0.21	63,63,63,63	0
57	MG	1A	3867	1/1	0.92	0.11	33,33,33,33	0
57	MG	1A	3190	1/1	0.92	0.12	46,46,46,46	0
57	MG	2a	1668	1/1	0.92	0.14	58,58,58,58	0
57	MG	1A	3382	1/1	0.92	0.20	59,59,59,59	0
57	MG	2A	3348	1/1	0.92	0.28	58,58,58,58	0
57	MG	1A	3874	1/1	0.92	0.14	52,52,52,52	0
57	MG	1a	1758	1/1	0.92	0.08	63,63,63,63	0
57	MG	2A	3638	1/1	0.92	0.07	68,68,68,68	0
57	MG	2a	1676	1/1	0.92	0.29	61,61,61,61	0
57	MG	2A	3351	1/1	0.92	0.24	57,57,57,57	0
57	MG	1Y	201	1/1	0.92	0.26	69,69,69,69	0
57	MG	1Y	202	1/1	0.92	0.35	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1Z	301	1/1	0.92	0.15	67,67,67,67	0
57	MG	2A	3355	1/1	0.92	0.12	42,42,42,42	0
57	MG	1A	3384	1/1	0.92	0.09	51,51,51,51	0
57	MG	1A	3632	1/1	0.92	0.10	29,29,29,29	0
57	MG	2a	1687	1/1	0.92	0.14	57,57,57,57	0
57	MG	1A	3385	1/1	0.92	0.11	63,63,63,63	0
57	MG	2A	3650	1/1	0.92	0.27	47,47,47,47	0
57	MG	2a	1690	1/1	0.92	0.12	66,66,66,66	0
57	MG	1a	1777	1/1	0.92	0.07	85,85,85,85	0
57	MG	1A	3639	1/1	0.92	0.18	61,61,61,61	0
57	MG	1A	4041	1/1	0.92	0.07	53,53,53,53	0
57	MG	2A	3656	1/1	0.92	0.13	56,56,56,56	0
57	MG	1A	3333	1/1	0.92	0.15	60,60,60,60	0
57	MG	1A	3157	1/1	0.92	0.15	52,52,52,52	0
57	MG	1A	3532	1/1	0.92	0.20	46,46,46,46	0
57	MG	2A	3663	1/1	0.92	0.12	66,66,66,66	0
57	MG	2a	1702	1/1	0.92	0.13	64,64,64,64	0
57	MG	1A	3016	1/1	0.92	0.20	66,66,66,66	0
57	MG	2A	3665	1/1	0.92	0.13	70,70,70,70	0
57	MG	2A	3666	1/1	0.92	0.15	72,72,72,72	0
57	MG	2A	3668	1/1	0.92	0.16	56,56,56,56	0
57	MG	1a	1794	1/1	0.92	0.14	57,57,57,57	0
57	MG	1A	3396	1/1	0.92	0.13	53,53,53,53	0
57	MG	2A	3376	1/1	0.92	0.21	62,62,62,62	0
57	MG	1A	3537	1/1	0.92	0.12	45,45,45,45	0
57	MG	2A	3175	1/1	0.92	0.23	65,65,65,65	0
57	MG	1A	3398	1/1	0.92	0.12	45,45,45,45	0
57	MG	2A	3685	1/1	0.92	0.13	88,88,88,88	0
57	MG	1A	4063	1/1	0.92	0.10	71,71,71,71	0
57	MG	2A	3689	1/1	0.92	0.16	54,54,54,54	0
57	MG	1A	3233	1/1	0.92	0.12	47,47,47,47	0
57	MG	2A	3388	1/1	0.92	0.25	66,66,66,66	0
57	MG	1A	3787	1/1	0.92	0.33	62,62,62,62	0
57	MG	2A	3696	1/1	0.92	0.13	73,73,73,73	0
57	MG	1A	3788	1/1	0.92	0.20	59,59,59,59	0
57	MG	1A	3341	1/1	0.92	0.15	35,35,35,35	0
57	MG	2a	1729	1/1	0.92	0.16	74,74,74,74	0
57	MG	2A	3395	1/1	0.92	0.20	58,58,58,58	0
57	MG	2A	3396	1/1	0.92	0.18	48,48,48,48	0
57	MG	2A	3397	1/1	0.92	0.28	62,62,62,62	0
57	MG	1a	1805	1/1	0.92	0.25	53,53,53,53	0
57	MG	2A	3187	1/1	0.92	0.09	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1745	1/1	0.92	0.11	75,75,75,75	0
57	MG	2A	3714	1/1	0.92	0.09	52,52,52,52	0
57	MG	2A	3188	1/1	0.92	0.18	51,51,51,51	0
57	MG	1A	3790	1/1	0.92	0.11	70,70,70,70	0
57	MG	2A	3192	1/1	0.92	0.14	45,45,45,45	0
57	MG	2a	1753	1/1	0.92	0.16	52,52,52,52	0
57	MG	1A	4074	1/1	0.92	0.12	62,62,62,62	0
57	MG	1A	3918	1/1	0.92	0.14	65,65,65,65	0
57	MG	1A	3920	1/1	0.92	0.16	52,52,52,52	0
57	MG	1A	4077	1/1	0.92	0.07	61,61,61,61	0
57	MG	1A	3791	1/1	0.92	0.12	40,40,40,40	0
57	MG	1a	1606	1/1	0.92	0.15	60,60,60,60	0
57	MG	1A	4083	1/1	0.92	0.17	31,31,31,31	0
57	MG	1e	201	1/1	0.92	0.16	72,72,72,72	0
57	MG	1h	201	1/1	0.92	0.07	66,66,66,66	0
57	MG	2A	3740	1/1	0.92	0.10	62,62,62,62	0
57	MG	2a	1766	1/1	0.92	0.26	61,61,61,61	0
57	MG	1A	3197	1/1	0.92	0.14	39,39,39,39	0
57	MG	2A	3210	1/1	0.92	0.19	63,63,63,63	0
57	MG	2A	3746	1/1	0.92	0.11	55,55,55,55	0
57	MG	1l	3201	1/1	0.92	0.18	60,60,60,60	0
57	MG	1A	3406	1/1	0.92	0.29	41,41,41,41	0
57	MG	2A	3752	1/1	0.92	0.19	71,71,71,71	0
57	MG	2a	1774	1/1	0.92	0.18	68,68,68,68	0
57	MG	1A	3302	1/1	0.92	0.12	54,54,54,54	0
57	MG	1A	3093	1/1	0.92	0.11	47,47,47,47	0
57	MG	1A	3126	1/1	0.92	0.17	48,48,48,48	0
57	MG	2a	1778	1/1	0.92	0.21	56,56,56,56	0
57	MG	2A	3218	1/1	0.92	0.10	58,58,58,58	0
57	MG	2A	3220	1/1	0.92	0.10	63,63,63,63	0
57	MG	1A	4091	1/1	0.92	0.17	40,40,40,40	0
57	MG	1A	3275	1/1	0.92	0.07	53,53,53,53	0
57	MG	2a	1784	1/1	0.92	0.25	65,65,65,65	0
57	MG	1A	3416	1/1	0.92	0.23	67,67,67,67	0
57	MG	1A	4094	1/1	0.92	0.21	42,42,42,42	0
57	MG	1a	1635	1/1	0.92	0.12	49,49,49,49	0
57	MG	1A	3417	1/1	0.92	0.15	45,45,45,45	0
57	MG	2A	3458	1/1	0.92	0.11	46,46,46,46	0
57	MG	1A	3938	1/1	0.92	0.11	66,66,66,66	0
57	MG	1A	3133	1/1	0.92	0.11	48,48,48,48	0
57	MG	1A	3942	1/1	0.92	0.09	31,31,31,31	0
57	MG	1a	1641	1/1	0.92	0.16	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3943	1/1	0.92	0.09	33,33,33,33	0
57	MG	2a	1799	1/1	0.92	0.25	60,60,60,60	0
57	MG	1a	1645	1/1	0.92	0.21	54,54,54,54	0
57	MG	2A	3780	1/1	0.92	0.18	67,67,67,67	0
57	MG	2A	3004	1/1	0.92	0.18	50,50,50,50	0
57	MG	2A	3475	1/1	0.92	0.07	46,46,46,46	0
57	MG	2a	1806	1/1	0.92	0.17	53,53,53,53	0
57	MG	2A	3476	1/1	0.92	0.12	71,71,71,71	0
57	MG	2A	3005	1/1	0.92	0.20	56,56,56,56	0
57	MG	1B	206	1/1	0.92	0.10	47,47,47,47	0
57	MG	1A	3681	1/1	0.92	0.16	62,62,62,62	0
57	MG	1B	209	1/1	0.92	0.25	57,57,57,57	0
57	MG	1A	3946	1/1	0.92	0.10	28,28,28,28	0
57	MG	1A	3104	1/1	0.92	0.26	29,29,29,29	0
57	MG	1A	3563	1/1	0.92	0.10	25,25,25,25	0
57	MG	1A	3480	1/1	0.92	0.11	52,52,52,52	0
57	MG	2d	301	1/1	0.92	0.10	69,69,69,69	0
57	MG	2A	3027	1/1	0.92	0.12	45,45,45,45	0
57	MG	2A	3489	1/1	0.92	0.16	60,60,60,60	0
57	MG	1A	3042	1/1	0.92	0.23	35,35,35,35	0
57	MG	2B	205	1/1	0.92	0.25	57,57,57,57	0
57	MG	2A	3033	1/1	0.92	0.17	55,55,55,55	0
57	MG	1A	3957	1/1	0.92	0.06	26,26,26,26	0
57	MG	2A	3036	1/1	0.92	0.18	66,66,66,66	0
57	MG	2A	3038	1/1	0.92	0.18	70,70,70,70	0
57	MG	1A	3698	1/1	0.92	0.08	25,25,25,25	0
57	MG	2B	212	1/1	0.92	0.23	65,65,65,65	0
57	MG	2A	3040	1/1	0.92	0.14	60,60,60,60	0
57	MG	2A	3041	1/1	0.92	0.16	62,62,62,62	0
57	MG	2A	3505	1/1	0.92	0.19	59,59,59,59	0
57	MG	1A	3816	1/1	0.92	0.32	41,41,41,41	0
57	MG	1A	3817	1/1	0.92	0.15	61,61,61,61	0
57	MG	1A	3369	1/1	0.92	0.14	55,55,55,55	0
57	MG	1A	3315	1/1	0.92	0.17	61,61,61,61	0
57	MG	1A	3974	1/1	0.92	0.09	62,62,62,62	0
57	MG	2A	3051	1/1	0.92	0.20	56,56,56,56	0
57	MG	1a	1669	1/1	0.92	0.21	64,64,64,64	0
57	MG	1A	3579	1/1	0.92	0.08	34,34,34,34	0
57	MG	1A	3582	1/1	0.92	0.11	51,51,51,51	0
57	MG	1D	312	1/1	0.92	0.14	39,39,39,39	0
57	MG	2x	109	1/1	0.92	0.13	70,70,70,70	0
57	MG	1a	1674	1/1	0.92	0.24	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3520	1/1	0.92	0.12	41,41,41,41	0
57	MG	2E	308	1/1	0.93	0.11	61,61,61,61	0
57	MG	2A	3016	1/1	0.93	0.20	39,39,39,39	0
57	MG	1A	3361	1/1	0.93	0.29	33,33,33,33	0
57	MG	1A	3813	1/1	0.93	0.12	32,32,32,32	0
57	MG	2F	307	1/1	0.93	0.25	51,51,51,51	0
57	MG	1B	205	1/1	0.93	0.25	58,58,58,58	0
57	MG	1A	3691	1/1	0.93	0.09	45,45,45,45	0
57	MG	1A	3948	1/1	0.93	0.13	40,40,40,40	0
57	MG	1a	1643	1/1	0.93	0.23	67,67,67,67	0
57	MG	2A	3029	1/1	0.93	0.22	48,48,48,48	0
57	MG	2Q	201	1/1	0.93	0.08	65,65,65,65	0
57	MG	1a	1644	1/1	0.93	0.12	49,49,49,49	0
57	MG	2R	201	1/1	0.93	0.33	50,50,50,50	0
57	MG	1A	3567	1/1	0.93	0.09	30,30,30,30	0
57	MG	1B	210	1/1	0.93	0.17	51,51,51,51	0
57	MG	1B	211	1/1	0.93	0.27	64,64,64,64	0
57	MG	1B	212	1/1	0.93	0.18	60,60,60,60	0
57	MG	1A	3002	1/1	0.93	0.12	60,60,60,60	0
57	MG	1A	3951	1/1	0.93	0.15	52,52,52,52	0
57	MG	1a	1653	1/1	0.93	0.23	50,50,50,50	0
57	MG	1a	1656	1/1	0.93	0.14	49,49,49,49	0
57	MG	2A	3272	1/1	0.93	0.14	52,52,52,52	0
57	MG	2A	3273	1/1	0.93	0.18	70,70,70,70	0
57	MG	1A	3569	1/1	0.93	0.11	39,39,39,39	0
57	MG	1A	3820	1/1	0.93	0.14	56,56,56,56	0
57	MG	1A	3059	1/1	0.93	0.19	44,44,44,44	0
57	MG	2A	3049	1/1	0.93	0.15	67,67,67,67	0
57	MG	27	102	1/1	0.93	0.10	57,57,57,57	0
57	MG	1A	3182	1/1	0.93	0.12	51,51,51,51	0
57	MG	1A	3578	1/1	0.93	0.17	35,35,35,35	0
57	MG	2A	3052	1/1	0.93	0.16	59,59,59,59	0
57	MG	1A	3487	1/1	0.93	0.18	41,41,41,41	0
57	MG	1A	3581	1/1	0.93	0.10	39,39,39,39	0
57	MG	2A	3555	1/1	0.93	0.18	50,50,50,50	0
57	MG	2A	3556	1/1	0.93	0.13	62,62,62,62	0
57	MG	1A	3421	1/1	0.93	0.18	52,52,52,52	0
57	MG	2a	1604	1/1	0.93	0.28	73,73,73,73	0
57	MG	1B	230	1/1	0.93	0.09	49,49,49,49	0
57	MG	2A	3287	1/1	0.93	0.28	58,58,58,58	0
57	MG	2a	1607	1/1	0.93	0.43	69,69,69,69	0
57	MG	1a	1667	1/1	0.93	0.08	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3063	1/1	0.93	0.12	53,53,53,53	0
57	MG	1A	3712	1/1	0.93	0.14	61,61,61,61	0
57	MG	1A	3831	1/1	0.93	0.13	41,41,41,41	0
57	MG	1A	3978	1/1	0.93	0.09	66,66,66,66	0
57	MG	1A	3715	1/1	0.93	0.06	20,20,20,20	0
57	MG	1a	1672	1/1	0.93	0.27	70,70,70,70	0
57	MG	1A	3834	1/1	0.93	0.14	49,49,49,49	0
57	MG	1A	3836	1/1	0.93	0.21	40,40,40,40	0
57	MG	1A	3716	1/1	0.93	0.11	44,44,44,44	0
57	MG	2A	3075	1/1	0.93	0.15	57,57,57,57	0
57	MG	2A	3076	1/1	0.93	0.09	52,52,52,52	0
57	MG	2A	3577	1/1	0.93	0.12	53,53,53,53	0
57	MG	1A	3986	1/1	0.93	0.09	41,41,41,41	0
57	MG	1E	308	1/1	0.93	0.18	40,40,40,40	0
57	MG	1A	3094	1/1	0.93	0.21	66,66,66,66	0
57	MG	2A	3081	1/1	0.93	0.07	52,52,52,52	0
57	MG	2A	3583	1/1	0.93	0.09	43,43,43,43	0
57	MG	1a	1685	1/1	0.93	0.23	61,61,61,61	0
57	MG	2A	3585	1/1	0.93	0.27	57,57,57,57	0
57	MG	1A	3006	1/1	0.93	0.17	55,55,55,55	0
57	MG	2A	3589	1/1	0.93	0.12	54,54,54,54	0
57	MG	2A	3308	1/1	0.93	0.25	70,70,70,70	0
57	MG	2A	3084	1/1	0.93	0.09	41,41,41,41	0
57	MG	1a	1687	1/1	0.93	0.32	55,55,55,55	0
57	MG	2A	3595	1/1	0.93	0.20	56,56,56,56	0
57	MG	2A	3311	1/1	0.93	0.11	65,65,65,65	0
57	MG	1F	303	1/1	0.93	0.12	31,31,31,31	0
57	MG	1A	3843	1/1	0.93	0.09	31,31,31,31	0
57	MG	1A	3586	1/1	0.93	0.06	33,33,33,33	0
57	MG	2A	3602	1/1	0.93	0.08	31,31,31,31	0
57	MG	1F	307	1/1	0.93	0.09	38,38,38,38	0
57	MG	1a	1693	1/1	0.93	0.13	61,61,61,61	0
57	MG	1F	309	1/1	0.93	0.22	29,29,29,29	0
57	MG	1F	311	1/1	0.93	0.09	46,46,46,46	0
57	MG	2a	1651	1/1	0.93	0.15	67,67,67,67	0
57	MG	2A	3096	1/1	0.93	0.12	62,62,62,62	0
57	MG	1F	312	1/1	0.93	0.16	54,54,54,54	0
57	MG	1A	3253	1/1	0.93	0.09	60,60,60,60	0
57	MG	1A	3590	1/1	0.93	0.08	24,24,24,24	0
57	MG	1A	3316	1/1	0.93	0.08	55,55,55,55	0
57	MG	1A	3595	1/1	0.93	0.10	36,36,36,36	0
57	MG	2A	3104	1/1	0.93	0.23	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1664	1/1	0.93	0.15	64,64,64,64	0
57	MG	1a	1708	1/1	0.93	0.17	60,60,60,60	0
57	MG	2A	3109	1/1	0.93	0.16	45,45,45,45	0
57	MG	1G	204	1/1	0.93	0.14	62,62,62,62	0
57	MG	2A	3629	1/1	0.93	0.12	61,61,61,61	0
57	MG	2A	3332	1/1	0.93	0.21	39,39,39,39	0
57	MG	1A	4000	1/1	0.93	0.09	33,33,33,33	0
57	MG	2A	3113	1/1	0.93	0.11	52,52,52,52	0
57	MG	2a	1674	1/1	0.93	0.27	59,59,59,59	0
57	MG	2A	3335	1/1	0.93	0.30	62,62,62,62	0
57	MG	2A	3336	1/1	0.93	0.23	47,47,47,47	0
57	MG	1A	4006	1/1	0.93	0.08	59,59,59,59	0
57	MG	2A	3637	1/1	0.93	0.11	54,54,54,54	0
57	MG	2A	3115	1/1	0.93	0.11	61,61,61,61	0
57	MG	1N	201	1/1	0.93	0.17	45,45,45,45	0
57	MG	2A	3342	1/1	0.93	0.31	54,54,54,54	0
57	MG	1A	3285	1/1	0.93	0.28	52,52,52,52	0
57	MG	2A	3120	1/1	0.93	0.09	53,53,53,53	0
57	MG	1N	205	1/1	0.93	0.11	44,44,44,44	0
57	MG	1A	3256	1/1	0.93	0.07	56,56,56,56	0
57	MG	2A	3646	1/1	0.93	0.10	56,56,56,56	0
57	MG	2A	3124	1/1	0.93	0.25	46,46,46,46	0
57	MG	1A	3505	1/1	0.93	0.15	33,33,33,33	0
57	MG	2A	3129	1/1	0.93	0.16	41,41,41,41	0
57	MG	2a	1693	1/1	0.93	0.22	65,65,65,65	0
57	MG	1A	3288	1/1	0.93	0.18	42,42,42,42	0
57	MG	2A	3132	1/1	0.93	0.21	64,64,64,64	0
57	MG	1A	3603	1/1	0.93	0.10	32,32,32,32	0
57	MG	1P	203	1/1	0.93	0.27	32,32,32,32	0
57	MG	2A	3657	1/1	0.93	0.10	49,49,49,49	0
57	MG	1A	3377	1/1	0.93	0.12	37,37,37,37	0
57	MG	1a	1733	1/1	0.93	0.21	71,71,71,71	0
57	MG	2A	3660	1/1	0.93	0.10	42,42,42,42	0
57	MG	1A	3325	1/1	0.93	0.12	39,39,39,39	0
57	MG	1Q	206	1/1	0.93	0.13	43,43,43,43	0
57	MG	2A	3142	1/1	0.93	0.11	62,62,62,62	0
57	MG	1A	4014	1/1	0.93	0.18	29,29,29,29	0
57	MG	1R	204	1/1	0.93	0.11	30,30,30,30	0
57	MG	2a	1712	1/1	0.93	0.17	51,51,51,51	0
57	MG	1A	3612	1/1	0.93	0.10	46,46,46,46	0
57	MG	2A	3147	1/1	0.93	0.08	56,56,56,56	0
57	MG	2A	3674	1/1	0.93	0.09	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1741	1/1	0.93	0.09	58,58,58,58	0
57	MG	1A	3292	1/1	0.93	0.28	47,47,47,47	0
57	MG	1A	3513	1/1	0.93	0.17	50,50,50,50	0
57	MG	1S	202	1/1	0.93	0.10	54,54,54,54	0
57	MG	1a	1746	1/1	0.93	0.12	58,58,58,58	0
57	MG	2A	3681	1/1	0.93	0.06	40,40,40,40	0
57	MG	1A	3211	1/1	0.93	0.10	45,45,45,45	0
57	MG	2A	3378	1/1	0.93	0.16	59,59,59,59	0
57	MG	2a	1725	1/1	0.93	0.06	84,84,84,84	0
57	MG	1A	3873	1/1	0.93	0.19	42,42,42,42	0
57	MG	1a	1751	1/1	0.93	0.12	64,64,64,64	0
57	MG	1A	3518	1/1	0.93	0.12	54,54,54,54	0
57	MG	2A	3383	1/1	0.93	0.11	42,42,42,42	0
57	MG	1A	3875	1/1	0.93	0.07	31,31,31,31	0
57	MG	1A	3440	1/1	0.93	0.15	46,46,46,46	0
57	MG	1A	3878	1/1	0.93	0.07	48,48,48,48	0
57	MG	2A	3389	1/1	0.93	0.28	54,54,54,54	0
57	MG	2a	1742	1/1	0.93	0.13	47,47,47,47	0
57	MG	2A	3703	1/1	0.93	0.09	63,63,63,63	0
57	MG	1A	4036	1/1	0.93	0.15	50,50,50,50	0
57	MG	1A	3767	1/1	0.93	0.08	38,38,38,38	0
57	MG	2A	3710	1/1	0.93	0.14	58,58,58,58	0
57	MG	2a	1750	1/1	0.93	0.23	63,63,63,63	0
57	MG	2A	3393	1/1	0.93	0.17	43,43,43,43	0
57	MG	1A	3880	1/1	0.93	0.09	51,51,51,51	0
57	MG	1A	3330	1/1	0.93	0.17	39,39,39,39	0
57	MG	2A	3170	1/1	0.93	0.18	62,62,62,62	0
57	MG	1a	1770	1/1	0.93	0.09	53,53,53,53	0
57	MG	1X	104	1/1	0.93	0.10	40,40,40,40	0
57	MG	1A	3116	1/1	0.93	0.26	45,45,45,45	0
57	MG	2A	3727	1/1	0.93	0.14	50,50,50,50	0
57	MG	1A	3156	1/1	0.93	0.31	35,35,35,35	0
57	MG	1A	3895	1/1	0.93	0.08	53,53,53,53	0
57	MG	10	101	1/1	0.93	0.20	43,43,43,43	0
57	MG	1A	3334	1/1	0.93	0.10	53,53,53,53	0
57	MG	1A	4046	1/1	0.93	0.11	43,43,43,43	0
57	MG	2A	3409	1/1	0.93	0.11	54,54,54,54	0
57	MG	1A	3389	1/1	0.93	0.20	38,38,38,38	0
57	MG	1A	4049	1/1	0.93	0.10	44,44,44,44	0
57	MG	1A	3780	1/1	0.93	0.08	37,37,37,37	0
57	MG	1A	3782	1/1	0.93	0.08	34,34,34,34	0
57	MG	2A	3742	1/1	0.93	0.17	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	10	110	1/1	0.93	0.06	42,42,42,42	0
57	MG	1A	3904	1/1	0.93	0.08	74,74,74,74	0
57	MG	2A	3191	1/1	0.93	0.20	56,56,56,56	0
57	MG	1A	3534	1/1	0.93	0.07	40,40,40,40	0
57	MG	1A	3391	1/1	0.93	0.12	36,36,36,36	0
57	MG	1A	3648	1/1	0.93	0.09	20,20,20,20	0
57	MG	2a	1780	1/1	0.93	0.23	62,62,62,62	0
57	MG	1A	3215	1/1	0.93	0.12	48,48,48,48	0
57	MG	1A	3910	1/1	0.93	0.19	67,67,67,67	0
57	MG	2A	3197	1/1	0.93	0.25	58,58,58,58	0
57	MG	1A	4069	1/1	0.93	0.08	63,63,63,63	0
57	MG	2A	3434	1/1	0.93	0.09	38,38,38,38	0
57	MG	1A	4071	1/1	0.93	0.13	59,59,59,59	0
57	MG	2A	3763	1/1	0.93	0.11	60,60,60,60	0
57	MG	2A	3438	1/1	0.93	0.11	69,69,69,69	0
57	MG	15	102	1/1	0.93	0.15	36,36,36,36	0
57	MG	2A	3440	1/1	0.93	0.14	55,55,55,55	0
57	MG	2A	3201	1/1	0.93	0.12	59,59,59,59	0
57	MG	2A	3203	1/1	0.93	0.23	54,54,54,54	0
57	MG	2A	3445	1/1	0.93	0.11	36,36,36,36	0
57	MG	2A	3204	1/1	0.93	0.21	48,48,48,48	0
57	MG	1A	3337	1/1	0.93	0.28	36,36,36,36	0
57	MG	2A	3206	1/1	0.93	0.26	45,45,45,45	0
57	MG	1A	3297	1/1	0.93	0.21	58,58,58,58	0
57	MG	2A	3778	1/1	0.93	0.07	60,60,60,60	0
57	MG	16	101	1/1	0.93	0.11	52,52,52,52	0
57	MG	1A	3166	1/1	0.93	0.18	60,60,60,60	0
57	MG	18	105	1/1	0.93	0.16	50,50,50,50	0
57	MG	18	106	1/1	0.93	0.17	53,53,53,53	0
57	MG	2A	3466	1/1	0.93	0.10	40,40,40,40	0
57	MG	1A	3544	1/1	0.93	0.13	27,27,27,27	0
57	MG	1A	3919	1/1	0.93	0.09	51,51,51,51	0
57	MG	2A	3472	1/1	0.93	0.09	47,47,47,47	0
57	MG	1A	3665	1/1	0.93	0.13	43,43,43,43	0
57	MG	1A	3792	1/1	0.93	0.07	28,28,28,28	0
57	MG	1A	3465	1/1	0.93	0.07	52,52,52,52	0
57	MG	1A	3300	1/1	0.93	0.12	56,56,56,56	0
57	MG	1A	3925	1/1	0.93	0.14	56,56,56,56	0
57	MG	2B	201	1/1	0.93	0.18	69,69,69,69	0
57	MG	1a	1608	1/1	0.93	0.10	52,52,52,52	0
57	MG	2A	3224	1/1	0.93	0.34	65,65,65,65	0
57	MG	1A	3342	1/1	0.93	0.16	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3343	1/1	0.93	0.11	45,45,45,45	0
57	MG	1x	102	1/1	0.93	0.17	70,70,70,70	0
57	MG	1A	3469	1/1	0.93	0.24	29,29,29,29	0
57	MG	1A	3273	1/1	0.93	0.17	51,51,51,51	0
57	MG	1A	3407	1/1	0.93	0.17	43,43,43,43	0
57	MG	2A	3232	1/1	0.93	0.12	66,66,66,66	0
57	MG	1A	3303	1/1	0.93	0.19	56,56,56,56	0
57	MG	1A	3304	1/1	0.93	0.21	45,45,45,45	0
57	MG	1x	109	1/1	0.93	0.29	71,71,71,71	0
57	MG	1A	3176	1/1	0.93	0.17	48,48,48,48	0
57	MG	1a	1627	1/1	0.93	0.27	63,63,63,63	0
57	MG	1A	4097	1/1	0.93	0.08	46,46,46,46	0
57	MG	1y	101	1/1	0.93	0.13	55,55,55,55	0
57	MG	1a	1630	1/1	0.93	0.48	71,71,71,71	0
57	MG	1a	1633	1/1	0.93	0.17	58,58,58,58	0
57	MG	1A	3359	1/1	0.93	0.27	36,36,36,36	0
57	MG	2x	106	1/1	0.93	0.11	67,67,67,67	0
57	MG	1A	4100	1/1	0.93	0.26	53,53,53,53	0
57	MG	2A	3008	1/1	0.93	0.21	49,49,49,49	0
57	MG	1A	3686	1/1	0.93	0.09	48,48,48,48	0
57	MG	2A	3251	1/1	0.93	0.15	62,62,62,62	0
57	MG	2A	3015	1/1	0.93	0.21	58,58,58,58	0
59	TYK	2A	3798	64/64	0.93	0.11	32,46,61,66	0
57	MG	1A	3554	1/1	0.94	0.19	63,63,63,63	0
57	MG	2A	3172	1/1	0.94	0.10	56,56,56,56	0
57	MG	27	101	1/1	0.94	0.24	59,59,59,59	0
57	MG	1e	202	1/1	0.94	0.16	58,58,58,58	0
57	MG	1A	3682	1/1	0.94	0.10	57,57,57,57	0
57	MG	1B	219	1/1	0.94	0.09	34,34,34,34	0
57	MG	1a	1631	1/1	0.94	0.19	59,59,59,59	0
57	MG	2A	3601	1/1	0.94	0.11	68,68,68,68	0
57	MG	1A	3241	1/1	0.94	0.10	49,49,49,49	0
57	MG	2A	3178	1/1	0.94	0.08	67,67,67,67	0
57	MG	1A	3195	1/1	0.94	0.08	34,34,34,34	0
57	MG	2A	3362	1/1	0.94	0.08	50,50,50,50	0
57	MG	1B	222	1/1	0.94	0.12	56,56,56,56	0
57	MG	1B	223	1/1	0.94	0.11	58,58,58,58	0
57	MG	2A	3611	1/1	0.94	0.09	55,55,55,55	0
57	MG	1A	3070	1/1	0.94	0.06	33,33,33,33	0
57	MG	1B	226	1/1	0.94	0.08	45,45,45,45	0
57	MG	1A	3471	1/1	0.94	0.32	40,40,40,40	0
57	MG	1A	3826	1/1	0.94	0.11	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3372	1/1	0.94	0.12	59,59,59,59	0
57	MG	2A	3189	1/1	0.94	0.16	64,64,64,64	0
57	MG	2A	3622	1/1	0.94	0.13	48,48,48,48	0
57	MG	2A	3625	1/1	0.94	0.10	50,50,50,50	0
57	MG	2A	3375	1/1	0.94	0.09	69,69,69,69	0
57	MG	1A	3403	1/1	0.94	0.17	42,42,42,42	0
57	MG	1A	3828	1/1	0.94	0.22	38,38,38,38	0
57	MG	1A	3695	1/1	0.94	0.08	44,44,44,44	0
57	MG	1A	3244	1/1	0.94	0.10	59,59,59,59	0
57	MG	1A	3344	1/1	0.94	0.21	45,45,45,45	0
57	MG	1D	309	1/1	0.94	0.16	52,52,52,52	0
57	MG	1A	3566	1/1	0.94	0.07	52,52,52,52	0
57	MG	2a	1627	1/1	0.94	0.23	45,45,45,45	0
57	MG	1a	1649	1/1	0.94	0.15	46,46,46,46	0
57	MG	1A	3476	1/1	0.94	0.10	49,49,49,49	0
57	MG	1A	3077	1/1	0.94	0.15	36,36,36,36	0
57	MG	1A	3408	1/1	0.94	0.21	46,46,46,46	0
57	MG	2A	3391	1/1	0.94	0.19	61,61,61,61	0
57	MG	2A	3003	1/1	0.94	0.23	57,57,57,57	0
57	MG	1a	1655	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3838	1/1	0.94	0.08	36,36,36,36	0
57	MG	1A	3022	1/1	0.94	0.04	17,17,17,17	0
57	MG	1A	3571	1/1	0.94	0.09	43,43,43,43	0
57	MG	2A	3011	1/1	0.94	0.12	46,46,46,46	0
57	MG	1A	3411	1/1	0.94	0.10	58,58,58,58	0
57	MG	2A	3014	1/1	0.94	0.11	50,50,50,50	0
57	MG	2A	3212	1/1	0.94	0.10	58,58,58,58	0
57	MG	2A	3401	1/1	0.94	0.06	42,42,42,42	0
57	MG	2A	3402	1/1	0.94	0.24	71,71,71,71	0
57	MG	2a	1646	1/1	0.94	0.26	61,61,61,61	0
57	MG	1A	3994	1/1	0.94	0.08	29,29,29,29	0
57	MG	1A	3050	1/1	0.94	0.07	45,45,45,45	0
57	MG	1A	3845	1/1	0.94	0.08	29,29,29,29	0
57	MG	1A	3353	1/1	0.94	0.17	55,55,55,55	0
57	MG	1A	3202	1/1	0.94	0.15	36,36,36,36	0
57	MG	1A	3719	1/1	0.94	0.08	38,38,38,38	0
57	MG	2a	1653	1/1	0.94	0.12	47,47,47,47	0
57	MG	2A	3661	1/1	0.94	0.10	41,41,41,41	0
57	MG	2A	3219	1/1	0.94	0.14	49,49,49,49	0
57	MG	2a	1656	1/1	0.94	0.26	63,63,63,63	0
57	MG	1A	3486	1/1	0.94	0.25	43,43,43,43	0
57	MG	2a	1658	1/1	0.94	0.21	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1F	313	1/1	0.94	0.16	32,32,32,32	0
57	MG	2A	3028	1/1	0.94	0.13	50,50,50,50	0
57	MG	1A	3052	1/1	0.94	0.08	51,51,51,51	0
57	MG	1A	3360	1/1	0.94	0.09	57,57,57,57	0
57	MG	1A	3856	1/1	0.94	0.11	49,49,49,49	0
57	MG	1A	3725	1/1	0.94	0.12	27,27,27,27	0
57	MG	2a	1667	1/1	0.94	0.11	66,66,66,66	0
57	MG	1A	3490	1/1	0.94	0.23	49,49,49,49	0
57	MG	1A	3103	1/1	0.94	0.29	34,34,34,34	0
57	MG	1a	1675	1/1	0.94	0.36	58,58,58,58	0
57	MG	1a	1676	1/1	0.94	0.07	73,73,73,73	0
57	MG	1a	1677	1/1	0.94	0.22	41,41,41,41	0
57	MG	2A	3432	1/1	0.94	0.07	30,30,30,30	0
57	MG	2A	3683	1/1	0.94	0.13	72,72,72,72	0
57	MG	2A	3684	1/1	0.94	0.19	50,50,50,50	0
57	MG	2A	3433	1/1	0.94	0.08	45,45,45,45	0
57	MG	2A	3042	1/1	0.94	0.21	36,36,36,36	0
57	MG	2A	3435	1/1	0.94	0.17	69,69,69,69	0
57	MG	2a	1681	1/1	0.94	0.19	35,35,35,35	0
57	MG	2a	1682	1/1	0.94	0.35	60,60,60,60	0
57	MG	1A	3492	1/1	0.94	0.10	24,24,24,24	0
57	MG	1A	3208	1/1	0.94	0.08	50,50,50,50	0
57	MG	2A	3694	1/1	0.94	0.12	64,64,64,64	0
57	MG	1a	1680	1/1	0.94	0.24	40,40,40,40	0
57	MG	1a	1681	1/1	0.94	0.14	57,57,57,57	0
57	MG	1A	3254	1/1	0.94	0.13	34,34,34,34	0
57	MG	2A	3442	1/1	0.94	0.11	41,41,41,41	0
57	MG	2A	3443	1/1	0.94	0.08	44,44,44,44	0
57	MG	1A	3255	1/1	0.94	0.13	46,46,46,46	0
57	MG	2A	3704	1/1	0.94	0.07	72,72,72,72	0
57	MG	1A	3127	1/1	0.94	0.24	41,41,41,41	0
57	MG	1A	4025	1/1	0.94	0.07	53,53,53,53	0
57	MG	2A	3053	1/1	0.94	0.17	58,58,58,58	0
57	MG	1A	4027	1/1	0.94	0.14	49,49,49,49	0
57	MG	2A	3712	1/1	0.94	0.11	40,40,40,40	0
57	MG	2A	3452	1/1	0.94	0.08	39,39,39,39	0
57	MG	2A	3056	1/1	0.94	0.16	73,73,73,73	0
57	MG	1A	3499	1/1	0.94	0.07	58,58,58,58	0
57	MG	2a	1703	1/1	0.94	0.18	64,64,64,64	0
57	MG	2A	3719	1/1	0.94	0.07	56,56,56,56	0
57	MG	2a	1706	1/1	0.94	0.17	61,61,61,61	0
57	MG	2A	3249	1/1	0.94	0.16	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1P	201	1/1	0.94	0.27	32,32,32,32	0
57	MG	1A	3167	1/1	0.94	0.08	45,45,45,45	0
57	MG	2A	3060	1/1	0.94	0.10	50,50,50,50	0
57	MG	2A	3061	1/1	0.94	0.09	37,37,37,37	0
57	MG	1P	204	1/1	0.94	0.35	28,28,28,28	0
57	MG	1A	3750	1/1	0.94	0.09	53,53,53,53	0
57	MG	1A	3501	1/1	0.94	0.24	32,32,32,32	0
57	MG	2a	1715	1/1	0.94	0.45	60,60,60,60	0
57	MG	1Q	205	1/1	0.94	0.12	46,46,46,46	0
57	MG	1A	3174	1/1	0.94	0.10	32,32,32,32	0
57	MG	1A	3129	1/1	0.94	0.11	39,39,39,39	0
57	MG	2A	3068	1/1	0.94	0.25	44,44,44,44	0
57	MG	1A	3610	1/1	0.94	0.07	41,41,41,41	0
57	MG	1A	3611	1/1	0.94	0.10	42,42,42,42	0
57	MG	2A	3072	1/1	0.94	0.07	57,57,57,57	0
57	MG	1A	3763	1/1	0.94	0.06	32,32,32,32	0
57	MG	1A	3882	1/1	0.94	0.08	43,43,43,43	0
57	MG	1A	3429	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	3613	1/1	0.94	0.10	43,43,43,43	0
57	MG	1A	3177	1/1	0.94	0.14	54,54,54,54	0
57	MG	1A	3216	1/1	0.94	0.08	53,53,53,53	0
57	MG	1A	3004	1/1	0.94	0.10	25,25,25,25	0
57	MG	2A	3755	1/1	0.94	0.17	62,62,62,62	0
57	MG	2a	1733	1/1	0.94	0.13	72,72,72,72	0
57	MG	1A	4048	1/1	0.94	0.13	61,61,61,61	0
57	MG	2a	1735	1/1	0.94	0.08	52,52,52,52	0
57	MG	1A	3771	1/1	0.94	0.18	73,73,73,73	0
57	MG	2A	3758	1/1	0.94	0.19	50,50,50,50	0
57	MG	2a	1741	1/1	0.94	0.10	77,77,77,77	0
57	MG	1A	3038	1/1	0.94	0.20	36,36,36,36	0
57	MG	2A	3499	1/1	0.94	0.11	54,54,54,54	0
57	MG	1A	3903	1/1	0.94	0.10	61,61,61,61	0
57	MG	1V	201	1/1	0.94	0.13	28,28,28,28	0
57	MG	1a	1729	1/1	0.94	0.26	45,45,45,45	0
57	MG	1V	204	1/1	0.94	0.14	49,49,49,49	0
57	MG	1A	3516	1/1	0.94	0.14	33,33,33,33	0
57	MG	1A	3627	1/1	0.94	0.07	43,43,43,43	0
57	MG	1A	3779	1/1	0.94	0.08	30,30,30,30	0
57	MG	1a	1736	1/1	0.94	0.08	54,54,54,54	0
57	MG	1A	3180	1/1	0.94	0.13	50,50,50,50	0
57	MG	2A	3510	1/1	0.94	0.12	51,51,51,51	0
57	MG	2A	3511	1/1	0.94	0.12	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3435	1/1	0.94	0.13	56,56,56,56	0
57	MG	1A	3524	1/1	0.94	0.06	37,37,37,37	0
57	MG	1A	3912	1/1	0.94	0.12	64,64,64,64	0
57	MG	1A	3525	1/1	0.94	0.08	39,39,39,39	0
57	MG	2A	3782	1/1	0.94	0.08	54,54,54,54	0
57	MG	1A	3379	1/1	0.94	0.25	47,47,47,47	0
57	MG	1A	3645	1/1	0.94	0.08	29,29,29,29	0
57	MG	1A	3917	1/1	0.94	0.07	52,52,52,52	0
57	MG	1A	3110	1/1	0.94	0.17	35,35,35,35	0
57	MG	2A	3107	1/1	0.94	0.10	70,70,70,70	0
57	MG	2A	3790	1/1	0.94	0.12	60,60,60,60	0
57	MG	1A	3327	1/1	0.94	0.11	59,59,59,59	0
57	MG	1A	3531	1/1	0.94	0.07	42,42,42,42	0
57	MG	2A	3793	1/1	0.94	0.07	64,64,64,64	0
57	MG	2A	3524	1/1	0.94	0.10	37,37,37,37	0
57	MG	2A	3111	1/1	0.94	0.23	57,57,57,57	0
57	MG	2A	3300	1/1	0.94	0.11	64,64,64,64	0
57	MG	1a	1749	1/1	0.94	0.08	73,73,73,73	0
57	MG	1A	3649	1/1	0.94	0.05	28,28,28,28	0
57	MG	2A	3532	1/1	0.94	0.09	38,38,38,38	0
57	MG	1A	4079	1/1	0.94	0.08	48,48,48,48	0
57	MG	1a	1754	1/1	0.94	0.08	64,64,64,64	0
57	MG	1A	4082	1/1	0.94	0.29	33,33,33,33	0
57	MG	2A	3118	1/1	0.94	0.11	49,49,49,49	0
57	MG	2a	1786	1/1	0.94	0.18	68,68,68,68	0
57	MG	2B	207	1/1	0.94	0.09	65,65,65,65	0
57	MG	1l	105	1/1	0.94	0.10	53,53,53,53	0
57	MG	1A	3147	1/1	0.94	0.26	38,38,38,38	0
57	MG	1A	3224	1/1	0.94	0.20	50,50,50,50	0
57	MG	2A	3545	1/1	0.94	0.11	50,50,50,50	0
57	MG	1A	3111	1/1	0.94	0.16	39,39,39,39	0
57	MG	1A	3447	1/1	0.94	0.23	50,50,50,50	0
57	MG	1A	4087	1/1	0.94	0.13	51,51,51,51	0
57	MG	1A	3660	1/1	0.94	0.06	16,16,16,16	0
57	MG	1A	3929	1/1	0.94	0.08	65,65,65,65	0
57	MG	2B	217	1/1	0.94	0.32	71,71,71,71	0
57	MG	1A	3661	1/1	0.94	0.13	46,46,46,46	0
57	MG	2a	1802	1/1	0.94	0.19	55,55,55,55	0
57	MG	2B	219	1/1	0.94	0.13	62,62,62,62	0
57	MG	2D	301	1/1	0.94	0.08	42,42,42,42	0
57	MG	1A	3797	1/1	0.94	0.06	36,36,36,36	0
57	MG	1A	3332	1/1	0.94	0.32	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3136	1/1	0.94	0.11	32,32,32,32	0
57	MG	2a	1809	1/1	0.94	0.13	78,78,78,78	0
57	MG	1A	3234	1/1	0.94	0.09	52,52,52,52	0
57	MG	1a	1783	1/1	0.94	0.17	64,64,64,64	0
57	MG	1A	3390	1/1	0.94	0.22	37,37,37,37	0
57	MG	2E	302	1/1	0.94	0.11	55,55,55,55	0
57	MG	1a	1790	1/1	0.94	0.25	74,74,74,74	0
57	MG	2a	1817	1/1	0.94	0.14	54,54,54,54	0
57	MG	2E	305	1/1	0.94	0.10	63,63,63,63	0
57	MG	2A	3141	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	4096	1/1	0.94	0.09	50,50,50,50	0
57	MG	2d	302	1/1	0.94	0.22	56,56,56,56	0
57	MG	2A	3327	1/1	0.94	0.17	39,39,39,39	0
57	MG	19	101	1/1	0.94	0.20	52,52,52,52	0
57	MG	2F	301	1/1	0.94	0.09	47,47,47,47	0
57	MG	1A	3458	1/1	0.94	0.07	55,55,55,55	0
57	MG	2F	303	1/1	0.94	0.20	54,54,54,54	0
57	MG	1A	3940	1/1	0.94	0.17	51,51,51,51	0
57	MG	2F	306	1/1	0.94	0.16	48,48,48,48	0
57	MG	2q	201	1/1	0.94	0.09	77,77,77,77	0
57	MG	1A	3941	1/1	0.94	0.13	18,18,18,18	0
57	MG	2t	201	1/1	0.94	0.12	58,58,58,58	0
57	MG	1a	1797	1/1	0.94	0.12	66,66,66,66	0
57	MG	1A	3187	1/1	0.94	0.35	37,37,37,37	0
57	MG	1A	3460	1/1	0.94	0.06	51,51,51,51	0
57	MG	1A	3672	1/1	0.94	0.18	63,63,63,63	0
57	MG	2A	3575	1/1	0.94	0.13	60,60,60,60	0
57	MG	1A	3673	1/1	0.94	0.09	37,37,37,37	0
57	MG	1A	3809	1/1	0.94	0.19	45,45,45,45	0
57	MG	2w	105	1/1	0.94	0.20	51,51,51,51	0
57	MG	1a	1612	1/1	0.94	0.16	66,66,66,66	0
57	MG	1a	1613	1/1	0.94	0.11	62,62,62,62	0
57	MG	1A	3392	1/1	0.94	0.11	49,49,49,49	0
57	MG	1A	3189	1/1	0.94	0.35	38,38,38,38	0
57	MG	1a	1808	1/1	0.94	0.13	67,67,67,67	0
57	MG	1a	1616	1/1	0.94	0.12	61,61,61,61	0
57	MG	1A	3549	1/1	0.94	0.38	59,59,59,59	0
57	MG	1A	3112	1/1	0.94	0.18	30,30,30,30	0
57	MG	2A	3588	1/1	0.94	0.12	60,60,60,60	0
57	MG	1A	3953	1/1	0.94	0.12	60,60,60,60	0
57	MG	1A	3115	1/1	0.94	0.12	38,38,38,38	0
57	MG	1A	3956	1/1	0.94	0.18	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	K	1A	3512	1/1	0.94	0.10	54,54,54,54	0
57	MG	2A	3592	1/1	0.94	0.12	36,36,36,36	0
60	ZN	24	501	1/1	0.94	0.14	126,126,126,126	0
57	MG	1A	3024	1/1	0.95	0.16	35,35,35,35	0
57	MG	1A	3075	1/1	0.95	0.13	33,33,33,33	0
57	MG	2A	3669	1/1	0.95	0.13	73,73,73,73	0
57	MG	2A	3670	1/1	0.95	0.10	48,48,48,48	0
57	MG	1a	1750	1/1	0.95	0.07	64,64,64,64	0
57	MG	2A	3672	1/1	0.95	0.08	65,65,65,65	0
57	MG	1A	3226	1/1	0.95	0.19	31,31,31,31	0
57	MG	2A	3456	1/1	0.95	0.16	51,51,51,51	0
57	MG	2A	3265	1/1	0.95	0.11	60,60,60,60	0
57	MG	2A	3677	1/1	0.95	0.06	60,60,60,60	0
57	MG	17	105	1/1	0.95	0.09	50,50,50,50	0
57	MG	18	103	1/1	0.95	0.16	33,33,33,33	0
57	MG	1A	3231	1/1	0.95	0.22	42,42,42,42	0
57	MG	2a	1641	1/1	0.95	0.16	67,67,67,67	0
57	MG	2A	3269	1/1	0.95	0.16	66,66,66,66	0
57	MG	1a	1756	1/1	0.95	0.09	64,64,64,64	0
57	MG	1A	3833	1/1	0.95	0.15	32,32,32,32	0
57	MG	2a	1645	1/1	0.95	0.13	70,70,70,70	0
57	MG	1A	3968	1/1	0.95	0.05	37,37,37,37	0
57	MG	2A	3686	1/1	0.95	0.06	55,55,55,55	0
57	MG	2A	3471	1/1	0.95	0.09	45,45,45,45	0
57	MG	2A	3688	1/1	0.95	0.09	50,50,50,50	0
57	MG	2A	3098	1/1	0.95	0.15	49,49,49,49	0
57	MG	1A	3415	1/1	0.95	0.10	55,55,55,55	0
57	MG	1A	3972	1/1	0.95	0.07	46,46,46,46	0
57	MG	1A	3835	1/1	0.95	0.10	25,25,25,25	0
57	MG	1A	3076	1/1	0.95	0.19	42,42,42,42	0
57	MG	2A	3103	1/1	0.95	0.38	68,68,68,68	0
57	MG	1A	3289	1/1	0.95	0.38	56,56,56,56	0
57	MG	2A	3698	1/1	0.95	0.17	54,54,54,54	0
57	MG	1A	3291	1/1	0.95	0.09	61,61,61,61	0
57	MG	1A	3130	1/1	0.95	0.08	42,42,42,42	0
57	MG	1A	3503	1/1	0.95	0.10	44,44,44,44	0
57	MG	1a	1609	1/1	0.95	0.32	56,56,56,56	0
57	MG	2A	3705	1/1	0.95	0.13	51,51,51,51	0
57	MG	2A	3706	1/1	0.95	0.07	39,39,39,39	0
57	MG	1A	3734	1/1	0.95	0.06	27,27,27,27	0
57	MG	1a	1782	1/1	0.95	0.10	54,54,54,54	0
57	MG	1A	3983	1/1	0.95	0.06	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3606	1/1	0.95	0.06	31,31,31,31	0
57	MG	1A	3737	1/1	0.95	0.07	50,50,50,50	0
57	MG	2A	3493	1/1	0.95	0.07	64,64,64,64	0
57	MG	1A	3351	1/1	0.95	0.23	47,47,47,47	0
57	MG	2A	3117	1/1	0.95	0.08	54,54,54,54	0
57	MG	1A	3352	1/1	0.95	0.07	47,47,47,47	0
57	MG	1a	1793	1/1	0.95	0.17	65,65,65,65	0
57	MG	1a	1620	1/1	0.95	0.07	50,50,50,50	0
57	MG	2a	1678	1/1	0.95	0.14	55,55,55,55	0
57	MG	1A	3851	1/1	0.95	0.06	24,24,24,24	0
57	MG	1A	3508	1/1	0.95	0.18	36,36,36,36	0
57	MG	1A	3745	1/1	0.95	0.06	39,39,39,39	0
57	MG	2A	3126	1/1	0.95	0.15	61,61,61,61	0
57	MG	1A	3101	1/1	0.95	0.06	31,31,31,31	0
57	MG	1A	3186	1/1	0.95	0.27	33,33,33,33	0
57	MG	2A	3734	1/1	0.95	0.07	24,24,24,24	0
57	MG	1D	302	1/1	0.95	0.23	40,40,40,40	0
57	MG	1a	1628	1/1	0.95	0.11	43,43,43,43	0
57	MG	1D	303	1/1	0.95	0.17	39,39,39,39	0
57	MG	1D	305	1/1	0.95	0.07	41,41,41,41	0
57	MG	2A	3512	1/1	0.95	0.08	53,53,53,53	0
57	MG	1A	3102	1/1	0.95	0.20	40,40,40,40	0
57	MG	1A	3998	1/1	0.95	0.12	34,34,34,34	0
57	MG	1A	3143	1/1	0.95	0.24	39,39,39,39	0
57	MG	1A	3753	1/1	0.95	0.10	22,22,22,22	0
57	MG	1E	303	1/1	0.95	0.17	36,36,36,36	0
57	MG	2A	3312	1/1	0.95	0.25	69,69,69,69	0
57	MG	2A	3751	1/1	0.95	0.07	65,65,65,65	0
57	MG	1A	4005	1/1	0.95	0.08	26,26,26,26	0
57	MG	1A	3035	1/1	0.95	0.07	29,29,29,29	0
57	MG	2a	1701	1/1	0.95	0.12	51,51,51,51	0
57	MG	1A	3862	1/1	0.95	0.13	47,47,47,47	0
57	MG	1a	1813	1/1	0.95	0.06	47,47,47,47	0
57	MG	1A	3145	1/1	0.95	0.38	39,39,39,39	0
57	MG	1A	3146	1/1	0.95	0.16	34,34,34,34	0
57	MG	1F	301	1/1	0.95	0.11	34,34,34,34	0
57	MG	2A	3527	1/1	0.95	0.12	59,59,59,59	0
57	MG	1F	302	1/1	0.95	0.11	33,33,33,33	0
57	MG	1A	3366	1/1	0.95	0.08	44,44,44,44	0
57	MG	1A	3626	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3760	1/1	0.95	0.07	24,24,24,24	0
57	MG	2A	3533	1/1	0.95	0.06	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3534	1/1	0.95	0.17	63,63,63,63	0
57	MG	1A	3871	1/1	0.95	0.10	24,24,24,24	0
57	MG	1r	101	1/1	0.95	0.11	69,69,69,69	0
57	MG	1F	308	1/1	0.95	0.09	50,50,50,50	0
57	MG	2A	3773	1/1	0.95	0.14	70,70,70,70	0
57	MG	1A	3081	1/1	0.95	0.18	37,37,37,37	0
57	MG	2A	3540	1/1	0.95	0.08	48,48,48,48	0
57	MG	1w	102	1/1	0.95	0.10	49,49,49,49	0
57	MG	1A	4017	1/1	0.95	0.07	43,43,43,43	0
57	MG	1A	3764	1/1	0.95	0.36	30,30,30,30	0
57	MG	2A	3331	1/1	0.95	0.32	48,48,48,48	0
57	MG	2A	3546	1/1	0.95	0.11	46,46,46,46	0
57	MG	1A	3048	1/1	0.95	0.10	27,27,27,27	0
57	MG	2a	1727	1/1	0.95	0.09	71,71,71,71	0
57	MG	1A	3108	1/1	0.95	0.10	37,37,37,37	0
57	MG	1A	3370	1/1	0.95	0.15	52,52,52,52	0
57	MG	1A	3768	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3036	1/1	0.95	0.15	28,28,28,28	0
57	MG	1x	105	1/1	0.95	0.16	63,63,63,63	0
57	MG	2A	3789	1/1	0.95	0.13	55,55,55,55	0
57	MG	1A	3306	1/1	0.95	0.29	58,58,58,58	0
57	MG	2a	1738	1/1	0.95	0.06	75,75,75,75	0
57	MG	1G	205	1/1	0.95	0.10	49,49,49,49	0
57	MG	1A	3443	1/1	0.95	0.17	43,43,43,43	0
57	MG	1A	3200	1/1	0.95	0.10	36,36,36,36	0
57	MG	1x	110	1/1	0.95	0.07	22,22,22,22	0
57	MG	1a	1664	1/1	0.95	0.13	64,64,64,64	0
57	MG	1A	4031	1/1	0.95	0.11	40,40,40,40	0
57	MG	2A	3179	1/1	0.95	0.37	65,65,65,65	0
57	MG	1A	3249	1/1	0.95	0.13	40,40,40,40	0
57	MG	1A	3775	1/1	0.95	0.08	45,45,45,45	0
57	MG	1A	3892	1/1	0.95	0.12	62,62,62,62	0
57	MG	1O	203	1/1	0.95	0.18	55,55,55,55	0
57	MG	1A	3201	1/1	0.95	0.14	49,49,49,49	0
57	MG	2a	1755	1/1	0.95	0.11	46,46,46,46	0
57	MG	2A	3186	1/1	0.95	0.10	57,57,57,57	0
57	MG	1A	3777	1/1	0.95	0.06	26,26,26,26	0
57	MG	2A	3569	1/1	0.95	0.09	61,61,61,61	0
57	MG	1A	3310	1/1	0.95	0.12	51,51,51,51	0
57	MG	2a	1760	1/1	0.95	0.19	54,54,54,54	0
57	MG	1A	3312	1/1	0.95	0.16	49,49,49,49	0
57	MG	2A	3010	1/1	0.95	0.07	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3781	1/1	0.95	0.08	31,31,31,31	0
57	MG	1A	3452	1/1	0.95	0.08	65,65,65,65	0
57	MG	1A	3060	1/1	0.95	0.18	39,39,39,39	0
57	MG	1A	3029	1/1	0.95	0.28	31,31,31,31	0
57	MG	1A	3457	1/1	0.95	0.17	39,39,39,39	0
57	MG	1A	3113	1/1	0.95	0.11	34,34,34,34	0
57	MG	2A	3581	1/1	0.95	0.09	64,64,64,64	0
57	MG	1A	3160	1/1	0.95	0.14	35,35,35,35	0
57	MG	2A	3020	1/1	0.95	0.14	49,49,49,49	0
57	MG	2A	3022	1/1	0.95	0.28	47,47,47,47	0
57	MG	1R	202	1/1	0.95	0.19	37,37,37,37	0
57	MG	1A	3548	1/1	0.95	0.09	36,36,36,36	0
57	MG	2A	3202	1/1	0.95	0.18	50,50,50,50	0
57	MG	2D	307	1/1	0.95	0.15	68,68,68,68	0
57	MG	1a	1683	1/1	0.95	0.17	55,55,55,55	0
57	MG	1A	3911	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3383	1/1	0.95	0.24	54,54,54,54	0
57	MG	1A	3318	1/1	0.95	0.25	54,54,54,54	0
57	MG	1A	3209	1/1	0.95	0.30	44,44,44,44	0
57	MG	2A	3381	1/1	0.95	0.18	50,50,50,50	0
57	MG	2A	3208	1/1	0.95	0.07	54,54,54,54	0
57	MG	2A	3031	1/1	0.95	0.12	47,47,47,47	0
57	MG	2A	3384	1/1	0.95	0.08	63,63,63,63	0
57	MG	1A	3669	1/1	0.95	0.07	61,61,61,61	0
57	MG	2A	3211	1/1	0.95	0.11	49,49,49,49	0
57	MG	2a	1789	1/1	0.95	0.10	60,60,60,60	0
57	MG	2A	3387	1/1	0.95	0.14	53,53,53,53	0
57	MG	2F	304	1/1	0.95	0.09	49,49,49,49	0
57	MG	1A	3386	1/1	0.95	0.06	48,48,48,48	0
57	MG	1A	3555	1/1	0.95	0.21	54,54,54,54	0
57	MG	1A	3114	1/1	0.95	0.13	43,43,43,43	0
57	MG	1A	4070	1/1	0.95	0.10	45,45,45,45	0
57	MG	2a	1796	1/1	0.95	0.22	63,63,63,63	0
57	MG	1A	3051	1/1	0.95	0.08	54,54,54,54	0
57	MG	1a	1695	1/1	0.95	0.20	43,43,43,43	0
57	MG	2O	201	1/1	0.95	0.14	51,51,51,51	0
57	MG	1A	3322	1/1	0.95	0.32	39,39,39,39	0
57	MG	1A	3676	1/1	0.95	0.08	45,45,45,45	0
57	MG	1A	3091	1/1	0.95	0.09	32,32,32,32	0
57	MG	2Q	202	1/1	0.95	0.22	47,47,47,47	0
57	MG	1V	203	1/1	0.95	0.12	27,27,27,27	0
57	MG	1A	3092	1/1	0.95	0.15	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3618	1/1	0.95	0.08	47,47,47,47	0
57	MG	2A	3619	1/1	0.95	0.09	40,40,40,40	0
57	MG	1A	3562	1/1	0.95	0.07	46,46,46,46	0
57	MG	1a	1707	1/1	0.95	0.14	65,65,65,65	0
57	MG	1A	3393	1/1	0.95	0.17	47,47,47,47	0
57	MG	1W	204	1/1	0.95	0.09	38,38,38,38	0
57	MG	1A	3267	1/1	0.95	0.16	34,34,34,34	0
57	MG	20	101	1/1	0.95	0.07	63,63,63,63	0
57	MG	1a	1712	1/1	0.95	0.06	31,31,31,31	0
57	MG	1a	1716	1/1	0.95	0.07	69,69,69,69	0
57	MG	1A	3806	1/1	0.95	0.10	58,58,58,58	0
57	MG	1A	4080	1/1	0.95	0.17	43,43,43,43	0
57	MG	2A	3632	1/1	0.95	0.06	61,61,61,61	0
57	MG	1A	3931	1/1	0.95	0.07	72,72,72,72	0
57	MG	2A	3234	1/1	0.95	0.15	62,62,62,62	0
57	MG	1A	3119	1/1	0.95	0.20	32,32,32,32	0
57	MG	1a	1721	1/1	0.95	0.06	39,39,39,39	0
57	MG	2A	3237	1/1	0.95	0.30	53,53,53,53	0
57	MG	1A	3329	1/1	0.95	0.17	54,54,54,54	0
57	MG	1A	3397	1/1	0.95	0.16	42,42,42,42	0
57	MG	1a	1726	1/1	0.95	0.08	52,52,52,52	0
57	MG	2A	3241	1/1	0.95	0.23	63,63,63,63	0
57	MG	1A	3272	1/1	0.95	0.20	46,46,46,46	0
57	MG	1A	3812	1/1	0.95	0.12	18,18,18,18	0
57	MG	1A	3173	1/1	0.95	0.08	20,20,20,20	0
57	MG	1A	3217	1/1	0.95	0.10	22,22,22,22	0
57	MG	2A	3429	1/1	0.95	0.07	67,67,67,67	0
57	MG	1A	3574	1/1	0.95	0.13	13,13,13,13	0
57	MG	2A	3649	1/1	0.95	0.07	51,51,51,51	0
57	MG	11	101	1/1	0.95	0.41	39,39,39,39	0
57	MG	2A	3651	1/1	0.95	0.12	51,51,51,51	0
57	MG	2w	107	1/1	0.95	0.21	70,70,70,70	0
57	MG	1A	3402	1/1	0.95	0.07	61,61,61,61	0
57	MG	1A	3577	1/1	0.95	0.10	56,56,56,56	0
57	MG	2A	3654	1/1	0.95	0.08	58,58,58,58	0
57	MG	1A	3120	1/1	0.95	0.25	35,35,35,35	0
57	MG	1A	3066	1/1	0.95	0.18	31,31,31,31	0
57	MG	1A	3705	1/1	0.95	0.11	36,36,36,36	0
57	MG	1A	3005	1/1	0.95	0.09	45,45,45,45	0
57	MG	13	103	1/1	0.95	0.09	59,59,59,59	0
57	MG	1A	3824	1/1	0.95	0.09	42,42,42,42	0
57	MG	1A	3336	1/1	0.95	0.08	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3280	1/1	0.95	0.07	39,39,39,39	0
57	MG	1A	3095	1/1	0.95	0.06	42,42,42,42	0
59	TYK	1A	4101	64/64	0.95	0.09	16,30,46,51	0
57	MG	1A	3713	1/1	0.95	0.13	51,51,51,51	0
57	MG	2A	3447	1/1	0.95	0.10	41,41,41,41	0
57	MG	1U	206	1/1	0.96	0.18	33,33,33,33	0
57	MG	1a	1699	1/1	0.96	0.20	51,51,51,51	0
57	MG	2A	3048	1/1	0.96	0.09	48,48,48,48	0
57	MG	1U	207	1/1	0.96	0.24	38,38,38,38	0
57	MG	2a	1625	1/1	0.96	0.07	86,86,86,86	0
57	MG	2A	3437	1/1	0.96	0.05	33,33,33,33	0
57	MG	1a	1701	1/1	0.96	0.17	38,38,38,38	0
57	MG	1A	3453	1/1	0.96	0.27	48,48,48,48	0
57	MG	1A	3175	1/1	0.96	0.06	38,38,38,38	0
57	MG	1a	1705	1/1	0.96	0.11	55,55,55,55	0
57	MG	2A	3054	1/1	0.96	0.11	45,45,45,45	0
57	MG	1a	1706	1/1	0.96	0.31	63,63,63,63	0
57	MG	1A	3932	1/1	0.96	0.11	43,43,43,43	0
57	MG	1A	3818	1/1	0.96	0.12	41,41,41,41	0
57	MG	1A	3078	1/1	0.96	0.21	34,34,34,34	0
57	MG	1A	3298	1/1	0.96	0.21	39,39,39,39	0
57	MG	1A	3937	1/1	0.96	0.10	53,53,53,53	0
57	MG	1a	1713	1/1	0.96	0.12	37,37,37,37	0
57	MG	2A	3451	1/1	0.96	0.09	42,42,42,42	0
57	MG	1a	1715	1/1	0.96	0.14	57,57,57,57	0
57	MG	2A	3250	1/1	0.96	0.21	57,57,57,57	0
57	MG	1A	3720	1/1	0.96	0.07	29,29,29,29	0
57	MG	1W	205	1/1	0.96	0.06	35,35,35,35	0
57	MG	2A	3682	1/1	0.96	0.07	67,67,67,67	0
57	MG	2A	3459	1/1	0.96	0.13	38,38,38,38	0
57	MG	1W	206	1/1	0.96	0.13	28,28,28,28	0
57	MG	2A	3461	1/1	0.96	0.10	57,57,57,57	0
57	MG	2A	3462	1/1	0.96	0.07	31,31,31,31	0
57	MG	1X	102	1/1	0.96	0.12	37,37,37,37	0
57	MG	1A	3721	1/1	0.96	0.09	42,42,42,42	0
57	MG	2A	3465	1/1	0.96	0.06	60,60,60,60	0
57	MG	1X	105	1/1	0.96	0.07	51,51,51,51	0
57	MG	1A	3530	1/1	0.96	0.09	41,41,41,41	0
57	MG	2A	3693	1/1	0.96	0.13	71,71,71,71	0
57	MG	2A	3468	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3117	1/1	0.96	0.22	37,37,37,37	0
57	MG	1a	1725	1/1	0.96	0.07	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3614	1/1	0.96	0.16	50,50,50,50	0
57	MG	1Z	302	1/1	0.96	0.25	47,47,47,47	0
57	MG	1A	3615	1/1	0.96	0.11	36,36,36,36	0
57	MG	2A	3701	1/1	0.96	0.04	46,46,46,46	0
57	MG	1A	3726	1/1	0.96	0.06	31,31,31,31	0
57	MG	1A	3616	1/1	0.96	0.05	25,25,25,25	0
57	MG	1A	3080	1/1	0.96	0.11	34,34,34,34	0
57	MG	10	106	1/1	0.96	0.27	64,64,64,64	0
57	MG	1A	3733	1/1	0.96	0.05	36,36,36,36	0
57	MG	1A	3399	1/1	0.96	0.25	34,34,34,34	0
57	MG	1A	3619	1/1	0.96	0.08	19,19,19,19	0
57	MG	1A	4090	1/1	0.96	0.31	31,31,31,31	0
57	MG	2a	1672	1/1	0.96	0.14	56,56,56,56	0
57	MG	1A	3346	1/1	0.96	0.14	38,38,38,38	0
57	MG	1A	3301	1/1	0.96	0.19	39,39,39,39	0
57	MG	1A	3148	1/1	0.96	0.06	32,32,32,32	0
57	MG	2A	3488	1/1	0.96	0.10	52,52,52,52	0
57	MG	2A	3715	1/1	0.96	0.07	38,38,38,38	0
57	MG	1A	3955	1/1	0.96	0.08	16,16,16,16	0
57	MG	2A	3089	1/1	0.96	0.10	46,46,46,46	0
57	MG	2A	3090	1/1	0.96	0.09	51,51,51,51	0
57	MG	1A	3625	1/1	0.96	0.05	21,21,21,21	0
57	MG	1A	3021	1/1	0.96	0.07	47,47,47,47	0
57	MG	2A	3726	1/1	0.96	0.06	61,61,61,61	0
57	MG	1A	3181	1/1	0.96	0.15	39,39,39,39	0
57	MG	2A	3280	1/1	0.96	0.14	47,47,47,47	0
57	MG	1A	4098	1/1	0.96	0.10	51,51,51,51	0
57	MG	1A	3631	1/1	0.96	0.05	17,17,17,17	0
57	MG	1A	3009	1/1	0.96	0.04	22,22,22,22	0
57	MG	1A	3963	1/1	0.96	0.06	34,34,34,34	0
57	MG	1A	3964	1/1	0.96	0.10	24,24,24,24	0
57	MG	2A	3736	1/1	0.96	0.05	56,56,56,56	0
57	MG	1A	3965	1/1	0.96	0.05	32,32,32,32	0
57	MG	15	105	1/1	0.96	0.13	43,43,43,43	0
57	MG	2a	1694	1/1	0.96	0.16	63,63,63,63	0
57	MG	1A	3749	1/1	0.96	0.10	47,47,47,47	0
57	MG	1A	3543	1/1	0.96	0.18	55,55,55,55	0
57	MG	17	101	1/1	0.96	0.05	32,32,32,32	0
57	MG	2A	3105	1/1	0.96	0.23	55,55,55,55	0
57	MG	1A	3847	1/1	0.96	0.07	42,42,42,42	0
57	MG	2A	3744	1/1	0.96	0.14	43,43,43,43	0
57	MG	1A	3354	1/1	0.96	0.20	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3747	1/1	0.96	0.08	58,58,58,58	0
57	MG	2A	3108	1/1	0.96	0.12	40,40,40,40	0
57	MG	18	101	1/1	0.96	0.18	53,53,53,53	0
57	MG	2a	1705	1/1	0.96	0.16	44,44,44,44	0
57	MG	2A	3750	1/1	0.96	0.07	59,59,59,59	0
57	MG	18	102	1/1	0.96	0.12	39,39,39,39	0
57	MG	1A	3973	1/1	0.96	0.04	54,54,54,54	0
57	MG	18	104	1/1	0.96	0.18	41,41,41,41	0
57	MG	1a	1771	1/1	0.96	0.09	45,45,45,45	0
57	MG	1A	3183	1/1	0.96	0.19	45,45,45,45	0
57	MG	1a	1775	1/1	0.96	0.06	62,62,62,62	0
57	MG	1A	3154	1/1	0.96	0.13	30,30,30,30	0
57	MG	1A	3473	1/1	0.96	0.30	38,38,38,38	0
57	MG	1A	3155	1/1	0.96	0.14	27,27,27,27	0
57	MG	2A	3525	1/1	0.96	0.08	35,35,35,35	0
57	MG	1A	3260	1/1	0.96	0.29	47,47,47,47	0
57	MG	1A	3980	1/1	0.96	0.06	54,54,54,54	0
57	MG	1A	3063	1/1	0.96	0.04	31,31,31,31	0
57	MG	2A	3122	1/1	0.96	0.09	44,44,44,44	0
57	MG	1a	1784	1/1	0.96	0.07	46,46,46,46	0
57	MG	1a	1785	1/1	0.96	0.10	59,59,59,59	0
57	MG	1a	1788	1/1	0.96	0.20	50,50,50,50	0
57	MG	2A	3770	1/1	0.96	0.10	58,58,58,58	0
57	MG	1A	3761	1/1	0.96	0.10	20,20,20,20	0
57	MG	1A	3762	1/1	0.96	0.05	37,37,37,37	0
57	MG	2A	3130	1/1	0.96	0.15	43,43,43,43	0
57	MG	1A	3984	1/1	0.96	0.08	43,43,43,43	0
57	MG	1A	3311	1/1	0.96	0.13	54,54,54,54	0
57	MG	2A	3133	1/1	0.96	0.15	60,60,60,60	0
57	MG	1A	3650	1/1	0.96	0.07	61,61,61,61	0
57	MG	1B	225	1/1	0.96	0.08	37,37,37,37	0
57	MG	1A	3988	1/1	0.96	0.06	51,51,51,51	0
57	MG	2A	3781	1/1	0.96	0.06	52,52,52,52	0
57	MG	1A	3263	1/1	0.96	0.20	39,39,39,39	0
57	MG	1A	3266	1/1	0.96	0.23	28,28,28,28	0
57	MG	1A	3041	1/1	0.96	0.16	30,30,30,30	0
57	MG	1A	3017	1/1	0.96	0.15	28,28,28,28	0
57	MG	1A	3658	1/1	0.96	0.12	31,31,31,31	0
57	MG	2a	1744	1/1	0.96	0.17	64,64,64,64	0
57	MG	1a	1621	1/1	0.96	0.05	43,43,43,43	0
57	MG	1A	3659	1/1	0.96	0.04	23,23,23,23	0
57	MG	1a	1803	1/1	0.96	0.07	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3145	1/1	0.96	0.06	55,55,55,55	0
57	MG	1A	3483	1/1	0.96	0.14	35,35,35,35	0
57	MG	1B	234	1/1	0.96	0.06	37,37,37,37	0
57	MG	2a	1752	1/1	0.96	0.09	53,53,53,53	0
57	MG	2A	3148	1/1	0.96	0.25	46,46,46,46	0
57	MG	1D	301	1/1	0.96	0.16	36,36,36,36	0
57	MG	2A	3150	1/1	0.96	0.13	63,63,63,63	0
57	MG	2A	3338	1/1	0.96	0.08	39,39,39,39	0
57	MG	1A	3772	1/1	0.96	0.08	30,30,30,30	0
57	MG	1A	3054	1/1	0.96	0.06	28,28,28,28	0
57	MG	1A	3662	1/1	0.96	0.06	27,27,27,27	0
57	MG	1D	308	1/1	0.96	0.11	47,47,47,47	0
57	MG	1A	3420	1/1	0.96	0.17	43,43,43,43	0
57	MG	1D	310	1/1	0.96	0.15	26,26,26,26	0
57	MG	1A	4001	1/1	0.96	0.07	29,29,29,29	0
57	MG	1A	4003	1/1	0.96	0.07	45,45,45,45	0
57	MG	1A	3191	1/1	0.96	0.06	40,40,40,40	0
57	MG	1A	3877	1/1	0.96	0.14	33,33,33,33	0
57	MG	2a	1767	1/1	0.96	0.39	69,69,69,69	0
57	MG	2A	3571	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	3274	1/1	0.96	0.07	37,37,37,37	0
57	MG	1E	306	1/1	0.96	0.11	23,23,23,23	0
57	MG	1A	3778	1/1	0.96	0.09	28,28,28,28	0
57	MG	1a	1640	1/1	0.96	0.34	61,61,61,61	0
57	MG	1m	3001	1/1	0.96	0.13	58,58,58,58	0
57	MG	2A	3169	1/1	0.96	0.12	40,40,40,40	0
57	MG	1A	3228	1/1	0.96	0.16	24,24,24,24	0
57	MG	1A	3230	1/1	0.96	0.23	28,28,28,28	0
57	MG	1A	3192	1/1	0.96	0.13	29,29,29,29	0
57	MG	1A	3883	1/1	0.96	0.09	45,45,45,45	0
57	MG	1w	101	1/1	0.96	0.13	43,43,43,43	0
57	MG	1A	3376	1/1	0.96	0.06	42,42,42,42	0
57	MG	1A	3323	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	3888	1/1	0.96	0.06	70,70,70,70	0
57	MG	2A	3587	1/1	0.96	0.15	68,68,68,68	0
57	MG	1A	3891	1/1	0.96	0.07	33,33,33,33	0
57	MG	1A	3232	1/1	0.96	0.05	46,46,46,46	0
57	MG	2A	3366	1/1	0.96	0.17	46,46,46,46	0
57	MG	1A	3893	1/1	0.96	0.10	43,43,43,43	0
57	MG	1A	3109	1/1	0.96	0.05	33,33,33,33	0
57	MG	1A	3573	1/1	0.96	0.07	35,35,35,35	0
57	MG	2A	3370	1/1	0.96	0.16	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3183	1/1	0.96	0.19	56,56,56,56	0
57	MG	1a	1654	1/1	0.96	0.14	61,61,61,61	0
57	MG	1A	3194	1/1	0.96	0.07	22,22,22,22	0
57	MG	1A	3161	1/1	0.96	0.06	38,38,38,38	0
57	MG	2A	3600	1/1	0.96	0.08	58,58,58,58	0
57	MG	1A	3027	1/1	0.96	0.32	32,32,32,32	0
57	MG	1A	3902	1/1	0.96	0.06	47,47,47,47	0
57	MG	1G	201	1/1	0.96	0.14	39,39,39,39	0
57	MG	1A	3071	1/1	0.96	0.33	47,47,47,47	0
57	MG	1A	4032	1/1	0.96	0.13	40,40,40,40	0
57	MG	1A	3436	1/1	0.96	0.14	46,46,46,46	0
57	MG	2A	3607	1/1	0.96	0.09	50,50,50,50	0
57	MG	1A	4034	1/1	0.96	0.15	48,48,48,48	0
57	MG	2A	3610	1/1	0.96	0.08	39,39,39,39	0
57	MG	1A	3504	1/1	0.96	0.22	37,37,37,37	0
57	MG	1A	3132	1/1	0.96	0.15	29,29,29,29	0
57	MG	2Q	203	1/1	0.96	0.05	48,48,48,48	0
57	MG	1A	3506	1/1	0.96	0.17	34,34,34,34	0
57	MG	1A	3689	1/1	0.96	0.08	56,56,56,56	0
57	MG	2A	3006	1/1	0.96	0.06	40,40,40,40	0
57	MG	2a	1813	1/1	0.96	0.13	45,45,45,45	0
57	MG	1A	3073	1/1	0.96	0.10	31,31,31,31	0
57	MG	1A	3046	1/1	0.96	0.06	35,35,35,35	0
57	MG	1O	202	1/1	0.96	0.12	50,50,50,50	0
57	MG	1A	3387	1/1	0.96	0.08	51,51,51,51	0
57	MG	2a	1819	1/1	0.96	0.07	69,69,69,69	0
57	MG	1A	3290	1/1	0.96	0.06	35,35,35,35	0
57	MG	2A	3623	1/1	0.96	0.12	69,69,69,69	0
57	MG	2X	101	1/1	0.96	0.06	65,65,65,65	0
57	MG	1A	3169	1/1	0.96	0.26	29,29,29,29	0
57	MG	1A	4045	1/1	0.96	0.10	44,44,44,44	0
57	MG	1A	3593	1/1	0.96	0.07	22,22,22,22	0
57	MG	1P	202	1/1	0.96	0.22	26,26,26,26	0
57	MG	23	102	1/1	0.96	0.06	54,54,54,54	0
57	MG	1A	3172	1/1	0.96	0.10	35,35,35,35	0
57	MG	1A	3596	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	3047	1/1	0.96	0.17	34,34,34,34	0
57	MG	1Q	201	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	3028	1/1	0.96	0.07	41,41,41,41	0
57	MG	1A	3706	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	4052	1/1	0.96	0.05	50,50,50,50	0
57	MG	1A	4054	1/1	0.96	0.12	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	4056	1/1	0.96	0.07	50,50,50,50	0
57	MG	2w	101	1/1	0.96	0.22	66,66,66,66	0
57	MG	1A	4057	1/1	0.96	0.07	51,51,51,51	0
57	MG	28	105	1/1	0.96	0.08	63,63,63,63	0
57	MG	2A	3411	1/1	0.96	0.08	52,52,52,52	0
57	MG	1A	4058	1/1	0.96	0.06	35,35,35,35	0
57	MG	2A	3032	1/1	0.96	0.07	25,25,25,25	0
57	MG	1A	3450	1/1	0.96	0.05	43,43,43,43	0
57	MG	2A	3034	1/1	0.96	0.21	60,60,60,60	0
57	MG	2A	3416	1/1	0.96	0.09	35,35,35,35	0
57	MG	1a	1689	1/1	0.96	0.07	53,53,53,53	0
57	MG	1A	3522	1/1	0.96	0.28	38,38,38,38	0
57	MG	1A	4061	1/1	0.96	0.06	40,40,40,40	0
57	MG	2A	3420	1/1	0.96	0.15	48,48,48,48	0
57	MG	1A	4062	1/1	0.96	0.14	48,48,48,48	0
57	MG	1A	3451	1/1	0.96	0.17	46,46,46,46	0
57	MG	1A	3926	1/1	0.96	0.14	61,61,61,61	0
57	MG	2A	3228	1/1	0.96	0.09	54,54,54,54	0
57	MG	1A	3604	1/1	0.96	0.07	29,29,29,29	0
57	MG	2a	1615	1/1	0.96	0.32	62,62,62,62	0
57	MG	1A	3207	1/1	0.96	0.11	36,36,36,36	0
57	MG	1A	3714	1/1	0.96	0.08	51,51,51,51	0
60	ZN	2Y	202	1/1	0.96	0.05	105,105,105,105	0
57	MG	2A	3045	1/1	0.96	0.12	55,55,55,55	0
57	MG	1U	201	1/1	0.97	0.13	30,30,30,30	0
57	MG	2A	3422	1/1	0.97	0.11	59,59,59,59	0
57	MG	1A	3521	1/1	0.97	0.14	40,40,40,40	0
57	MG	1U	203	1/1	0.97	0.16	53,53,53,53	0
57	MG	1U	204	1/1	0.97	0.13	35,35,35,35	0
57	MG	2A	3426	1/1	0.97	0.06	44,44,44,44	0
57	MG	1A	3137	1/1	0.97	0.13	51,51,51,51	0
57	MG	1A	3339	1/1	0.97	0.16	48,48,48,48	0
57	MG	1A	3592	1/1	0.97	0.07	27,27,27,27	0
57	MG	2A	3125	1/1	0.97	0.17	44,44,44,44	0
57	MG	2A	3431	1/1	0.97	0.07	53,53,53,53	0
57	MG	1n	101	1/1	0.97	0.15	46,46,46,46	0
57	MG	2A	3127	1/1	0.97	0.18	44,44,44,44	0
57	MG	1A	3138	1/1	0.97	0.12	57,57,57,57	0
57	MG	1A	3594	1/1	0.97	0.11	58,58,58,58	0
57	MG	1A	3087	1/1	0.97	0.10	27,27,27,27	0
57	MG	1V	202	1/1	0.97	0.16	36,36,36,36	0
57	MG	1A	3470	1/1	0.97	0.20	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3212	1/1	0.97	0.07	45,45,45,45	0
57	MG	1A	3684	1/1	0.97	0.15	50,50,50,50	0
57	MG	1A	3685	1/1	0.97	0.08	44,44,44,44	0
57	MG	1W	202	1/1	0.97	0.09	57,57,57,57	0
57	MG	1W	203	1/1	0.97	0.19	33,33,33,33	0
57	MG	2A	3285	1/1	0.97	0.07	58,58,58,58	0
57	MG	1B	202	1/1	0.97	0.17	49,49,49,49	0
57	MG	1A	3188	1/1	0.97	0.28	31,31,31,31	0
57	MG	1A	3599	1/1	0.97	0.04	16,16,16,16	0
57	MG	2A	3621	1/1	0.97	0.07	34,34,34,34	0
57	MG	1A	3020	1/1	0.97	0.13	26,26,26,26	0
57	MG	1A	3425	1/1	0.97	0.20	37,37,37,37	0
57	MG	1B	207	1/1	0.97	0.07	42,42,42,42	0
57	MG	1A	3693	1/1	0.97	0.07	52,52,52,52	0
57	MG	2A	3453	1/1	0.97	0.10	38,38,38,38	0
57	MG	1A	3884	1/1	0.97	0.06	45,45,45,45	0
57	MG	1A	3065	1/1	0.97	0.06	14,14,14,14	0
57	MG	1A	3168	1/1	0.97	0.09	37,37,37,37	0
57	MG	1A	3605	1/1	0.97	0.04	27,27,27,27	0
57	MG	1A	3697	1/1	0.97	0.07	53,53,53,53	0
57	MG	1A	3090	1/1	0.97	0.19	37,37,37,37	0
57	MG	10	104	1/1	0.97	0.11	44,44,44,44	0
57	MG	1B	215	1/1	0.97	0.05	55,55,55,55	0
57	MG	2A	3154	1/1	0.97	0.09	60,60,60,60	0
57	MG	1A	3699	1/1	0.97	0.11	29,29,29,29	0
57	MG	1A	4002	1/1	0.97	0.05	34,34,34,34	0
57	MG	1A	3700	1/1	0.97	0.07	24,24,24,24	0
57	MG	2D	304	1/1	0.97	0.05	27,27,27,27	0
57	MG	1A	3535	1/1	0.97	0.15	28,28,28,28	0
57	MG	2A	3469	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	3171	1/1	0.97	0.07	34,34,34,34	0
57	MG	1a	1702	1/1	0.97	0.11	38,38,38,38	0
57	MG	1A	3349	1/1	0.97	0.09	40,40,40,40	0
57	MG	2A	3162	1/1	0.97	0.06	34,34,34,34	0
57	MG	2E	303	1/1	0.97	0.10	43,43,43,43	0
57	MG	1A	3350	1/1	0.97	0.17	24,24,24,24	0
57	MG	1A	3032	1/1	0.97	0.38	27,27,27,27	0
57	MG	1A	3801	1/1	0.97	0.05	53,53,53,53	0
57	MG	1A	3482	1/1	0.97	0.19	37,37,37,37	0
57	MG	1A	3905	1/1	0.97	0.07	62,62,62,62	0
57	MG	2A	3479	1/1	0.97	0.06	39,39,39,39	0
57	MG	2A	3480	1/1	0.97	0.07	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1736	1/1	0.97	0.21	56,56,56,56	0
57	MG	1A	3542	1/1	0.97	0.08	37,37,37,37	0
57	MG	12	103	1/1	0.97	0.10	43,43,43,43	0
57	MG	2A	3021	1/1	0.97	0.08	44,44,44,44	0
57	MG	13	101	1/1	0.97	0.05	36,36,36,36	0
57	MG	13	102	1/1	0.97	0.10	39,39,39,39	0
57	MG	2A	3024	1/1	0.97	0.11	39,39,39,39	0
57	MG	1A	3250	1/1	0.97	0.15	51,51,51,51	0
57	MG	2a	1746	1/1	0.97	0.09	64,64,64,64	0
57	MG	1A	4016	1/1	0.97	0.04	25,25,25,25	0
57	MG	13	105	1/1	0.97	0.06	52,52,52,52	0
57	MG	1A	3317	1/1	0.97	0.26	41,41,41,41	0
57	MG	1A	3286	1/1	0.97	0.10	31,31,31,31	0
57	MG	1A	3107	1/1	0.97	0.10	33,33,33,33	0
57	MG	1A	3043	1/1	0.97	0.08	42,42,42,42	0
57	MG	2A	3667	1/1	0.97	0.06	50,50,50,50	0
57	MG	1A	3441	1/1	0.97	0.12	64,64,64,64	0
57	MG	1A	3913	1/1	0.97	0.05	43,43,43,43	0
57	MG	1A	3489	1/1	0.97	0.18	38,38,38,38	0
57	MG	1A	3811	1/1	0.97	0.06	64,64,64,64	0
57	MG	17	102	1/1	0.97	0.11	33,33,33,33	0
57	MG	2A	3673	1/1	0.97	0.06	49,49,49,49	0
57	MG	1D	306	1/1	0.97	0.06	29,29,29,29	0
57	MG	1A	3037	1/1	0.97	0.16	32,32,32,32	0
57	MG	1a	1730	1/1	0.97	0.08	54,54,54,54	0
57	MG	1A	3624	1/1	0.97	0.05	29,29,29,29	0
57	MG	2W	202	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3551	1/1	0.97	0.07	33,33,33,33	0
57	MG	1A	3010	1/1	0.97	0.08	31,31,31,31	0
57	MG	1A	3225	1/1	0.97	0.10	61,61,61,61	0
57	MG	1A	3324	1/1	0.97	0.20	30,30,30,30	0
57	MG	1A	3365	1/1	0.97	0.18	42,42,42,42	0
57	MG	1A	3819	1/1	0.97	0.05	43,43,43,43	0
57	MG	1A	3083	1/1	0.97	0.12	39,39,39,39	0
57	MG	1A	3637	1/1	0.97	0.08	45,45,45,45	0
57	MG	1A	3730	1/1	0.97	0.05	22,22,22,22	0
57	MG	1A	3638	1/1	0.97	0.05	31,31,31,31	0
57	MG	1A	3496	1/1	0.97	0.26	54,54,54,54	0
57	MG	1A	3640	1/1	0.97	0.07	22,22,22,22	0
57	MG	1A	4043	1/1	0.97	0.15	55,55,55,55	0
57	MG	2A	3691	1/1	0.97	0.08	57,57,57,57	0
57	MG	1a	1607	1/1	0.97	0.27	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3735	1/1	0.97	0.09	25,25,25,25	0
57	MG	1A	3497	1/1	0.97	0.11	47,47,47,47	0
57	MG	1A	3560	1/1	0.97	0.07	21,21,21,21	0
57	MG	1A	3644	1/1	0.97	0.06	26,26,26,26	0
57	MG	1A	3448	1/1	0.97	0.11	37,37,37,37	0
57	MG	1A	3404	1/1	0.97	0.16	37,37,37,37	0
57	MG	2A	3528	1/1	0.97	0.04	36,36,36,36	0
57	MG	1F	310	1/1	0.97	0.09	29,29,29,29	0
57	MG	1A	3743	1/1	0.97	0.04	38,38,38,38	0
57	MG	2A	3361	1/1	0.97	0.20	54,54,54,54	0
57	MG	1a	1617	1/1	0.97	0.13	45,45,45,45	0
57	MG	1a	1759	1/1	0.97	0.05	67,67,67,67	0
57	MG	1a	1619	1/1	0.97	0.05	51,51,51,51	0
57	MG	1A	3128	1/1	0.97	0.04	36,36,36,36	0
57	MG	1A	3564	1/1	0.97	0.12	53,53,53,53	0
57	MG	1A	4053	1/1	0.97	0.13	24,24,24,24	0
57	MG	2A	3070	1/1	0.97	0.11	28,28,28,28	0
57	MG	1A	3229	1/1	0.97	0.09	45,45,45,45	0
57	MG	1a	1766	1/1	0.97	0.11	64,64,64,64	0
57	MG	2A	3371	1/1	0.97	0.07	24,24,24,24	0
57	MG	1a	1768	1/1	0.97	0.06	53,53,53,53	0
57	MG	2A	3544	1/1	0.97	0.13	50,50,50,50	0
57	MG	2a	1803	1/1	0.97	0.12	61,61,61,61	0
57	MG	2A	3373	1/1	0.97	0.40	42,42,42,42	0
57	MG	2a	1621	1/1	0.97	0.19	61,61,61,61	0
57	MG	2a	1622	1/1	0.97	0.08	59,59,59,59	0
57	MG	1A	4055	1/1	0.97	0.08	58,58,58,58	0
57	MG	2A	3721	1/1	0.97	0.13	64,64,64,64	0
57	MG	1A	3502	1/1	0.97	0.06	28,28,28,28	0
57	MG	1A	3015	1/1	0.97	0.16	37,37,37,37	0
57	MG	2A	3724	1/1	0.97	0.10	56,56,56,56	0
57	MG	1A	3055	1/1	0.97	0.22	49,49,49,49	0
57	MG	1A	3839	1/1	0.97	0.06	30,30,30,30	0
57	MG	2A	3079	1/1	0.97	0.09	58,58,58,58	0
57	MG	1A	3751	1/1	0.97	0.06	23,23,23,23	0
57	MG	1A	3655	1/1	0.97	0.06	28,28,28,28	0
57	MG	2A	3732	1/1	0.97	0.07	64,64,64,64	0
57	MG	1A	3842	1/1	0.97	0.05	23,23,23,23	0
57	MG	1a	1781	1/1	0.97	0.09	53,53,53,53	0
57	MG	2a	1821	1/1	0.97	0.06	66,66,66,66	0
57	MG	1A	3409	1/1	0.97	0.26	39,39,39,39	0
57	MG	1A	3455	1/1	0.97	0.17	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	4065	1/1	0.97	0.11	51,51,51,51	0
57	MG	1A	3952	1/1	0.97	0.04	48,48,48,48	0
57	MG	1a	1786	1/1	0.97	0.05	53,53,53,53	0
57	MG	1a	1787	1/1	0.97	0.05	52,52,52,52	0
57	MG	1A	3756	1/1	0.97	0.05	39,39,39,39	0
57	MG	2A	3563	1/1	0.97	0.09	71,71,71,71	0
57	MG	1A	4068	1/1	0.97	0.15	36,36,36,36	0
57	MG	1A	3261	1/1	0.97	0.17	33,33,33,33	0
57	MG	2A	3745	1/1	0.97	0.09	57,57,57,57	0
57	MG	1A	3131	1/1	0.97	0.08	28,28,28,28	0
57	MG	1A	3086	1/1	0.97	0.09	59,59,59,59	0
57	MG	1A	3850	1/1	0.97	0.09	21,21,21,21	0
57	MG	1A	3959	1/1	0.97	0.06	53,53,53,53	0
57	MG	1A	3264	1/1	0.97	0.05	49,49,49,49	0
57	MG	1A	3265	1/1	0.97	0.18	40,40,40,40	0
57	MG	2A	3572	1/1	0.97	0.10	56,56,56,56	0
57	MG	1A	3205	1/1	0.97	0.06	48,48,48,48	0
57	MG	1Q	203	1/1	0.97	0.14	52,52,52,52	0
57	MG	1A	3664	1/1	0.97	0.07	38,38,38,38	0
57	MG	1A	3100	1/1	0.97	0.08	41,41,41,41	0
57	MG	1A	3515	1/1	0.97	0.11	31,31,31,31	0
57	MG	1A	3857	1/1	0.97	0.06	34,34,34,34	0
57	MG	2a	1660	1/1	0.97	0.17	42,42,42,42	0
57	MG	1R	201	1/1	0.97	0.18	43,43,43,43	0
57	MG	2a	1662	1/1	0.97	0.09	51,51,51,51	0
57	MG	1A	4081	1/1	0.97	0.07	57,57,57,57	0
57	MG	1R	203	1/1	0.97	0.36	38,38,38,38	0
57	MG	1A	3967	1/1	0.97	0.07	28,28,28,28	0
57	MG	1A	3464	1/1	0.97	0.19	29,29,29,29	0
57	MG	1A	3969	1/1	0.97	0.08	37,37,37,37	0
57	MG	1A	3517	1/1	0.97	0.14	23,23,23,23	0
57	MG	1A	3134	1/1	0.97	0.10	41,41,41,41	0
57	MG	1A	3520	1/1	0.97	0.22	40,40,40,40	0
57	MG	1A	3587	1/1	0.97	0.04	41,41,41,41	0
57	MG	1A	3588	1/1	0.97	0.04	18,18,18,18	0
60	ZN	14	102	1/1	0.97	0.07	100,100,100,100	0
57	MG	2A	3772	1/1	0.97	0.04	49,49,49,49	0
57	MG	1A	3976	1/1	0.97	0.06	57,57,57,57	0
57	MG	1D	307	1/1	0.98	0.16	36,36,36,36	0
57	MG	1A	3692	1/1	0.98	0.05	46,46,46,46	0
57	MG	1U	208	1/1	0.98	0.29	37,37,37,37	0
57	MG	2A	3446	1/1	0.98	0.07	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1618	1/1	0.98	0.04	36,36,36,36	0
57	MG	1A	3074	1/1	0.98	0.11	42,42,42,42	0
57	MG	1A	3752	1/1	0.98	0.05	20,20,20,20	0
57	MG	1A	3642	1/1	0.98	0.07	29,29,29,29	0
57	MG	1A	3008	1/1	0.98	0.04	26,26,26,26	0
57	MG	1E	301	1/1	0.98	0.24	36,36,36,36	0
57	MG	1A	3236	1/1	0.98	0.18	36,36,36,36	0
57	MG	2A	3454	1/1	0.98	0.09	35,35,35,35	0
57	MG	2A	3455	1/1	0.98	0.10	35,35,35,35	0
57	MG	2A	3152	1/1	0.98	0.10	58,58,58,58	0
57	MG	1a	1709	1/1	0.98	0.06	41,41,41,41	0
57	MG	1A	3003	1/1	0.98	0.04	22,22,22,22	0
57	MG	1E	304	1/1	0.98	0.14	29,29,29,29	0
57	MG	1A	3149	1/1	0.98	0.11	37,37,37,37	0
57	MG	1A	3519	1/1	0.98	0.17	35,35,35,35	0
57	MG	1A	3150	1/1	0.98	0.16	48,48,48,48	0
57	MG	1A	3240	1/1	0.98	0.06	48,48,48,48	0
57	MG	1A	3007	1/1	0.98	0.05	35,35,35,35	0
57	MG	1X	101	1/1	0.98	0.22	40,40,40,40	0
57	MG	1A	3945	1/1	0.98	0.07	26,26,26,26	0
57	MG	1X	103	1/1	0.98	0.05	44,44,44,44	0
57	MG	1A	3651	1/1	0.98	0.09	28,28,28,28	0
57	MG	1A	3602	1/1	0.98	0.14	24,24,24,24	0
57	MG	1f	201	1/1	0.98	0.10	41,41,41,41	0
57	MG	1A	4015	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3011	1/1	0.98	0.12	48,48,48,48	0
57	MG	1A	3269	1/1	0.98	0.08	30,30,30,30	0
57	MG	1F	306	1/1	0.98	0.20	36,36,36,36	0
57	MG	1A	3355	1/1	0.98	0.31	27,27,27,27	0
57	MG	1A	4019	1/1	0.98	0.05	41,41,41,41	0
57	MG	1A	3710	1/1	0.98	0.07	19,19,19,19	0
57	MG	1A	4021	1/1	0.98	0.09	19,19,19,19	0
57	MG	1A	3270	1/1	0.98	0.17	33,33,33,33	0
57	MG	1A	3527	1/1	0.98	0.23	34,34,34,34	0
57	MG	1A	3890	1/1	0.98	0.03	31,31,31,31	0
57	MG	1A	4026	1/1	0.98	0.05	46,46,46,46	0
57	MG	2A	3594	1/1	0.98	0.05	65,65,65,65	0
57	MG	2A	3708	1/1	0.98	0.11	39,39,39,39	0
57	MG	2A	3377	1/1	0.98	0.04	37,37,37,37	0
57	MG	1a	1650	1/1	0.98	0.08	44,44,44,44	0
57	MG	1A	3357	1/1	0.98	0.23	27,27,27,27	0
57	MG	1A	3609	1/1	0.98	0.06	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3358	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3958	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3894	1/1	0.98	0.03	54,54,54,54	0
57	MG	1A	3153	1/1	0.98	0.11	32,32,32,32	0
57	MG	1a	1744	1/1	0.98	0.06	43,43,43,43	0
57	MG	1A	3896	1/1	0.98	0.03	36,36,36,36	0
57	MG	1A	3079	1/1	0.98	0.30	33,33,33,33	0
57	MG	2A	3497	1/1	0.98	0.04	40,40,40,40	0
57	MG	1A	3105	1/1	0.98	0.06	40,40,40,40	0
57	MG	2a	1797	1/1	0.98	0.17	54,54,54,54	0
57	MG	1N	202	1/1	0.98	0.04	45,45,45,45	0
57	MG	2A	3725	1/1	0.98	0.06	42,42,42,42	0
57	MG	2A	3500	1/1	0.98	0.08	59,59,59,59	0
57	MG	2A	3093	1/1	0.98	0.05	28,28,28,28	0
57	MG	2A	3728	1/1	0.98	0.07	36,36,36,36	0
57	MG	1N	203	1/1	0.98	0.04	44,44,44,44	0
57	MG	1A	3362	1/1	0.98	0.04	29,29,29,29	0
57	MG	1A	3221	1/1	0.98	0.13	42,42,42,42	0
57	MG	1A	3901	1/1	0.98	0.04	53,53,53,53	0
57	MG	1a	1753	1/1	0.98	0.05	66,66,66,66	0
57	MG	2A	3002	1/1	0.98	0.27	49,49,49,49	0
57	MG	1A	3013	1/1	0.98	0.12	29,29,29,29	0
57	MG	1A	3135	1/1	0.98	0.10	33,33,33,33	0
57	MG	1A	3069	1/1	0.98	0.06	27,27,27,27	0
57	MG	1a	1757	1/1	0.98	0.06	45,45,45,45	0
57	MG	1A	3121	1/1	0.98	0.16	33,33,33,33	0
57	MG	2A	3624	1/1	0.98	0.06	33,33,33,33	0
57	MG	2a	1815	1/1	0.98	0.05	67,67,67,67	0
57	MG	1A	3971	1/1	0.98	0.07	38,38,38,38	0
57	MG	2A	3009	1/1	0.98	0.04	40,40,40,40	0
57	MG	2A	3404	1/1	0.98	0.07	63,63,63,63	0
57	MG	1A	3671	1/1	0.98	0.06	21,21,21,21	0
57	MG	2X	102	1/1	0.98	0.12	48,48,48,48	0
57	MG	2Y	201	1/1	0.98	0.16	60,60,60,60	0
57	MG	1A	3539	1/1	0.98	0.19	49,49,49,49	0
57	MG	2A	3012	1/1	0.98	0.06	48,48,48,48	0
57	MG	2A	3306	1/1	0.98	0.06	43,43,43,43	0
57	MG	1a	1762	1/1	0.98	0.06	64,64,64,64	0
57	MG	23	101	1/1	0.98	0.06	58,58,58,58	0
57	MG	1A	3728	1/1	0.98	0.05	54,54,54,54	0
57	MG	1B	216	1/1	0.98	0.15	38,38,38,38	0
57	MG	1A	3729	1/1	0.98	0.09	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3580	1/1	0.98	0.07	27,27,27,27	0
57	MG	2A	3018	1/1	0.98	0.11	33,33,33,33	0
57	MG	1A	3731	1/1	0.98	0.05	40,40,40,40	0
57	MG	1a	1769	1/1	0.98	0.09	58,58,58,58	0
57	MG	1A	3622	1/1	0.98	0.05	39,39,39,39	0
57	MG	2A	3641	1/1	0.98	0.20	41,41,41,41	0
57	MG	1A	3846	1/1	0.98	0.07	46,46,46,46	0
57	MG	1A	3044	1/1	0.98	0.05	35,35,35,35	0
57	MG	2A	3421	1/1	0.98	0.07	39,39,39,39	0
57	MG	2A	3761	1/1	0.98	0.06	57,57,57,57	0
57	MG	1a	1773	1/1	0.98	0.04	63,63,63,63	0
57	MG	1A	3227	1/1	0.98	0.13	29,29,29,29	0
57	MG	1A	3141	1/1	0.98	0.15	32,32,32,32	0
57	MG	1A	3142	1/1	0.98	0.06	32,32,32,32	0
57	MG	1A	3585	1/1	0.98	0.07	56,56,56,56	0
57	MG	1A	3738	1/1	0.98	0.09	48,48,48,48	0
57	MG	1A	3628	1/1	0.98	0.06	36,36,36,36	0
57	MG	1A	3629	1/1	0.98	0.04	21,21,21,21	0
57	MG	1A	3741	1/1	0.98	0.09	47,47,47,47	0
57	MG	1A	3437	1/1	0.98	0.07	45,45,45,45	0
57	MG	1A	3438	1/1	0.98	0.06	45,45,45,45	0
57	MG	1A	3744	1/1	0.98	0.05	42,42,42,42	0
57	MG	1A	3284	1/1	0.98	0.14	41,41,41,41	0
57	MG	2a	1731	1/1	0.98	0.04	70,70,70,70	0
57	MG	2A	3037	1/1	0.98	0.06	52,52,52,52	0
57	MG	1A	3030	1/1	0.98	0.09	22,22,22,22	0
57	MG	1A	3995	1/1	0.98	0.07	37,37,37,37	0
57	MG	1A	3164	1/1	0.98	0.10	17,17,17,17	0
57	MG	1a	1611	1/1	0.98	0.05	29,29,29,29	0
57	MG	1D	304	1/1	0.98	0.08	22,22,22,22	0
57	MG	1A	3072	1/1	0.98	0.12	39,39,39,39	0
57	MG	1A	3053	1/1	0.98	0.07	33,33,33,33	0
60	ZN	29	102	1/1	0.98	0.04	78,78,78,78	0
60	ZN	2n	501	1/1	0.98	0.04	86,86,86,86	0
61	SF4	2d	303	8/8	0.98	0.04	67,73,84,84	0
57	MG	1A	3268	1/1	0.99	0.14	33,33,33,33	0
57	MG	2A	3490	1/1	0.99	0.06	35,35,35,35	0
57	MG	2A	3716	1/1	0.99	0.07	37,37,37,37	0
57	MG	1Q	202	1/1	0.99	0.03	35,35,35,35	0
57	MG	2a	1743	1/1	0.99	0.09	69,69,69,69	0
57	MG	2A	3718	1/1	0.99	0.04	51,51,51,51	0
57	MG	2A	3492	1/1	0.99	0.04	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3921	1/1	0.99	0.03	27,27,27,27	0
57	MG	2A	3337	1/1	0.99	0.05	32,32,32,32	0
57	MG	1A	3031	1/1	0.99	0.11	23,23,23,23	0
57	MG	1X	106	1/1	0.99	0.05	34,34,34,34	0
57	MG	1A	3886	1/1	0.99	0.03	12,12,12,12	0
57	MG	1a	1735	1/1	0.99	0.10	58,58,58,58	0
57	MG	2A	3786	1/1	0.99	0.03	64,64,64,64	0
57	MG	1A	3067	1/1	0.99	0.04	16,16,16,16	0
57	MG	1A	3098	1/1	0.99	0.21	35,35,35,35	0
57	MG	1A	3553	1/1	0.99	0.29	31,31,31,31	0
57	MG	1A	3426	1/1	0.99	0.07	43,43,43,43	0
57	MG	1A	3703	1/1	0.99	0.07	46,46,46,46	0
57	MG	2A	3616	1/1	0.99	0.04	49,49,49,49	0
57	MG	1A	4004	1/1	0.99	0.03	41,41,41,41	0
57	MG	1A	3652	1/1	0.99	0.05	40,40,40,40	0
57	MG	1A	3572	1/1	0.99	0.04	21,21,21,21	0
57	MG	1A	3678	1/1	0.99	0.04	16,16,16,16	0
57	MG	1A	3630	1/1	0.99	0.07	26,26,26,26	0
57	MG	1A	3860	1/1	0.99	0.04	36,36,36,36	0
57	MG	1A	3708	1/1	0.99	0.04	42,42,42,42	0
57	MG	1A	3935	1/1	0.99	0.04	39,39,39,39	0
57	MG	2A	3406	1/1	0.99	0.06	65,65,65,65	0
57	MG	1A	3799	1/1	0.99	0.06	32,32,32,32	0
57	MG	1A	3136	1/1	0.99	0.06	16,16,16,16	0
57	MG	1A	3062	1/1	0.99	0.11	30,30,30,30	0
57	MG	1A	3633	1/1	0.99	0.04	27,27,27,27	0
57	MG	1A	3634	1/1	0.99	0.05	20,20,20,20	0
57	MG	1A	3635	1/1	0.99	0.02	26,26,26,26	0
57	MG	1A	3869	1/1	0.99	0.03	25,25,25,25	0
57	MG	1A	3870	1/1	0.99	0.03	26,26,26,26	0
57	MG	1A	3575	1/1	0.99	0.06	29,29,29,29	0
57	MG	1A	3012	1/1	0.99	0.03	23,23,23,23	0
57	MG	1A	4022	1/1	0.99	0.05	22,22,22,22	0
57	MG	1A	3687	1/1	0.99	0.06	21,21,21,21	0
57	MG	1A	3717	1/1	0.99	0.07	41,41,41,41	0
57	MG	1a	1714	1/1	0.99	0.08	45,45,45,45	0
57	MG	1A	3688	1/1	0.99	0.05	21,21,21,21	0
57	MG	1A	3122	1/1	0.99	0.18	32,32,32,32	0
57	MG	1A	3987	1/1	0.99	0.03	21,21,21,21	0
57	MG	15	103	1/1	0.99	0.32	28,28,28,28	0
57	MG	2A	3700	1/1	0.99	0.03	47,47,47,47	0
57	MG	1a	1767	1/1	0.99	0.04	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3170	1/1	0.99	0.14	27,27,27,27	0
57	MG	1A	3462	1/1	0.99	0.19	39,39,39,39	0
57	MG	2A	3535	1/1	0.99	0.08	38,38,38,38	0
57	MG	1A	3140	1/1	0.99	0.12	32,32,32,32	0
57	MG	1a	1722	1/1	0.99	0.05	35,35,35,35	0
57	MG	2A	3766	1/1	0.99	0.05	54,54,54,54	0
57	MG	1A	3014	1/1	0.99	0.04	28,28,28,28	0
57	MG	1a	1632	1/1	0.99	0.09	23,23,23,23	0
60	ZN	1Y	203	1/1	0.99	0.03	68,68,68,68	0
57	MG	1a	1774	1/1	0.99	0.03	44,44,44,44	0
60	ZN	15	107	1/1	0.99	0.03	43,43,43,43	0
60	ZN	16	102	1/1	0.99	0.03	44,44,44,44	0
60	ZN	19	102	1/1	0.99	0.04	42,42,42,42	0
60	ZN	1n	102	1/1	0.99	0.03	57,57,57,57	0
57	MG	1A	3279	1/1	0.99	0.20	30,30,30,30	0
57	MG	1A	3206	1/1	0.99	0.11	39,39,39,39	0
60	ZN	25	105	1/1	0.99	0.04	57,57,57,57	0
60	ZN	26	501	1/1	0.99	0.03	61,61,61,61	0
57	MG	17	103	1/1	0.99	0.05	29,29,29,29	0
57	MG	2a	1737	1/1	0.99	0.03	52,52,52,52	0
61	SF4	1d	501	8/8	0.99	0.06	56,62,68,68	0
57	MG	1A	3040	1/1	0.99	0.06	35,35,35,35	0
57	MG	2A	3608	1/1	1.00	0.02	32,32,32,32	0
57	MG	2A	3496	1/1	1.00	0.05	33,33,33,33	0
57	MG	1A	3889	1/1	1.00	0.04	23,23,23,23	0
57	MG	1a	1776	1/1	1.00	0.05	49,49,49,49	0
57	MG	1A	3864	1/1	1.00	0.06	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.