



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2025 – 09:11 PM EDT

PDB ID : 5W4K
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with Klebsazolicin and bound to mRNA and A-, P- and E-site tRNAs at 2.7Å resolution
Authors : Metelev, M.; Osterman, I.A.; Ghilarov, D.; Khabibullina, N.F.; Yakimov, A.; Shabalin, K.; Utkina, I.; Travin, D.Y.; Komarova, E.S.; Serebryakova, M.; Artamonova, T.; Khodorkovskii, M.; Konevega, A.L.; Sergiev, P.V.; Severinov, K.; Polikanov, Y.S.
Deposited on : 2017-06-12
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)

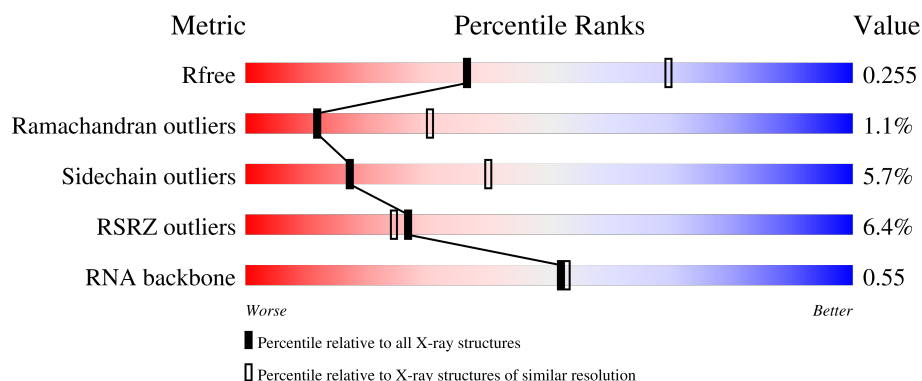
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


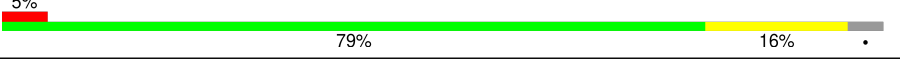

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3333 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)
RNA backbone	3690	1028 (2.94-2.46)

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	
1	2A	2915	
2	1B	121	

Continued on next page...



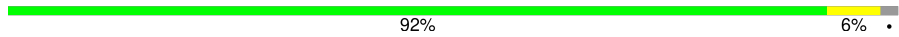
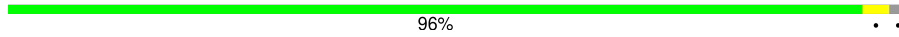

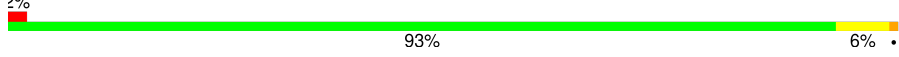
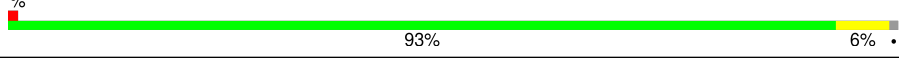
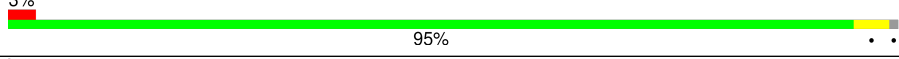
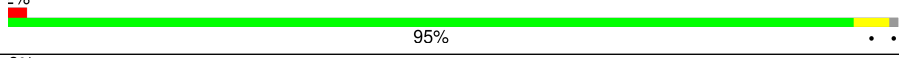
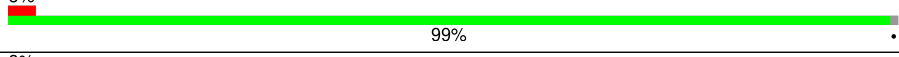
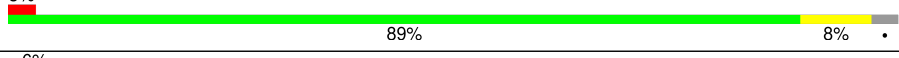
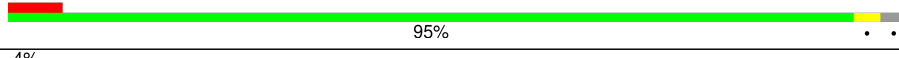


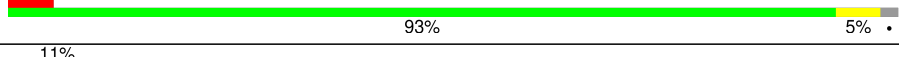
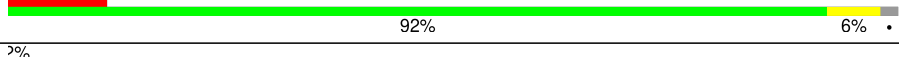
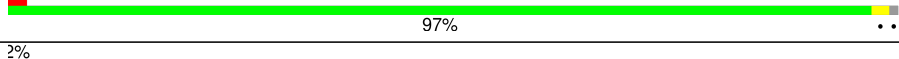
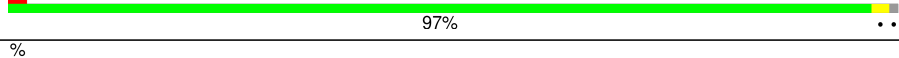
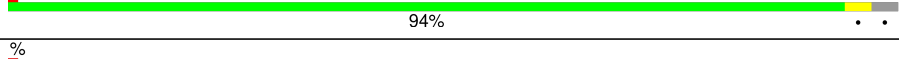
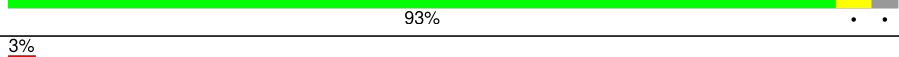
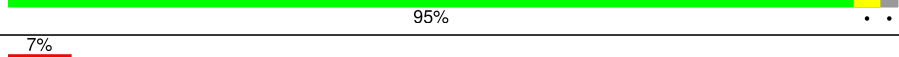
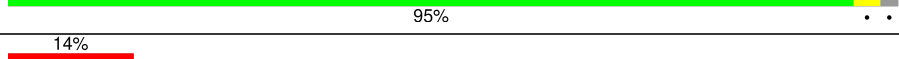

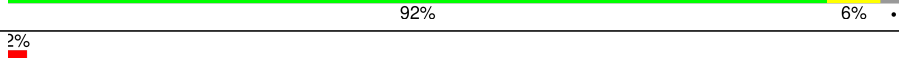
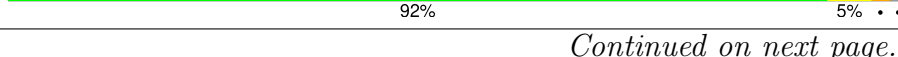
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

Continued from previous page...

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





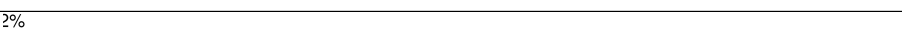


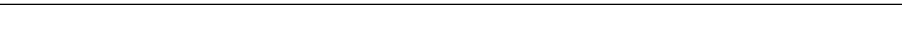
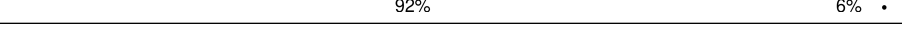
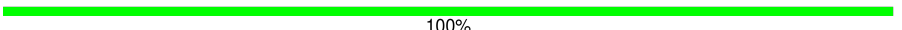

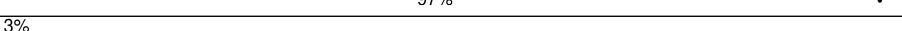


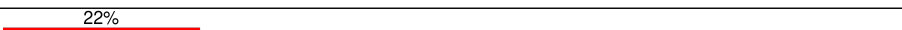




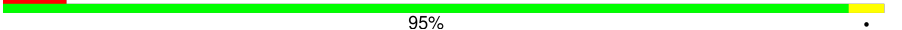





Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	25	60	 92% 7% .
28	16	54	 87% 11% .
28	26	54	 93% 6% .
29	17	49	 2% 88% 10% .
29	27	49	 2% 90% 8% .
30	18	65	 88% 11% .
30	28	65	 92% 6% .
31	19	37	 100%
31	29	37	 8% 97% .
32	1a	1521	 3% 82% 16% ..
33	1b	256	 14% 84% 6% 10%
33	2b	256	 22% 83% 7% 10%
34	1c	239	 2% 83% . 14%
34	2c	239	 28% 85% . 14%
35	1d	209	 7% 95% .
35	2d	209	 9% 93% 6%
36	1e	162	 % 86% 5% 9%
36	2e	162	 17% 87% . 9%
37	1f	101	 96% . .
37	2f	101	 % 96% . .
38	1g	156	 6% 94% 6% .
38	2g	156	 10% 94% 5% .
39	1h	138	 2% 96% . .
39	2h	138	 6% 96% . .
40	1i	128	 6% 95% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1y	76	
56	2y	76	
57	2a	1521	
58	A	18	
58	B	18	

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
59	MG	1A	3515	-	-	-	X
59	MG	1a	3435	-	-	-	X
59	MG	1y	104	-	-	-	X
59	MG	2a	3118	-	-	-	X

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 302030 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			

- 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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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 mRNA.

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

Continued on next page...

Continued from previous page...

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

- Molecule 54 is a RNA chain called tRNA, A-site and E-site tRNAs.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0
			1592	713	285	518	74	2		
54	2w	72	Total	C	N	O	P	S	0	0
			1544	690	278	502	72	2		

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		
55	2x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 56 is a RNA chain called tRNA.

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

- Molecule 57 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	2a	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

- Molecule 58 is a protein called Klebsazolicin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	A	18	Total	C	N	O	S	0	0	0
			115	64	23	25	3			
58	B	18	Total	C	N	O	S	0	0	0
			115	64	23	25	3			

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1229	Total Mg 1229 1229	0	0
59	1B	38	Total Mg 38 38	0	0
59	1D	13	Total Mg 13 13	0	0
59	1E	14	Total Mg 14 14	0	0
59	1F	10	Total Mg 10 10	0	0
59	1G	5	Total Mg 5 5	0	0
59	1I	1	Total Mg 1 1	0	0
59	1N	9	Total Mg 9 9	0	0
59	1O	6	Total Mg 6 6	0	0
59	1P	4	Total Mg 4 4	0	0
59	1Q	6	Total Mg 6 6	0	0
59	1R	3	Total Mg 3 3	0	0
59	1S	3	Total Mg 3 3	0	0
59	1T	2	Total Mg 2 2	0	0
59	1U	5	Total Mg 5 5	0	0
59	1V	2	Total Mg 2 2	0	0
59	1W	5	Total Mg 5 5	0	0
59	1X	5	Total Mg 5 5	0	0
59	1Y	3	Total Mg 3 3	0	0
59	1Z	4	Total Mg 4 4	0	0
59	10	8	Total Mg 8 8	0	0
59	11	3	Total Mg 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	12	2	Total 2	Mg 2	0	0
59	13	3	Total 3	Mg 3	0	0
59	15	2	Total 2	Mg 2	0	0
59	16	3	Total 3	Mg 3	0	0
59	17	2	Total 2	Mg 2	0	0
59	18	3	Total 3	Mg 3	0	0
59	19	1	Total 1	Mg 1	0	0
59	1a	278	Total 278	Mg 278	0	0
59	1b	2	Total 2	Mg 2	0	0
59	1d	1	Total 1	Mg 1	0	0
59	1e	1	Total 1	Mg 1	0	0
59	1f	3	Total 3	Mg 3	0	0
59	1k	1	Total 1	Mg 1	0	0
59	1l	3	Total 3	Mg 3	0	0
59	1n	2	Total 2	Mg 2	0	0
59	1p	1	Total 1	Mg 1	0	0
59	1s	1	Total 1	Mg 1	0	0
59	1t	1	Total 1	Mg 1	0	0
59	1v	1	Total 1	Mg 1	0	0
59	1w	12	Total 12	Mg 12	0	0
59	1x	17	Total 17	Mg 17	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1y	5	Total 5	Mg 5	0	0
59	2A	848	Total 848	Mg 848	0	0
59	2B	22	Total 22	Mg 22	0	0
59	2D	5	Total 5	Mg 5	0	0
59	2E	7	Total 7	Mg 7	0	0
59	2F	4	Total 4	Mg 4	0	0
59	2G	1	Total 1	Mg 1	0	0
59	2N	1	Total 1	Mg 1	0	0
59	2O	2	Total 2	Mg 2	0	0
59	2P	1	Total 1	Mg 1	0	0
59	2Q	4	Total 4	Mg 4	0	0
59	2R	3	Total 3	Mg 3	0	0
59	2S	1	Total 1	Mg 1	0	0
59	2T	3	Total 3	Mg 3	0	0
59	2U	4	Total 4	Mg 4	0	0
59	2V	1	Total 1	Mg 1	0	0
59	2X	2	Total 2	Mg 2	0	0
59	2Z	1	Total 1	Mg 1	0	0
59	20	3	Total 3	Mg 3	0	0
59	23	2	Total 2	Mg 2	0	0
59	25	3	Total 3	Mg 3	0	0

Continued on next page...

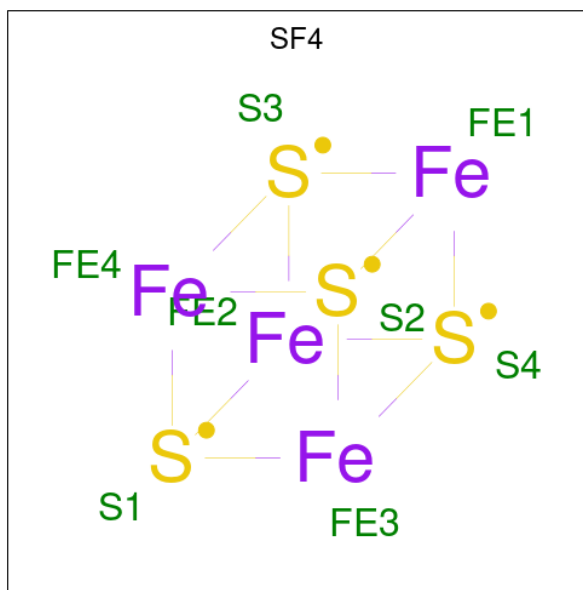
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	27	1	Total 1	Mg 1	0	0
59	28	2	Total 2	Mg 2	0	0
59	2a	239	Total 239	Mg 239	0	0
59	2d	1	Total 1	Mg 1	0	0
59	2e	1	Total 1	Mg 1	0	0
59	2f	2	Total 2	Mg 2	0	0
59	2g	1	Total 1	Mg 1	0	0
59	2j	2	Total 2	Mg 2	0	0
59	2k	1	Total 1	Mg 1	0	0
59	2l	2	Total 2	Mg 2	0	0
59	2p	1	Total 1	Mg 1	0	0
59	2q	5	Total 5	Mg 5	0	0
59	2r	1	Total 1	Mg 1	0	0
59	2t	1	Total 1	Mg 1	0	0
59	2v	4	Total 4	Mg 4	0	0
59	2w	7	Total 7	Mg 7	0	0
59	2x	4	Total 4	Mg 4	0	0
59	2y	7	Total 7	Mg 7	0	0
59	A	1	Total 1	Mg 1	0	0
59	B	1	Total 1	Mg 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1Y	1	Total Zn 1 1	0	0
60	14	1	Total Zn 1 1	0	0
60	15	1	Total Zn 1 1	0	0
60	16	1	Total Zn 1 1	0	0
60	19	1	Total Zn 1 1	0	0
60	1n	1	Total Zn 1 1	0	0
60	2Y	1	Total Zn 1 1	0	0
60	24	1	Total Zn 1 1	0	0
60	25	1	Total Zn 1 1	0	0
60	26	1	Total Zn 1 1	0	0
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

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



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

- Molecule 62 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2A	1	Total	K	0	0
			1	1		

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1A	2636	Total	O	0	0
			2636	2636		
63	1B	71	Total	O	0	0
			71	71		
63	1D	31	Total	O	0	0
			31	31		
63	1E	35	Total	O	0	0
			35	35		
63	1F	18	Total	O	0	0
			18	18		
63	1G	6	Total	O	0	0
			6	6		
63	1H	3	Total	O	0	0
			3	3		
63	1I	2	Total	O	0	0
			2	2		
63	1N	10	Total	O	0	0
			10	10		
63	1O	8	Total	O	0	0
			8	8		
63	1P	23	Total	O	0	0
			23	23		
63	1Q	16	Total	O	0	0
			16	16		
63	1R	14	Total	O	0	0
			14	14		
63	1S	4	Total	O	0	0
			4	4		
63	1T	9	Total	O	0	0
			9	9		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1U	13	Total 13	O 13	0	0
63	1V	9	Total 9	O 9	0	0
63	1W	11	Total 11	O 11	0	0
63	1X	8	Total 8	O 8	0	0
63	1Y	7	Total 7	O 7	0	0
63	1Z	2	Total 2	O 2	0	0
63	10	12	Total 12	O 12	0	0
63	11	13	Total 13	O 13	0	0
63	12	4	Total 4	O 4	0	0
63	13	5	Total 5	O 5	0	0
63	14	1	Total 1	O 1	0	0
63	15	5	Total 5	O 5	0	0
63	16	5	Total 5	O 5	0	0
63	17	9	Total 9	O 9	0	0
63	18	13	Total 13	O 13	0	0
63	19	1	Total 1	O 1	0	0
63	1a	523	Total 523	O 523	0	0
63	1b	1	Total 1	O 1	0	0
63	1d	3	Total 3	O 3	0	0
63	1e	3	Total 3	O 3	0	0
63	1g	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1k	3	Total 3	O 3	0	0
63	1l	10	Total 10	O 10	0	0
63	1m	1	Total 1	O 1	0	0
63	1o	2	Total 2	O 2	0	0
63	1p	1	Total 1	O 1	0	0
63	1q	4	Total 4	O 4	0	0
63	1r	1	Total 1	O 1	0	0
63	1t	2	Total 2	O 2	0	0
63	1v	6	Total 6	O 6	0	0
63	1w	26	Total 26	O 26	0	0
63	1x	18	Total 18	O 18	0	0
63	1y	2	Total 2	O 2	0	0
63	2A	1602	Total 1602	O 1602	0	0
63	2B	28	Total 28	O 28	0	0
63	2D	29	Total 29	O 29	0	0
63	2E	15	Total 15	O 15	0	0
63	2F	20	Total 20	O 20	0	0
63	2I	4	Total 4	O 4	0	0
63	2N	2	Total 2	O 2	0	0
63	2P	15	Total 15	O 15	0	0
63	2Q	2	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	2R	5	Total 5	O 5	0	0
63	2T	6	Total 6	O 6	0	0
63	2U	6	Total 6	O 6	0	0
63	2V	4	Total 4	O 4	0	0
63	2W	4	Total 4	O 4	0	0
63	2X	4	Total 4	O 4	0	0
63	2Y	1	Total 1	O 1	0	0
63	2Z	2	Total 2	O 2	0	0
63	20	5	Total 5	O 5	0	0
63	21	14	Total 14	O 14	0	0
63	22	1	Total 1	O 1	0	0
63	23	2	Total 2	O 2	0	0
63	25	4	Total 4	O 4	0	0
63	27	7	Total 7	O 7	0	0
63	28	7	Total 7	O 7	0	0
63	29	1	Total 1	O 1	0	0
63	2a	389	Total 389	O 389	0	0
63	2d	3	Total 3	O 3	0	0
63	2e	3	Total 3	O 3	0	0
63	2f	1	Total 1	O 1	0	0
63	2g	1	Total 1	O 1	0	0

Continued on next page...

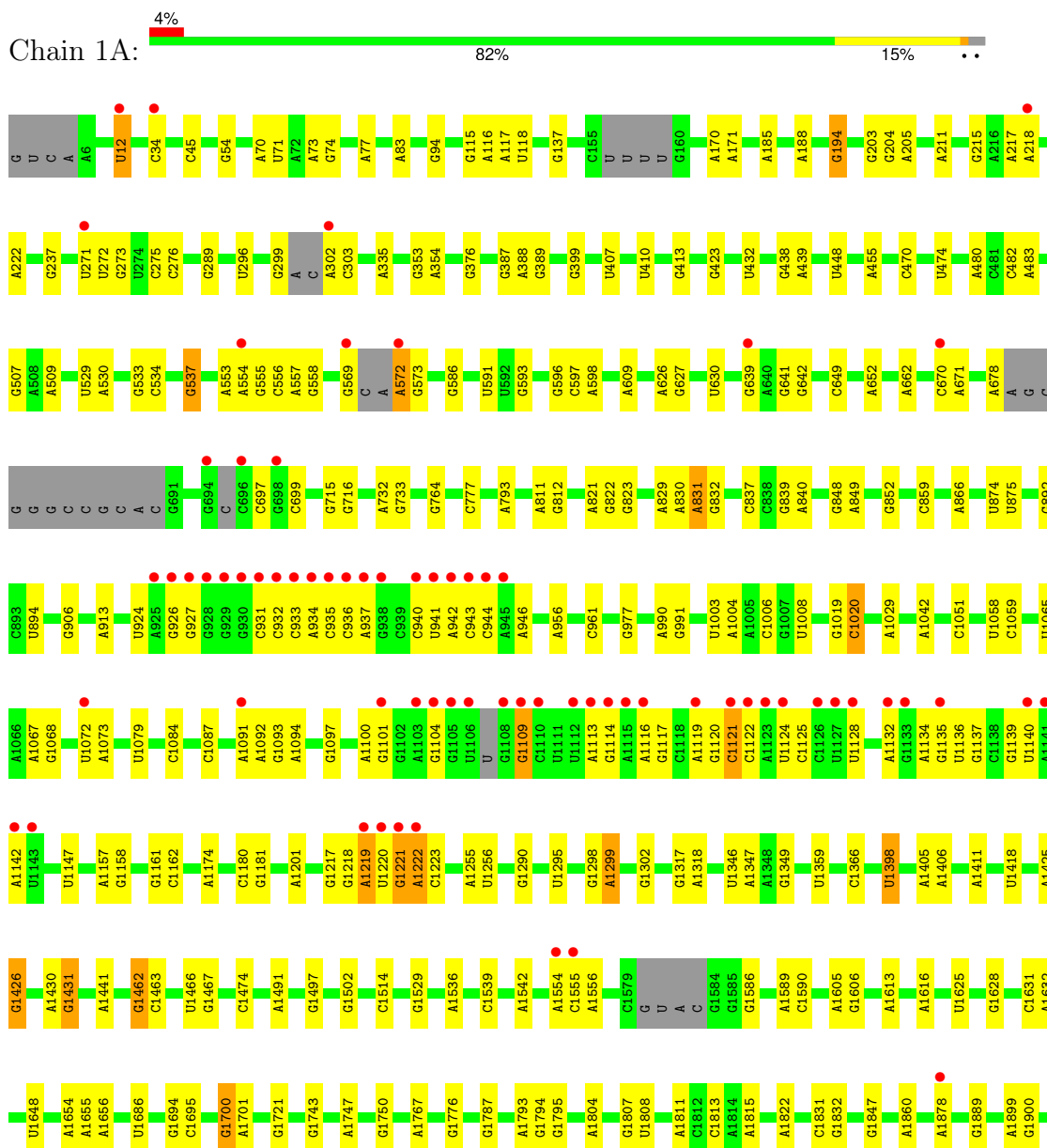
Continued from previous page...

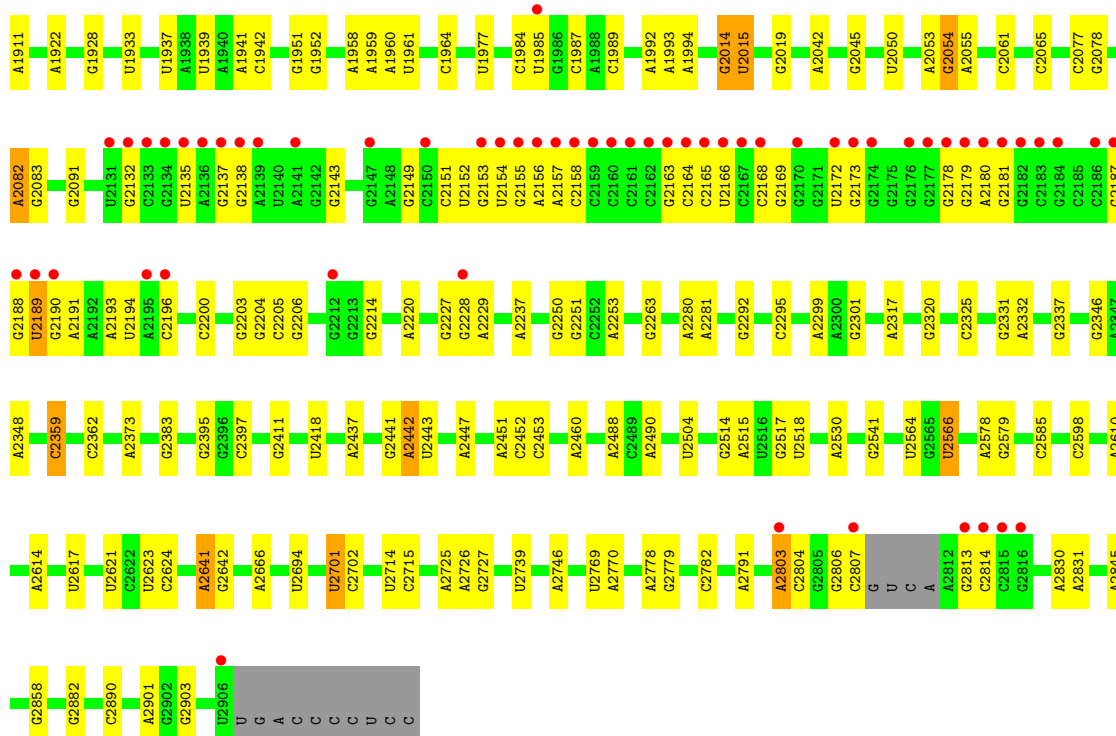
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	2h	2	Total	O	0	0
			2	2		
63	2i	1	Total	O	0	0
			1	1		
63	2j	4	Total	O	0	0
			4	4		
63	2l	5	Total	O	0	0
			5	5		
63	2o	1	Total	O	0	0
			1	1		
63	2p	3	Total	O	0	0
			3	3		
63	2q	2	Total	O	0	0
			2	2		
63	2r	1	Total	O	0	0
			1	1		
63	2t	3	Total	O	0	0
			3	3		
63	2u	1	Total	O	0	0
			1	1		
63	2v	1	Total	O	0	0
			1	1		
63	2w	3	Total	O	0	0
			3	3		
63	2x	10	Total	O	0	0
			10	10		
63	2y	20	Total	O	0	0
			20	20		
63	A	4	Total	O	0	0
			4	4		
63	B	2	Total	O	0	0
			2	2		

3 Residue-property plots [i](#)

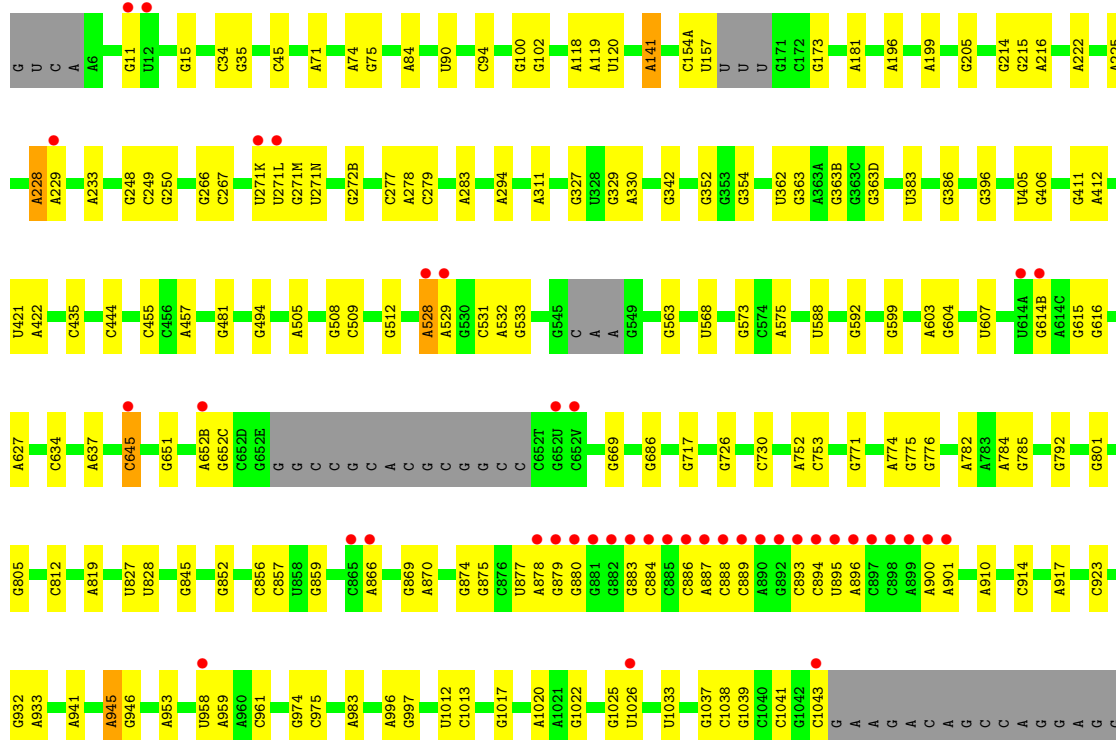
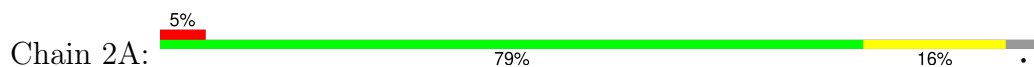
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

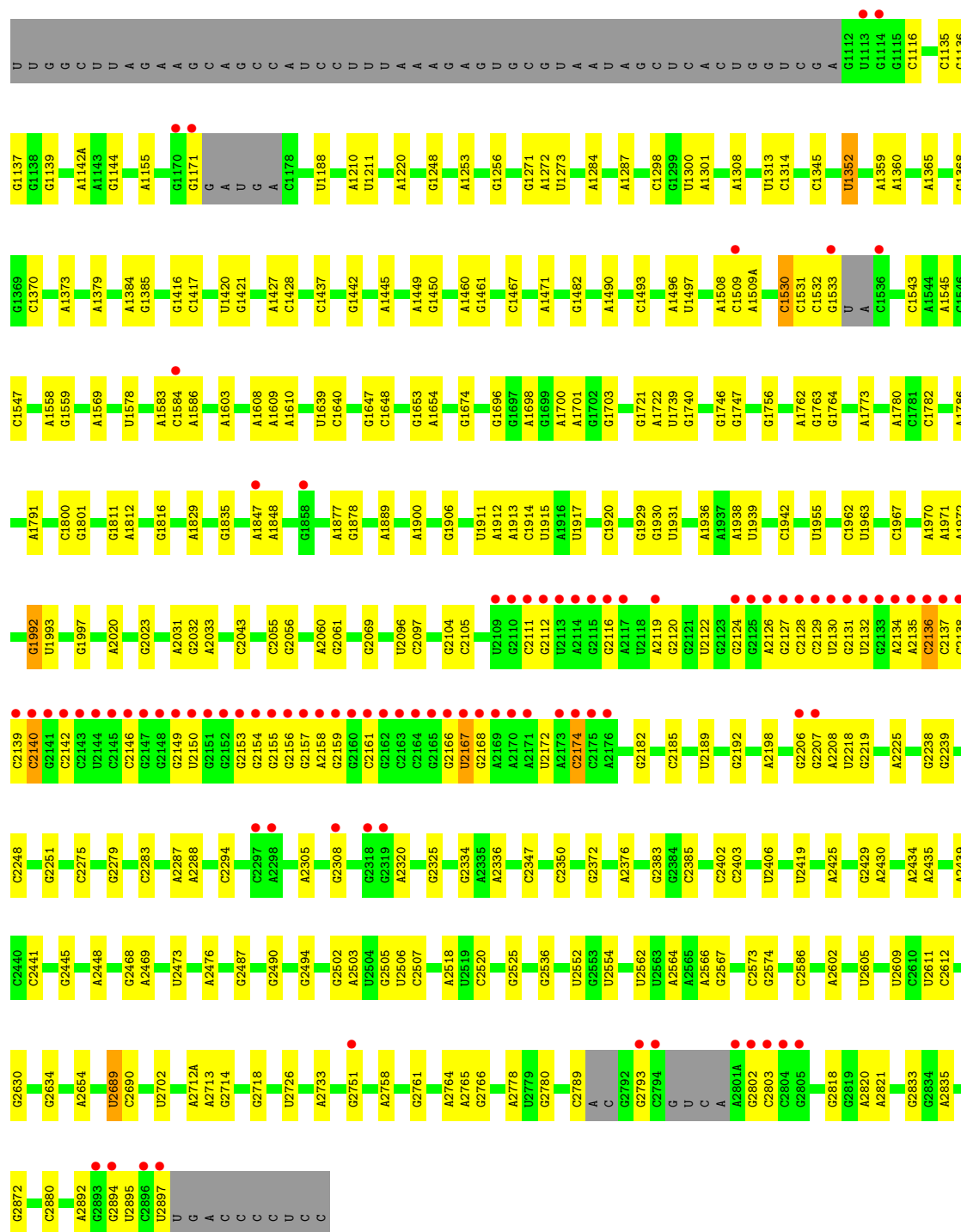
• Molecule 1: 23S Ribosomal RNA





• Molecule 1: 23S Ribosomal RNA



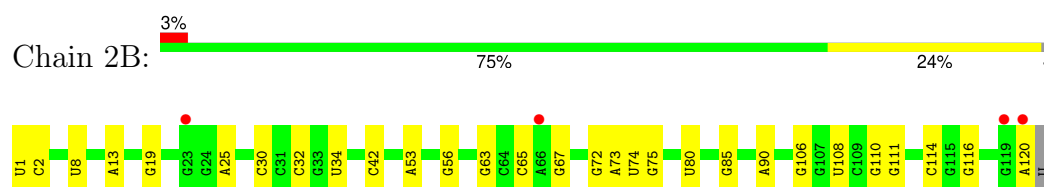


• Molecule 2: 5S Ribosomal RNA

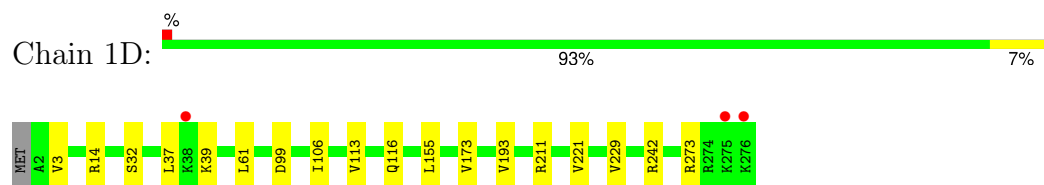
Chain 1B: 90% 8%



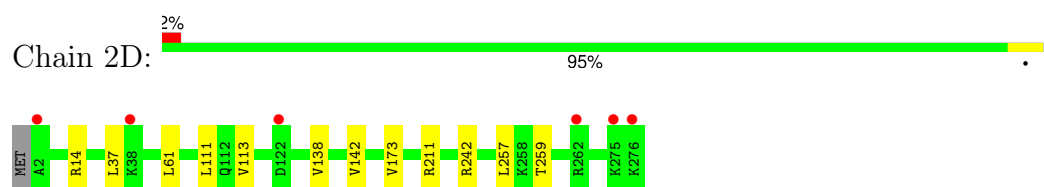
• Molecule 2: 5S Ribosomal RNA



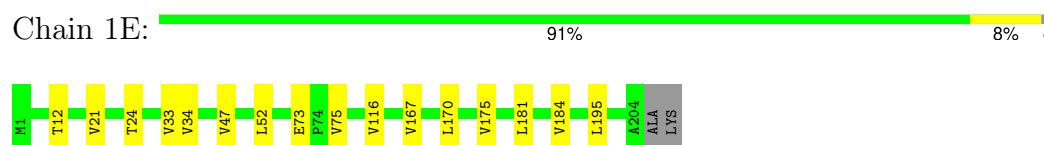
- Molecule 3: 50S ribosomal protein L2



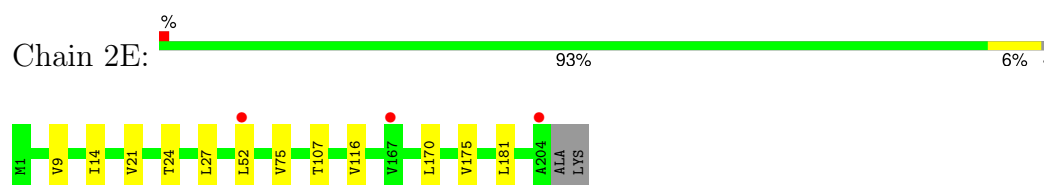
- Molecule 3: 50S ribosomal protein L2



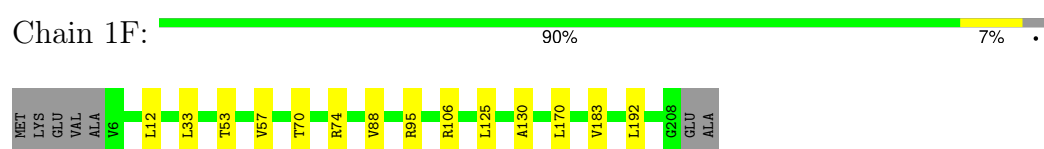
- Molecule 4: 50S ribosomal protein L3



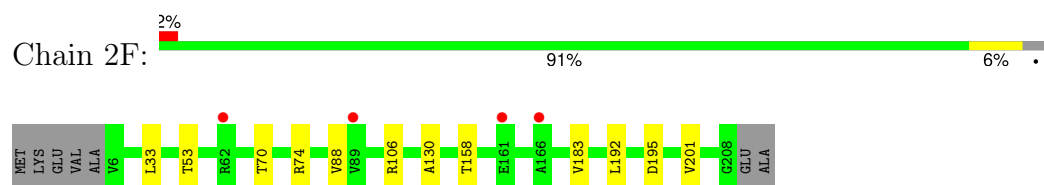
- Molecule 4: 50S ribosomal protein L3



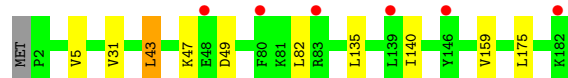
- Molecule 5: 50S ribosomal protein L4



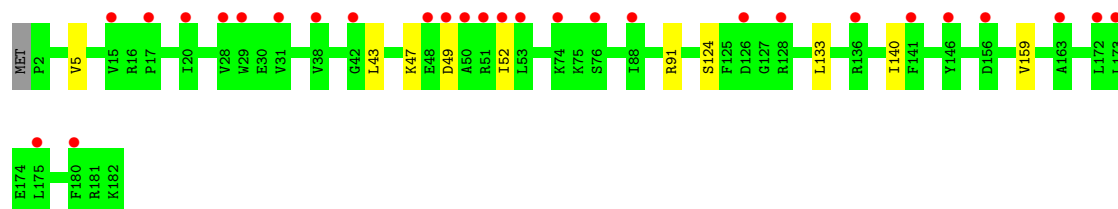
- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5



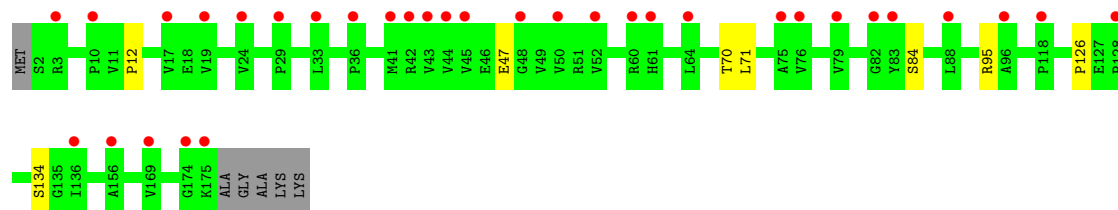
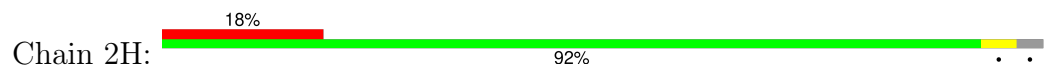
- Molecule 6: 50S ribosomal protein L5



- Molecule 7: 50S ribosomal protein L6



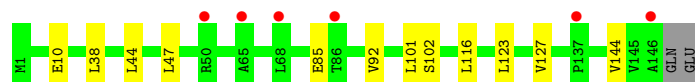
- Molecule 7: 50S ribosomal protein L6



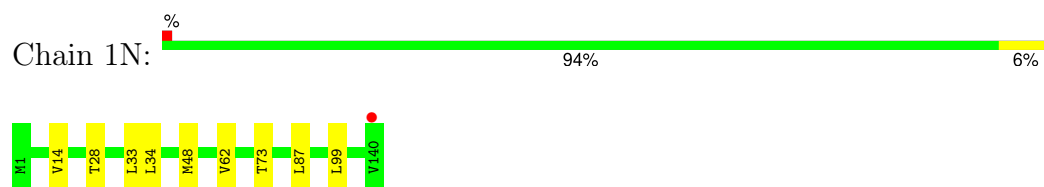
- Molecule 8: 50S ribosomal protein L9



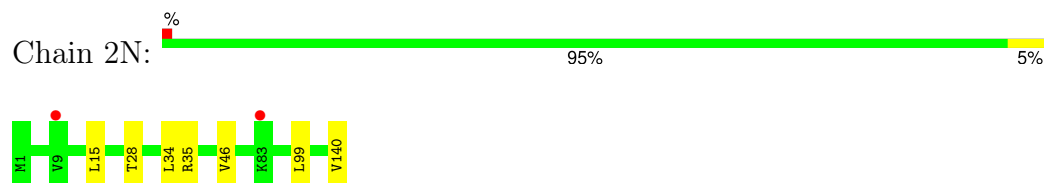
- Molecule 8: 50S ribosomal protein L9



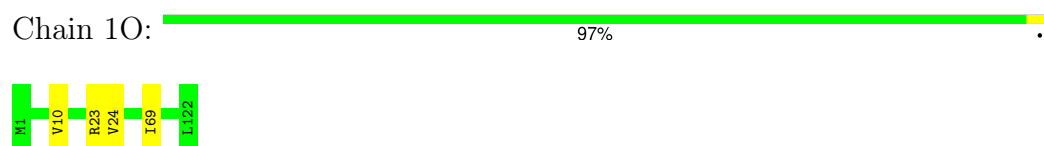
• Molecule 9: 50S ribosomal protein L13



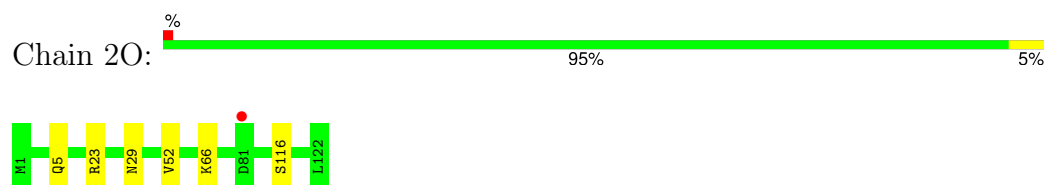
• Molecule 9: 50S ribosomal protein L13



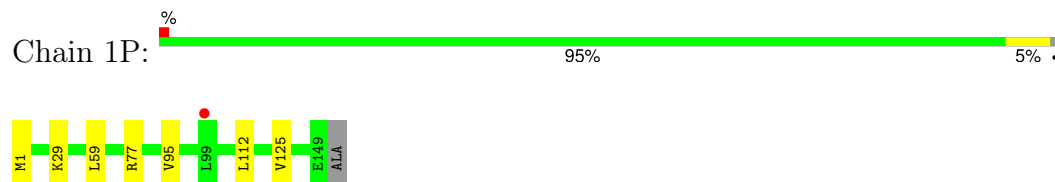
• Molecule 10: 50S ribosomal protein L14



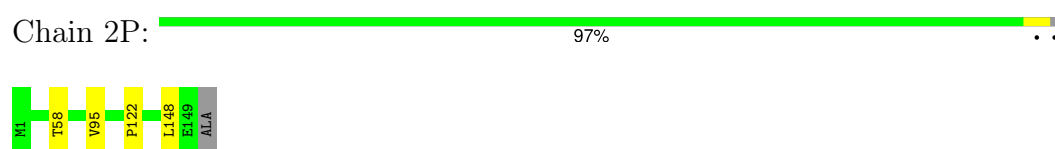
• Molecule 10: 50S ribosomal protein L14



• Molecule 11: 50S ribosomal protein L15

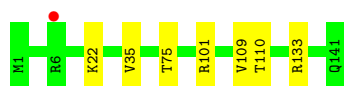


• Molecule 11: 50S ribosomal protein L15



• Molecule 12: 50S ribosomal protein L16





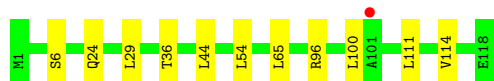
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



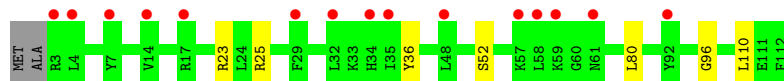
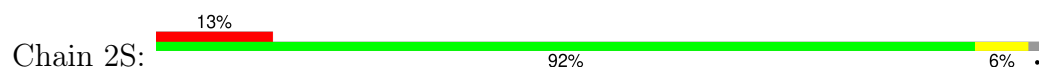
- Molecule 13: 50S ribosomal protein L17



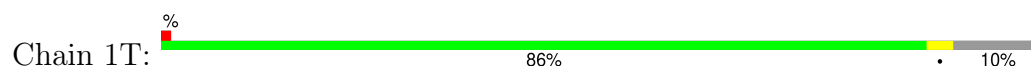
- Molecule 14: 50S ribosomal protein L18



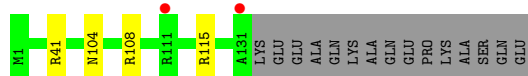
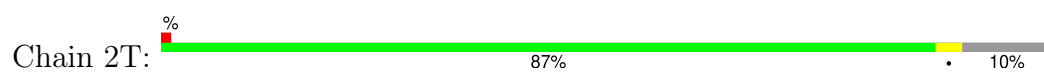
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



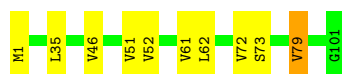
- Molecule 16: 50S ribosomal protein L20



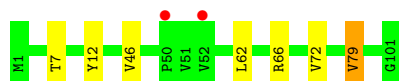
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



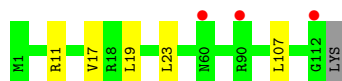
- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22



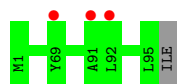
- Molecule 18: 50S ribosomal protein L22



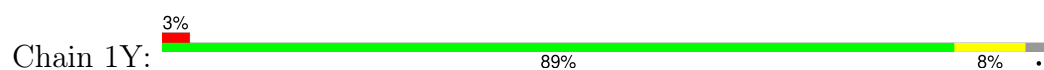
- Molecule 19: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L23



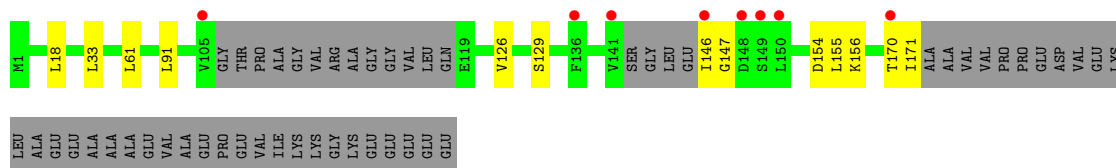
- Molecule 20: 50S ribosomal protein L24



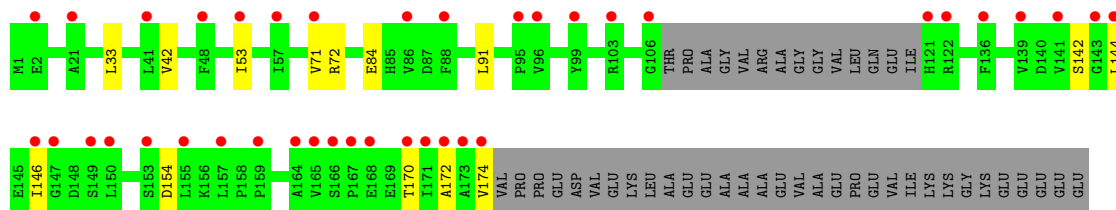
- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25



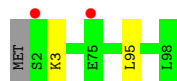
- Molecule 22: 50S ribosomal protein L27



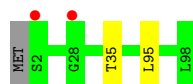
- Molecule 22: 50S ribosomal protein L27



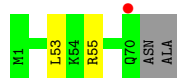
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



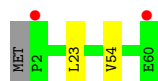
- Molecule 24: 50S ribosomal protein L29



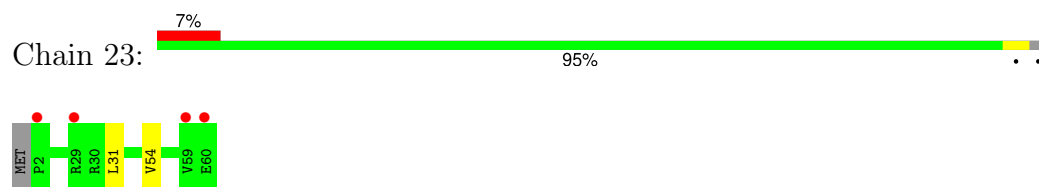
- Molecule 24: 50S ribosomal protein L29



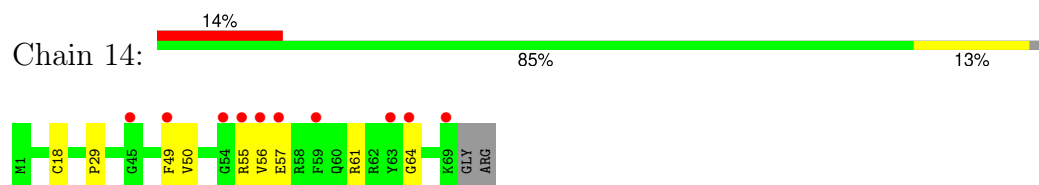
- Molecule 25: 50S ribosomal protein L30



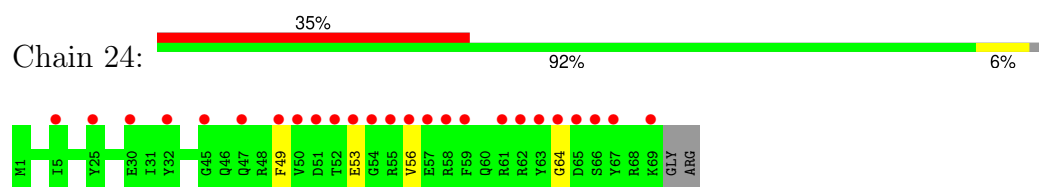
- Molecule 25: 50S ribosomal protein L30



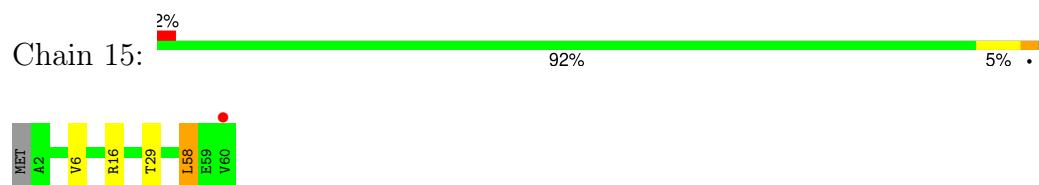
- Molecule 26: 50S ribosomal protein L31



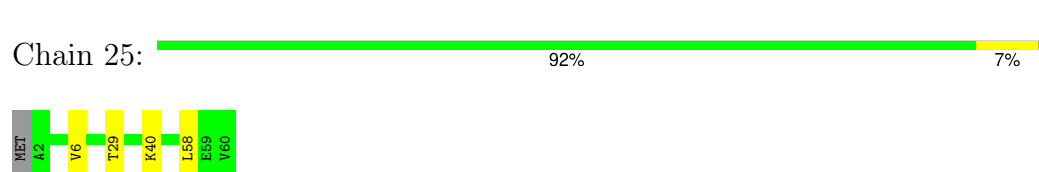
- Molecule 26: 50S ribosomal protein L31



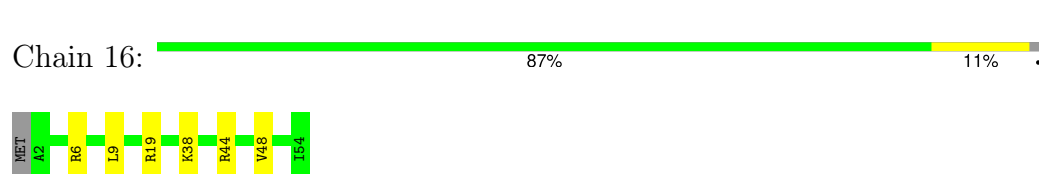
- Molecule 27: 50S ribosomal protein L32



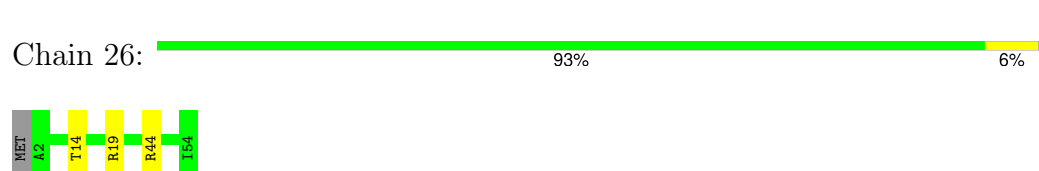
- Molecule 27: 50S ribosomal protein L32



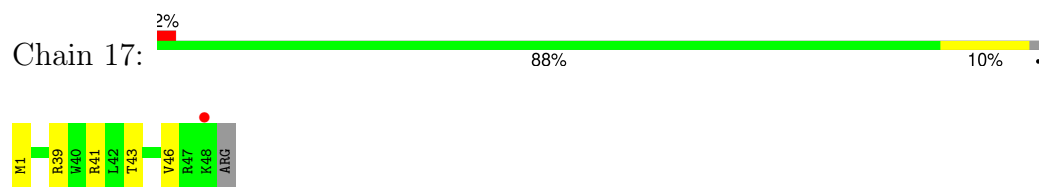
- Molecule 28: 50S ribosomal protein L33



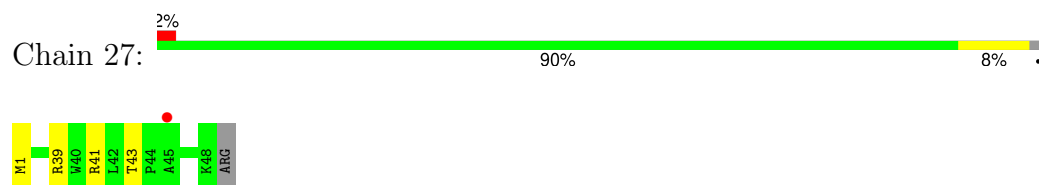
- Molecule 28: 50S ribosomal protein L33



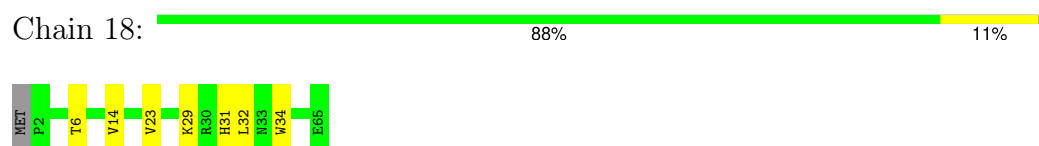
- Molecule 29: 50S ribosomal protein L34



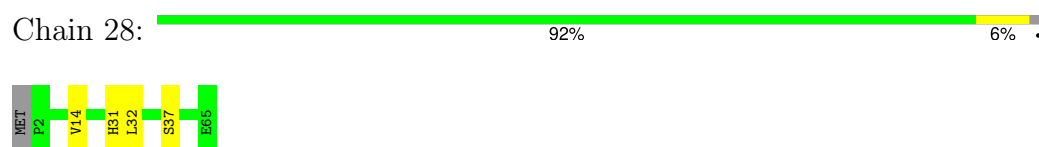
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35

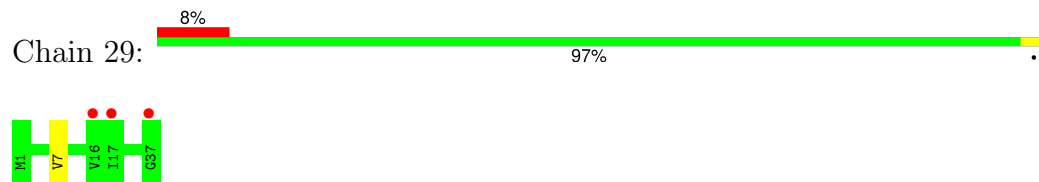


- Molecule 31: 50S ribosomal protein L36

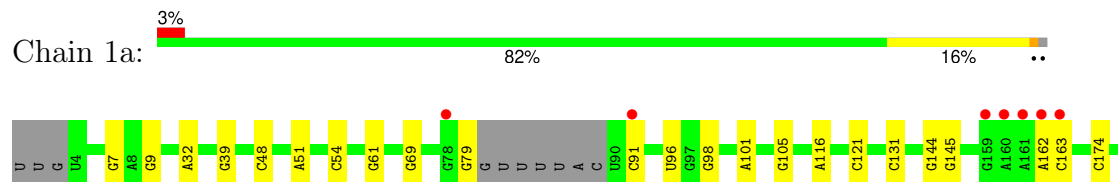


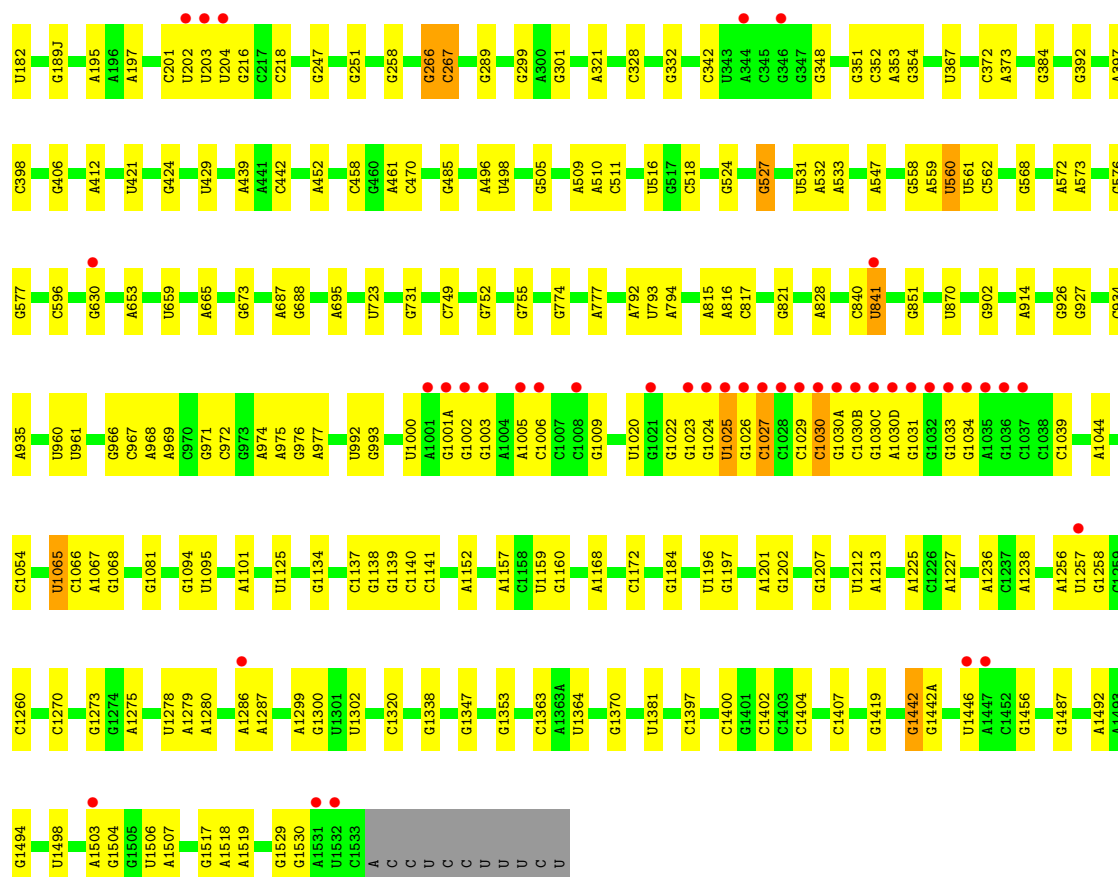
There are no outlier residues recorded for this chain.

- Molecule 31: 50S ribosomal protein L36

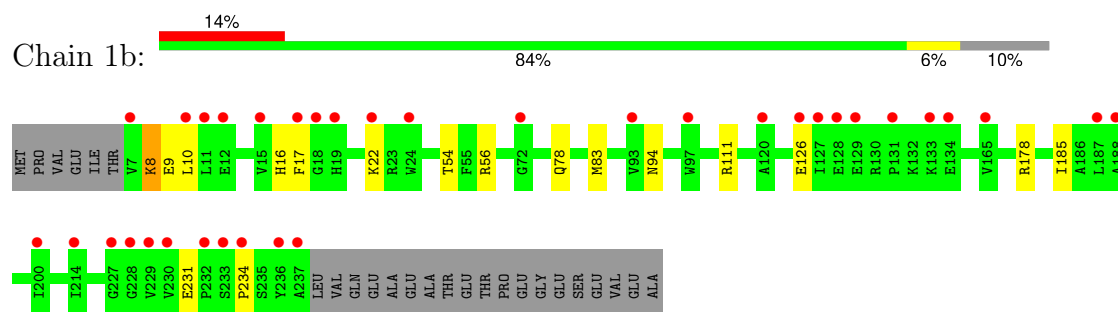


- Molecule 32: 16S Ribosomal RNA

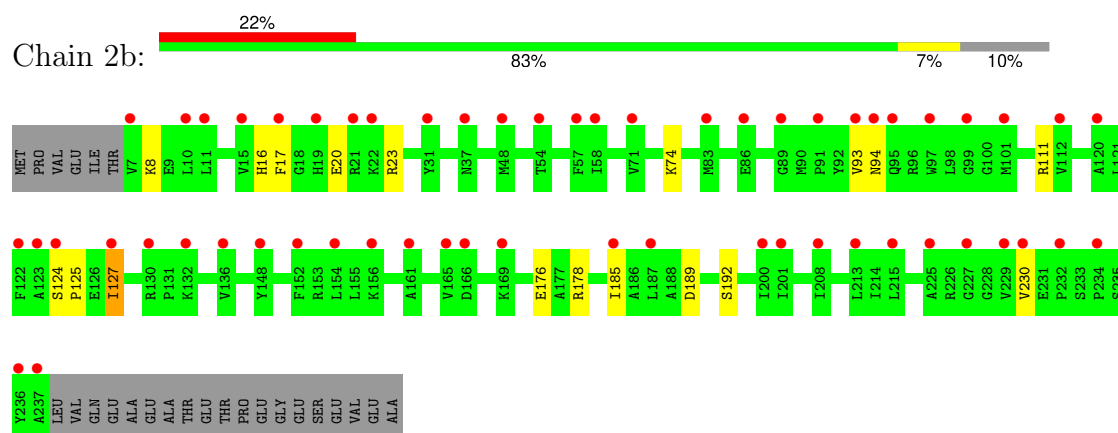




• Molecule 33: 30S ribosomal protein S2

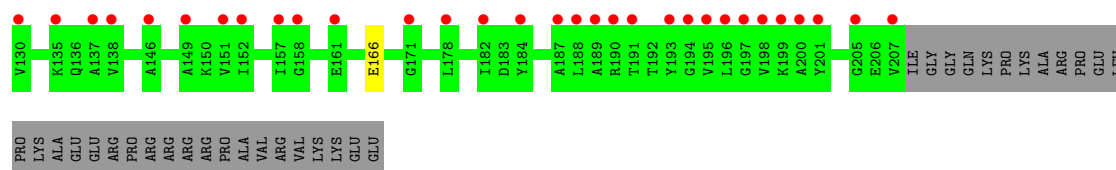


• Molecule 33: 30S ribosomal protein S2



- [illegible]

- [illegible]



- | Met |
|------|
| G2 |
| I5 |
| L19 |
| C31 |
| R59 |
| I70 |
| S83 |
| R107 |
| F110 |
| L135 |
| E150 |
| M154 |
| I158 |
| A164 |
| G167 |
| R168 |
| K169 |
| V170 |
| W173 |
| V178 |
| E179 |
| G180 |
| L194 |
| A195 |
| L196 |
| R209 |

- [illegible]

- [illegible]

- | MET | PRO | GLU | THR |
|------|-----|-----|-----|
| D5 | | | |
| M10 | | | |
| I11 | | | |
| L12 | | | |
| I13 | | | |
| A17 | | | |
| Q20 | | | |
| A21 | | | |
| G22 | | | |
| R25 | | | |
| L31 | | | |
| V32 | | | |
| V33 | | | |
| V34 | | | |
| V41 | | | |
| V51 | | | |
| A54 | | | |
| E68 | | | |
| G74 | | | |
| T75 | | | |
| I80 | | | |
| G85 | | | |
| A94 | | | |
| V100 | | | |
| I109 | | | |
| L110 | | | |
| E111 | | | |
| L112 | | | |
| A113 | | | |
| G114 | | | |
| V115 | | | |
| I116 | | | |
| L118 | | | |
| T120 | | | |
| S125 | | | |
| V133 | | | |

LYS
GLY
GLU
ALA
HIS
ALA
GLN
ALA
GLN
GLY

- Molecule 37: 30S ribosomal protein S6

Chain 1f:  96% ..

H1
L21
V40
L45
N100
ALA

- Molecule 37: 30S ribosomal protein S6

Chain 2f:  96% ..

H1
L21
V40
V72
S93
N100
ALA

- Molecule 38: 30S ribosomal protein S7

Chain 1g:  94% 6% ..

MET
A2
D15
L16
L59
R79
V80
G81
G82
A83
N84
R85
L104
R111
R114
R115
H153
W156

- Molecule 38: 30S ribosomal protein S7

Chain 2g:  94% 10% 5% ..

MET
A2
R3
R4
R5
R6
A7
Q13
L16
V17
R76
S77
R78
R79
V80
G81
G82
A83
N84
Y85
A152
W156

- Molecule 39: 30S ribosomal protein S8

Chain 1h:  96% ..

MET
L2
T3
D4
D25
V26
L63
I80
R85
L112
W138

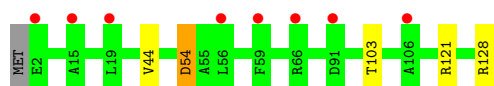
- Molecule 39: 30S ribosomal protein S8

Chain 2h:  96% ..

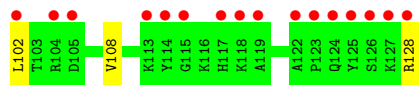
MET
L2
T3
R14
V51
D52
V53
P67
R85
G90
R102
G108
L112
R122
E123
A124
W138

- Molecule 40: 30S ribosomal protein S9

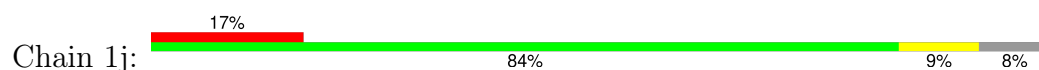
Chain 1i:  95% ..



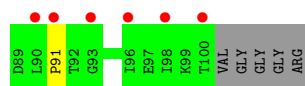
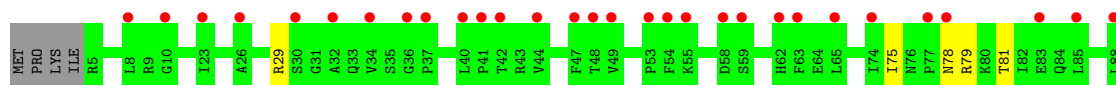
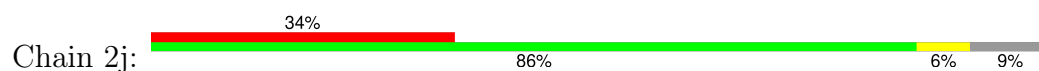
- Molecule 40: 30S ribosomal protein S9



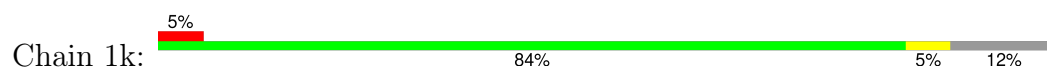
- Molecule 41: 30S ribosomal protein S10



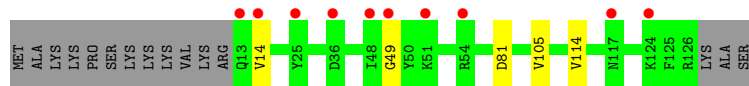
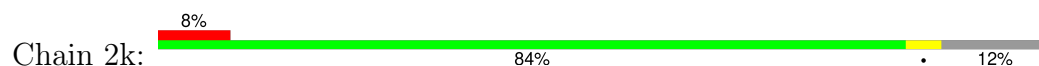
- Molecule 41: 30S ribosomal protein S10



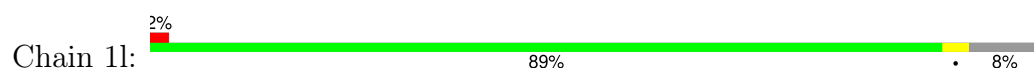
- Molecule 42: 30S ribosomal protein S11



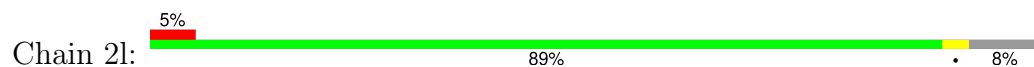
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12



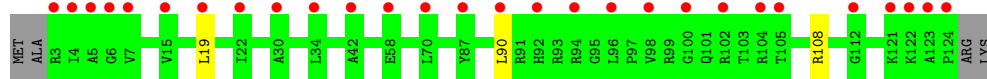
- Molecule 43: 30S ribosomal protein S12



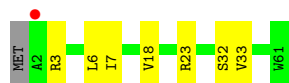
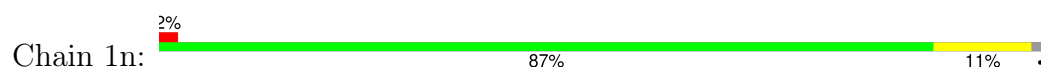
- Molecule 44: 30S ribosomal protein S13



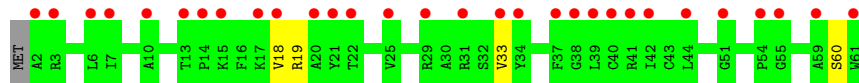
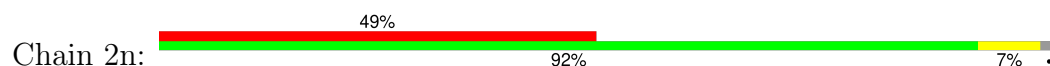
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



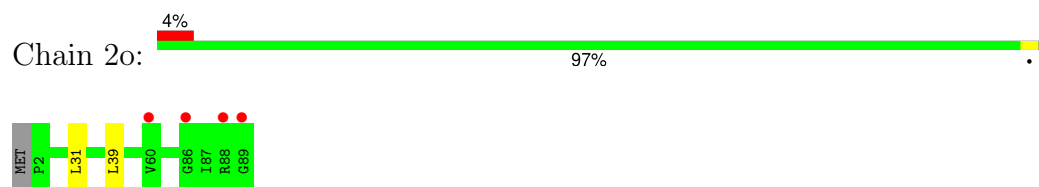
- Molecule 45: 30S ribosomal protein S14 type Z



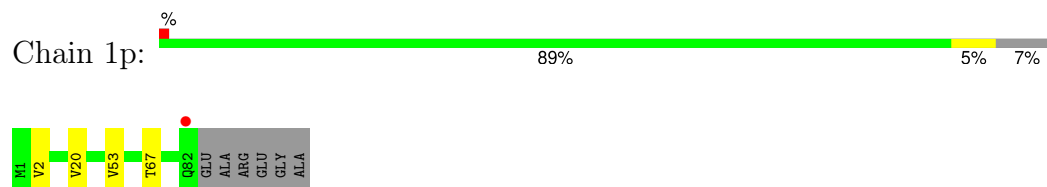
- Molecule 46: 30S ribosomal protein S15



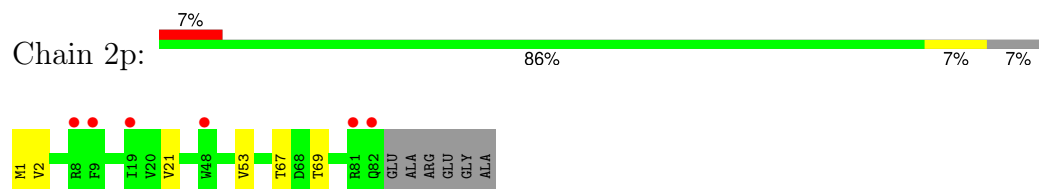
- Molecule 46: 30S ribosomal protein S15



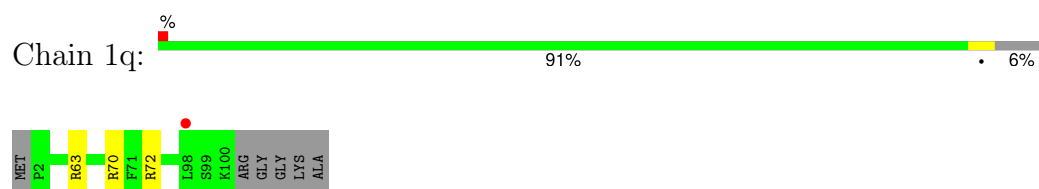
- Molecule 47: 30S ribosomal protein S16



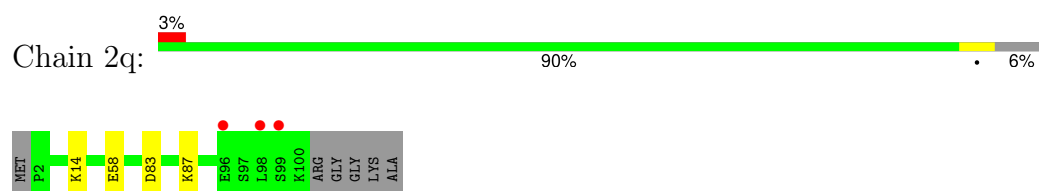
- Molecule 47: 30S ribosomal protein S16



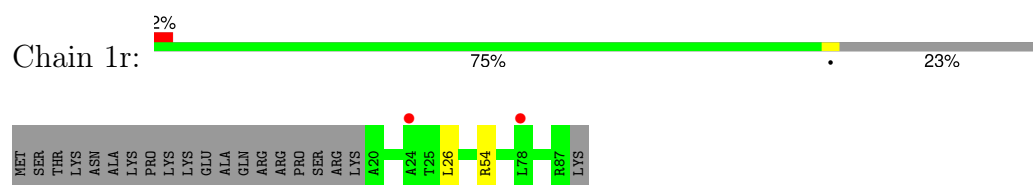
- Molecule 48: 30S ribosomal protein S17



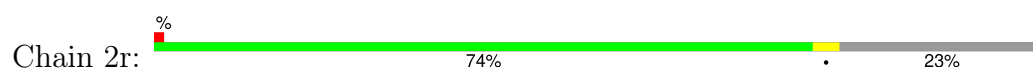
- Molecule 48: 30S ribosomal protein S17

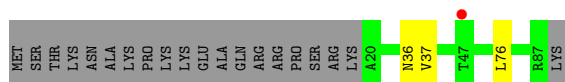


- Molecule 49: 30S ribosomal protein S18

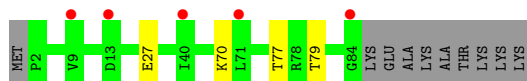
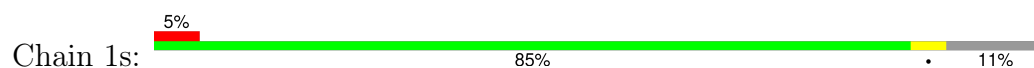


- Molecule 49: 30S ribosomal protein S18

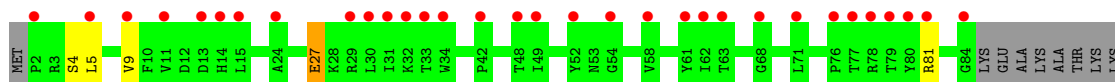
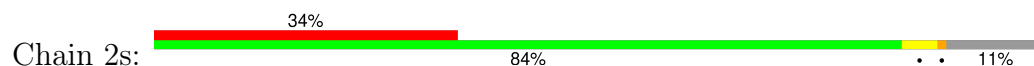




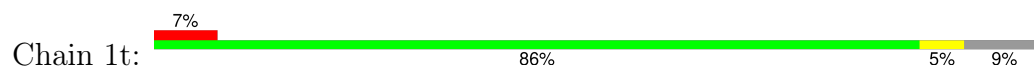
- Molecule 50: 30S ribosomal protein S19



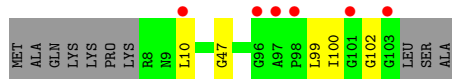
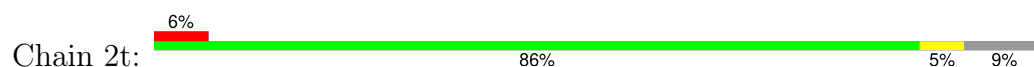
- Molecule 50: 30S ribosomal protein S19



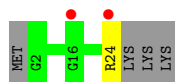
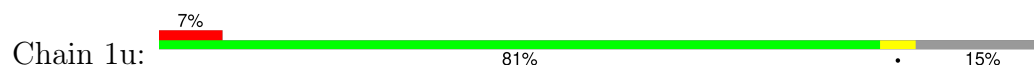
- Molecule 51: 30S ribosomal protein S20



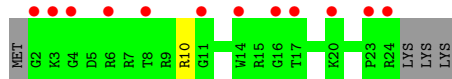
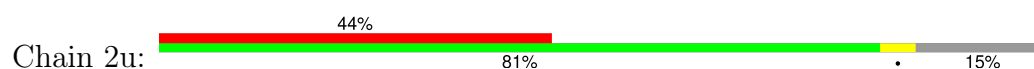
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: mRNA



- Molecule 53: mRNA



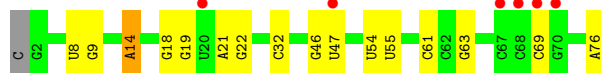
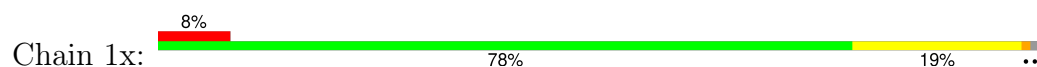
- Molecule 54: tRNA, A-site and E-site tRNAs



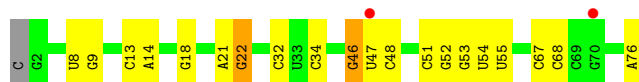
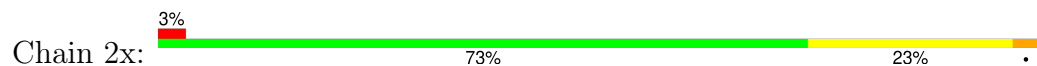
- Molecule 54: tRNA, A-site and E-site tRNAs



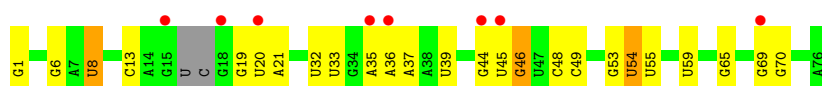
- Molecule 55: P-site tRNA



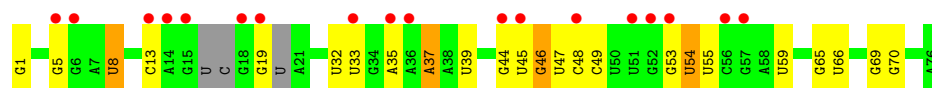
- Molecule 55: P-site tRNA



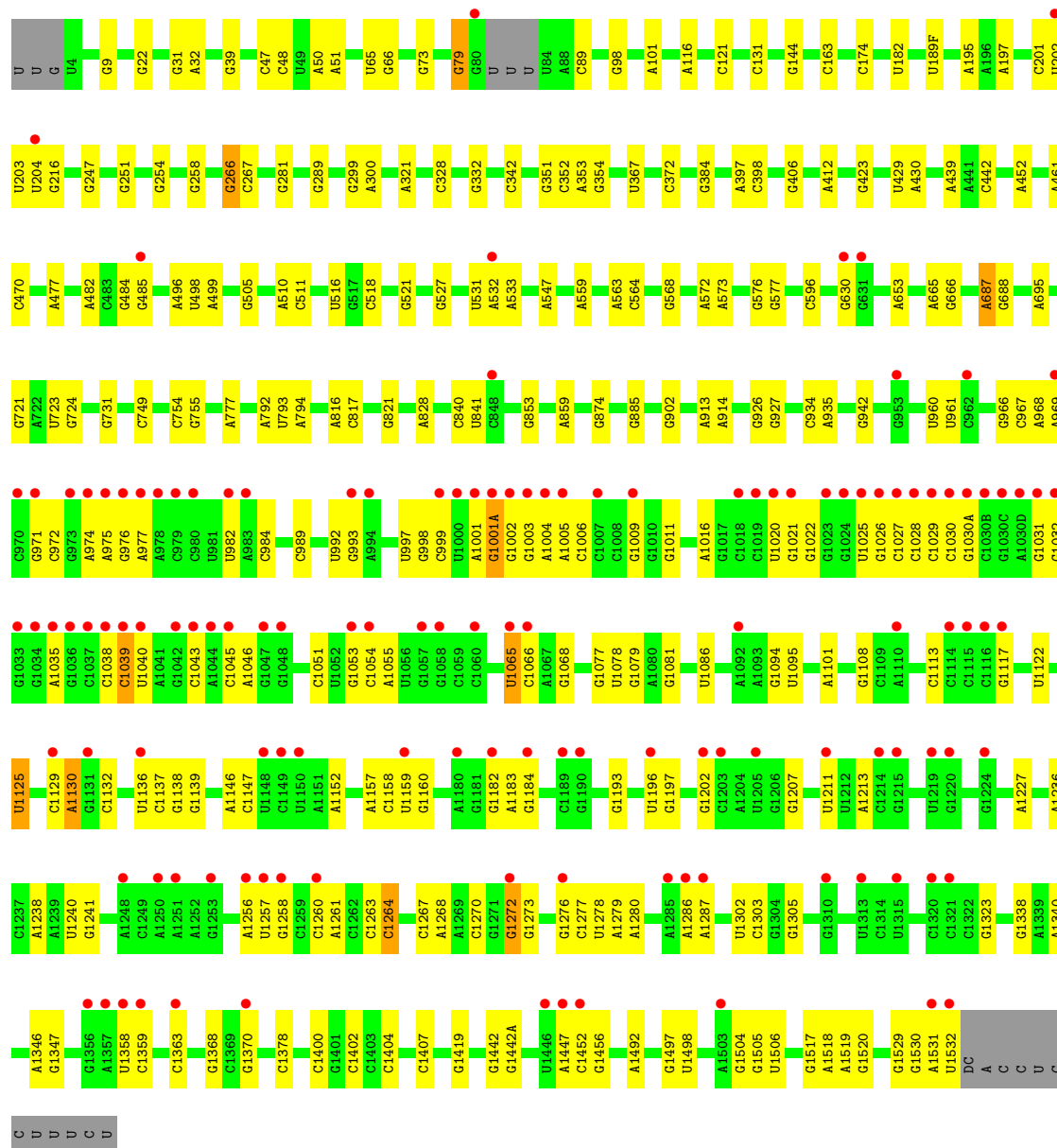
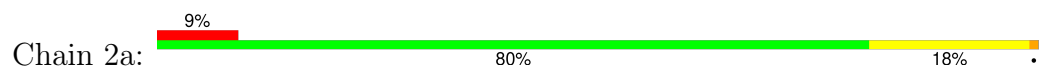
- Molecule 56: tRNA



- Molecule 56: tRNA



- Molecule 57: 16S Ribosomal RNA

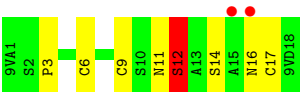


- Molecule 58: Klebsazolicin





● Molecule 58: Klebsazolicin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.64Å 449.06Å 622.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	155.50 – 2.70 155.50 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (155.50-2.70) 99.3 (155.50-2.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.207 , 0.252 0.211 , 0.255	Depositor DCC
R_{free} test set	78960 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 70.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	302030	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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: 2MA, ZN, BB9, SF4, MG, 5MC, UR3, K, M2G, 5MU, 0TD, 4OC, OMG, G7M, 2MG, MIA, 4SU, MA6, PSU, 9VA, 2MU, 9VD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1A	0.54	0/69009	0.98	82/107712 (0.1%)
1	2A	0.41	0/67293	0.88	41/105034 (0.0%)
2	1B	0.46	1/2882 (0.0%)	0.88	0/4494
2	2B	0.41	1/2879 (0.0%)	0.87	1/4487 (0.0%)
3	1D	0.36	0/2186	0.57	0/2944
3	2D	0.33	0/2186	0.54	0/2944
4	1E	0.36	0/1592	0.54	0/2149
4	2E	0.31	0/1592	0.50	0/2149
5	1F	0.34	0/1619	0.57	0/2193
5	2F	0.30	0/1615	0.49	0/2188
6	1G	0.29	0/1448	0.49	0/1957
6	2G	0.30	0/1453	0.52	0/1963
7	1H	0.33	0/1356	0.50	0/1834
7	2H	0.29	0/1356	0.45	0/1834
8	1I	0.29	0/1112	0.51	0/1514
8	2I	0.27	0/1079	0.50	0/1475
9	1N	0.34	0/1144	0.53	0/1543
9	2N	0.29	0/1144	0.46	0/1543
10	1O	0.38	0/943	0.56	0/1269
10	2O	0.34	0/943	0.52	0/1269
11	1P	0.34	0/1152	0.56	0/1533
11	2P	0.31	0/1152	0.52	0/1533
12	1Q	0.35	0/1143	0.54	0/1527
12	2Q	0.30	0/1143	0.48	0/1527
13	1R	0.33	0/982	0.54	0/1312
13	2R	0.27	0/982	0.53	0/1312
14	1S	0.32	0/883	0.56	0/1176
14	2S	0.32	0/880	0.47	0/1172
15	1T	0.35	0/1105	0.54	0/1477
15	2T	0.29	0/1097	0.46	0/1468
16	1U	0.39	0/977	0.55	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.31	0/977	0.46	0/1301
17	1V	0.38	0/782	0.57	0/1049
17	2V	0.30	0/782	0.51	0/1049
18	1W	0.35	0/897	0.54	0/1205
18	2W	0.32	0/897	0.49	0/1205
19	1X	0.38	0/764	0.57	0/1025
19	2X	0.31	0/764	0.48	0/1025
20	1Y	0.36	0/819	0.57	1/1095 (0.1%)
20	2Y	0.32	0/819	0.53	0/1095
21	1Z	0.32	0/1267	0.53	0/1717
21	2Z	0.30	0/1299	0.50	0/1763
22	10	0.37	0/662	0.58	0/881
22	20	0.30	0/662	0.50	0/881
23	11	0.35	0/762	0.53	0/1014
23	21	0.32	0/762	0.53	0/1014
24	12	0.32	0/590	0.49	0/781
24	22	0.28	0/590	0.42	0/781
25	13	0.32	0/474	0.53	0/635
25	23	0.28	0/469	0.46	0/630
26	14	0.35	0/565	0.53	0/761
26	24	0.31	0/545	0.50	0/737
27	15	0.35	0/469	0.59	1/635 (0.2%)
27	25	0.32	0/469	0.50	0/635
28	16	0.35	0/460	0.55	0/613
28	26	0.29	0/456	0.49	0/608
29	17	0.34	0/426	0.54	0/561
29	27	0.31	0/426	0.52	0/561
30	18	0.32	0/525	0.55	0/691
30	28	0.30	0/525	0.49	0/691
31	19	0.34	0/310	0.53	0/407
31	29	0.30	0/310	0.52	0/407
32	1a	0.39	0/35795	0.89	39/55864 (0.1%)
33	1b	0.29	0/1881	0.48	0/2542
33	2b	0.31	0/1860	0.47	0/2518
34	1c	0.29	0/1572	0.47	0/2126
34	2c	0.29	0/1566	0.46	0/2119
35	1d	0.30	0/1685	0.49	0/2262
35	2d	0.29	0/1704	0.47	0/2284
36	1e	0.31	0/1145	0.51	0/1543
36	2e	0.31	0/1149	0.51	0/1548
37	1f	0.30	0/823	0.47	0/1115
37	2f	0.31	0/829	0.48	0/1123
38	1g	0.28	0/1250	0.44	0/1679

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	2g	0.28	0/1254	0.44	0/1683
39	1h	0.28	0/1108	0.48	0/1494
39	2h	0.28	0/1108	0.46	0/1494
40	1i	0.29	0/1002	0.50	0/1346
40	2i	0.30	0/997	0.50	0/1343
41	1j	0.28	0/722	0.48	0/982
41	2j	0.30	0/727	0.52	0/988
42	1k	0.29	0/844	0.48	0/1145
42	2k	0.29	0/848	0.48	0/1149
43	1l	0.31	0/937	0.53	0/1260
43	2l	0.29	0/937	0.49	0/1260
44	1m	0.29	0/969	0.49	0/1302
44	2m	0.28	0/961	0.51	0/1291
45	1n	0.30	0/501	0.48	0/664
45	2n	0.32	0/501	0.50	0/664
46	1o	0.28	0/739	0.43	0/985
46	2o	0.26	0/739	0.42	0/985
47	1p	0.28	0/697	0.51	0/939
47	2p	0.29	0/693	0.50	0/935
48	1q	0.30	0/836	0.48	0/1117
48	2q	0.30	0/836	0.47	0/1117
49	1r	0.28	0/560	0.48	0/746
49	2r	0.28	0/560	0.44	0/746
50	1s	0.28	0/667	0.54	0/900
50	2s	0.30	0/661	0.54	0/893
51	1t	0.28	0/730	0.47	0/965
51	2t	0.28	0/729	0.43	0/965
52	1u	0.27	0/203	0.44	0/266
52	2u	0.36	0/203	0.48	0/266
53	1v	0.42	0/310	0.86	0/480
53	2v	0.47	0/310	0.86	0/480
54	1w	0.54	1/1606 (0.1%)	1.09	0/2497
54	2w	0.51	0/1556	1.13	4/2418 (0.2%)
55	1x	0.55	1/1725 (0.1%)	1.13	13/2689 (0.5%)
55	2x	0.46	0/1725	1.06	7/2689 (0.3%)
56	1y	0.72	6/1632 (0.4%)	1.22	13/2540 (0.5%)
56	2y	0.75	6/1609 (0.4%)	1.24	12/2502 (0.5%)
57	2a	0.38	3/35886 (0.0%)	0.90	50/56005 (0.1%)
58	A	2.13	4/74 (5.4%)	2.00	5/97 (5.2%)
58	B	2.13	3/74 (4.1%)	2.04	4/97 (4.1%)
All	All	0.42	26/316886 (0.0%)	0.84	273/474393 (0.1%)

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
26	24	0	1
33	1b	0	1
50	2s	0	1
58	A	1	0
58	B	1	0
All	All	2	3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	37	A	C5-C4	13.66	1.48	1.38
56	1y	37	A	C5-C4	13.39	1.48	1.38
58	B	12	SER	CA-CB	-13.07	1.33	1.52
58	A	12	SER	CA-CB	-12.57	1.34	1.52
56	2y	1	G	OP3-P	-10.39	1.48	1.61
56	1y	1	G	OP3-P	-10.30	1.48	1.61
2	2B	1	U	OP3-P	-10.05	1.49	1.61
54	1w	1	G	OP3-P	-10.03	1.49	1.61
2	1B	1	U	OP3-P	-9.80	1.49	1.61
57	2a	1272	G	N1-C2	-9.26	1.30	1.37
56	2y	37	A	C5-C6	9.05	1.49	1.41
56	1y	37	A	C5-C6	8.92	1.49	1.41
57	2a	1272	G	C6-N1	-8.85	1.33	1.39
58	B	12	SER	CA-C	-7.53	1.33	1.52
58	A	12	SER	CA-C	-7.29	1.34	1.52
56	1y	37	A	C8-N7	6.86	1.36	1.31
56	2y	37	A	C8-N7	6.80	1.36	1.31
56	2y	37	A	N7-C5	-6.56	1.35	1.39
58	A	12	SER	N-CA	-6.48	1.33	1.46
58	B	12	SER	N-CA	-6.44	1.33	1.46
56	1y	37	A	N7-C5	-6.31	1.35	1.39
58	A	12	SER	CB-OG	-6.19	1.34	1.42
56	1y	37	A	N9-C4	-5.51	1.34	1.37
56	2y	37	A	N9-C4	-5.27	1.34	1.37
57	2a	1263	C	N3-C4	-5.20	1.30	1.33
55	1x	22	G	N7-C5	5.10	1.42	1.39

All (273) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2a	1263	C	N1-C2-O2	22.88	132.63	118.90
57	2a	1272	G	N3-C2-N2	20.83	134.48	119.90
56	2y	37	A	C2-N3-C4	20.81	121.00	110.60
56	1y	37	A	C2-N3-C4	20.56	120.88	110.60
57	2a	1272	G	C5-C6-O6	20.05	140.63	128.60
57	2a	1272	G	N1-C2-N2	-18.59	99.47	116.20
57	2a	1263	C	C2-N3-C4	14.28	127.04	119.90
57	2a	1263	C	N3-C2-O2	-13.11	112.72	121.90
57	2a	1272	G	N1-C6-O6	-12.89	112.16	119.90
56	2y	37	A	N1-C2-N3	-12.78	122.91	129.30
1	1A	1132	A	N1-C6-N6	-12.72	110.97	118.60
56	1y	37	A	N1-C2-N3	-12.44	123.08	129.30
56	2y	37	A	N3-C4-C5	-11.59	118.69	126.80
56	1y	37	A	N3-C4-C5	-11.35	118.85	126.80
1	1A	1686	U	O5'-P-OP2	-10.96	95.84	105.70
32	1a	1027	C	C5-C4-N4	10.85	127.79	120.20
32	1a	1027	C	N3-C2-O2	-10.81	114.33	121.90
1	1A	1121	C	N1-C2-O2	10.74	125.34	118.90
1	1A	1121	C	C2-N3-C4	10.60	125.20	119.90
57	2a	1272	G	C6-N1-C2	10.44	131.36	125.10
1	2A	2136	C	N1-C2-O2	9.82	124.79	118.90
56	2y	37	A	N3-C4-N9	9.80	135.24	127.40
57	2a	1263	C	C5-C6-N1	9.43	125.72	121.00
56	1y	37	A	N3-C4-N9	9.18	134.74	127.40
1	1A	1109	G	C5-C6-O6	8.94	133.96	128.60
57	2a	1263	C	C5-C4-N4	8.91	126.44	120.20
1	1A	537	G	O4'-C1'-N9	8.91	115.33	108.20
57	2a	1001(A)	G	N3-C4-N9	8.86	131.31	126.00
55	1x	46	G	C6-N1-C2	-8.76	119.84	125.10
56	1y	37	A	C4-C5-N7	-8.76	106.32	110.70
57	2a	1272	G	C5-C6-N1	-8.68	107.16	111.50
55	1x	14	A	C4-C5-C6	8.67	121.33	117.00
1	1A	1109	G	C6-N1-C2	8.49	130.19	125.10
56	1y	33	U	C2-N1-C1'	8.34	127.71	117.70
1	1A	2189	U	C2-N1-C1'	8.27	127.62	117.70
32	1a	1027	C	N3-C4-C5	-8.23	118.61	121.90
55	1x	14	A	C5-N7-C8	8.17	107.98	103.90
56	2y	37	A	C4-C5-N7	-8.09	106.65	110.70
32	1a	1025	U	N1-C2-O2	8.03	128.42	122.80
1	2A	2473	U	C2-N1-C1'	7.99	127.29	117.70
32	1a	1027	C	C6-N1-C2	-7.96	117.12	120.30
1	1A	2694	U	O5'-P-OP2	-7.94	98.56	105.70
57	2a	1263	C	N3-C4-N4	-7.85	112.50	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2B	80	U	O4'-C1'-N1	7.84	114.48	108.20
56	2y	33	U	C2-N1-C1'	7.83	127.09	117.70
32	1a	1034	G	N3-C2-N2	7.81	125.37	119.90
1	1A	215	G	O4'-C1'-N9	7.81	114.44	108.20
56	1y	37	A	C5-N7-C8	7.71	107.76	103.90
55	1x	22	G	C5-N7-C8	-7.71	100.45	104.30
32	1a	1034	G	N9-C4-C5	-7.64	102.34	105.40
57	2a	1272	G	C2-N3-C4	-7.63	108.08	111.90
1	1A	591	U	C5-C4-O4	-7.62	121.33	125.90
1	1A	1807	G	O5'-P-OP2	-7.56	98.89	105.70
32	1a	1030(B)	C	C2-N1-C1'	7.53	127.08	118.80
57	2a	1263	C	C2-N1-C1'	7.53	127.08	118.80
1	1A	1109	G	N3-C2-N2	7.51	125.16	119.90
1	1A	2504	U	O5'-P-OP1	-7.43	99.02	105.70
1	1A	1132	A	C5-C6-N6	7.37	129.60	123.70
55	2x	14	A	C5-N7-C8	7.34	107.57	103.90
1	1A	2189	U	N1-C2-O2	7.30	127.91	122.80
58	B	12	SER	CB-CA-C	7.27	123.92	110.10
32	1a	1027	C	N1-C2-O2	7.26	123.25	118.90
57	2a	1263	C	C6-N1-C2	-7.15	117.44	120.30
1	1A	2189	U	N3-C2-O2	-7.14	117.20	122.20
58	A	12	SER	CB-CA-C	7.13	123.65	110.10
56	2y	37	A	C5-N7-C8	7.10	107.45	103.90
57	2a	1039	C	C5-C4-N4	-7.07	115.25	120.20
1	1A	2807	C	N1-C2-O2	7.04	123.12	118.90
55	1x	14	A	C5-C6-N1	-6.98	114.21	117.70
1	2A	2136	C	N3-C2-O2	-6.94	117.04	121.90
55	2x	14	A	C4-C5-C6	6.94	120.47	117.00
1	2A	2473	U	N1-C2-O2	6.87	127.61	122.80
1	1A	1222	A	O5'-P-OP1	-6.84	99.54	105.70
32	1a	1034	G	N3-C4-N9	6.84	130.10	126.00
1	2A	2248	C	O5'-P-OP2	-6.81	99.57	105.70
32	1a	1034	G	C4-C5-N7	6.80	113.52	110.80
57	2a	1001(A)	G	C4-N9-C1'	6.75	135.28	126.50
1	1A	2566	U	O5'-P-OP1	-6.74	99.64	105.70
57	2a	1263	C	C4-C5-C6	-6.73	114.03	117.40
57	2a	79	G	C5-C6-O6	6.69	132.62	128.60
1	2A	2473	U	N3-C2-O2	-6.68	117.52	122.20
58	A	11	ASN	C-N-CA	-6.68	105.00	121.70
54	2w	50	U	C5-C4-O4	-6.67	121.90	125.90
1	1A	2050	U	N3-C4-O4	-6.61	114.77	119.40
56	1y	33	U	N1-C2-O2	6.59	127.41	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2y	37	A	C8-N9-C4	6.58	108.43	105.80
57	2a	1263	C	N1-C2-N3	-6.55	114.61	119.20
1	1A	1815	A	O5'-P-OP2	-6.54	99.81	105.70
32	1a	558	G	O5'-P-OP1	-6.54	99.82	105.70
1	1A	892	G	O4'-C1'-N9	6.52	113.42	108.20
57	2a	1039	C	C2-N1-C1'	6.51	125.96	118.80
1	2A	2140	C	N1-C2-O2	6.49	122.79	118.90
56	1y	37	A	C8-N9-C4	6.49	108.39	105.80
32	1a	1030(B)	C	C6-N1-C2	-6.47	117.71	120.30
58	B	11	ASN	C-N-CA	-6.46	105.55	121.70
55	1x	22	G	C4-C5-C6	-6.41	114.95	118.80
1	2A	2139	C	C2-N1-C1'	6.37	125.81	118.80
1	1A	2359	C	N1-C2-O2	6.35	122.71	118.90
1	2A	2140	C	C2-N1-C1'	6.32	125.75	118.80
1	1A	848	G	O5'-P-OP2	-6.31	100.02	105.70
32	1a	1027	C	N3-C4-N4	-6.30	113.59	118.00
1	2A	512	G	O4'-C1'-N9	6.28	113.23	108.20
57	2a	1001(A)	G	N3-C4-C5	-6.28	125.46	128.60
32	1a	267	C	O5'-P-OP1	-6.27	100.06	105.70
57	2a	1001(A)	G	C8-N9-C1'	-6.26	118.86	127.00
56	1y	33	U	C6-N1-C1'	-6.26	112.43	121.20
57	2a	1272	G	C4-N9-C1'	6.26	134.64	126.50
1	1A	2701	U	P-O3'-C3'	6.26	127.21	119.70
57	2a	1272	G	C8-N9-C1'	-6.24	118.89	127.00
1	1A	2858	G	O4'-C1'-N9	6.24	113.19	108.20
32	1a	1030(B)	C	N1-C2-O2	6.22	122.64	118.90
55	2x	46	G	C6-N1-C2	-6.20	121.38	125.10
57	2a	754	C	C2-N1-C1'	6.19	125.61	118.80
55	1x	22	G	N3-C4-N9	-6.19	122.28	126.00
32	1a	299	G	C5-C6-O6	-6.19	124.89	128.60
1	1A	840	A	O5'-P-OP2	-6.15	100.17	105.70
1	2A	1313	U	C2-N1-C1'	6.12	125.05	117.70
1	2A	1352	U	O5'-P-OP1	-6.11	100.20	105.70
1	1A	2383	G	C5-C6-N1	6.09	114.55	111.50
1	2A	945	A	N1-C6-N6	6.07	122.24	118.60
56	2y	37	A	C6-N1-C2	6.07	122.24	118.60
57	2a	1001(A)	G	C6-C5-N7	-6.07	126.76	130.40
32	1a	1030	C	N1-C2-O2	6.06	122.53	118.90
1	2A	2167	U	C2-N1-C1'	6.03	124.94	117.70
55	1x	46	G	C5-C6-N1	6.01	114.50	111.50
1	2A	2149	G	N3-C4-N9	5.99	129.59	126.00
57	2a	299	G	C5-C6-O6	-5.99	125.01	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	894	U	C2-N1-C1'	5.96	124.86	117.70
32	1a	1002	G	C4-N9-C1'	5.96	134.25	126.50
1	2A	1992	G	P-O3'-C3'	5.96	126.86	119.70
1	2A	2167	U	N1-C2-O2	5.96	126.97	122.80
1	2A	1698	A	O4'-C1'-N9	5.95	112.96	108.20
32	1a	266	G	P-O3'-C3'	5.92	126.80	119.70
1	1A	1128	U	N3-C4-O4	-5.89	115.27	119.40
1	1A	2641	A	P-O3'-C3'	5.87	126.74	119.70
57	2a	754	C	N1-C2-O2	5.85	122.41	118.90
57	2a	1039	C	N3-C4-N4	5.85	122.10	118.00
1	1A	2014	G	C8-N9-C4	-5.85	104.06	106.40
32	1a	1030	C	C2-N3-C4	5.84	122.82	119.90
1	2A	141	A	N7-C8-N9	5.83	116.71	113.80
1	1A	1121	C	C5-C4-N4	5.83	124.28	120.20
55	1x	22	G	N7-C8-N9	5.83	116.01	113.10
1	1A	1128	U	N3-C4-C5	5.82	118.09	114.60
55	1x	22	G	C8-N9-C1'	5.82	134.57	127.00
32	1a	1025	U	N3-C2-O2	-5.82	118.12	122.20
54	2w	25	C	C5-C4-N4	5.82	124.27	120.20
56	1y	37	A	C6-N1-C2	5.79	122.07	118.60
1	1A	1958	A	O4'-C1'-N9	5.75	112.80	108.20
1	1A	593	G	C5-C6-O6	-5.74	125.15	128.60
56	2y	47	U	C2-N1-C1'	5.74	124.59	117.70
1	1A	194	G	O5'-P-OP2	-5.73	100.54	105.70
1	1A	399	G	O4'-C1'-N9	5.73	112.78	108.20
56	1y	37	A	C6-C5-N7	5.72	136.31	132.30
57	2a	266	G	P-O3'-C3'	5.72	126.56	119.70
1	1A	1462	G	O4'-C1'-N9	5.71	112.77	108.20
57	2a	1043	C	N1-C2-O2	5.70	122.32	118.90
1	2A	141	A	C8-N9-C4	-5.69	103.53	105.80
1	1A	1221	G	OP1-P-O3'	5.66	117.66	105.20
1	1A	1295	U	O5'-P-OP1	-5.66	100.61	105.70
32	1a	1067	A	P-O3'-C3'	5.65	126.47	119.70
32	1a	1002	G	C8-N9-C1'	-5.64	119.67	127.00
1	1A	2014	G	P-O3'-C3'	5.63	126.46	119.70
1	1A	1398	U	O5'-P-OP1	-5.63	100.63	105.70
1	2A	228	A	P-O3'-C3'	5.63	126.45	119.70
1	1A	1431	G	O4'-C1'-N9	5.61	112.68	108.20
32	1a	841	U	C5-C6-N1	5.60	125.50	122.70
1	2A	1639	U	O5'-P-OP2	-5.59	100.67	105.70
1	1A	2189	U	C5-C6-N1	5.59	125.49	122.70
1	1A	2015	U	O5'-P-OP1	-5.58	100.67	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	14	A	C4-N9-C1'	5.57	136.32	126.30
1	2A	2139	C	N1-C2-O2	5.56	122.24	118.90
55	2x	46	G	N3-C2-N2	-5.55	116.01	119.90
57	2a	1130	A	O5'-P-OP1	-5.55	100.71	105.70
57	2a	687	A	P-O3'-C3'	5.54	126.34	119.70
1	2A	1530	C	P-O3'-C3'	5.51	126.32	119.70
1	1A	1219	A	P-O3'-C3'	5.51	126.31	119.70
20	1Y	54	LYS	C-N-CA	5.50	135.46	121.70
57	2a	65	U	P-O3'-C3'	5.50	126.30	119.70
57	2a	1028	C	C2-N3-C4	5.48	122.64	119.90
27	15	58	LEU	CA-CB-CG	5.48	127.90	115.30
58	A	4	GLY	N-CA-C	-5.47	99.42	113.10
32	1a	1027	C	C6-N1-C1'	5.47	127.37	120.80
1	1A	572	A	P-O3'-C3'	5.47	126.26	119.70
57	2a	299	G	N1-C6-O6	5.47	123.18	119.90
32	1a	1034	G	C8-N9-C1'	-5.46	119.91	127.00
1	1A	2082	A	C8-N9-C4	5.46	107.98	105.80
57	2a	1001(A)	G	N9-C4-C5	-5.44	103.22	105.40
58	B	3	PRO	N-CA-C	5.43	126.22	112.10
1	2A	2139	C	C6-N1-C1'	-5.43	114.29	120.80
1	1A	2803	A	C2-N3-C4	5.42	113.31	110.60
1	1A	961	C	N1-C2-O2	5.42	122.15	118.90
55	1x	14	A	C4-C5-N7	-5.42	107.99	110.70
1	1A	1359	U	N3-C2-O2	-5.42	118.41	122.20
1	1A	410	U	C2-N1-C1'	-5.41	111.21	117.70
58	B	12	SER	N-CA-C	5.40	125.57	111.00
1	2A	2174	C	N1-C2-O2	5.38	122.13	118.90
55	1x	14	A	C8-N9-C1'	-5.37	118.03	127.70
1	2A	2128	C	C2-N3-C4	5.36	122.58	119.90
56	1y	37	A	N7-C8-N9	-5.36	111.12	113.80
55	2x	14	A	C5-C6-N1	-5.36	115.02	117.70
1	2A	2167	U	N3-C2-O2	-5.35	118.45	122.20
1	2A	383	U	O4'-C1'-N1	5.35	112.48	108.20
57	2a	254	G	O5'-P-OP1	-5.35	100.89	105.70
32	1a	266	G	O4'-C1'-N9	-5.34	103.92	108.20
56	2y	33	U	C6-N1-C1'	-5.34	113.72	121.20
1	1A	1020	C	N1-C2-O2	-5.32	115.71	118.90
1	1A	2442	A	C2-N3-C4	5.31	113.26	110.60
1	1A	2610	A	O5'-P-OP1	-5.31	100.92	105.70
57	2a	1505	G	N3-C4-N9	-5.31	122.81	126.00
1	1A	1648	U	N3-C4-O4	-5.30	115.69	119.40
1	1A	649	C	O5'-P-OP1	-5.28	100.95	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	22	G	C5-N7-C8	-5.27	101.66	104.30
1	2A	528	A	P-O3'-C3'	5.27	126.02	119.70
57	2a	1039	C	C6-N1-C1'	-5.27	114.48	120.80
1	1A	2331	G	C5-N7-C8	-5.26	101.67	104.30
58	A	3	PRO	C-N-CA	5.25	133.32	122.30
1	1A	1694	G	O4'-C1'-N9	-5.24	104.00	108.20
1	2A	801	G	O5'-P-OP2	-5.24	100.99	105.70
1	1A	1441	A	C8-N9-C4	5.23	107.89	105.80
1	2A	2149	G	C4-N9-C1'	5.23	133.30	126.50
1	1A	2359	C	N3-C2-O2	-5.23	118.24	121.90
1	2A	845	G	O4'-C1'-N9	5.22	112.38	108.20
1	1A	12	U	C2-N1-C1'	5.22	123.97	117.70
57	2a	913	A	P-O3'-C3'	5.22	125.96	119.70
54	2w	50	U	N3-C4-O4	5.21	123.05	119.40
1	2A	845	G	C4-N9-C1'	5.20	133.27	126.50
1	1A	1700	G	P-O3'-C3'	5.20	125.94	119.70
1	1A	2331	G	O4'-C1'-N9	5.19	112.35	108.20
57	2a	1125	U	C2-N1-C1'	5.18	123.92	117.70
1	2A	2689	U	P-O3'-C3'	5.18	125.91	119.70
1	2A	1298	C	O5'-P-OP2	-5.17	101.04	105.70
1	2A	2149	G	C8-N9-C1'	-5.17	120.27	127.00
1	1A	831	A	O4'-C1'-N9	5.17	112.34	108.20
32	1a	560	U	C3'-C2'-C1'	5.17	105.64	101.50
57	2a	1264	C	N1-C2-O2	5.17	122.00	118.90
58	A	12	SER	N-CA-C	5.17	124.95	111.00
55	2x	34	C	C2-N1-C1'	5.16	124.48	118.80
57	2a	563	A	O4'-C1'-N9	5.16	112.33	108.20
1	1A	1219	A	OP1-P-O3'	5.16	116.54	105.20
56	2y	33	U	N1-C2-O2	5.15	126.40	122.80
1	1A	591	U	N3-C4-C5	5.14	117.68	114.60
57	2a	299	G	C4-C5-N7	5.13	112.85	110.80
32	1a	1225	A	C5-C6-N6	5.13	127.80	123.70
57	2a	1065	U	P-O3'-C3'	5.13	125.86	119.70
1	1A	1128	U	C2-N3-C4	-5.13	123.92	127.00
1	1A	2054	G	C5-N7-C8	5.13	106.86	104.30
32	1a	1030(B)	C	C5-C6-N1	5.13	123.56	121.00
1	1A	1109	G	C5-C6-N1	-5.12	108.94	111.50
57	2a	1001(A)	G	C4-C5-N7	5.12	112.85	110.80
1	1A	849	A	O5'-P-OP1	-5.12	101.09	105.70
32	1a	1030(B)	C	N3-C2-O2	-5.12	118.32	121.90
1	1A	1700	G	C8-N9-C4	-5.11	104.36	106.40
1	2A	2473	U	C6-N1-C1'	-5.11	114.05	121.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2253	A	OP1-P-O3'	5.11	116.43	105.20
1	1A	1298	G	N3-C4-N9	-5.10	122.94	126.00
1	2A	645	C	C2-N1-C1'	5.09	124.40	118.80
1	1A	715	G	OP2-P-O3'	5.08	116.38	105.20
32	1a	560	U	C2-N1-C1'	5.08	123.80	117.70
1	1A	1426	G	O5'-P-OP2	-5.07	101.14	105.70
1	1A	1121	C	C5-C6-N1	5.06	123.53	121.00
32	1a	1225	A	C6-N1-C2	5.06	121.64	118.60
32	1a	1034	G	C4-N9-C1'	5.06	133.07	126.50
1	2A	645	C	N1-C2-O2	5.05	121.93	118.90
57	2a	1039	C	C5-C6-N1	5.04	123.52	121.00
1	1A	2189	U	C6-N1-C2	-5.04	117.98	121.00
32	1a	1065	U	P-O3'-C3'	5.03	125.74	119.70
1	1A	1808	U	OP1-P-O3'	5.03	116.26	105.20
32	1a	1030	C	C5-C4-N4	5.02	123.72	120.20
32	1a	1020	U	C2-N1-C1'	5.01	123.72	117.70
1	2A	228	A	OP1-P-O3'	5.01	116.22	105.20
1	1A	1299	A	N7-C8-N9	-5.01	111.30	113.80
32	1a	1442	G	C2-N3-C4	5.00	114.40	111.90
54	2w	10	G	C5-C6-N1	-5.00	109.00	111.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
58	A	12	SER	CA
58	B	12	SER	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	8	LYS	Peptide
26	24	56	VAL	Peptide
50	2s	27	GLU	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	261 (96%)	12 (4%)	0	100	100
3	2D	273/276 (99%)	259 (95%)	14 (5%)	0	100	100
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	25	49
4	2E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	25	49
5	1F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	25	49
5	2F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	25	49
6	1G	179/182 (98%)	168 (94%)	8 (4%)	3 (2%)	7	20
6	2G	179/182 (98%)	162 (90%)	13 (7%)	4 (2%)	5	15
7	1H	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	22	45
7	2H	172/180 (96%)	156 (91%)	13 (8%)	3 (2%)	7	20
8	1I	144/148 (97%)	130 (90%)	13 (9%)	1 (1%)	19	42
8	2I	144/148 (97%)	129 (90%)	13 (9%)	2 (1%)	9	24
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
10	1O	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
10	2O	120/122 (98%)	112 (93%)	6 (5%)	2 (2%)	7	20
11	1P	147/150 (98%)	134 (91%)	12 (8%)	1 (1%)	19	42
11	2P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	19	42
12	1Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
12	2Q	139/141 (99%)	130 (94%)	6 (4%)	3 (2%)	5	15
13	1R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
13	2R	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
14	2S	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	14	35
15	1T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	16	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	13	33
17	2V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	13	33
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	110 (100%)	0	0	100	100
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	12	30
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	1Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	13	33
20	2Y	105/110 (96%)	100 (95%)	4 (4%)	1 (1%)	13	33
21	1Z	148/206 (72%)	134 (90%)	12 (8%)	2 (1%)	9	24
21	2Z	156/206 (76%)	138 (88%)	15 (10%)	3 (2%)	6	17
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
22	20	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	12	30
23	21	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	57 (100%)	0	0	100	100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	1
26	24	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	8	22
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	194 (85%)	26 (11%)	9 (4%)	2	5
33	2b	229/256 (90%)	201 (88%)	21 (9%)	7 (3%)	3	8
34	1c	204/239 (85%)	188 (92%)	13 (6%)	3 (2%)	8	22
34	2c	204/239 (85%)	178 (87%)	24 (12%)	2 (1%)	13	33
35	1d	206/209 (99%)	193 (94%)	11 (5%)	2 (1%)	13	33
35	2d	206/209 (99%)	189 (92%)	14 (7%)	3 (2%)	8	22
36	1e	146/162 (90%)	135 (92%)	8 (6%)	3 (2%)	5	15
36	2e	146/162 (90%)	134 (92%)	10 (7%)	2 (1%)	9	24
37	1f	98/101 (97%)	94 (96%)	3 (3%)	1 (1%)	13	33
37	2f	98/101 (97%)	94 (96%)	3 (3%)	1 (1%)	13	33
38	1g	153/156 (98%)	142 (93%)	10 (6%)	1 (1%)	19	42
38	2g	153/156 (98%)	140 (92%)	9 (6%)	4 (3%)	4	11
39	1h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
39	2h	135/138 (98%)	118 (87%)	17 (13%)	0	100	100
40	1i	125/128 (98%)	109 (87%)	14 (11%)	2 (2%)	8	21
40	2i	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
41	1j	95/105 (90%)	84 (88%)	6 (6%)	5 (5%)	1	3
41	2j	94/105 (90%)	79 (84%)	10 (11%)	5 (5%)	1	3
42	1k	112/129 (87%)	105 (94%)	6 (5%)	1 (1%)	14	35
42	2k	112/129 (87%)	105 (94%)	5 (4%)	2 (2%)	7	18
43	1l	119/132 (90%)	114 (96%)	5 (4%)	0	100	100
43	2l	119/132 (90%)	110 (92%)	9 (8%)	0	100	100
44	1m	121/126 (96%)	111 (92%)	9 (7%)	1 (1%)	16	38
44	2m	120/126 (95%)	108 (90%)	12 (10%)	0	100	100
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	51 (88%)	5 (9%)	2 (3%)	3	7
46	1o	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	11	28
46	2o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
47	1p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	10	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	70 (88%)	9 (11%)	1 (1%)	10	26
48	1q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
49	1r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	8	22
50	1s	81/93 (87%)	72 (89%)	8 (10%)	1 (1%)	11	28
50	2s	81/93 (87%)	68 (84%)	10 (12%)	3 (4%)	2	6
51	1t	94/106 (89%)	85 (90%)	5 (5%)	4 (4%)	2	4
51	2t	94/106 (89%)	85 (90%)	4 (4%)	5 (5%)	1	3
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	15 (71%)	6 (29%)	0	100	100
58	A	12/18 (67%)	5 (42%)	5 (42%)	2 (17%)	0	0
58	B	12/18 (67%)	6 (50%)	4 (33%)	2 (17%)	0	0
All	All	11394/12164 (94%)	10597 (93%)	676 (6%)	121 (1%)	12	30

All (121) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	47	LYS
7	1H	126	PRO
8	1I	10	GLU
20	1Y	55	TYR
23	1I	3	LYS
33	1b	10	LEU
33	1b	17	PHE
40	1i	54	ASP
41	1j	79	ARG
51	1t	100	ILE
5	2F	130	ALA
6	2G	47	LYS
7	2H	47	GLU
7	2H	126	PRO
20	2Y	55	TYR
38	2g	6	ARG
50	2s	81	ARG
51	2t	10	LEU
51	2t	47	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
58	A	12	SER
5	1F	130	ALA
15	1T	37	GLY
19	1X	93	GLU
21	1Z	156	LYS
33	1b	22	LYS
33	1b	126	GLU
36	1e	85	GLY
41	1j	55	LYS
44	1m	67	GLU
51	1t	47	GLY
6	2G	49	ASP
6	2G	124	SER
8	2I	10	GLU
10	2O	5	GLN
12	2Q	17	LEU
17	2V	79	VAL
21	2Z	172	ALA
33	2b	17	PHE
34	2c	95	THR
41	2j	29	ARG
41	2j	75	ILE
42	2k	49	GLY
49	2r	36	ASN
51	2t	100	ILE
58	A	16	ASN
58	B	12	SER
58	B	16	ASN
26	14	18	CYS
33	1b	8	LYS
37	1f	40	VAL
41	1j	77	PRO
46	1o	19	PRO
51	1t	10	LEU
7	2H	12	PRO
8	2I	85	GLU
14	2S	96	GLY
21	2Z	142	SER
33	2b	8	LYS
33	2b	20	GLU
35	2d	178	VAL
35	2d	179	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	2g	4	ARG
41	2j	78	ASN
50	2s	27	GLU
51	2t	99	LEU
4	1E	52	LEU
6	1G	49	ASP
26	14	55	ARG
26	14	57	GLU
26	14	64	GLY
34	1c	65	ALA
36	1e	86	ALA
38	1g	80	VAL
41	1j	29	ARG
41	1j	78	ASN
50	1s	27	GLU
4	2E	52	LEU
33	2b	16	HIS
33	2b	74	LYS
33	2b	125	PRO
36	2e	85	GLY
38	2g	80	VAL
45	2n	19	ARG
50	2s	9	VAL
6	1G	43	LEU
11	1P	29	LYS
17	1V	79	VAL
21	1Z	147	GLY
33	1b	9	GLU
33	1b	16	HIS
33	1b	231	GLU
35	1d	178	VAL
35	1d	179	GLU
10	2O	29	ASN
12	2Q	16	ARG
26	24	64	GLY
36	2e	112	LEU
41	2j	79	ARG
6	2G	52	ILE
11	2P	122	PRO
21	2Z	146	ILE
34	2c	66	VAL
45	2n	60	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1c	66	VAL
42	1k	105	VAL
47	1p	53	VAL
12	2Q	15	GLY
33	2b	127	ILE
42	2k	105	VAL
35	2d	171	GLY
51	2t	102	GLY
51	1t	102	GLY
38	2g	17	VAL
41	2j	91	PRO
47	2p	53	VAL
26	14	29	PRO
33	1b	234	PRO
36	1e	69	VAL
40	1i	44	VAL
37	2f	40	VAL
34	1c	81	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%)	197 (92%)	18 (8%)	9	22
3	2D	215/218 (99%)	203 (94%)	12 (6%)	17	41
4	1E	164/166 (99%)	149 (91%)	15 (9%)	7	19
4	2E	164/166 (99%)	153 (93%)	11 (7%)	13	33
5	1F	160/166 (96%)	147 (92%)	13 (8%)	9	23
5	2F	159/166 (96%)	148 (93%)	11 (7%)	13	31
6	1G	143/156 (92%)	135 (94%)	8 (6%)	17	41
6	2G	143/156 (92%)	137 (96%)	6 (4%)	25	53
7	1H	144/148 (97%)	138 (96%)	6 (4%)	25	53
7	2H	144/148 (97%)	139 (96%)	5 (4%)	31	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	1I	113/124 (91%)	103 (91%)	10 (9%)	8	20
8	2I	105/124 (85%)	95 (90%)	10 (10%)	7	17
9	1N	118/119 (99%)	109 (92%)	9 (8%)	11	27
9	2N	118/119 (99%)	111 (94%)	7 (6%)	16	38
10	1O	100/100 (100%)	96 (96%)	4 (4%)	27	55
10	2O	100/100 (100%)	96 (96%)	4 (4%)	27	55
11	1P	115/116 (99%)	109 (95%)	6 (5%)	19	44
11	2P	115/116 (99%)	112 (97%)	3 (3%)	41	70
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	15	35
12	2Q	111/111 (100%)	103 (93%)	8 (7%)	12	30
13	1R	101/101 (100%)	89 (88%)	12 (12%)	4	10
13	2R	101/101 (100%)	90 (89%)	11 (11%)	5	13
14	1S	86/88 (98%)	78 (91%)	8 (9%)	7	18
14	2S	85/88 (97%)	79 (93%)	6 (7%)	12	30
15	1T	115/127 (91%)	111 (96%)	4 (4%)	31	60
15	2T	113/127 (89%)	109 (96%)	4 (4%)	31	60
16	1U	93/94 (99%)	86 (92%)	7 (8%)	11	28
16	2U	93/94 (99%)	90 (97%)	3 (3%)	34	63
17	1V	80/82 (98%)	70 (88%)	10 (12%)	3	9
17	2V	80/82 (98%)	73 (91%)	7 (9%)	8	20
18	1W	90/92 (98%)	83 (92%)	7 (8%)	10	26
18	2W	90/92 (98%)	85 (94%)	5 (6%)	17	41
19	1X	77/78 (99%)	74 (96%)	3 (4%)	27	56
19	2X	77/78 (99%)	77 (100%)	0	100	100
20	1Y	85/91 (93%)	78 (92%)	7 (8%)	9	23
20	2Y	85/91 (93%)	83 (98%)	2 (2%)	44	73
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	9	23
21	2Z	137/179 (76%)	126 (92%)	11 (8%)	10	24
22	10	65/67 (97%)	61 (94%)	4 (6%)	15	36
22	20	65/67 (97%)	60 (92%)	5 (8%)	10	26
23	11	80/83 (96%)	79 (99%)	1 (1%)	65	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	21	80/83 (96%)	78 (98%)	2 (2%)	42	72
24	12	65/67 (97%)	63 (97%)	2 (3%)	35	64
24	22	65/67 (97%)	62 (95%)	3 (5%)	23	49
25	13	51/52 (98%)	49 (96%)	2 (4%)	27	56
25	23	50/52 (96%)	48 (96%)	2 (4%)	27	55
26	14	59/63 (94%)	55 (93%)	4 (7%)	13	32
26	24	53/63 (84%)	51 (96%)	2 (4%)	28	56
27	15	50/52 (96%)	46 (92%)	4 (8%)	10	24
27	25	50/52 (96%)	46 (92%)	4 (8%)	10	24
28	16	51/52 (98%)	45 (88%)	6 (12%)	4	10
28	26	50/52 (96%)	47 (94%)	3 (6%)	16	38
29	17	41/42 (98%)	36 (88%)	5 (12%)	4	9
29	27	41/42 (98%)	37 (90%)	4 (10%)	6	16
30	18	54/55 (98%)	47 (87%)	7 (13%)	3	8
30	28	54/55 (98%)	50 (93%)	4 (7%)	11	28
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	67
33	1b	192/220 (87%)	184 (96%)	8 (4%)	25	53
33	2b	187/220 (85%)	175 (94%)	12 (6%)	14	34
34	1c	142/188 (76%)	137 (96%)	5 (4%)	31	60
34	2c	140/188 (74%)	138 (99%)	2 (1%)	62	84
35	1d	169/181 (93%)	160 (95%)	9 (5%)	19	43
35	2d	173/181 (96%)	161 (93%)	12 (7%)	13	31
36	1e	113/123 (92%)	108 (96%)	5 (4%)	24	51
36	2e	114/123 (93%)	109 (96%)	5 (4%)	24	51
37	1f	84/90 (93%)	82 (98%)	2 (2%)	44	73
37	2f	85/90 (94%)	83 (98%)	2 (2%)	44	73
38	1g	119/127 (94%)	111 (93%)	8 (7%)	13	33
38	2g	120/127 (94%)	116 (97%)	4 (3%)	33	62
39	1h	114/119 (96%)	109 (96%)	5 (4%)	24	51
39	2h	114/119 (96%)	109 (96%)	5 (4%)	24	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	1i	90/99 (91%)	86 (96%)	4 (4%)	24	51
40	2i	89/99 (90%)	80 (90%)	9 (10%)	6	15
41	1j	66/92 (72%)	62 (94%)	4 (6%)	15	36
41	2j	69/92 (75%)	68 (99%)	1 (1%)	62	84
42	1k	82/99 (83%)	77 (94%)	5 (6%)	15	36
42	2k	83/99 (84%)	80 (96%)	3 (4%)	30	59
43	1l	96/108 (89%)	93 (97%)	3 (3%)	35	64
43	2l	96/108 (89%)	93 (97%)	3 (3%)	35	64
44	1m	93/101 (92%)	84 (90%)	9 (10%)	6	17
44	2m	92/101 (91%)	89 (97%)	3 (3%)	33	62
45	1n	49/50 (98%)	42 (86%)	7 (14%)	2	7
45	2n	49/50 (98%)	47 (96%)	2 (4%)	26	54
46	1o	78/80 (98%)	73 (94%)	5 (6%)	14	34
46	2o	78/80 (98%)	76 (97%)	2 (3%)	41	70
47	1p	69/74 (93%)	66 (96%)	3 (4%)	25	52
47	2p	68/74 (92%)	63 (93%)	5 (7%)	11	28
48	1q	94/97 (97%)	91 (97%)	3 (3%)	34	63
48	2q	94/97 (97%)	90 (96%)	4 (4%)	25	52
49	1r	59/77 (77%)	57 (97%)	2 (3%)	32	61
49	2r	59/77 (77%)	57 (97%)	2 (3%)	32	61
50	1s	69/80 (86%)	66 (96%)	3 (4%)	25	52
50	2s	67/80 (84%)	65 (97%)	2 (3%)	36	65
51	1t	70/82 (85%)	69 (99%)	1 (1%)	62	84
51	2t	70/82 (85%)	70 (100%)	0	100	100
52	1u	18/22 (82%)	17 (94%)	1 (6%)	17	41
52	2u	18/22 (82%)	17 (94%)	1 (6%)	17	41
58	A	9/9 (100%)	7 (78%)	2 (22%)	1	2
58	B	9/9 (100%)	7 (78%)	2 (22%)	1	2
All	All	9321/10082 (92%)	8790 (94%)	531 (6%)	17	40

All (531) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	14	ARG
3	1D	32	SER
3	1D	37	LEU
3	1D	39	LYS
3	1D	61	LEU
3	1D	99	ASP
3	1D	106	ILE
3	1D	113	VAL
3	1D	116	GLN
3	1D	155	LEU
3	1D	173	VAL
3	1D	193	VAL
3	1D	211	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	273	ARG
4	1E	12	THR
4	1E	21	VAL
4	1E	24	THR
4	1E	33	VAL
4	1E	34	VAL
4	1E	47	VAL
4	1E	73	GLU
4	1E	75	VAL
4	1E	116	VAL
4	1E	167	VAL
4	1E	170	LEU
4	1E	175	VAL
4	1E	181	LEU
4	1E	184	VAL
4	1E	195	LEU
5	1F	12	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	70	THR
5	1F	74	ARG
5	1F	88	VAL
5	1F	95	ARG
5	1F	106	ARG
5	1F	125	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1F	170	LEU
5	1F	183	VAL
5	1F	192	LEU
6	1G	5	VAL
6	1G	31	VAL
6	1G	43	LEU
6	1G	82	LEU
6	1G	135	LEU
6	1G	140	ILE
6	1G	159	VAL
6	1G	175	LEU
7	1H	15	VAL
7	1H	23	ARG
7	1H	71	LEU
7	1H	81	GLU
7	1H	134	SER
7	1H	139	GLN
8	1I	9	LEU
8	1I	12	LEU
8	1I	38	LEU
8	1I	47	LEU
8	1I	77	LEU
8	1I	101	LEU
8	1I	109	ILE
8	1I	116	LEU
8	1I	123	LEU
8	1I	140	LEU
9	1N	14	VAL
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	48	MET
9	1N	62	VAL
9	1N	73	THR
9	1N	87	LEU
9	1N	99	LEU
10	1O	10	VAL
10	1O	23	ARG
10	1O	24	VAL
10	1O	69	ILE
11	1P	1	MET
11	1P	59	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	1P	77	ARG
11	1P	95	VAL
11	1P	112	LEU
11	1P	125	VAL
12	1Q	22	LYS
12	1Q	35	VAL
12	1Q	75	THR
12	1Q	101	ARG
12	1Q	109	VAL
12	1Q	110	THR
12	1Q	133	ARG
13	1R	6	SER
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	96	ARG
13	1R	100	LEU
13	1R	111	LEU
13	1R	114	VAL
14	1S	14	VAL
14	1S	25	ARG
14	1S	36	TYR
14	1S	46	VAL
14	1S	69	VAL
14	1S	73	LEU
14	1S	85	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	67	SER
15	1T	95	ARG
15	1T	96	ARG
16	1U	8	VAL
16	1U	31	SER
16	1U	50	ARG
16	1U	74	LEU
16	1U	77	SER
16	1U	85	LYS
16	1U	95	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	1V	1	MET
17	1V	35	LEU
17	1V	46	VAL
17	1V	51	VAL
17	1V	52	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	73	SER
17	1V	79	VAL
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	23	LEU
18	1W	63	ASP
18	1W	92	ARG
18	1W	107	LEU
19	1X	35	THR
19	1X	52	VAL
19	1X	81	VAL
20	1Y	7	VAL
20	1Y	64	GLU
20	1Y	72	VAL
20	1Y	90	LEU
20	1Y	97	ARG
20	1Y	99	CYS
20	1Y	107	ASP
21	1Z	18	LEU
21	1Z	33	LEU
21	1Z	61	LEU
21	1Z	91	LEU
21	1Z	126	VAL
21	1Z	129	SER
21	1Z	146	ILE
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	170	THR
21	1Z	171	ILE
22	10	10	THR
22	10	14	ARG
22	10	39	ARG
22	10	74	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	11	95	LEU
24	12	53	LEU
24	12	55	ARG
25	13	23	LEU
25	13	54	VAL
26	14	49	PHE
26	14	50	VAL
26	14	56	VAL
26	14	61	ARG
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
27	15	58	LEU
28	16	6	ARG
28	16	9	LEU
28	16	19	ARG
28	16	38	LYS
28	16	44	ARG
28	16	48	VAL
29	17	1	MET
29	17	39	ARG
29	17	41	ARG
29	17	43	THR
29	17	46	VAL
30	18	6	THR
30	18	14	VAL
30	18	23	VAL
30	18	29	LYS
30	18	31	HIS
30	18	32	LEU
30	18	34	TRP
33	1b	54	THR
33	1b	56	ARG
33	1b	78	GLN
33	1b	83	MET
33	1b	94	ASN
33	1b	111	ARG
33	1b	178	ARG
33	1b	185	ILE
34	1c	3	ASN
34	1c	112	SER
34	1c	115	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1c	195	VAL
34	1c	206	GLU
35	1d	5	ILE
35	1d	19	LEU
35	1d	31	CYS
35	1d	59	ARG
35	1d	70	ILE
35	1d	107	ARG
35	1d	135	LEU
35	1d	178	VAL
35	1d	196	LEU
36	1e	16	THR
36	1e	20	GLN
36	1e	41	VAL
36	1e	67	VAL
36	1e	91	LEU
37	1f	21	LEU
37	1f	45	LEU
38	1g	15	ASP
38	1g	16	LEU
38	1g	59	LEU
38	1g	79	ARG
38	1g	104	LEU
38	1g	111	ARG
38	1g	114	ARG
38	1g	115	ARG
39	1h	25	ASP
39	1h	26	VAL
39	1h	63	LEU
39	1h	85	ARG
39	1h	112	LEU
40	1i	54	ASP
40	1i	103	THR
40	1i	121	ARG
40	1i	128	ARG
41	1j	38	ILE
41	1j	43	ARG
41	1j	81	THR
41	1j	92	THR
42	1k	33	THR
42	1k	48	ILE
42	1k	87	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	1k	109	VAL
42	1k	114	VAL
43	1l	33	ARG
43	1l	83	VAL
43	1l	113	ARG
44	1m	14	ARG
44	1m	19	LEU
44	1m	43	THR
44	1m	49	THR
44	1m	70	LEU
44	1m	102	ARG
44	1m	104	ARG
44	1m	105	THR
44	1m	117	VAL
45	1n	3	ARG
45	1n	6	LEU
45	1n	7	ILE
45	1n	18	VAL
45	1n	23	ARG
45	1n	32	SER
45	1n	33	VAL
46	1o	5	LYS
46	1o	39	LEU
46	1o	56	LEU
46	1o	65	ARG
46	1o	87	ILE
47	1p	2	VAL
47	1p	20	VAL
47	1p	67	THR
48	1q	63	ARG
48	1q	70	ARG
48	1q	72	ARG
49	1r	26	LEU
49	1r	54	ARG
50	1s	70	LYS
50	1s	77	THR
50	1s	79	THR
51	1t	8	ARG
52	1u	24	ARG
3	2D	14	ARG
3	2D	37	LEU
3	2D	61	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2D	111	LEU
3	2D	113	VAL
3	2D	138	VAL
3	2D	142	VAL
3	2D	173	VAL
3	2D	211	ARG
3	2D	242	ARG
3	2D	257	LEU
3	2D	259	THR
4	2E	9	VAL
4	2E	14	ILE
4	2E	21	VAL
4	2E	24	THR
4	2E	27	LEU
4	2E	75	VAL
4	2E	107	THR
4	2E	116	VAL
4	2E	170	LEU
4	2E	175	VAL
4	2E	181	LEU
5	2F	33	LEU
5	2F	53	THR
5	2F	70	THR
5	2F	74	ARG
5	2F	88	VAL
5	2F	106	ARG
5	2F	158	THR
5	2F	183	VAL
5	2F	192	LEU
5	2F	195	ASP
5	2F	201	VAL
6	2G	5	VAL
6	2G	43	LEU
6	2G	91	ARG
6	2G	133	LEU
6	2G	140	ILE
6	2G	159	VAL
7	2H	70	THR
7	2H	71	LEU
7	2H	84	SER
7	2H	95	ARG
7	2H	134	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	2I	38	LEU
8	2I	44	LEU
8	2I	47	LEU
8	2I	92	VAL
8	2I	101	LEU
8	2I	102	SER
8	2I	116	LEU
8	2I	123	LEU
8	2I	127	VAL
8	2I	144	VAL
9	2N	15	LEU
9	2N	28	THR
9	2N	34	LEU
9	2N	35	ARG
9	2N	46	VAL
9	2N	99	LEU
9	2N	140	VAL
10	2O	23	ARG
10	2O	52	VAL
10	2O	66	LYS
10	2O	116	SER
11	2P	58	THR
11	2P	95	VAL
11	2P	148	LEU
12	2Q	1	MET
12	2Q	35	VAL
12	2Q	38	GLU
12	2Q	60	ARG
12	2Q	75	THR
12	2Q	109	VAL
12	2Q	110	THR
12	2Q	133	ARG
13	2R	6	SER
13	2R	24	GLN
13	2R	29	LEU
13	2R	36	THR
13	2R	44	LEU
13	2R	54	LEU
13	2R	65	LEU
13	2R	96	ARG
13	2R	100	LEU
13	2R	111	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	2R	114	VAL
14	2S	23	ARG
14	2S	25	ARG
14	2S	36	TYR
14	2S	52	SER
14	2S	80	LEU
14	2S	110	LEU
15	2T	41	ARG
15	2T	104	ASN
15	2T	108	ARG
15	2T	115	ARG
16	2U	8	VAL
16	2U	31	SER
16	2U	74	LEU
17	2V	7	THR
17	2V	12	TYR
17	2V	46	VAL
17	2V	62	LEU
17	2V	66	ARG
17	2V	72	VAL
17	2V	79	VAL
18	2W	11	ARG
18	2W	17	VAL
18	2W	19	LEU
18	2W	23	LEU
18	2W	107	LEU
20	2Y	49	VAL
20	2Y	97	ARG
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	53	ILE
21	2Z	71	VAL
21	2Z	72	ARG
21	2Z	84	GLU
21	2Z	91	LEU
21	2Z	144	LEU
21	2Z	154	ASP
21	2Z	170	THR
21	2Z	174	VAL
22	20	9	SER
22	20	14	ARG
22	20	27	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	20	39	ARG
22	20	74	ARG
23	21	35	THR
23	21	95	LEU
24	22	28	LYS
24	22	52	ASP
24	22	59	ARG
25	23	31	LEU
25	23	54	VAL
26	24	49	PHE
26	24	53	GLU
27	25	6	VAL
27	25	29	THR
27	25	40	LYS
27	25	58	LEU
28	26	14	THR
28	26	19	ARG
28	26	44	ARG
29	27	1	MET
29	27	39	ARG
29	27	41	ARG
29	27	43	THR
30	28	14	VAL
30	28	31	HIS
30	28	32	LEU
30	28	37	SER
31	29	7	VAL
33	2b	23	ARG
33	2b	93	VAL
33	2b	94	ASN
33	2b	111	ARG
33	2b	124	SER
33	2b	127	ILE
33	2b	176	GLU
33	2b	178	ARG
33	2b	185	ILE
33	2b	189	ASP
33	2b	192	SER
33	2b	230	VAL
34	2c	128	PHE
34	2c	166	GLU
35	2d	31	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2d	83	SER
35	2d	107	ARG
35	2d	108	LEU
35	2d	135	LEU
35	2d	150	GLU
35	2d	170	VAL
35	2d	175	SER
35	2d	178	VAL
35	2d	181	MET
35	2d	208	SER
35	2d	209	ARG
36	2e	41	VAL
36	2e	68	GLU
36	2e	75	THR
36	2e	111	GLU
36	2e	120	THR
37	2f	72	VAL
37	2f	93	SER
38	2g	13	GLN
38	2g	16	LEU
38	2g	78	ARG
38	2g	79	ARG
39	2h	3	THR
39	2h	14	ARG
39	2h	51	VAL
39	2h	85	ARG
39	2h	112	LEU
40	2i	3	GLN
40	2i	14	VAL
40	2i	53	VAL
40	2i	64	THR
40	2i	71	SER
40	2i	75	ASP
40	2i	102	LEU
40	2i	108	VAL
40	2i	128	ARG
41	2j	81	THR
42	2k	14	VAL
42	2k	81	ASP
42	2k	114	VAL
43	2l	83	VAL
43	2l	113	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	2l	117	ARG
44	2m	19	LEU
44	2m	90	LEU
44	2m	108	ARG
45	2n	18	VAL
45	2n	33	VAL
46	2o	31	LEU
46	2o	39	LEU
47	2p	1	MET
47	2p	2	VAL
47	2p	21	VAL
47	2p	67	THR
47	2p	69	THR
48	2q	14	LYS
48	2q	58	GLU
48	2q	83	ASP
48	2q	87	LYS
49	2r	37	VAL
49	2r	76	LEU
50	2s	4	SER
50	2s	5	LEU
52	2u	10	ARG
58	A	12	SER
58	A	14	SER
58	B	12	SER
58	B	14	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	126	GLN
5	1F	203	GLN
6	1G	26	GLN
12	1Q	57	HIS
14	1S	95	HIS
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
20	1Y	43	ASN
21	1Z	73	GLN
21	1Z	151	HIS
22	10	50	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	11	56	GLN
25	13	32	GLN
34	1c	6	HIS
34	1c	37	GLN
34	1c	162	GLN
35	1d	42	GLN
35	1d	77	ASN
35	1d	119	GLN
35	1d	123	HIS
35	1d	125	HIS
36	1e	78	HIS
37	1f	100	ASN
38	1g	28	ASN
40	1i	3	GLN
40	1i	31	GLN
40	1i	58	HIS
40	1i	87	GLN
40	1i	124	GLN
41	1j	56	HIS
43	1l	99	HIS
45	1n	49	HIS
46	1o	28	GLN
47	1p	13	HIS
50	1s	23	ASN
50	1s	69	HIS
50	1s	83	HIS
51	1t	16	HIS
3	2D	87	ASN
4	2E	48	GLN
5	2F	69	HIS
6	2G	66	GLN
12	2Q	123	HIS
13	2R	31	HIS
13	2R	71	GLN
17	2V	80	GLN
18	2W	60	ASN
19	2X	31	HIS
21	2Z	73	GLN
22	20	50	ASN
23	21	56	GLN
25	23	32	GLN
26	24	46	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	2b	40	HIS
33	2b	94	ASN
34	2c	6	HIS
34	2c	102	ASN
35	2d	125	HIS
36	2e	78	HIS
37	2f	73	ASN
37	2f	100	ASN
38	2g	28	ASN
38	2g	86	GLN
38	2g	109	ASN
40	2i	3	GLN
40	2i	58	HIS
40	2i	87	GLN
41	2j	56	HIS
44	2m	77	ASN
46	2o	62	GLN
49	2r	63	GLN
50	2s	23	ASN
50	2s	47	HIS
50	2s	69	HIS
50	2s	83	HIS
58	A	5	ASN
58	B	5	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	407 (14%)	38 (1%)
1	2A	2788/2915 (95%)	458 (16%)	25 (0%)
2	1B	120/121 (99%)	10 (8%)	1 (0%)
2	2B	118/121 (97%)	27 (22%)	0
32	1a	1494/1521 (98%)	227 (15%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	1 (8%)	0
54	1w	71/76 (93%)	23 (32%)	0
54	2w	68/76 (89%)	22 (32%)	0
55	1x	75/77 (97%)	10 (13%)	0
55	2x	75/77 (97%)	14 (18%)	0
56	1y	72/76 (94%)	19 (26%)	0
56	2y	70/76 (92%)	18 (25%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
57	2a	1498/1521 (98%)	260 (17%)	0
All	All	9334/9620 (97%)	1498 (16%)	64 (0%)

All (1498) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	54	G
1	1A	70	A
1	1A	71	U
1	1A	73	A
1	1A	74	G
1	1A	77	A
1	1A	83	A
1	1A	94	G
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	137	G
1	1A	170	A
1	1A	171	A
1	1A	185	A
1	1A	188	A
1	1A	194	G
1	1A	203	G
1	1A	204	G
1	1A	205	A
1	1A	211	A
1	1A	217	A
1	1A	218	A
1	1A	222	A
1	1A	237	G
1	1A	271	U
1	1A	272	U
1	1A	273	G
1	1A	275	C
1	1A	276	C
1	1A	289	G
1	1A	296	U
1	1A	299	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	303	C
1	1A	335	A
1	1A	353	G
1	1A	354	A
1	1A	376	G
1	1A	387	G
1	1A	388	A
1	1A	389	G
1	1A	407	U
1	1A	413	G
1	1A	423	G
1	1A	432	U
1	1A	438	G
1	1A	439	A
1	1A	448	U
1	1A	455	A
1	1A	470	C
1	1A	474	U
1	1A	480	A
1	1A	482	C
1	1A	483	A
1	1A	507	G
1	1A	529	U
1	1A	530	A
1	1A	533	G
1	1A	534	C
1	1A	537	G
1	1A	553	A
1	1A	554	A
1	1A	555	G
1	1A	556	C
1	1A	557	A
1	1A	558	G
1	1A	569	G
1	1A	573	G
1	1A	586	G
1	1A	596	G
1	1A	597	C
1	1A	598	A
1	1A	609	A
1	1A	626	A
1	1A	627	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	630	U
1	1A	639	G
1	1A	641	G
1	1A	642	G
1	1A	652	A
1	1A	662	A
1	1A	670	C
1	1A	671	A
1	1A	678	A
1	1A	697	C
1	1A	699	C
1	1A	716	G
1	1A	733	G
1	1A	764	G
1	1A	777	C
1	1A	811	A
1	1A	812	G
1	1A	822	G
1	1A	823	G
1	1A	829	A
1	1A	830	A
1	1A	831	A
1	1A	832	G
1	1A	837	C
1	1A	839	G
1	1A	852	G
1	1A	859	C
1	1A	866	A
1	1A	874	U
1	1A	875	U
1	1A	906	G
1	1A	913	A
1	1A	924	U
1	1A	926	G
1	1A	927	G
1	1A	931	C
1	1A	932	C
1	1A	933	C
1	1A	934	A
1	1A	935	C
1	1A	936	C
1	1A	937	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	940	C
1	1A	942	A
1	1A	943	C
1	1A	944	C
1	1A	946	A
1	1A	956	A
1	1A	977	G
1	1A	990	A
1	1A	991	G
1	1A	1003	U
1	1A	1004	A
1	1A	1006	C
1	1A	1008	U
1	1A	1019	G
1	1A	1020	C
1	1A	1029	A
1	1A	1042	A
1	1A	1051	C
1	1A	1058	U
1	1A	1059	C
1	1A	1068	G
1	1A	1072	U
1	1A	1073	A
1	1A	1079	U
1	1A	1084	C
1	1A	1087	C
1	1A	1091	A
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1097	G
1	1A	1100	A
1	1A	1101	G
1	1A	1104	G
1	1A	1109	G
1	1A	1113	A
1	1A	1114	G
1	1A	1116	A
1	1A	1117	G
1	1A	1119	A
1	1A	1120	G
1	1A	1121	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1122	C
1	1A	1124	U
1	1A	1125	C
1	1A	1134	A
1	1A	1135	G
1	1A	1136	U
1	1A	1137	G
1	1A	1139	G
1	1A	1140	U
1	1A	1142	A
1	1A	1147	U
1	1A	1157	A
1	1A	1158	G
1	1A	1161	G
1	1A	1162	C
1	1A	1174	A
1	1A	1180	C
1	1A	1181	G
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1222	A
1	1A	1223	C
1	1A	1256	U
1	1A	1290	G
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1346	U
1	1A	1347	A
1	1A	1349	G
1	1A	1366	C
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1418	U
1	1A	1426	G
1	1A	1430	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1431	G
1	1A	1462	G
1	1A	1463	C
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1491	A
1	1A	1497	G
1	1A	1502	G
1	1A	1514	C
1	1A	1529	G
1	1A	1536	A
1	1A	1539	C
1	1A	1542	A
1	1A	1554	A
1	1A	1555	C
1	1A	1556	A
1	1A	1586	G
1	1A	1589	A
1	1A	1590	C
1	1A	1605	A
1	1A	1606	G
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1628	G
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1655	A
1	1A	1656	A
1	1A	1695	C
1	1A	1701	A
1	1A	1721	G
1	1A	1743	G
1	1A	1747	A
1	1A	1750	G
1	1A	1767	A
1	1A	1776	G
1	1A	1787	G
1	1A	1794	G
1	1A	1795	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1804	A
1	1A	1811	A
1	1A	1813	C
1	1A	1822	A
1	1A	1831	C
1	1A	1832	G
1	1A	1847	G
1	1A	1860	A
1	1A	1878	A
1	1A	1889	G
1	1A	1899	A
1	1A	1900	G
1	1A	1911	A
1	1A	1922	A
1	1A	1928	G
1	1A	1941	A
1	1A	1951	G
1	1A	1952	G
1	1A	1959	A
1	1A	1960	A
1	1A	1977	U
1	1A	1985	U
1	1A	1987	C
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2014	G
1	1A	2015	U
1	1A	2019	G
1	1A	2042	A
1	1A	2045	G
1	1A	2053	A
1	1A	2054	G
1	1A	2055	A
1	1A	2061	C
1	1A	2065	C
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2091	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2132	G
1	1A	2135	U
1	1A	2137	G
1	1A	2138	G
1	1A	2143	G
1	1A	2149	G
1	1A	2151	C
1	1A	2152	U
1	1A	2153	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2157	A
1	1A	2158	C
1	1A	2163	G
1	1A	2164	C
1	1A	2165	C
1	1A	2166	U
1	1A	2168	C
1	1A	2169	G
1	1A	2172	U
1	1A	2173	G
1	1A	2178	G
1	1A	2179	G
1	1A	2180	A
1	1A	2181	G
1	1A	2187	G
1	1A	2188	G
1	1A	2189	U
1	1A	2190	G
1	1A	2191	A
1	1A	2193	A
1	1A	2194	U
1	1A	2196	C
1	1A	2200	C
1	1A	2204	G
1	1A	2206	G
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G
1	1A	2228	G
1	1A	2229	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2237	A
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A
1	1A	2292	G
1	1A	2295	C
1	1A	2299	A
1	1A	2301	G
1	1A	2317	A
1	1A	2320	G
1	1A	2325	C
1	1A	2332	A
1	1A	2337	G
1	1A	2346	G
1	1A	2348	A
1	1A	2359	C
1	1A	2362	C
1	1A	2373	A
1	1A	2395	G
1	1A	2397	C
1	1A	2411	G
1	1A	2418	U
1	1A	2437	A
1	1A	2441	G
1	1A	2442	A
1	1A	2443	U
1	1A	2447	A
1	1A	2451	A
1	1A	2452	C
1	1A	2453	C
1	1A	2460	A
1	1A	2488	A
1	1A	2490	A
1	1A	2514	G
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2541	G
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2585	C
1	1A	2598	C
1	1A	2614	A
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2641	A
1	1A	2642	G
1	1A	2666	A
1	1A	2701	U
1	1A	2702	C
1	1A	2714	U
1	1A	2715	C
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2746	A
1	1A	2770	A
1	1A	2778	A
1	1A	2779	G
1	1A	2782	C
1	1A	2791	A
1	1A	2803	A
1	1A	2804	C
1	1A	2806	G
1	1A	2813	G
1	1A	2814	C
1	1A	2830	A
1	1A	2831	A
1	1A	2845	A
1	1A	2882	G
1	1A	2890	C
1	1A	2901	A
1	1A	2903	G
2	1B	2	C
2	1B	15	A
2	1B	45	A
2	1B	50	G
2	1B	52	A
2	1B	56	G
2	1B	67	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1B	73	A
2	1B	106	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	51	A
32	1a	54	C
32	1a	61	G
32	1a	69	G
32	1a	79	G
32	1a	91	C
32	1a	96	U
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	145	G
32	1a	162	A
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	218	C
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	301	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	342	C
32	1a	348	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	392	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	421	U
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	524	G
32	1a	527	G7M
32	1a	531	U
32	1a	532	A
32	1a	533	A
32	1a	547	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	562	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	630	G
32	1a	653	A
32	1a	659	U
32	1a	665	A
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	752	G
32	1a	755	G
32	1a	774	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	870	U
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	1000	U
32	1a	1001(A)	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1030(D)	A
32	1a	1031	G
32	1a	1033	G
32	1a	1039	C
32	1a	1044	A
32	1a	1054	C
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1125	U
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1141	C
32	1a	1152	A
32	1a	1157	A
32	1a	1159	U
32	1a	1160	G
32	1a	1168	A
32	1a	1172	C
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C
32	1a	1273	G
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1320	C
32	1a	1338	G
32	1a	1347	G
32	1a	1353	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1381	U
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	24	A
54	1w	2	C
54	1w	6	G
54	1w	7	A
54	1w	8	4SU
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	45	U
54	1w	46	G7M
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	62	C
54	1w	67	C
54	1w	68	C
54	1w	69	G
54	1w	70	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	1w	72	C
54	1w	73	A
54	1w	74	C
55	1x	9	G
55	1x	14	A
55	1x	18	G
55	1x	19	G
55	1x	21	A
55	1x	47	U
55	1x	61	C
55	1x	63	G
55	1x	69	C
55	1x	76	A
56	1y	6	G
56	1y	8	4SU
56	1y	13	C
56	1y	19	G
56	1y	20	U
56	1y	21	A
56	1y	35	A
56	1y	36	A
56	1y	44	G
56	1y	45	U
56	1y	46	G7M
56	1y	48	C
56	1y	49	C
56	1y	53	G
56	1y	54	5MU
56	1y	59	U
56	1y	65	G
56	1y	69	G
56	1y	70	G
1	2A	11	G
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	94	C
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	141	A
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	233	A
1	2A	248	G
1	2A	249	C
1	2A	250	G
1	2A	266	G
1	2A	267	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	279	C
1	2A	283	A
1	2A	294	A
1	2A	311	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	342	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	352	G
1	2A	354	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	363(D)	G
1	2A	386	G
1	2A	396	G
1	2A	405	U
1	2A	406	G
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	422	A
1	2A	435	C
1	2A	444	C
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	494	G
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	528	A
1	2A	529	A
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	588	U
1	2A	592	G
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	651	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	852	G
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	870	A
1	2A	874	G
1	2A	875	G
1	2A	877	U
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	883	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	914	C
1	2A	917	A
1	2A	923	C
1	2A	932	G
1	2A	933	A
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	997	G
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1020	A
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1037	G
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1116	C
1	2A	1135	C
1	2A	1136	G
1	2A	1137	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1144	G
1	2A	1155	A
1	2A	1171	G
1	2A	1188	U
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1248	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1284	A
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1308	A
1	2A	1314	C
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1373	A
1	2A	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1460	A
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1543	C
1	2A	1545	A
1	2A	1547	C
1	2A	1558	A
1	2A	1559	G
1	2A	1569	A
1	2A	1578	U
1	2A	1583	A
1	2A	1584	C
1	2A	1586	A
1	2A	1603	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C
1	2A	1647	G
1	2A	1648	C
1	2A	1653	G
1	2A	1654	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1740	G
1	2A	1746	G
1	2A	1747	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1811	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1900	A
1	2A	1906	G
1	2A	1912	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1931	U
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2096	U
1	2A	2097	C
1	2A	2104	G
1	2A	2105	C
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2130	U
1	2A	2131	G
1	2A	2132	U
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C
1	2A	2146	C
1	2A	2150	U
1	2A	2153	G
1	2A	2154	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2159	G
1	2A	2161	C
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2174	C
1	2A	2182	G
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2219	G
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2294	C
1	2A	2305	A
1	2A	2308	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2372	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2402	C
1	2A	2403	C
1	2A	2406	U
1	2A	2419	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2434	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2468	G
1	2A	2469	A
1	2A	2476	A
1	2A	2487	G
1	2A	2490	G
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2536	G
1	2A	2554	U
1	2A	2562	U
1	2A	2564	A
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2574	G
1	2A	2586	C
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2712(A)	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2758	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2780	G
1	2A	2789	C
1	2A	2793	G
1	2A	2802	G
1	2A	2803	C
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2872	G
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	2B	2	C
2	2B	8	U
2	2B	13	A
2	2B	19	G
2	2B	25	A
2	2B	30	C
2	2B	32	C
2	2B	34	U
2	2B	42	C
2	2B	53	A
2	2B	56	G
2	2B	63	G
2	2B	65	C
2	2B	67	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2B	72	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	90	A
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	111	G
2	2B	114	C
2	2B	116	G
2	2B	120	A
57	2a	9	G
57	2a	22	G
57	2a	31	G
57	2a	32	A
57	2a	39	G
57	2a	47	C
57	2a	48	C
57	2a	50	A
57	2a	51	A
57	2a	66	G
57	2a	73	G
57	2a	79	G
57	2a	89	C
57	2a	98	G
57	2a	101	A
57	2a	116	A
57	2a	121	C
57	2a	131	C
57	2a	144	G
57	2a	163	C
57	2a	174	C
57	2a	182	U
57	2a	189(F)	U
57	2a	195	A
57	2a	197	A
57	2a	201	C
57	2a	202	U
57	2a	203	U
57	2a	204	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	2a	216	G
57	2a	247	G
57	2a	251	G
57	2a	258	G
57	2a	266	G
57	2a	267	C
57	2a	281	G
57	2a	289	G
57	2a	300	A
57	2a	321	A
57	2a	328	C
57	2a	332	G
57	2a	342	C
57	2a	351	G
57	2a	352	C
57	2a	353	A
57	2a	354	G
57	2a	367	U
57	2a	372	C
57	2a	384	G
57	2a	397	A
57	2a	398	C
57	2a	406	G
57	2a	412	A
57	2a	423	G
57	2a	429	U
57	2a	430	A
57	2a	439	A
57	2a	442	C
57	2a	452	A
57	2a	461	A
57	2a	470	C
57	2a	477	A
57	2a	482	A
57	2a	484	G
57	2a	485	G
57	2a	496	A
57	2a	498	U
57	2a	499	A
57	2a	505	G
57	2a	510	A
57	2a	511	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	2a	518	C
57	2a	521	G
57	2a	531	U
57	2a	532	A
57	2a	533	A
57	2a	547	A
57	2a	559	A
57	2a	564	C
57	2a	568	G
57	2a	572	A
57	2a	573	A
57	2a	576	G
57	2a	577	G
57	2a	596	C
57	2a	630	G
57	2a	653	A
57	2a	665	A
57	2a	666	G
57	2a	687	A
57	2a	688	G
57	2a	695	A
57	2a	721	G
57	2a	723	U
57	2a	724	G
57	2a	731	G
57	2a	749	C
57	2a	755	G
57	2a	777	A
57	2a	792	A
57	2a	793	U
57	2a	794	A
57	2a	816	A
57	2a	817	C
57	2a	821	G
57	2a	828	A
57	2a	840	C
57	2a	841	U
57	2a	853	G
57	2a	859	A
57	2a	874	G
57	2a	885	G
57	2a	902	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	2a	914	A
57	2a	926	G
57	2a	927	G
57	2a	934	C
57	2a	935	A
57	2a	942	G
57	2a	960	U
57	2a	961	U
57	2a	968	A
57	2a	969	A
57	2a	971	G
57	2a	972	C
57	2a	974	A
57	2a	975	A
57	2a	976	G
57	2a	977	A
57	2a	982	U
57	2a	984	C
57	2a	989	C
57	2a	992	U
57	2a	993	G
57	2a	997	U
57	2a	998	G
57	2a	999	C
57	2a	1001	A
57	2a	1001(A)	G
57	2a	1002	G
57	2a	1003	G
57	2a	1004	A
57	2a	1005	A
57	2a	1006	C
57	2a	1009	G
57	2a	1011	G
57	2a	1016	A
57	2a	1020	U
57	2a	1021	G
57	2a	1022	G
57	2a	1025	U
57	2a	1026	G
57	2a	1027	C
57	2a	1029	C
57	2a	1030	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	2a	1030(A)	G
57	2a	1031	G
57	2a	1032	G
57	2a	1035	A
57	2a	1038	C
57	2a	1039	C
57	2a	1040	U
57	2a	1045	C
57	2a	1046	A
57	2a	1051	C
57	2a	1053	G
57	2a	1054	C
57	2a	1055	A
57	2a	1065	U
57	2a	1066	C
57	2a	1068	G
57	2a	1077	G
57	2a	1078	U
57	2a	1079	G
57	2a	1081	G
57	2a	1086	U
57	2a	1094	G
57	2a	1095	U
57	2a	1101	A
57	2a	1108	G
57	2a	1113	C
57	2a	1117	G
57	2a	1122	U
57	2a	1125	U
57	2a	1129	C
57	2a	1130	A
57	2a	1132	C
57	2a	1136	U
57	2a	1137	C
57	2a	1138	G
57	2a	1139	G
57	2a	1146	A
57	2a	1147	C
57	2a	1152	A
57	2a	1157	A
57	2a	1158	C
57	2a	1159	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	2a	1160	G
57	2a	1182	G
57	2a	1183	A
57	2a	1184	G
57	2a	1193	G
57	2a	1196	U
57	2a	1197	G
57	2a	1202	G
57	2a	1211	U
57	2a	1213	A
57	2a	1227	A
57	2a	1236	A
57	2a	1238	A
57	2a	1240	U
57	2a	1241	G
57	2a	1256	A
57	2a	1257	U
57	2a	1258	G
57	2a	1260	C
57	2a	1261	A
57	2a	1264	C
57	2a	1267	C
57	2a	1268	A
57	2a	1270	C
57	2a	1272	G
57	2a	1273	G
57	2a	1276	G
57	2a	1277	C
57	2a	1278	U
57	2a	1279	A
57	2a	1280	A
57	2a	1286	A
57	2a	1287	A
57	2a	1302	U
57	2a	1303	C
57	2a	1305	G
57	2a	1323	G
57	2a	1338	G
57	2a	1340	A
57	2a	1346	A
57	2a	1347	G
57	2a	1358	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	2a	1359	C
57	2a	1363	C
57	2a	1368	G
57	2a	1370	G
57	2a	1378	C
57	2a	1419	G
57	2a	1442	G
57	2a	1442(A)	G
57	2a	1447	A
57	2a	1452	C
57	2a	1456	G
57	2a	1492	A
57	2a	1497	G
57	2a	1504	G
57	2a	1506	U
57	2a	1517	G
57	2a	1520	G
57	2a	1529	G
57	2a	1530	G
57	2a	1531	A
57	2a	1532	U
53	2v	13	A
54	2w	3	C
54	2w	4	C
54	2w	5	G
54	2w	6	G
54	2w	8	4SU
54	2w	11	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	27	G
54	2w	46	G7M
54	2w	47	U
54	2w	48	C
54	2w	50	U
54	2w	62	C
54	2w	64	A
54	2w	65	G
54	2w	68	C
54	2w	69	G
54	2w	70	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	2w	73	A
54	2w	74	C
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	21	A
55	2x	22	G
55	2x	46	G
55	2x	47	U
55	2x	48	C
55	2x	51	C
55	2x	52	G
55	2x	53	G
55	2x	67	C
55	2x	68	C
55	2x	76	A
56	2y	5	G
56	2y	8	4SU
56	2y	13	C
56	2y	19	G
56	2y	35	A
56	2y	37	A
56	2y	44	G
56	2y	45	U
56	2y	46	G7M
56	2y	48	C
56	2y	49	C
56	2y	53	G
56	2y	54	5MU
56	2y	59	U
56	2y	65	G
56	2y	66	U
56	2y	69	G
56	2y	70	G

All (64) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	115	G
1	1A	185	A
1	1A	271	U
1	1A	302	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	509	A
1	1A	572	A
1	1A	596	G
1	1A	716	G
1	1A	732	A
1	1A	793	A
1	1A	811	A
1	1A	821	A
1	1A	913	A
1	1A	941	U
1	1A	1003	U
1	1A	1019	G
1	1A	1065	U
1	1A	1067	A
1	1A	1093	G
1	1A	1201	A
1	1A	1219	A
1	1A	1221	G
1	1A	1255	A
1	1A	1425	A
1	1A	1554	A
1	1A	1654	A
1	1A	1700	G
1	1A	1793	A
1	1A	2014	G
1	1A	2156	A
1	1A	2203	G
1	1A	2205	C
1	1A	2418	U
1	1A	2442	A
1	1A	2451	A
1	1A	2641	A
1	1A	2701	U
1	1A	2769	U
2	1B	1	U
1	2A	34	C
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	528	A
1	2A	752	A
1	2A	774	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	958	U
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1608	A
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2689	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	G7M	1a	527	59,32	20,26,27	2.75	3 (15%)	16,39,42	0.89	1 (6%)
55	PSU	2x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.02	4 (19%)
1	4OC	2A	1920	1	19,22,24	0.76	0	25,31,35	0.88	1 (4%)
43	0TD	2l	92	43	8,9,10	4.58	1 (12%)	6,11,13	3.35	3 (50%)
55	4SU	2x	8	55,59	18,21,22	2.08	4 (22%)	25,30,33	1.47	6 (24%)
1	PSU	2A	1917	1	18,21,22	1.38	2 (11%)	21,30,33	2.04	3 (14%)
54	PSU	2w	32	54	18,21,22	1.32	2 (11%)	21,30,33	1.95	4 (19%)
55	5MC	1x	32	55	19,22,23	1.63	3 (15%)	26,32,35	1.22	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	1A	1984	59,1	19,22,23	1.61	3 (15%)	26,32,35	1.10	2 (7%)
1	OMG	2A	2251	55,59,1	19,26,27	0.92	1 (5%)	21,38,41	1.10	2 (9%)
56	4SU	1y	8	56	18,21,22	1.75	5 (27%)	25,30,33	1.99	5 (20%)
1	2MU	1A	2564	59,1	19,22,24	1.22	2 (10%)	25,31,36	2.05	6 (24%)
32	5MC	1a	1404	32	19,22,23	1.73	3 (15%)	26,32,35	1.20	4 (15%)
32	PSU	1a	516	59,32	18,21,22	1.35	3 (16%)	21,30,33	1.97	5 (23%)
58	BB9	A	6	58	2,5,6	4.24	1 (50%)	1,5,7	2.55	1 (100%)
54	MIA	2w	37	54	19,27,32	1.94	2 (10%)	18,39,47	1.51	4 (22%)
1	PSU	1A	1939	1	18,21,22	1.35	2 (11%)	21,30,33	2.07	3 (14%)
1	5MU	1A	1961	1	19,22,23	1.41	5 (26%)	27,32,35	2.38	6 (22%)
32	M2G	1a	966	32	20,27,28	1.33	2 (10%)	19,40,43	1.06	2 (10%)
57	5MC	2a	1404	57	19,22,23	1.70	3 (15%)	26,32,35	1.22	3 (11%)
54	MIA	1w	37	54	24,31,32	2.22	3 (12%)	22,44,47	2.47	6 (27%)
57	UR3	2a	1498	57	19,22,23	1.02	1 (5%)	26,32,35	1.79	3 (11%)
58	BB9	A	9	58	2,5,6	4.61	1 (50%)	1,5,7	2.56	1 (100%)
1	2MA	2A	2503	59,1	18,25,26	0.72	0	20,37,40	1.86	4 (20%)
1	5MC	1A	1964	59,1	19,22,23	1.46	3 (15%)	26,32,35	1.12	2 (7%)
32	5MC	1a	1400	32	19,22,23	1.61	3 (15%)	26,32,35	1.15	3 (11%)
58	BB9	B	17	58	2,5,6	4.30	1 (50%)	1,5,7	4.14	1 (100%)
54	PSU	1w	32	59,54	18,21,22	1.35	2 (11%)	21,30,33	1.93	3 (14%)
56	5MU	2y	54	56	19,22,23	1.52	5 (26%)	27,32,35	2.02	9 (33%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	1.06	1 (4%)
32	5MC	1a	967	32	19,22,23	1.58	2 (10%)	26,32,35	1.05	2 (7%)
57	G7M	2a	527	57,59	20,26,27	2.68	4 (20%)	16,39,42	0.90	1 (6%)
32	2MG	1a	1207	32	18,26,27	0.92	1 (5%)	16,38,41	1.63	4 (25%)
57	MA6	2a	1519	57	19,26,27	1.21	2 (10%)	18,38,41	2.03	4 (22%)
32	MA6	1a	1518	32	19,26,27	1.11	2 (10%)	18,38,41	2.19	5 (27%)
1	2MU	2A	2552	59,1	19,22,24	1.29	2 (10%)	25,31,36	2.02	6 (24%)
57	5MC	2a	1407	57	19,22,23	1.50	3 (15%)	26,32,35	1.22	3 (11%)
57	5MC	2a	967	57	19,22,23	1.74	3 (15%)	26,32,35	1.09	2 (7%)
1	5MC	2A	1942	1	19,22,23	1.64	3 (15%)	26,32,35	1.16	2 (7%)
56	PSU	1y	32	56	18,21,22	1.40	2 (11%)	21,30,33	1.96	3 (14%)
57	2MG	2a	1207	57	18,26,27	0.91	1 (5%)	16,38,41	1.41	3 (18%)
54	5MU	1w	54	54	19,22,23	1.36	5 (26%)	27,32,35	2.11	7 (25%)
54	PSU	2w	39	54	18,21,22	1.40	2 (11%)	21,30,33	1.76	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	5MU	2w	54	54	19,22,23	1.38	5 (26%)	27,32,35	1.72	6 (22%)
56	G7M	1y	46	56	20,26,27	2.70	4 (20%)	16,39,42	0.84	1 (6%)
1	2MA	1A	2515	59,1	18,25,26	0.70	0	20,37,40	2.10	4 (20%)
58	BB9	B	9	58	2,5,6	4.94	1 (50%)	1,5,7	2.89	1 (100%)
56	PSU	1y	55	56	18,21,22	1.41	2 (11%)	21,30,33	2.07	3 (14%)
54	PSU	1w	39	54	18,21,22	1.36	2 (11%)	21,30,33	1.92	3 (14%)
55	5MU	2x	54	55	19,22,23	1.42	5 (26%)	27,32,35	2.18	6 (22%)
1	5MU	2A	1915	1	19,22,23	1.45	6 (31%)	27,32,35	2.20	5 (18%)
1	PSU	1A	2617	59,1	18,21,22	1.39	3 (16%)	21,30,33	2.12	4 (19%)
1	4OC	1A	1942	1	19,22,24	0.78	0	25,31,35	0.95	1 (4%)
54	PSU	2w	55	54	18,21,22	1.40	2 (11%)	21,30,33	2.05	3 (14%)
58	BB9	A	17	58	2,5,6	4.59	1 (50%)	1,5,7	4.29	1 (100%)
55	PSU	1x	55	55,59	18,21,22	1.31	2 (11%)	21,30,33	2.04	4 (19%)
56	PSU	2y	39	56	18,21,22	1.29	2 (11%)	21,30,33	2.00	3 (14%)
54	PSU	1w	55	54	18,21,22	1.43	2 (11%)	21,30,33	2.01	4 (19%)
32	UR3	1a	1498	32	19,22,23	1.07	1 (5%)	26,32,35	1.79	4 (15%)
56	G7M	2y	46	56	20,26,27	2.76	4 (20%)	16,39,42	0.83	1 (6%)
1	5MU	2A	1939	59,1	19,22,23	1.43	5 (26%)	27,32,35	2.38	6 (22%)
1	OMG	1A	2263	55,59,1	19,26,27	0.91	1 (5%)	21,38,41	1.04	1 (4%)
57	PSU	2a	516	57	18,21,22	1.31	2 (11%)	21,30,33	2.05	4 (19%)
1	PSU	2A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	1.98	4 (19%)
54	G7M	1w	46	54	20,26,27	2.73	4 (20%)	16,39,42	0.87	1 (6%)
56	PSU	2y	32	56	18,21,22	1.37	2 (11%)	21,30,33	1.92	4 (19%)
56	5MU	1y	54	56	19,22,23	1.49	5 (26%)	27,32,35	1.81	5 (18%)
1	5MU	1A	1937	1	19,22,23	1.39	4 (21%)	27,32,35	2.28	6 (22%)
56	PSU	2y	55	56	18,21,22	1.36	2 (11%)	21,30,33	2.04	3 (14%)
54	G7M	2w	46	54	20,26,27	2.69	3 (15%)	16,39,42	1.18	1 (6%)
55	5MU	1x	54	55,59	19,22,23	1.44	6 (31%)	27,32,35	2.00	7 (25%)
55	5MC	2x	32	55	19,22,23	1.64	2 (10%)	26,32,35	1.19	3 (11%)
58	BB9	B	6	58	2,5,6	4.08	1 (50%)	1,5,7	2.75	1 (100%)
56	4SU	2y	8	56,59	18,21,22	1.75	4 (22%)	25,30,33	2.11	4 (16%)
54	4SU	2w	8	54	18,21,22	1.68	4 (22%)	25,30,33	2.49	5 (20%)
57	M2G	2a	966	57	20,27,28	1.37	3 (15%)	19,40,43	1.08	2 (10%)
57	5MC	2a	1400	57	19,22,23	1.71	3 (15%)	26,32,35	1.25	3 (11%)
55	4SU	1x	8	55	18,21,22	2.12	5 (27%)	25,30,33	1.66	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	MA6	1a	1519	32	19,26,27	1.11	2 (10%)	18,38,41	1.99	5 (27%)
1	PSU	1A	1933	1	18,21,22	1.43	2 (11%)	21,30,33	2.06	3 (14%)
56	PSU	1y	39	56	18,21,22	1.34	2 (11%)	21,30,33	2.00	4 (19%)
54	4SU	1w	8	54	18,21,22	1.76	5 (27%)	25,30,33	1.89	4 (16%)
32	5MC	1a	1407	32	19,22,23	1.48	3 (15%)	26,32,35	1.13	2 (7%)
57	MA6	2a	1518	57	19,26,27	1.17	2 (10%)	18,38,41	2.27	5 (27%)
57	4OC	2a	1402	57	20,23,24	0.77	0	25,32,35	1.06	2 (8%)
1	5MC	2A	1962	59,1	19,22,23	1.70	3 (15%)	26,32,35	1.18	3 (11%)
43	0TD	1l	92	43	8,9,10	4.50	1 (12%)	6,11,13	2.36	2 (33%)
1	PSU	2A	2605	1	18,21,22	1.35	2 (11%)	21,30,33	2.10	5 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	G7M	1a	527	59,32	-	3/3/25/26	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
55	4SU	2x	8	55,59	-	1/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1984	59,1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,59,1	-	0/5/27/28	0/3/3/3
56	4SU	1y	8	56	-	2/7/25/26	0/2/2/2
1	2MU	1A	2564	59,1	-	0/9/27/28	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	59,32	-	0/7/25/26	0/2/2/2
58	BB9	A	6	58	-	0/0/4/6	-
54	MIA	2w	37	54	-	2/7/29/34	0/3/3/3
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1961	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
57	5MC	2a	1404	57	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	2/11/33/34	0/3/3/3
57	UR3	2a	1498	57	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	BB9	A	9	58	-	0/0/4/6	-
1	2MA	2A	2503	59,1	-	1/3/25/26	0/3/3/3
1	5MC	1A	1964	59,1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
58	BB9	B	17	58	-	0/0/4/6	-
54	PSU	1w	32	59,54	-	0/7/25/26	0/2/2/2
56	5MU	2y	54	56	-	3/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
57	G7M	2a	527	57,59	-	3/3/25/26	0/3/3/3
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
57	MA6	2a	1519	57	-	4/7/29/30	0/3/3/3
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
1	2MU	2A	2552	59,1	-	0/9/27/28	0/2/2/2
57	5MC	2a	1407	57	-	0/7/25/26	0/2/2/2
57	5MC	2a	967	57	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
57	2MG	2a	1207	57	-	2/5/27/28	0/3/3/3
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
56	G7M	1y	46	56	-	1/3/25/26	0/3/3/3
1	2MA	1A	2515	59,1	-	1/3/25/26	0/3/3/3
58	BB9	B	9	58	-	0/0/4/6	-
56	PSU	1y	55	56	-	1/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	59,1	-	0/7/25/26	0/2/2/2
1	4OC	1A	1942	1	-	1/9/27/30	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
58	BB9	A	17	58	-	0/0/4/6	-
55	PSU	1x	55	55,59	-	0/7/25/26	0/2/2/2
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
56	G7M	2y	46	56	-	1/3/25/26	0/3/3/3
1	5MU	2A	1939	59,1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2263	55,59,1	-	0/5/27/28	0/3/3/3
57	PSU	2a	516	57	-	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	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	3/3/25/26	0/3/3/3
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	2/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	0/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	3/3/25/26	0/3/3/3
55	5MU	1x	54	55,59	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
58	BB9	B	6	58	-	0/0/4/6	-
56	4SU	2y	8	56,59	-	2/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
57	M2G	2a	966	57	-	0/7/29/30	0/3/3/3
57	5MC	2a	1400	57	-	4/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
57	MA6	2a	1518	57	-	3/7/29/30	0/3/3/3
57	4OC	2a	1402	57	-	2/9/29/30	0/2/2/2
1	5MC	2A	1962	59,1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2

All (222) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.66	1.69	1.82
43	1l	92	0TD	CB-SB	-12.29	1.69	1.82
32	1a	527	G7M	C8-N9	7.96	1.47	1.33
56	2y	46	G7M	C8-N9	7.79	1.47	1.33
54	1w	46	G7M	C8-N9	7.78	1.47	1.33
56	1y	46	G7M	C8-N9	7.70	1.47	1.33
57	2a	527	G7M	C8-N9	7.70	1.47	1.33
54	2w	46	G7M	C8-N9	7.63	1.47	1.33
54	2w	46	G7M	C8-N7	7.55	1.46	1.33
32	1a	527	G7M	C8-N7	7.36	1.46	1.33
57	2a	527	G7M	C8-N7	7.24	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	37	MIA	C2-S10	-7.24	1.69	1.75
54	1w	46	G7M	C8-N7	7.20	1.46	1.33
56	1y	46	G7M	C8-N7	7.12	1.46	1.33
56	2y	46	G7M	C8-N7	7.09	1.46	1.33
54	1w	37	MIA	C13-C14	6.96	1.53	1.32
58	B	9	BB9	C-CA	-6.95	1.33	1.45
54	1w	37	MIA	C2-S10	-6.94	1.70	1.75
58	A	9	BB9	C-CA	-6.48	1.34	1.45
57	2a	967	5MC	C5-C4	6.43	1.49	1.44
58	A	17	BB9	C-CA	-6.42	1.34	1.45
57	2a	1400	5MC	C5-C4	6.31	1.48	1.44
1	2A	1962	5MC	C5-C4	6.29	1.48	1.44
57	2a	1404	5MC	C5-C4	6.22	1.48	1.44
32	1a	1404	5MC	C5-C4	6.12	1.48	1.44
58	B	17	BB9	C-CA	-6.01	1.35	1.45
58	A	6	BB9	C-CA	-5.96	1.35	1.45
1	2A	1942	5MC	C5-C4	5.88	1.48	1.44
55	1x	32	5MC	C5-C4	5.81	1.48	1.44
1	1A	1984	5MC	C5-C4	5.81	1.48	1.44
55	2x	32	5MC	C5-C4	5.80	1.48	1.44
32	1a	1400	5MC	C5-C4	5.78	1.48	1.44
58	B	6	BB9	C-CA	-5.74	1.35	1.45
32	1a	967	5MC	C5-C4	5.62	1.48	1.44
32	1a	1407	5MC	C5-C4	5.29	1.48	1.44
57	2a	1407	5MC	C5-C4	5.10	1.48	1.44
1	1A	1964	5MC	C5-C4	4.99	1.47	1.44
55	2x	8	4SU	C4-N3	-4.94	1.32	1.37
56	2y	46	G7M	C5-C4	4.89	1.48	1.39
54	2w	8	4SU	C4-S4	-4.79	1.60	1.68
55	1x	8	4SU	C4-N3	-4.78	1.32	1.37
56	2y	8	4SU	C4-S4	-4.74	1.60	1.68
56	1y	46	G7M	C5-C4	4.73	1.48	1.39
32	1a	527	G7M	C5-C4	4.71	1.48	1.39
54	1w	8	4SU	C4-S4	-4.66	1.60	1.68
54	1w	46	G7M	C5-C4	4.64	1.48	1.39
55	1x	8	4SU	C4-S4	-4.45	1.60	1.68
55	2x	8	4SU	C4-S4	-4.42	1.60	1.68
56	1y	8	4SU	C4-S4	-4.42	1.60	1.68
54	2w	46	G7M	C5-C4	4.35	1.47	1.39
57	2a	527	G7M	C5-C4	4.31	1.47	1.39
57	2a	966	M2G	C2-N3	4.24	1.36	1.30
54	1w	55	PSU	C6-C5	4.17	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	1y	32	PSU	C6-C5	4.03	1.39	1.35
56	2y	55	PSU	C6-C5	3.96	1.39	1.35
56	2y	32	PSU	C6-C5	3.95	1.39	1.35
54	2w	55	PSU	C6-C5	3.89	1.39	1.35
56	1y	55	PSU	C6-C5	3.86	1.39	1.35
55	1x	8	4SU	C2-N3	-3.81	1.31	1.38
32	1a	966	M2G	C2-N3	3.69	1.35	1.30
56	1y	39	PSU	C6-C5	3.68	1.39	1.35
54	2w	39	PSU	C6-C5	3.63	1.39	1.35
1	1A	1933	PSU	C6-C5	3.62	1.39	1.35
55	2x	55	PSU	C6-C5	3.62	1.39	1.35
56	2y	39	PSU	C6-C5	3.58	1.39	1.35
54	1w	32	PSU	C6-C5	3.55	1.39	1.35
1	2A	1911	PSU	C6-C5	3.52	1.39	1.35
1	1A	1939	PSU	C6-C5	3.50	1.39	1.35
54	1w	39	PSU	C6-C5	3.48	1.39	1.35
1	2A	2605	PSU	C6-C5	3.45	1.39	1.35
55	2x	8	4SU	C2-N3	-3.44	1.32	1.38
1	2A	1917	PSU	C6-C5	3.41	1.39	1.35
57	2a	516	PSU	C6-C5	3.39	1.39	1.35
54	2w	32	PSU	C6-C5	3.36	1.39	1.35
56	2y	54	5MU	C2-N1	3.28	1.43	1.38
55	1x	8	4SU	C5-C4	-3.28	1.38	1.42
56	1y	8	4SU	C4-N3	-3.25	1.34	1.37
32	1a	516	PSU	C6-C5	3.23	1.38	1.35
54	1w	8	4SU	C4-N3	-3.16	1.34	1.37
56	1y	54	5MU	C6-C5	3.13	1.39	1.34
32	1a	966	M2G	C2-N2	3.12	1.40	1.35
55	1x	55	PSU	C6-C5	3.12	1.38	1.35
57	2a	1519	MA6	C6-C5	3.11	1.49	1.44
1	1A	1961	5MU	C4-N3	-3.03	1.33	1.38
57	2a	1518	MA6	C6-C5	3.03	1.49	1.44
55	2x	54	5MU	C6-C5	2.97	1.39	1.34
1	1A	2564	2MU	C4-N3	-2.95	1.33	1.38
55	1x	32	5MC	C6-C5	2.91	1.39	1.34
1	2A	1939	5MU	C4-N3	-2.90	1.33	1.38
56	2y	8	4SU	C4-N3	-2.88	1.34	1.37
55	2x	32	5MC	C6-C5	2.87	1.39	1.34
57	2a	1407	5MC	C6-C5	2.87	1.39	1.34
32	1a	1400	5MC	C6-C5	2.87	1.39	1.34
32	1a	967	5MC	C6-C5	2.86	1.39	1.34
55	2x	8	4SU	C5-C4	-2.86	1.39	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1915	5MU	C6-C5	2.82	1.39	1.34
56	2y	54	5MU	C6-C5	2.81	1.39	1.34
1	2A	2552	2MU	C4-N3	-2.81	1.33	1.38
57	2a	966	M2G	C2-N2	2.80	1.40	1.35
57	2a	967	5MC	C6-C5	2.78	1.39	1.34
55	1x	54	5MU	C6-C5	2.78	1.39	1.34
1	2A	1939	5MU	C6-C5	2.78	1.39	1.34
54	2w	54	5MU	C6-C5	2.78	1.39	1.34
57	2a	1404	5MC	C6-C5	2.76	1.39	1.34
32	1a	1518	MA6	C6-C5	2.73	1.49	1.44
1	2A	1911	PSU	C4-N3	-2.70	1.33	1.38
55	1x	54	5MU	C4-N3	-2.69	1.33	1.38
1	1A	1961	5MU	C2-N3	-2.69	1.33	1.38
1	1A	1937	5MU	C4-N3	-2.68	1.33	1.38
32	1a	516	PSU	C4-N3	-2.68	1.33	1.38
54	2w	37	MIA	C6-C5	2.68	1.49	1.44
1	1A	2617	PSU	C4-N3	-2.67	1.33	1.38
57	2a	1400	5MC	C6-C5	2.67	1.39	1.34
54	1w	39	PSU	C4-N3	-2.67	1.33	1.38
1	2A	1915	5MU	C2-N1	2.66	1.42	1.38
54	2w	54	5MU	C4-N3	-2.65	1.33	1.38
1	2A	1942	5MC	C6-C5	2.65	1.38	1.34
54	2w	39	PSU	C4-N3	-2.64	1.33	1.38
32	1a	1404	5MC	C6-C5	2.63	1.38	1.34
1	1A	1933	PSU	C4-N3	-2.63	1.33	1.38
1	2A	1915	5MU	C4-N3	-2.60	1.34	1.38
56	1y	54	5MU	C4-N3	-2.60	1.34	1.38
54	1w	54	5MU	C6-C5	2.60	1.38	1.34
1	1A	2617	PSU	C6-C5	2.59	1.38	1.35
54	2w	8	4SU	C4-N3	-2.58	1.34	1.37
56	1y	54	5MU	C4-C5	2.58	1.49	1.44
1	1A	1937	5MU	C2-N1	2.58	1.42	1.38
1	1A	1937	5MU	C6-C5	2.58	1.38	1.34
1	1A	1961	5MU	C6-C5	2.57	1.38	1.34
55	2x	54	5MU	C4-N3	-2.54	1.34	1.38
1	1A	2617	PSU	C2-N1	-2.54	1.33	1.36
1	1A	1961	5MU	C6-N1	-2.53	1.33	1.38
32	1a	1498	UR3	C2-N1	2.53	1.42	1.38
1	2A	1939	5MU	C6-N1	-2.52	1.33	1.38
54	2w	55	PSU	C4-N3	-2.52	1.34	1.38
1	1A	1964	5MC	C6-C5	2.52	1.38	1.34
1	2A	1939	5MU	C2-N3	-2.51	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1962	5MC	C6-C5	2.51	1.38	1.34
54	1w	37	MIA	C6-C5	2.51	1.48	1.44
32	1a	1404	5MC	C6-N1	-2.50	1.33	1.38
1	2A	1915	5MU	C4-C5	2.50	1.48	1.44
1	2A	2605	PSU	C4-N3	-2.50	1.34	1.38
54	1w	32	PSU	C4-N3	-2.49	1.34	1.38
56	2y	54	5MU	C4-N3	-2.49	1.34	1.38
54	1w	54	5MU	C4-C5	2.48	1.48	1.44
55	1x	54	5MU	C4-C5	2.48	1.48	1.44
56	1y	8	4SU	C2-N1	2.48	1.42	1.38
1	1A	1984	5MC	C6-N1	-2.48	1.33	1.38
56	2y	8	4SU	C5-C4	-2.48	1.39	1.42
1	2A	1917	PSU	C4-N3	-2.48	1.34	1.38
56	2y	54	5MU	C4-C5	2.48	1.48	1.44
32	1a	1407	5MC	C6-C5	2.47	1.38	1.34
54	2w	8	4SU	C5-C4	-2.47	1.39	1.42
55	2x	54	5MU	C4-C5	2.47	1.48	1.44
1	1A	1964	5MC	C6-N1	-2.46	1.33	1.38
54	1w	46	G7M	C6-N1	-2.46	1.34	1.37
1	1A	1984	5MC	C6-C5	2.46	1.38	1.34
56	2y	46	G7M	C6-N1	-2.45	1.34	1.37
54	1w	8	4SU	C5-C4	-2.45	1.39	1.42
55	1x	55	PSU	C4-N3	-2.44	1.34	1.38
56	1y	39	PSU	C4-N3	-2.44	1.34	1.38
54	2w	32	PSU	C4-N3	-2.44	1.34	1.38
56	2y	55	PSU	C4-N3	-2.43	1.34	1.38
54	1w	54	5MU	C4-N3	-2.40	1.34	1.38
56	1y	55	PSU	C4-N3	-2.40	1.34	1.38
1	2A	2251	OMG	C6-N1	-2.39	1.34	1.37
1	2A	2552	2MU	C5-C4	2.39	1.48	1.43
1	1A	2564	2MU	C2-N3	-2.38	1.33	1.38
56	1y	54	5MU	C2-N1	2.37	1.42	1.38
56	2y	8	4SU	C2-N1	2.37	1.42	1.38
55	2x	55	PSU	C4-N3	-2.36	1.34	1.38
56	1y	32	PSU	C4-N3	-2.36	1.34	1.38
57	2a	527	G7M	C6-N1	-2.34	1.34	1.37
32	1a	1207	2MG	C6-N1	-2.34	1.34	1.37
56	1y	8	4SU	C5-C4	-2.32	1.39	1.42
55	1x	32	5MC	C6-N1	-2.32	1.34	1.38
55	2x	54	5MU	C2-N1	2.32	1.42	1.38
1	1A	1961	5MU	C4-C5	2.32	1.48	1.44
1	2A	1962	5MC	C6-N1	-2.31	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1937	5MU	C6-N1	-2.29	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.29	1.34	1.38
32	1a	1519	MA6	C6-C5	2.29	1.48	1.44
56	1y	54	5MU	C2-N3	-2.28	1.34	1.38
54	2w	8	4SU	C2-N1	2.27	1.42	1.38
56	2y	32	PSU	C4-N3	-2.26	1.34	1.38
57	2a	1498	UR3	C2-N1	2.26	1.41	1.38
57	2a	1400	5MC	C6-N1	-2.26	1.34	1.38
57	2a	1518	MA6	C6-N1	2.25	1.35	1.32
57	2a	1207	2MG	C6-N1	-2.24	1.34	1.37
1	1A	1939	PSU	C4-N3	-2.24	1.34	1.38
55	1x	54	5MU	C2-N1	2.23	1.42	1.38
54	1w	55	PSU	C4-N3	-2.22	1.34	1.38
54	2w	54	5MU	C4-C5	2.21	1.48	1.44
57	2a	516	PSU	C4-N3	-2.20	1.34	1.38
57	2a	1407	5MC	C6-N1	-2.19	1.34	1.38
57	2a	1519	MA6	C6-N1	2.18	1.35	1.32
56	2y	39	PSU	C4-N3	-2.18	1.34	1.38
1	1A	2263	OMG	C6-N1	-2.17	1.34	1.37
1	2A	1939	5MU	C4-C5	2.17	1.48	1.44
57	2a	966	M2G	C6-N1	-2.17	1.34	1.37
57	2a	1404	5MC	C6-N1	-2.16	1.34	1.38
54	1w	8	4SU	C2-N1	2.15	1.41	1.38
32	1a	1407	5MC	C6-N1	-2.14	1.34	1.38
55	1x	8	4SU	O2-C2	2.13	1.26	1.23
56	2y	54	5MU	C2-N3	-2.13	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.12	1.34	1.38
32	1a	516	PSU	C2-N3	-2.07	1.34	1.37
55	1x	54	5MU	C2-N3	-2.07	1.34	1.38
55	1x	54	5MU	C6-N1	-2.06	1.34	1.38
54	1w	54	5MU	C6-N1	-2.06	1.34	1.38
56	1y	8	4SU	C6-C5	2.06	1.39	1.35
54	1w	8	4SU	C2-N3	-2.05	1.34	1.38
57	2a	967	5MC	C6-N1	-2.05	1.34	1.38
54	1w	54	5MU	C2-N1	2.05	1.41	1.38
1	2A	1915	5MU	C2-N3	-2.04	1.34	1.38
32	1a	1519	MA6	C6-N1	2.04	1.35	1.32
56	1y	46	G7M	C6-N1	-2.03	1.34	1.37
32	1a	1400	5MC	C6-N1	-2.03	1.34	1.38
54	2w	54	5MU	C2-N3	-2.03	1.34	1.38
55	2x	54	5MU	C6-N1	-2.03	1.34	1.38
32	1a	1518	MA6	C6-N1	2.02	1.35	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	54	5MU	C2-N1	2.01	1.41	1.38

All (300) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	37	MIA	C12-C13-C14	-9.00	110.85	127.01
54	2w	8	4SU	C4-N3-C2	-7.73	119.90	127.31
57	2a	1498	UR3	C4-N3-C2	-7.14	118.83	124.58
43	2l	92	0TD	CSB-SB-CB	-7.10	89.59	102.36
1	1A	2515	2MA	C2-N3-C4	7.02	121.13	115.46
32	1a	1498	UR3	C4-N3-C2	-6.76	119.14	124.58
56	1y	55	PSU	N1-C2-N3	6.60	122.13	115.17
1	2A	1917	PSU	N1-C2-N3	6.43	121.95	115.17
1	1A	1933	PSU	N1-C2-N3	6.34	121.86	115.17
55	2x	55	PSU	N1-C2-N3	6.34	121.85	115.17
56	2y	55	PSU	N1-C2-N3	6.32	121.83	115.17
1	2A	2503	2MA	C2-N3-C4	6.30	120.55	115.46
54	2w	55	PSU	N1-C2-N3	6.27	121.79	115.17
57	2a	516	PSU	N1-C2-N3	6.23	121.74	115.17
56	1y	32	PSU	N1-C2-N3	6.22	121.73	115.17
56	1y	39	PSU	N1-C2-N3	6.21	121.72	115.17
1	2A	2605	PSU	N1-C2-N3	6.19	121.70	115.17
1	2A	1911	PSU	N1-C2-N3	6.19	121.70	115.17
1	1A	2617	PSU	N1-C2-N3	6.18	121.69	115.17
57	2a	1518	MA6	C2-N1-C6	6.14	122.86	116.84
55	1x	55	PSU	N1-C2-N3	6.12	121.62	115.17
54	2w	8	4SU	C5-C4-N3	6.09	120.41	114.75
56	2y	8	4SU	C4-N3-C2	-6.08	121.48	127.31
1	1A	1939	PSU	N1-C2-N3	6.07	121.57	115.17
54	2w	32	PSU	N1-C2-N3	6.04	121.54	115.17
56	2y	39	PSU	N1-C2-N3	6.02	121.52	115.17
1	1A	2564	2MU	N3-C2-N1	5.95	122.63	114.89
1	2A	1939	5MU	C4-N3-C2	-5.92	119.58	127.34
54	1w	55	PSU	N1-C2-N3	5.91	121.40	115.17
32	1a	516	PSU	N1-C2-N3	5.90	121.39	115.17
54	1w	32	PSU	N1-C2-N3	5.90	121.39	115.17
32	1a	1518	MA6	C2-N1-C6	5.88	122.61	116.84
56	2y	32	PSU	N1-C2-N3	5.86	121.35	115.17
56	1y	8	4SU	C4-N3-C2	-5.85	121.70	127.31
54	1w	39	PSU	N1-C2-N3	5.83	121.31	115.17
1	1A	1961	5MU	C4-N3-C2	-5.76	119.79	127.34
1	1A	1961	5MU	C5-C4-N3	5.63	120.21	115.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2y	8	4SU	C5-C4-N3	5.61	119.97	114.75
55	2x	54	5MU	N3-C2-N1	5.53	122.09	114.89
1	2A	2552	2MU	N3-C2-N1	5.53	122.09	114.89
1	1A	1937	5MU	C4-N3-C2	-5.53	120.09	127.34
54	2w	39	PSU	N1-C2-N3	5.46	120.93	115.17
54	1w	8	4SU	C4-N3-C2	-5.42	122.11	127.31
1	2A	1915	5MU	C4-N3-C2	-5.37	120.29	127.34
1	2A	1939	5MU	C5-C4-N3	5.34	119.97	115.32
55	2x	54	5MU	C4-N3-C2	-5.33	120.36	127.34
1	2A	2552	2MU	C4-N3-C2	-5.28	120.06	126.61
1	1A	1937	5MU	C5-C4-N3	5.26	119.90	115.32
1	2A	1915	5MU	N3-C2-N1	5.20	121.66	114.89
1	2A	1939	5MU	N3-C2-N1	5.18	121.63	114.89
54	1w	54	5MU	C4-N3-C2	-5.10	120.65	127.34
1	1A	1937	5MU	O4-C4-C5	-5.10	119.08	124.92
57	2a	1519	MA6	C2-N1-C6	5.07	121.81	116.84
1	2A	1939	5MU	C5-C6-N1	-5.01	117.87	123.31
1	1A	1937	5MU	N3-C2-N1	5.01	121.41	114.89
54	1w	8	4SU	C5-C4-N3	4.97	119.38	114.75
1	1A	1961	5MU	N3-C2-N1	4.93	121.31	114.89
54	1w	54	5MU	N3-C2-N1	4.87	121.23	114.89
1	2A	1915	5MU	C5-C4-N3	4.82	119.52	115.32
55	1x	54	5MU	N3-C2-N1	4.82	121.16	114.89
55	1x	54	5MU	C4-N3-C2	-4.80	121.05	127.34
1	1A	2564	2MU	C4-N3-C2	-4.76	120.70	126.61
56	1y	54	5MU	N3-C2-N1	4.67	120.97	114.89
1	1A	1961	5MU	C5-C6-N1	-4.67	118.24	123.31
56	1y	8	4SU	C5-C4-N3	4.66	119.08	114.75
1	2A	2605	PSU	C4-N3-C2	-4.51	120.15	126.37
56	2y	54	5MU	C5-C4-N3	4.46	119.20	115.32
54	2w	8	4SU	C5-C4-S4	-4.44	119.23	124.31
1	1A	2617	PSU	O2-C2-N1	-4.43	118.22	122.79
1	2A	1939	5MU	O4-C4-C5	-4.43	119.85	124.92
54	2w	37	MIA	C12-N6-C6	-4.41	118.76	122.85
54	2w	8	4SU	N3-C2-N1	4.41	120.63	114.89
32	1a	1519	MA6	C2-N1-C6	4.41	121.16	116.84
54	1w	54	5MU	C5-C4-N3	4.40	119.14	115.32
1	1A	2564	2MU	O2-C2-N1	-4.34	117.14	122.80
1	1A	1939	PSU	O2-C2-N1	-4.34	118.31	122.79
56	2y	54	5MU	C4-N3-C2	-4.31	121.69	127.34
58	A	17	BB9	O-C-CA	-4.29	120.01	125.39
55	2x	54	5MU	C5-C4-N3	4.25	119.02	115.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1y	54	5MU	C4-N3-C2	-4.23	121.79	127.34
57	2a	516	PSU	C4-N3-C2	-4.23	120.55	126.37
55	1x	55	PSU	C4-N3-C2	-4.21	120.56	126.37
1	1A	1961	5MU	O4-C4-C5	-4.21	120.10	124.92
54	2w	54	5MU	N3-C2-N1	4.19	120.35	114.89
55	1x	54	5MU	C5-C4-N3	4.18	118.96	115.32
56	1y	39	PSU	C4-N3-C2	-4.16	120.64	126.37
56	1y	8	4SU	N3-C2-N1	4.16	120.31	114.89
55	2x	54	5MU	O4-C4-C5	-4.14	120.18	124.92
32	1a	516	PSU	C4-N3-C2	-4.14	120.67	126.37
55	2x	55	PSU	C4-N3-C2	-4.14	120.67	126.37
58	B	17	BB9	O-C-CA	-4.14	120.20	125.39
54	2w	55	PSU	C4-N3-C2	-4.13	120.68	126.37
1	2A	1915	5MU	O4-C4-C5	-4.13	120.19	124.92
1	1A	2617	PSU	C4-N3-C2	-4.13	120.68	126.37
56	2y	39	PSU	C4-N3-C2	-4.12	120.70	126.37
56	2y	54	5MU	N3-C2-N1	4.10	120.22	114.89
54	1w	54	5MU	O4-C4-C5	-4.10	120.23	124.92
43	1l	92	0TD	CSB-SB-CB	-4.07	95.05	102.36
1	1A	1939	PSU	C4-N3-C2	-4.06	120.77	126.37
54	2w	32	PSU	C4-N3-C2	-4.05	120.79	126.37
56	1y	55	PSU	O2-C2-N1	-4.04	118.62	122.79
56	2y	55	PSU	C4-N3-C2	-4.03	120.82	126.37
55	1x	8	4SU	C6-C5-C4	-4.01	116.48	119.95
54	1w	37	MIA	C15-C14-C13	-4.00	110.66	122.66
1	1A	1933	PSU	C4-N3-C2	-4.00	120.87	126.37
1	1A	1933	PSU	O2-C2-N1	-4.00	118.67	122.79
1	2A	1917	PSU	O2-C2-N1	-3.96	118.71	122.79
1	2A	1911	PSU	C4-N3-C2	-3.96	120.92	126.37
56	2y	8	4SU	C5-C4-S4	-3.94	119.81	124.31
57	2a	1518	MA6	C9-N6-C6	-3.93	108.55	119.40
57	2a	1518	MA6	N3-C2-N1	-3.89	123.39	128.67
57	2a	1400	5MC	C5-C6-N1	-3.88	119.09	123.31
1	2A	1917	PSU	C4-N3-C2	-3.82	121.11	126.37
54	2w	54	5MU	C4-N3-C2	-3.81	122.34	127.34
57	2a	1519	MA6	C9-N6-C6	-3.80	108.92	119.40
54	1w	32	PSU	C4-N3-C2	-3.78	121.17	126.37
56	1y	32	PSU	C4-N3-C2	-3.77	121.18	126.37
54	1w	39	PSU	C4-N3-C2	-3.75	121.21	126.37
55	1x	32	5MC	C5-C6-N1	-3.74	119.25	123.31
54	1w	55	PSU	O2-C2-N1	-3.74	118.93	122.79
57	2a	516	PSU	O2-C2-N1	-3.73	118.94	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2y	54	5MU	O4-C4-C5	-3.73	120.65	124.92
55	1x	8	4SU	O2-C2-N1	3.72	127.64	122.80
56	2y	55	PSU	O2-C2-N1	-3.71	118.96	122.79
56	1y	55	PSU	C4-N3-C2	-3.71	121.27	126.37
54	1w	32	PSU	O2-C2-N1	-3.69	118.98	122.79
56	2y	8	4SU	N3-C2-N1	3.69	119.69	114.89
55	1x	55	PSU	O2-C2-N1	-3.69	118.98	122.79
32	1a	1518	MA6	N3-C2-N1	-3.68	123.67	128.67
1	2A	1962	5MC	C5-C6-N1	-3.67	119.33	123.31
32	1a	1519	MA6	C9-N6-C6	-3.66	109.29	119.40
56	2y	39	PSU	O2-C2-N1	-3.66	119.02	122.79
56	1y	54	5MU	C5-C4-N3	3.62	118.47	115.32
1	1A	1961	5MU	O2-C2-N1	-3.60	118.11	122.80
54	1w	8	4SU	N3-C2-N1	3.60	119.58	114.89
32	1a	1207	2MG	N1-C2-N2	3.59	120.23	116.56
56	2y	32	PSU	C4-N3-C2	-3.59	121.43	126.37
55	2x	54	5MU	C5-C6-N1	-3.54	119.47	123.31
55	1x	54	5MU	C5-C6-N1	-3.53	119.48	123.31
55	2x	32	5MC	C5-C6-N1	-3.50	119.51	123.31
54	1w	37	MIA	C16-C14-C13	-3.48	112.21	122.66
55	1x	54	5MU	O4-C4-C5	-3.48	120.94	124.92
32	1a	1519	MA6	N3-C2-N1	-3.48	123.95	128.67
57	2a	1519	MA6	N3-C2-N1	-3.47	123.96	128.67
57	2a	1518	MA6	C4-C5-N7	-3.47	105.67	109.34
54	1w	55	PSU	C4-N3-C2	-3.46	121.60	126.37
56	2y	32	PSU	O2-C2-N1	-3.46	119.22	122.79
55	2x	8	4SU	C5-C4-N3	3.45	117.96	114.75
1	2A	1915	5MU	C5-C6-N1	-3.45	119.57	123.31
1	1A	1964	5MC	C5-C6-N1	-3.44	119.58	123.31
54	2w	54	5MU	O4-C4-C5	-3.44	120.98	124.92
57	2a	1519	MA6	C4-C5-N7	-3.42	105.72	109.34
54	2w	54	5MU	C5-C4-N3	3.42	118.30	115.32
1	2A	1939	5MU	O2-C2-N1	-3.42	118.34	122.80
1	1A	1984	5MC	C5-C6-N1	-3.42	119.60	123.31
54	1w	39	PSU	O2-C2-N1	-3.42	119.27	122.79
57	2a	1407	5MC	C5-C4-N3	-3.40	118.27	121.75
55	1x	8	4SU	C5-C4-N3	3.40	117.91	114.75
54	1w	54	5MU	C5-C6-N1	-3.40	119.62	123.31
57	2a	967	5MC	C5-C6-N1	-3.39	119.63	123.31
54	2w	39	PSU	C4-N3-C2	-3.38	121.71	126.37
56	1y	54	5MU	C5-C6-N1	-3.37	119.65	123.31
57	2a	1407	5MC	C5-C6-N1	-3.37	119.65	123.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2a	1404	5MC	C5-C6-N1	-3.35	119.67	123.31
56	1y	32	PSU	O2-C2-N1	-3.33	119.36	122.79
32	1a	1518	MA6	C9-N6-C6	-3.33	110.23	119.40
1	2A	2552	2MU	O2-C2-N1	-3.31	118.48	122.80
57	2a	1498	UR3	C5-C4-N3	3.31	119.40	115.04
54	2w	32	PSU	O2-C2-N1	-3.29	119.40	122.79
32	1a	1207	2MG	C8-N7-C5	3.28	108.14	102.55
54	2w	55	PSU	O2-C2-N1	-3.27	119.41	122.79
32	1a	1407	5MC	C5-C6-N1	-3.27	119.77	123.31
32	1a	1498	UR3	C5-C4-N3	3.26	119.34	115.04
54	1w	8	4SU	C5-C4-S4	-3.25	120.60	124.31
32	1a	1518	MA6	C4-C5-N7	-3.23	105.92	109.34
1	2A	1942	5MC	C5-C4-N3	-3.21	118.46	121.75
43	1l	92	0TD	OD2-CG-CB	3.20	120.06	113.15
56	1y	54	5MU	O4-C4-C5	-3.19	121.26	124.92
32	1a	967	5MC	C5-C6-N1	-3.18	119.86	123.31
1	1A	1937	5MU	C5-C6-N1	-3.14	119.91	123.31
56	1y	8	4SU	C5-C4-S4	-3.11	120.75	124.31
32	1a	1400	5MC	C5-C6-N1	-3.10	119.94	123.31
1	2A	2552	2MU	C5-C4-N3	3.09	119.13	114.80
43	2l	92	0TD	OD2-CG-CB	3.08	119.80	113.15
55	1x	32	5MC	C5-C4-N3	-3.05	118.63	121.75
56	2y	54	5MU	C5-C6-N1	-3.04	120.01	123.31
32	1a	1404	5MC	C5-C4-N3	-3.04	118.64	121.75
54	1w	54	5MU	O2-C2-N1	-3.04	118.84	122.80
1	2A	1911	PSU	O2-C2-N1	-3.04	119.66	122.79
32	1a	1207	2MG	N2-C2-N3	-3.03	116.65	120.51
32	1a	1519	MA6	C4-C5-N7	-3.01	106.16	109.34
55	2x	55	PSU	O2-C2-N1	-3.00	119.70	122.79
1	2A	2605	PSU	O2-C2-N1	-2.99	119.70	122.79
1	2A	2251	OMG	C8-N7-C5	2.98	107.63	102.55
55	2x	54	5MU	O2-C2-N1	-2.98	118.92	122.80
56	1y	39	PSU	O2-C2-N1	-2.97	119.72	122.79
55	2x	8	4SU	C1'-N1-C2	2.97	122.92	117.59
1	1A	2515	2MA	C2-N1-C6	2.96	122.66	118.10
32	1a	1519	MA6	N1-C6-N6	2.93	120.22	116.83
57	2a	1207	2MG	C8-N7-C5	2.92	107.53	102.55
1	1A	2263	OMG	C8-N7-C5	2.92	107.52	102.55
58	B	9	BB9	O-C-CA	-2.89	121.76	125.39
1	1A	2564	2MU	C2'-C1'-N1	-2.86	108.81	114.24
32	1a	1400	5MC	C5-C4-N3	-2.86	118.83	121.75
55	1x	8	4SU	C1'-N1-C2	2.85	122.72	117.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2y	54	5MU	C1'-N1-C2	2.84	122.70	117.59
32	1a	516	PSU	O2-C2-N1	-2.84	119.86	122.79
32	1a	1404	5MC	C5-C6-N1	-2.81	120.26	123.31
57	2a	966	M2G	C8-N7-C5	2.79	107.31	102.55
56	2y	54	5MU	C1'-N1-C6	-2.79	116.55	121.15
57	2a	1404	5MC	C5-C4-N3	-2.79	118.89	121.75
32	1a	966	M2G	C8-N7-C5	2.78	107.29	102.55
54	2w	54	5MU	C5-C6-N1	-2.76	120.32	123.31
54	1w	37	MIA	C2-N1-C6	2.75	122.31	117.42
58	B	6	BB9	O-C-CA	-2.75	121.95	125.39
32	1a	1407	5MC	C5-C4-N3	-2.74	118.95	121.75
57	2a	527	G7M	CN7-N7-C8	-2.74	112.27	125.43
1	1A	1964	5MC	C5-C4-N3	-2.73	118.96	121.75
1	2A	2552	2MU	C2'-C1'-N1	-2.73	109.07	114.24
32	1a	1498	UR3	C3U-N3-C4	2.71	121.62	117.87
54	2w	46	G7M	CN7-N7-C8	-2.69	112.50	125.43
54	2w	37	MIA	C4-C5-N7	-2.67	106.52	109.34
56	1y	46	G7M	CN7-N7-C8	-2.64	112.73	125.43
55	2x	32	5MC	O2-C2-N3	-2.64	118.17	122.33
1	1A	2515	2MA	C4-C5-N7	-2.63	106.56	109.34
54	1w	37	MIA	C4-C5-N7	-2.61	106.57	109.34
54	1w	55	PSU	C6-C5-C4	-2.61	116.42	118.17
56	2y	46	G7M	CN7-N7-C8	-2.60	112.91	125.43
1	2A	1962	5MC	C5-C4-N3	-2.60	119.09	121.75
57	2a	1207	2MG	N1-C2-N2	2.60	119.21	116.56
55	2x	8	4SU	O2-C2-N1	2.59	126.17	122.80
32	1a	527	G7M	CN7-N7-C8	-2.59	112.95	125.43
1	2A	1942	5MC	C5-C6-N1	-2.59	120.50	123.31
54	1w	37	MIA	N3-C2-N1	-2.57	122.33	127.03
54	2w	37	MIA	C2-N1-C6	2.57	121.98	117.42
58	A	9	BB9	O-C-CA	-2.56	122.18	125.39
54	2w	8	4SU	C1'-N1-C2	2.56	122.19	117.59
32	1a	1402	4OC	C6-C5-C4	2.56	120.08	117.00
57	2a	967	5MC	C5-C4-N3	-2.55	119.14	121.75
58	A	6	BB9	O-C-CA	-2.55	122.19	125.39
1	1A	1937	5MU	O2-C2-N1	-2.55	119.48	122.80
1	2A	2605	PSU	C5-C6-N1	-2.55	118.61	122.14
56	2y	54	5MU	O2-C2-N3	-2.53	116.82	121.49
55	2x	8	4SU	C6-C5-C4	-2.53	117.76	119.95
1	1A	2564	2MU	C5-C4-N3	2.52	118.33	114.80
1	2A	2552	2MU	O4-C4-C5	-2.51	120.83	125.16
57	2a	1518	MA6	C10-N6-C9	-2.50	108.14	116.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	32	5MC	C5-C4-N3	-2.50	119.19	121.75
1	2A	2503	2MA	C4-C5-N7	-2.47	106.73	109.34
54	2w	39	PSU	O2-C2-N1	-2.45	120.26	122.79
32	1a	967	5MC	C5-C4-N3	-2.45	119.24	121.75
55	1x	8	4SU	O2-C2-N3	-2.45	116.98	121.49
55	1x	8	4SU	S4-C4-N3	-2.44	117.66	120.20
57	2a	1404	5MC	O2-C2-N3	-2.44	118.49	122.33
1	1A	1942	4OC	O2-C2-N3	-2.43	118.50	122.33
57	2a	1402	4OC	C6-C5-C4	2.43	119.92	117.00
57	2a	1207	2MG	N2-C2-N3	-2.42	117.42	120.51
1	1A	2515	2MA	C5-C6-N1	-2.42	117.98	120.84
55	2x	8	4SU	O2-C2-N3	-2.42	117.03	121.49
55	1x	54	5MU	O2-C2-N1	-2.41	119.66	122.80
54	1w	46	G7M	CN7-N7-C8	-2.39	113.93	125.43
1	2A	2503	2MA	C2-N1-C6	2.38	121.75	118.10
1	1A	1984	5MC	C5-C4-N3	-2.37	119.33	121.75
57	2a	1400	5MC	C5-C4-N3	-2.35	119.35	121.75
55	2x	55	PSU	C5-C6-N1	-2.33	118.91	122.14
32	1a	1404	5MC	CM5-C5-C6	-2.32	119.71	122.85
1	1A	2564	2MU	O4-C4-C5	-2.29	121.22	125.16
43	2l	92	0TD	OD1-CG-CB	-2.28	117.67	122.44
57	2a	1400	5MC	O2-C2-N3	-2.27	118.75	122.33
57	2a	1498	UR3	C3U-N3-C4	2.27	121.01	117.87
55	2x	8	4SU	S4-C4-N3	-2.26	117.84	120.20
54	1w	54	5MU	C5M-C5-C4	2.24	121.17	118.78
54	2w	32	PSU	C5-C6-N1	-2.24	119.04	122.14
32	1a	1400	5MC	O2-C2-N3	-2.23	118.82	122.33
32	1a	1404	5MC	O2-C2-N3	-2.21	118.84	122.33
54	2w	54	5MU	O2-C2-N1	-2.20	119.94	122.80
54	2w	37	MIA	N3-C2-N1	-2.20	123.01	127.03
32	1a	1518	MA6	C10-N6-C6	-2.19	113.37	119.40
32	1a	516	PSU	C5-C6-N1	-2.18	119.12	122.14
32	1a	1498	UR3	C1'-N1-C2	2.17	120.60	117.04
56	1y	39	PSU	C5-C6-N1	-2.15	119.16	122.14
56	2y	32	PSU	C6-C5-C4	-2.14	116.73	118.17
56	2y	54	5MU	C5M-C5-C4	2.14	121.06	118.78
1	2A	2251	OMG	C5-C6-N1	2.13	118.14	114.07
55	1x	55	PSU	C5-C6-N1	-2.12	119.20	122.14
57	2a	516	PSU	O4'-C1'-C2'	2.11	108.07	105.15
1	2A	1911	PSU	O4'-C1'-C2'	2.10	108.06	105.15
1	2A	1920	4OC	O2-C2-N3	-2.10	119.03	122.33
32	1a	516	PSU	O4'-C1'-C2'	2.09	108.05	105.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1962	5MC	CM5-C5-C6	-2.08	120.04	122.85
57	2a	1407	5MC	O2-C2-N3	-2.07	119.06	122.33
57	2a	1402	4OC	O2-C2-N3	-2.07	119.06	122.33
56	1y	8	4SU	C1'-N1-C2	2.06	121.29	117.59
57	2a	966	M2G	C5-C6-N1	2.06	118.00	114.07
1	1A	2617	PSU	C5-C6-N1	-2.04	119.31	122.14
32	1a	1207	2MG	CM2-N2-C2	-2.03	119.28	123.65
1	2A	2503	2MA	O4'-C1'-N9	-2.03	106.06	108.75
55	1x	54	5MU	C5M-C5-C4	2.01	120.93	118.78
1	2A	2605	PSU	O4-C4-C5	-2.01	119.02	124.01
32	1a	966	M2G	O6-C6-C5	-2.00	120.35	124.32

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	37	MIA	C12-C13-C14-C15
54	1w	37	MIA	C12-C13-C14-C16
56	1y	8	4SU	O4'-C4'-C5'-O5'
56	1y	46	G7M	C4'-C5'-O5'-P
56	1y	54	5MU	O4'-C4'-C5'-O5'
56	2y	54	5MU	C3'-C4'-C5'-O5'
56	2y	54	5MU	O4'-C4'-C5'-O5'
57	2a	1207	2MG	N1-C2-N2-CM2
57	2a	1207	2MG	N3-C2-N2-CM2
57	2a	1518	MA6	C5-C6-N6-C9
57	2a	1519	MA6	O4'-C4'-C5'-O5'
56	2y	8	4SU	C3'-C4'-C5'-O5'
56	2y	8	4SU	O4'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
54	2w	46	G7M	O4'-C4'-C5'-O5'
54	2w	46	G7M	C3'-C4'-C5'-O5'
56	1y	8	4SU	C3'-C4'-C5'-O5'
57	2a	1402	4OC	O4'-C4'-C5'-O5'
57	2a	1518	MA6	N1-C6-N6-C9
32	1a	1402	4OC	O4'-C4'-C5'-O5'
56	1y	54	5MU	C3'-C4'-C5'-O5'
57	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
57	2a	527	G7M	C3'-C4'-C5'-O5'
54	1w	46	G7M	C4'-C5'-O5'-P
56	2y	46	G7M	C4'-C5'-O5'-P
57	2a	1402	4OC	C3'-C4'-C5'-O5'
54	1w	46	G7M	C3'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
57	2a	1400	5MC	C2'-C1'-N1-C6
1	2A	1917	PSU	O4'-C4'-C5'-O5'
54	1w	46	G7M	O4'-C4'-C5'-O5'
57	2a	1518	MA6	C5-C6-N6-C10
56	1y	55	PSU	O4'-C1'-C5-C4
57	2a	527	G7M	O4'-C4'-C5'-O5'
54	2w	46	G7M	C4'-C5'-O5'-P
57	2a	1519	MA6	C4'-C5'-O5'-P
57	2a	1400	5MC	O4'-C1'-N1-C6
32	1a	527	G7M	C4'-C5'-O5'-P
57	2a	527	G7M	C4'-C5'-O5'-P
32	1a	1519	MA6	C4'-C5'-O5'-P
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
54	2w	37	MIA	N1-C6-N6-C12
57	2a	1400	5MC	O4'-C1'-N1-C2
54	2w	37	MIA	C5-C6-N6-C12
1	1A	2515	2MA	C4'-C5'-O5'-P
57	2a	1519	MA6	N1-C6-N6-C9
1	1A	1942	4OC	C2'-C1'-N1-C2
55	2x	8	4SU	C2'-C1'-N1-C2
56	2y	54	5MU	C2'-C1'-N1-C2
57	2a	1400	5MC	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2940 ligands modelled in this entry, 2938 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
61	SF4	2d	501	35	0,12,12	-	-	-		
61	SF4	1d	501	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	SF4	2d	501	35	-	-	0/6/5/5
61	SF4	1d	501	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	-0.62	128 (4%) 39 37	13, 29, 85, 99	0
1	2A	2789/2915 (95%)	-0.02	132 (4%) 37 35	25, 51, 87, 102	0
2	1B	120/121 (99%)	-0.52	0 100 100	23, 41, 55, 80	0
2	2B	120/121 (99%)	0.94	4 (3%) 49 47	55, 72, 80, 89	0
3	1D	275/276 (99%)	-0.37	3 (1%) 77 77	14, 29, 45, 72	0
3	2D	275/276 (99%)	0.05	6 (2%) 62 61	25, 43, 57, 71	0
4	1E	204/206 (99%)	-0.41	0 100 100	14, 32, 53, 71	0
4	2E	204/206 (99%)	0.24	3 (1%) 71 71	28, 53, 65, 73	0
5	1F	203/210 (96%)	-0.33	0 100 100	15, 35, 60, 77	0
5	2F	203/210 (96%)	0.31	4 (1%) 64 64	30, 61, 75, 83	0
6	1G	181/182 (99%)	0.23	6 (3%) 49 47	33, 50, 66, 81	0
6	2G	181/182 (99%)	1.38	28 (15%) 6 6	62, 73, 81, 89	0
7	1H	174/180 (96%)	0.01	3 (1%) 69 68	31, 45, 59, 63	0
7	2H	174/180 (96%)	1.40	33 (18%) 4 4	65, 78, 84, 88	0
8	1I	146/148 (98%)	0.62	1 (0%) 84 83	37, 66, 76, 80	0
8	2I	146/148 (98%)	0.73	6 (4%) 42 40	48, 65, 75, 81	0
9	1N	140/140 (100%)	-0.34	1 (0%) 84 83	18, 31, 53, 63	0
9	2N	140/140 (100%)	0.55	2 (1%) 73 73	40, 57, 71, 79	0
10	1O	122/122 (100%)	-0.37	0 100 100	21, 32, 48, 54	0
10	2O	122/122 (100%)	0.24	1 (0%) 82 82	41, 53, 63, 68	0
11	1P	149/150 (99%)	-0.20	1 (0%) 84 83	14, 37, 63, 72	0
11	2P	149/150 (99%)	0.37	0 100 100	29, 61, 75, 82	0
12	1Q	141/141 (100%)	-0.37	1 (0%) 84 83	21, 32, 50, 67	0
12	2Q	141/141 (100%)	0.82	11 (7%) 20 19	40, 61, 72, 76	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%)	-0.52	0 100 100	18, 27, 41, 48	0
13	2R	118/118 (100%)	-0.01	1 (0%) 82 82	34, 45, 55, 65	0
14	1S	110/112 (98%)	-0.11	0 100 100	30, 41, 54, 59	0
14	2S	110/112 (98%)	1.17	15 (13%) 8 7	56, 67, 75, 80	0
15	1T	131/146 (89%)	-0.12	2 (1%) 71 71	24, 35, 61, 70	0
15	2T	131/146 (89%)	0.36	2 (1%) 71 71	44, 55, 73, 77	0
16	1U	116/118 (98%)	-0.71	0 100 100	15, 23, 37, 54	0
16	2U	116/118 (98%)	0.34	0 100 100	38, 55, 69, 76	0
17	1V	101/101 (100%)	-0.51	0 100 100	15, 32, 47, 57	0
17	2V	101/101 (100%)	0.74	2 (1%) 64 64	35, 64, 70, 75	0
18	1W	112/113 (99%)	-0.54	1 (0%) 81 80	17, 25, 44, 78	0
18	2W	112/113 (99%)	0.08	3 (2%) 56 54	31, 42, 59, 87	0
19	1X	95/96 (98%)	-0.27	2 (2%) 63 63	17, 31, 52, 73	0
19	2X	95/96 (98%)	0.37	3 (3%) 50 48	38, 53, 65, 76	0
20	1Y	107/110 (97%)	-0.02	3 (2%) 55 53	28, 42, 62, 77	0
20	2Y	107/110 (97%)	0.87	7 (6%) 26 24	50, 65, 73, 80	0
21	1Z	154/206 (74%)	0.44	8 (5%) 34 31	33, 56, 77, 85	0
21	2Z	160/206 (77%)	1.50	39 (24%) 2 2	63, 76, 86, 89	0
22	10	83/85 (97%)	-0.12	4 (4%) 36 35	22, 29, 51, 60	0
22	20	83/85 (97%)	0.99	9 (10%) 12 12	39, 58, 67, 74	0
23	11	97/98 (98%)	-0.05	2 (2%) 63 63	20, 36, 62, 70	0
23	21	97/98 (98%)	0.40	2 (2%) 63 63	33, 49, 69, 73	0
24	12	70/72 (97%)	-0.05	1 (1%) 73 73	29, 41, 53, 67	0
24	22	70/72 (97%)	0.39	1 (1%) 73 73	52, 63, 71, 76	0
25	13	59/60 (98%)	-0.39	2 (3%) 48 46	17, 28, 50, 75	0
25	23	59/60 (98%)	0.65	4 (6%) 25 23	46, 58, 75, 84	0
26	14	69/71 (97%)	0.72	10 (14%) 7 6	41, 65, 81, 87	0
26	24	69/71 (97%)	1.75	25 (36%) 1 1	71, 79, 87, 89	0
27	15	59/60 (98%)	-0.58	1 (1%) 69 68	15, 24, 44, 53	0
27	25	59/60 (98%)	-0.07	0 100 100	31, 46, 56, 72	0
28	16	53/54 (98%)	-0.46	0 100 100	25, 34, 49, 56	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%)	0.42	0 100 100	42, 54, 63, 68	0
29	17	48/49 (97%)	-0.50	1 (2%) 63 63	16, 22, 47, 54	0
29	27	48/49 (97%)	-0.12	1 (2%) 63 63	27, 34, 57, 66	0
30	18	64/65 (98%)	-0.53	0 100 100	21, 26, 36, 48	0
30	28	64/65 (98%)	0.29	0 100 100	40, 49, 57, 60	0
31	19	37/37 (100%)	-0.42	0 100 100	22, 31, 48, 53	0
31	29	37/37 (100%)	1.08	3 (8%) 19 18	55, 63, 72, 73	0
32	1a	1488/1521 (97%)	0.17	48 (3%) 50 48	28, 57, 86, 101	0
33	1b	231/256 (90%)	1.08	35 (15%) 6 6	57, 72, 82, 90	0
33	2b	231/256 (90%)	1.49	57 (24%) 2 2	67, 80, 86, 91	0
34	1c	206/239 (86%)	0.70	5 (2%) 59 58	51, 64, 75, 82	0
34	2c	206/239 (86%)	1.64	66 (32%) 1 1	67, 78, 83, 88	0
35	1d	208/209 (99%)	0.82	14 (6%) 25 23	49, 61, 73, 81	0
35	2d	208/209 (99%)	1.03	19 (9%) 16 15	56, 66, 74, 81	0
36	1e	148/162 (91%)	0.44	2 (1%) 73 73	44, 55, 68, 72	0
36	2e	148/162 (91%)	1.39	28 (18%) 4 4	60, 72, 79, 84	0
37	1f	100/101 (99%)	0.49	0 100 100	44, 60, 69, 77	0
37	2f	100/101 (99%)	0.43	1 (1%) 79 79	50, 61, 69, 78	0
38	1g	155/156 (99%)	0.40	9 (5%) 30 28	46, 61, 74, 86	0
38	2g	155/156 (99%)	0.96	15 (9%) 15 14	62, 71, 80, 85	0
39	1h	137/138 (99%)	0.54	3 (2%) 62 61	48, 58, 65, 72	0
39	2h	137/138 (99%)	1.03	8 (5%) 30 28	60, 71, 76, 81	0
40	1i	127/128 (99%)	0.74	8 (6%) 27 25	47, 67, 76, 80	0
40	2i	127/128 (99%)	1.76	47 (37%) 1 1	66, 76, 82, 84	0
41	1j	97/105 (92%)	1.19	18 (18%) 4 4	48, 70, 80, 85	0
41	2j	96/105 (91%)	1.92	36 (37%) 1 1	70, 79, 87, 91	0
42	1k	114/129 (88%)	0.51	6 (5%) 33 31	36, 57, 68, 76	0
42	2k	114/129 (88%)	0.87	10 (8%) 17 16	48, 65, 74, 78	0
43	1l	121/132 (91%)	0.21	3 (2%) 58 57	36, 45, 57, 62	0
43	2l	121/132 (91%)	0.72	7 (5%) 30 28	48, 61, 71, 76	0
44	1m	123/126 (97%)	0.37	4 (3%) 49 47	46, 60, 69, 73	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	2m	122/126 (96%)	1.50	28 (22%) 2 3	65, 75, 80, 82	0
45	1n	60/61 (98%)	0.51	1 (1%) 69 68	50, 57, 66, 69	0
45	2n	60/61 (98%)	2.14	30 (50%) 0 1	70, 77, 81, 83	0
46	1o	88/89 (98%)	0.40	5 (5%) 30 28	42, 56, 67, 74	0
46	2o	88/89 (98%)	0.70	4 (4%) 39 37	53, 67, 75, 77	0
47	1p	82/88 (93%)	0.76	1 (1%) 76 76	48, 59, 69, 71	0
47	2p	82/88 (93%)	0.82	6 (7%) 22 20	55, 63, 70, 73	0
48	1q	99/105 (94%)	0.41	1 (1%) 79 79	47, 58, 70, 72	0
48	2q	99/105 (94%)	0.73	3 (3%) 52 50	56, 65, 74, 79	0
49	1r	68/88 (77%)	0.41	2 (2%) 54 52	49, 58, 70, 72	0
49	2r	68/88 (77%)	0.55	1 (1%) 71 71	53, 64, 74, 79	0
50	1s	83/93 (89%)	0.57	5 (6%) 29 27	52, 62, 70, 77	0
50	2s	83/93 (89%)	1.99	32 (38%) 1 1	71, 79, 85, 86	0
51	1t	96/106 (90%)	0.78	7 (7%) 22 20	49, 60, 71, 77	0
51	2t	96/106 (90%)	0.70	6 (6%) 27 25	54, 64, 75, 77	0
52	1u	23/27 (85%)	0.85	2 (8%) 17 16	53, 57, 63, 66	0
52	2u	23/27 (85%)	2.00	12 (52%) 0 1	68, 73, 77, 79	0
53	1v	13/24 (54%)	0.37	2 (15%) 6 6	41, 47, 71, 95	0
53	2v	13/24 (54%)	1.71	4 (30%) 1 2	59, 72, 89, 91	0
54	1w	67/76 (88%)	1.32	17 (25%) 2 2	34, 80, 94, 98	0
54	2w	65/76 (85%)	1.85	25 (38%) 1 1	52, 89, 95, 101	0
55	1x	72/77 (93%)	0.36	6 (8%) 19 17	28, 59, 75, 84	0
55	2x	72/77 (93%)	0.88	2 (2%) 55 53	43, 72, 83, 85	0
56	1y	68/76 (89%)	1.08	8 (11%) 10 10	28, 84, 91, 95	0
56	2y	67/76 (88%)	1.55	18 (26%) 2 2	46, 90, 94, 97	0
57	2a	1491/1521 (98%)	0.72	132 (8%) 17 16	42, 70, 89, 101	0
58	A	13/18 (72%)	0.03	2 (15%) 6 6	17, 21, 65, 77	0
58	B	13/18 (72%)	0.88	2 (15%) 6 6	32, 35, 69, 80	0
All	All	20903/21784 (95%)	0.28	1341 (6%) 27 24	13, 56, 83, 102	0

All (1341) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	2l	2	SER	7.6
45	1n	2	ALA	6.9
57	2a	1030(B)	C	6.2
1	2A	883	G	6.1
38	1g	80	VAL	6.1
45	2n	2	ALA	5.6
33	2b	237	ALA	5.5
57	2a	1030(A)	G	5.4
44	2m	104	ARG	5.2
54	2w	71	G	5.1
1	2A	896	A	5.1
21	1Z	141	VAL	5.1
1	2A	2155	G	5.0
6	1G	182	LYS	4.9
50	2s	13	ASP	4.9
54	1w	70	G	4.9
1	2A	2146	C	4.8
57	2a	1033	G	4.8
26	24	65	ASP	4.7
1	2A	2145	C	4.7
50	2s	79	THR	4.6
40	2i	14	VAL	4.6
32	1a	1447	A	4.5
57	2a	1030	C	4.5
54	1w	71	G	4.5
6	2G	48	GLU	4.5
25	23	60	GLU	4.4
57	2a	1034	G	4.4
1	2A	1536	C	4.4
50	2s	29	ARG	4.4
1	2A	2159	G	4.4
44	2m	102	ARG	4.4
38	2g	80	VAL	4.3
57	2a	1036	G	4.3
3	1D	276	LYS	4.3
1	1A	932	C	4.3
3	2D	38	LYS	4.3
34	2c	182	ILE	4.3
1	2A	882	G	4.3
31	29	37	GLY	4.3
38	2g	82	GLY	4.3
3	1D	275	LYS	4.2
40	2i	126	SER	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	28	VAL	4.2
32	1a	1531	A	4.2
38	1g	82	GLY	4.2
45	2n	39	LEU	4.2
1	1A	2167	C	4.2
15	1T	131	ALA	4.1
53	2v	24	A	4.1
18	2W	112	GLY	4.1
18	2W	60	ASN	4.1
1	1A	944	C	4.1
12	2Q	22	LYS	4.1
1	1A	926	G	4.1
6	2G	50	ALA	4.0
1	1A	931	C	4.0
23	1l	2	SER	4.0
41	2j	65	LEU	4.0
1	2A	2133	G	4.0
32	1a	1035	A	4.0
44	2m	123	ALA	4.0
32	1a	1030	C	4.0
35	2d	164	ALA	4.0
32	1a	1503	A	4.0
54	1w	1	G	4.0
41	2j	47	PHE	4.0
7	1H	2	SER	4.0
3	2D	275	LYS	4.0
45	2n	34	TYR	4.0
1	2A	2160	G	4.0
32	1a	1003	G	4.0
41	2j	32	ALA	3.9
19	1X	95	LEU	3.9
33	1b	237	ALA	3.9
1	2A	2156	G	3.9
45	2n	6	LEU	3.9
1	1A	943	C	3.9
38	2g	84	ASN	3.9
54	2w	70	G	3.9
26	24	59	PHE	3.9
54	1w	72	C	3.9
54	2w	72	C	3.9
33	2b	236	TYR	3.9
35	1d	169	LYS	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	884	C	3.8
26	24	56	VAL	3.8
57	2a	1202	G	3.8
38	2g	81	GLY	3.8
41	1j	33	GLN	3.8
14	2S	3	ARG	3.8
26	14	63	TYR	3.8
1	2A	885	C	3.8
32	1a	204	U	3.8
52	2u	11	GLY	3.8
1	2A	2112	G	3.8
32	1a	1030(A)	G	3.8
51	1t	103	GLY	3.8
21	1Z	146	ILE	3.8
57	2a	1038	C	3.7
21	2Z	146	ILE	3.7
32	1a	1257	U	3.7
50	1s	84	GLY	3.7
15	1T	130	ALA	3.7
34	2c	188	LEU	3.7
50	2s	71	LEU	3.7
34	2c	62	ASP	3.7
32	1a	1030(C)	G	3.7
54	2w	4	C	3.7
57	2a	1035	A	3.7
22	20	84	LEU	3.7
1	2A	2154	G	3.7
32	1a	1023	G	3.7
32	1a	1036	G	3.7
1	2A	2144	U	3.7
34	2c	195	VAL	3.7
45	2n	33	VAL	3.7
21	2Z	170	THR	3.7
26	24	63	TYR	3.6
1	1A	1140	U	3.6
1	2A	886	C	3.6
36	2e	10	MET	3.6
54	1w	4	C	3.6
22	10	6	GLY	3.6
1	1A	2180	A	3.6
35	2d	154	ASN	3.6
42	2k	54	ARG	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	97	TRP	3.6
32	1a	1025	U	3.6
32	1a	1034	G	3.6
21	2Z	144	LEU	3.6
33	2b	165	VAL	3.6
1	1A	2135	U	3.6
32	1a	1532	U	3.6
1	1A	1133	G	3.6
1	2A	2127	G	3.6
1	2A	2147	G	3.6
32	1a	163	C	3.6
27	15	60	VAL	3.6
45	2n	18	VAL	3.6
50	2s	77	THR	3.6
33	1b	11	LEU	3.5
20	1Y	1	MET	3.5
1	2A	898	C	3.5
1	2A	2111	C	3.5
40	2i	102	LEU	3.5
38	2g	83	ALA	3.5
41	1j	32	ALA	3.5
44	2m	124	PRO	3.5
1	2A	2113	U	3.5
1	2A	2166	G	3.5
44	2m	5	ALA	3.5
52	2u	2	GLY	3.5
26	24	49	PHE	3.5
53	2v	14	A	3.5
1	2A	897	C	3.5
1	2A	2139	C	3.5
57	2a	1027	C	3.5
1	1A	927	G	3.5
1	1A	1221	G	3.5
1	2A	2149	G	3.5
57	2a	1001(A)	G	3.5
1	1A	1127	U	3.5
56	1y	20	U	3.5
21	2Z	168	GLU	3.4
21	2Z	172	ALA	3.4
38	1g	83	ALA	3.4
58	A	15	ALA	3.4
53	2v	13	A	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	889	C	3.4
54	2w	13	C	3.4
54	2w	67	C	3.4
57	2a	1149	C	3.4
1	2A	2802	G	3.4
38	2g	7	ALA	3.4
41	2j	34	VAL	3.4
58	B	16	ASN	3.4
22	10	3	HIS	3.4
32	1a	1030(D)	A	3.4
6	1G	48	GLU	3.4
32	1a	1029	C	3.4
1	1A	1114	G	3.4
1	1A	2134	G	3.4
1	1A	2181	G	3.4
57	2a	1021	G	3.4
21	2Z	173	ALA	3.4
33	2b	136	VAL	3.4
34	2c	157	ILE	3.4
34	2c	198	VAL	3.4
40	2i	10	ARG	3.4
1	1A	925	A	3.4
1	2A	652(B)	A	3.4
54	2w	73	A	3.4
57	2a	1447	A	3.4
32	1a	1030(B)	C	3.4
31	29	17	ILE	3.4
50	2s	9	VAL	3.4
57	2a	1257	U	3.4
1	1A	930	G	3.4
1	2A	2115	G	3.4
45	2n	3	ARG	3.4
1	1A	935	C	3.3
41	2j	8	LEU	3.3
57	2a	1532	U	3.3
1	1A	929	G	3.3
1	2A	2168	G	3.3
57	2a	1026	G	3.3
50	2s	80	TYR	3.3
52	2u	14	TRP	3.3
7	2H	136	ILE	3.3
33	1b	127	ILE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	2e	33	VAL	3.3
1	1A	942	A	3.3
1	2A	2158	A	3.3
53	2v	12	A	3.3
41	2j	78	ASN	3.3
1	1A	696	C	3.3
21	2Z	167	PRO	3.3
33	2b	234	PRO	3.3
45	2n	7	ILE	3.3
32	1a	1001(A)	G	3.3
32	1a	1024	G	3.3
32	1a	1032	G	3.3
33	2b	7	VAL	3.3
57	2a	1030(C)	G	3.3
12	2Q	104	PHE	3.3
26	24	57	GLU	3.3
32	1a	1286	A	3.3
54	1w	73	A	3.3
1	1A	1124	U	3.3
1	1A	1121	C	3.3
32	1a	91	C	3.3
33	1b	22	LYS	3.3
42	2k	49	GLY	3.3
35	2d	73	ARG	3.3
1	2A	2308	G	3.3
32	1a	346	G	3.3
32	1a	1031	G	3.3
32	1a	1033	G	3.3
26	24	66	SER	3.2
1	2A	887	A	3.2
1	2A	2119	A	3.2
42	2k	25	TYR	3.2
33	2b	230	VAL	3.2
19	2X	92	LEU	3.2
35	1d	194	LEU	3.2
37	2f	21	LEU	3.2
1	1A	936	C	3.2
1	2A	2896	C	3.2
26	24	64	GLY	3.2
41	2j	59	SER	3.2
41	1j	86	MET	3.2
54	1w	69	G	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	81	ILE	3.2
1	2A	899	A	3.2
1	2A	2173	A	3.2
53	1v	12	A	3.2
26	24	54	GLY	3.2
40	1i	91	ASP	3.2
45	2n	38	GLY	3.2
1	1A	1110	C	3.2
40	2i	49	PRO	3.2
3	2D	2	ALA	3.2
1	1A	1105	G	3.2
57	2a	1004	A	3.2
1	1A	271	U	3.2
1	1A	1143	U	3.2
1	2A	1026	U	3.2
21	1Z	149	SER	3.2
1	1A	2160	C	3.2
29	27	45	ALA	3.2
32	1a	1028	C	3.2
35	1d	170	VAL	3.2
40	2i	124	GLN	3.2
6	2G	136	ARG	3.2
33	2b	21	ARG	3.2
45	2n	21	TYR	3.2
36	2e	85	GLY	3.2
50	2s	84	GLY	3.2
56	2y	18	G	3.1
1	1A	2141	A	3.1
1	2A	2169	A	3.1
34	2c	8	ILE	3.1
57	2a	1357	A	3.1
41	2j	90	LEU	3.1
7	2H	45	VAL	3.1
43	2l	18	VAL	3.1
38	1g	85	TYR	3.1
26	24	53	GLU	3.1
14	2S	59	LYS	3.1
40	2i	11	LYS	3.1
44	2m	122	LYS	3.1
21	2Z	21	ALA	3.1
1	1A	928	G	3.1
1	2A	879	G	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	880	G	3.1
21	2Z	174	VAL	3.1
54	2w	15	G	3.1
1	1A	945	A	3.1
1	2A	2126	A	3.1
40	2i	91	ASP	3.1
1	1A	2164	C	3.1
1	2A	2137	C	3.1
1	2A	2175	C	3.1
33	1b	126	GLU	3.1
40	2i	19	LEU	3.1
41	2j	40	LEU	3.1
44	1m	2	ALA	3.1
6	2G	76	SER	3.1
12	2Q	6	ARG	3.1
34	2c	2	GLY	3.1
1	1A	1141	A	3.1
32	1a	162	A	3.1
57	2a	1002	G	3.1
57	2a	1531	A	3.1
22	20	68	GLU	3.1
35	2d	179	GLU	3.1
39	2h	2	LEU	3.1
42	2k	117	ASN	3.1
1	2A	888	C	3.1
32	1a	1027	C	3.1
41	2j	44	VAL	3.1
34	2c	9	GLY	3.1
38	2g	85	TYR	3.1
56	2y	33	U	3.0
32	1a	1001	A	3.0
56	2y	36	A	3.0
57	2a	1286	A	3.0
41	2j	100	THR	3.0
32	1a	1002	G	3.0
38	1g	84	ASN	3.0
7	2H	52	VAL	3.0
33	2b	15	VAL	3.0
36	2e	22	GLY	3.0
57	2a	1116	C	3.0
34	2c	193	TYR	3.0
44	2m	87	TYR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	185	ILE	3.0
57	2a	1446	U	3.0
21	2Z	96	VAL	3.0
58	B	15	ALA	3.0
1	2A	11	G	3.0
1	2A	1171	G	3.0
19	1X	94	GLY	3.0
36	2e	114	GLY	3.0
1	1A	2158	C	3.0
54	2w	2	C	3.0
12	2Q	2	LEU	3.0
21	2Z	157	LEU	3.0
34	2c	32	LEU	3.0
50	2s	49	ILE	3.0
45	2n	13	THR	3.0
34	2c	129	ALA	3.0
38	1g	2	ALA	3.0
54	2w	45	U	3.0
20	2Y	54	LYS	3.0
50	2s	2	PRO	3.0
1	1A	2163	G	3.0
1	1A	2178	G	3.0
56	2y	15	G	3.0
34	2c	201	TYR	3.0
22	20	43	THR	3.0
46	1o	88	ARG	3.0
1	1A	1555	C	3.0
1	1A	2807	C	3.0
33	1b	7	VAL	3.0
34	1c	207	VAL	3.0
40	2i	28	VAL	3.0
57	2a	1260	C	3.0
33	2b	152	PHE	3.0
33	2b	187	LEU	2.9
50	2s	5	LEU	2.9
41	2j	74	ILE	2.9
41	2j	96	ILE	2.9
46	2o	88	ARG	2.9
1	2A	881	G	2.9
57	2a	976	G	2.9
1	1A	1122	C	2.9
1	1A	2133	C	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2168	C	2.9
1	2A	2803	C	2.9
1	2A	2132	U	2.9
6	2G	52	ILE	2.9
1	2A	2134	A	2.9
6	2G	15	VAL	2.9
26	14	56	VAL	2.9
1	1A	2137	G	2.9
1	2A	2116	G	2.9
54	2w	5	G	2.9
57	2a	630	G	2.9
57	2a	993	G	2.9
57	2a	1031	G	2.9
57	2a	1032	G	2.9
50	2s	15	LEU	2.9
1	1A	933	C	2.9
1	2A	894	C	2.9
1	2A	1509	C	2.9
21	2Z	171	ILE	2.9
1	1A	2154	U	2.9
1	1A	2172	U	2.9
40	2i	9	ARG	2.9
43	1l	64	TYR	2.9
36	2e	21	ALA	2.9
45	2n	25	VAL	2.9
1	1A	2136	A	2.9
57	2a	1030(D)	A	2.9
51	2t	103	GLY	2.9
45	2n	44	LEU	2.9
34	2c	79	ARG	2.9
40	2i	20	ARG	2.9
45	2n	31	ARG	2.9
52	2u	6	ARG	2.9
1	1A	2155	G	2.9
1	2A	1533	G	2.9
6	2G	146	TYR	2.9
57	2a	1150	U	2.9
47	2p	82	GLN	2.9
21	1Z	148	ASP	2.9
26	24	51	ASP	2.9
33	1b	17	PHE	2.9
41	2j	63	PHE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	14	54	GLY	2.9
41	2j	10	GLY	2.9
43	1l	63	GLY	2.9
44	2m	6	GLY	2.9
1	1A	1115	A	2.9
1	2A	2176	A	2.9
32	1a	160	A	2.9
35	2d	188	LEU	2.9
44	1m	104	ARG	2.8
21	1Z	170	THR	2.8
50	2s	24	ALA	2.8
1	2A	2157	G	2.8
1	2A	2136	C	2.8
46	2o	86	GLY	2.8
57	2a	1029	C	2.8
3	1D	38	LYS	2.8
43	2l	126	LYS	2.8
1	1A	572	A	2.8
34	2c	128	PHE	2.8
41	2j	37	PRO	2.8
14	2S	35	ILE	2.8
26	24	58	ARG	2.8
1	1A	639	G	2.8
1	1A	1108	G	2.8
1	2A	2151	G	2.8
57	2a	1131	G	2.8
57	2a	1114	C	2.8
33	1b	233	SER	2.8
6	2G	31	VAL	2.8
26	24	50	VAL	2.8
33	1b	229	VAL	2.8
1	2A	2114	A	2.8
8	2I	146	ALA	2.8
40	2i	122	ALA	2.8
6	1G	146	TYR	2.8
33	1b	236	TYR	2.8
39	2h	67	PRO	2.8
40	2i	62	TYR	2.8
34	2c	194	GLY	2.8
35	1d	167	GLY	2.8
36	2e	5	ASP	2.8
6	2G	128	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
55	1x	47	U	2.8
45	2n	40	CYS	2.8
1	1A	2174	G	2.8
32	1a	1026	G	2.8
57	2a	1042	G	2.8
57	2a	1117	G	2.8
33	2b	123	ALA	2.8
34	2c	189	ALA	2.8
7	2H	36	PRO	2.8
40	2i	90	PRO	2.8
43	2l	64	TYR	2.8
1	2A	1847	A	2.8
26	24	62	ARG	2.8
35	2d	132	ARG	2.8
41	1j	4	ILE	2.7
21	2Z	141	VAL	2.7
21	2Z	149	SER	2.7
22	20	30	VAL	2.7
33	2b	112	VAL	2.7
34	2c	138	VAL	2.7
40	1i	106	ALA	2.7
21	2Z	41	LEU	2.7
51	1t	10	LEU	2.7
35	2d	87	GLY	2.7
1	1A	1135	G	2.7
1	2A	2165	G	2.7
34	2c	39	ILE	2.7
36	2e	51	VAL	2.7
40	2i	119	ALA	2.7
1	1A	1072	U	2.7
34	2c	190	ARG	2.7
50	2s	68	GLY	2.7
34	2c	124	ILE	2.7
1	1A	34	C	2.7
54	1w	3	C	2.7
57	2a	979	C	2.7
57	2a	1045	C	2.7
1	2A	2153	G	2.7
54	2w	10	G	2.7
55	1x	70	G	2.7
57	2a	1003	G	2.7
1	1A	1113	A	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	878	A	2.7
1	2A	2801(A)	A	2.7
32	1a	161	A	2.7
33	2b	71	VAL	2.7
36	2e	115	VAL	2.7
57	2a	1001	A	2.7
34	2c	73	PRO	2.7
34	2c	137	ALA	2.7
40	1i	59	PHE	2.7
41	2j	85	LEU	2.7
48	2q	99	SER	2.7
50	1s	71	LEU	2.7
52	2u	8	THR	2.7
7	1H	3	ARG	2.7
22	20	3	HIS	2.7
1	2A	2167	U	2.7
21	2Z	53	ILE	2.7
34	2c	17	ASP	2.7
40	2i	105	ASP	2.7
1	1A	2162	C	2.7
1	2A	1043	C	2.7
1	2A	2297	C	2.7
5	2F	166	ALA	2.7
47	2p	9	PHE	2.7
36	2e	120	THR	2.7
1	1A	2179	G	2.7
1	1A	2187	G	2.7
1	2A	892	G	2.7
1	2A	2131	G	2.7
1	2A	2319	G	2.7
54	1w	44	G	2.7
57	2a	631	G	2.7
57	2a	1024	G	2.7
57	2a	1224	G	2.7
57	2a	1272	G	2.7
38	2g	5	ARG	2.7
52	2u	24	ARG	2.7
26	14	45	GLY	2.7
33	1b	228	GLY	2.7
41	2j	93	GLY	2.7
46	1o	87	ILE	2.7
50	2s	31	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
56	2y	45	U	2.6
9	2N	83	LYS	2.6
41	2j	55	LYS	2.6
7	2H	17	VAL	2.6
34	2c	207	VAL	2.6
44	2m	7	VAL	2.6
14	2S	4	LEU	2.6
26	14	59	PHE	2.6
33	2b	225	ALA	2.6
34	2c	200	ALA	2.6
35	1d	195	ALA	2.6
45	2n	14	PRO	2.6
5	2F	62	ARG	2.6
33	1b	19	HIS	2.6
1	1A	2161	C	2.6
1	1A	2186	C	2.6
1	2A	2128	C	2.6
33	2b	124	SER	2.6
36	2e	74	GLY	2.6
54	1w	2	C	2.6
57	2a	1503	A	2.6
54	2w	6	G	2.6
54	2w	18	G	2.6
54	2w	44	G	2.6
56	1y	44	G	2.6
57	2a	1058	G	2.6
57	2a	1182	G	2.6
7	2H	175	LYS	2.6
55	2x	47	U	2.6
31	29	16	VAL	2.6
34	2c	68	VAL	2.6
34	2c	99	VAL	2.6
36	2e	12	LEU	2.6
39	2h	53	VAL	2.6
42	2k	14	VAL	2.6
50	1s	9	VAL	2.6
25	23	2	PRO	2.6
22	20	2	ALA	2.6
34	2c	92	ALA	2.6
45	2n	22	THR	2.6
34	2c	197	GLY	2.6
34	2c	77	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	2e	125	SER	2.6
40	1i	2	GLU	2.6
1	1A	2159	C	2.6
40	2i	92	TYR	2.6
1	1A	302	A	2.6
1	1A	934	A	2.6
1	1A	2157	A	2.6
32	1a	1005	A	2.6
41	1j	76	ASN	2.6
1	2A	2162	G	2.6
8	2I	68	LEU	2.6
14	2S	32	LEU	2.6
21	2Z	159	PRO	2.6
34	2c	196	LEU	2.6
44	2m	15	VAL	2.6
24	12	70	GLN	2.6
1	2A	614(A)	U	2.6
7	2H	96	ALA	2.6
22	20	69	PHE	2.6
34	2c	149	ALA	2.6
57	2a	1219	U	2.6
50	2s	63	THR	2.6
33	2b	208	ILE	2.6
41	2j	23	ILE	2.6
26	24	69	LYS	2.6
14	2S	92	TYR	2.6
50	2s	61	TYR	2.6
34	2c	36	ASP	2.6
50	2s	30	LEU	2.6
1	2A	2138	C	2.6
32	1a	1037	C	2.6
33	2b	232	PRO	2.6
41	2j	91	PRO	2.6
36	2e	20	GLN	2.6
54	2w	3	C	2.6
57	2a	980	C	2.6
57	2a	1019	C	2.6
57	2a	1115	C	2.6
4	2E	204	ALA	2.6
12	2Q	121	ALA	2.6
26	14	55	ARG	2.6
26	24	55	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	218	A	2.6
1	1A	1116	A	2.6
1	2A	2117	A	2.6
1	1A	2906	U	2.6
6	2G	20	ILE	2.6
34	2c	5	ILE	2.6
46	1o	89	GLY	2.6
1	1A	2212	G	2.6
32	1a	78	G	2.6
57	2a	1053	G	2.6
57	2a	1356	G	2.6
7	2H	41	MET	2.5
21	2Z	166	SER	2.5
34	2c	4	LYS	2.5
34	2c	52	LEU	2.5
42	1k	36	ASP	2.5
33	1b	230	VAL	2.5
41	1j	34	VAL	2.5
46	1o	19	PRO	2.5
15	2T	111	ARG	2.5
35	2d	47	ARG	2.5
41	1j	79	ARG	2.5
45	2n	29	ARG	2.5
15	2T	131	ALA	2.5
35	1d	158	ILE	2.5
40	2i	115	GLY	2.5
41	1j	31	GLY	2.5
50	2s	62	ILE	2.5
1	2A	895	U	2.5
54	2w	66	U	2.5
1	1A	938	G	2.5
1	1A	2184	G	2.5
1	2A	614(B)	G	2.5
1	2A	1114	G	2.5
1	2A	2125	G	2.5
1	2A	2893	G	2.5
33	2b	11	LEU	2.5
44	2m	70	LEU	2.5
48	2q	98	LEU	2.5
7	2H	19	VAL	2.5
8	2I	137	PRO	2.5
9	2N	9	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	2e	25	ARG	2.5
40	2i	17	VAL	2.5
40	2i	86	VAL	2.5
34	1c	107	GLN	2.5
44	2m	94	ARG	2.5
43	2l	32	PHE	2.5
20	2Y	44	ILE	2.5
8	2I	86	THR	2.5
33	1b	12	GLU	2.5
1	2A	2143	C	2.5
41	2j	30	SER	2.5
57	2a	1054	C	2.5
1	1A	2156	A	2.5
1	2A	229	A	2.5
1	2A	890	A	2.5
57	2a	1256	A	2.5
33	2b	215	LEU	2.5
40	1i	19	LEU	2.5
56	1y	45	U	2.5
57	2a	1020	U	2.5
7	2H	76	VAL	2.5
26	24	25	TYR	2.5
46	2o	60	VAL	2.5
50	2s	81	ARG	2.5
6	1G	80	PHE	2.5
1	2A	2805	G	2.5
32	1a	1021	G	2.5
57	2a	1023	G	2.5
3	2D	276	LYS	2.5
50	2s	32	LYS	2.5
34	2c	158	GLY	2.5
35	2d	23	GLY	2.5
36	1e	85	GLY	2.5
26	24	30	GLU	2.5
33	1b	129	GLU	2.5
7	2H	88	LEU	2.5
7	2H	29	PRO	2.5
38	1g	79	ARG	2.5
41	2j	77	PRO	2.5
36	2e	34	VAL	2.5
1	1A	1112	U	2.5
1	1A	1123	A	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1142	A	2.5
1	1A	1222	A	2.5
1	2A	645	C	2.5
1	2A	901	A	2.5
1	2A	2161	C	2.5
1	2A	2170	A	2.5
21	2Z	99	TYR	2.5
33	2b	148	TYR	2.5
50	2s	52	TYR	2.5
54	2w	11	C	2.5
56	1y	35	A	2.5
56	1y	36	A	2.5
57	2a	1018	C	2.5
57	2a	1148	U	2.5
21	2Z	164	ALA	2.5
33	1b	120	ALA	2.5
34	2c	65	ALA	2.5
35	2d	161	ASN	2.5
41	1j	74	ILE	2.5
34	2c	15	THR	2.5
1	1A	2173	G	2.4
1	1A	2228	G	2.4
54	2w	19	G	2.4
57	2a	1253	G	2.4
21	1Z	150	LEU	2.4
6	2G	51	ARG	2.4
33	2b	91	PRO	2.4
38	2g	4	ARG	2.4
39	2h	102	ARG	2.4
50	2s	76	PRO	2.4
7	2H	43	VAL	2.4
21	2Z	71	VAL	2.4
43	1l	18	VAL	2.4
12	2Q	103	MET	2.4
21	2Z	136	PHE	2.4
22	20	5	LYS	2.4
33	2b	22	LYS	2.4
33	2b	83	MET	2.4
34	2c	6	HIS	2.4
33	1b	188	ALA	2.4
34	2c	184	TYR	2.4
6	2G	88	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	2k	36	ASP	2.4
1	1A	1128	U	2.4
1	2A	2897	U	2.4
57	2a	1025	U	2.4
57	2a	1358	U	2.4
1	1A	670	C	2.4
1	1A	937	A	2.4
1	1A	1103	A	2.4
1	1A	2183	C	2.4
45	2n	55	GLY	2.4
41	2j	42	THR	2.4
57	2a	999	C	2.4
33	2b	10	LEU	2.4
41	2j	88	LEU	2.4
17	2V	50	PRO	2.4
26	24	61	ARG	2.4
40	2i	104	ARG	2.4
1	1A	2132	G	2.4
1	1A	2177	G	2.4
1	1A	2816	G	2.4
1	2A	2148	G	2.4
1	2A	2207	G	2.4
1	2A	2793	G	2.4
4	2E	167	VAL	2.4
40	2i	127	LYS	2.4
56	2y	5	G	2.4
14	2S	29	PHE	2.4
39	1h	80	ILE	2.4
40	2i	125	TYR	2.4
44	2m	100	GLY	2.4
57	2a	1205	U	2.4
1	1A	1091	A	2.4
1	1A	2803	A	2.4
1	2A	528	A	2.4
34	2c	33	LEU	2.4
51	2t	10	LEU	2.4
57	2a	969	A	2.4
57	2a	975	A	2.4
1	1A	1126	C	2.4
1	2A	865	C	2.4
1	2A	893	C	2.4
1	2A	2174	C	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1008	C	2.4
56	2y	56	C	2.4
57	2a	1037	C	2.4
21	2Z	122	ARG	2.4
35	1d	173	TRP	2.4
35	2d	166	LYS	2.4
40	2i	95	LYS	2.4
6	2G	180	PHE	2.4
35	2d	160	GLN	2.4
41	2j	54	PHE	2.4
51	1t	100	ILE	2.4
20	2Y	55	TYR	2.4
21	2Z	106	GLY	2.4
23	2l	28	GLY	2.4
43	2l	63	GLY	2.4
52	2u	4	GLY	2.4
52	2u	16	GLY	2.4
1	2A	652(U)	G	2.4
54	1w	10	G	2.4
54	2w	69	G	2.4
57	2a	1220	G	2.4
40	2i	7	THR	2.4
6	2G	173	LEU	2.4
6	2G	175	LEU	2.4
21	2Z	150	LEU	2.4
38	2g	16	LEU	2.4
1	1A	2166	U	2.4
25	23	29	ARG	2.4
32	1a	1446	U	2.4
54	1w	66	U	2.4
12	2Q	1	MET	2.4
40	2i	113	LYS	2.4
51	2t	98	PRO	2.4
1	1A	1119	A	2.4
7	2H	79	VAL	2.4
21	1Z	105	VAL	2.4
33	1b	24	TRP	2.4
50	2s	11	VAL	2.4
54	2w	14	A	2.4
1	1A	940	C	2.4
1	1A	2815	C	2.4
33	2b	122	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	1w	67	C	2.4
54	2w	61	C	2.4
55	1x	68	C	2.4
57	2a	1039	C	2.4
12	2Q	136	ALA	2.4
33	1b	214	ILE	2.4
34	2c	187	ALA	2.4
36	2e	13	ILE	2.4
38	2g	152	ALA	2.4
12	2Q	30	GLY	2.4
33	1b	18	GLY	2.4
41	1j	93	GLY	2.4
44	2m	112	GLY	2.4
50	2s	54	GLY	2.4
50	1s	13	ASP	2.4
26	24	52	THR	2.3
50	2s	48	THR	2.3
33	1b	128	GLU	2.3
35	2d	194	LEU	2.3
39	1h	112	LEU	2.3
40	2i	99	LEU	2.3
18	2W	90	ARG	2.3
21	2Z	103	ARG	2.3
38	2g	3	ARG	2.3
38	2g	79	ARG	2.3
1	1A	1104	G	2.3
1	1A	2176	G	2.3
1	1A	2182	G	2.3
1	1A	2188	G	2.3
44	1m	124	PRO	2.3
50	2s	42	PRO	2.3
55	2x	70	G	2.3
56	2y	44	G	2.3
7	2H	169	VAL	2.3
21	2Z	121	HIS	2.3
1	2A	2109	U	2.3
1	2A	2150	U	2.3
33	2b	17	PHE	2.3
35	2d	173	TRP	2.3
1	1A	1132	A	2.3
32	1a	344	A	2.3
54	1w	7	A	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
57	2a	1287	A	2.3
7	2H	48	GLY	2.3
7	2H	174	GLY	2.3
14	2S	7	TYR	2.3
40	2i	5	TYR	2.3
55	1x	69	C	2.3
57	2a	1129	C	2.3
57	2a	1189	C	2.3
14	2S	61	ASN	2.3
41	2j	58	ASP	2.3
58	A	16	ASN	2.3
14	2S	58	LEU	2.3
34	2c	47	LEU	2.3
33	1b	134	GLU	2.3
43	2l	41	ARG	2.3
52	1u	24	ARG	2.3
45	2n	54	PRO	2.3
7	2H	61	HIS	2.3
44	2m	92	HIS	2.3
9	1N	140	VAL	2.3
21	2Z	139	VAL	2.3
33	2b	229	VAL	2.3
42	1k	14	VAL	2.3
6	2G	29	TRP	2.3
33	1b	97	TRP	2.3
33	2b	200	ILE	2.3
36	2e	109	ILE	2.3
1	1A	12	U	2.3
1	1A	1985	U	2.3
1	2A	2110	G	2.3
7	2H	75	ALA	2.3
32	1a	630	G	2.3
56	2y	53	G	2.3
57	2a	485	G	2.3
57	2a	1315	U	2.3
35	1d	180	GLY	2.3
35	2d	167	GLY	2.3
39	2h	106	GLY	2.3
33	1b	187	LEU	2.3
34	1c	87	LEU	2.3
40	2i	79	LEU	2.3
42	1k	25	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
48	1q	98	LEU	2.3
1	1A	1554	A	2.3
7	1H	13	LYS	2.3
23	11	75	GLU	2.3
25	13	60	GLU	2.3
57	2a	1044	A	2.3
35	1d	168	ARG	2.3
6	2G	17	PRO	2.3
57	2a	962	C	2.3
57	2a	1321	C	2.3
57	2a	1452	C	2.3
5	2F	89	VAL	2.3
42	1k	48	ILE	2.3
33	2b	161	ALA	2.3
34	2c	53	ALA	2.3
45	2n	20	ALA	2.3
51	2t	97	ALA	2.3
6	2G	42	GLY	2.3
18	1W	112	GLY	2.3
1	1A	941	U	2.3
32	1a	202	U	2.3
42	2k	124	LYS	2.3
34	1c	193	TYR	2.3
1	1A	698	G	2.3
1	1A	1109	G	2.3
1	2A	2124	G	2.3
33	2b	166	ASP	2.3
40	2i	2	GLU	2.3
49	2r	47	THR	2.3
56	1y	69	G	2.3
57	2a	1370	G	2.3
33	2b	19	HIS	2.3
41	2j	62	HIS	2.3
57	2a	1005	A	2.3
57	2a	1092	A	2.3
25	23	59	VAL	2.3
33	2b	95	GLN	2.3
34	2c	116	VAL	2.3
36	2e	100	VAL	2.3
1	1A	2150	C	2.3
1	2A	2140	C	2.3
35	1d	110	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	147	GLY	2.3
33	2b	99	GLY	2.3
6	2G	53	LEU	2.3
22	10	5	LYS	2.2
29	17	48	LYS	2.2
36	2e	31	LEU	2.3
45	2n	15	LYS	2.2
40	2i	128	ARG	2.2
26	14	57	GLU	2.2
20	1Y	92	ASN	2.2
33	2b	31	TYR	2.2
33	2b	86	GLU	2.2
40	2i	114	TYR	2.2
1	1A	2131	U	2.2
52	2u	23	PRO	2.2
56	2y	51	U	2.2
14	2S	34	HIS	2.2
38	1g	153	HIS	2.2
1	1A	569	G	2.2
1	1A	2138	G	2.2
1	2A	2894	G	2.2
2	2B	119	G	2.2
33	1b	165	VAL	2.2
34	2c	130	VAL	2.2
54	2w	65	G	2.2
56	1y	18	G	2.2
57	2a	1190	G	2.2
34	2c	152	ILE	2.2
36	1e	13	ILE	2.2
41	1j	75	ILE	2.2
1	1A	2139	A	2.2
57	2a	1248	A	2.2
33	2b	89	GLY	2.2
33	2b	101	MET	2.2
34	2c	199	LYS	2.2
45	2n	51	GLY	2.2
51	1t	74	LYS	2.2
36	2e	119	LEU	2.2
44	2m	19	LEU	2.2
44	2m	34	LEU	2.2
1	2A	2163	C	2.2
1	2A	2164	C	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
57	2a	1043	C	2.2
57	2a	1203	C	2.2
6	1G	83	ARG	2.2
7	2H	3	ARG	2.2
35	1d	150	GLU	2.2
33	2b	54	THR	2.2
35	1d	154	ASN	2.2
40	2i	4	TYR	2.2
46	1o	69	TYR	2.2
1	1A	1220	U	2.2
1	2A	271(K)	U	2.2
1	2A	1113	U	2.2
14	2S	14	VAL	2.2
32	1a	841	U	2.2
57	2a	1211	U	2.2
26	24	47	GLN	2.2
26	24	5	ILE	2.2
33	2b	57	PHE	2.2
47	1p	82	GLN	2.2
36	2e	118	ILE	2.2
47	2p	19	ILE	2.2
20	2Y	34	LYS	2.2
36	2e	54	ALA	2.2
40	2i	13	ALA	2.2
40	2i	118	LYS	2.2
6	1G	139	LEU	2.2
7	2H	64	LEU	2.2
7	2H	82	GLY	2.2
11	1P	99	LEU	2.2
38	1g	81	GLY	2.2
44	2m	90	LEU	2.2
51	2t	101	GLY	2.2
14	2S	17	ARG	2.2
32	1a	159	G	2.2
41	1j	29	ARG	2.2
56	1y	15	G	2.2
56	2y	6	G	2.2
57	2a	971	G	2.2
57	2a	1047	G	2.2
57	2a	1215	G	2.2
1	1A	554	A	2.2
1	1A	2195	A	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
57	2a	977	A	2.2
57	2a	978	A	2.2
35	1d	83	SER	2.2
7	2H	10	PRO	2.2
33	1b	232	PRO	2.2
41	2j	48	THR	2.2
1	1A	2196	C	2.2
56	2y	13	C	2.2
57	2a	1060	C	2.2
57	2a	1066	C	2.2
57	2a	1320	C	2.2
10	2O	81	ASP	2.2
8	1I	109	ILE	2.2
20	2Y	57	GLN	2.2
21	2Z	48	PHE	2.2
21	2Z	165	VAL	2.2
26	14	49	PHE	2.2
44	2m	98	VAL	2.2
45	2n	37	PHE	2.2
50	2s	58	VAL	2.2
33	2b	127	ILE	2.2
34	2c	14	ILE	2.2
33	1b	133	LYS	2.2
35	2d	86	LYS	2.2
42	2k	51	LYS	2.2
1	1A	2189	U	2.2
1	2A	271(L)	U	2.2
1	2A	2130	U	2.2
33	2b	48	MET	2.2
34	2c	61	ALA	2.2
40	2i	82	ALA	2.2
41	2j	26	ALA	2.2
54	1w	20	U	2.2
54	1w	45	U	2.2
57	2a	1136	U	2.2
57	2a	1159	U	2.2
57	2a	1196	U	2.2
21	2Z	155	LEU	2.2
34	2c	87	LEU	2.2
7	2H	42	ARG	2.2
8	2I	50	ARG	2.2
21	2Z	143	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	14	64	GLY	2.2
33	1b	72	GLY	2.2
39	2h	90	GLY	2.2
39	2h	122	ARG	2.2
51	1t	98	PRO	2.2
52	2u	17	THR	2.2
1	2A	900	A	2.2
50	2s	14	HIS	2.2
56	2y	14	A	2.2
56	2y	35	A	2.2
1	1A	694	G	2.2
1	1A	2153	G	2.2
1	2A	2318	G	2.2
36	2e	133	TYR	2.2
57	2a	953	G	2.2
57	2a	973	G	2.2
57	2a	1258	G	2.2
57	2a	1276	G	2.2
3	2D	122	ASP	2.2
34	1c	62	ASP	2.2
7	2H	24	VAL	2.2
21	2Z	57	ILE	2.2
33	1b	15	VAL	2.2
33	2b	201	ILE	2.2
36	2e	41	VAL	2.2
41	1j	6	ILE	2.2
41	2j	49	VAL	2.2
50	1s	40	ILE	2.2
1	1A	2814	C	2.2
34	2c	135	LYS	2.2
57	2a	848	C	2.2
4	2E	52	LEU	2.2
22	10	7	LEU	2.2
34	2c	24	ALA	2.2
33	2b	130	ARG	2.2
34	2c	205	GLY	2.2
46	2o	89	GLY	2.2
51	2t	96	GLY	2.2
47	2p	48	TRP	2.1
57	2a	1000	U	2.1
57	2a	1040	U	2.1
57	2a	1065	U	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	123	PRO	2.1
41	2j	53	PRO	2.1
35	2d	20	TYR	2.1
7	2H	44	VAL	2.1
21	2Z	86	VAL	2.1
22	20	45	PHE	2.1
24	22	70	GLN	2.1
33	2b	132	LYS	2.1
41	1j	72	VAL	2.1
44	2m	4	ILE	2.1
45	2n	17	LYS	2.1
1	1A	1219	A	2.1
1	2A	2135	A	2.1
2	2B	120	A	2.1
1	2A	1170	G	2.1
1	2A	2751	G	2.1
14	2S	48	LEU	2.1
33	2b	213	LEU	2.1
44	2m	96	LEU	2.1
56	2y	19	G	2.1
56	2y	52	G	2.1
57	2a	1057	G	2.1
7	2H	156	ALA	2.1
45	2n	10	ALA	2.1
44	1m	102	ARG	2.1
45	2n	41	ARG	2.1
26	24	45	GLY	2.1
40	2i	67	GLY	2.1
1	2A	2794	C	2.1
55	1x	67	C	2.1
50	2s	34	TRP	2.1
1	2A	12	U	2.1
6	2G	74	LYS	2.1
33	2b	37	ASN	2.1
6	2G	49	ASP	2.1
6	2G	141	PHE	2.1
21	1Z	136	PHE	2.1
33	1b	93	VAL	2.1
33	2b	93	VAL	2.1
34	2c	23	TYR	2.1
40	2i	41	VAL	2.1
41	1j	98	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	1k	75	TYR	2.1
33	1b	10	LEU	2.1
3	2D	262	ARG	2.1
33	2b	120	ALA	2.1
38	2g	2	ALA	2.1
40	2i	15	ALA	2.1
44	2m	30	ALA	2.1
47	2p	81	ARG	2.1
34	2c	171	GLY	2.1
53	1v	13	A	2.1
54	2w	7	A	2.1
57	2a	532	A	2.1
57	2a	983	A	2.1
57	2a	1180	A	2.1
1	2A	2141	G	2.1
1	2A	2152	G	2.1
21	2Z	95	PRO	2.1
34	2c	161	GLU	2.1
41	1j	77	PRO	2.1
57	2a	1009	G	2.1
57	2a	1184	G	2.1
57	2a	1310	G	2.1
40	2i	117	HIS	2.1
1	2A	2129	C	2.1
32	1a	1006	C	2.1
44	2m	105	THR	2.1
57	2a	1007	C	2.1
57	2a	1214	C	2.1
1	1A	1106	U	2.1
32	1a	203	U	2.1
6	2G	38	VAL	2.1
33	2b	58	ILE	2.1
34	2c	151	VAL	2.1
41	2j	98	ILE	2.1
42	2k	48	ILE	2.1
26	24	32	TYR	2.1
49	1r	78	LEU	2.1
36	2e	17	ALA	2.1
36	2e	94	ALA	2.1
40	1i	15	ALA	2.1
44	2m	3	ARG	2.1
45	2n	59	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	2Q	15	GLY	2.1
33	1b	234	PRO	2.1
35	2d	37	PRO	2.1
44	2m	58	GLU	2.1
1	2A	866	A	2.1
1	2A	2298	A	2.1
45	2n	61	TRP	2.1
57	2a	1110	A	2.1
14	2S	57	LYS	2.1
26	14	69	LYS	2.1
40	2i	97	LYS	2.1
52	2u	20	LYS	2.1
50	2s	33	THR	2.1
33	1b	200	ILE	2.1
44	2m	22	ILE	2.1
45	2n	42	ILE	2.1
1	1A	2147	G	2.1
1	1A	2170	G	2.1
1	2A	1858	G	2.1
2	2B	23	G	2.1
17	2V	52	VAL	2.1
21	2Z	88	PHE	2.1
40	2i	44	VAL	2.1
40	2i	101	PHE	2.1
41	1j	24	VAL	2.1
42	2k	13	GLN	2.1
56	2y	57	G	2.1
57	2a	1048	G	2.1
1	2A	1584	C	2.1
1	2A	2142	C	2.1
1	2A	2804	C	2.1
34	2c	178	LEU	2.1
35	2d	21	LEU	2.1
40	1i	56	LEU	2.1
1	2A	958	U	2.1
6	2G	156	ASP	2.1
26	24	67	TYR	2.1
57	2a	1028	C	2.1
7	2H	60	ARG	2.1
38	2g	76	ARG	2.1
47	2p	8	ARG	2.1
50	2s	78	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
57	2a	1313	U	2.1
6	2G	163	ALA	2.1
13	2R	101	ALA	2.1
34	2c	146	ALA	2.1
39	2h	124	ALA	2.1
44	2m	42	ALA	2.1
51	1t	102	GLY	2.1
7	2H	118	PRO	2.0
20	2Y	53	PRO	2.0
33	1b	131	PRO	2.0
41	2j	83	GLU	2.0
48	2q	96	GLU	2.0
33	2b	156	LYS	2.0
52	2u	3	LYS	2.0
12	2Q	7	MET	2.0
34	2c	191	THR	2.0
41	1j	38	ILE	2.0
7	2H	50	VAL	2.0
21	2Z	153	SER	2.0
42	1k	13	GLN	2.0
51	1t	70	SER	2.0
54	2w	26	A	2.0
57	2a	974	A	2.0
57	2a	1251	A	2.0
33	2b	154	LEU	2.0
34	2c	48	TYR	2.0
39	1h	4	ASP	2.0
8	2I	65	ALA	2.0
19	2X	91	ALA	2.0
49	1r	24	ALA	2.0
1	1A	1101	G	2.0
1	1A	2190	G	2.0
1	1A	2813	G	2.0
1	2A	2206	G	2.0
33	1b	227	GLY	2.0
33	2b	227	GLY	2.0
41	2j	36	GLY	2.0
52	1u	16	GLY	2.0
55	1x	20	U	2.0
57	2a	80	G	2.0
57	2a	202	U	2.0
57	2a	204	U	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
57	2a	982	U	2.0
1	1A	2165	C	2.0
1	2A	652(V)	C	2.0
54	1w	68	C	2.0
56	2y	48	C	2.0
57	2a	970	C	2.0
57	2a	1359	C	2.0
57	2a	1363	C	2.0
7	2H	128	PRO	2.0
25	13	2	PRO	2.0
41	2j	41	PRO	2.0
5	2F	161	GLU	2.0
20	1Y	91	GLU	2.0
21	2Z	2	GLU	2.0
33	2b	169	LYS	2.0
44	2m	121	LYS	2.0
20	2Y	1	MET	2.0
34	2c	67	THR	2.0
36	2e	80	ILE	2.0
40	2i	27	THR	2.0
6	2G	172	LEU	2.0
7	2H	33	LEU	2.0
43	2l	55	VAL	2.0
12	1Q	6	ARG	2.0
34	2c	88	ARG	2.0
40	1i	66	ARG	2.0
33	2b	94	ASN	2.0
1	1A	1878	A	2.0
1	2A	529	A	2.0
1	2A	2171	A	2.0
2	2B	66	A	2.0
6	2G	126	ASP	2.0
7	2H	83	TYR	2.0
19	2X	69	TYR	2.0
35	1d	164	ALA	2.0
57	2a	994	A	2.0
57	2a	1250	A	2.0
57	2a	1285	A	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	PSU	2y	55	20/21	0.46	0.18	89,99,107,116	0
54	G7M	2w	46	24/25	0.52	0.17	80,88,101,118	0
56	5MU	2y	54	21/22	0.54	0.16	86,91,105,122	0
56	G7M	2y	46	24/25	0.54	0.18	82,90,99,118	0
56	G7M	1y	46	24/25	0.55	0.18	80,88,98,108	0
54	G7M	1w	46	24/25	0.58	0.18	70,80,100,123	0
56	PSU	1y	55	20/21	0.62	0.14	84,90,100,105	0
56	5MU	1y	54	21/22	0.66	0.15	76,85,92,104	0
56	4SU	2y	8	20/21	0.67	0.14	85,90,98,107	0
56	PSU	2y	32	20/21	0.74	0.14	74,82,94,96	0
54	4SU	2w	8	20/21	0.75	0.12	82,88,103,107	0
58	BB9	B	17	6/7	0.75	0.31	68,79,86,100	0
56	4SU	1y	8	20/21	0.77	0.14	83,88,102,104	0
54	PSU	2w	55	20/21	0.78	0.12	73,83,90,98	0
56	PSU	2y	39	20/21	0.79	0.14	72,80,86,98	0
54	4SU	1w	8	20/21	0.79	0.14	72,81,89,91	0
55	5MU	2x	54	21/22	0.82	0.14	70,77,80,92	0
55	PSU	2x	55	20/21	0.83	0.13	69,73,79,80	0
57	2MG	2a	1207	24/25	0.84	0.14	72,80,87,88	0
56	PSU	1y	32	20/21	0.84	0.13	70,78,86,87	0
54	PSU	2w	32	20/21	0.85	0.12	70,77,85,91	0
54	5MU	2w	54	21/22	0.86	0.11	67,75,81,86	0
43	0TD	1l	92	10/11	0.86	0.16	41,42,49,76	0
58	BB9	A	17	6/7	0.86	0.19	54,69,80,92	0
55	4SU	2x	8	20/21	0.86	0.12	70,75,79,81	0
56	PSU	1y	39	20/21	0.87	0.11	69,73,78,82	0
43	0TD	2l	92	10/11	0.87	0.16	58,62,66,84	0
57	M2G	2a	966	25/26	0.87	0.15	56,62,75,78	0
54	PSU	1w	55	20/21	0.89	0.10	53,69,78,80	0
57	5MC	2a	967	21/22	0.91	0.12	60,65,76,77	0
55	5MC	2x	32	21/22	0.91	0.13	62,66,70,75	0
57	PSU	2a	516	20/21	0.91	0.11	58,66,72,72	0
1	5MU	2A	1915	21/22	0.91	0.10	58,65,68,73	0
55	5MU	1x	54	21/22	0.92	0.10	54,61,65,73	0
57	5MC	2a	1400	21/22	0.92	0.14	58,64,70,74	0
57	4OC	2a	1402	22/23	0.92	0.12	48,57,64,65	0
1	PSU	2A	1911	20/21	0.92	0.10	50,55,60,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	PSU	1w	32	20/21	0.92	0.10	53,59,72,72	0
1	PSU	2A	1917	20/21	0.93	0.09	51,60,68,71	0
54	MIA	2w	37	25/30	0.93	0.10	63,70,76,77	0
57	G7M	2a	527	24/25	0.93	0.11	46,55,64,74	0
57	5MC	2a	1404	21/22	0.93	0.10	46,51,59,64	0
57	5MC	2a	1407	21/22	0.93	0.11	38,49,54,63	0
54	PSU	2w	39	20/21	0.93	0.10	65,72,79,80	0
55	PSU	1x	55	20/21	0.93	0.09	52,56,67,69	0
1	4OC	2A	1920	21/23	0.94	0.09	50,55,58,59	0
1	5MU	1A	1937	21/22	0.94	0.10	39,44,52,54	0
32	2MG	1a	1207	24/25	0.94	0.10	50,60,65,66	0
55	4SU	1x	8	20/21	0.95	0.09	48,55,66,78	0
57	UR3	2a	1498	21/22	0.95	0.11	44,50,56,60	0
57	MA6	2a	1518	24/25	0.95	0.10	42,58,62,63	0
57	MA6	2a	1519	24/25	0.95	0.12	47,54,62,63	0
54	5MU	1w	54	21/22	0.95	0.08	45,59,64,65	0
1	5MC	2A	1962	21/22	0.95	0.08	31,43,52,61	0
55	5MC	1x	32	21/22	0.96	0.09	39,46,52,57	0
1	PSU	1A	1939	20/21	0.96	0.09	36,41,45,46	0
32	MA6	1a	1519	24/25	0.96	0.09	30,35,38,42	0
1	5MC	2A	1942	21/22	0.96	0.09	39,50,56,63	0
54	MIA	1w	37	29/30	0.96	0.09	36,44,57,62	0
32	PSU	1a	516	20/21	0.96	0.07	45,49,50,51	0
32	G7M	1a	527	24/25	0.96	0.08	31,38,45,46	0
32	M2G	1a	966	25/26	0.96	0.10	39,44,51,60	0
1	OMG	2A	2251	24/25	0.97	0.07	33,37,41,47	0
1	2MA	2A	2503	23/24	0.97	0.09	26,30,33,36	0
1	PSU	2A	2605	20/21	0.97	0.08	24,33,36,37	0
1	4OC	1A	1942	21/23	0.97	0.07	29,34,37,40	0
1	5MC	1A	1964	21/22	0.97	0.07	24,31,36,43	0
32	5MC	1a	967	21/22	0.97	0.08	42,45,51,54	0
1	PSU	1A	1933	20/21	0.97	0.08	31,38,41,42	0
32	5MC	1a	1400	21/22	0.97	0.07	30,41,43,48	0
32	4OC	1a	1402	22/23	0.97	0.07	33,38,43,44	0
1	5MU	2A	1939	21/22	0.97	0.08	30,33,39,42	0
54	PSU	1w	39	20/21	0.97	0.08	44,50,59,59	0
32	5MC	1a	1404	21/22	0.97	0.07	29,33,37,40	0
32	5MC	1a	1407	21/22	0.97	0.07	27,33,37,40	0
1	5MC	1A	1984	21/22	0.98	0.05	18,26,30,37	0
1	2MU	1A	2564	21/23	0.98	0.07	16,22,26,31	0
1	PSU	1A	2617	20/21	0.98	0.06	15,18,23,24	0
1	5MU	1A	1961	21/22	0.98	0.07	15,20,24,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	UR3	1a	1498	21/22	0.98	0.06	27,33,37,39	0
58	BB9	A	6	6/7	0.98	0.05	20,21,22,23	0
58	BB9	B	9	6/7	0.98	0.07	32,35,36,37	0
1	2MU	2A	2552	21/23	0.98	0.07	32,37,41,46	0
32	MA6	1a	1518	24/25	0.98	0.07	25,33,36,39	0
58	BB9	A	9	6/7	0.99	0.05	14,16,16,19	0
1	OMG	1A	2263	24/25	0.99	0.04	15,19,22,25	0
1	2MA	1A	2515	23/24	0.99	0.05	10,14,17,22	0
58	BB9	B	6	6/7	0.99	0.05	23,30,33,35	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2j	8002	1/1	0.36	0.17	85,85,85,85	0
59	MG	1A	3445	1/1	0.43	0.31	55,55,55,55	0
59	MG	2a	3113	1/1	0.44	0.31	69,69,69,69	0
59	MG	2A	3528	1/1	0.45	0.32	81,81,81,81	0
59	MG	2A	3447	1/1	0.53	0.18	57,57,57,57	0
59	MG	1A	4115	1/1	0.55	0.23	60,60,60,60	0
59	MG	2A	3259	1/1	0.56	0.19	82,82,82,82	0
59	MG	2A	3781	1/1	0.56	0.25	63,63,63,63	0
59	MG	2y	3005	1/1	0.56	0.19	98,98,98,98	0
59	MG	1w	111	1/1	0.58	0.30	80,80,80,80	0
59	MG	2A	3075	1/1	0.59	0.22	73,73,73,73	0
59	MG	1a	3548	1/1	0.59	0.34	74,74,74,74	0
59	MG	2A	3520	1/1	0.61	0.18	79,79,79,79	0
59	MG	2v	103	1/1	0.61	0.32	70,70,70,70	0
59	MG	1y	104	1/1	0.61	0.40	80,80,80,80	0
59	MG	1A	3819	1/1	0.62	0.15	23,23,23,23	0
59	MG	1y	102	1/1	0.62	0.18	77,77,77,77	0
59	MG	2a	3221	1/1	0.62	0.30	76,76,76,76	0
59	MG	1y	105	1/1	0.63	0.17	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3619	1/1	0.63	0.24	60,60,60,60	0
59	MG	1B	229	1/1	0.64	0.16	69,69,69,69	0
59	MG	2a	3211	1/1	0.64	0.28	65,65,65,65	0
59	MG	2U	202	1/1	0.65	0.25	69,69,69,69	0
59	MG	1B	225	1/1	0.65	0.17	59,59,59,59	0
59	MG	2a	3206	1/1	0.65	0.21	74,74,74,74	0
59	MG	1A	3420	1/1	0.65	0.21	60,60,60,60	0
59	MG	1a	3482	1/1	0.67	0.28	52,52,52,52	0
59	MG	2A	3191	1/1	0.68	0.20	59,59,59,59	0
59	MG	1a	3358	1/1	0.68	0.26	73,73,73,73	0
59	MG	1A	4118	1/1	0.68	0.18	69,69,69,69	0
59	MG	2j	8001	1/1	0.69	0.15	63,63,63,63	0
59	MG	1Z	303	1/1	0.69	0.10	69,69,69,69	0
59	MG	1A	3926	1/1	0.69	0.19	22,22,22,22	0
59	MG	2w	3004	1/1	0.69	0.17	75,75,75,75	0
59	MG	2a	3180	1/1	0.69	0.24	74,74,74,74	0
59	MG	1B	220	1/1	0.70	0.24	66,66,66,66	0
59	MG	2A	3265	1/1	0.70	0.37	73,73,73,73	0
59	MG	2A	3733	1/1	0.70	0.23	71,71,71,71	0
59	MG	2A	3146	1/1	0.70	0.21	78,78,78,78	0
59	MG	1y	103	1/1	0.70	0.21	88,88,88,88	0
59	MG	2A	3774	1/1	0.71	0.23	64,64,64,64	0
59	MG	2A	3588	1/1	0.71	0.19	60,60,60,60	0
59	MG	2B	3003	1/1	0.71	0.28	71,71,71,71	0
59	MG	2A	3611	1/1	0.71	0.14	66,66,66,66	0
59	MG	2A	3307	1/1	0.71	0.29	60,60,60,60	0
59	MG	2A	3622	1/1	0.71	0.25	58,58,58,58	0
59	MG	1a	3421	1/1	0.71	0.20	64,64,64,64	0
59	MG	2y	3007	1/1	0.71	0.15	78,78,78,78	0
59	MG	1A	3405	1/1	0.72	0.12	55,55,55,55	0
59	MG	1A	3265	1/1	0.72	0.16	51,51,51,51	0
59	MG	2a	3212	1/1	0.72	0.26	73,73,73,73	0
59	MG	2A	3535	1/1	0.72	0.14	63,63,63,63	0
59	MG	1A	3395	1/1	0.72	0.20	54,54,54,54	0
59	MG	2S	8001	1/1	0.72	0.19	73,73,73,73	0
59	MG	1Y	503	1/1	0.72	0.13	69,69,69,69	0
59	MG	2w	3003	1/1	0.72	0.16	74,74,74,74	0
59	MG	2a	3037	1/1	0.72	0.30	74,74,74,74	0
59	MG	2A	3018	1/1	0.72	0.23	71,71,71,71	0
59	MG	1A	3722	1/1	0.72	0.28	72,72,72,72	0
59	MG	2a	3215	1/1	0.73	0.34	75,75,75,75	0
59	MG	2A	3689	1/1	0.73	0.14	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3725	1/1	0.73	0.17	64,64,64,64	0
59	MG	1A	3702	1/1	0.73	0.14	20,20,20,20	0
59	MG	2A	3347	1/1	0.73	0.20	57,57,57,57	0
59	MG	2a	3182	1/1	0.73	0.20	67,67,67,67	0
59	MG	2A	3253	1/1	0.73	0.20	61,61,61,61	0
59	MG	2x	103	1/1	0.73	0.30	74,74,74,74	0
59	MG	1A	4072	1/1	0.73	0.17	55,55,55,55	0
59	MG	1a	3536	1/1	0.73	0.22	58,58,58,58	0
59	MG	2a	3235	1/1	0.74	0.24	80,80,80,80	0
59	MG	2a	3133	1/1	0.74	0.16	67,67,67,67	0
59	MG	1a	3557	1/1	0.74	0.27	63,63,63,63	0
59	MG	1s	3001	1/1	0.74	0.25	62,62,62,62	0
59	MG	1A	4011	1/1	0.74	0.20	59,59,59,59	0
59	MG	1x	116	1/1	0.74	0.12	70,70,70,70	0
59	MG	1A	3902	1/1	0.74	0.14	45,45,45,45	0
59	MG	2A	3726	1/1	0.74	0.19	56,56,56,56	0
59	MG	2A	3085	1/1	0.74	0.15	62,62,62,62	0
59	MG	1a	3416	1/1	0.75	0.37	62,62,62,62	0
59	MG	1A	3578	1/1	0.75	0.18	73,73,73,73	0
59	MG	1a	3426	1/1	0.75	0.37	55,55,55,55	0
59	MG	2g	8001	1/1	0.75	0.11	74,74,74,74	0
59	MG	2A	3539	1/1	0.75	0.16	57,57,57,57	0
59	MG	2a	3118	1/1	0.75	0.50	71,71,71,71	0
59	MG	2A	3555	1/1	0.75	0.23	61,61,61,61	0
59	MG	2A	3765	1/1	0.75	0.18	70,70,70,70	0
59	MG	2A	3769	1/1	0.75	0.21	56,56,56,56	0
59	MG	2A	3247	1/1	0.75	0.30	52,52,52,52	0
59	MG	1A	3454	1/1	0.75	0.13	55,55,55,55	0
59	MG	2A	3494	1/1	0.75	0.15	58,58,58,58	0
59	MG	1a	3396	1/1	0.76	0.20	62,62,62,62	0
59	MG	1w	112	1/1	0.76	0.11	65,65,65,65	0
59	MG	2A	3531	1/1	0.76	0.17	57,57,57,57	0
59	MG	1a	3492	1/1	0.76	0.12	75,75,75,75	0
59	MG	2A	3771	1/1	0.76	0.15	67,67,67,67	0
59	MG	2A	3289	1/1	0.76	0.18	70,70,70,70	0
59	MG	2a	3220	1/1	0.76	0.31	65,65,65,65	0
59	MG	1A	3166	1/1	0.76	0.24	54,54,54,54	0
59	MG	2A	3789	1/1	0.76	0.23	66,66,66,66	0
59	MG	2A	3795	1/1	0.76	0.23	66,66,66,66	0
59	MG	2A	3836	1/1	0.76	0.28	65,65,65,65	0
59	MG	2A	3209	1/1	0.76	0.20	60,60,60,60	0
59	MG	2q	205	1/1	0.76	0.26	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3596	1/1	0.76	0.19	60,60,60,60	0
59	MG	2A	3376	1/1	0.76	0.16	54,54,54,54	0
59	MG	2A	3402	1/1	0.76	0.27	57,57,57,57	0
59	MG	2w	3007	1/1	0.76	0.23	72,72,72,72	0
59	MG	2A	3427	1/1	0.76	0.19	49,49,49,49	0
59	MG	2A	3246	1/1	0.76	0.20	67,67,67,67	0
59	MG	2A	3051	1/1	0.76	0.23	67,67,67,67	0
59	MG	2A	3658	1/1	0.77	0.17	68,68,68,68	0
59	MG	1A	4174	1/1	0.77	0.25	52,52,52,52	0
59	MG	1a	3435	1/1	0.77	0.41	76,76,76,76	0
59	MG	2A	3516	1/1	0.77	0.31	64,64,64,64	0
59	MG	2a	3210	1/1	0.77	0.21	65,65,65,65	0
59	MG	2A	3517	1/1	0.77	0.23	58,58,58,58	0
59	MG	1a	3330	1/1	0.77	0.17	58,58,58,58	0
59	MG	2A	3260	1/1	0.77	0.22	76,76,76,76	0
59	MG	1A	3798	1/1	0.77	0.31	44,44,44,44	0
59	MG	2A	3273	1/1	0.77	0.23	66,66,66,66	0
59	MG	2A	3100	1/1	0.77	0.22	65,65,65,65	0
59	MG	2A	3290	1/1	0.77	0.12	67,67,67,67	0
59	MG	2A	3558	1/1	0.77	0.14	56,56,56,56	0
59	MG	2A	3126	1/1	0.77	0.23	59,59,59,59	0
59	MG	1A	3449	1/1	0.77	0.13	54,54,54,54	0
59	MG	2v	102	1/1	0.77	0.29	69,69,69,69	0
59	MG	2A	3597	1/1	0.77	0.19	65,65,65,65	0
59	MG	1A	3292	1/1	0.77	0.20	71,71,71,71	0
59	MG	2a	3002	1/1	0.77	0.20	73,73,73,73	0
59	MG	1A	3515	1/1	0.77	0.48	71,71,71,71	0
59	MG	2a	3093	1/1	0.77	0.30	71,71,71,71	0
59	MG	1a	3572	1/1	0.77	0.15	63,63,63,63	0
59	MG	2A	3626	1/1	0.77	0.15	68,68,68,68	0
59	MG	2A	3731	1/1	0.78	0.18	72,72,72,72	0
59	MG	1A	3429	1/1	0.78	0.18	50,50,50,50	0
59	MG	2A	3760	1/1	0.78	0.27	61,61,61,61	0
59	MG	1A	3410	1/1	0.78	0.19	58,58,58,58	0
59	MG	2a	3205	1/1	0.78	0.19	60,60,60,60	0
59	MG	2A	3073	1/1	0.78	0.23	63,63,63,63	0
59	MG	1a	3578	1/1	0.78	0.14	59,59,59,59	0
59	MG	2A	3080	1/1	0.78	0.22	74,74,74,74	0
59	MG	1B	222	1/1	0.78	0.20	50,50,50,50	0
59	MG	1w	109	1/1	0.78	0.19	68,68,68,68	0
59	MG	2A	3792	1/1	0.78	0.17	63,63,63,63	0
59	MG	1A	3577	1/1	0.78	0.19	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	3801	1/1	0.78	0.09	34,34,34,34	0
59	MG	1A	4106	1/1	0.78	0.18	58,58,58,58	0
59	MG	2B	3015	1/1	0.78	0.23	64,64,64,64	0
59	MG	2F	301	1/1	0.78	0.31	70,70,70,70	0
59	MG	2I	202	1/1	0.78	0.16	71,71,71,71	0
59	MG	2R	203	1/1	0.78	0.19	52,52,52,52	0
59	MG	1A	4111	1/1	0.78	0.17	63,63,63,63	0
59	MG	2A	3243	1/1	0.78	0.20	66,66,66,66	0
59	MG	1A	3806	1/1	0.78	0.25	47,47,47,47	0
59	MG	2a	3036	1/1	0.78	0.17	71,71,71,71	0
59	MG	1A	3344	1/1	0.78	0.23	57,57,57,57	0
59	MG	1a	3553	1/1	0.78	0.29	60,60,60,60	0
59	MG	2a	3108	1/1	0.78	0.25	62,62,62,62	0
59	MG	2A	3005	1/1	0.78	0.19	62,62,62,62	0
59	MG	1A	3997	1/1	0.79	0.17	41,41,41,41	0
59	MG	2A	3325	1/1	0.79	0.30	68,68,68,68	0
59	MG	18	101	1/1	0.79	0.24	62,62,62,62	0
59	MG	1A	4145	1/1	0.79	0.12	45,45,45,45	0
59	MG	2a	3216	1/1	0.79	0.36	63,63,63,63	0
59	MG	1x	114	1/1	0.79	0.26	58,58,58,58	0
59	MG	2A	3573	1/1	0.79	0.17	64,64,64,64	0
59	MG	2a	3005	1/1	0.79	0.33	74,74,74,74	0
59	MG	2A	3587	1/1	0.79	0.14	62,62,62,62	0
59	MG	2A	3768	1/1	0.79	0.18	58,58,58,58	0
59	MG	1A	3479	1/1	0.79	0.33	69,69,69,69	0
59	MG	2a	3101	1/1	0.79	0.29	59,59,59,59	0
59	MG	1A	4063	1/1	0.79	0.12	45,45,45,45	0
59	MG	2A	3448	1/1	0.79	0.25	70,70,70,70	0
59	MG	2A	3097	1/1	0.79	0.38	74,74,74,74	0
59	MG	1A	3892	1/1	0.79	0.15	62,62,62,62	0
59	MG	1A	3645	1/1	0.79	0.30	63,63,63,63	0
59	MG	2w	3006	1/1	0.79	0.10	72,72,72,72	0
59	MG	1A	3911	1/1	0.79	0.13	62,62,62,62	0
59	MG	2a	3199	1/1	0.79	0.16	58,58,58,58	0
59	MG	2y	3002	1/1	0.79	0.14	80,80,80,80	0
59	MG	2A	3636	1/1	0.79	0.19	64,64,64,64	0
59	MG	1A	3740	1/1	0.79	0.19	49,49,49,49	0
59	MG	2A	3029	1/1	0.80	0.29	66,66,66,66	0
59	MG	2A	3105	1/1	0.80	0.12	54,54,54,54	0
59	MG	2a	3183	1/1	0.80	0.18	65,65,65,65	0
59	MG	1A	4077	1/1	0.80	0.21	59,59,59,59	0
59	MG	2A	3462	1/1	0.80	0.14	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3599	1/1	0.80	0.19	65,65,65,65	0
59	MG	1a	3543	1/1	0.80	0.17	68,68,68,68	0
59	MG	2A	3813	1/1	0.80	0.18	62,62,62,62	0
59	MG	2A	3161	1/1	0.80	0.19	67,67,67,67	0
59	MG	2A	3275	1/1	0.80	0.25	66,66,66,66	0
59	MG	1a	3425	1/1	0.80	0.23	58,58,58,58	0
59	MG	2B	3020	1/1	0.80	0.10	80,80,80,80	0
59	MG	2A	3524	1/1	0.80	0.19	51,51,51,51	0
59	MG	1a	3550	1/1	0.80	0.24	78,78,78,78	0
59	MG	2A	3663	1/1	0.80	0.14	60,60,60,60	0
59	MG	2A	3240	1/1	0.80	0.20	62,62,62,62	0
59	MG	2A	3312	1/1	0.80	0.15	55,55,55,55	0
59	MG	2A	3084	1/1	0.80	0.34	76,76,76,76	0
59	MG	2a	3017	1/1	0.80	0.25	76,76,76,76	0
59	MG	2A	3547	1/1	0.80	0.28	67,67,67,67	0
59	MG	1a	3393	1/1	0.80	0.15	70,70,70,70	0
59	MG	2a	3046	1/1	0.80	0.15	70,70,70,70	0
59	MG	2A	3742	1/1	0.80	0.16	69,69,69,69	0
59	MG	2w	3005	1/1	0.80	0.12	73,73,73,73	0
59	MG	2A	3748	1/1	0.80	0.19	55,55,55,55	0
59	MG	2a	3106	1/1	0.80	0.35	67,67,67,67	0
59	MG	2A	3022	1/1	0.80	0.14	46,46,46,46	0
59	MG	2A	3564	1/1	0.80	0.20	54,54,54,54	0
59	MG	2A	3249	1/1	0.80	0.15	62,62,62,62	0
59	MG	2A	3583	1/1	0.80	0.15	48,48,48,48	0
59	MG	1A	3907	1/1	0.81	0.18	74,74,74,74	0
59	MG	1a	3549	1/1	0.81	0.31	67,67,67,67	0
59	MG	2A	3255	1/1	0.81	0.34	65,65,65,65	0
59	MG	1A	3360	1/1	0.81	0.14	42,42,42,42	0
59	MG	2A	3758	1/1	0.81	0.33	63,63,63,63	0
59	MG	1A	3382	1/1	0.81	0.23	57,57,57,57	0
59	MG	1A	3948	1/1	0.81	0.13	69,69,69,69	0
59	MG	2a	3146	1/1	0.81	0.20	79,79,79,79	0
59	MG	1a	3567	1/1	0.81	0.10	83,83,83,83	0
59	MG	1A	3193	1/1	0.81	0.16	56,56,56,56	0
59	MG	1A	3647	1/1	0.81	0.23	56,56,56,56	0
59	MG	1a	3418	1/1	0.81	0.29	64,64,64,64	0
59	MG	2A	3775	1/1	0.81	0.15	63,63,63,63	0
59	MG	1a	3420	1/1	0.81	0.21	65,65,65,65	0
59	MG	1A	3503	1/1	0.81	0.19	53,53,53,53	0
59	MG	1A	3869	1/1	0.81	0.12	54,54,54,54	0
59	MG	2A	3793	1/1	0.81	0.20	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3346	1/1	0.81	0.22	62,62,62,62	0
59	MG	2A	3143	1/1	0.81	0.21	77,77,77,77	0
59	MG	1A	3178	1/1	0.81	0.20	61,61,61,61	0
59	MG	2A	3377	1/1	0.81	0.16	36,36,36,36	0
59	MG	2B	3008	1/1	0.81	0.22	66,66,66,66	0
59	MG	2A	3605	1/1	0.81	0.22	55,55,55,55	0
59	MG	2B	3018	1/1	0.81	0.19	62,62,62,62	0
59	MG	1B	230	1/1	0.81	0.18	59,59,59,59	0
59	MG	2B	3022	1/1	0.81	0.26	72,72,72,72	0
59	MG	2A	3413	1/1	0.81	0.12	43,43,43,43	0
59	MG	2A	3188	1/1	0.81	0.20	53,53,53,53	0
59	MG	1a	3462	1/1	0.81	0.24	72,72,72,72	0
59	MG	1E	312	1/1	0.81	0.12	56,56,56,56	0
59	MG	1a	3489	1/1	0.81	0.13	85,85,85,85	0
59	MG	2a	3003	1/1	0.81	0.25	54,54,54,54	0
59	MG	2A	3480	1/1	0.81	0.13	24,24,24,24	0
59	MG	2A	3687	1/1	0.81	0.12	39,39,39,39	0
59	MG	2a	3019	1/1	0.81	0.32	63,63,63,63	0
59	MG	1P	203	1/1	0.81	0.14	49,49,49,49	0
59	MG	1A	4095	1/1	0.81	0.26	61,61,61,61	0
59	MG	1A	3732	1/1	0.81	0.17	60,60,60,60	0
59	MG	2a	3035	1/1	0.82	0.16	57,57,57,57	0
59	MG	2A	3675	1/1	0.82	0.14	51,51,51,51	0
59	MG	1A	3745	1/1	0.82	0.19	48,48,48,48	0
59	MG	2a	3044	1/1	0.82	0.22	66,66,66,66	0
59	MG	1a	3424	1/1	0.82	0.20	66,66,66,66	0
59	MG	2a	3066	1/1	0.82	0.22	54,54,54,54	0
59	MG	2a	3081	1/1	0.82	0.19	67,67,67,67	0
59	MG	2a	3092	1/1	0.82	0.29	61,61,61,61	0
59	MG	2A	3708	1/1	0.82	0.17	29,29,29,29	0
59	MG	2a	3098	1/1	0.82	0.26	69,69,69,69	0
59	MG	2A	3193	1/1	0.82	0.23	40,40,40,40	0
59	MG	1a	3305	1/1	0.82	0.14	54,54,54,54	0
59	MG	2A	3218	1/1	0.82	0.21	63,63,63,63	0
59	MG	2A	3457	1/1	0.82	0.15	65,65,65,65	0
59	MG	2A	3223	1/1	0.82	0.11	59,59,59,59	0
59	MG	2A	3233	1/1	0.82	0.33	66,66,66,66	0
59	MG	2a	3134	1/1	0.82	0.13	80,80,80,80	0
59	MG	1B	231	1/1	0.82	0.23	63,63,63,63	0
59	MG	2a	3176	1/1	0.82	0.37	75,75,75,75	0
59	MG	2A	3044	1/1	0.82	0.15	62,62,62,62	0
59	MG	2a	3181	1/1	0.82	0.18	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1a	3336	1/1	0.82	0.28	60,60,60,60	0
59	MG	2A	3067	1/1	0.82	0.19	55,55,55,55	0
59	MG	1b	3001	1/1	0.82	0.12	74,74,74,74	0
59	MG	1l	203	1/1	0.82	0.23	64,64,64,64	0
59	MG	1A	3249	1/1	0.82	0.12	43,43,43,43	0
59	MG	2a	3209	1/1	0.82	0.19	57,57,57,57	0
59	MG	2A	3258	1/1	0.82	0.25	68,68,68,68	0
59	MG	1a	3362	1/1	0.82	0.14	51,51,51,51	0
59	MG	1a	3369	1/1	0.82	0.19	64,64,64,64	0
59	MG	2A	3262	1/1	0.82	0.17	56,56,56,56	0
59	MG	2A	3264	1/1	0.82	0.19	60,60,60,60	0
59	MG	2A	3087	1/1	0.82	0.20	53,53,53,53	0
59	MG	2A	3272	1/1	0.82	0.23	44,44,44,44	0
59	MG	2A	3089	1/1	0.82	0.21	78,78,78,78	0
59	MG	2a	3238	1/1	0.82	0.17	62,62,62,62	0
59	MG	1a	3370	1/1	0.82	0.30	67,67,67,67	0
59	MG	2A	3287	1/1	0.82	0.33	65,65,65,65	0
59	MG	1a	3508	1/1	0.82	0.15	51,51,51,51	0
59	MG	2B	3016	1/1	0.82	0.24	77,77,77,77	0
59	MG	1F	310	1/1	0.82	0.23	47,47,47,47	0
59	MG	2A	3295	1/1	0.82	0.18	58,58,58,58	0
59	MG	1A	4117	1/1	0.82	0.16	63,63,63,63	0
59	MG	1V	202	1/1	0.82	0.12	54,54,54,54	0
59	MG	1A	4019	1/1	0.82	0.36	33,33,33,33	0
59	MG	2A	3154	1/1	0.82	0.32	58,58,58,58	0
59	MG	1A	3340	1/1	0.82	0.35	46,46,46,46	0
59	MG	2A	3162	1/1	0.82	0.14	56,56,56,56	0
59	MG	2A	3651	1/1	0.82	0.13	72,72,72,72	0
59	MG	2A	3169	1/1	0.82	0.19	53,53,53,53	0
59	MG	2A	3399	1/1	0.82	0.17	55,55,55,55	0
59	MG	2A	3669	1/1	0.82	0.12	69,69,69,69	0
59	MG	1A	4141	1/1	0.83	0.14	36,36,36,36	0
59	MG	2A	3776	1/1	0.83	0.16	56,56,56,56	0
59	MG	2A	3594	1/1	0.83	0.12	64,64,64,64	0
59	MG	1O	3006	1/1	0.83	0.12	64,64,64,64	0
59	MG	1A	3904	1/1	0.83	0.13	58,58,58,58	0
59	MG	1a	3402	1/1	0.83	0.24	60,60,60,60	0
59	MG	1a	3415	1/1	0.83	0.34	56,56,56,56	0
59	MG	1A	3508	1/1	0.83	0.14	53,53,53,53	0
59	MG	2a	3163	1/1	0.83	0.11	91,91,91,91	0
59	MG	2A	3438	1/1	0.83	0.26	77,77,77,77	0
59	MG	2A	3845	1/1	0.83	0.52	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	4178	1/1	0.83	0.17	60,60,60,60	0
59	MG	1A	4179	1/1	0.83	0.20	60,60,60,60	0
59	MG	2A	3629	1/1	0.83	0.16	67,67,67,67	0
59	MG	2a	3193	1/1	0.83	0.18	70,70,70,70	0
59	MG	2A	3634	1/1	0.83	0.17	41,41,41,41	0
59	MG	1A	3656	1/1	0.83	0.20	57,57,57,57	0
59	MG	2A	3170	1/1	0.83	0.20	60,60,60,60	0
59	MG	2a	3208	1/1	0.83	0.16	63,63,63,63	0
59	MG	2A	3474	1/1	0.83	0.22	55,55,55,55	0
59	MG	1A	3378	1/1	0.83	0.29	62,62,62,62	0
59	MG	2R	202	1/1	0.83	0.24	61,61,61,61	0
59	MG	1A	3521	1/1	0.83	0.12	54,54,54,54	0
59	MG	2A	3285	1/1	0.83	0.12	52,52,52,52	0
59	MG	2A	3286	1/1	0.83	0.34	58,58,58,58	0
59	MG	20	3001	1/1	0.83	0.26	66,66,66,66	0
59	MG	25	104	1/1	0.83	0.12	61,61,61,61	0
59	MG	1A	3955	1/1	0.83	0.10	68,68,68,68	0
59	MG	1a	3345	1/1	0.83	0.35	62,62,62,62	0
59	MG	1a	3350	1/1	0.83	0.23	61,61,61,61	0
59	MG	2a	3009	1/1	0.83	0.36	67,67,67,67	0
59	MG	1A	3223	1/1	0.83	0.19	40,40,40,40	0
59	MG	1A	3489	1/1	0.83	0.12	33,33,33,33	0
59	MG	1x	112	1/1	0.83	0.15	47,47,47,47	0
59	MG	2A	3088	1/1	0.83	0.17	65,65,65,65	0
59	MG	2A	3329	1/1	0.83	0.12	59,59,59,59	0
59	MG	2A	3557	1/1	0.83	0.13	53,53,53,53	0
59	MG	1a	3363	1/1	0.83	0.27	50,50,50,50	0
59	MG	2a	3064	1/1	0.83	0.29	70,70,70,70	0
59	MG	1A	3271	1/1	0.83	0.35	35,35,35,35	0
59	MG	2A	3348	1/1	0.83	0.25	66,66,66,66	0
59	MG	2a	3082	1/1	0.83	0.24	65,65,65,65	0
59	MG	2A	3354	1/1	0.83	0.21	61,61,61,61	0
59	MG	2y	3003	1/1	0.83	0.11	83,83,83,83	0
59	MG	2A	3584	1/1	0.83	0.18	52,52,52,52	0
59	MG	2A	3366	1/1	0.83	0.35	70,70,70,70	0
59	MG	2A	3309	1/1	0.84	0.15	57,57,57,57	0
59	MG	1A	3958	1/1	0.84	0.15	45,45,45,45	0
59	MG	2A	3559	1/1	0.84	0.16	38,38,38,38	0
59	MG	2A	3313	1/1	0.84	0.25	54,54,54,54	0
59	MG	1A	3338	1/1	0.84	0.17	42,42,42,42	0
59	MG	1A	3673	1/1	0.84	0.16	33,33,33,33	0
59	MG	2a	3110	1/1	0.84	0.16	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2a	3112	1/1	0.84	0.22	51,51,51,51	0
59	MG	2A	3778	1/1	0.84	0.22	63,63,63,63	0
59	MG	2a	3116	1/1	0.84	0.26	65,65,65,65	0
59	MG	2A	3338	1/1	0.84	0.47	66,66,66,66	0
59	MG	1A	3828	1/1	0.84	0.12	46,46,46,46	0
59	MG	1A	3518	1/1	0.84	0.39	63,63,63,63	0
59	MG	2a	3138	1/1	0.84	0.11	88,88,88,88	0
59	MG	1a	3544	1/1	0.84	0.24	66,66,66,66	0
59	MG	1A	3113	1/1	0.84	0.20	37,37,37,37	0
59	MG	2a	3166	1/1	0.84	0.16	65,65,65,65	0
59	MG	1A	4074	1/1	0.84	0.17	63,63,63,63	0
59	MG	1A	3284	1/1	0.84	0.12	37,37,37,37	0
59	MG	1a	3391	1/1	0.84	0.17	55,55,55,55	0
59	MG	2A	3606	1/1	0.84	0.13	73,73,73,73	0
59	MG	2B	3007	1/1	0.84	0.17	69,69,69,69	0
59	MG	2a	3187	1/1	0.84	0.14	71,71,71,71	0
59	MG	2A	3390	1/1	0.84	0.21	60,60,60,60	0
59	MG	2a	3198	1/1	0.84	0.20	56,56,56,56	0
59	MG	1A	3138	1/1	0.84	0.23	59,59,59,59	0
59	MG	1A	3641	1/1	0.84	0.17	40,40,40,40	0
59	MG	1D	313	1/1	0.84	0.30	34,34,34,34	0
59	MG	1a	3405	1/1	0.84	0.17	47,47,47,47	0
59	MG	1A	4110	1/1	0.84	0.13	62,62,62,62	0
59	MG	2D	304	1/1	0.84	0.60	44,44,44,44	0
59	MG	1A	3910	1/1	0.84	0.16	64,64,64,64	0
59	MG	2A	3637	1/1	0.84	0.11	61,61,61,61	0
59	MG	2A	3095	1/1	0.84	0.22	60,60,60,60	0
59	MG	1A	3746	1/1	0.84	0.18	48,48,48,48	0
59	MG	2A	3662	1/1	0.84	0.20	69,69,69,69	0
59	MG	1A	3788	1/1	0.84	0.23	27,27,27,27	0
59	MG	1A	3310	1/1	0.84	0.33	40,40,40,40	0
59	MG	2a	3236	1/1	0.84	0.09	75,75,75,75	0
59	MG	28	102	1/1	0.84	0.29	58,58,58,58	0
59	MG	1A	4127	1/1	0.84	0.28	44,44,44,44	0
59	MG	2A	3128	1/1	0.84	0.17	50,50,50,50	0
59	MG	1x	103	1/1	0.84	0.17	60,60,60,60	0
59	MG	1A	4131	1/1	0.84	0.18	40,40,40,40	0
59	MG	2a	3013	1/1	0.84	0.24	68,68,68,68	0
59	MG	1A	4135	1/1	0.84	0.28	40,40,40,40	0
59	MG	2a	3018	1/1	0.84	0.20	67,67,67,67	0
59	MG	1A	4138	1/1	0.84	0.14	76,76,76,76	0
59	MG	1a	3329	1/1	0.84	0.40	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1a	3478	1/1	0.84	0.12	68,68,68,68	0
59	MG	2A	3292	1/1	0.84	0.20	66,66,66,66	0
59	MG	1A	3328	1/1	0.84	0.28	27,27,27,27	0
59	MG	2A	3749	1/1	0.84	0.18	55,55,55,55	0
59	MG	2x	104	1/1	0.84	0.21	71,71,71,71	0
59	MG	2A	3306	1/1	0.84	0.30	60,60,60,60	0
59	MG	2A	3551	1/1	0.84	0.15	60,60,60,60	0
59	MG	2y	3004	1/1	0.84	0.12	66,66,66,66	0
59	MG	2A	3761	1/1	0.84	0.18	61,61,61,61	0
59	MG	2A	3178	1/1	0.84	0.20	50,50,50,50	0
59	MG	2A	3336	1/1	0.85	0.35	57,57,57,57	0
59	MG	1A	3177	1/1	0.85	0.21	47,47,47,47	0
59	MG	2A	3173	1/1	0.85	0.19	62,62,62,62	0
59	MG	1A	3952	1/1	0.85	0.13	48,48,48,48	0
59	MG	1A	4124	1/1	0.85	0.12	56,56,56,56	0
59	MG	2A	3189	1/1	0.85	0.14	54,54,54,54	0
59	MG	2A	3365	1/1	0.85	0.15	56,56,56,56	0
59	MG	1A	3809	1/1	0.85	0.12	48,48,48,48	0
59	MG	2A	3654	1/1	0.85	0.14	62,62,62,62	0
59	MG	1A	3252	1/1	0.85	0.10	28,28,28,28	0
59	MG	2a	3053	1/1	0.85	0.19	58,58,58,58	0
59	MG	2a	3055	1/1	0.85	0.31	58,58,58,58	0
59	MG	2A	3198	1/1	0.85	0.13	71,71,71,71	0
59	MG	1A	3971	1/1	0.85	0.10	45,45,45,45	0
59	MG	2a	3073	1/1	0.85	0.26	71,71,71,71	0
59	MG	2A	3667	1/1	0.85	0.18	47,47,47,47	0
59	MG	2A	3211	1/1	0.85	0.24	61,61,61,61	0
59	MG	1A	4137	1/1	0.85	0.22	64,64,64,64	0
59	MG	1a	3436	1/1	0.85	0.32	56,56,56,56	0
59	MG	2A	3414	1/1	0.85	0.09	43,43,43,43	0
59	MG	2A	3422	1/1	0.85	0.14	67,67,67,67	0
59	MG	2A	3712	1/1	0.85	0.12	40,40,40,40	0
59	MG	2a	3107	1/1	0.85	0.28	68,68,68,68	0
59	MG	2A	3224	1/1	0.85	0.10	49,49,49,49	0
59	MG	1A	3988	1/1	0.85	0.17	62,62,62,62	0
59	MG	2A	3236	1/1	0.85	0.33	57,57,57,57	0
59	MG	1a	3466	1/1	0.85	0.34	72,72,72,72	0
59	MG	2A	3455	1/1	0.85	0.18	65,65,65,65	0
59	MG	2A	3747	1/1	0.85	0.30	61,61,61,61	0
59	MG	2a	3122	1/1	0.85	0.24	67,67,67,67	0
59	MG	2A	3242	1/1	0.85	0.20	56,56,56,56	0
59	MG	1a	3472	1/1	0.85	0.28	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3471	1/1	0.85	0.30	58,58,58,58	0
59	MG	1A	3990	1/1	0.85	0.21	46,46,46,46	0
59	MG	2a	3153	1/1	0.85	0.10	80,80,80,80	0
59	MG	2a	3158	1/1	0.85	0.13	71,71,71,71	0
59	MG	2a	3160	1/1	0.85	0.13	73,73,73,73	0
59	MG	1A	3995	1/1	0.85	0.19	49,49,49,49	0
59	MG	2A	3764	1/1	0.85	0.16	38,38,38,38	0
59	MG	2A	3486	1/1	0.85	0.23	61,61,61,61	0
59	MG	2A	3491	1/1	0.85	0.13	53,53,53,53	0
59	MG	1A	3629	1/1	0.85	0.10	17,17,17,17	0
59	MG	2A	3770	1/1	0.85	0.20	53,53,53,53	0
59	MG	1A	3850	1/1	0.85	0.16	46,46,46,46	0
59	MG	1A	3857	1/1	0.85	0.11	22,22,22,22	0
59	MG	1a	3511	1/1	0.85	0.15	46,46,46,46	0
59	MG	1A	3254	1/1	0.85	0.24	64,64,64,64	0
59	MG	2A	3526	1/1	0.85	0.14	54,54,54,54	0
59	MG	2a	3204	1/1	0.85	0.30	62,62,62,62	0
59	MG	1A	3126	1/1	0.85	0.27	29,29,29,29	0
59	MG	1A	4073	1/1	0.85	0.14	40,40,40,40	0
59	MG	2A	3791	1/1	0.85	0.13	62,62,62,62	0
59	MG	1a	3381	1/1	0.85	0.23	62,62,62,62	0
59	MG	1a	3385	1/1	0.85	0.34	57,57,57,57	0
59	MG	2A	3542	1/1	0.85	0.10	52,52,52,52	0
59	MG	2A	3543	1/1	0.85	0.12	46,46,46,46	0
59	MG	1a	3388	1/1	0.85	0.35	61,61,61,61	0
59	MG	1A	3102	1/1	0.85	0.13	46,46,46,46	0
59	MG	2a	3217	1/1	0.85	0.20	58,58,58,58	0
59	MG	2a	3219	1/1	0.85	0.14	73,73,73,73	0
59	MG	1A	3758	1/1	0.85	0.11	37,37,37,37	0
59	MG	1a	3394	1/1	0.85	0.25	61,61,61,61	0
59	MG	2a	3229	1/1	0.85	0.26	60,60,60,60	0
59	MG	1A	3773	1/1	0.85	0.09	57,57,57,57	0
59	MG	2B	3010	1/1	0.85	0.24	60,60,60,60	0
59	MG	2A	3110	1/1	0.85	0.19	60,60,60,60	0
59	MG	2A	3119	1/1	0.85	0.21	61,61,61,61	0
59	MG	2A	3566	1/1	0.85	0.12	71,71,71,71	0
59	MG	1A	3909	1/1	0.85	0.19	58,58,58,58	0
59	MG	2A	3291	1/1	0.85	0.31	74,74,74,74	0
59	MG	2p	3001	1/1	0.85	0.21	63,63,63,63	0
59	MG	2q	201	1/1	0.85	0.16	50,50,50,50	0
59	MG	1A	3087	1/1	0.85	0.22	56,56,56,56	0
59	MG	2A	3585	1/1	0.85	0.17	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2O	8001	1/1	0.85	0.15	53,53,53,53	0
59	MG	2Q	3004	1/1	0.85	0.16	45,45,45,45	0
59	MG	1a	3409	1/1	0.85	0.15	74,74,74,74	0
59	MG	1a	3410	1/1	0.85	0.21	59,59,59,59	0
59	MG	2A	3150	1/1	0.85	0.14	42,42,42,42	0
59	MG	1v	3001	1/1	0.85	0.14	60,60,60,60	0
59	MG	1a	3414	1/1	0.85	0.32	57,57,57,57	0
59	MG	1A	3526	1/1	0.85	0.23	59,59,59,59	0
59	MG	2A	3315	1/1	0.85	0.34	63,63,63,63	0
59	MG	2A	3168	1/1	0.85	0.14	59,59,59,59	0
59	MG	1A	3678	1/1	0.85	0.22	57,57,57,57	0
59	MG	2A	3614	1/1	0.85	0.15	63,63,63,63	0
59	MG	2a	3006	1/1	0.85	0.50	76,76,76,76	0
59	MG	1A	3132	1/1	0.86	0.16	30,30,30,30	0
59	MG	2A	3234	1/1	0.86	0.32	64,64,64,64	0
59	MG	1A	4125	1/1	0.86	0.19	40,40,40,40	0
59	MG	2a	3059	1/1	0.86	0.13	53,53,53,53	0
59	MG	1A	3487	1/1	0.86	0.12	55,55,55,55	0
59	MG	2a	3065	1/1	0.86	0.19	58,58,58,58	0
59	MG	2A	3458	1/1	0.86	0.10	53,53,53,53	0
59	MG	1A	3652	1/1	0.86	0.13	35,35,35,35	0
59	MG	2a	3074	1/1	0.86	0.14	64,64,64,64	0
59	MG	2a	3080	1/1	0.86	0.19	58,58,58,58	0
59	MG	1A	3289	1/1	0.86	0.35	29,29,29,29	0
59	MG	1a	3325	1/1	0.86	0.18	50,50,50,50	0
59	MG	2a	3087	1/1	0.86	0.29	65,65,65,65	0
59	MG	2a	3088	1/1	0.86	0.21	61,61,61,61	0
59	MG	2a	3089	1/1	0.86	0.25	67,67,67,67	0
59	MG	1a	3439	1/1	0.86	0.16	63,63,63,63	0
59	MG	1a	3453	1/1	0.86	0.13	64,64,64,64	0
59	MG	2A	3250	1/1	0.86	0.13	56,56,56,56	0
59	MG	2A	3755	1/1	0.86	0.25	64,64,64,64	0
59	MG	2a	3105	1/1	0.86	0.19	64,64,64,64	0
59	MG	2A	3492	1/1	0.86	0.11	44,44,44,44	0
59	MG	1a	3326	1/1	0.86	0.34	56,56,56,56	0
59	MG	2A	3079	1/1	0.86	0.23	60,60,60,60	0
59	MG	1A	3062	1/1	0.86	0.24	47,47,47,47	0
59	MG	1A	3861	1/1	0.86	0.10	39,39,39,39	0
59	MG	1a	3335	1/1	0.86	0.18	57,57,57,57	0
59	MG	1A	3413	1/1	0.86	0.25	49,49,49,49	0
59	MG	1A	4036	1/1	0.86	0.10	46,46,46,46	0
59	MG	1A	3103	1/1	0.86	0.13	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2a	3131	1/1	0.86	0.12	77,77,77,77	0
59	MG	2A	3271	1/1	0.86	0.16	71,71,71,71	0
59	MG	1a	3504	1/1	0.86	0.12	57,57,57,57	0
59	MG	1a	3354	1/1	0.86	0.14	66,66,66,66	0
59	MG	1A	3377	1/1	0.86	0.12	62,62,62,62	0
59	MG	1a	3361	1/1	0.86	0.19	68,68,68,68	0
59	MG	2A	3783	1/1	0.86	0.11	73,73,73,73	0
59	MG	2A	3788	1/1	0.86	0.15	57,57,57,57	0
59	MG	1A	3440	1/1	0.86	0.18	70,70,70,70	0
59	MG	1A	4187	1/1	0.86	0.20	47,47,47,47	0
59	MG	2A	3556	1/1	0.86	0.13	60,60,60,60	0
59	MG	2a	3179	1/1	0.86	0.20	64,64,64,64	0
59	MG	2A	3288	1/1	0.86	0.10	67,67,67,67	0
59	MG	2A	3794	1/1	0.86	0.15	61,61,61,61	0
59	MG	1A	4188	1/1	0.86	0.27	55,55,55,55	0
59	MG	2A	3798	1/1	0.86	0.17	57,57,57,57	0
59	MG	2a	3186	1/1	0.86	0.41	69,69,69,69	0
59	MG	2A	3806	1/1	0.86	0.12	54,54,54,54	0
59	MG	2A	3809	1/1	0.86	0.12	55,55,55,55	0
59	MG	1B	204	1/1	0.86	0.28	48,48,48,48	0
59	MG	1a	3372	1/1	0.86	0.22	64,64,64,64	0
59	MG	2A	3145	1/1	0.86	0.22	62,62,62,62	0
59	MG	1a	3374	1/1	0.86	0.22	53,53,53,53	0
59	MG	2A	3582	1/1	0.86	0.14	29,29,29,29	0
59	MG	2A	3297	1/1	0.86	0.19	52,52,52,52	0
59	MG	1a	3380	1/1	0.86	0.17	48,48,48,48	0
59	MG	2B	3011	1/1	0.86	0.21	62,62,62,62	0
59	MG	2A	3151	1/1	0.86	0.19	74,74,74,74	0
59	MG	1B	217	1/1	0.86	0.12	41,41,41,41	0
59	MG	2A	3159	1/1	0.86	0.27	62,62,62,62	0
59	MG	2B	3019	1/1	0.86	0.15	61,61,61,61	0
59	MG	1A	3314	1/1	0.86	0.15	47,47,47,47	0
59	MG	1A	3556	1/1	0.86	0.14	30,30,30,30	0
59	MG	2A	3324	1/1	0.86	0.24	53,53,53,53	0
59	MG	2A	3165	1/1	0.86	0.16	61,61,61,61	0
59	MG	2a	3223	1/1	0.86	0.22	69,69,69,69	0
59	MG	1A	4082	1/1	0.86	0.11	50,50,50,50	0
59	MG	1A	3561	1/1	0.86	0.15	48,48,48,48	0
59	MG	1A	3129	1/1	0.86	0.16	36,36,36,36	0
59	MG	2A	3613	1/1	0.86	0.14	36,36,36,36	0
59	MG	2f	3002	1/1	0.86	0.21	69,69,69,69	0
59	MG	1A	3394	1/1	0.86	0.14	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1a	3401	1/1	0.86	0.11	48,48,48,48	0
59	MG	2U	204	1/1	0.86	0.27	49,49,49,49	0
59	MG	2A	3179	1/1	0.86	0.13	46,46,46,46	0
59	MG	2A	3625	1/1	0.86	0.21	67,67,67,67	0
59	MG	1B	232	1/1	0.86	0.11	67,67,67,67	0
59	MG	1a	3404	1/1	0.86	0.43	65,65,65,65	0
59	MG	1A	3617	1/1	0.86	0.11	47,47,47,47	0
59	MG	1A	4112	1/1	0.86	0.14	56,56,56,56	0
59	MG	1A	3461	1/1	0.86	0.12	58,58,58,58	0
59	MG	1A	3638	1/1	0.86	0.11	28,28,28,28	0
59	MG	1A	3468	1/1	0.86	0.34	41,41,41,41	0
59	MG	2A	3216	1/1	0.86	0.16	47,47,47,47	0
59	MG	1P	204	1/1	0.86	0.21	41,41,41,41	0
59	MG	2x	102	1/1	0.86	0.18	64,64,64,64	0
59	MG	1R	203	1/1	0.86	0.16	33,33,33,33	0
59	MG	2a	3027	1/1	0.86	0.35	63,63,63,63	0
59	MG	2y	3001	1/1	0.86	0.15	65,65,65,65	0
59	MG	1S	3001	1/1	0.86	0.30	39,39,39,39	0
59	MG	2A	3225	1/1	0.86	0.18	53,53,53,53	0
59	MG	2A	3428	1/1	0.86	0.16	63,63,63,63	0
59	MG	2A	3231	1/1	0.86	0.11	75,75,75,75	0
59	MG	2a	3045	1/1	0.86	0.23	58,58,58,58	0
59	MG	16	104	1/1	0.87	0.23	43,43,43,43	0
59	MG	2A	3745	1/1	0.87	0.14	48,48,48,48	0
59	MG	1A	3303	1/1	0.87	0.20	50,50,50,50	0
59	MG	2A	3060	1/1	0.87	0.23	63,63,63,63	0
59	MG	2A	3473	1/1	0.87	0.20	63,63,63,63	0
59	MG	1A	3573	1/1	0.87	0.10	32,32,32,32	0
59	MG	2A	3757	1/1	0.87	0.18	54,54,54,54	0
59	MG	1a	3427	1/1	0.87	0.15	64,64,64,64	0
59	MG	1a	3315	1/1	0.87	0.15	48,48,48,48	0
59	MG	2a	3091	1/1	0.87	0.17	77,77,77,77	0
59	MG	1a	3322	1/1	0.87	0.28	51,51,51,51	0
59	MG	1A	3388	1/1	0.87	0.19	47,47,47,47	0
59	MG	2A	3083	1/1	0.87	0.26	61,61,61,61	0
59	MG	1A	3767	1/1	0.87	0.13	53,53,53,53	0
59	MG	1A	3033	1/1	0.87	0.27	57,57,57,57	0
59	MG	1A	3775	1/1	0.87	0.17	46,46,46,46	0
59	MG	1a	3331	1/1	0.87	0.41	60,60,60,60	0
59	MG	1A	3973	1/1	0.87	0.11	28,28,28,28	0
59	MG	1A	3986	1/1	0.87	0.12	61,61,61,61	0
59	MG	1A	3612	1/1	0.87	0.12	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3274	1/1	0.87	0.30	59,59,59,59	0
59	MG	2A	3779	1/1	0.87	0.13	67,67,67,67	0
59	MG	2A	3538	1/1	0.87	0.18	47,47,47,47	0
59	MG	2A	3782	1/1	0.87	0.11	60,60,60,60	0
59	MG	1a	3490	1/1	0.87	0.13	57,57,57,57	0
59	MG	1A	3226	1/1	0.87	0.28	56,56,56,56	0
59	MG	1A	3800	1/1	0.87	0.15	30,30,30,30	0
59	MG	1a	3505	1/1	0.87	0.11	56,56,56,56	0
59	MG	1A	3628	1/1	0.87	0.08	21,21,21,21	0
59	MG	2A	3553	1/1	0.87	0.20	63,63,63,63	0
59	MG	1A	3485	1/1	0.87	0.26	41,41,41,41	0
59	MG	1A	4012	1/1	0.87	0.21	53,53,53,53	0
59	MG	1A	4205	1/1	0.87	0.16	45,45,45,45	0
59	MG	2A	3801	1/1	0.87	0.13	55,55,55,55	0
59	MG	1a	3364	1/1	0.87	0.28	53,53,53,53	0
59	MG	1A	3269	1/1	0.87	0.33	27,27,27,27	0
59	MG	1B	212	1/1	0.87	0.12	42,42,42,42	0
59	MG	2A	3565	1/1	0.87	0.15	49,49,49,49	0
59	MG	2A	3837	1/1	0.87	0.16	61,61,61,61	0
59	MG	2A	3298	1/1	0.87	0.25	41,41,41,41	0
59	MG	2A	3300	1/1	0.87	0.26	46,46,46,46	0
59	MG	2A	3574	1/1	0.87	0.20	56,56,56,56	0
59	MG	2a	3188	1/1	0.87	0.12	64,64,64,64	0
59	MG	1A	3810	1/1	0.87	0.11	38,38,38,38	0
59	MG	1A	4045	1/1	0.87	0.12	53,53,53,53	0
59	MG	1B	221	1/1	0.87	0.19	52,52,52,52	0
59	MG	2a	3202	1/1	0.87	0.23	67,67,67,67	0
59	MG	1a	3562	1/1	0.87	0.22	63,63,63,63	0
59	MG	1A	4057	1/1	0.87	0.14	50,50,50,50	0
59	MG	1a	3384	1/1	0.87	0.20	46,46,46,46	0
59	MG	1A	3232	1/1	0.87	0.14	51,51,51,51	0
59	MG	1A	3644	1/1	0.87	0.09	56,56,56,56	0
59	MG	2A	3327	1/1	0.87	0.26	62,62,62,62	0
59	MG	2A	3172	1/1	0.87	0.17	54,54,54,54	0
59	MG	2E	303	1/1	0.87	0.28	53,53,53,53	0
59	MG	1A	3835	1/1	0.87	0.14	51,51,51,51	0
59	MG	2F	303	1/1	0.87	0.47	54,54,54,54	0
59	MG	2G	3001	1/1	0.87	0.25	64,64,64,64	0
59	MG	1A	3277	1/1	0.87	0.13	48,48,48,48	0
59	MG	2A	3344	1/1	0.87	0.19	56,56,56,56	0
59	MG	1A	4076	1/1	0.87	0.09	43,43,43,43	0
59	MG	1w	104	1/1	0.87	0.14	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1w	108	1/1	0.87	0.19	59,59,59,59	0
59	MG	1B	233	1/1	0.87	0.16	64,64,64,64	0
59	MG	1A	3237	1/1	0.87	0.16	52,52,52,52	0
59	MG	2Z	8001	1/1	0.87	0.22	68,68,68,68	0
59	MG	1A	3350	1/1	0.87	0.17	57,57,57,57	0
59	MG	2A	3628	1/1	0.87	0.13	43,43,43,43	0
59	MG	2A	3367	1/1	0.87	0.17	52,52,52,52	0
59	MG	2A	3368	1/1	0.87	0.14	63,63,63,63	0
59	MG	1A	4085	1/1	0.87	0.16	64,64,64,64	0
59	MG	1x	111	1/1	0.87	0.20	65,65,65,65	0
59	MG	2A	3639	1/1	0.87	0.10	47,47,47,47	0
59	MG	2A	3380	1/1	0.87	0.12	41,41,41,41	0
59	MG	2t	3001	1/1	0.87	0.17	53,53,53,53	0
59	MG	2A	3652	1/1	0.87	0.14	60,60,60,60	0
59	MG	2A	3215	1/1	0.87	0.13	49,49,49,49	0
59	MG	2w	3002	1/1	0.87	0.19	73,73,73,73	0
59	MG	1A	3516	1/1	0.87	0.20	49,49,49,49	0
59	MG	1a	3406	1/1	0.87	0.22	50,50,50,50	0
59	MG	1A	3671	1/1	0.87	0.14	57,57,57,57	0
59	MG	1A	3045	1/1	0.87	0.13	53,53,53,53	0
59	MG	1a	3412	1/1	0.87	0.22	51,51,51,51	0
59	MG	2x	101	1/1	0.87	0.18	72,72,72,72	0
59	MG	1A	3441	1/1	0.87	0.10	62,62,62,62	0
59	MG	1A	3001	1/1	0.87	0.11	35,35,35,35	0
59	MG	1A	3533	1/1	0.87	0.13	51,51,51,51	0
59	MG	2A	3441	1/1	0.87	0.11	29,29,29,29	0
59	MG	1A	3300	1/1	0.87	0.12	42,42,42,42	0
59	MG	2A	3239	1/1	0.87	0.21	61,61,61,61	0
59	MG	2A	3452	1/1	0.87	0.23	56,56,56,56	0
59	MG	1A	3560	1/1	0.87	0.12	45,45,45,45	0
59	MG	1l	101	1/1	0.87	0.16	45,45,45,45	0
59	MG	1a	3487	1/1	0.88	0.21	62,62,62,62	0
59	MG	2A	3099	1/1	0.88	0.15	51,51,51,51	0
59	MG	1A	3201	1/1	0.88	0.17	55,55,55,55	0
59	MG	1A	3824	1/1	0.88	0.08	35,35,35,35	0
59	MG	1A	4003	1/1	0.88	0.13	54,54,54,54	0
59	MG	2A	3600	1/1	0.88	0.15	55,55,55,55	0
59	MG	2A	3601	1/1	0.88	0.15	60,60,60,60	0
59	MG	2A	3602	1/1	0.88	0.12	51,51,51,51	0
59	MG	1a	3493	1/1	0.88	0.17	51,51,51,51	0
59	MG	2a	3014	1/1	0.88	0.19	57,57,57,57	0
59	MG	2A	3122	1/1	0.88	0.38	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	4005	1/1	0.88	0.18	52,52,52,52	0
59	MG	2A	3127	1/1	0.88	0.37	57,57,57,57	0
59	MG	1a	3359	1/1	0.88	0.21	66,66,66,66	0
59	MG	2a	3030	1/1	0.88	0.21	60,60,60,60	0
59	MG	2a	3031	1/1	0.88	0.19	57,57,57,57	0
59	MG	2a	3034	1/1	0.88	0.21	53,53,53,53	0
59	MG	2A	3318	1/1	0.88	0.27	53,53,53,53	0
59	MG	2A	3320	1/1	0.88	0.25	59,59,59,59	0
59	MG	1A	3699	1/1	0.88	0.11	37,37,37,37	0
59	MG	1A	4190	1/1	0.88	0.30	42,42,42,42	0
59	MG	1a	3535	1/1	0.88	0.16	59,59,59,59	0
59	MG	1A	3833	1/1	0.88	0.08	36,36,36,36	0
59	MG	2A	3332	1/1	0.88	0.43	64,64,64,64	0
59	MG	1A	3081	1/1	0.88	0.23	51,51,51,51	0
59	MG	2A	3153	1/1	0.88	0.15	57,57,57,57	0
59	MG	2A	3340	1/1	0.88	0.28	59,59,59,59	0
59	MG	1a	3366	1/1	0.88	0.17	57,57,57,57	0
59	MG	1a	3367	1/1	0.88	0.25	53,53,53,53	0
59	MG	1A	3843	1/1	0.88	0.14	19,19,19,19	0
59	MG	1B	214	1/1	0.88	0.09	55,55,55,55	0
59	MG	2A	3350	1/1	0.88	0.30	57,57,57,57	0
59	MG	2A	3352	1/1	0.88	0.09	64,64,64,64	0
59	MG	1A	3844	1/1	0.88	0.17	35,35,35,35	0
59	MG	2a	3085	1/1	0.88	0.24	69,69,69,69	0
59	MG	2A	3361	1/1	0.88	0.10	66,66,66,66	0
59	MG	2A	3671	1/1	0.88	0.18	66,66,66,66	0
59	MG	2A	3362	1/1	0.88	0.09	57,57,57,57	0
59	MG	2A	3686	1/1	0.88	0.09	48,48,48,48	0
59	MG	1A	4048	1/1	0.88	0.07	33,33,33,33	0
59	MG	1a	3559	1/1	0.88	0.19	69,69,69,69	0
59	MG	2A	3690	1/1	0.88	0.15	37,37,37,37	0
59	MG	1a	3561	1/1	0.88	0.14	62,62,62,62	0
59	MG	2a	3102	1/1	0.88	0.16	66,66,66,66	0
59	MG	2A	3171	1/1	0.88	0.10	44,44,44,44	0
59	MG	2A	3718	1/1	0.88	0.11	52,52,52,52	0
59	MG	2A	3722	1/1	0.88	0.12	72,72,72,72	0
59	MG	1A	4052	1/1	0.88	0.17	60,60,60,60	0
59	MG	1a	3565	1/1	0.88	0.16	35,35,35,35	0
59	MG	2a	3111	1/1	0.88	0.26	54,54,54,54	0
59	MG	2A	3174	1/1	0.88	0.11	60,60,60,60	0
59	MG	1A	3846	1/1	0.88	0.14	57,57,57,57	0
59	MG	2a	3114	1/1	0.88	0.37	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3739	1/1	0.88	0.19	49,49,49,49	0
59	MG	1A	3849	1/1	0.88	0.14	54,54,54,54	0
59	MG	2A	3183	1/1	0.88	0.26	52,52,52,52	0
59	MG	2A	3185	1/1	0.88	0.12	53,53,53,53	0
59	MG	1A	3424	1/1	0.88	0.18	53,53,53,53	0
59	MG	1A	3730	1/1	0.88	0.09	33,33,33,33	0
59	MG	2a	3135	1/1	0.88	0.16	60,60,60,60	0
59	MG	2A	3751	1/1	0.88	0.19	50,50,50,50	0
59	MG	2A	3752	1/1	0.88	0.10	61,61,61,61	0
59	MG	1f	3003	1/1	0.88	0.30	57,57,57,57	0
59	MG	1l	202	1/1	0.88	0.11	82,82,82,82	0
59	MG	1A	3321	1/1	0.88	0.12	49,49,49,49	0
59	MG	2A	3205	1/1	0.88	0.37	73,73,73,73	0
59	MG	2A	3207	1/1	0.88	0.09	56,56,56,56	0
59	MG	2a	3174	1/1	0.88	0.15	74,74,74,74	0
59	MG	2A	3208	1/1	0.88	0.13	71,71,71,71	0
59	MG	1A	4075	1/1	0.88	0.14	21,21,21,21	0
59	MG	2A	3210	1/1	0.88	0.17	62,62,62,62	0
59	MG	1A	3504	1/1	0.88	0.22	53,53,53,53	0
59	MG	1B	236	1/1	0.88	0.12	57,57,57,57	0
59	MG	1a	3399	1/1	0.88	0.17	42,42,42,42	0
59	MG	1D	310	1/1	0.88	0.16	43,43,43,43	0
59	MG	1w	110	1/1	0.88	0.13	81,81,81,81	0
59	MG	1D	312	1/1	0.88	0.10	49,49,49,49	0
59	MG	2A	3477	1/1	0.88	0.21	57,57,57,57	0
59	MG	2a	3196	1/1	0.88	0.14	63,63,63,63	0
59	MG	1A	3889	1/1	0.88	0.07	22,22,22,22	0
59	MG	2A	3481	1/1	0.88	0.11	37,37,37,37	0
59	MG	1A	3436	1/1	0.88	0.35	34,34,34,34	0
59	MG	2A	3487	1/1	0.88	0.13	48,48,48,48	0
59	MG	2A	3786	1/1	0.88	0.21	55,55,55,55	0
59	MG	1A	3896	1/1	0.88	0.15	54,54,54,54	0
59	MG	1A	4091	1/1	0.88	0.16	42,42,42,42	0
59	MG	1A	3021	1/1	0.88	0.24	67,67,67,67	0
59	MG	2A	3507	1/1	0.88	0.13	33,33,33,33	0
59	MG	2A	3510	1/1	0.88	0.10	58,58,58,58	0
59	MG	1A	3291	1/1	0.88	0.11	43,43,43,43	0
59	MG	1A	4109	1/1	0.88	0.12	42,42,42,42	0
59	MG	2A	3796	1/1	0.88	0.15	70,70,70,70	0
59	MG	1A	3392	1/1	0.88	0.11	52,52,52,52	0
59	MG	2A	3799	1/1	0.88	0.17	60,60,60,60	0
59	MG	1A	3642	1/1	0.88	0.13	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	3774	1/1	0.88	0.10	52,52,52,52	0
59	MG	1A	3227	1/1	0.88	0.18	50,50,50,50	0
59	MG	2a	3226	1/1	0.88	0.23	59,59,59,59	0
59	MG	10	106	1/1	0.88	0.24	63,63,63,63	0
59	MG	2A	3828	1/1	0.88	0.12	60,60,60,60	0
59	MG	1A	3778	1/1	0.88	0.12	38,38,38,38	0
59	MG	1A	3783	1/1	0.88	0.12	64,64,64,64	0
59	MG	2A	3032	1/1	0.88	0.28	54,54,54,54	0
59	MG	2A	3033	1/1	0.88	0.17	58,58,58,58	0
59	MG	2B	3006	1/1	0.88	0.27	66,66,66,66	0
59	MG	2A	3041	1/1	0.88	0.29	60,60,60,60	0
59	MG	2A	3545	1/1	0.88	0.13	61,61,61,61	0
59	MG	1A	4122	1/1	0.88	0.12	44,44,44,44	0
59	MG	2A	3550	1/1	0.88	0.10	56,56,56,56	0
59	MG	2q	203	1/1	0.88	0.19	53,53,53,53	0
59	MG	1A	3949	1/1	0.88	0.12	52,52,52,52	0
59	MG	1a	3429	1/1	0.88	0.24	61,61,61,61	0
59	MG	1A	3074	1/1	0.88	0.40	28,28,28,28	0
59	MG	2A	3068	1/1	0.88	0.16	52,52,52,52	0
59	MG	2A	3069	1/1	0.88	0.27	45,45,45,45	0
59	MG	1A	3794	1/1	0.88	0.10	57,57,57,57	0
59	MG	1A	3399	1/1	0.88	0.30	67,67,67,67	0
59	MG	2E	301	1/1	0.88	0.15	66,66,66,66	0
59	MG	1a	3441	1/1	0.88	0.11	53,53,53,53	0
59	MG	1A	3462	1/1	0.88	0.10	50,50,50,50	0
59	MG	1a	3459	1/1	0.88	0.11	66,66,66,66	0
59	MG	2A	3568	1/1	0.88	0.13	74,74,74,74	0
59	MG	2A	3571	1/1	0.88	0.13	68,68,68,68	0
59	MG	1A	3349	1/1	0.88	0.09	49,49,49,49	0
59	MG	1A	3155	1/1	0.88	0.16	61,61,61,61	0
59	MG	1A	3569	1/1	0.88	0.13	42,42,42,42	0
59	MG	1a	3476	1/1	0.88	0.09	55,55,55,55	0
59	MG	1A	3677	1/1	0.88	0.10	10,10,10,10	0
59	MG	1A	4162	1/1	0.88	0.14	54,54,54,54	0
59	MG	2A	3293	1/1	0.88	0.20	55,55,55,55	0
59	MG	2A	3640	1/1	0.89	0.13	49,49,49,49	0
59	MG	2a	3015	1/1	0.89	0.12	66,66,66,66	0
59	MG	2A	3641	1/1	0.89	0.16	75,75,75,75	0
59	MG	1A	3426	1/1	0.89	0.15	46,46,46,46	0
59	MG	1w	102	1/1	0.89	0.17	63,63,63,63	0
59	MG	2a	3025	1/1	0.89	0.28	52,52,52,52	0
59	MG	1A	4086	1/1	0.89	0.10	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2a	3028	1/1	0.89	0.22	64,64,64,64	0
59	MG	1A	3769	1/1	0.89	0.18	48,48,48,48	0
59	MG	1F	302	1/1	0.89	0.20	50,50,50,50	0
59	MG	2A	3199	1/1	0.89	0.13	54,54,54,54	0
59	MG	2A	3204	1/1	0.89	0.24	58,58,58,58	0
59	MG	2A	3410	1/1	0.89	0.10	25,25,25,25	0
59	MG	1A	3367	1/1	0.89	0.14	59,59,59,59	0
59	MG	2a	3038	1/1	0.89	0.19	78,78,78,78	0
59	MG	2a	3042	1/1	0.89	0.08	70,70,70,70	0
59	MG	2a	3043	1/1	0.89	0.26	66,66,66,66	0
59	MG	2A	3674	1/1	0.89	0.30	61,61,61,61	0
59	MG	1a	3407	1/1	0.89	0.12	36,36,36,36	0
59	MG	1O	3003	1/1	0.89	0.15	54,54,54,54	0
59	MG	1A	3433	1/1	0.89	0.15	56,56,56,56	0
59	MG	1x	109	1/1	0.89	0.15	68,68,68,68	0
59	MG	2a	3058	1/1	0.89	0.24	70,70,70,70	0
59	MG	2A	3434	1/1	0.89	0.09	24,24,24,24	0
59	MG	2A	3702	1/1	0.89	0.10	64,64,64,64	0
59	MG	2A	3706	1/1	0.89	0.09	70,70,70,70	0
59	MG	2A	3436	1/1	0.89	0.09	28,28,28,28	0
59	MG	1A	3375	1/1	0.89	0.13	29,29,29,29	0
59	MG	1A	3308	1/1	0.89	0.17	53,53,53,53	0
59	MG	2a	3079	1/1	0.89	0.29	67,67,67,67	0
59	MG	1Q	203	1/1	0.89	0.17	51,51,51,51	0
59	MG	1Q	204	1/1	0.89	0.14	46,46,46,46	0
59	MG	1A	3918	1/1	0.89	0.09	27,27,27,27	0
59	MG	1A	3921	1/1	0.89	0.11	37,37,37,37	0
59	MG	1A	3924	1/1	0.89	0.14	22,22,22,22	0
59	MG	2A	3737	1/1	0.89	0.12	47,47,47,47	0
59	MG	1A	3188	1/1	0.89	0.23	37,37,37,37	0
59	MG	1A	3930	1/1	0.89	0.14	71,71,71,71	0
59	MG	2A	3468	1/1	0.89	0.10	32,32,32,32	0
59	MG	2A	3470	1/1	0.89	0.17	53,53,53,53	0
59	MG	2a	3095	1/1	0.89	0.10	52,52,52,52	0
59	MG	2a	3097	1/1	0.89	0.17	48,48,48,48	0
59	MG	1A	3787	1/1	0.89	0.13	49,49,49,49	0
59	MG	1A	3276	1/1	0.89	0.12	52,52,52,52	0
59	MG	2A	3023	1/1	0.89	0.08	35,35,35,35	0
59	MG	1a	3428	1/1	0.89	0.24	56,56,56,56	0
59	MG	1A	3106	1/1	0.89	0.23	33,33,33,33	0
59	MG	17	101	1/1	0.89	0.14	49,49,49,49	0
59	MG	1A	4126	1/1	0.89	0.13	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2a	3109	1/1	0.89	0.25	55,55,55,55	0
59	MG	1A	3649	1/1	0.89	0.10	55,55,55,55	0
59	MG	1a	3314	1/1	0.89	0.10	53,53,53,53	0
59	MG	1A	3544	1/1	0.89	0.09	44,44,44,44	0
59	MG	1A	4134	1/1	0.89	0.14	52,52,52,52	0
59	MG	1A	3654	1/1	0.89	0.13	54,54,54,54	0
59	MG	1A	3655	1/1	0.89	0.15	42,42,42,42	0
59	MG	1a	3327	1/1	0.89	0.22	60,60,60,60	0
59	MG	2a	3119	1/1	0.89	0.22	68,68,68,68	0
59	MG	1A	3982	1/1	0.89	0.12	57,57,57,57	0
59	MG	2A	3773	1/1	0.89	0.10	40,40,40,40	0
59	MG	1a	3477	1/1	0.89	0.16	67,67,67,67	0
59	MG	1A	3545	1/1	0.89	0.12	21,21,21,21	0
59	MG	2A	3082	1/1	0.89	0.14	44,44,44,44	0
59	MG	2A	3527	1/1	0.89	0.15	65,65,65,65	0
59	MG	1A	3657	1/1	0.89	0.17	67,67,67,67	0
59	MG	1A	4155	1/1	0.89	0.11	54,54,54,54	0
59	MG	2A	3533	1/1	0.89	0.12	55,55,55,55	0
59	MG	1A	3812	1/1	0.89	0.16	57,57,57,57	0
59	MG	1A	3109	1/1	0.89	0.19	46,46,46,46	0
59	MG	1a	3346	1/1	0.89	0.29	57,57,57,57	0
59	MG	2a	3170	1/1	0.89	0.18	49,49,49,49	0
59	MG	1A	3331	1/1	0.89	0.11	41,41,41,41	0
59	MG	1a	3495	1/1	0.89	0.14	63,63,63,63	0
59	MG	1A	3286	1/1	0.89	0.17	64,64,64,64	0
59	MG	2A	3546	1/1	0.89	0.16	60,60,60,60	0
59	MG	1A	3110	1/1	0.89	0.08	29,29,29,29	0
59	MG	1A	3690	1/1	0.89	0.13	14,14,14,14	0
59	MG	1A	3044	1/1	0.89	0.12	45,45,45,45	0
59	MG	2a	3185	1/1	0.89	0.09	64,64,64,64	0
59	MG	1a	3525	1/1	0.89	0.11	76,76,76,76	0
59	MG	1A	3255	1/1	0.89	0.17	54,54,54,54	0
59	MG	1A	3711	1/1	0.89	0.11	34,34,34,34	0
59	MG	1a	3542	1/1	0.89	0.12	53,53,53,53	0
59	MG	2a	3195	1/1	0.89	0.14	54,54,54,54	0
59	MG	2A	3808	1/1	0.89	0.12	54,54,54,54	0
59	MG	1A	4037	1/1	0.89	0.11	40,40,40,40	0
59	MG	1a	3365	1/1	0.89	0.14	62,62,62,62	0
59	MG	2A	3814	1/1	0.89	0.10	44,44,44,44	0
59	MG	2a	3203	1/1	0.89	0.18	57,57,57,57	0
59	MG	2A	3816	1/1	0.89	0.13	43,43,43,43	0
59	MG	2A	3299	1/1	0.89	0.24	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3829	1/1	0.89	0.17	60,60,60,60	0
59	MG	2A	3831	1/1	0.89	0.34	39,39,39,39	0
59	MG	2A	3140	1/1	0.89	0.35	72,72,72,72	0
59	MG	2A	3303	1/1	0.89	0.13	50,50,50,50	0
59	MG	2A	3844	1/1	0.89	0.27	48,48,48,48	0
59	MG	1B	213	1/1	0.89	0.16	43,43,43,43	0
59	MG	2a	3214	1/1	0.89	0.26	68,68,68,68	0
59	MG	2A	3569	1/1	0.89	0.20	59,59,59,59	0
59	MG	1A	3187	1/1	0.89	0.09	39,39,39,39	0
59	MG	1A	3584	1/1	0.89	0.11	33,33,33,33	0
59	MG	2A	3310	1/1	0.89	0.20	53,53,53,53	0
59	MG	2A	3147	1/1	0.89	0.22	53,53,53,53	0
59	MG	1B	218	1/1	0.89	0.14	36,36,36,36	0
59	MG	2B	3012	1/1	0.89	0.14	63,63,63,63	0
59	MG	2B	3014	1/1	0.89	0.18	67,67,67,67	0
59	MG	2a	3228	1/1	0.89	0.20	56,56,56,56	0
59	MG	1A	3594	1/1	0.89	0.08	15,15,15,15	0
59	MG	2a	3234	1/1	0.89	0.21	62,62,62,62	0
59	MG	1a	3373	1/1	0.89	0.24	59,59,59,59	0
59	MG	2B	3017	1/1	0.89	0.15	57,57,57,57	0
59	MG	1A	3603	1/1	0.89	0.10	39,39,39,39	0
59	MG	1A	3741	1/1	0.89	0.15	46,46,46,46	0
59	MG	1A	3876	1/1	0.89	0.15	60,60,60,60	0
59	MG	1A	3883	1/1	0.89	0.12	52,52,52,52	0
59	MG	2A	3164	1/1	0.89	0.23	56,56,56,56	0
59	MG	1a	3571	1/1	0.89	0.12	57,57,57,57	0
59	MG	1A	3353	1/1	0.89	0.20	51,51,51,51	0
59	MG	1a	3575	1/1	0.89	0.23	55,55,55,55	0
59	MG	1A	3228	1/1	0.89	0.19	56,56,56,56	0
59	MG	2A	3343	1/1	0.89	0.25	60,60,60,60	0
59	MG	1A	3893	1/1	0.89	0.20	39,39,39,39	0
59	MG	2O	8002	1/1	0.89	0.14	48,48,48,48	0
59	MG	1d	502	1/1	0.89	0.27	52,52,52,52	0
59	MG	2w	3001	1/1	0.89	0.21	56,56,56,56	0
59	MG	1A	3895	1/1	0.89	0.10	39,39,39,39	0
59	MG	1B	235	1/1	0.89	0.12	63,63,63,63	0
59	MG	2A	3618	1/1	0.89	0.33	36,36,36,36	0
59	MG	2A	3176	1/1	0.89	0.13	44,44,44,44	0
59	MG	2A	3177	1/1	0.89	0.20	63,63,63,63	0
59	MG	2A	3623	1/1	0.89	0.11	51,51,51,51	0
59	MG	1A	4078	1/1	0.89	0.09	58,58,58,58	0
59	MG	2A	3357	1/1	0.89	0.14	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3627	1/1	0.89	0.13	53,53,53,53	0
59	MG	2A	3359	1/1	0.89	0.09	48,48,48,48	0
59	MG	1n	503	1/1	0.89	0.15	49,49,49,49	0
59	MG	2A	3180	1/1	0.89	0.15	53,53,53,53	0
59	MG	1p	101	1/1	0.89	0.18	48,48,48,48	0
59	MG	1A	3622	1/1	0.89	0.13	17,17,17,17	0
59	MG	2a	3012	1/1	0.89	0.16	63,63,63,63	0
59	MG	2A	3186	1/1	0.89	0.26	64,64,64,64	0
59	MG	1A	4098	1/1	0.90	0.14	37,37,37,37	0
59	MG	2a	3052	1/1	0.90	0.18	52,52,52,52	0
59	MG	1A	4102	1/1	0.90	0.14	50,50,50,50	0
59	MG	1A	4104	1/1	0.90	0.14	53,53,53,53	0
59	MG	2a	3057	1/1	0.90	0.21	60,60,60,60	0
59	MG	1A	3977	1/1	0.90	0.12	37,37,37,37	0
59	MG	1A	3078	1/1	0.90	0.21	48,48,48,48	0
59	MG	2a	3062	1/1	0.90	0.12	54,54,54,54	0
59	MG	2a	3063	1/1	0.90	0.20	55,55,55,55	0
59	MG	2A	3530	1/1	0.90	0.11	35,35,35,35	0
59	MG	1a	3344	1/1	0.90	0.21	56,56,56,56	0
59	MG	1A	3143	1/1	0.90	0.26	56,56,56,56	0
59	MG	2a	3067	1/1	0.90	0.15	56,56,56,56	0
59	MG	1A	3326	1/1	0.90	0.12	49,49,49,49	0
59	MG	2A	3301	1/1	0.90	0.27	41,41,41,41	0
59	MG	2a	3078	1/1	0.90	0.21	70,70,70,70	0
59	MG	1a	3430	1/1	0.90	0.16	69,69,69,69	0
59	MG	2A	3766	1/1	0.90	0.09	53,53,53,53	0
59	MG	1A	3376	1/1	0.90	0.14	48,48,48,48	0
59	MG	1a	3353	1/1	0.90	0.25	58,58,58,58	0
59	MG	2a	3084	1/1	0.90	0.11	71,71,71,71	0
59	MG	1A	3071	1/1	0.90	0.38	34,34,34,34	0
59	MG	1A	3586	1/1	0.90	0.14	49,49,49,49	0
59	MG	2A	3311	1/1	0.90	0.19	44,44,44,44	0
59	MG	1x	102	1/1	0.90	0.31	59,59,59,59	0
59	MG	2a	3090	1/1	0.90	0.11	65,65,65,65	0
59	MG	1a	3443	1/1	0.90	0.28	49,49,49,49	0
59	MG	2A	3314	1/1	0.90	0.32	60,60,60,60	0
59	MG	1A	3589	1/1	0.90	0.10	40,40,40,40	0
59	MG	2A	3317	1/1	0.90	0.18	51,51,51,51	0
59	MG	1A	3330	1/1	0.90	0.34	36,36,36,36	0
59	MG	1a	3460	1/1	0.90	0.18	58,58,58,58	0
59	MG	1A	4009	1/1	0.90	0.09	71,71,71,71	0
59	MG	1A	3674	1/1	0.90	0.08	14,14,14,14	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3181	1/1	0.90	0.23	57,57,57,57	0
59	MG	1A	3595	1/1	0.90	0.08	18,18,18,18	0
59	MG	2A	3567	1/1	0.90	0.12	63,63,63,63	0
59	MG	1E	305	1/1	0.90	0.18	42,42,42,42	0
59	MG	2A	3335	1/1	0.90	0.10	56,56,56,56	0
59	MG	1A	3510	1/1	0.90	0.16	41,41,41,41	0
59	MG	1A	3380	1/1	0.90	0.09	33,33,33,33	0
59	MG	1F	309	1/1	0.90	0.09	36,36,36,36	0
59	MG	2A	3579	1/1	0.90	0.15	32,32,32,32	0
59	MG	2A	3341	1/1	0.90	0.29	53,53,53,53	0
59	MG	1A	3693	1/1	0.90	0.12	13,13,13,13	0
59	MG	2A	3192	1/1	0.90	0.16	46,46,46,46	0
59	MG	2A	3021	1/1	0.90	0.17	54,54,54,54	0
59	MG	1a	3371	1/1	0.90	0.15	55,55,55,55	0
59	MG	2a	3124	1/1	0.90	0.13	62,62,62,62	0
59	MG	2a	3126	1/1	0.90	0.08	59,59,59,59	0
59	MG	2A	3810	1/1	0.90	0.11	59,59,59,59	0
59	MG	1G	3004	1/1	0.90	0.08	40,40,40,40	0
59	MG	2A	3591	1/1	0.90	0.20	63,63,63,63	0
59	MG	2A	3201	1/1	0.90	0.23	43,43,43,43	0
59	MG	2A	3202	1/1	0.90	0.13	51,51,51,51	0
59	MG	2a	3141	1/1	0.90	0.16	56,56,56,56	0
59	MG	1O	3001	1/1	0.90	0.11	54,54,54,54	0
59	MG	2a	3150	1/1	0.90	0.10	57,57,57,57	0
59	MG	2a	3151	1/1	0.90	0.10	73,73,73,73	0
59	MG	1A	3274	1/1	0.90	0.22	51,51,51,51	0
59	MG	2a	3157	1/1	0.90	0.11	77,77,77,77	0
59	MG	1A	3332	1/1	0.90	0.21	35,35,35,35	0
59	MG	2A	3035	1/1	0.90	0.26	67,67,67,67	0
59	MG	2A	3843	1/1	0.90	0.09	63,63,63,63	0
59	MG	2A	3037	1/1	0.90	0.21	59,59,59,59	0
59	MG	2A	3038	1/1	0.90	0.21	48,48,48,48	0
59	MG	2A	3846	1/1	0.90	0.13	38,38,38,38	0
59	MG	1a	3499	1/1	0.90	0.12	61,61,61,61	0
59	MG	2a	3177	1/1	0.90	0.13	58,58,58,58	0
59	MG	2A	3607	1/1	0.90	0.10	30,30,30,30	0
59	MG	1A	3623	1/1	0.90	0.10	15,15,15,15	0
59	MG	1a	3382	1/1	0.90	0.09	63,63,63,63	0
59	MG	2A	3375	1/1	0.90	0.10	45,45,45,45	0
59	MG	2A	3053	1/1	0.90	0.28	61,61,61,61	0
59	MG	2A	3219	1/1	0.90	0.09	54,54,54,54	0
59	MG	1A	4053	1/1	0.90	0.25	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1a	3510	1/1	0.90	0.13	53,53,53,53	0
59	MG	1A	3296	1/1	0.90	0.10	55,55,55,55	0
59	MG	1a	3514	1/1	0.90	0.11	50,50,50,50	0
59	MG	2A	3405	1/1	0.90	0.10	65,65,65,65	0
59	MG	2A	3232	1/1	0.90	0.17	63,63,63,63	0
59	MG	1a	3386	1/1	0.90	0.25	50,50,50,50	0
59	MG	2A	3630	1/1	0.90	0.19	66,66,66,66	0
59	MG	1A	4148	1/1	0.90	0.28	60,60,60,60	0
59	MG	2D	305	1/1	0.90	0.32	44,44,44,44	0
59	MG	2A	3235	1/1	0.90	0.31	62,62,62,62	0
59	MG	2E	302	1/1	0.90	0.12	38,38,38,38	0
59	MG	1a	3389	1/1	0.90	0.14	48,48,48,48	0
59	MG	2E	306	1/1	0.90	0.11	29,29,29,29	0
59	MG	1a	3537	1/1	0.90	0.09	46,46,46,46	0
59	MG	1a	3539	1/1	0.90	0.14	50,50,50,50	0
59	MG	1A	4060	1/1	0.90	0.15	27,27,27,27	0
59	MG	1A	3022	1/1	0.90	0.14	39,39,39,39	0
59	MG	1T	8001	1/1	0.90	0.13	43,43,43,43	0
59	MG	2Q	3002	1/1	0.90	0.25	48,48,48,48	0
59	MG	2A	3653	1/1	0.90	0.17	60,60,60,60	0
59	MG	2A	3445	1/1	0.90	0.13	42,42,42,42	0
59	MG	1A	3261	1/1	0.90	0.14	48,48,48,48	0
59	MG	1A	4176	1/1	0.90	0.14	15,15,15,15	0
59	MG	2T	201	1/1	0.90	0.16	54,54,54,54	0
59	MG	2A	3451	1/1	0.90	0.12	46,46,46,46	0
59	MG	1A	3455	1/1	0.90	0.18	51,51,51,51	0
59	MG	1A	3306	1/1	0.90	0.23	47,47,47,47	0
59	MG	1a	3556	1/1	0.90	0.09	46,46,46,46	0
59	MG	2A	3256	1/1	0.90	0.23	53,53,53,53	0
59	MG	1A	3837	1/1	0.90	0.17	48,48,48,48	0
59	MG	2A	3682	1/1	0.90	0.10	56,56,56,56	0
59	MG	2A	3685	1/1	0.90	0.12	62,62,62,62	0
59	MG	2d	502	1/1	0.90	0.17	59,59,59,59	0
59	MG	2A	3466	1/1	0.90	0.20	55,55,55,55	0
59	MG	1a	3558	1/1	0.90	0.12	63,63,63,63	0
59	MG	2a	3007	1/1	0.90	0.22	66,66,66,66	0
59	MG	1A	3839	1/1	0.90	0.26	25,25,25,25	0
59	MG	1A	3643	1/1	0.90	0.12	42,42,42,42	0
59	MG	2A	3111	1/1	0.90	0.14	60,60,60,60	0
59	MG	1A	3400	1/1	0.90	0.13	51,51,51,51	0
59	MG	2q	202	1/1	0.90	0.19	57,57,57,57	0
59	MG	2A	3266	1/1	0.90	0.09	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1a	3408	1/1	0.90	0.50	60,60,60,60	0
59	MG	2r	3001	1/1	0.90	0.20	77,77,77,77	0
59	MG	2A	3717	1/1	0.90	0.09	63,63,63,63	0
59	MG	2v	101	1/1	0.90	0.25	49,49,49,49	0
59	MG	1B	201	1/1	0.90	0.17	44,44,44,44	0
59	MG	2a	3023	1/1	0.90	0.37	54,54,54,54	0
59	MG	1A	3752	1/1	0.90	0.09	27,27,27,27	0
59	MG	1B	208	1/1	0.90	0.24	63,63,63,63	0
59	MG	1a	3413	1/1	0.90	0.23	54,54,54,54	0
59	MG	2A	3728	1/1	0.90	0.08	24,24,24,24	0
59	MG	2A	3141	1/1	0.90	0.12	38,38,38,38	0
59	MG	2a	3033	1/1	0.90	0.17	56,56,56,56	0
59	MG	1A	3959	1/1	0.90	0.12	55,55,55,55	0
59	MG	2A	3735	1/1	0.90	0.22	62,62,62,62	0
59	MG	2A	3736	1/1	0.90	0.17	58,58,58,58	0
59	MG	1A	3970	1/1	0.90	0.08	41,41,41,41	0
59	MG	1A	3283	1/1	0.90	0.12	45,45,45,45	0
59	MG	2a	3040	1/1	0.90	0.24	47,47,47,47	0
59	MG	2a	3041	1/1	0.90	0.17	63,63,63,63	0
59	MG	2A	3740	1/1	0.90	0.10	48,48,48,48	0
59	MG	2A	3511	1/1	0.90	0.17	50,50,50,50	0
59	MG	1e	3001	1/1	0.90	0.12	67,67,67,67	0
59	MG	2y	3006	1/1	0.90	0.08	89,89,89,89	0
59	MG	1A	3263	1/1	0.90	0.12	45,45,45,45	0
59	MG	1E	314	1/1	0.91	0.17	47,47,47,47	0
59	MG	1A	3124	1/1	0.91	0.10	29,29,29,29	0
59	MG	2A	3378	1/1	0.91	0.26	55,55,55,55	0
59	MG	2A	3194	1/1	0.91	0.34	38,38,38,38	0
59	MG	2A	3388	1/1	0.91	0.17	60,60,60,60	0
59	MG	1A	3077	1/1	0.91	0.14	42,42,42,42	0
59	MG	1A	3724	1/1	0.91	0.14	46,46,46,46	0
59	MG	2A	3684	1/1	0.91	0.07	33,33,33,33	0
59	MG	1G	3003	1/1	0.91	0.07	56,56,56,56	0
59	MG	2A	3404	1/1	0.91	0.13	48,48,48,48	0
59	MG	1A	3381	1/1	0.91	0.15	41,41,41,41	0
59	MG	1I	3001	1/1	0.91	0.12	62,62,62,62	0
59	MG	1N	3004	1/1	0.91	0.11	41,41,41,41	0
59	MG	1A	3175	1/1	0.91	0.14	44,44,44,44	0
59	MG	1A	4090	1/1	0.91	0.14	34,34,34,34	0
59	MG	2a	3047	1/1	0.91	0.21	60,60,60,60	0
59	MG	1A	3898	1/1	0.91	0.14	49,49,49,49	0
59	MG	1A	3585	1/1	0.91	0.09	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1x	117	1/1	0.91	0.12	63,63,63,63	0
59	MG	2A	3213	1/1	0.91	0.31	52,52,52,52	0
59	MG	2A	3214	1/1	0.91	0.13	58,58,58,58	0
59	MG	1A	3387	1/1	0.91	0.19	45,45,45,45	0
59	MG	1A	3905	1/1	0.91	0.07	71,71,71,71	0
59	MG	2A	3446	1/1	0.91	0.12	44,44,44,44	0
59	MG	1A	3020	1/1	0.91	0.08	45,45,45,45	0
59	MG	1A	3341	1/1	0.91	0.11	45,45,45,45	0
59	MG	2A	3221	1/1	0.91	0.18	59,59,59,59	0
59	MG	1A	3343	1/1	0.91	0.09	43,43,43,43	0
59	MG	2A	3017	1/1	0.91	0.20	39,39,39,39	0
59	MG	1A	3470	1/1	0.91	0.26	47,47,47,47	0
59	MG	2a	3076	1/1	0.91	0.32	56,56,56,56	0
59	MG	2a	3077	1/1	0.91	0.23	57,57,57,57	0
59	MG	1T	8002	1/1	0.91	0.15	51,51,51,51	0
59	MG	2A	3741	1/1	0.91	0.15	60,60,60,60	0
59	MG	1A	3051	1/1	0.91	0.21	49,49,49,49	0
59	MG	1A	3481	1/1	0.91	0.09	38,38,38,38	0
59	MG	2A	3024	1/1	0.91	0.12	43,43,43,43	0
59	MG	2A	3469	1/1	0.91	0.22	60,60,60,60	0
59	MG	2A	3025	1/1	0.91	0.09	42,42,42,42	0
59	MG	2A	3026	1/1	0.91	0.15	32,32,32,32	0
59	MG	2A	3472	1/1	0.91	0.21	50,50,50,50	0
59	MG	2A	3754	1/1	0.91	0.21	64,64,64,64	0
59	MG	2A	3237	1/1	0.91	0.12	59,59,59,59	0
59	MG	1A	3482	1/1	0.91	0.13	42,42,42,42	0
59	MG	1a	3438	1/1	0.91	0.21	55,55,55,55	0
59	MG	2A	3478	1/1	0.91	0.17	56,56,56,56	0
59	MG	2A	3241	1/1	0.91	0.21	66,66,66,66	0
59	MG	1A	3053	1/1	0.91	0.18	44,44,44,44	0
59	MG	2A	3483	1/1	0.91	0.16	36,36,36,36	0
59	MG	2A	3485	1/1	0.91	0.11	36,36,36,36	0
59	MG	10	107	1/1	0.91	0.13	38,38,38,38	0
59	MG	2a	3103	1/1	0.91	0.17	62,62,62,62	0
59	MG	2a	3104	1/1	0.91	0.27	54,54,54,54	0
59	MG	1A	3626	1/1	0.91	0.10	24,24,24,24	0
59	MG	1A	3942	1/1	0.91	0.18	45,45,45,45	0
59	MG	1A	3076	1/1	0.91	0.17	30,30,30,30	0
59	MG	1A	3782	1/1	0.91	0.11	60,60,60,60	0
59	MG	2A	3497	1/1	0.91	0.11	30,30,30,30	0
59	MG	2A	3498	1/1	0.91	0.09	45,45,45,45	0
59	MG	2A	3501	1/1	0.91	0.16	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3777	1/1	0.91	0.10	55,55,55,55	0
59	MG	2A	3252	1/1	0.91	0.15	58,58,58,58	0
59	MG	1a	3302	1/1	0.91	0.23	53,53,53,53	0
59	MG	2A	3780	1/1	0.91	0.21	62,62,62,62	0
59	MG	1A	3404	1/1	0.91	0.17	34,34,34,34	0
59	MG	2A	3513	1/1	0.91	0.14	67,67,67,67	0
59	MG	2A	3057	1/1	0.91	0.22	51,51,51,51	0
59	MG	2A	3785	1/1	0.91	0.12	53,53,53,53	0
59	MG	2a	3125	1/1	0.91	0.15	79,79,79,79	0
59	MG	2A	3058	1/1	0.91	0.09	45,45,45,45	0
59	MG	2a	3127	1/1	0.91	0.09	74,74,74,74	0
59	MG	1A	3490	1/1	0.91	0.24	58,58,58,58	0
59	MG	2A	3522	1/1	0.91	0.11	48,48,48,48	0
59	MG	2A	3062	1/1	0.91	0.27	43,43,43,43	0
59	MG	2A	3261	1/1	0.91	0.06	59,59,59,59	0
59	MG	1a	3475	1/1	0.91	0.16	48,48,48,48	0
59	MG	1A	3493	1/1	0.91	0.34	55,55,55,55	0
59	MG	1a	3321	1/1	0.91	0.14	50,50,50,50	0
59	MG	1A	3351	1/1	0.91	0.11	31,31,31,31	0
59	MG	2A	3270	1/1	0.91	0.14	62,62,62,62	0
59	MG	1A	3966	1/1	0.91	0.12	44,44,44,44	0
59	MG	2a	3156	1/1	0.91	0.10	77,77,77,77	0
59	MG	2A	3077	1/1	0.91	0.14	46,46,46,46	0
59	MG	1a	3484	1/1	0.91	0.12	41,41,41,41	0
59	MG	2a	3159	1/1	0.91	0.18	62,62,62,62	0
59	MG	1A	3968	1/1	0.91	0.08	27,27,27,27	0
59	MG	1A	3796	1/1	0.91	0.15	45,45,45,45	0
59	MG	2A	3281	1/1	0.91	0.23	67,67,67,67	0
59	MG	2A	3284	1/1	0.91	0.12	59,59,59,59	0
59	MG	1A	3406	1/1	0.91	0.12	50,50,50,50	0
59	MG	1A	3506	1/1	0.91	0.09	41,41,41,41	0
59	MG	2A	3822	1/1	0.91	0.09	33,33,33,33	0
59	MG	1A	3409	1/1	0.91	0.17	51,51,51,51	0
59	MG	1A	3153	1/1	0.91	0.27	25,25,25,25	0
59	MG	1A	3984	1/1	0.91	0.09	10,10,10,10	0
59	MG	1a	3341	1/1	0.91	0.17	50,50,50,50	0
59	MG	1A	3358	1/1	0.91	0.25	49,49,49,49	0
59	MG	2A	3840	1/1	0.91	0.10	30,30,30,30	0
59	MG	1A	3650	1/1	0.91	0.13	36,36,36,36	0
59	MG	1A	3989	1/1	0.91	0.12	49,49,49,49	0
59	MG	2A	3560	1/1	0.91	0.07	61,61,61,61	0
59	MG	2a	3192	1/1	0.91	0.15	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3294	1/1	0.91	0.20	47,47,47,47	0
59	MG	2B	3001	1/1	0.91	0.28	53,53,53,53	0
59	MG	1A	3651	1/1	0.91	0.12	37,37,37,37	0
59	MG	2B	3004	1/1	0.91	0.07	53,53,53,53	0
59	MG	2A	3104	1/1	0.91	0.16	52,52,52,52	0
59	MG	1A	4184	1/1	0.91	0.14	31,31,31,31	0
59	MG	1A	3415	1/1	0.91	0.17	45,45,45,45	0
59	MG	1A	3821	1/1	0.91	0.07	21,21,21,21	0
59	MG	1A	3823	1/1	0.91	0.14	59,59,59,59	0
59	MG	1A	3319	1/1	0.91	0.08	38,38,38,38	0
59	MG	2A	3305	1/1	0.91	0.19	52,52,52,52	0
59	MG	1A	4210	1/1	0.91	0.18	30,30,30,30	0
59	MG	2A	3581	1/1	0.91	0.07	51,51,51,51	0
59	MG	1A	4221	1/1	0.91	0.28	31,31,31,31	0
59	MG	2A	3308	1/1	0.91	0.19	50,50,50,50	0
59	MG	1A	3825	1/1	0.91	0.19	27,27,27,27	0
59	MG	2A	3137	1/1	0.91	0.29	60,60,60,60	0
59	MG	1A	3197	1/1	0.91	0.23	32,32,32,32	0
59	MG	1a	3546	1/1	0.91	0.16	46,46,46,46	0
59	MG	2A	3590	1/1	0.91	0.10	35,35,35,35	0
59	MG	1A	3830	1/1	0.91	0.11	40,40,40,40	0
59	MG	2A	3593	1/1	0.91	0.09	37,37,37,37	0
59	MG	1B	209	1/1	0.91	0.21	58,58,58,58	0
59	MG	1a	3368	1/1	0.91	0.35	63,63,63,63	0
59	MG	1A	4013	1/1	0.91	0.09	50,50,50,50	0
59	MG	2A	3598	1/1	0.91	0.11	63,63,63,63	0
59	MG	2F	304	1/1	0.91	0.11	74,74,74,74	0
59	MG	1A	4014	1/1	0.91	0.08	65,65,65,65	0
59	MG	1A	3368	1/1	0.91	0.13	39,39,39,39	0
59	MG	2a	3237	1/1	0.91	0.21	56,56,56,56	0
59	MG	1A	3427	1/1	0.91	0.19	43,43,43,43	0
59	MG	1A	3666	1/1	0.91	0.11	49,49,49,49	0
59	MG	2A	3326	1/1	0.91	0.18	46,46,46,46	0
59	MG	1a	3560	1/1	0.91	0.10	53,53,53,53	0
59	MG	1A	4039	1/1	0.91	0.08	50,50,50,50	0
59	MG	1a	3377	1/1	0.91	0.27	61,61,61,61	0
59	MG	2k	3001	1/1	0.91	0.26	50,50,50,50	0
59	MG	1A	3536	1/1	0.91	0.15	48,48,48,48	0
59	MG	1A	3842	1/1	0.91	0.10	15,15,15,15	0
59	MG	1A	3537	1/1	0.91	0.12	49,49,49,49	0
59	MG	1B	226	1/1	0.91	0.12	56,56,56,56	0
59	MG	1A	3370	1/1	0.91	0.23	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	4056	1/1	0.91	0.10	43,43,43,43	0
59	MG	1A	3431	1/1	0.91	0.09	45,45,45,45	0
59	MG	1b	3002	1/1	0.91	0.18	69,69,69,69	0
59	MG	1A	4059	1/1	0.91	0.18	57,57,57,57	0
59	MG	2a	3004	1/1	0.91	0.24	56,56,56,56	0
59	MG	1A	3154	1/1	0.91	0.17	42,42,42,42	0
59	MG	1f	3001	1/1	0.91	0.18	29,29,29,29	0
59	MG	1A	4061	1/1	0.91	0.13	40,40,40,40	0
59	MG	2a	3008	1/1	0.91	0.20	63,63,63,63	0
59	MG	1A	3680	1/1	0.91	0.13	53,53,53,53	0
59	MG	2a	3011	1/1	0.91	0.23	53,53,53,53	0
59	MG	1A	3209	1/1	0.91	0.15	41,41,41,41	0
59	MG	2A	3358	1/1	0.91	0.25	56,56,56,56	0
59	MG	1a	3398	1/1	0.91	0.27	58,58,58,58	0
59	MG	1A	3438	1/1	0.91	0.14	57,57,57,57	0
59	MG	1A	3697	1/1	0.91	0.10	18,18,18,18	0
59	MG	2A	3364	1/1	0.91	0.15	63,63,63,63	0
59	MG	1t	3001	1/1	0.91	0.13	43,43,43,43	0
59	MG	1A	3262	1/1	0.91	0.22	41,41,41,41	0
59	MG	2a	3024	1/1	0.91	0.26	59,59,59,59	0
59	MG	1E	308	1/1	0.91	0.25	59,59,59,59	0
59	MG	2A	3190	1/1	0.91	0.14	37,37,37,37	0
59	MG	1A	3572	1/1	0.91	0.09	38,38,38,38	0
59	MG	2a	3029	1/1	0.91	0.26	58,58,58,58	0
59	MG	1A	3173	1/1	0.92	0.09	36,36,36,36	0
59	MG	1A	3442	1/1	0.92	0.16	63,63,63,63	0
59	MG	1A	3305	1/1	0.92	0.11	50,50,50,50	0
59	MG	1a	3397	1/1	0.92	0.14	60,60,60,60	0
59	MG	2A	3003	1/1	0.92	0.34	61,61,61,61	0
59	MG	1A	3574	1/1	0.92	0.18	52,52,52,52	0
59	MG	2Q	3003	1/1	0.92	0.12	54,54,54,54	0
59	MG	1A	3091	1/1	0.92	0.06	17,17,17,17	0
59	MG	2R	201	1/1	0.92	0.14	63,63,63,63	0
59	MG	1a	3400	1/1	0.92	0.19	54,54,54,54	0
59	MG	1A	3307	1/1	0.92	0.12	50,50,50,50	0
59	MG	2A	3267	1/1	0.92	0.10	55,55,55,55	0
59	MG	1B	234	1/1	0.92	0.12	54,54,54,54	0
59	MG	2T	202	1/1	0.92	0.18	61,61,61,61	0
59	MG	1A	3125	1/1	0.92	0.26	32,32,32,32	0
59	MG	1A	4065	1/1	0.92	0.09	45,45,45,45	0
59	MG	1D	302	1/1	0.92	0.15	17,17,17,17	0
59	MG	1A	4066	1/1	0.92	0.12	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	23	102	1/1	0.92	0.11	45,45,45,45	0
59	MG	2A	3028	1/1	0.92	0.13	25,25,25,25	0
59	MG	28	101	1/1	0.92	0.34	54,54,54,54	0
59	MG	1A	4067	1/1	0.92	0.14	36,36,36,36	0
59	MG	2a	3001	1/1	0.92	0.08	52,52,52,52	0
59	MG	2A	3283	1/1	0.92	0.11	60,60,60,60	0
59	MG	1A	4070	1/1	0.92	0.08	33,33,33,33	0
59	MG	1E	301	1/1	0.92	0.12	33,33,33,33	0
59	MG	1A	3728	1/1	0.92	0.13	16,16,16,16	0
59	MG	1E	307	1/1	0.92	0.15	40,40,40,40	0
59	MG	1A	3729	1/1	0.92	0.12	11,11,11,11	0
59	MG	1A	3891	1/1	0.92	0.07	15,15,15,15	0
59	MG	2A	3042	1/1	0.92	0.11	43,43,43,43	0
59	MG	1A	3100	1/1	0.92	0.22	23,23,23,23	0
59	MG	1A	3186	1/1	0.92	0.26	35,35,35,35	0
59	MG	2A	3052	1/1	0.92	0.16	56,56,56,56	0
59	MG	1A	3386	1/1	0.92	0.10	47,47,47,47	0
59	MG	2A	3055	1/1	0.92	0.07	24,24,24,24	0
59	MG	1A	3591	1/1	0.92	0.09	26,26,26,26	0
59	MG	1A	3742	1/1	0.92	0.08	29,29,29,29	0
59	MG	1A	4083	1/1	0.92	0.11	68,68,68,68	0
59	MG	2a	3021	1/1	0.92	0.13	62,62,62,62	0
59	MG	2a	3022	1/1	0.92	0.17	62,62,62,62	0
59	MG	1A	3899	1/1	0.92	0.11	50,50,50,50	0
59	MG	2A	3603	1/1	0.92	0.11	49,49,49,49	0
59	MG	2A	3065	1/1	0.92	0.12	47,47,47,47	0
59	MG	2A	3066	1/1	0.92	0.14	54,54,54,54	0
59	MG	2A	3304	1/1	0.92	0.35	56,56,56,56	0
59	MG	1A	3128	1/1	0.92	0.20	30,30,30,30	0
59	MG	2A	3612	1/1	0.92	0.12	44,44,44,44	0
59	MG	1N	3009	1/1	0.92	0.16	28,28,28,28	0
59	MG	1A	4088	1/1	0.92	0.12	42,42,42,42	0
59	MG	2A	3617	1/1	0.92	0.11	40,40,40,40	0
59	MG	2A	3072	1/1	0.92	0.12	42,42,42,42	0
59	MG	1A	3474	1/1	0.92	0.20	55,55,55,55	0
59	MG	2A	3621	1/1	0.92	0.11	57,57,57,57	0
59	MG	1a	3434	1/1	0.92	0.17	48,48,48,48	0
59	MG	2A	3076	1/1	0.92	0.13	37,37,37,37	0
59	MG	1A	3596	1/1	0.92	0.09	54,54,54,54	0
59	MG	1A	4093	1/1	0.92	0.10	40,40,40,40	0
59	MG	1A	3753	1/1	0.92	0.09	25,25,25,25	0
59	MG	1A	4096	1/1	0.92	0.32	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3316	1/1	0.92	0.26	49,49,49,49	0
59	MG	1A	3754	1/1	0.92	0.19	32,32,32,32	0
59	MG	1R	201	1/1	0.92	0.10	28,28,28,28	0
59	MG	2a	3049	1/1	0.92	0.14	55,55,55,55	0
59	MG	1a	3448	1/1	0.92	0.21	60,60,60,60	0
59	MG	1A	3597	1/1	0.92	0.10	34,34,34,34	0
59	MG	1a	3454	1/1	0.92	0.10	46,46,46,46	0
59	MG	1a	3458	1/1	0.92	0.13	51,51,51,51	0
59	MG	1A	3762	1/1	0.92	0.14	48,48,48,48	0
59	MG	2A	3096	1/1	0.92	0.18	55,55,55,55	0
59	MG	2a	3061	1/1	0.92	0.16	60,60,60,60	0
59	MG	2A	3330	1/1	0.92	0.14	53,53,53,53	0
59	MG	1S	3002	1/1	0.92	0.18	48,48,48,48	0
59	MG	1A	3915	1/1	0.92	0.08	24,24,24,24	0
59	MG	2A	3655	1/1	0.92	0.08	62,62,62,62	0
59	MG	1A	3036	1/1	0.92	0.17	23,23,23,23	0
59	MG	2A	3337	1/1	0.92	0.17	44,44,44,44	0
59	MG	2a	3068	1/1	0.92	0.17	52,52,52,52	0
59	MG	2a	3069	1/1	0.92	0.35	68,68,68,68	0
59	MG	2A	3102	1/1	0.92	0.17	41,41,41,41	0
59	MG	2A	3664	1/1	0.92	0.12	68,68,68,68	0
59	MG	2A	3666	1/1	0.92	0.10	62,62,62,62	0
59	MG	1a	3467	1/1	0.92	0.14	53,53,53,53	0
59	MG	1U	202	1/1	0.92	0.18	27,27,27,27	0
59	MG	2A	3109	1/1	0.92	0.14	43,43,43,43	0
59	MG	1A	3480	1/1	0.92	0.10	40,40,40,40	0
59	MG	2A	3345	1/1	0.92	0.17	59,59,59,59	0
59	MG	2A	3677	1/1	0.92	0.10	63,63,63,63	0
59	MG	2A	3678	1/1	0.92	0.15	64,64,64,64	0
59	MG	1Y	502	1/1	0.92	0.18	53,53,53,53	0
59	MG	2a	3086	1/1	0.92	0.25	60,60,60,60	0
59	MG	1A	3770	1/1	0.92	0.11	40,40,40,40	0
59	MG	1Z	302	1/1	0.92	0.14	48,48,48,48	0
59	MG	2A	3349	1/1	0.92	0.09	50,50,50,50	0
59	MG	2A	3124	1/1	0.92	0.18	32,32,32,32	0
59	MG	1A	3771	1/1	0.92	0.07	33,33,33,33	0
59	MG	2A	3353	1/1	0.92	0.19	57,57,57,57	0
59	MG	2A	3692	1/1	0.92	0.09	40,40,40,40	0
59	MG	2A	3695	1/1	0.92	0.11	53,53,53,53	0
59	MG	1a	3483	1/1	0.92	0.14	58,58,58,58	0
59	MG	1A	3325	1/1	0.92	0.25	31,31,31,31	0
59	MG	2a	3099	1/1	0.92	0.25	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3707	1/1	0.92	0.15	64,64,64,64	0
59	MG	1A	4116	1/1	0.92	0.11	50,50,50,50	0
59	MG	1A	3936	1/1	0.92	0.09	19,19,19,19	0
59	MG	12	3001	1/1	0.92	0.09	40,40,40,40	0
59	MG	13	3001	1/1	0.92	0.08	39,39,39,39	0
59	MG	1A	3057	1/1	0.92	0.06	26,26,26,26	0
59	MG	2A	3724	1/1	0.92	0.16	34,34,34,34	0
59	MG	1a	3494	1/1	0.92	0.10	48,48,48,48	0
59	MG	1A	4121	1/1	0.92	0.11	30,30,30,30	0
59	MG	1A	3264	1/1	0.92	0.10	56,56,56,56	0
59	MG	19	101	1/1	0.92	0.14	46,46,46,46	0
59	MG	2A	3732	1/1	0.92	0.11	47,47,47,47	0
59	MG	1A	3396	1/1	0.92	0.10	46,46,46,46	0
59	MG	2A	3734	1/1	0.92	0.10	54,54,54,54	0
59	MG	1a	3506	1/1	0.92	0.11	59,59,59,59	0
59	MG	2a	3117	1/1	0.92	0.27	53,53,53,53	0
59	MG	2A	3155	1/1	0.92	0.16	44,44,44,44	0
59	MG	1a	3507	1/1	0.92	0.09	64,64,64,64	0
59	MG	2a	3120	1/1	0.92	0.10	51,51,51,51	0
59	MG	2A	3738	1/1	0.92	0.20	60,60,60,60	0
59	MG	1a	3303	1/1	0.92	0.17	55,55,55,55	0
59	MG	2A	3381	1/1	0.92	0.16	17,17,17,17	0
59	MG	2A	3385	1/1	0.92	0.13	63,63,63,63	0
59	MG	2A	3386	1/1	0.92	0.12	45,45,45,45	0
59	MG	1a	3304	1/1	0.92	0.20	58,58,58,58	0
59	MG	1A	3781	1/1	0.92	0.14	42,42,42,42	0
59	MG	2A	3391	1/1	0.92	0.10	41,41,41,41	0
59	MG	1A	3195	1/1	0.92	0.12	48,48,48,48	0
59	MG	2A	3166	1/1	0.92	0.27	56,56,56,56	0
59	MG	1A	3105	1/1	0.92	0.12	30,30,30,30	0
59	MG	1a	3531	1/1	0.92	0.07	49,49,49,49	0
59	MG	2a	3148	1/1	0.92	0.12	73,73,73,73	0
59	MG	1A	4130	1/1	0.92	0.10	65,65,65,65	0
59	MG	2A	3412	1/1	0.92	0.09	40,40,40,40	0
59	MG	1A	3786	1/1	0.92	0.08	26,26,26,26	0
59	MG	2a	3154	1/1	0.92	0.14	42,42,42,42	0
59	MG	1a	3324	1/1	0.92	0.20	57,57,57,57	0
59	MG	2A	3415	1/1	0.92	0.10	36,36,36,36	0
59	MG	2A	3763	1/1	0.92	0.14	66,66,66,66	0
59	MG	2A	3416	1/1	0.92	0.09	34,34,34,34	0
59	MG	1A	3015	1/1	0.92	0.12	43,43,43,43	0
59	MG	1A	3494	1/1	0.92	0.21	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2a	3164	1/1	0.92	0.08	75,75,75,75	0
59	MG	1A	3789	1/1	0.92	0.12	56,56,56,56	0
59	MG	1A	3019	1/1	0.92	0.17	33,33,33,33	0
59	MG	2a	3173	1/1	0.92	0.18	61,61,61,61	0
59	MG	1a	3545	1/1	0.92	0.07	46,46,46,46	0
59	MG	1A	3339	1/1	0.92	0.12	45,45,45,45	0
59	MG	1A	3505	1/1	0.92	0.10	51,51,51,51	0
59	MG	1a	3334	1/1	0.92	0.20	49,49,49,49	0
59	MG	2A	3182	1/1	0.92	0.19	61,61,61,61	0
59	MG	1A	4147	1/1	0.92	0.14	50,50,50,50	0
59	MG	2A	3184	1/1	0.92	0.20	45,45,45,45	0
59	MG	1a	3551	1/1	0.92	0.17	54,54,54,54	0
59	MG	1A	3275	1/1	0.92	0.11	38,38,38,38	0
59	MG	1a	3555	1/1	0.92	0.09	47,47,47,47	0
59	MG	1a	3337	1/1	0.92	0.30	55,55,55,55	0
59	MG	1A	4151	1/1	0.92	0.10	45,45,45,45	0
59	MG	2a	3189	1/1	0.92	0.20	57,57,57,57	0
59	MG	2a	3191	1/1	0.92	0.15	55,55,55,55	0
59	MG	1a	3343	1/1	0.92	0.15	40,40,40,40	0
59	MG	1A	3211	1/1	0.92	0.22	47,47,47,47	0
59	MG	1A	4156	1/1	0.92	0.17	37,37,37,37	0
59	MG	2A	3787	1/1	0.92	0.11	58,58,58,58	0
59	MG	1A	3212	1/1	0.92	0.13	49,49,49,49	0
59	MG	1A	3808	1/1	0.92	0.22	33,33,33,33	0
59	MG	2a	3200	1/1	0.92	0.12	65,65,65,65	0
59	MG	2a	3201	1/1	0.92	0.21	46,46,46,46	0
59	MG	1a	3351	1/1	0.92	0.15	42,42,42,42	0
59	MG	2A	3200	1/1	0.92	0.22	37,37,37,37	0
59	MG	1a	3566	1/1	0.92	0.11	57,57,57,57	0
59	MG	1A	3511	1/1	0.92	0.23	51,51,51,51	0
59	MG	2A	3203	1/1	0.92	0.30	61,61,61,61	0
59	MG	1a	3569	1/1	0.92	0.16	66,66,66,66	0
59	MG	2A	3797	1/1	0.92	0.12	49,49,49,49	0
59	MG	1A	3214	1/1	0.92	0.15	46,46,46,46	0
59	MG	1a	3355	1/1	0.92	0.22	51,51,51,51	0
59	MG	1A	3218	1/1	0.92	0.20	38,38,38,38	0
59	MG	2a	3213	1/1	0.92	0.13	66,66,66,66	0
59	MG	1A	3222	1/1	0.92	0.09	38,38,38,38	0
59	MG	1a	3360	1/1	0.92	0.11	45,45,45,45	0
59	MG	1A	3425	1/1	0.92	0.08	49,49,49,49	0
59	MG	1A	3523	1/1	0.92	0.12	37,37,37,37	0
59	MG	2A	3812	1/1	0.92	0.09	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	4007	1/1	0.92	0.16	54,54,54,54	0
59	MG	2A	3493	1/1	0.92	0.08	29,29,29,29	0
59	MG	2a	3222	1/1	0.92	0.17	57,57,57,57	0
59	MG	1A	4194	1/1	0.92	0.24	33,33,33,33	0
59	MG	1A	4197	1/1	0.92	0.25	25,25,25,25	0
59	MG	2A	3827	1/1	0.92	0.13	62,62,62,62	0
59	MG	2A	3217	1/1	0.92	0.15	48,48,48,48	0
59	MG	2a	3232	1/1	0.92	0.20	60,60,60,60	0
59	MG	1A	3082	1/1	0.92	0.17	48,48,48,48	0
59	MG	1A	4010	1/1	0.92	0.13	50,50,50,50	0
59	MG	2A	3835	1/1	0.92	0.08	48,48,48,48	0
59	MG	1n	502	1/1	0.92	0.29	58,58,58,58	0
59	MG	1A	3665	1/1	0.92	0.21	51,51,51,51	0
59	MG	2A	3838	1/1	0.92	0.18	51,51,51,51	0
59	MG	1A	4229	1/1	0.92	0.10	24,24,24,24	0
59	MG	2A	3842	1/1	0.92	0.32	46,46,46,46	0
59	MG	2A	3514	1/1	0.92	0.20	35,35,35,35	0
59	MG	1A	3290	1/1	0.92	0.19	37,37,37,37	0
59	MG	2A	3226	1/1	0.92	0.09	53,53,53,53	0
59	MG	2l	201	1/1	0.92	0.10	65,65,65,65	0
59	MG	1B	203	1/1	0.92	0.19	49,49,49,49	0
59	MG	2A	3521	1/1	0.92	0.14	42,42,42,42	0
59	MG	1A	3670	1/1	0.92	0.12	43,43,43,43	0
59	MG	1A	3832	1/1	0.92	0.16	47,47,47,47	0
59	MG	2A	3525	1/1	0.92	0.16	55,55,55,55	0
59	MG	1A	3111	1/1	0.92	0.13	56,56,56,56	0
59	MG	1A	4021	1/1	0.92	0.08	27,27,27,27	0
59	MG	1a	3378	1/1	0.92	0.21	63,63,63,63	0
59	MG	1A	4025	1/1	0.92	0.09	37,37,37,37	0
59	MG	2A	3238	1/1	0.92	0.28	53,53,53,53	0
59	MG	2B	3013	1/1	0.92	0.24	63,63,63,63	0
59	MG	2v	104	1/1	0.92	0.17	52,52,52,52	0
59	MG	2A	3532	1/1	0.92	0.10	53,53,53,53	0
59	MG	1A	3359	1/1	0.92	0.17	56,56,56,56	0
59	MG	1A	3163	1/1	0.92	0.10	48,48,48,48	0
59	MG	1A	3002	1/1	0.92	0.13	53,53,53,53	0
59	MG	1A	4043	1/1	0.92	0.11	39,39,39,39	0
59	MG	2A	3540	1/1	0.92	0.14	48,48,48,48	0
59	MG	1x	104	1/1	0.92	0.14	61,61,61,61	0
59	MG	2B	3021	1/1	0.92	0.25	68,68,68,68	0
59	MG	1A	3167	1/1	0.92	0.10	38,38,38,38	0
59	MG	2D	302	1/1	0.92	0.11	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1x	110	1/1	0.92	0.14	59,59,59,59	0
59	MG	1a	3387	1/1	0.92	0.24	40,40,40,40	0
59	MG	1A	3439	1/1	0.92	0.14	39,39,39,39	0
59	MG	1B	223	1/1	0.92	0.16	45,45,45,45	0
59	MG	1a	3390	1/1	0.92	0.28	53,53,53,53	0
59	MG	1A	3302	1/1	0.92	0.14	54,54,54,54	0
59	MG	2E	307	1/1	0.92	0.11	62,62,62,62	0
59	MG	2A	3554	1/1	0.92	0.19	62,62,62,62	0
59	MG	2a	3010	1/1	0.93	0.24	62,62,62,62	0
59	MG	2A	3139	1/1	0.93	0.14	33,33,33,33	0
59	MG	1A	3951	1/1	0.93	0.08	52,52,52,52	0
59	MG	1A	3446	1/1	0.93	0.16	35,35,35,35	0
59	MG	1A	3447	1/1	0.93	0.29	38,38,38,38	0
59	MG	2A	3144	1/1	0.93	0.15	65,65,65,65	0
59	MG	2a	3016	1/1	0.93	0.08	46,46,46,46	0
59	MG	1a	3541	1/1	0.93	0.19	61,61,61,61	0
59	MG	1a	3333	1/1	0.93	0.23	54,54,54,54	0
59	MG	1A	3575	1/1	0.93	0.07	13,13,13,13	0
59	MG	2a	3020	1/1	0.93	0.20	61,61,61,61	0
59	MG	1A	3760	1/1	0.93	0.17	32,32,32,32	0
59	MG	1A	4153	1/1	0.93	0.09	49,49,49,49	0
59	MG	2A	3648	1/1	0.93	0.14	60,60,60,60	0
59	MG	2A	3152	1/1	0.93	0.20	48,48,48,48	0
59	MG	1A	3962	1/1	0.93	0.18	55,55,55,55	0
59	MG	1A	3174	1/1	0.93	0.08	23,23,23,23	0
59	MG	1A	3967	1/1	0.93	0.10	42,42,42,42	0
59	MG	2A	3156	1/1	0.93	0.11	39,39,39,39	0
59	MG	2A	3157	1/1	0.93	0.20	47,47,47,47	0
59	MG	2A	3158	1/1	0.93	0.11	50,50,50,50	0
59	MG	2A	3360	1/1	0.93	0.13	50,50,50,50	0
59	MG	1A	4168	1/1	0.93	0.08	36,36,36,36	0
59	MG	1A	3452	1/1	0.93	0.17	32,32,32,32	0
59	MG	1A	4175	1/1	0.93	0.12	36,36,36,36	0
59	MG	1a	3554	1/1	0.93	0.13	58,58,58,58	0
59	MG	1A	3768	1/1	0.93	0.14	56,56,56,56	0
59	MG	1A	3133	1/1	0.93	0.09	41,41,41,41	0
59	MG	1A	3097	1/1	0.93	0.08	35,35,35,35	0
59	MG	2A	3370	1/1	0.93	0.07	54,54,54,54	0
59	MG	2A	3372	1/1	0.93	0.23	50,50,50,50	0
59	MG	2A	3680	1/1	0.93	0.15	55,55,55,55	0
59	MG	1A	3457	1/1	0.93	0.30	55,55,55,55	0
59	MG	1A	4185	1/1	0.93	0.17	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1a	3356	1/1	0.93	0.09	41,41,41,41	0
59	MG	1A	3459	1/1	0.93	0.09	58,58,58,58	0
59	MG	2a	3051	1/1	0.93	0.21	55,55,55,55	0
59	MG	1A	3317	1/1	0.93	0.27	32,32,32,32	0
59	MG	1a	3564	1/1	0.93	0.09	54,54,54,54	0
59	MG	2A	3175	1/1	0.93	0.10	63,63,63,63	0
59	MG	1A	3593	1/1	0.93	0.09	18,18,18,18	0
59	MG	2A	3387	1/1	0.93	0.09	47,47,47,47	0
59	MG	2A	3696	1/1	0.93	0.08	73,73,73,73	0
59	MG	2A	3699	1/1	0.93	0.08	38,38,38,38	0
59	MG	1A	4191	1/1	0.93	0.10	27,27,27,27	0
59	MG	1A	4193	1/1	0.93	0.08	14,14,14,14	0
59	MG	1A	3777	1/1	0.93	0.12	45,45,45,45	0
59	MG	2A	3397	1/1	0.93	0.07	23,23,23,23	0
59	MG	1A	3318	1/1	0.93	0.10	49,49,49,49	0
59	MG	1A	3464	1/1	0.93	0.17	51,51,51,51	0
59	MG	1A	3216	1/1	0.93	0.13	36,36,36,36	0
59	MG	1a	3576	1/1	0.93	0.18	53,53,53,53	0
59	MG	2A	3407	1/1	0.93	0.09	34,34,34,34	0
59	MG	1A	3469	1/1	0.93	0.21	33,33,33,33	0
59	MG	1A	4223	1/1	0.93	0.13	39,39,39,39	0
59	MG	1A	4228	1/1	0.93	0.28	34,34,34,34	0
59	MG	2A	3729	1/1	0.93	0.09	57,57,57,57	0
59	MG	2A	3730	1/1	0.93	0.07	53,53,53,53	0
59	MG	1A	3599	1/1	0.93	0.12	21,21,21,21	0
59	MG	1A	3600	1/1	0.93	0.08	21,21,21,21	0
59	MG	1A	3266	1/1	0.93	0.17	45,45,45,45	0
59	MG	2a	3083	1/1	0.93	0.14	59,59,59,59	0
59	MG	1A	3322	1/1	0.93	0.21	47,47,47,47	0
59	MG	2A	3423	1/1	0.93	0.09	33,33,33,33	0
59	MG	1A	3792	1/1	0.93	0.10	42,42,42,42	0
59	MG	1A	3476	1/1	0.93	0.31	44,44,44,44	0
59	MG	2A	3431	1/1	0.93	0.12	54,54,54,54	0
59	MG	1A	3795	1/1	0.93	0.10	23,23,23,23	0
59	MG	1A	3323	1/1	0.93	0.45	28,28,28,28	0
59	MG	1A	3389	1/1	0.93	0.27	36,36,36,36	0
59	MG	2A	3440	1/1	0.93	0.16	58,58,58,58	0
59	MG	2A	3744	1/1	0.93	0.10	47,47,47,47	0
59	MG	1A	4015	1/1	0.93	0.14	52,52,52,52	0
59	MG	2a	3096	1/1	0.93	0.47	56,56,56,56	0
59	MG	1A	4018	1/1	0.93	0.09	47,47,47,47	0
59	MG	1A	3799	1/1	0.93	0.15	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	3217	1/1	0.93	0.17	47,47,47,47	0
59	MG	1A	3270	1/1	0.93	0.09	45,45,45,45	0
59	MG	2A	3450	1/1	0.93	0.09	53,53,53,53	0
59	MG	1w	107	1/1	0.93	0.10	62,62,62,62	0
59	MG	2A	3206	1/1	0.93	0.24	50,50,50,50	0
59	MG	1A	4030	1/1	0.93	0.20	58,58,58,58	0
59	MG	1A	3802	1/1	0.93	0.23	31,31,31,31	0
59	MG	1A	3005	1/1	0.93	0.14	47,47,47,47	0
59	MG	2A	3459	1/1	0.93	0.19	55,55,55,55	0
59	MG	1A	3632	1/1	0.93	0.19	53,53,53,53	0
59	MG	1A	4041	1/1	0.93	0.08	42,42,42,42	0
59	MG	2A	3467	1/1	0.93	0.16	54,54,54,54	0
59	MG	2A	3212	1/1	0.93	0.11	49,49,49,49	0
59	MG	1A	3636	1/1	0.93	0.13	46,46,46,46	0
59	MG	1A	4044	1/1	0.93	0.10	54,54,54,54	0
59	MG	1A	3182	1/1	0.93	0.09	38,38,38,38	0
59	MG	1x	107	1/1	0.93	0.13	50,50,50,50	0
59	MG	1A	3639	1/1	0.93	0.08	51,51,51,51	0
59	MG	1A	3116	1/1	0.93	0.11	43,43,43,43	0
59	MG	1A	3225	1/1	0.93	0.27	64,64,64,64	0
59	MG	2a	3121	1/1	0.93	0.26	61,61,61,61	0
59	MG	1B	238	1/1	0.93	0.09	30,30,30,30	0
59	MG	1x	113	1/1	0.93	0.15	61,61,61,61	0
59	MG	1A	3822	1/1	0.93	0.06	11,11,11,11	0
59	MG	1A	3491	1/1	0.93	0.12	47,47,47,47	0
59	MG	1A	3039	1/1	0.93	0.05	22,22,22,22	0
59	MG	2A	3229	1/1	0.93	0.15	54,54,54,54	0
59	MG	2a	3132	1/1	0.93	0.09	68,68,68,68	0
59	MG	1A	3278	1/1	0.93	0.34	62,62,62,62	0
59	MG	2A	3490	1/1	0.93	0.09	30,30,30,30	0
59	MG	1A	3498	1/1	0.93	0.17	51,51,51,51	0
59	MG	2a	3136	1/1	0.93	0.08	64,64,64,64	0
59	MG	1A	3648	1/1	0.93	0.12	31,31,31,31	0
59	MG	2a	3140	1/1	0.93	0.11	68,68,68,68	0
59	MG	1A	3502	1/1	0.93	0.14	35,35,35,35	0
59	MG	1A	3049	1/1	0.93	0.14	54,54,54,54	0
59	MG	2A	3004	1/1	0.93	0.17	46,46,46,46	0
59	MG	1A	3161	1/1	0.93	0.15	25,25,25,25	0
59	MG	2A	3008	1/1	0.93	0.14	44,44,44,44	0
59	MG	2A	3505	1/1	0.93	0.12	35,35,35,35	0
59	MG	1E	313	1/1	0.93	0.22	34,34,34,34	0
59	MG	1A	3088	1/1	0.93	0.15	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3019	1/1	0.93	0.11	54,54,54,54	0
59	MG	1A	3411	1/1	0.93	0.17	48,48,48,48	0
59	MG	1F	307	1/1	0.93	0.11	44,44,44,44	0
59	MG	1A	3507	1/1	0.93	0.12	45,45,45,45	0
59	MG	2A	3800	1/1	0.93	0.09	62,62,62,62	0
59	MG	1a	3419	1/1	0.93	0.22	49,49,49,49	0
59	MG	1A	3233	1/1	0.93	0.16	51,51,51,51	0
59	MG	2a	3167	1/1	0.93	0.08	74,74,74,74	0
59	MG	2a	3169	1/1	0.93	0.15	51,51,51,51	0
59	MG	1A	3345	1/1	0.93	0.21	37,37,37,37	0
59	MG	2a	3171	1/1	0.93	0.09	55,55,55,55	0
59	MG	1A	3661	1/1	0.93	0.08	36,36,36,36	0
59	MG	2A	3523	1/1	0.93	0.13	63,63,63,63	0
59	MG	1A	3848	1/1	0.93	0.07	72,72,72,72	0
59	MG	1A	3089	1/1	0.93	0.07	28,28,28,28	0
59	MG	2a	3178	1/1	0.93	0.21	52,52,52,52	0
59	MG	1A	3513	1/1	0.93	0.12	44,44,44,44	0
59	MG	2A	3257	1/1	0.93	0.10	49,49,49,49	0
59	MG	2A	3819	1/1	0.93	0.09	47,47,47,47	0
59	MG	1A	3239	1/1	0.93	0.27	49,49,49,49	0
59	MG	1A	3242	1/1	0.93	0.24	24,24,24,24	0
59	MG	2a	3184	1/1	0.93	0.26	61,61,61,61	0
59	MG	1A	3517	1/1	0.93	0.19	41,41,41,41	0
59	MG	1a	3432	1/1	0.93	0.14	44,44,44,44	0
59	MG	1a	3433	1/1	0.93	0.43	61,61,61,61	0
59	MG	1A	4087	1/1	0.93	0.11	34,34,34,34	0
59	MG	2A	3045	1/1	0.93	0.09	49,49,49,49	0
59	MG	2A	3047	1/1	0.93	0.13	47,47,47,47	0
59	MG	2A	3048	1/1	0.93	0.20	53,53,53,53	0
59	MG	2A	3839	1/1	0.93	0.23	39,39,39,39	0
59	MG	2a	3194	1/1	0.93	0.15	68,68,68,68	0
59	MG	2A	3268	1/1	0.93	0.23	61,61,61,61	0
59	MG	2A	3049	1/1	0.93	0.09	44,44,44,44	0
59	MG	2A	3544	1/1	0.93	0.11	64,64,64,64	0
59	MG	1A	3246	1/1	0.93	0.12	47,47,47,47	0
59	MG	1A	4089	1/1	0.93	0.16	42,42,42,42	0
59	MG	1A	3675	1/1	0.93	0.17	21,21,21,21	0
59	MG	2A	3549	1/1	0.93	0.16	55,55,55,55	0
59	MG	1A	3356	1/1	0.93	0.09	38,38,38,38	0
59	MG	1A	3522	1/1	0.93	0.23	28,28,28,28	0
59	MG	2B	3005	1/1	0.93	0.29	61,61,61,61	0
59	MG	2A	3277	1/1	0.93	0.30	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2a	3207	1/1	0.93	0.22	55,55,55,55	0
59	MG	2A	3279	1/1	0.93	0.26	43,43,43,43	0
59	MG	1A	3428	1/1	0.93	0.22	56,56,56,56	0
59	MG	2B	3009	1/1	0.93	0.09	54,54,54,54	0
59	MG	1A	3688	1/1	0.93	0.13	43,43,43,43	0
59	MG	1A	3042	1/1	0.93	0.07	17,17,17,17	0
59	MG	1A	4099	1/1	0.93	0.10	50,50,50,50	0
59	MG	1A	3529	1/1	0.93	0.41	33,33,33,33	0
59	MG	1A	4103	1/1	0.93	0.12	42,42,42,42	0
59	MG	2A	3561	1/1	0.93	0.10	31,31,31,31	0
59	MG	1W	201	1/1	0.93	0.20	39,39,39,39	0
59	MG	1A	3530	1/1	0.93	0.08	32,32,32,32	0
59	MG	2A	3071	1/1	0.93	0.12	50,50,50,50	0
59	MG	1A	3430	1/1	0.93	0.23	32,32,32,32	0
59	MG	1A	3535	1/1	0.93	0.14	37,37,37,37	0
59	MG	2A	3074	1/1	0.93	0.07	49,49,49,49	0
59	MG	2a	3225	1/1	0.93	0.14	59,59,59,59	0
59	MG	2A	3570	1/1	0.93	0.09	64,64,64,64	0
59	MG	1A	3202	1/1	0.93	0.09	43,43,43,43	0
59	MG	1Z	304	1/1	0.93	0.21	50,50,50,50	0
59	MG	2a	3231	1/1	0.93	0.17	57,57,57,57	0
59	MG	10	105	1/1	0.93	0.14	40,40,40,40	0
59	MG	2A	3576	1/1	0.93	0.10	64,64,64,64	0
59	MG	1A	3714	1/1	0.93	0.07	10,10,10,10	0
59	MG	1A	3203	1/1	0.93	0.16	53,53,53,53	0
59	MG	2E	304	1/1	0.93	0.20	59,59,59,59	0
59	MG	2E	305	1/1	0.93	0.12	43,43,43,43	0
59	MG	2A	3081	1/1	0.93	0.08	45,45,45,45	0
59	MG	2e	3001	1/1	0.93	0.13	62,62,62,62	0
59	MG	1A	4113	1/1	0.93	0.07	35,35,35,35	0
59	MG	2A	3302	1/1	0.93	0.37	57,57,57,57	0
59	MG	11	103	1/1	0.93	0.16	70,70,70,70	0
59	MG	1A	3543	1/1	0.93	0.09	17,17,17,17	0
59	MG	1A	3362	1/1	0.93	0.11	53,53,53,53	0
59	MG	15	103	1/1	0.93	0.11	54,54,54,54	0
59	MG	1A	3366	1/1	0.93	0.14	58,58,58,58	0
59	MG	1A	3547	1/1	0.93	0.10	29,29,29,29	0
59	MG	2A	3094	1/1	0.93	0.14	43,43,43,43	0
59	MG	1A	3551	1/1	0.93	0.10	29,29,29,29	0
59	MG	1A	3734	1/1	0.93	0.12	45,45,45,45	0
59	MG	1A	3304	1/1	0.93	0.15	36,36,36,36	0
59	MG	1A	3206	1/1	0.93	0.12	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1a	3503	1/1	0.93	0.10	71,71,71,71	0
59	MG	1A	3258	1/1	0.93	0.15	26,26,26,26	0
59	MG	1A	3567	1/1	0.93	0.07	27,27,27,27	0
59	MG	2T	203	1/1	0.93	0.23	50,50,50,50	0
59	MG	1A	4128	1/1	0.93	0.12	53,53,53,53	0
59	MG	2U	203	1/1	0.93	0.24	56,56,56,56	0
59	MG	1A	4129	1/1	0.93	0.10	55,55,55,55	0
59	MG	1a	3317	1/1	0.93	0.07	41,41,41,41	0
59	MG	2A	3321	1/1	0.93	0.08	58,58,58,58	0
59	MG	2A	3608	1/1	0.93	0.14	60,60,60,60	0
59	MG	25	103	1/1	0.93	0.15	42,42,42,42	0
59	MG	1A	3372	1/1	0.93	0.20	37,37,37,37	0
59	MG	1A	3945	1/1	0.93	0.08	59,59,59,59	0
59	MG	1A	3947	1/1	0.93	0.13	58,58,58,58	0
59	MG	1a	3519	1/1	0.93	0.19	65,65,65,65	0
59	MG	1A	3748	1/1	0.93	0.29	24,24,24,24	0
59	MG	1A	3092	1/1	0.93	0.23	32,32,32,32	0
59	MG	2A	3331	1/1	0.93	0.08	58,58,58,58	0
59	MG	1a	3532	1/1	0.93	0.08	57,57,57,57	0
59	MG	2A	3334	1/1	0.93	0.18	61,61,61,61	0
59	MG	2A	3131	1/1	0.93	0.23	51,51,51,51	0
59	MG	1A	3950	1/1	0.93	0.14	47,47,47,47	0
59	MG	2A	3138	1/1	0.93	0.20	45,45,45,45	0
59	MG	1A	3897	1/1	0.94	0.09	38,38,38,38	0
59	MG	1A	3631	1/1	0.94	0.18	16,16,16,16	0
59	MG	1A	3285	1/1	0.94	0.14	42,42,42,42	0
59	MG	1A	3900	1/1	0.94	0.09	53,53,53,53	0
59	MG	1A	3763	1/1	0.94	0.12	46,46,46,46	0
59	MG	1A	3903	1/1	0.94	0.08	29,29,29,29	0
59	MG	1A	3765	1/1	0.94	0.15	33,33,33,33	0
59	MG	1A	3327	1/1	0.94	0.39	42,42,42,42	0
59	MG	1A	3443	1/1	0.94	0.23	49,49,49,49	0
59	MG	1D	301	1/1	0.94	0.22	24,24,24,24	0
59	MG	1A	3114	1/1	0.94	0.12	36,36,36,36	0
59	MG	1D	308	1/1	0.94	0.18	27,27,27,27	0
59	MG	1A	3288	1/1	0.94	0.22	50,50,50,50	0
59	MG	2A	3670	1/1	0.94	0.10	64,64,64,64	0
59	MG	1A	3149	1/1	0.94	0.07	20,20,20,20	0
59	MG	2A	3672	1/1	0.94	0.08	58,58,58,58	0
59	MG	1A	3913	1/1	0.94	0.11	21,21,21,21	0
59	MG	1A	3253	1/1	0.94	0.16	37,37,37,37	0
59	MG	2A	3676	1/1	0.94	0.08	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1E	302	1/1	0.94	0.11	47,47,47,47	0
59	MG	2A	3395	1/1	0.94	0.07	28,28,28,28	0
59	MG	2A	3187	1/1	0.94	0.45	37,37,37,37	0
59	MG	1A	3916	1/1	0.94	0.08	12,12,12,12	0
59	MG	2A	3400	1/1	0.94	0.08	21,21,21,21	0
59	MG	2A	3401	1/1	0.94	0.12	59,59,59,59	0
59	MG	1a	3392	1/1	0.94	0.21	45,45,45,45	0
59	MG	1A	3451	1/1	0.94	0.17	38,38,38,38	0
59	MG	1A	4092	1/1	0.94	0.13	45,45,45,45	0
59	MG	1A	3919	1/1	0.94	0.05	67,67,67,67	0
59	MG	1A	3527	1/1	0.94	0.16	22,22,22,22	0
59	MG	1A	3923	1/1	0.94	0.07	46,46,46,46	0
59	MG	2A	3197	1/1	0.94	0.17	50,50,50,50	0
59	MG	1F	301	1/1	0.94	0.14	50,50,50,50	0
59	MG	1A	3184	1/1	0.94	0.10	42,42,42,42	0
59	MG	1A	3079	1/1	0.94	0.13	46,46,46,46	0
59	MG	2A	3418	1/1	0.94	0.07	46,46,46,46	0
59	MG	1x	101	1/1	0.94	0.10	38,38,38,38	0
59	MG	1A	3780	1/1	0.94	0.07	10,10,10,10	0
59	MG	1A	3121	1/1	0.94	0.09	37,37,37,37	0
59	MG	1G	3002	1/1	0.94	0.16	53,53,53,53	0
59	MG	2A	3430	1/1	0.94	0.07	29,29,29,29	0
59	MG	1A	3534	1/1	0.94	0.08	38,38,38,38	0
59	MG	1x	108	1/1	0.94	0.23	53,53,53,53	0
59	MG	2A	3435	1/1	0.94	0.08	47,47,47,47	0
59	MG	1A	3456	1/1	0.94	0.09	50,50,50,50	0
59	MG	1A	3784	1/1	0.94	0.09	14,14,14,14	0
59	MG	1A	3391	1/1	0.94	0.14	41,41,41,41	0
59	MG	2a	3072	1/1	0.94	0.32	50,50,50,50	0
59	MG	1N	3005	1/1	0.94	0.12	51,51,51,51	0
59	MG	1N	3006	1/1	0.94	0.19	41,41,41,41	0
59	MG	1N	3007	1/1	0.94	0.27	49,49,49,49	0
59	MG	1x	115	1/1	0.94	0.12	56,56,56,56	0
59	MG	1A	3299	1/1	0.94	0.09	49,49,49,49	0
59	MG	1A	3393	1/1	0.94	0.16	47,47,47,47	0
59	MG	1A	3342	1/1	0.94	0.09	42,42,42,42	0
59	MG	1O	3005	1/1	0.94	0.13	40,40,40,40	0
59	MG	2A	3453	1/1	0.94	0.11	60,60,60,60	0
59	MG	1A	4114	1/1	0.94	0.14	57,57,57,57	0
59	MG	1A	3220	1/1	0.94	0.21	25,25,25,25	0
59	MG	2A	3220	1/1	0.94	0.18	68,68,68,68	0
59	MG	2A	3002	1/1	0.94	0.28	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	3221	1/1	0.94	0.15	40,40,40,40	0
59	MG	2A	3464	1/1	0.94	0.15	46,46,46,46	0
59	MG	2A	3465	1/1	0.94	0.11	54,54,54,54	0
59	MG	1a	3423	1/1	0.94	0.28	53,53,53,53	0
59	MG	1A	3043	1/1	0.94	0.12	21,21,21,21	0
59	MG	1A	3347	1/1	0.94	0.18	40,40,40,40	0
59	MG	2A	3227	1/1	0.94	0.20	47,47,47,47	0
59	MG	2A	3015	1/1	0.94	0.10	57,57,57,57	0
59	MG	2A	3756	1/1	0.94	0.11	51,51,51,51	0
59	MG	1A	3473	1/1	0.94	0.32	54,54,54,54	0
59	MG	1A	3965	1/1	0.94	0.09	46,46,46,46	0
59	MG	1A	3403	1/1	0.94	0.22	33,33,33,33	0
59	MG	2a	3100	1/1	0.94	0.26	51,51,51,51	0
59	MG	1A	3348	1/1	0.94	0.08	56,56,56,56	0
59	MG	1A	3157	1/1	0.94	0.11	37,37,37,37	0
59	MG	1a	3431	1/1	0.94	0.12	38,38,38,38	0
59	MG	2A	3479	1/1	0.94	0.09	26,26,26,26	0
59	MG	1A	3969	1/1	0.94	0.09	36,36,36,36	0
59	MG	1A	3068	1/1	0.94	0.18	53,53,53,53	0
59	MG	1U	204	1/1	0.94	0.06	36,36,36,36	0
59	MG	2A	3484	1/1	0.94	0.10	33,33,33,33	0
59	MG	1A	3803	1/1	0.94	0.18	33,33,33,33	0
59	MG	1A	3804	1/1	0.94	0.22	27,27,27,27	0
59	MG	1a	3437	1/1	0.94	0.34	58,58,58,58	0
59	MG	1X	3004	1/1	0.94	0.07	49,49,49,49	0
59	MG	2A	3245	1/1	0.94	0.12	48,48,48,48	0
59	MG	1A	3023	1/1	0.94	0.37	24,24,24,24	0
59	MG	2A	3036	1/1	0.94	0.09	49,49,49,49	0
59	MG	1a	3440	1/1	0.94	0.07	50,50,50,50	0
59	MG	2A	3496	1/1	0.94	0.13	49,49,49,49	0
59	MG	1A	3981	1/1	0.94	0.07	13,13,13,13	0
59	MG	2A	3251	1/1	0.94	0.08	40,40,40,40	0
59	MG	2A	3499	1/1	0.94	0.18	53,53,53,53	0
59	MG	1Y	504	1/1	0.94	0.24	45,45,45,45	0
59	MG	1a	3447	1/1	0.94	0.14	51,51,51,51	0
59	MG	2A	3254	1/1	0.94	0.07	47,47,47,47	0
59	MG	2A	3509	1/1	0.94	0.10	40,40,40,40	0
59	MG	1A	3352	1/1	0.94	0.08	43,43,43,43	0
59	MG	2a	3128	1/1	0.94	0.07	59,59,59,59	0
59	MG	1A	3483	1/1	0.94	0.12	56,56,56,56	0
59	MG	2A	3046	1/1	0.94	0.19	58,58,58,58	0
59	MG	1A	3985	1/1	0.94	0.10	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3515	1/1	0.94	0.08	39,39,39,39	0
59	MG	10	101	1/1	0.94	0.17	41,41,41,41	0
59	MG	1A	3686	1/1	0.94	0.08	29,29,29,29	0
59	MG	2A	3518	1/1	0.94	0.19	51,51,51,51	0
59	MG	2A	3519	1/1	0.94	0.13	62,62,62,62	0
59	MG	2A	3050	1/1	0.94	0.13	48,48,48,48	0
59	MG	2a	3143	1/1	0.94	0.08	43,43,43,43	0
59	MG	1A	4142	1/1	0.94	0.07	47,47,47,47	0
59	MG	2A	3263	1/1	0.94	0.20	47,47,47,47	0
59	MG	2a	3149	1/1	0.94	0.08	58,58,58,58	0
59	MG	2A	3803	1/1	0.94	0.08	50,50,50,50	0
59	MG	2A	3804	1/1	0.94	0.11	59,59,59,59	0
59	MG	2a	3152	1/1	0.94	0.07	65,65,65,65	0
59	MG	1a	3461	1/1	0.94	0.10	41,41,41,41	0
59	MG	1A	3052	1/1	0.94	0.25	45,45,45,45	0
59	MG	1A	3813	1/1	0.94	0.07	15,15,15,15	0
59	MG	2A	3056	1/1	0.94	0.14	56,56,56,56	0
59	MG	1A	3354	1/1	0.94	0.21	37,37,37,37	0
59	MG	2A	3269	1/1	0.94	0.12	50,50,50,50	0
59	MG	1a	3470	1/1	0.94	0.08	49,49,49,49	0
59	MG	2a	3162	1/1	0.94	0.09	55,55,55,55	0
59	MG	1a	3471	1/1	0.94	0.11	51,51,51,51	0
59	MG	1A	4149	1/1	0.94	0.10	47,47,47,47	0
59	MG	2a	3165	1/1	0.94	0.08	68,68,68,68	0
59	MG	2A	3820	1/1	0.94	0.17	35,35,35,35	0
59	MG	1a	3473	1/1	0.94	0.16	37,37,37,37	0
59	MG	2A	3823	1/1	0.94	0.18	47,47,47,47	0
59	MG	2A	3824	1/1	0.94	0.14	43,43,43,43	0
59	MG	1A	3991	1/1	0.94	0.12	40,40,40,40	0
59	MG	2a	3172	1/1	0.94	0.14	42,42,42,42	0
59	MG	13	3002	1/1	0.94	0.07	37,37,37,37	0
59	MG	1A	3579	1/1	0.94	0.08	30,30,30,30	0
59	MG	2a	3175	1/1	0.94	0.09	58,58,58,58	0
59	MG	1A	4154	1/1	0.94	0.07	38,38,38,38	0
59	MG	2A	3832	1/1	0.94	0.18	53,53,53,53	0
59	MG	2A	3834	1/1	0.94	0.08	42,42,42,42	0
59	MG	1A	3695	1/1	0.94	0.07	20,20,20,20	0
59	MG	1A	3488	1/1	0.94	0.08	45,45,45,45	0
59	MG	18	103	1/1	0.94	0.12	38,38,38,38	0
59	MG	1a	3486	1/1	0.94	0.13	59,59,59,59	0
59	MG	1A	3698	1/1	0.94	0.10	16,16,16,16	0
59	MG	1A	4164	1/1	0.94	0.08	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3841	1/1	0.94	0.08	59,59,59,59	0
59	MG	2A	3548	1/1	0.94	0.08	36,36,36,36	0
59	MG	1A	3075	1/1	0.94	0.28	29,29,29,29	0
59	MG	2A	3078	1/1	0.94	0.09	33,33,33,33	0
59	MG	1A	4172	1/1	0.94	0.30	44,44,44,44	0
59	MG	1A	3700	1/1	0.94	0.07	20,20,20,20	0
59	MG	2A	3847	1/1	0.94	0.31	37,37,37,37	0
59	MG	1a	3309	1/1	0.94	0.24	61,61,61,61	0
59	MG	1A	3416	1/1	0.94	0.14	52,52,52,52	0
59	MG	1a	3497	1/1	0.94	0.11	65,65,65,65	0
59	MG	1A	3709	1/1	0.94	0.07	20,20,20,20	0
59	MG	2a	3197	1/1	0.94	0.11	54,54,54,54	0
59	MG	1a	3501	1/1	0.94	0.07	57,57,57,57	0
59	MG	1A	3357	1/1	0.94	0.24	45,45,45,45	0
59	MG	1A	3713	1/1	0.94	0.12	49,49,49,49	0
59	MG	1A	3492	1/1	0.94	0.17	55,55,55,55	0
59	MG	2A	3562	1/1	0.94	0.10	57,57,57,57	0
59	MG	2A	3091	1/1	0.94	0.11	44,44,44,44	0
59	MG	2A	3093	1/1	0.94	0.27	56,56,56,56	0
59	MG	1A	3720	1/1	0.94	0.07	34,34,34,34	0
59	MG	1A	3037	1/1	0.94	0.18	37,37,37,37	0
59	MG	1A	3311	1/1	0.94	0.12	39,39,39,39	0
59	MG	1A	4189	1/1	0.94	0.10	44,44,44,44	0
59	MG	1A	3313	1/1	0.94	0.08	38,38,38,38	0
59	MG	1A	4024	1/1	0.94	0.09	46,46,46,46	0
59	MG	1A	4192	1/1	0.94	0.31	29,29,29,29	0
59	MG	2A	3103	1/1	0.94	0.25	62,62,62,62	0
59	MG	2A	3575	1/1	0.94	0.13	60,60,60,60	0
59	MG	1A	3500	1/1	0.94	0.11	54,54,54,54	0
59	MG	2D	301	1/1	0.94	0.21	47,47,47,47	0
59	MG	1a	3526	1/1	0.94	0.18	50,50,50,50	0
59	MG	1a	3527	1/1	0.94	0.07	62,62,62,62	0
59	MG	1a	3528	1/1	0.94	0.07	59,59,59,59	0
59	MG	1a	3530	1/1	0.94	0.08	62,62,62,62	0
59	MG	2A	3114	1/1	0.94	0.15	39,39,39,39	0
59	MG	2A	3117	1/1	0.94	0.14	60,60,60,60	0
59	MG	1A	4027	1/1	0.94	0.05	45,45,45,45	0
59	MG	1A	3847	1/1	0.94	0.06	25,25,25,25	0
59	MG	2A	3589	1/1	0.94	0.08	46,46,46,46	0
59	MG	1A	4203	1/1	0.94	0.20	33,33,33,33	0
59	MG	2A	3323	1/1	0.94	0.27	47,47,47,47	0
59	MG	2F	302	1/1	0.94	0.13	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	3204	1/1	0.94	0.20	23,23,23,23	0
59	MG	1a	3338	1/1	0.94	0.20	51,51,51,51	0
59	MG	1A	3363	1/1	0.94	0.13	30,30,30,30	0
59	MG	1a	3540	1/1	0.94	0.07	36,36,36,36	0
59	MG	2A	3328	1/1	0.94	0.28	51,51,51,51	0
59	MG	2P	201	1/1	0.94	0.25	51,51,51,51	0
59	MG	2Q	3001	1/1	0.94	0.07	52,52,52,52	0
59	MG	1A	4212	1/1	0.94	0.11	32,32,32,32	0
59	MG	1A	3234	1/1	0.94	0.10	33,33,33,33	0
59	MG	1A	3048	1/1	0.94	0.07	39,39,39,39	0
59	MG	1A	4225	1/1	0.94	0.19	34,34,34,34	0
59	MG	2A	3333	1/1	0.94	0.11	60,60,60,60	0
59	MG	1a	3348	1/1	0.94	0.20	41,41,41,41	0
59	MG	2A	3142	1/1	0.94	0.11	58,58,58,58	0
59	MG	1a	3349	1/1	0.94	0.11	45,45,45,45	0
59	MG	1a	3547	1/1	0.94	0.09	48,48,48,48	0
59	MG	1A	3859	1/1	0.94	0.08	37,37,37,37	0
59	MG	2U	201	1/1	0.94	0.15	47,47,47,47	0
59	MG	1A	3860	1/1	0.94	0.07	37,37,37,37	0
59	MG	2q	204	1/1	0.94	0.10	70,70,70,70	0
59	MG	1A	3608	1/1	0.94	0.10	16,16,16,16	0
59	MG	2A	3148	1/1	0.94	0.13	65,65,65,65	0
59	MG	2V	201	1/1	0.94	0.18	60,60,60,60	0
59	MG	2X	3001	1/1	0.94	0.16	59,59,59,59	0
59	MG	2A	3615	1/1	0.94	0.09	46,46,46,46	0
59	MG	1A	3058	1/1	0.94	0.10	50,50,50,50	0
59	MG	1A	3874	1/1	0.94	0.10	13,13,13,13	0
59	MG	1A	3744	1/1	0.94	0.08	44,44,44,44	0
59	MG	1a	3357	1/1	0.94	0.13	58,58,58,58	0
59	MG	1A	3880	1/1	0.94	0.10	64,64,64,64	0
59	MG	1A	3881	1/1	0.94	0.15	47,47,47,47	0
59	MG	1A	4058	1/1	0.94	0.13	47,47,47,47	0
59	MG	1A	3210	1/1	0.94	0.08	35,35,35,35	0
59	MG	1A	3884	1/1	0.94	0.11	41,41,41,41	0
59	MG	1A	3371	1/1	0.94	0.22	39,39,39,39	0
59	MG	1A	3509	1/1	0.94	0.17	40,40,40,40	0
59	MG	1A	4064	1/1	0.94	0.11	30,30,30,30	0
59	MG	2A	3631	1/1	0.94	0.17	54,54,54,54	0
59	MG	2A	3632	1/1	0.94	0.08	29,29,29,29	0
59	MG	1A	3625	1/1	0.94	0.12	63,63,63,63	0
59	MG	1A	3281	1/1	0.94	0.22	43,43,43,43	0
59	MG	1A	3139	1/1	0.94	0.09	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3167	1/1	0.94	0.34	57,57,57,57	0
59	MG	1A	3247	1/1	0.94	0.18	47,47,47,47	0
59	MG	1a	3570	1/1	0.94	0.20	47,47,47,47	0
59	MG	A	8001	1/1	0.94	0.10	57,57,57,57	0
59	MG	2A	3134	1/1	0.95	0.19	58,58,58,58	0
59	MG	1a	3307	1/1	0.95	0.27	51,51,51,51	0
59	MG	2A	3351	1/1	0.95	0.07	56,56,56,56	0
59	MG	1a	3308	1/1	0.95	0.07	44,44,44,44	0
59	MG	1A	3980	1/1	0.95	0.09	39,39,39,39	0
59	MG	1A	4152	1/1	0.95	0.08	21,21,21,21	0
59	MG	2A	3633	1/1	0.95	0.07	37,37,37,37	0
59	MG	2A	3355	1/1	0.95	0.13	44,44,44,44	0
59	MG	1A	3453	1/1	0.95	0.10	18,18,18,18	0
59	MG	1A	3194	1/1	0.95	0.20	45,45,45,45	0
59	MG	1a	3320	1/1	0.95	0.18	51,51,51,51	0
59	MG	1A	3983	1/1	0.95	0.11	63,63,63,63	0
59	MG	1A	3538	1/1	0.95	0.10	20,20,20,20	0
59	MG	2A	3643	1/1	0.95	0.06	48,48,48,48	0
59	MG	1a	3323	1/1	0.95	0.14	43,43,43,43	0
59	MG	2A	3363	1/1	0.95	0.14	47,47,47,47	0
59	MG	1A	4160	1/1	0.95	0.09	53,53,53,53	0
59	MG	1A	4161	1/1	0.95	0.06	35,35,35,35	0
59	MG	1A	3539	1/1	0.95	0.08	26,26,26,26	0
59	MG	2a	3026	1/1	0.95	0.27	47,47,47,47	0
59	MG	1A	3542	1/1	0.95	0.09	41,41,41,41	0
59	MG	2A	3656	1/1	0.95	0.06	40,40,40,40	0
59	MG	2A	3657	1/1	0.95	0.08	60,60,60,60	0
59	MG	1A	4167	1/1	0.95	0.05	19,19,19,19	0
59	MG	2A	3661	1/1	0.95	0.11	54,54,54,54	0
59	MG	2a	3032	1/1	0.95	0.08	54,54,54,54	0
59	MG	1A	3987	1/1	0.95	0.07	47,47,47,47	0
59	MG	1A	3807	1/1	0.95	0.13	21,21,21,21	0
59	MG	2A	3373	1/1	0.95	0.07	31,31,31,31	0
59	MG	2A	3665	1/1	0.95	0.10	38,38,38,38	0
59	MG	1a	3332	1/1	0.95	0.12	38,38,38,38	0
59	MG	1A	3384	1/1	0.95	0.08	40,40,40,40	0
59	MG	2a	3039	1/1	0.95	0.09	55,55,55,55	0
59	MG	1A	3385	1/1	0.95	0.17	39,39,39,39	0
59	MG	1A	3329	1/1	0.95	0.09	51,51,51,51	0
59	MG	1A	4177	1/1	0.95	0.19	29,29,29,29	0
59	MG	1A	3229	1/1	0.95	0.07	45,45,45,45	0
59	MG	2A	3673	1/1	0.95	0.07	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	3996	1/1	0.95	0.08	35,35,35,35	0
59	MG	1a	3339	1/1	0.95	0.14	54,54,54,54	0
59	MG	1a	3340	1/1	0.95	0.10	53,53,53,53	0
59	MG	1A	3679	1/1	0.95	0.07	50,50,50,50	0
59	MG	1a	3342	1/1	0.95	0.07	42,42,42,42	0
59	MG	2A	3679	1/1	0.95	0.11	79,79,79,79	0
59	MG	1A	4000	1/1	0.95	0.12	47,47,47,47	0
59	MG	2A	3392	1/1	0.95	0.07	58,58,58,58	0
59	MG	1A	4002	1/1	0.95	0.06	44,44,44,44	0
59	MG	1A	3815	1/1	0.95	0.10	25,25,25,25	0
59	MG	1A	3818	1/1	0.95	0.09	14,14,14,14	0
59	MG	2a	3060	1/1	0.95	0.20	49,49,49,49	0
59	MG	1A	4006	1/1	0.95	0.06	31,31,31,31	0
59	MG	1A	3230	1/1	0.95	0.23	40,40,40,40	0
59	MG	1A	3682	1/1	0.95	0.10	48,48,48,48	0
59	MG	2A	3403	1/1	0.95	0.10	38,38,38,38	0
59	MG	1A	3552	1/1	0.95	0.10	7,7,7,7	0
59	MG	1a	3568	1/1	0.95	0.06	53,53,53,53	0
59	MG	2A	3697	1/1	0.95	0.07	25,25,25,25	0
59	MG	1A	3687	1/1	0.95	0.16	54,54,54,54	0
59	MG	2A	3408	1/1	0.95	0.12	56,56,56,56	0
59	MG	2a	3071	1/1	0.95	0.14	51,51,51,51	0
59	MG	1A	4195	1/1	0.95	0.17	27,27,27,27	0
59	MG	1A	3231	1/1	0.95	0.17	39,39,39,39	0
59	MG	1A	3689	1/1	0.95	0.08	41,41,41,41	0
59	MG	1a	3573	1/1	0.95	0.20	37,37,37,37	0
59	MG	1A	3463	1/1	0.95	0.20	24,24,24,24	0
59	MG	1A	3691	1/1	0.95	0.13	39,39,39,39	0
59	MG	2A	3417	1/1	0.95	0.10	31,31,31,31	0
59	MG	1A	4016	1/1	0.95	0.11	24,24,24,24	0
59	MG	1A	4213	1/1	0.95	0.14	24,24,24,24	0
59	MG	1A	4017	1/1	0.95	0.09	44,44,44,44	0
59	MG	1A	3333	1/1	0.95	0.16	35,35,35,35	0
59	MG	1A	3564	1/1	0.95	0.05	26,26,26,26	0
59	MG	1A	3334	1/1	0.95	0.11	39,39,39,39	0
59	MG	1A	3335	1/1	0.95	0.11	46,46,46,46	0
59	MG	2A	3433	1/1	0.95	0.08	38,38,38,38	0
59	MG	1A	3336	1/1	0.95	0.07	36,36,36,36	0
59	MG	1B	202	1/1	0.95	0.23	37,37,37,37	0
59	MG	1A	4026	1/1	0.95	0.08	45,45,45,45	0
59	MG	2A	3437	1/1	0.95	0.14	48,48,48,48	0
59	MG	1A	3156	1/1	0.95	0.11	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3196	1/1	0.95	0.10	51,51,51,51	0
59	MG	2a	3094	1/1	0.95	0.15	48,48,48,48	0
59	MG	1B	205	1/1	0.95	0.10	40,40,40,40	0
59	MG	2A	3443	1/1	0.95	0.07	30,30,30,30	0
59	MG	1A	3034	1/1	0.95	0.07	27,27,27,27	0
59	MG	1A	4031	1/1	0.95	0.09	47,47,47,47	0
59	MG	1B	210	1/1	0.95	0.09	51,51,51,51	0
59	MG	1w	101	1/1	0.95	0.11	56,56,56,56	0
59	MG	1B	211	1/1	0.95	0.30	52,52,52,52	0
59	MG	1w	103	1/1	0.95	0.14	56,56,56,56	0
59	MG	1a	3375	1/1	0.95	0.12	37,37,37,37	0
59	MG	1w	105	1/1	0.95	0.11	39,39,39,39	0
59	MG	1w	106	1/1	0.95	0.15	61,61,61,61	0
59	MG	2A	3753	1/1	0.95	0.13	52,52,52,52	0
59	MG	1a	3376	1/1	0.95	0.17	62,62,62,62	0
59	MG	1A	4033	1/1	0.95	0.06	45,45,45,45	0
59	MG	1A	3705	1/1	0.95	0.07	17,17,17,17	0
59	MG	1a	3379	1/1	0.95	0.08	49,49,49,49	0
59	MG	1A	3708	1/1	0.95	0.08	37,37,37,37	0
59	MG	1B	215	1/1	0.95	0.06	44,44,44,44	0
59	MG	1A	3398	1/1	0.95	0.11	49,49,49,49	0
59	MG	1A	3198	1/1	0.95	0.21	27,27,27,27	0
59	MG	2a	3115	1/1	0.95	0.27	59,59,59,59	0
59	MG	1B	219	1/1	0.95	0.05	28,28,28,28	0
59	MG	1A	4042	1/1	0.95	0.07	42,42,42,42	0
59	MG	1x	105	1/1	0.95	0.17	47,47,47,47	0
59	MG	2A	3767	1/1	0.95	0.13	59,59,59,59	0
59	MG	1A	3236	1/1	0.95	0.18	34,34,34,34	0
59	MG	1A	3402	1/1	0.95	0.12	42,42,42,42	0
59	MG	1A	3717	1/1	0.95	0.06	21,21,21,21	0
59	MG	2a	3123	1/1	0.95	0.16	55,55,55,55	0
59	MG	1A	3199	1/1	0.95	0.07	32,32,32,32	0
59	MG	2A	3772	1/1	0.95	0.11	35,35,35,35	0
59	MG	1A	4049	1/1	0.95	0.07	36,36,36,36	0
59	MG	1A	3721	1/1	0.95	0.08	14,14,14,14	0
59	MG	1A	3159	1/1	0.95	0.18	32,32,32,32	0
59	MG	1A	4054	1/1	0.95	0.20	57,57,57,57	0
59	MG	1a	3395	1/1	0.95	0.07	40,40,40,40	0
59	MG	2A	3482	1/1	0.95	0.08	40,40,40,40	0
59	MG	1A	3723	1/1	0.95	0.12	53,53,53,53	0
59	MG	2A	3230	1/1	0.95	0.12	42,42,42,42	0
59	MG	1A	3127	1/1	0.95	0.19	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	3875	1/1	0.95	0.14	54,54,54,54	0
59	MG	2a	3139	1/1	0.95	0.08	65,65,65,65	0
59	MG	1A	3107	1/1	0.95	0.27	32,32,32,32	0
59	MG	2A	3784	1/1	0.95	0.09	56,56,56,56	0
59	MG	2A	3488	1/1	0.95	0.23	54,54,54,54	0
59	MG	2a	3144	1/1	0.95	0.17	50,50,50,50	0
59	MG	1A	3877	1/1	0.95	0.06	44,44,44,44	0
59	MG	1A	3879	1/1	0.95	0.08	51,51,51,51	0
59	MG	2A	3001	1/1	0.95	0.32	49,49,49,49	0
59	MG	1A	3407	1/1	0.95	0.13	46,46,46,46	0
59	MG	1A	3294	1/1	0.95	0.12	30,30,30,30	0
59	MG	1D	305	1/1	0.95	0.11	29,29,29,29	0
59	MG	1A	3295	1/1	0.95	0.07	47,47,47,47	0
59	MG	1A	3164	1/1	0.95	0.26	27,27,27,27	0
59	MG	2A	3013	1/1	0.95	0.10	47,47,47,47	0
59	MG	2A	3500	1/1	0.95	0.11	27,27,27,27	0
59	MG	1A	3886	1/1	0.95	0.06	38,38,38,38	0
59	MG	2A	3503	1/1	0.95	0.06	32,32,32,32	0
59	MG	2A	3504	1/1	0.95	0.10	27,27,27,27	0
59	MG	2a	3161	1/1	0.95	0.10	72,72,72,72	0
59	MG	2A	3244	1/1	0.95	0.17	47,47,47,47	0
59	MG	1A	4068	1/1	0.95	0.06	38,38,38,38	0
59	MG	2A	3508	1/1	0.95	0.10	43,43,43,43	0
59	MG	1A	3888	1/1	0.95	0.06	31,31,31,31	0
59	MG	2A	3805	1/1	0.95	0.11	53,53,53,53	0
59	MG	1a	3411	1/1	0.95	0.28	47,47,47,47	0
59	MG	1A	3735	1/1	0.95	0.06	20,20,20,20	0
59	MG	1A	3298	1/1	0.95	0.16	57,57,57,57	0
59	MG	1A	3165	1/1	0.95	0.29	22,22,22,22	0
59	MG	1A	3250	1/1	0.95	0.11	49,49,49,49	0
59	MG	1A	3894	1/1	0.95	0.06	43,43,43,43	0
59	MG	1A	3743	1/1	0.95	0.10	38,38,38,38	0
59	MG	1A	3495	1/1	0.95	0.07	46,46,46,46	0
59	MG	1A	4079	1/1	0.95	0.15	68,68,68,68	0
59	MG	2A	3031	1/1	0.95	0.22	44,44,44,44	0
59	MG	1A	3496	1/1	0.95	0.18	50,50,50,50	0
59	MG	1F	306	1/1	0.95	0.09	40,40,40,40	0
59	MG	1A	3013	1/1	0.95	0.23	44,44,44,44	0
59	MG	1A	4084	1/1	0.95	0.11	45,45,45,45	0
59	MG	1A	3499	1/1	0.95	0.07	46,46,46,46	0
59	MG	1A	3751	1/1	0.95	0.07	21,21,21,21	0
59	MG	1A	3614	1/1	0.95	0.06	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	3615	1/1	0.95	0.17	55,55,55,55	0
59	MG	2A	3529	1/1	0.95	0.11	47,47,47,47	0
59	MG	2A	3043	1/1	0.95	0.12	57,57,57,57	0
59	MG	1A	3422	1/1	0.95	0.19	56,56,56,56	0
59	MG	1N	3001	1/1	0.95	0.28	52,52,52,52	0
59	MG	2a	3190	1/1	0.95	0.19	56,56,56,56	0
59	MG	1A	3756	1/1	0.95	0.07	26,26,26,26	0
59	MG	1A	3619	1/1	0.95	0.07	19,19,19,19	0
59	MG	1A	3908	1/1	0.95	0.07	55,55,55,55	0
59	MG	1A	3759	1/1	0.95	0.12	41,41,41,41	0
59	MG	1A	3423	1/1	0.95	0.10	41,41,41,41	0
59	MG	2A	3541	1/1	0.95	0.12	30,30,30,30	0
59	MG	1A	3761	1/1	0.95	0.13	49,49,49,49	0
59	MG	1A	4097	1/1	0.95	0.11	45,45,45,45	0
59	MG	1A	3014	1/1	0.95	0.14	38,38,38,38	0
59	MG	2A	3054	1/1	0.95	0.08	43,43,43,43	0
59	MG	2A	3280	1/1	0.95	0.08	49,49,49,49	0
59	MG	2B	3002	1/1	0.95	0.33	56,56,56,56	0
59	MG	1A	3028	1/1	0.95	0.05	34,34,34,34	0
59	MG	1A	3137	1/1	0.95	0.20	43,43,43,43	0
59	MG	1A	3766	1/1	0.95	0.06	21,21,21,21	0
59	MG	1a	3444	1/1	0.95	0.14	33,33,33,33	0
59	MG	2A	3059	1/1	0.95	0.06	37,37,37,37	0
59	MG	2A	3552	1/1	0.95	0.06	54,54,54,54	0
59	MG	1a	3446	1/1	0.95	0.08	48,48,48,48	0
59	MG	1A	3040	1/1	0.95	0.12	30,30,30,30	0
59	MG	1A	3259	1/1	0.95	0.21	41,41,41,41	0
59	MG	1a	3449	1/1	0.95	0.12	53,53,53,53	0
59	MG	1A	4107	1/1	0.95	0.11	17,17,17,17	0
59	MG	1A	3630	1/1	0.95	0.08	16,16,16,16	0
59	MG	1A	3215	1/1	0.95	0.28	33,33,33,33	0
59	MG	1A	3925	1/1	0.95	0.07	10,10,10,10	0
59	MG	1S	3003	1/1	0.95	0.06	61,61,61,61	0
59	MG	1A	3065	1/1	0.95	0.30	37,37,37,37	0
59	MG	1A	3772	1/1	0.95	0.20	46,46,46,46	0
59	MG	1A	3140	1/1	0.95	0.25	28,28,28,28	0
59	MG	1A	3432	1/1	0.95	0.20	47,47,47,47	0
59	MG	1a	3468	1/1	0.95	0.13	51,51,51,51	0
59	MG	2a	3224	1/1	0.95	0.19	58,58,58,58	0
59	MG	1A	3943	1/1	0.95	0.08	33,33,33,33	0
59	MG	1A	3364	1/1	0.95	0.28	34,34,34,34	0
59	MG	1W	202	1/1	0.95	0.09	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	3640	1/1	0.95	0.11	25,25,25,25	0
59	MG	2A	3572	1/1	0.95	0.08	24,24,24,24	0
59	MG	1A	4119	1/1	0.95	0.08	22,22,22,22	0
59	MG	2a	3233	1/1	0.95	0.08	50,50,50,50	0
59	MG	1A	3365	1/1	0.95	0.22	40,40,40,40	0
59	MG	1A	3779	1/1	0.95	0.17	36,36,36,36	0
59	MG	1A	3180	1/1	0.95	0.08	39,39,39,39	0
59	MG	2A	3086	1/1	0.95	0.18	30,30,30,30	0
59	MG	2A	3580	1/1	0.95	0.09	29,29,29,29	0
59	MG	1A	3115	1/1	0.95	0.07	24,24,24,24	0
59	MG	1A	3145	1/1	0.95	0.10	44,44,44,44	0
59	MG	2f	3001	1/1	0.95	0.09	38,38,38,38	0
59	MG	1A	3519	1/1	0.95	0.13	46,46,46,46	0
59	MG	2A	3090	1/1	0.95	0.17	53,53,53,53	0
59	MG	10	103	1/1	0.95	0.11	35,35,35,35	0
59	MG	1A	3050	1/1	0.95	0.15	31,31,31,31	0
59	MG	1A	3004	1/1	0.95	0.10	47,47,47,47	0
59	MG	1A	3224	1/1	0.95	0.14	49,49,49,49	0
59	MG	2A	3319	1/1	0.95	0.24	36,36,36,36	0
59	MG	1a	3491	1/1	0.95	0.08	75,75,75,75	0
59	MG	1A	3964	1/1	0.95	0.10	36,36,36,36	0
59	MG	2A	3322	1/1	0.95	0.34	42,42,42,42	0
59	MG	1A	3525	1/1	0.95	0.21	48,48,48,48	0
59	MG	1A	3444	1/1	0.95	0.10	45,45,45,45	0
59	MG	1A	4136	1/1	0.95	0.08	50,50,50,50	0
59	MG	1A	3272	1/1	0.95	0.12	36,36,36,36	0
59	MG	13	3003	1/1	0.95	0.10	42,42,42,42	0
59	MG	1A	3273	1/1	0.95	0.19	49,49,49,49	0
59	MG	2A	3106	1/1	0.95	0.09	57,57,57,57	0
59	MG	2A	3107	1/1	0.95	0.23	44,44,44,44	0
59	MG	2A	3604	1/1	0.95	0.12	46,46,46,46	0
59	MG	1A	4139	1/1	0.95	0.06	28,28,28,28	0
59	MG	1A	4140	1/1	0.95	0.05	31,31,31,31	0
59	MG	1A	3324	1/1	0.95	0.19	39,39,39,39	0
59	MG	18	102	1/1	0.95	0.22	37,37,37,37	0
59	MG	1A	3084	1/1	0.95	0.09	31,31,31,31	0
59	MG	1A	3192	1/1	0.95	0.21	27,27,27,27	0
59	MG	23	101	1/1	0.95	0.12	51,51,51,51	0
59	MG	2A	3121	1/1	0.95	0.19	49,49,49,49	0
59	MG	1a	3301	1/1	0.95	0.24	49,49,49,49	0
59	MG	2A	3339	1/1	0.95	0.33	50,50,50,50	0
59	MG	27	3001	1/1	0.95	0.28	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	3972	1/1	0.95	0.11	24,24,24,24	0
59	MG	2A	3125	1/1	0.95	0.07	30,30,30,30	0
59	MG	1A	3086	1/1	0.95	0.07	31,31,31,31	0
59	MG	1a	3517	1/1	0.95	0.07	60,60,60,60	0
59	MG	1A	3664	1/1	0.95	0.06	46,46,46,46	0
59	MG	2A	3130	1/1	0.95	0.24	46,46,46,46	0
59	MG	1A	4150	1/1	0.95	0.07	35,35,35,35	0
59	MG	2A	3133	1/1	0.95	0.16	48,48,48,48	0
59	MG	B	3001	1/1	0.95	0.14	46,46,46,46	0
59	MG	2A	3389	1/1	0.96	0.07	33,33,33,33	0
59	MG	1a	3577	1/1	0.96	0.08	50,50,50,50	0
59	MG	1A	3621	1/1	0.96	0.11	25,25,25,25	0
59	MG	1A	3267	1/1	0.96	0.13	42,42,42,42	0
59	MG	1A	3747	1/1	0.96	0.15	26,26,26,26	0
59	MG	2A	3396	1/1	0.96	0.07	41,41,41,41	0
59	MG	2A	3660	1/1	0.96	0.07	76,76,76,76	0
59	MG	1A	3369	1/1	0.96	0.28	31,31,31,31	0
59	MG	2A	3398	1/1	0.96	0.16	50,50,50,50	0
59	MG	1A	3750	1/1	0.96	0.09	42,42,42,42	0
59	MG	1A	3624	1/1	0.96	0.05	14,14,14,14	0
59	MG	1A	3032	1/1	0.96	0.20	26,26,26,26	0
59	MG	1A	3141	1/1	0.96	0.10	26,26,26,26	0
59	MG	1A	3320	1/1	0.96	0.09	41,41,41,41	0
59	MG	1A	3755	1/1	0.96	0.07	24,24,24,24	0
59	MG	1A	3901	1/1	0.96	0.06	59,59,59,59	0
59	MG	1A	3142	1/1	0.96	0.17	36,36,36,36	0
59	MG	1A	4069	1/1	0.96	0.08	48,48,48,48	0
59	MG	2A	3409	1/1	0.96	0.10	50,50,50,50	0
59	MG	1A	3183	1/1	0.96	0.08	39,39,39,39	0
59	MG	1A	3056	1/1	0.96	0.11	24,24,24,24	0
59	MG	1A	3144	1/1	0.96	0.41	35,35,35,35	0
59	MG	1A	3633	1/1	0.96	0.08	22,22,22,22	0
59	MG	1A	3634	1/1	0.96	0.06	12,12,12,12	0
59	MG	1A	3635	1/1	0.96	0.07	8,8,8,8	0
59	MG	1A	3764	1/1	0.96	0.06	54,54,54,54	0
59	MG	1A	3520	1/1	0.96	0.13	16,16,16,16	0
59	MG	2A	3420	1/1	0.96	0.09	28,28,28,28	0
59	MG	2A	3421	1/1	0.96	0.14	42,42,42,42	0
59	MG	1A	3379	1/1	0.96	0.10	37,37,37,37	0
59	MG	1A	3914	1/1	0.96	0.06	21,21,21,21	0
59	MG	2A	3424	1/1	0.96	0.08	31,31,31,31	0
59	MG	2A	3195	1/1	0.96	0.21	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	3094	1/1	0.96	0.25	28,28,28,28	0
59	MG	2A	3429	1/1	0.96	0.07	56,56,56,56	0
59	MG	1D	306	1/1	0.96	0.15	40,40,40,40	0
59	MG	1A	3448	1/1	0.96	0.28	36,36,36,36	0
59	MG	1A	3917	1/1	0.96	0.09	15,15,15,15	0
59	MG	2A	3700	1/1	0.96	0.07	35,35,35,35	0
59	MG	1A	3524	1/1	0.96	0.14	31,31,31,31	0
59	MG	2a	3056	1/1	0.96	0.08	47,47,47,47	0
59	MG	2A	3704	1/1	0.96	0.06	53,53,53,53	0
59	MG	1A	3146	1/1	0.96	0.13	34,34,34,34	0
59	MG	1A	3190	1/1	0.96	0.10	39,39,39,39	0
59	MG	1A	3191	1/1	0.96	0.15	45,45,45,45	0
59	MG	2A	3709	1/1	0.96	0.07	46,46,46,46	0
59	MG	1A	3279	1/1	0.96	0.14	45,45,45,45	0
59	MG	2A	3715	1/1	0.96	0.09	61,61,61,61	0
59	MG	2A	3439	1/1	0.96	0.06	32,32,32,32	0
59	MG	1x	106	1/1	0.96	0.20	57,57,57,57	0
59	MG	2A	3719	1/1	0.96	0.06	64,64,64,64	0
59	MG	2A	3720	1/1	0.96	0.06	42,42,42,42	0
59	MG	1E	306	1/1	0.96	0.13	31,31,31,31	0
59	MG	1A	3646	1/1	0.96	0.06	8,8,8,8	0
59	MG	2A	3444	1/1	0.96	0.10	31,31,31,31	0
59	MG	1A	3280	1/1	0.96	0.08	39,39,39,39	0
59	MG	1E	309	1/1	0.96	0.09	47,47,47,47	0
59	MG	1E	310	1/1	0.96	0.11	34,34,34,34	0
59	MG	1E	311	1/1	0.96	0.10	15,15,15,15	0
59	MG	2A	3449	1/1	0.96	0.11	17,17,17,17	0
59	MG	1A	3776	1/1	0.96	0.07	55,55,55,55	0
59	MG	1A	3931	1/1	0.96	0.06	64,64,64,64	0
59	MG	1A	3932	1/1	0.96	0.05	49,49,49,49	0
59	MG	1A	3933	1/1	0.96	0.08	25,25,25,25	0
59	MG	1A	3934	1/1	0.96	0.07	16,16,16,16	0
59	MG	1F	304	1/1	0.96	0.12	21,21,21,21	0
59	MG	1A	3531	1/1	0.96	0.24	28,28,28,28	0
59	MG	1A	4100	1/1	0.96	0.08	50,50,50,50	0
59	MG	1F	308	1/1	0.96	0.09	45,45,45,45	0
59	MG	2A	3463	1/1	0.96	0.09	43,43,43,43	0
59	MG	1A	3940	1/1	0.96	0.06	27,27,27,27	0
59	MG	1A	3095	1/1	0.96	0.09	23,23,23,23	0
59	MG	1A	3282	1/1	0.96	0.19	36,36,36,36	0
59	MG	2A	3746	1/1	0.96	0.09	48,48,48,48	0
59	MG	1A	3944	1/1	0.96	0.07	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	3151	1/1	0.96	0.06	15,15,15,15	0
59	MG	1G	3005	1/1	0.96	0.09	51,51,51,51	0
59	MG	2A	3009	1/1	0.96	0.05	31,31,31,31	0
59	MG	2A	3010	1/1	0.96	0.06	36,36,36,36	0
59	MG	1A	4108	1/1	0.96	0.06	32,32,32,32	0
59	MG	1A	3458	1/1	0.96	0.08	38,38,38,38	0
59	MG	1a	3417	1/1	0.96	0.33	50,50,50,50	0
59	MG	1N	3002	1/1	0.96	0.09	44,44,44,44	0
59	MG	1N	3003	1/1	0.96	0.25	37,37,37,37	0
59	MG	1A	3096	1/1	0.96	0.14	32,32,32,32	0
59	MG	2A	3759	1/1	0.96	0.08	52,52,52,52	0
59	MG	1A	3460	1/1	0.96	0.13	50,50,50,50	0
59	MG	1A	3119	1/1	0.96	0.07	33,33,33,33	0
59	MG	2A	3762	1/1	0.96	0.09	47,47,47,47	0
59	MG	1A	3540	1/1	0.96	0.10	47,47,47,47	0
59	MG	1A	3659	1/1	0.96	0.14	50,50,50,50	0
59	MG	1A	3953	1/1	0.96	0.06	64,64,64,64	0
59	MG	2A	3027	1/1	0.96	0.11	39,39,39,39	0
59	MG	1O	3002	1/1	0.96	0.30	41,41,41,41	0
59	MG	1A	3541	1/1	0.96	0.09	20,20,20,20	0
59	MG	2A	3030	1/1	0.96	0.12	50,50,50,50	0
59	MG	1A	3235	1/1	0.96	0.18	34,34,34,34	0
59	MG	1A	3337	1/1	0.96	0.18	48,48,48,48	0
59	MG	2A	3248	1/1	0.96	0.14	52,52,52,52	0
59	MG	1A	3287	1/1	0.96	0.20	38,38,38,38	0
59	MG	1A	4120	1/1	0.96	0.06	33,33,33,33	0
59	MG	2A	3495	1/1	0.96	0.13	37,37,37,37	0
59	MG	1Q	201	1/1	0.96	0.07	25,25,25,25	0
59	MG	1A	3070	1/1	0.96	0.12	25,25,25,25	0
59	MG	1A	3397	1/1	0.96	0.18	38,38,38,38	0
59	MG	2A	3040	1/1	0.96	0.14	40,40,40,40	0
59	MG	1Q	205	1/1	0.96	0.06	37,37,37,37	0
59	MG	1Q	206	1/1	0.96	0.07	39,39,39,39	0
59	MG	2A	3502	1/1	0.96	0.15	42,42,42,42	0
59	MG	1A	4123	1/1	0.96	0.07	46,46,46,46	0
59	MG	1A	3549	1/1	0.96	0.07	40,40,40,40	0
59	MG	2a	3129	1/1	0.96	0.09	75,75,75,75	0
59	MG	1A	3123	1/1	0.96	0.23	28,28,28,28	0
59	MG	1A	3472	1/1	0.96	0.10	26,26,26,26	0
59	MG	1a	3442	1/1	0.96	0.13	59,59,59,59	0
59	MG	1A	3676	1/1	0.96	0.06	29,29,29,29	0
59	MG	1A	3554	1/1	0.96	0.12	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3790	1/1	0.96	0.12	37,37,37,37	0
59	MG	1A	3555	1/1	0.96	0.09	48,48,48,48	0
59	MG	1A	3238	1/1	0.96	0.23	41,41,41,41	0
59	MG	1A	3805	1/1	0.96	0.26	30,30,30,30	0
59	MG	1U	205	1/1	0.96	0.22	29,29,29,29	0
59	MG	2a	3142	1/1	0.96	0.06	67,67,67,67	0
59	MG	1a	3450	1/1	0.96	0.14	51,51,51,51	0
59	MG	1a	3452	1/1	0.96	0.06	40,40,40,40	0
59	MG	1A	3974	1/1	0.96	0.07	17,17,17,17	0
59	MG	1A	3975	1/1	0.96	0.15	23,23,23,23	0
59	MG	1a	3455	1/1	0.96	0.06	27,27,27,27	0
59	MG	1a	3456	1/1	0.96	0.14	32,32,32,32	0
59	MG	1A	3098	1/1	0.96	0.20	30,30,30,30	0
59	MG	2A	3802	1/1	0.96	0.07	35,35,35,35	0
59	MG	1W	203	1/1	0.96	0.19	29,29,29,29	0
59	MG	2A	3276	1/1	0.96	0.12	32,32,32,32	0
59	MG	2A	3063	1/1	0.96	0.06	40,40,40,40	0
59	MG	1X	3001	1/1	0.96	0.13	30,30,30,30	0
59	MG	2A	3807	1/1	0.96	0.09	38,38,38,38	0
59	MG	1A	3979	1/1	0.96	0.06	35,35,35,35	0
59	MG	1A	3681	1/1	0.96	0.05	23,23,23,23	0
59	MG	2A	3282	1/1	0.96	0.30	54,54,54,54	0
59	MG	1A	3240	1/1	0.96	0.17	31,31,31,31	0
59	MG	1A	3478	1/1	0.96	0.27	42,42,42,42	0
59	MG	2A	3070	1/1	0.96	0.07	42,42,42,42	0
59	MG	1Z	301	1/1	0.96	0.11	34,34,34,34	0
59	MG	2A	3817	1/1	0.96	0.12	32,32,32,32	0
59	MG	2A	3818	1/1	0.96	0.07	63,63,63,63	0
59	MG	2A	3534	1/1	0.96	0.13	58,58,58,58	0
59	MG	1A	3565	1/1	0.96	0.06	28,28,28,28	0
59	MG	2A	3536	1/1	0.96	0.10	41,41,41,41	0
59	MG	1A	3158	1/1	0.96	0.12	44,44,44,44	0
59	MG	1A	4144	1/1	0.96	0.10	42,42,42,42	0
59	MG	2A	3825	1/1	0.96	0.07	42,42,42,42	0
59	MG	2A	3826	1/1	0.96	0.07	54,54,54,54	0
59	MG	1A	3568	1/1	0.96	0.07	15,15,15,15	0
59	MG	10	102	1/1	0.96	0.09	43,43,43,43	0
59	MG	1A	3099	1/1	0.96	0.19	31,31,31,31	0
59	MG	2A	3830	1/1	0.96	0.23	32,32,32,32	0
59	MG	10	104	1/1	0.96	0.05	39,39,39,39	0
59	MG	1A	3817	1/1	0.96	0.06	31,31,31,31	0
59	MG	1A	3570	1/1	0.96	0.11	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3296	1/1	0.96	0.15	33,33,33,33	0
59	MG	1A	3346	1/1	0.96	0.20	52,52,52,52	0
59	MG	10	108	1/1	0.96	0.04	39,39,39,39	0
59	MG	1A	3820	1/1	0.96	0.08	13,13,13,13	0
59	MG	11	102	1/1	0.96	0.07	25,25,25,25	0
59	MG	1A	3017	1/1	0.96	0.05	28,28,28,28	0
59	MG	1A	3992	1/1	0.96	0.05	30,30,30,30	0
59	MG	1A	3994	1/1	0.96	0.06	31,31,31,31	0
59	MG	1A	3696	1/1	0.96	0.09	30,30,30,30	0
59	MG	1A	3297	1/1	0.96	0.06	43,43,43,43	0
59	MG	1A	3484	1/1	0.96	0.19	27,27,27,27	0
59	MG	16	101	1/1	0.96	0.10	32,32,32,32	0
59	MG	1A	3083	1/1	0.96	0.16	36,36,36,36	0
59	MG	2A	3848	1/1	0.96	0.12	47,47,47,47	0
59	MG	1A	4001	1/1	0.96	0.10	37,37,37,37	0
59	MG	1A	4163	1/1	0.96	0.16	53,53,53,53	0
59	MG	1A	3205	1/1	0.96	0.20	24,24,24,24	0
59	MG	1A	3072	1/1	0.96	0.13	34,34,34,34	0
59	MG	2A	3098	1/1	0.96	0.20	47,47,47,47	0
59	MG	1A	3831	1/1	0.96	0.24	17,17,17,17	0
59	MG	1A	4171	1/1	0.96	0.24	26,26,26,26	0
59	MG	2A	3101	1/1	0.96	0.10	27,27,27,27	0
59	MG	1A	3704	1/1	0.96	0.08	13,13,13,13	0
59	MG	1A	4173	1/1	0.96	0.35	36,36,36,36	0
59	MG	1A	3581	1/1	0.96	0.06	22,22,22,22	0
59	MG	1A	3707	1/1	0.96	0.07	57,57,57,57	0
59	MG	1a	3512	1/1	0.96	0.07	45,45,45,45	0
59	MG	1a	3306	1/1	0.96	0.16	48,48,48,48	0
59	MG	1A	3836	1/1	0.96	0.07	36,36,36,36	0
59	MG	1a	3518	1/1	0.96	0.07	32,32,32,32	0
59	MG	1A	3583	1/1	0.96	0.07	50,50,50,50	0
59	MG	1A	3301	1/1	0.96	0.27	37,37,37,37	0
59	MG	2A	3115	1/1	0.96	0.30	36,36,36,36	0
59	MG	1a	3313	1/1	0.96	0.23	42,42,42,42	0
59	MG	1A	3208	1/1	0.96	0.19	33,33,33,33	0
59	MG	2a	3218	1/1	0.96	0.07	63,63,63,63	0
59	MG	2A	3120	1/1	0.96	0.13	34,34,34,34	0
59	MG	1A	4183	1/1	0.96	0.06	34,34,34,34	0
59	MG	1A	3104	1/1	0.96	0.26	32,32,32,32	0
59	MG	2D	303	1/1	0.96	0.04	20,20,20,20	0
59	MG	2A	3123	1/1	0.96	0.21	46,46,46,46	0
59	MG	1a	3319	1/1	0.96	0.05	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	3417	1/1	0.96	0.18	36,36,36,36	0
59	MG	1A	3715	1/1	0.96	0.06	62,62,62,62	0
59	MG	2a	3227	1/1	0.96	0.18	45,45,45,45	0
59	MG	1A	3590	1/1	0.96	0.09	40,40,40,40	0
59	MG	1A	3719	1/1	0.96	0.05	44,44,44,44	0
59	MG	2a	3230	1/1	0.96	0.07	68,68,68,68	0
59	MG	2A	3129	1/1	0.96	0.17	48,48,48,48	0
59	MG	1A	3418	1/1	0.96	0.17	22,22,22,22	0
59	MG	1A	3355	1/1	0.96	0.12	30,30,30,30	0
59	MG	2A	3342	1/1	0.96	0.06	41,41,41,41	0
59	MG	1A	4022	1/1	0.96	0.08	39,39,39,39	0
59	MG	1A	3026	1/1	0.96	0.37	28,28,28,28	0
59	MG	2A	3135	1/1	0.96	0.16	58,58,58,58	0
59	MG	2A	3136	1/1	0.96	0.20	33,33,33,33	0
59	MG	1A	3060	1/1	0.96	0.31	26,26,26,26	0
59	MG	1A	3168	1/1	0.96	0.37	38,38,38,38	0
59	MG	1A	3726	1/1	0.96	0.06	14,14,14,14	0
59	MG	1A	4198	1/1	0.96	0.12	22,22,22,22	0
59	MG	1A	3864	1/1	0.96	0.08	43,43,43,43	0
59	MG	1A	3868	1/1	0.96	0.06	30,30,30,30	0
59	MG	2A	3610	1/1	0.96	0.19	40,40,40,40	0
59	MG	1A	4207	1/1	0.96	0.15	26,26,26,26	0
59	MG	1A	4032	1/1	0.96	0.08	48,48,48,48	0
59	MG	1A	3169	1/1	0.96	0.08	34,34,34,34	0
59	MG	1A	4034	1/1	0.96	0.07	61,61,61,61	0
59	MG	1A	4215	1/1	0.96	0.36	31,31,31,31	0
59	MG	1A	4218	1/1	0.96	0.17	24,24,24,24	0
59	MG	2A	3149	1/1	0.96	0.14	29,29,29,29	0
59	MG	1A	3871	1/1	0.96	0.05	54,54,54,54	0
59	MG	2A	3620	1/1	0.96	0.14	50,50,50,50	0
59	MG	1A	4222	1/1	0.96	0.25	31,31,31,31	0
59	MG	1A	3135	1/1	0.96	0.19	22,22,22,22	0
59	MG	1A	4038	1/1	0.96	0.10	25,25,25,25	0
59	MG	1A	3501	1/1	0.96	0.16	41,41,41,41	0
59	MG	1A	3361	1/1	0.96	0.09	35,35,35,35	0
59	MG	1a	3347	1/1	0.96	0.13	40,40,40,40	0
59	MG	1A	3733	1/1	0.96	0.04	47,47,47,47	0
59	MG	1A	3607	1/1	0.96	0.04	17,17,17,17	0
59	MG	25	102	1/1	0.96	0.18	53,53,53,53	0
59	MG	1A	3309	1/1	0.96	0.12	56,56,56,56	0
59	MG	2A	3160	1/1	0.96	0.06	48,48,48,48	0
59	MG	1A	3736	1/1	0.96	0.11	15,15,15,15	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1a	3352	1/1	0.96	0.17	42,42,42,42	0
59	MG	2A	3163	1/1	0.96	0.07	57,57,57,57	0
59	MG	1A	4046	1/1	0.96	0.09	36,36,36,36	0
59	MG	2A	3379	1/1	0.96	0.07	24,24,24,24	0
59	MG	2A	3638	1/1	0.96	0.11	55,55,55,55	0
59	MG	1B	206	1/1	0.96	0.26	50,50,50,50	0
59	MG	1A	3018	1/1	0.96	0.05	8,8,8,8	0
59	MG	2A	3383	1/1	0.96	0.14	31,31,31,31	0
59	MG	1A	3064	1/1	0.96	0.12	19,19,19,19	0
59	MG	2A	3645	1/1	0.96	0.06	51,51,51,51	0
59	MG	1A	3176	1/1	0.96	0.07	35,35,35,35	0
59	MG	2A	3649	1/1	0.96	0.08	47,47,47,47	0
59	MG	1A	3090	1/1	0.96	0.11	29,29,29,29	0
59	MG	1A	3316	1/1	0.96	0.11	15,15,15,15	0
60	ZN	24	501	1/1	0.96	0.10	111,111,111,111	0
60	ZN	2n	501	1/1	0.96	0.06	90,90,90,90	0
59	MG	1A	3475	1/1	0.97	0.12	53,53,53,53	0
59	MG	2A	3007	1/1	0.97	0.13	40,40,40,40	0
59	MG	2A	3371	1/1	0.97	0.06	48,48,48,48	0
59	MG	1a	3451	1/1	0.97	0.10	43,43,43,43	0
59	MG	1A	3038	1/1	0.97	0.10	30,30,30,30	0
59	MG	1A	3978	1/1	0.97	0.06	38,38,38,38	0
59	MG	1A	4094	1/1	0.97	0.10	35,35,35,35	0
59	MG	2A	3014	1/1	0.97	0.06	29,29,29,29	0
59	MG	1A	3477	1/1	0.97	0.10	31,31,31,31	0
59	MG	1A	3251	1/1	0.97	0.17	47,47,47,47	0
59	MG	1A	3867	1/1	0.97	0.05	36,36,36,36	0
59	MG	1A	3108	1/1	0.97	0.27	26,26,26,26	0
59	MG	1A	3598	1/1	0.97	0.06	24,24,24,24	0
59	MG	1A	3080	1/1	0.97	0.12	16,16,16,16	0
59	MG	1A	3873	1/1	0.97	0.04	30,30,30,30	0
59	MG	1a	3463	1/1	0.97	0.16	44,44,44,44	0
59	MG	1A	3196	1/1	0.97	0.17	26,26,26,26	0
59	MG	1a	3310	1/1	0.97	0.09	19,19,19,19	0
59	MG	1a	3312	1/1	0.97	0.11	62,62,62,62	0
59	MG	1A	3602	1/1	0.97	0.06	19,19,19,19	0
59	MG	1A	3390	1/1	0.97	0.09	43,43,43,43	0
59	MG	1A	3054	1/1	0.97	0.11	24,24,24,24	0
59	MG	1a	3316	1/1	0.97	0.10	40,40,40,40	0
59	MG	1a	3474	1/1	0.97	0.07	42,42,42,42	0
59	MG	1A	3257	1/1	0.97	0.12	24,24,24,24	0
59	MG	2A	3034	1/1	0.97	0.08	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1B	224	1/1	0.97	0.17	52,52,52,52	0
59	MG	1A	3610	1/1	0.97	0.06	19,19,19,19	0
59	MG	1A	3055	1/1	0.97	0.15	50,50,50,50	0
59	MG	1a	3481	1/1	0.97	0.10	44,44,44,44	0
59	MG	2A	3039	1/1	0.97	0.14	23,23,23,23	0
59	MG	1B	228	1/1	0.97	0.06	30,30,30,30	0
59	MG	1A	3993	1/1	0.97	0.05	20,20,20,20	0
59	MG	1A	3613	1/1	0.97	0.09	36,36,36,36	0
59	MG	1a	3485	1/1	0.97	0.06	49,49,49,49	0
59	MG	1A	3694	1/1	0.97	0.08	29,29,29,29	0
59	MG	1A	3885	1/1	0.97	0.10	47,47,47,47	0
59	MG	1A	3486	1/1	0.97	0.21	31,31,31,31	0
59	MG	1A	3998	1/1	0.97	0.06	13,13,13,13	0
59	MG	2A	3228	1/1	0.97	0.05	36,36,36,36	0
59	MG	2A	3833	1/1	0.97	0.07	47,47,47,47	0
59	MG	1A	3887	1/1	0.97	0.08	50,50,50,50	0
59	MG	2A	3616	1/1	0.97	0.08	37,37,37,37	0
59	MG	1A	3147	1/1	0.97	0.36	26,26,26,26	0
59	MG	1B	237	1/1	0.97	0.07	39,39,39,39	0
59	MG	1A	3260	1/1	0.97	0.06	32,32,32,32	0
59	MG	1A	3200	1/1	0.97	0.16	37,37,37,37	0
59	MG	1a	3496	1/1	0.97	0.12	66,66,66,66	0
59	MG	1A	4004	1/1	0.97	0.07	43,43,43,43	0
59	MG	1a	3498	1/1	0.97	0.07	63,63,63,63	0
59	MG	2A	3624	1/1	0.97	0.06	44,44,44,44	0
59	MG	2A	3426	1/1	0.97	0.06	23,23,23,23	0
59	MG	1D	303	1/1	0.97	0.19	35,35,35,35	0
59	MG	1a	3500	1/1	0.97	0.07	64,64,64,64	0
59	MG	1D	304	1/1	0.97	0.14	38,38,38,38	0
59	MG	1A	3293	1/1	0.97	0.10	49,49,49,49	0
59	MG	1A	3148	1/1	0.97	0.20	26,26,26,26	0
59	MG	2A	3432	1/1	0.97	0.08	26,26,26,26	0
59	MG	2A	3061	1/1	0.97	0.10	42,42,42,42	0
59	MG	1A	3112	1/1	0.97	0.15	33,33,33,33	0
59	MG	1A	4008	1/1	0.97	0.10	54,54,54,54	0
59	MG	2A	3635	1/1	0.97	0.08	62,62,62,62	0
59	MG	1A	3785	1/1	0.97	0.10	18,18,18,18	0
59	MG	1A	3150	1/1	0.97	0.14	30,30,30,30	0
59	MG	1A	3401	1/1	0.97	0.07	28,28,28,28	0
59	MG	1A	3706	1/1	0.97	0.04	28,28,28,28	0
59	MG	1E	303	1/1	0.97	0.22	33,33,33,33	0
59	MG	1E	304	1/1	0.97	0.13	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3642	1/1	0.97	0.12	63,63,63,63	0
59	MG	2A	3442	1/1	0.97	0.12	24,24,24,24	0
59	MG	1A	3548	1/1	0.97	0.07	38,38,38,38	0
59	MG	1A	3101	1/1	0.97	0.19	30,30,30,30	0
59	MG	1A	4132	1/1	0.97	0.13	37,37,37,37	0
59	MG	1a	3520	1/1	0.97	0.06	60,60,60,60	0
59	MG	1a	3522	1/1	0.97	0.07	66,66,66,66	0
59	MG	1a	3524	1/1	0.97	0.05	71,71,71,71	0
59	MG	1A	4133	1/1	0.97	0.05	35,35,35,35	0
59	MG	1A	3030	1/1	0.97	0.16	14,14,14,14	0
59	MG	1A	3710	1/1	0.97	0.06	18,18,18,18	0
59	MG	1A	3093	1/1	0.97	0.06	35,35,35,35	0
59	MG	1A	3797	1/1	0.97	0.15	35,35,35,35	0
59	MG	2A	3659	1/1	0.97	0.06	66,66,66,66	0
59	MG	2A	3454	1/1	0.97	0.07	36,36,36,36	0
59	MG	1A	3268	1/1	0.97	0.13	32,32,32,32	0
59	MG	1A	3134	1/1	0.97	0.16	24,24,24,24	0
59	MG	1a	3533	1/1	0.97	0.06	59,59,59,59	0
59	MG	2a	3168	1/1	0.97	0.19	54,54,54,54	0
59	MG	1a	3534	1/1	0.97	0.06	45,45,45,45	0
59	MG	1A	3066	1/1	0.97	0.16	27,27,27,27	0
59	MG	1A	4023	1/1	0.97	0.04	49,49,49,49	0
59	MG	1A	3557	1/1	0.97	0.04	23,23,23,23	0
59	MG	1F	305	1/1	0.97	0.18	27,27,27,27	0
59	MG	1A	4143	1/1	0.97	0.12	16,16,16,16	0
59	MG	1A	3558	1/1	0.97	0.07	15,15,15,15	0
59	MG	2A	3092	1/1	0.97	0.13	32,32,32,32	0
59	MG	1A	3559	1/1	0.97	0.10	28,28,28,28	0
59	MG	2N	8001	1/1	0.97	0.08	45,45,45,45	0
59	MG	1A	4146	1/1	0.97	0.07	26,26,26,26	0
59	MG	1A	3637	1/1	0.97	0.06	18,18,18,18	0
59	MG	1G	3001	1/1	0.97	0.14	32,32,32,32	0
59	MG	1A	4029	1/1	0.97	0.06	46,46,46,46	0
59	MG	1A	3408	1/1	0.97	0.20	32,32,32,32	0
59	MG	2A	3476	1/1	0.97	0.07	43,43,43,43	0
59	MG	1A	3136	1/1	0.97	0.24	26,26,26,26	0
59	MG	1A	3185	1/1	0.97	0.22	36,36,36,36	0
59	MG	2A	3683	1/1	0.97	0.08	53,53,53,53	0
59	MG	1A	3725	1/1	0.97	0.07	41,41,41,41	0
59	MG	1A	3117	1/1	0.97	0.21	25,25,25,25	0
59	MG	1a	3552	1/1	0.97	0.13	55,55,55,55	0
59	MG	1A	4035	1/1	0.97	0.10	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	3566	1/1	0.97	0.06	13,13,13,13	0
59	MG	1A	3412	1/1	0.97	0.09	37,37,37,37	0
59	MG	1A	4159	1/1	0.97	0.09	34,34,34,34	0
59	MG	2A	3694	1/1	0.97	0.05	28,28,28,28	0
59	MG	1A	3922	1/1	0.97	0.08	41,41,41,41	0
59	MG	1A	3118	1/1	0.97	0.23	33,33,33,33	0
59	MG	1N	3008	1/1	0.97	0.09	36,36,36,36	0
59	MG	2A	3489	1/1	0.97	0.07	32,32,32,32	0
59	MG	2A	3112	1/1	0.97	0.05	33,33,33,33	0
59	MG	20	3003	1/1	0.97	0.11	50,50,50,50	0
59	MG	2A	3113	1/1	0.97	0.11	38,38,38,38	0
59	MG	1A	4040	1/1	0.97	0.06	36,36,36,36	0
59	MG	2A	3705	1/1	0.97	0.06	49,49,49,49	0
59	MG	1A	3731	1/1	0.97	0.07	33,33,33,33	0
59	MG	1a	3383	1/1	0.97	0.22	43,43,43,43	0
59	MG	1a	3563	1/1	0.97	0.11	50,50,50,50	0
59	MG	1A	3414	1/1	0.97	0.06	42,42,42,42	0
59	MG	2A	3710	1/1	0.97	0.08	34,34,34,34	0
59	MG	2A	3711	1/1	0.97	0.06	50,50,50,50	0
59	MG	1A	3008	1/1	0.97	0.04	16,16,16,16	0
59	MG	1A	3929	1/1	0.97	0.10	52,52,52,52	0
59	MG	1A	3162	1/1	0.97	0.30	30,30,30,30	0
59	MG	1P	201	1/1	0.97	0.21	23,23,23,23	0
59	MG	1P	202	1/1	0.97	0.33	25,25,25,25	0
59	MG	1A	3243	1/1	0.97	0.35	28,28,28,28	0
59	MG	1A	4047	1/1	0.97	0.13	31,31,31,31	0
59	MG	1A	3512	1/1	0.97	0.10	40,40,40,40	0
59	MG	1Q	202	1/1	0.97	0.11	37,37,37,37	0
59	MG	2A	3506	1/1	0.97	0.14	42,42,42,42	0
59	MG	1A	3739	1/1	0.97	0.32	26,26,26,26	0
59	MG	1A	3009	1/1	0.97	0.09	25,25,25,25	0
59	MG	2A	3132	1/1	0.97	0.07	21,21,21,21	0
59	MG	1A	3514	1/1	0.97	0.30	53,53,53,53	0
59	MG	1A	3939	1/1	0.97	0.06	36,36,36,36	0
59	MG	1A	3419	1/1	0.97	0.24	30,30,30,30	0
59	MG	1R	202	1/1	0.97	0.43	33,33,33,33	0
59	MG	1A	4181	1/1	0.97	0.27	33,33,33,33	0
59	MG	1A	4182	1/1	0.97	0.21	23,23,23,23	0
59	MG	1A	3941	1/1	0.97	0.08	30,30,30,30	0
59	MG	1A	3466	1/1	0.97	0.22	24,24,24,24	0
59	MG	1k	201	1/1	0.97	0.12	39,39,39,39	0
59	MG	1l	201	1/1	0.97	0.13	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	3829	1/1	0.97	0.08	38,38,38,38	0
59	MG	1A	3580	1/1	0.97	0.05	23,23,23,23	0
59	MG	1A	3467	1/1	0.97	0.09	28,28,28,28	0
59	MG	1A	4062	1/1	0.97	0.06	34,34,34,34	0
59	MG	1A	3122	1/1	0.97	0.23	28,28,28,28	0
59	MG	2a	3239	1/1	0.97	0.13	42,42,42,42	0
59	MG	1V	201	1/1	0.97	0.14	33,33,33,33	0
59	MG	1A	3658	1/1	0.97	0.05	39,39,39,39	0
59	MG	1A	3421	1/1	0.97	0.13	33,33,33,33	0
59	MG	1A	3660	1/1	0.97	0.07	40,40,40,40	0
59	MG	1A	3248	1/1	0.97	0.13	36,36,36,36	0
59	MG	1W	205	1/1	0.97	0.17	23,23,23,23	0
59	MG	1A	3838	1/1	0.97	0.13	26,26,26,26	0
59	MG	1A	3471	1/1	0.97	0.11	30,30,30,30	0
59	MG	1A	3954	1/1	0.97	0.07	49,49,49,49	0
59	MG	1A	4201	1/1	0.97	0.08	32,32,32,32	0
59	MG	1A	4071	1/1	0.97	0.08	50,50,50,50	0
59	MG	2A	3537	1/1	0.97	0.18	59,59,59,59	0
59	MG	1A	4204	1/1	0.97	0.09	29,29,29,29	0
59	MG	1a	3422	1/1	0.97	0.17	50,50,50,50	0
59	MG	1A	3587	1/1	0.97	0.07	51,51,51,51	0
59	MG	1A	3588	1/1	0.97	0.07	30,30,30,30	0
59	MG	1A	4208	1/1	0.97	0.31	29,29,29,29	0
59	MG	1A	3667	1/1	0.97	0.07	36,36,36,36	0
59	MG	2a	3048	1/1	0.97	0.16	42,42,42,42	0
59	MG	1A	4211	1/1	0.97	0.14	23,23,23,23	0
59	MG	1A	3960	1/1	0.97	0.07	16,16,16,16	0
59	MG	1A	3845	1/1	0.97	0.20	33,33,33,33	0
59	MG	1A	3963	1/1	0.97	0.07	37,37,37,37	0
59	MG	1A	3669	1/1	0.97	0.06	38,38,38,38	0
59	MG	1A	4219	1/1	0.97	0.18	32,32,32,32	0
59	MG	1A	4220	1/1	0.97	0.12	24,24,24,24	0
59	MG	1A	3757	1/1	0.97	0.04	39,39,39,39	0
59	MG	1A	4081	1/1	0.97	0.04	14,14,14,14	0
59	MG	1A	3219	1/1	0.97	0.07	51,51,51,51	0
59	MG	1A	3383	1/1	0.97	0.11	38,38,38,38	0
59	MG	12	3002	1/1	0.97	0.13	36,36,36,36	0
59	MG	1A	4227	1/1	0.97	0.17	32,32,32,32	0
59	MG	1A	3315	1/1	0.97	0.20	34,34,34,34	0
59	MG	1A	3851	1/1	0.97	0.09	43,43,43,43	0
59	MG	1y	101	1/1	0.97	0.14	32,32,32,32	0
59	MG	15	102	1/1	0.97	0.12	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	3852	1/1	0.97	0.12	36,36,36,36	0
59	MG	1A	3853	1/1	0.97	0.05	33,33,33,33	0
59	MG	2a	3070	1/1	0.97	0.16	60,60,60,60	0
59	MG	1a	3445	1/1	0.97	0.09	32,32,32,32	0
59	MG	16	103	1/1	0.97	0.07	49,49,49,49	0
59	MG	1A	3856	1/1	0.97	0.06	39,39,39,39	0
60	ZN	14	501	1/1	0.97	0.06	87,87,87,87	0
59	MG	1A	3592	1/1	0.97	0.04	17,17,17,17	0
59	MG	1A	3858	1/1	0.97	0.07	22,22,22,22	0
62	K	2A	3849	1/1	0.97	0.06	47,47,47,47	0
59	MG	17	102	1/1	0.98	0.07	46,46,46,46	0
59	MG	1A	3668	1/1	0.98	0.05	38,38,38,38	0
59	MG	1A	3890	1/1	0.98	0.05	50,50,50,50	0
59	MG	1D	307	1/1	0.98	0.19	24,24,24,24	0
59	MG	2A	3668	1/1	0.98	0.09	43,43,43,43	0
59	MG	1A	3609	1/1	0.98	0.04	17,17,17,17	0
59	MG	1D	309	1/1	0.98	0.10	37,37,37,37	0
59	MG	1A	4165	1/1	0.98	0.09	9,9,9,9	0
59	MG	1D	311	1/1	0.98	0.21	19,19,19,19	0
59	MG	1A	4166	1/1	0.98	0.08	11,11,11,11	0
59	MG	1A	3085	1/1	0.98	0.17	15,15,15,15	0
59	MG	1A	3738	1/1	0.98	0.03	27,27,27,27	0
59	MG	1A	4169	1/1	0.98	0.10	22,22,22,22	0
59	MG	2A	3356	1/1	0.98	0.11	18,18,18,18	0
59	MG	2A	3512	1/1	0.98	0.05	45,45,45,45	0
59	MG	1A	4170	1/1	0.98	0.11	23,23,23,23	0
59	MG	1A	3611	1/1	0.98	0.06	17,17,17,17	0
59	MG	2A	3681	1/1	0.98	0.06	62,62,62,62	0
59	MG	1A	3672	1/1	0.98	0.04	42,42,42,42	0
59	MG	1a	3311	1/1	0.98	0.04	45,45,45,45	0
59	MG	1A	3035	1/1	0.98	0.27	24,24,24,24	0
59	MG	1A	3181	1/1	0.98	0.23	25,25,25,25	0
59	MG	2A	3222	1/1	0.98	0.07	45,45,45,45	0
59	MG	1A	3562	1/1	0.98	0.08	18,18,18,18	0
59	MG	2A	3688	1/1	0.98	0.07	38,38,38,38	0
59	MG	1A	4080	1/1	0.98	0.10	28,28,28,28	0
59	MG	1A	3563	1/1	0.98	0.05	37,37,37,37	0
59	MG	2A	3691	1/1	0.98	0.04	29,29,29,29	0
59	MG	2a	3130	1/1	0.98	0.06	79,79,79,79	0
59	MG	1A	3814	1/1	0.98	0.04	22,22,22,22	0
59	MG	2A	3693	1/1	0.98	0.10	32,32,32,32	0
59	MG	1a	3318	1/1	0.98	0.04	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3369	1/1	0.98	0.04	67,67,67,67	0
59	MG	1A	3027	1/1	0.98	0.21	30,30,30,30	0
59	MG	1A	4180	1/1	0.98	0.20	28,28,28,28	0
59	MG	2a	3137	1/1	0.98	0.07	68,68,68,68	0
59	MG	2A	3698	1/1	0.98	0.05	49,49,49,49	0
59	MG	1A	3207	1/1	0.98	0.20	24,24,24,24	0
59	MG	1A	3620	1/1	0.98	0.07	15,15,15,15	0
59	MG	2A	3374	1/1	0.98	0.07	49,49,49,49	0
59	MG	1f	3002	1/1	0.98	0.09	33,33,33,33	0
59	MG	1A	3120	1/1	0.98	0.11	10,10,10,10	0
59	MG	1A	3749	1/1	0.98	0.03	26,26,26,26	0
59	MG	1A	3450	1/1	0.98	0.21	31,31,31,31	0
59	MG	2a	3147	1/1	0.98	0.04	59,59,59,59	0
59	MG	1A	3047	1/1	0.98	0.05	19,19,19,19	0
59	MG	1A	3683	1/1	0.98	0.04	29,29,29,29	0
59	MG	1a	3328	1/1	0.98	0.12	17,17,17,17	0
59	MG	2A	3382	1/1	0.98	0.04	58,58,58,58	0
59	MG	1A	3160	1/1	0.98	0.30	36,36,36,36	0
59	MG	2A	3714	1/1	0.98	0.06	66,66,66,66	0
59	MG	2A	3384	1/1	0.98	0.07	28,28,28,28	0
59	MG	2a	3155	1/1	0.98	0.05	72,72,72,72	0
59	MG	2A	3716	1/1	0.98	0.07	56,56,56,56	0
59	MG	1A	3073	1/1	0.98	0.17	26,26,26,26	0
59	MG	1A	3912	1/1	0.98	0.09	47,47,47,47	0
59	MG	1A	3826	1/1	0.98	0.06	42,42,42,42	0
59	MG	1A	3571	1/1	0.98	0.10	13,13,13,13	0
59	MG	2A	3721	1/1	0.98	0.03	17,17,17,17	0
59	MG	1A	3627	1/1	0.98	0.05	28,28,28,28	0
59	MG	1A	3003	1/1	0.98	0.07	16,16,16,16	0
59	MG	1A	4196	1/1	0.98	0.22	29,29,29,29	0
59	MG	2A	3108	1/1	0.98	0.08	43,43,43,43	0
59	MG	2A	3393	1/1	0.98	0.06	27,27,27,27	0
59	MG	2A	3394	1/1	0.98	0.04	40,40,40,40	0
59	MG	1A	3528	1/1	0.98	0.12	35,35,35,35	0
59	MG	1A	3007	1/1	0.98	0.12	17,17,17,17	0
59	MG	1A	4199	1/1	0.98	0.19	32,32,32,32	0
59	MG	1A	4200	1/1	0.98	0.25	27,27,27,27	0
59	MG	2X	3002	1/1	0.98	0.08	47,47,47,47	0
59	MG	1a	3464	1/1	0.98	0.03	31,31,31,31	0
59	MG	1A	3189	1/1	0.98	0.27	43,43,43,43	0
59	MG	20	3002	1/1	0.98	0.09	51,51,51,51	0
59	MG	1A	4202	1/1	0.98	0.19	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	2A	3116	1/1	0.98	0.25	35,35,35,35	0
59	MG	1A	4101	1/1	0.98	0.08	41,41,41,41	0
59	MG	2A	3118	1/1	0.98	0.18	37,37,37,37	0
59	MG	1A	3920	1/1	0.98	0.06	45,45,45,45	0
59	MG	2A	3406	1/1	0.98	0.07	39,39,39,39	0
59	MG	2A	3563	1/1	0.98	0.05	52,52,52,52	0
59	MG	2A	3743	1/1	0.98	0.05	40,40,40,40	0
59	MG	1A	3576	1/1	0.98	0.12	9,9,9,9	0
59	MG	1A	4206	1/1	0.98	0.17	21,21,21,21	0
59	MG	1A	3241	1/1	0.98	0.16	24,24,24,24	0
59	MG	1A	4105	1/1	0.98	0.09	53,53,53,53	0
59	MG	2A	3411	1/1	0.98	0.06	40,40,40,40	0
59	MG	1A	4209	1/1	0.98	0.13	21,21,21,21	0
59	MG	2A	3750	1/1	0.98	0.06	51,51,51,51	0
59	MG	1O	3004	1/1	0.98	0.06	48,48,48,48	0
59	MG	1A	3061	1/1	0.98	0.09	8,8,8,8	0
59	MG	1A	3031	1/1	0.98	0.27	24,24,24,24	0
59	MG	1a	3479	1/1	0.98	0.08	48,48,48,48	0
59	MG	1a	3480	1/1	0.98	0.04	37,37,37,37	0
59	MG	1A	3244	1/1	0.98	0.18	24,24,24,24	0
59	MG	2A	3419	1/1	0.98	0.06	28,28,28,28	0
59	MG	2A	3577	1/1	0.98	0.06	36,36,36,36	0
59	MG	1A	3841	1/1	0.98	0.04	24,24,24,24	0
59	MG	1A	4214	1/1	0.98	0.30	36,36,36,36	0
59	MG	1A	3927	1/1	0.98	0.09	12,12,12,12	0
59	MG	1A	4216	1/1	0.98	0.08	24,24,24,24	0
59	MG	1A	4217	1/1	0.98	0.14	35,35,35,35	0
59	MG	2A	3425	1/1	0.98	0.09	47,47,47,47	0
59	MG	1A	3497	1/1	0.98	0.19	38,38,38,38	0
59	MG	2A	3586	1/1	0.98	0.04	46,46,46,46	0
59	MG	1a	3488	1/1	0.98	0.05	39,39,39,39	0
59	MG	1A	4020	1/1	0.98	0.15	34,34,34,34	0
59	MG	2A	3278	1/1	0.98	0.17	40,40,40,40	0
59	MG	1A	3701	1/1	0.98	0.04	17,17,17,17	0
59	MG	1A	3582	1/1	0.98	0.03	24,24,24,24	0
59	MG	2A	3592	1/1	0.98	0.04	23,23,23,23	0
59	MG	1A	3703	1/1	0.98	0.07	55,55,55,55	0
59	MG	1A	3245	1/1	0.98	0.24	21,21,21,21	0
59	MG	1A	4224	1/1	0.98	0.04	23,23,23,23	0
59	MG	1A	3063	1/1	0.98	0.06	15,15,15,15	0
59	MG	1A	4226	1/1	0.98	0.08	24,24,24,24	0
59	MG	1A	3935	1/1	0.98	0.04	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	3012	1/1	0.98	0.09	18,18,18,18	0
59	MG	1A	4028	1/1	0.98	0.10	50,50,50,50	0
59	MG	1U	201	1/1	0.98	0.20	27,27,27,27	0
59	MG	1A	3937	1/1	0.98	0.06	22,22,22,22	0
59	MG	2A	3011	1/1	0.98	0.07	38,38,38,38	0
59	MG	2A	3012	1/1	0.98	0.05	35,35,35,35	0
59	MG	1a	3502	1/1	0.98	0.06	67,67,67,67	0
59	MG	1U	203	1/1	0.98	0.22	22,22,22,22	0
59	MG	1A	3041	1/1	0.98	0.08	20,20,20,20	0
59	MG	2A	3609	1/1	0.98	0.03	44,44,44,44	0
59	MG	1A	3465	1/1	0.98	0.18	27,27,27,27	0
59	MG	1A	3131	1/1	0.98	0.30	33,33,33,33	0
59	MG	1A	3171	1/1	0.98	0.06	25,25,25,25	0
59	MG	2A	3020	1/1	0.98	0.05	24,24,24,24	0
59	MG	1A	3172	1/1	0.98	0.04	25,25,25,25	0
59	MG	2a	3050	1/1	0.98	0.04	54,54,54,54	0
59	MG	1a	3509	1/1	0.98	0.05	61,61,61,61	0
59	MG	1B	207	1/1	0.98	0.04	32,32,32,32	0
59	MG	1A	3855	1/1	0.98	0.07	51,51,51,51	0
59	MG	2a	3054	1/1	0.98	0.17	41,41,41,41	0
59	MG	1W	204	1/1	0.98	0.13	32,32,32,32	0
59	MG	2A	3456	1/1	0.98	0.05	50,50,50,50	0
59	MG	1A	3712	1/1	0.98	0.05	43,43,43,43	0
59	MG	1a	3516	1/1	0.98	0.10	64,64,64,64	0
59	MG	1A	3024	1/1	0.98	0.25	19,19,19,19	0
59	MG	1X	3002	1/1	0.98	0.06	28,28,28,28	0
59	MG	1X	3003	1/1	0.98	0.14	32,32,32,32	0
59	MG	1A	3546	1/1	0.98	0.05	37,37,37,37	0
59	MG	1X	3005	1/1	0.98	0.06	26,26,26,26	0
59	MG	1A	3434	1/1	0.98	0.14	21,21,21,21	0
59	MG	1A	3716	1/1	0.98	0.04	34,34,34,34	0
59	MG	1A	3435	1/1	0.98	0.22	28,28,28,28	0
59	MG	1A	3862	1/1	0.98	0.05	38,38,38,38	0
59	MG	1A	3863	1/1	0.98	0.04	9,9,9,9	0
59	MG	2A	3811	1/1	0.98	0.09	62,62,62,62	0
59	MG	1a	3529	1/1	0.98	0.05	53,53,53,53	0
59	MG	1A	3718	1/1	0.98	0.06	39,39,39,39	0
59	MG	1A	3865	1/1	0.98	0.04	42,42,42,42	0
59	MG	1A	3067	1/1	0.98	0.11	19,19,19,19	0
59	MG	2A	3475	1/1	0.98	0.04	48,48,48,48	0
59	MG	2a	3075	1/1	0.98	0.17	33,33,33,33	0
59	MG	1A	3550	1/1	0.98	0.06	14,14,14,14	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	3437	1/1	0.98	0.13	48,48,48,48	0
59	MG	1A	3961	1/1	0.98	0.04	37,37,37,37	0
59	MG	2A	3821	1/1	0.98	0.06	35,35,35,35	0
59	MG	1A	4050	1/1	0.98	0.08	45,45,45,45	0
59	MG	1A	3870	1/1	0.98	0.04	29,29,29,29	0
59	MG	1a	3538	1/1	0.98	0.09	44,44,44,44	0
59	MG	1A	3312	1/1	0.98	0.23	33,33,33,33	0
59	MG	1A	3872	1/1	0.98	0.09	48,48,48,48	0
59	MG	2A	3647	1/1	0.98	0.07	39,39,39,39	0
59	MG	1a	3403	1/1	0.98	0.10	28,28,28,28	0
59	MG	1A	3553	1/1	0.98	0.05	20,20,20,20	0
59	MG	2A	3650	1/1	0.98	0.14	60,60,60,60	0
59	MG	1A	3790	1/1	0.98	0.13	35,35,35,35	0
59	MG	1A	3791	1/1	0.98	0.04	34,34,34,34	0
59	MG	1A	3373	1/1	0.98	0.12	29,29,29,29	0
59	MG	1A	3793	1/1	0.98	0.09	46,46,46,46	0
59	MG	1A	3601	1/1	0.98	0.05	12,12,12,12	0
59	MG	1A	3152	1/1	0.98	0.07	25,25,25,25	0
59	MG	1A	3727	1/1	0.98	0.08	15,15,15,15	0
59	MG	1A	3016	1/1	0.98	0.03	20,20,20,20	0
59	MG	1A	3604	1/1	0.98	0.05	27,27,27,27	0
59	MG	1A	3605	1/1	0.98	0.05	14,14,14,14	0
60	ZN	2Y	501	1/1	0.98	0.04	86,86,86,86	0
59	MG	1A	3606	1/1	0.98	0.07	17,17,17,17	0
60	ZN	29	501	1/1	0.98	0.04	69,69,69,69	0
59	MG	1A	3256	1/1	0.98	0.06	27,27,27,27	0
61	SF4	2d	501	8/8	0.98	0.05	56,66,80,82	0
59	MG	1A	3069	1/1	0.98	0.12	28,28,28,28	0
59	MG	1A	4051	1/1	0.99	0.04	38,38,38,38	0
59	MG	1A	3046	1/1	0.99	0.08	28,28,28,28	0
59	MG	1A	3816	1/1	0.99	0.07	35,35,35,35	0
59	MG	2A	3006	1/1	0.99	0.06	30,30,30,30	0
59	MG	1A	3840	1/1	0.99	0.04	16,16,16,16	0
59	MG	2A	3595	1/1	0.99	0.04	34,34,34,34	0
59	MG	1A	4055	1/1	0.99	0.06	32,32,32,32	0
59	MG	2A	3713	1/1	0.99	0.04	29,29,29,29	0
59	MG	1A	3011	1/1	0.99	0.21	16,16,16,16	0
59	MG	1B	216	1/1	0.99	0.09	38,38,38,38	0
59	MG	1A	3130	1/1	0.99	0.16	32,32,32,32	0
59	MG	2A	3064	1/1	0.99	0.11	16,16,16,16	0
59	MG	1A	3006	1/1	0.99	0.04	23,23,23,23	0
59	MG	1A	3956	1/1	0.99	0.06	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1A	3957	1/1	0.99	0.03	33,33,33,33	0
59	MG	1A	3684	1/1	0.99	0.04	28,28,28,28	0
59	MG	2A	3016	1/1	0.99	0.07	21,21,21,21	0
59	MG	2A	3723	1/1	0.99	0.03	47,47,47,47	0
59	MG	1A	3685	1/1	0.99	0.04	14,14,14,14	0
59	MG	1A	3059	1/1	0.99	0.15	10,10,10,10	0
59	MG	1A	3025	1/1	0.99	0.12	21,21,21,21	0
59	MG	2A	3727	1/1	0.99	0.04	31,31,31,31	0
59	MG	1A	3213	1/1	0.99	0.20	27,27,27,27	0
59	MG	1A	3374	1/1	0.99	0.16	27,27,27,27	0
59	MG	1F	303	1/1	0.99	0.03	24,24,24,24	0
59	MG	1B	227	1/1	0.99	0.05	31,31,31,31	0
59	MG	1a	3457	1/1	0.99	0.07	28,28,28,28	0
59	MG	1A	3029	1/1	0.99	0.08	29,29,29,29	0
59	MG	1A	3827	1/1	0.99	0.05	23,23,23,23	0
59	MG	1A	3999	1/1	0.99	0.03	20,20,20,20	0
59	MG	1A	3878	1/1	0.99	0.02	38,38,38,38	0
59	MG	1A	3906	1/1	0.99	0.07	36,36,36,36	0
59	MG	1A	3170	1/1	0.99	0.15	10,10,10,10	0
59	MG	1A	3692	1/1	0.99	0.07	37,37,37,37	0
59	MG	1a	3465	1/1	0.99	0.03	26,26,26,26	0
59	MG	1A	3938	1/1	0.99	0.02	22,22,22,22	0
59	MG	1A	3854	1/1	0.99	0.04	52,52,52,52	0
59	MG	1a	3513	1/1	0.99	0.03	61,61,61,61	0
59	MG	2A	3461	1/1	0.99	0.03	27,27,27,27	0
59	MG	1A	4186	1/1	0.99	0.09	27,27,27,27	0
59	MG	1a	3515	1/1	0.99	0.04	39,39,39,39	0
59	MG	1a	3469	1/1	0.99	0.06	48,48,48,48	0
59	MG	1A	3882	1/1	0.99	0.07	45,45,45,45	0
59	MG	1A	3179	1/1	0.99	0.05	25,25,25,25	0
59	MG	1A	3616	1/1	0.99	0.09	16,16,16,16	0
59	MG	1A	3532	1/1	0.99	0.22	25,25,25,25	0
59	MG	1a	3521	1/1	0.99	0.04	46,46,46,46	0
59	MG	2A	3815	1/1	0.99	0.03	56,56,56,56	0
59	MG	1A	3976	1/1	0.99	0.10	56,56,56,56	0
59	MG	1a	3523	1/1	0.99	0.02	54,54,54,54	0
59	MG	1A	3811	1/1	0.99	0.04	30,30,30,30	0
59	MG	1a	3574	1/1	0.99	0.05	43,43,43,43	0
59	MG	1A	3834	1/1	0.99	0.06	34,34,34,34	0
59	MG	1A	3946	1/1	0.99	0.03	46,46,46,46	0
59	MG	1A	3618	1/1	0.99	0.04	16,16,16,16	0
59	MG	1A	4157	1/1	0.99	0.04	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	ZN	1Y	501	1/1	0.99	0.02	58,58,58,58	0
59	MG	1A	4158	1/1	0.99	0.07	20,20,20,20	0
60	ZN	15	101	1/1	0.99	0.04	34,34,34,34	0
60	ZN	16	102	1/1	0.99	0.05	36,36,36,36	0
59	MG	1A	3662	1/1	0.99	0.05	15,15,15,15	0
59	MG	2A	3701	1/1	0.99	0.03	26,26,26,26	0
60	ZN	25	101	1/1	0.99	0.03	49,49,49,49	0
60	ZN	26	501	1/1	0.99	0.03	57,57,57,57	0
59	MG	2A	3644	1/1	0.99	0.04	69,69,69,69	0
59	MG	2A	3703	1/1	0.99	0.04	30,30,30,30	0
61	SF4	1d	501	8/8	0.99	0.06	52,55,64,66	0
59	MG	1A	3663	1/1	0.99	0.05	14,14,14,14	0
59	MG	2A	3646	1/1	0.99	0.04	53,53,53,53	0
60	ZN	1n	501	1/1	1.00	0.02	54,54,54,54	0
59	MG	1A	3737	1/1	1.00	0.03	34,34,34,34	0
59	MG	2A	3460	1/1	1.00	0.04	25,25,25,25	0
59	MG	1A	3928	1/1	1.00	0.02	16,16,16,16	0
59	MG	2a	3145	1/1	1.00	0.04	45,45,45,45	0
59	MG	1A	3653	1/1	1.00	0.03	12,12,12,12	0
59	MG	1A	3010	1/1	1.00	0.04	16,16,16,16	0
59	MG	2A	3578	1/1	1.00	0.04	25,25,25,25	0
59	MG	1A	3866	1/1	1.00	0.05	15,15,15,15	0
60	ZN	19	102	1/1	1.00	0.07	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.