Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2025 – 07:18 PM EDT

PDB ID	:	9O3K / pdb_00009o3k
Title	:	Crystal structure of the wild-type Thermus thermophilus 70S ribosome in complex with macrolide erythromycin, mRNA, aminoacylated A-site Lys-tRNAlys, P-site fMAC-peptidyl-tRNAmet, and deacylated E-site tRNAlys at 2.70A resolution
Authors	:	Syroegin, E.A.; Aleksandrova, E.V.; Kruglov, A.A.; Paranjpe, M.N.; Svetlov, M.S.; Polikanov, Y.S.
Deposited on	:	2025-04-07
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:

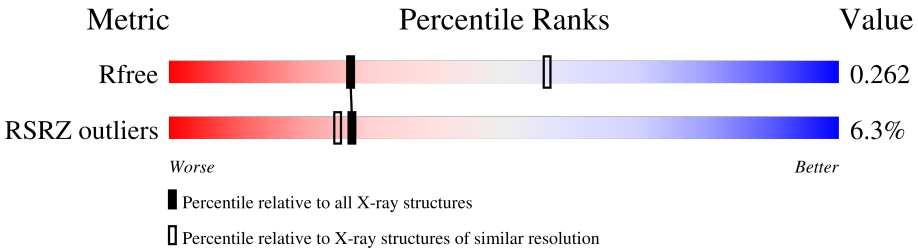
MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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)
RSRZ outliers	164620	3333 (2.70-2.70)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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
58	MG	1U	212	-	-	-	X
58	MG	2a	1613	-	-	-	X

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

2 Entry composition (i)

There are 63 unique types of molecules in this entry. The entry contains 298915 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 933	C 588	N 171	O 170	S 4	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called MET-LYS-mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			283	128	59	83	13			
53	2v	11	Total	C	N	O	P	0	0	0
			239	108	49	71	11			

- Molecule 54 is a RNA chain called A-site Aminoacyl-tRNA Lys-tRNAlys.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1599	718	282	524	74	1			
54	2w	74	Total	C	N	O	P	S	0	0	0
			1599	718	282	524	74	1			

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA fMAC-tRNAcys RNA-part.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			

- Molecule 56 is a protein called P-site Peptidyl-tRNA fMAC-tRNAcys Peptide-part.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1z	3	Total	C	N	O	S	0	0	0
			21	12	3	4	2			
56	2z	3	Total	C	N	O	S	0	0	0
			21	12	3	4	2			

- Molecule 57 is a RNA chain called E-site Deacylated tRNAlys.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
57	1y	74	Total	C	N	O	P	S	0	0	0
			1577	705	277	520	74	1			
57	2y	74	Total	C	N	O	P	S	0	0	0
			1577	705	277	520	74	1			

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1096	Total	Mg	0	0
			1096	1096		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1B	35	Total Mg 35 35	0	0
58	1D	11	Total Mg 11 11	0	0
58	1E	13	Total Mg 13 13	0	0
58	1F	12	Total Mg 12 12	0	0
58	1G	4	Total Mg 4 4	0	0
58	1H	1	Total Mg 1 1	0	0
58	1I	1	Total Mg 1 1	0	0
58	1N	5	Total Mg 5 5	0	0
58	1O	5	Total Mg 5 5	0	0
58	1P	8	Total Mg 8 8	0	0
58	1Q	7	Total Mg 7 7	0	0
58	1R	6	Total Mg 6 6	0	0
58	1S	2	Total Mg 2 2	0	0
58	1T	2	Total Mg 2 2	0	0
58	1U	12	Total Mg 12 12	0	0
58	1V	7	Total Mg 7 7	0	0
58	1W	7	Total Mg 7 7	0	0
58	1X	5	Total Mg 5 5	0	0
58	1Y	4	Total Mg 4 4	0	0
58	1Z	2	Total Mg 2 2	0	0
58	10	9	Total Mg 9 9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	11	4	Total Mg 4 4	0	0
58	12	2	Total Mg 2 2	0	0
58	13	3	Total Mg 3 3	0	0
58	14	1	Total Mg 1 1	0	0
58	15	4	Total Mg 4 4	0	0
58	16	1	Total Mg 1 1	0	0
58	17	5	Total Mg 5 5	0	0
58	18	7	Total Mg 7 7	0	0
58	19	1	Total Mg 1 1	0	0
58	1a	213	Total Mg 213 213	0	0
58	1b	1	Total Mg 1 1	0	0
58	1d	2	Total Mg 2 2	0	0
58	1e	2	Total Mg 2 2	0	0
58	1f	2	Total Mg 2 2	0	0
58	1k	1	Total Mg 1 1	0	0
58	1l	2	Total Mg 2 2	0	0
58	1m	1	Total Mg 1 1	0	0
58	1n	2	Total Mg 2 2	0	0
58	1p	1	Total Mg 1 1	0	0
58	1t	1	Total Mg 1 1	0	0
58	1v	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1w	7	Total Mg 7 7	0	0
58	1x	11	Total Mg 11 11	0	0
58	2A	687	Total Mg 687 687	0	0
58	2B	15	Total Mg 15 15	0	0
58	2D	6	Total Mg 6 6	0	0
58	2E	7	Total Mg 7 7	0	0
58	2F	4	Total Mg 4 4	0	0
58	2N	1	Total Mg 1 1	0	0
58	2O	1	Total Mg 1 1	0	0
58	2P	1	Total Mg 1 1	0	0
58	2Q	2	Total Mg 2 2	0	0
58	2R	3	Total Mg 3 3	0	0
58	2T	2	Total Mg 2 2	0	0
58	2V	1	Total Mg 1 1	0	0
58	2X	2	Total Mg 2 2	0	0
58	2Z	1	Total Mg 1 1	0	0
58	20	3	Total Mg 3 3	0	0
58	23	3	Total Mg 3 3	0	0
58	25	4	Total Mg 4 4	0	0
58	27	2	Total Mg 2 2	0	0
58	28	1	Total Mg 1 1	0	0

Continued on next page...

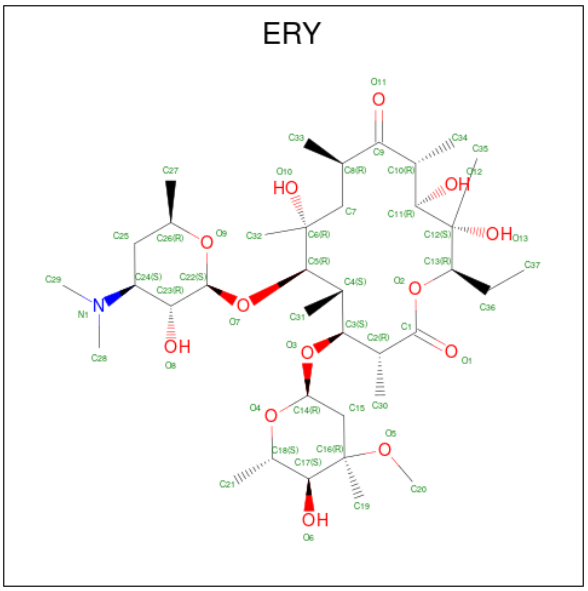
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	2a	222	Total Mg 222 222	0	0
58	2d	2	Total Mg 2 2	0	0
58	2e	1	Total Mg 1 1	0	0
58	2f	2	Total Mg 2 2	0	0
58	2g	1	Total Mg 1 1	0	0
58	2j	1	Total Mg 1 1	0	0
58	2l	6	Total Mg 6 6	0	0
58	2q	2	Total Mg 2 2	0	0
58	2r	1	Total Mg 1 1	0	0
58	2t	1	Total Mg 1 1	0	0
58	2v	2	Total Mg 2 2	0	0
58	2w	1	Total Mg 1 1	0	0
58	2x	5	Total Mg 5 5	0	0

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1	Total K 1 1	0	0
59	2x	1	Total K 1 1	0	0

- Molecule 60 is ERYTHROMYCIN A (CCD ID: ERY) (formula: $C_{37}H_{67}NO_{13}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1A	1	Total C N O 51 37 1 13	0	0
60	2A	1	Total C N O 51 37 1 13	0	0

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

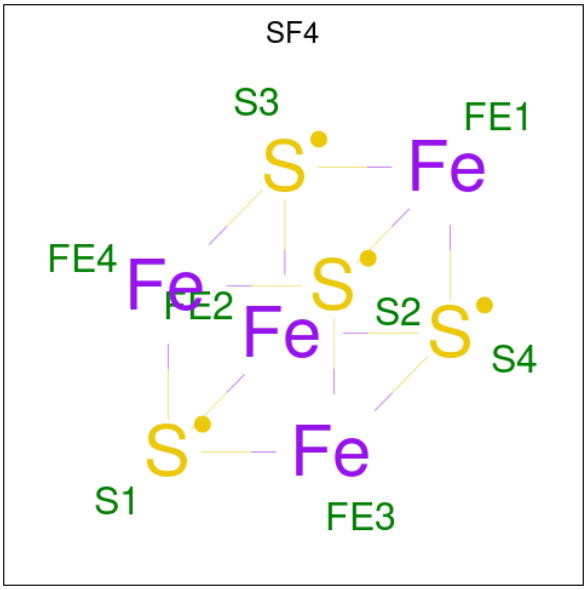
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1Y	1	Total Zn 1 1	0	0
61	14	1	Total Zn 1 1	0	0
61	15	1	Total Zn 1 1	0	0
61	16	1	Total Zn 1 1	0	0
61	19	1	Total Zn 1 1	0	0
61	1n	1	Total Zn 1 1	0	0
61	2Y	1	Total Zn 1 1	0	0
61	24	1	Total Zn 1 1	0	0
61	25	1	Total Zn 1 1	0	0
61	26	1	Total Zn 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	29	1	Total Zn 1 1	0	0
61	2n	1	Total Zn 1 1	0	0

- Molecule 62 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1d	1	Total Fe S 8 4 4	0	0
62	2d	1	Total Fe S 8 4 4	0	0

- Molecule 63 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1A	1715	Total O 1715 1715	0	0
63	1B	53	Total O 53 53	0	0
63	1D	28	Total O 28 28	0	0
63	1E	25	Total O 25 25	0	0
63	1F	13	Total O 13 13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1G	3	Total O 3 3	0	0
63	1H	2	Total O 2 2	0	0
63	1N	3	Total O 3 3	0	0
63	1O	4	Total O 4 4	0	0
63	1P	17	Total O 17 17	0	0
63	1Q	6	Total O 6 6	0	0
63	1R	12	Total O 12 12	0	0
63	1S	5	Total O 5 5	0	0
63	1T	5	Total O 5 5	0	0
63	1U	9	Total O 9 9	0	0
63	1V	9	Total O 9 9	0	0
63	1W	8	Total O 8 8	0	0
63	1X	7	Total O 7 7	0	0
63	1Y	2	Total O 2 2	0	0
63	1Z	1	Total O 1 1	0	0
63	10	9	Total O 9 9	0	0
63	11	8	Total O 8 8	0	0
63	12	3	Total O 3 3	0	0
63	13	4	Total O 4 4	0	0
63	15	6	Total O 6 6	0	0
63	16	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	17	9	Total O 9 9	0	0
63	18	9	Total O 9 9	0	0
63	1a	284	Total O 284 284	0	0
63	1e	1	Total O 1 1	0	0
63	1f	1	Total O 1 1	0	0
63	1i	1	Total O 1 1	0	0
63	1l	5	Total O 5 5	0	0
63	1m	2	Total O 2 2	0	0
63	1o	1	Total O 1 1	0	0
63	1q	2	Total O 2 2	0	0
63	1u	1	Total O 1 1	0	0
63	1v	5	Total O 5 5	0	0
63	1w	7	Total O 7 7	0	0
63	1x	6	Total O 6 6	0	0
63	1z	1	Total O 1 1	0	0
63	1y	1	Total O 1 1	0	0
63	2A	624	Total O 624 624	0	0
63	2B	12	Total O 12 12	0	0
63	2D	14	Total O 14 14	0	0
63	2E	5	Total O 5 5	0	0
63	2F	9	Total O 9 9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	2N	1	Total O 1 1	0	0
63	2O	1	Total O 1 1	0	0
63	2P	3	Total O 3 3	0	0
63	2Q	1	Total O 1 1	0	0
63	2R	1	Total O 1 1	0	0
63	2T	4	Total O 4 4	0	0
63	2U	1	Total O 1 1	0	0
63	2W	3	Total O 3 3	0	0
63	2Y	1	Total O 1 1	0	0
63	20	1	Total O 1 1	0	0
63	21	5	Total O 5 5	0	0
63	26	1	Total O 1 1	0	0
63	28	2	Total O 2 2	0	0
63	2a	161	Total O 161 161	0	0
63	2d	1	Total O 1 1	0	0
63	2e	2	Total O 2 2	0	0
63	2j	1	Total O 1 1	0	0
63	2l	4	Total O 4 4	0	0
63	2p	2	Total O 2 2	0	0
63	2v	1	Total O 1 1	0	0
63	2w	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	2x	2	Total O 2 2	0	0

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.69Å 447.93Å 622.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.21 – 2.70 152.21 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (152.21-2.70) 99.5 (152.21-2.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.217 , 0.262 0.219 , 0.262	Depositor DCC
R_{free} test set	79430 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	56.4	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 61.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	298915	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

86 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	M2G	2a	966	32	20,27,28	1.33	3 (15%)	19,40,43	1.08	2 (10%)
57	5MU	1y	54	57	19,22,23	1.41	5 (26%)	27,32,35	2.15	8 (29%)
32	5MC	1a	1404	32	19,22,23	1.79	3 (15%)	26,32,35	1.25	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	M2G	1a	966	32	20,27,28	1.37	3 (15%)	19,40,43	1.03	2 (10%)
32	4OC	2a	1402	58,32	20,23,24	0.77	0	25,32,35	1.09	2 (8%)
57	PSU	1y	39	57	18,21,22	1.39	2 (11%)	21,30,33	2.11	4 (19%)
1	PSU	1A	2605	58,1	18,21,22	1.41	4 (22%)	21,30,33	2.20	4 (19%)
1	2MA	1A	2503	58,1	18,25,26	0.76	0	20,37,40	2.03	4 (20%)
1	5MU	1A	1939	58,1	19,22,23	1.50	4 (21%)	27,32,35	2.08	6 (22%)
32	2MG	1a	1207	32	18,26,27	0.93	1 (5%)	16,38,41	1.57	4 (25%)
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.08	3 (14%)
55	PSU	1x	55	55	18,21,22	1.34	2 (11%)	21,30,33	2.12	4 (19%)
43	0TD	1l	92	43	8,9,10	4.54	1 (12%)	6,11,13	2.98	2 (33%)
57	PSU	2y	39	57	18,21,22	1.42	2 (11%)	21,30,33	1.77	2 (9%)
56	FME	2z	1	56	8,9,10	1.00	0	8,9,11	1.57	2 (25%)
55	5MC	1x	32	55	19,22,23	1.58	3 (15%)	26,32,35	1.19	2 (7%)
57	G7M	1y	46	57	20,26,27	1.36	2 (10%)	16,39,42	0.56	0
1	PSU	2A	2605	1	18,21,22	1.40	3 (16%)	21,30,33	2.01	4 (19%)
57	T6A	2y	37	57	17,24,35	0.82	1 (5%)	16,35,52	1.24	2 (12%)
57	G7M	2y	46	57	20,26,27	1.32	2 (10%)	16,39,42	0.65	0
32	5MC	2a	1404	32	19,22,23	1.68	3 (15%)	26,32,35	1.19	3 (11%)
1	OMG	2A	2251	55,1	19,26,27	0.89	1 (5%)	21,38,41	1.10	2 (9%)
55	8AN	1x	76	58,55	17,24,25	1.14	2 (11%)	13,35,38	2.99	2 (15%)
54	PSU	1w	55	54	18,21,22	1.37	1 (5%)	21,30,33	2.00	4 (19%)
32	UR3	1a	1498	32	19,22,23	1.00	0	26,32,35	1.64	2 (7%)
1	5MU	1A	1915	1	19,22,23	1.43	6 (31%)	27,32,35	2.12	7 (25%)
54	T6A	1w	37	54	26,34,35	0.95	1 (3%)	28,49,52	1.77	4 (14%)
32	PSU	2a	516	32	18,21,22	1.37	2 (11%)	21,30,33	2.03	5 (23%)
1	OMU	2A	2552	58,1	19,22,23	1.12	2 (10%)	25,31,34	1.88	5 (20%)
55	4SU	2x	8	55	18,21,22	2.13	6 (33%)	25,30,33	1.32	4 (16%)
55	5MU	2x	54	55	19,22,23	1.38	6 (31%)	27,32,35	2.03	6 (22%)
32	MA6	1a	1518	32	19,26,27	1.02	2 (10%)	18,38,41	1.90	3 (16%)
54	G7M	1w	46	54	20,26,27	1.20	1 (5%)	16,39,42	0.67	0
1	OMC	2A	1920	1	19,22,23	0.79	0	25,31,34	0.91	1 (4%)
32	PSU	1a	516	32	18,21,22	1.36	3 (16%)	21,30,33	1.89	4 (19%)
1	2MA	2A	2503	58,1	18,25,26	0.72	0	20,37,40	1.94	4 (20%)
1	5MC	1A	1942	1	19,22,23	1.64	3 (15%)	26,32,35	1.19	3 (11%)
32	5MC	2a	1400	32	19,22,23	1.71	3 (15%)	26,32,35	1.27	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	2A	1917	1	18,21,22	1.40	2 (11%)	21,30,33	1.96	3 (14%)
32	MA6	1a	1519	32	19,26,27	1.04	2 (10%)	18,38,41	2.00	3 (16%)
32	5MC	2a	967	32	19,22,23	1.77	3 (15%)	26,32,35	1.19	3 (11%)
32	5MC	1a	1407	32	19,22,23	1.54	3 (15%)	26,32,35	1.14	3 (11%)
32	UR3	2a	1498	32	19,22,23	1.03	2 (10%)	26,32,35	1.65	3 (11%)
55	4SU	1x	8	55	18,21,22	2.29	5 (27%)	25,30,33	1.60	6 (24%)
32	G7M	1a	527	58,32	20,26,27	1.22	2 (10%)	16,39,42	0.61	0
55	5MU	1x	54	55	19,22,23	1.43	5 (26%)	27,32,35	1.94	5 (18%)
1	PSU	2A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	1.99	3 (14%)
57	T6A	1y	37	57	17,24,35	0.81	0	16,35,52	1.23	2 (12%)
54	PSU	2w	39	54	18,21,22	1.29	2 (11%)	21,30,33	2.09	3 (14%)
1	OMC	1A	1920	1	19,22,23	0.78	0	25,31,34	0.93	1 (4%)
54	5MU	2w	54	54	19,22,23	1.54	6 (31%)	27,32,35	1.75	5 (18%)
54	PSU	1w	39	54	18,21,22	1.35	2 (11%)	21,30,33	1.98	4 (19%)
32	5MC	1a	967	32	19,22,23	1.50	3 (15%)	26,32,35	1.07	2 (7%)
32	5MC	2a	1407	32	19,22,23	1.57	3 (15%)	26,32,35	1.18	3 (11%)
54	A1B8A	2w	76	54	26,33,34	1.14	3 (11%)	23,46,49	1.57	1 (4%)
1	5MC	2A	1962	58,1	19,22,23	1.64	3 (15%)	26,32,35	1.15	2 (7%)
32	2MG	2a	1207	32	18,26,27	0.92	0	16,38,41	1.59	3 (18%)
43	0TD	2l	92	43	8,9,10	4.44	2 (25%)	6,11,13	6.78	1 (16%)
1	5MC	1A	1962	58,1	19,22,23	1.80	3 (15%)	26,32,35	1.20	3 (11%)
1	5MU	2A	1939	1	19,22,23	1.39	5 (26%)	27,32,35	2.25	6 (22%)
1	PSU	1A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	2.14	3 (14%)
32	G7M	2a	527	58,32	20,26,27	1.17	1 (5%)	16,39,42	0.59	0
32	5MC	1a	1400	32	19,22,23	1.61	3 (15%)	26,32,35	1.21	3 (11%)
1	5MU	2A	1915	1	19,22,23	1.49	5 (26%)	27,32,35	2.04	5 (18%)
54	PSU	2w	55	54	18,21,22	1.33	2 (11%)	21,30,33	1.96	4 (19%)
1	5MC	2A	1942	1	19,22,23	1.58	3 (15%)	26,32,35	1.11	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	1.01	1 (4%)
55	8AN	2x	76	58,55,59	17,24,25	1.13	2 (11%)	13,35,38	2.75	3 (23%)
54	T6A	2w	37	54,53	26,34,35	0.96	1 (3%)	28,49,52	1.82	5 (17%)
54	U8U	1w	34	54,53	20,24,25	1.42	2 (10%)	22,34,37	1.17	4 (18%)
32	MA6	2a	1519	32	19,26,27	1.02	2 (10%)	18,38,41	1.89	3 (16%)
55	PSU	2x	55	55	18,21,22	1.34	2 (11%)	21,30,33	2.03	4 (19%)
57	5MU	2y	54	57	19,22,23	1.49	5 (26%)	27,32,35	1.61	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
57	PSU	1y	55	57	18,21,22	1.39	2 (11%)	21,30,33	2.01	3 (14%)
55	5MC	2x	32	55	19,22,23	1.69	3 (15%)	26,32,35	1.25	4 (15%)
56	FME	1z	1	56	8,9,10	0.95	1 (12%)	8,9,11	2.12	2 (25%)
32	MA6	2a	1518	32	19,26,27	1.01	2 (10%)	18,38,41	1.96	3 (16%)
57	PSU	2y	55	57	18,21,22	1.37	2 (11%)	21,30,33	2.00	3 (14%)
57	U8U	2y	34	57	17,21,25	1.56	3 (17%)	21,30,37	1.49	3 (14%)
54	5MU	1w	54	54	19,22,23	1.33	4 (21%)	27,32,35	2.68	6 (22%)
54	U8U	2w	34	54,32,53	20,24,25	1.48	3 (15%)	22,34,37	1.73	2 (9%)
1	OMU	1A	2552	58,1	19,22,23	1.22	3 (15%)	25,31,34	1.85	5 (20%)
54	A1B8A	1w	76	54	26,33,34	1.19	3 (11%)	23,46,49	1.55	1 (4%)
1	OMG	1A	2251	58,55,1	19,26,27	0.94	1 (5%)	21,38,41	1.16	3 (14%)
54	G7M	2w	46	54	20,26,27	1.22	1 (5%)	16,39,42	0.98	1 (6%)
57	U8U	1y	34	57	17,21,25	1.56	4 (23%)	21,30,37	1.48	3 (14%)

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	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
57	5MU	1y	54	57	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	4OC	2a	1402	58,32	-	2/9/29/30	0/2/2/2
57	PSU	1y	39	57	-	4/7/25/26	0/2/2/2
1	PSU	1A	2605	58,1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	58,1	-	0/3/25/26	0/3/3/3
1	5MU	1A	1939	58,1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
57	PSU	2y	39	57	-	0/7/25/26	0/2/2/2
56	FME	2z	1	56	-	2/7/9/11	-
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
57	G7M	1y	46	57	-	0/3/25/26	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
57	T6A	2y	37	57	-	1/3/25/42	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	G7M	2y	46	57	-	0/3/25/26	0/3/3/3
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/5/27/28	0/3/3/3
55	8AN	1x	76	58,55	-	3/3/25/26	0/3/3/3
54	PSU	1w	55	54	-	2/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
54	T6A	1w	37	54	-	6/19/41/42	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	58,1	-	0/9/27/28	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
54	G7M	1w	46	54	-	0/3/25/26	0/3/3/3
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	58,1	-	0/3/25/26	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	2/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	58,32	-	2/3/25/26	0/3/3/3
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
57	T6A	1y	37	57	-	1/3/25/42	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
54	5MU	2w	54	54	-	3/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
54	A1B8A	2w	76	54	-	3/16/38/39	0/3/3/3
1	5MC	2A	1962	58,1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	1/5/27/28	0/3/3/3
43	0TD	2l	92	43	-	4/7/12/14	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1A	1962	58,1	-	2/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	58,32	-	3/3/25/26	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
55	8AN	2x	76	58,55,59	-	3/3/25/26	0/3/3/3
54	T6A	2w	37	54,53	-	9/19/41/42	0/3/3/3
54	U8U	1w	34	54,53	-	2/10/28/29	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
57	5MU	2y	54	57	-	0/7/25/26	0/2/2/2
57	PSU	1y	55	57	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
56	FME	1z	1	56	-	3/7/9/11	-
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
57	PSU	2y	55	57	-	0/7/25/26	0/2/2/2
57	U8U	2y	34	57	-	0/7/25/29	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
54	U8U	2w	34	54,32,53	-	6/10/28/29	0/2/2/2
1	OMU	1A	2552	58,1	-	0/9/27/28	0/2/2/2
54	A1B8A	1w	76	54	-	6/16/38/39	0/3/3/3
1	OMG	1A	2251	58,55,1	-	0/5/27/28	0/3/3/3
54	G7M	2w	46	54	-	1/3/25/26	0/3/3/3
57	U8U	1y	34	57	-	0/7/25/29	0/2/2/2

All (205) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.29	1.69	1.82
43	2l	92	0TD	CB-SB	-12.04	1.70	1.82
1	1A	1962	5MC	C5-C4	6.74	1.49	1.44
32	2a	967	5MC	C5-C4	6.60	1.49	1.44
32	1a	1404	5MC	C5-C4	6.56	1.49	1.44
32	2a	1400	5MC	C5-C4	6.35	1.48	1.44
32	2a	1404	5MC	C5-C4	6.07	1.48	1.44
55	2x	32	5MC	C5-C4	6.05	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1942	5MC	C5-C4	5.94	1.48	1.44
1	2A	1962	5MC	C5-C4	5.79	1.48	1.44
32	1a	1400	5MC	C5-C4	5.77	1.48	1.44
1	2A	1942	5MC	C5-C4	5.57	1.48	1.44
32	1a	1407	5MC	C5-C4	5.54	1.48	1.44
32	2a	1407	5MC	C5-C4	5.54	1.48	1.44
55	1x	8	4SU	C4-N3	-5.53	1.31	1.37
55	1x	32	5MC	C5-C4	5.44	1.48	1.44
32	1a	967	5MC	C5-C4	5.27	1.48	1.44
55	2x	8	4SU	C4-N3	-5.06	1.32	1.37
54	1w	34	U8U	C2-S2	-4.71	1.60	1.67
55	1x	8	4SU	C4-S4	-4.67	1.60	1.68
55	2x	8	4SU	C4-S4	-4.64	1.60	1.68
57	2y	34	U8U	C2-S2	-4.55	1.60	1.67
54	2w	34	U8U	C2-S2	-4.49	1.60	1.67
57	1y	34	U8U	C2-S2	-4.44	1.60	1.67
54	1w	55	PSU	C6-C5	4.17	1.39	1.35
57	1y	46	G7M	C5-C4	4.10	1.47	1.39
32	1a	966	M2G	C2-N3	4.10	1.36	1.30
32	2a	966	M2G	C2-N3	4.06	1.36	1.30
57	2y	39	PSU	C6-C5	4.05	1.39	1.35
57	2y	46	G7M	C5-C4	4.05	1.47	1.39
57	1y	55	PSU	C6-C5	4.04	1.39	1.35
55	1x	8	4SU	C5-C4	-3.99	1.37	1.42
54	1w	76	A1B8A	O4'-C1'	3.96	1.46	1.40
54	2w	55	PSU	C6-C5	3.95	1.39	1.35
57	2y	55	PSU	C6-C5	3.85	1.39	1.35
32	1a	527	G7M	C5-C4	3.83	1.46	1.39
54	1w	46	G7M	C5-C4	3.75	1.46	1.39
54	2w	46	G7M	C5-C4	3.72	1.46	1.39
57	1y	39	PSU	C6-C5	3.69	1.39	1.35
1	2A	1917	PSU	C6-C5	3.67	1.39	1.35
54	1w	39	PSU	C6-C5	3.67	1.39	1.35
1	1A	1917	PSU	C6-C5	3.65	1.39	1.35
55	1x	55	PSU	C6-C5	3.62	1.39	1.35
32	2a	516	PSU	C6-C5	3.60	1.39	1.35
55	1x	8	4SU	C2-N3	-3.57	1.31	1.38
32	2a	527	G7M	C5-C4	3.53	1.46	1.39
54	2w	76	A1B8A	O4'-C1'	3.43	1.45	1.40
54	2w	39	PSU	C6-C5	3.43	1.39	1.35
55	2x	55	PSU	C6-C5	3.41	1.39	1.35
54	2w	34	U8U	C6-N1	-3.36	1.32	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2605	PSU	C6-C5	3.34	1.39	1.35
1	2A	1911	PSU	C6-C5	3.31	1.39	1.35
1	1A	1911	PSU	C6-C5	3.23	1.38	1.35
54	2w	54	5MU	C6-C5	3.23	1.39	1.34
1	1A	1939	5MU	C4-N3	-3.21	1.32	1.38
55	2x	8	4SU	C5-C4	-3.18	1.38	1.42
32	1a	516	PSU	C6-C5	3.17	1.38	1.35
1	2A	1915	5MU	C6-C5	2.99	1.39	1.34
1	2A	1942	5MC	C6-C5	2.97	1.39	1.34
55	1x	32	5MC	C6-C5	2.97	1.39	1.34
57	2y	54	5MU	C6-C5	2.97	1.39	1.34
1	1A	2605	PSU	C4-N3	-2.96	1.33	1.38
32	2a	1404	5MC	C6-C5	2.90	1.39	1.34
55	2x	8	4SU	C2-N3	-2.89	1.32	1.38
1	2A	2605	PSU	C4-N3	-2.88	1.33	1.38
54	2w	54	5MU	C2-N1	2.85	1.42	1.38
1	1A	1939	5MU	C2-N3	-2.85	1.33	1.38
1	1A	1939	5MU	C6-C5	2.82	1.39	1.34
57	1y	54	5MU	C4-C5	2.82	1.49	1.44
1	2A	1915	5MU	C2-N1	2.80	1.42	1.38
32	1a	966	M2G	C2-N2	2.80	1.40	1.35
1	2A	1939	5MU	C4-N3	-2.78	1.33	1.38
55	2x	54	5MU	C6-C5	2.77	1.39	1.34
1	1A	1915	5MU	C6-C5	2.75	1.39	1.34
55	2x	32	5MC	C6-C5	2.74	1.39	1.34
55	1x	54	5MU	C6-C5	2.74	1.39	1.34
1	2A	1939	5MU	C6-C5	2.74	1.39	1.34
54	1w	34	U8U	C4-N3	-2.74	1.33	1.38
57	2y	54	5MU	C4-N3	-2.74	1.33	1.38
57	1y	54	5MU	C6-C5	2.73	1.39	1.34
55	1x	54	5MU	C4-N3	-2.71	1.33	1.38
32	2a	966	M2G	C2-N2	2.69	1.40	1.35
1	2A	1962	5MC	C6-C5	2.68	1.39	1.34
32	1a	1404	5MC	C6-N1	-2.68	1.33	1.38
1	2A	1911	PSU	C4-N3	-2.67	1.33	1.38
1	1A	2552	OMU	C4-N3	-2.67	1.34	1.38
32	2a	967	5MC	C6-C5	2.67	1.39	1.34
1	1A	1915	5MU	C4-C5	2.67	1.49	1.44
1	2A	1915	5MU	C4-C5	2.66	1.49	1.44
57	1y	34	U8U	C4-N3	-2.65	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.64	1.33	1.38
1	1A	1911	PSU	C4-N3	-2.64	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	76	8AN	C6-C5	-2.62	1.33	1.43
32	1a	1404	5MC	C6-C5	2.62	1.38	1.34
57	2y	39	PSU	C4-N3	-2.62	1.33	1.38
32	1a	1400	5MC	C6-C5	2.62	1.38	1.34
57	2y	54	5MU	C2-N1	2.62	1.42	1.38
54	2w	54	5MU	C4-N3	-2.60	1.34	1.38
55	1x	76	8AN	C6-C5	-2.60	1.33	1.43
32	2a	1407	5MC	C6-C5	2.60	1.38	1.34
54	1w	54	5MU	C2-N1	2.59	1.42	1.38
1	2A	1917	PSU	C4-N3	-2.58	1.34	1.38
1	1A	1915	5MU	C4-N3	-2.57	1.34	1.38
32	1a	516	PSU	C4-N3	-2.57	1.34	1.38
54	2w	37	T6A	C6-C5	2.56	1.48	1.44
1	2A	2251	OMG	C6-N1	-2.56	1.33	1.37
1	2A	1962	5MC	C6-N1	-2.56	1.33	1.38
54	1w	76	A1B8A	C6-C5	-2.55	1.33	1.43
54	1w	39	PSU	C4-N3	-2.55	1.34	1.38
1	1A	1942	5MC	C6-N1	-2.54	1.33	1.38
54	2w	76	A1B8A	C6-C5	-2.53	1.34	1.43
57	2y	34	U8U	C5-C4	2.53	1.49	1.43
1	1A	2251	OMG	C6-N1	-2.53	1.33	1.37
57	1y	34	U8U	C5-C4	2.52	1.49	1.43
1	1A	1942	5MC	C6-C5	2.51	1.38	1.34
57	1y	55	PSU	C4-N3	-2.50	1.34	1.38
1	1A	1939	5MU	C6-N1	-2.50	1.33	1.38
32	2a	1400	5MC	C6-C5	2.50	1.38	1.34
55	2x	54	5MU	C4-N3	-2.49	1.34	1.38
55	2x	55	PSU	C4-N3	-2.49	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.49	1.34	1.37
57	2y	54	5MU	C4-C5	2.49	1.48	1.44
1	2A	1915	5MU	C4-N3	-2.48	1.34	1.38
32	1a	966	M2G	C6-N1	-2.47	1.34	1.37
32	1a	967	5MC	C6-C5	2.47	1.38	1.34
32	1a	1518	MA6	C6-C5	-2.46	1.41	1.44
1	2A	1939	5MU	C6-N1	-2.45	1.33	1.38
55	1x	32	5MC	C6-N1	-2.44	1.33	1.38
55	2x	32	5MC	C6-N1	-2.43	1.33	1.38
54	1w	54	5MU	C6-C5	2.42	1.38	1.34
1	1A	1962	5MC	C6-C5	2.42	1.38	1.34
54	2w	54	5MU	O2-C2	2.42	1.27	1.23
54	1w	54	5MU	C4-C5	2.42	1.48	1.44
55	2x	54	5MU	C4-C5	2.41	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	39	PSU	C4-N3	-2.41	1.34	1.38
1	1A	1917	PSU	C4-N3	-2.40	1.34	1.38
32	1a	1407	5MC	C6-C5	2.40	1.38	1.34
55	1x	54	5MU	C4-C5	2.39	1.48	1.44
57	1y	54	5MU	C2-N1	2.38	1.42	1.38
55	1x	54	5MU	C2-N1	2.38	1.42	1.38
1	1A	2605	PSU	C6-C5	2.37	1.37	1.35
1	1A	1915	5MU	C2-N1	2.37	1.42	1.38
1	1A	2605	PSU	C2-N3	-2.36	1.33	1.37
32	2a	1407	5MC	C6-N1	-2.35	1.34	1.38
32	2a	1518	MA6	C6-C5	-2.35	1.41	1.44
32	1a	1400	5MC	C6-N1	-2.35	1.34	1.38
57	2y	34	U8U	C4-N3	-2.35	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.35	1.34	1.38
54	1w	54	5MU	C6-N1	-2.34	1.34	1.38
32	2a	516	PSU	C4-N3	-2.34	1.34	1.38
55	1x	8	4SU	O2-C2	2.33	1.27	1.23
32	1a	967	5MC	C6-N1	-2.33	1.34	1.38
32	2a	1498	UR3	C2-N1	2.33	1.41	1.38
1	2A	2552	OMU	C4-N3	-2.32	1.34	1.38
32	2a	1519	MA6	C6-C5	-2.32	1.41	1.44
57	1y	46	G7M	C6-N1	-2.31	1.34	1.37
55	2x	8	4SU	O2-C2	2.31	1.27	1.23
57	1y	39	PSU	C4-N3	-2.31	1.34	1.38
32	1a	1519	MA6	C6-C5	-2.30	1.41	1.44
55	1x	55	PSU	C4-N3	-2.29	1.34	1.38
1	1A	2552	OMU	C2-N3	-2.29	1.34	1.38
1	1A	2552	OMU	C5-C4	-2.28	1.38	1.43
54	2w	34	U8U	C4-N3	-2.28	1.34	1.38
54	1w	37	T6A	C6-C5	2.27	1.48	1.44
32	1a	1407	5MC	C6-N1	-2.26	1.34	1.38
54	2w	54	5MU	C4-C5	2.25	1.48	1.44
55	2x	76	8AN	C5-N7	-2.23	1.31	1.39
1	2A	1939	5MU	C2-N3	-2.22	1.34	1.38
32	2a	966	M2G	C6-N1	-2.20	1.34	1.37
32	2a	1404	5MC	C6-N1	-2.19	1.34	1.38
1	2A	2605	PSU	C2-N3	-2.19	1.33	1.37
32	2a	967	5MC	C6-N1	-2.19	1.34	1.38
57	2y	46	G7M	C6-N1	-2.18	1.34	1.37
1	2A	1939	5MU	C4-C5	2.16	1.48	1.44
57	1y	54	5MU	C6-N1	-2.15	1.34	1.38
1	1A	2605	PSU	C2-N1	-2.14	1.33	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	54	5MU	C2-N3	-2.14	1.34	1.38
57	2y	54	5MU	C2-N3	-2.14	1.34	1.38
54	2w	55	PSU	C4-N3	-2.13	1.34	1.38
32	1a	527	G7M	C6-N1	-2.13	1.34	1.37
54	2w	76	A1B8A	C5-N7	-2.13	1.32	1.39
1	2A	1942	5MC	C6-N1	-2.13	1.34	1.38
57	1y	54	5MU	C4-N3	-2.12	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.12	1.34	1.38
57	2y	55	PSU	C4-N3	-2.11	1.34	1.38
32	2a	1518	MA6	C6-N1	2.11	1.35	1.32
54	1w	76	A1B8A	C5-N7	-2.11	1.32	1.39
55	2x	54	5MU	C2-N3	-2.10	1.34	1.38
1	1A	1915	5MU	C6-N1	-2.08	1.34	1.38
32	2a	1519	MA6	C6-N1	2.07	1.35	1.32
55	2x	8	4SU	C2-N1	2.07	1.41	1.38
43	2l	92	0TD	CB-CA	2.06	1.55	1.54
55	2x	54	5MU	C6-N1	-2.06	1.34	1.38
57	1y	34	U8U	C6-C5	2.05	1.39	1.35
32	1a	516	PSU	C2-N3	-2.05	1.34	1.37
55	1x	76	8AN	C5-N7	-2.04	1.32	1.39
32	1a	1519	MA6	C6-N1	2.04	1.35	1.32
32	2a	1498	UR3	C6-C5	2.03	1.39	1.35
32	1a	1518	MA6	C6-N1	2.03	1.35	1.32
57	2y	37	T6A	C2-N3	2.03	1.35	1.32
56	1z	1	FME	CN-N	2.03	1.39	1.33
54	2w	54	5MU	C6-N1	-2.01	1.34	1.38
55	2x	54	5MU	C2-N1	2.01	1.41	1.38
1	1A	1915	5MU	C2-N3	-2.00	1.34	1.38
1	2A	2552	OMU	C6-C5	2.00	1.39	1.35

All (273) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	16.41	131.87	102.36
55	1x	76	8AN	C4'-O4'-C1'	-8.03	102.57	109.92
54	1w	37	T6A	C2-N1-C6	7.09	122.11	116.60
1	2A	2503	2MA	C2-N3-C4	6.87	121.01	115.46
1	1A	2503	2MA	C2-N3-C4	6.83	120.98	115.46
1	1A	2605	PSU	N1-C2-N3	6.81	122.35	115.17
54	1w	54	5MU	C4-N3-C2	-6.78	118.45	127.34
54	2w	37	T6A	C2-N1-C6	6.76	121.85	116.60
57	1y	39	PSU	N1-C2-N3	6.68	122.22	115.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	-6.67	90.37	102.36
1	1A	1911	PSU	N1-C2-N3	6.65	122.18	115.17
54	1w	54	5MU	O4-C4-C5	-6.62	117.35	124.92
55	1x	55	PSU	N1-C2-N3	6.59	122.11	115.17
32	1a	1498	UR3	C4-N3-C2	-6.53	119.33	124.58
1	1A	1917	PSU	N1-C2-N3	6.52	122.04	115.17
55	2x	76	8AN	C4'-O4'-C1'	-6.51	103.96	109.92
54	2w	76	A1B8A	N3-C2-N1	-6.49	119.86	128.67
55	1x	76	8AN	N3-C2-N1	-6.48	119.88	128.67
55	2x	76	8AN	N3-C2-N1	-6.44	119.93	128.67
54	1w	76	A1B8A	N3-C2-N1	-6.41	119.97	128.67
32	2a	1498	UR3	C4-N3-C2	-6.39	119.44	124.58
54	2w	39	PSU	N1-C2-N3	6.33	121.85	115.17
57	1y	55	PSU	N1-C2-N3	6.31	121.82	115.17
32	2a	516	PSU	N1-C2-N3	6.27	121.78	115.17
55	2x	55	PSU	N1-C2-N3	6.25	121.76	115.17
1	2A	1917	PSU	N1-C2-N3	6.22	121.73	115.17
54	1w	39	PSU	N1-C2-N3	6.20	121.71	115.17
57	2y	55	PSU	N1-C2-N3	6.18	121.68	115.17
1	2A	2605	PSU	N1-C2-N3	6.17	121.67	115.17
1	2A	1911	PSU	N1-C2-N3	6.10	121.61	115.17
54	2w	34	U8U	C1'-N1-C6	-6.04	111.20	121.15
32	1a	516	PSU	N1-C2-N3	5.78	121.26	115.17
32	1a	1519	MA6	N3-C2-N1	-5.74	120.88	128.67
54	1w	55	PSU	N1-C2-N3	5.69	121.17	115.17
54	1w	54	5MU	N3-C2-N1	5.69	122.29	114.89
32	2a	1518	MA6	N3-C2-N1	-5.62	121.05	128.67
1	2A	1939	5MU	C4-N3-C2	-5.60	120.00	127.34
54	1w	54	5MU	C5-C4-N3	5.60	120.19	115.32
32	1a	1518	MA6	N3-C2-N1	-5.57	121.11	128.67
54	2w	55	PSU	N1-C2-N3	5.53	121.00	115.17
57	2y	39	PSU	N1-C2-N3	5.32	120.78	115.17
1	1A	1915	5MU	N3-C2-N1	5.29	121.77	114.89
57	1y	54	5MU	C4-N3-C2	-5.27	120.43	127.34
1	2A	1939	5MU	N3-C2-N1	5.26	121.74	114.89
32	2a	1519	MA6	N3-C2-N1	-5.23	121.57	128.67
1	1A	1915	5MU	C4-N3-C2	-5.14	120.61	127.34
1	2A	1915	5MU	N3-C2-N1	5.07	121.49	114.89
32	2a	1518	MA6	C2-N1-C6	5.04	121.79	116.84
57	2y	34	U8U	C2-N3-C4	-5.04	121.13	127.33
55	2x	54	5MU	N3-C2-N1	5.03	121.44	114.89
1	1A	1939	5MU	C4-N3-C2	-5.02	120.76	127.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	1y	34	U8U	C2-N3-C4	-5.01	121.17	127.33
1	1A	1939	5MU	N3-C2-N1	4.93	121.31	114.89
1	2A	1915	5MU	C4-N3-C2	-4.93	120.88	127.34
1	2A	2552	OMU	C4-N3-C2	-4.91	120.51	126.61
55	2x	54	5MU	C4-N3-C2	-4.90	120.92	127.34
57	1y	54	5MU	N3-C2-N1	4.88	121.24	114.89
32	1a	1519	MA6	C2-N1-C6	4.84	121.59	116.84
1	1A	2552	OMU	C4-N3-C2	-4.82	120.63	126.61
1	2A	1939	5MU	C5-C4-N3	4.78	119.47	115.32
1	1A	1939	5MU	C5-C4-N3	4.75	119.45	115.32
56	1z	1	FME	CA-N-CN	4.70	130.06	122.82
55	1x	54	5MU	N3-C2-N1	4.69	120.99	114.89
32	1a	1518	MA6	C2-N1-C6	4.67	121.42	116.84
1	1A	2552	OMU	N3-C2-N1	4.64	120.93	114.89
54	2w	39	PSU	C4-N3-C2	-4.58	120.06	126.37
55	1x	54	5MU	C4-N3-C2	-4.57	121.34	127.34
1	1A	2605	PSU	C4-N3-C2	-4.53	120.14	126.37
57	1y	54	5MU	C5-C4-N3	4.52	119.25	115.32
1	2A	2552	OMU	N3-C2-N1	4.52	120.77	114.89
32	2a	1519	MA6	C2-N1-C6	4.48	121.23	116.84
54	2w	34	U8U	C-C5-C6	-4.41	114.59	121.21
57	2y	55	PSU	O2-C2-N1	-4.40	118.26	122.79
54	1w	55	PSU	O2-C2-N1	-4.37	118.28	122.79
57	1y	39	PSU	O2-C2-N1	-4.37	118.29	122.79
1	1A	1915	5MU	C5-C4-N3	4.36	119.11	115.32
1	2A	1939	5MU	O4-C4-C5	-4.35	119.94	124.92
55	2x	55	PSU	C4-N3-C2	-4.35	120.38	126.37
1	1A	1911	PSU	C4-N3-C2	-4.33	120.40	126.37
1	1A	1917	PSU	C4-N3-C2	-4.24	120.53	126.37
1	1A	1911	PSU	O2-C2-N1	-4.23	118.42	122.79
1	1A	1939	5MU	C5-C6-N1	-4.21	118.74	123.31
1	2A	1939	5MU	C5-C6-N1	-4.19	118.76	123.31
1	1A	2605	PSU	O2-C2-N1	-4.15	118.51	122.79
55	1x	55	PSU	C4-N3-C2	-4.14	120.67	126.37
1	2A	2605	PSU	C4-N3-C2	-4.14	120.67	126.37
32	2a	516	PSU	C4-N3-C2	-4.12	120.70	126.37
1	2A	1915	5MU	C5-C4-N3	4.09	118.88	115.32
54	1w	54	5MU	C5-C6-N1	-4.08	118.88	123.31
55	1x	54	5MU	C5-C4-N3	4.07	118.86	115.32
54	2w	54	5MU	N3-C2-N1	4.06	120.18	114.89
55	2x	54	5MU	C5-C4-N3	4.05	118.84	115.32
57	1y	54	5MU	O4-C4-C5	-4.00	120.34	124.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	8	4SU	C6-C5-C4	-3.98	116.50	119.95
57	1y	55	PSU	C4-N3-C2	-3.97	120.90	126.37
54	1w	39	PSU	C4-N3-C2	-3.96	120.91	126.37
54	2w	55	PSU	C4-N3-C2	-3.96	120.92	126.37
1	2A	1911	PSU	C4-N3-C2	-3.95	120.94	126.37
55	1x	55	PSU	O2-C2-N1	-3.92	118.75	122.79
57	1y	39	PSU	C4-N3-C2	-3.91	120.99	126.37
32	2a	1404	5MC	C5-C6-N1	-3.90	119.08	123.31
1	1A	1939	5MU	O4-C4-C5	-3.88	120.48	124.92
55	2x	54	5MU	O4-C4-C5	-3.87	120.49	124.92
54	2w	54	5MU	C4-N3-C2	-3.85	122.29	127.34
1	2A	1917	PSU	C4-N3-C2	-3.82	121.10	126.37
55	1x	32	5MC	C5-C6-N1	-3.77	119.22	123.31
1	2A	1915	5MU	O4-C4-C5	-3.76	120.61	124.92
54	2w	39	PSU	O2-C2-N1	-3.72	118.96	122.79
57	2y	54	5MU	N3-C2-N1	3.71	119.72	114.89
32	1a	516	PSU	C4-N3-C2	-3.71	121.26	126.37
54	2w	54	5MU	O4-C4-C5	-3.68	120.71	124.92
57	2y	55	PSU	C4-N3-C2	-3.67	121.32	126.37
1	1A	1915	5MU	O4-C4-C5	-3.66	120.73	124.92
54	2w	54	5MU	C5-C4-N3	3.64	118.49	115.32
54	1w	37	T6A	N3-C2-N1	-3.64	123.73	128.67
55	1x	54	5MU	O4-C4-C5	-3.62	120.77	124.92
1	1A	2552	OMU	C5-C4-N3	3.62	119.87	114.80
1	2A	2552	OMU	O2-C2-N1	-3.57	118.15	122.80
1	2A	1911	PSU	O2-C2-N1	-3.55	119.13	122.79
54	2w	37	T6A	N3-C2-N1	-3.53	123.88	128.67
57	1y	37	T6A	N3-C2-N1	-3.52	123.89	128.67
32	2a	1400	5MC	C5-C6-N1	-3.52	119.50	123.31
32	2a	1207	2MG	N1-C2-N2	3.49	120.13	116.56
32	1a	1400	5MC	C5-C6-N1	-3.49	119.53	123.31
32	2a	967	5MC	C5-C6-N1	-3.47	119.54	123.31
1	1A	1917	PSU	O2-C2-N1	-3.44	119.24	122.79
1	2A	2552	OMU	C5-C4-N3	3.44	119.61	114.80
1	1A	1962	5MC	C5-C6-N1	-3.41	119.61	123.31
56	2z	1	FME	CA-N-CN	3.41	128.06	122.82
55	2x	8	4SU	C5-C4-N3	3.40	117.92	114.75
55	1x	54	5MU	C5-C6-N1	-3.40	119.62	123.31
57	2y	54	5MU	C5-C4-N3	3.40	118.28	115.32
32	2a	1407	5MC	C5-C6-N1	-3.39	119.63	123.31
1	2A	1917	PSU	O2-C2-N1	-3.38	119.30	122.79
54	1w	55	PSU	C4-N3-C2	-3.37	121.72	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	54	5MU	C5-C6-N1	-3.37	119.65	123.31
57	1y	54	5MU	C5-C6-N1	-3.36	119.66	123.31
1	2A	1962	5MC	C5-C6-N1	-3.34	119.69	123.31
57	1y	55	PSU	O2-C2-N1	-3.29	119.40	122.79
55	1x	8	4SU	O2-C2-N1	3.28	127.07	122.80
57	2y	54	5MU	C4-N3-C2	-3.27	123.05	127.34
57	2y	37	T6A	N3-C2-N1	-3.27	124.24	128.67
54	2w	37	T6A	N6-C10-N11	3.26	118.26	113.77
56	1z	1	FME	C-CA-N	3.26	115.79	109.50
57	2y	39	PSU	C4-N3-C2	-3.25	121.89	126.37
32	2a	516	PSU	O2-C2-N1	-3.25	119.44	122.79
54	2w	55	PSU	O2-C2-N1	-3.25	119.44	122.79
1	2A	1942	5MC	C5-C6-N1	-3.22	119.81	123.31
32	1a	1404	5MC	C5-C6-N1	-3.20	119.83	123.31
32	1a	1207	2MG	N1-C2-N2	3.20	119.83	116.56
32	2a	1207	2MG	N2-C2-N3	-3.19	116.44	120.51
32	1a	967	5MC	C5-C6-N1	-3.14	119.90	123.31
1	2A	2251	OMG	C8-N7-C5	3.14	107.89	102.55
1	2A	1915	5MU	C5-C6-N1	-3.14	119.91	123.31
54	1w	34	U8U	C5-C4-N3	3.13	119.99	115.21
54	1w	39	PSU	O2-C2-N1	-3.12	119.57	122.79
55	1x	8	4SU	C1'-N1-C2	3.12	123.19	117.59
32	1a	516	PSU	O2-C2-N1	-3.11	119.58	122.79
32	1a	1207	2MG	C8-N7-C5	3.11	107.84	102.55
32	2a	1519	MA6	C4-C5-N7	-3.10	106.06	109.34
32	1a	1404	5MC	C5-C4-N3	-3.09	118.58	121.75
32	2a	1407	5MC	C5-C4-N3	-3.08	118.59	121.75
55	2x	32	5MC	C5-C6-N1	-3.07	119.98	123.31
1	1A	1915	5MU	C5-C6-N1	-3.02	120.03	123.31
1	2A	2605	PSU	O2-C2-N1	-3.02	119.67	122.79
1	1A	2552	OMU	O2-C2-N1	-3.02	118.87	122.80
1	1A	1942	5MC	C5-C6-N1	-2.99	120.06	123.31
32	1a	1498	UR3	C5-C4-N3	2.99	118.98	115.04
32	2a	1498	UR3	C5-C4-N3	2.99	118.98	115.04
57	2y	34	U8U	C5-C4-N3	2.98	118.97	114.80
32	2a	1207	2MG	C8-N7-C5	2.98	107.62	102.55
57	1y	34	U8U	C5-C4-N3	2.97	118.96	114.80
32	1a	1519	MA6	C4-C5-N7	-2.97	106.20	109.34
57	2y	37	T6A	C4-C5-N7	-2.96	106.20	109.34
1	2A	1942	5MC	C5-C4-N3	-2.96	118.72	121.75
55	2x	8	4SU	C1'-N1-C2	2.94	122.87	117.59
1	1A	2552	OMU	O4-C4-C5	-2.92	120.13	125.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2w	55	PSU	C6-C5-C4	-2.91	116.21	118.17
32	2a	966	M2G	C8-N7-C5	2.91	107.50	102.55
55	2x	32	5MC	C5-C4-N3	-2.91	118.78	121.75
57	2y	54	5MU	O4-C4-C5	-2.90	121.60	124.92
55	1x	32	5MC	C5-C4-N3	-2.89	118.79	121.75
55	1x	8	4SU	C5-C4-N3	2.89	117.44	114.75
1	2A	1939	5MU	O2-C2-N1	-2.87	119.07	122.80
55	2x	55	PSU	O2-C2-N1	-2.86	119.84	122.79
32	1a	1407	5MC	C5-C4-N3	-2.85	118.83	121.75
1	1A	1942	5MC	C5-C4-N3	-2.83	118.85	121.75
1	1A	2251	OMG	C8-N7-C5	2.83	107.36	102.55
32	1a	1407	5MC	C5-C6-N1	-2.80	120.27	123.31
32	1a	966	M2G	C8-N7-C5	2.80	107.31	102.55
32	1a	1518	MA6	C4-C5-N7	-2.79	106.39	109.34
1	1A	1962	5MC	CM5-C5-C6	-2.75	119.12	122.85
1	2A	2552	OMU	O4-C4-C5	-2.75	120.42	125.16
54	1w	54	5MU	O2-C2-N1	-2.73	119.25	122.80
1	1A	1962	5MC	C5-C4-N3	-2.72	118.97	121.75
32	2a	1518	MA6	C4-C5-N7	-2.71	106.47	109.34
1	1A	2503	2MA	C2-N1-C6	2.70	122.25	118.10
54	1w	34	U8U	O4-C4-C5	-2.70	120.17	124.71
32	1a	1207	2MG	N2-C2-N3	-2.70	117.07	120.51
1	2A	2503	2MA	C4-C5-N7	-2.70	106.49	109.34
54	2w	54	5MU	C5-C6-N1	-2.66	120.42	123.31
54	2w	37	T6A	C4-C5-N7	-2.66	106.53	109.34
32	1a	1400	5MC	C5-C4-N3	-2.66	119.03	121.75
55	2x	8	4SU	C6-C5-C4	-2.64	117.66	119.95
57	1y	54	5MU	C5M-C5-C4	2.64	121.60	118.78
55	2x	54	5MU	O2-C2-N1	-2.63	119.37	122.80
54	1w	55	PSU	C6-C5-C4	-2.61	116.42	118.17
57	2y	34	U8U	O4-C4-C5	-2.61	120.67	125.16
1	1A	2605	PSU	C5-C6-N1	-2.60	118.54	122.14
1	2A	1962	5MC	C5-C4-N3	-2.58	119.11	121.75
57	2y	54	5MU	C5-C6-N1	-2.58	120.51	123.31
1	1A	1915	5MU	O2-C2-N1	-2.58	119.44	122.80
1	2A	2503	2MA	C2-N1-C6	2.55	122.02	118.10
1	1A	2503	2MA	C5-C6-N1	-2.54	117.84	120.84
32	2a	967	5MC	C5-C4-N3	-2.52	119.17	121.75
32	2a	1400	5MC	O2-C2-N3	-2.51	118.37	122.33
55	2x	32	5MC	O2-C2-N3	-2.51	118.38	122.33
56	2z	1	FME	C-CA-N	2.49	114.30	109.50
1	1A	1915	5MU	C5M-C5-C4	2.49	121.44	118.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1402	4OC	O2-C2-N3	-2.48	118.42	122.33
1	1A	2503	2MA	C4-C5-N7	-2.48	106.72	109.34
32	2a	1402	4OC	C6-C5-C4	2.47	119.98	117.00
54	1w	37	T6A	C4-C5-N7	-2.47	106.73	109.34
32	1a	1407	5MC	O2-C2-N3	-2.46	118.45	122.33
55	2x	55	PSU	C5-C6-N1	-2.46	118.73	122.14
32	1a	1404	5MC	CM5-C5-C6	-2.44	119.55	122.85
54	1w	37	T6A	N6-C10-N11	2.43	117.11	113.77
57	1y	37	T6A	C4-C5-N7	-2.41	106.79	109.34
57	1y	34	U8U	O4-C4-C5	-2.39	121.03	125.16
1	1A	1942	5MC	CM5-C5-C6	-2.38	119.62	122.85
32	2a	1400	5MC	C5-C4-N3	-2.37	119.33	121.75
32	1a	1404	5MC	O2-C2-N3	-2.35	118.63	122.33
32	2a	1404	5MC	C5-C4-N3	-2.32	119.38	121.75
57	1y	54	5MU	O2-C2-N1	-2.32	119.78	122.80
32	1a	967	5MC	C5-C4-N3	-2.32	119.38	121.75
32	1a	1402	4OC	C6-C5-C4	2.30	119.77	117.00
32	2a	516	PSU	O4'-C1'-C2'	2.29	108.32	105.15
32	1a	1207	2MG	CM2-N2-C2	-2.27	118.77	123.65
1	1A	2251	OMG	O6-C6-C5	-2.26	119.84	124.32
57	1y	39	PSU	O4'-C1'-C2'	2.23	108.23	105.15
1	1A	2251	OMG	C5-C6-N1	2.21	118.29	114.07
54	2w	46	G7M	N2-C2-N3	-2.20	115.39	119.67
1	1A	1920	OMC	O2-C2-N3	-2.18	118.90	122.33
1	2A	2605	PSU	C5-C6-N1	-2.17	119.13	122.14
32	2a	966	M2G	C5-C6-N1	2.16	118.19	114.07
55	2x	76	8AN	O4'-C1'-N9	-2.14	105.91	108.75
54	1w	39	PSU	C5-C6-N1	-2.14	119.17	122.14
55	1x	8	4SU	C4-N3-C2	2.13	129.36	127.31
1	2A	2251	OMG	C5-C6-N1	2.13	118.14	114.07
54	2w	37	T6A	N6-C6-N1	2.13	121.11	118.71
55	2x	8	4SU	O2-C2-N1	2.13	125.56	122.80
32	2a	1400	5MC	CM5-C5-C6	-2.13	119.97	122.85
32	2a	1498	UR3	C6-N1-C2	-2.13	120.06	121.80
32	2a	1404	5MC	O2-C2-N3	-2.12	118.99	122.33
32	1a	966	M2G	C5-C6-N1	2.11	118.10	114.07
55	2x	32	5MC	C1'-N1-C6	-2.11	117.67	121.15
32	2a	967	5MC	O2-C2-N3	-2.10	119.01	122.33
32	1a	1400	5MC	O2-C2-N3	-2.10	119.01	122.33
54	1w	34	U8U	C5-C6-N1	-2.10	120.11	122.94
1	2A	2503	2MA	C5-C6-N1	-2.10	118.36	120.84
43	1l	92	0TD	OD2-CG-CB	2.09	117.68	113.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	34	U8U	C1'-N1-C6	-2.09	117.70	121.15
32	2a	516	PSU	C5-C6-N1	-2.09	119.24	122.14
57	2y	54	5MU	C5M-C5-C4	2.07	120.99	118.78
55	1x	55	PSU	C5-C6-N1	-2.06	119.27	122.14
57	2y	54	5MU	C1'-N1-C2	2.06	121.30	117.59
57	1y	54	5MU	C5M-C5-C6	-2.06	120.06	122.85
1	2A	1920	OMC	O2-C2-N3	-2.05	119.09	122.33
55	1x	8	4SU	S4-C4-N3	-2.05	118.06	120.20
32	2a	1407	5MC	O2-C2-N3	-2.03	119.13	122.33
32	2a	1400	5MC	C1'-N1-C6	-2.03	117.81	121.15
1	1A	1939	5MU	O2-C2-N1	-2.02	120.16	122.80
32	1a	516	PSU	C6-C5-C4	-2.01	116.82	118.17

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
57	1y	39	PSU	C2'-C1'-C5-C4
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
43	2l	92	0TD	O-C-CA-CB
55	2x	76	8AN	O4'-C4'-C5'-O5'
55	2x	76	8AN	C3'-C4'-C5'-O5'
54	1w	34	U8U	C5-C-N-CA
54	2w	34	U8U	N-C-C5-C4
54	2w	34	U8U	C5-C-N-CA
54	1w	37	T6A	O10-C10-N6-C6
54	1w	37	T6A	N11-C10-N6-C6
54	1w	37	T6A	C14-C12-C13-ODA
54	1w	37	T6A	C14-C12-C13-ODB
54	2w	37	T6A	O10-C10-N6-C6
54	2w	37	T6A	N11-C10-N6-C6
54	2w	37	T6A	N6-C10-N11-C12
54	2w	37	T6A	C13-C12-C14-O14
54	2w	37	T6A	C13-C12-C14-C15
54	1w	76	A1B8A	O4'-C4'-C5'-O5'
54	2w	76	A1B8A	O4'-C4'-C5'-O5'
56	1z	1	FME	C-CA-CB-CG
56	2z	1	FME	O-C-CA-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	2w	37	T6A	O10-C10-N11-C12
55	1x	76	8AN	C3'-C4'-C5'-O5'
54	2w	76	A1B8A	C3'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
54	1w	76	A1B8A	C-CA-CB-CG
55	1x	76	8AN	O4'-C4'-C5'-O5'
56	1z	1	FME	CA-CB-CG-SD
56	1z	1	FME	N-CA-CB-CG
54	1w	76	A1B8A	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
1	2A	1917	PSU	O4'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	2a	1400	5MC	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
54	2w	37	T6A	N11-C12-C14-C15
54	1w	37	T6A	N11-C12-C13-ODA
54	1w	37	T6A	N11-C12-C13-ODB
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	2a	1404	5MC	O4'-C4'-C5'-O5'
54	2w	34	U8U	C3'-C4'-C5'-O5'
54	2w	34	U8U	O4'-C4'-C5'-O5'
54	2w	54	5MU	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1404	5MC	C3'-C4'-C5'-O5'
54	2w	54	5MU	C3'-C4'-C5'-O5'
54	2w	76	A1B8A	CA-CB-CG-CD
54	1w	76	A1B8A	CA-CB-CG-CD
32	2a	527	G7M	O4'-C4'-C5'-O5'
32	2a	1207	2MG	O4'-C4'-C5'-O5'
57	1y	39	PSU	C3'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
54	1w	76	A1B8A	N-CA-CB-CG
57	1y	39	PSU	C4'-C5'-O5'-P
43	1l	92	0TD	SB-CB-CG-OD1
43	2l	92	0TD	SB-CB-CG-OD1
55	1x	76	8AN	C4'-C5'-O5'-P
55	2x	76	8AN	C4'-C5'-O5'-P
54	1w	55	PSU	O4'-C1'-C5-C4
32	2a	1402	4OC	C3'-C4'-C5'-O5'
57	1y	37	T6A	C4'-C5'-O5'-P
54	1w	76	A1B8A	CE-CD-CG-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
56	2z	1	FME	CA-CB-CG-SD
1	1A	1962	5MC	C2'-C1'-N1-C6
54	2w	46	G7M	C4'-C5'-O5'-P
54	2w	37	T6A	N11-C12-C14-O14
57	1y	39	PSU	O4'-C4'-C5'-O5'
1	2A	1917	PSU	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C4'-C5'-O5'-P
32	2a	527	G7M	C4'-C5'-O5'-P
43	2l	92	0TD	SB-CB-CG-OD2
54	2w	54	5MU	C4'-C5'-O5'-P
54	1w	55	PSU	O4'-C1'-C5-C6
1	1A	1962	5MC	O4'-C1'-N1-C6
54	1w	34	U8U	N-C-C5-C6
54	2w	34	U8U	N-C-C5-C6
57	2y	37	T6A	C3'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
54	2w	37	T6A	N11-C12-C13-ODB
32	1a	1402	4OC	C3'-C4'-C5'-O5'
1	1A	1920	OMC	C2'-C1'-N1-C2
54	2w	34	U8U	C2'-C1'-N1-C2
32	2a	1519	MA6	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

4.6 Ligand geometry (i)

Of 2540 ligands modelled in this entry, 2536 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
62	SF4	1d	303	35	0,12,12	-	-	-		
60	ERY	1A	4098	-	53,53,53	0.95	2 (3%)	82,82,82	1.49	12 (14%)
60	ERY	2A	3688	-	53,53,53	0.95	2 (3%)	82,82,82	1.36	9 (10%)
62	SF4	2d	303	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
62	SF4	1d	303	35	-	-	0/6/5/5
60	ERY	1A	4098	-	-	1/72/107/107	0/3/3/3
60	ERY	2A	3688	-	-	5/72/107/107	0/3/3/3
62	SF4	2d	303	35	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	2A	3688	ERY	O2-C1	4.85	1.45	1.34
60	1A	4098	ERY	O2-C1	4.77	1.45	1.34
60	1A	4098	ERY	O2-C13	-2.84	1.41	1.46
60	2A	3688	ERY	O2-C13	-2.41	1.42	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	2A	3688	ERY	C13-O2-C1	-5.08	109.32	118.20
60	1A	4098	ERY	O3-C3-C4	3.97	112.91	108.23
60	1A	4098	ERY	C6-C5-C4	-3.69	108.53	113.89
60	2A	3688	ERY	O5-C16-C15	-3.66	107.32	112.95
60	2A	3688	ERY	O5-C16-C17	3.58	109.05	103.86
60	2A	3688	ERY	O2-C1-C2	3.58	119.17	111.53
60	1A	4098	ERY	C13-O2-C1	-3.43	112.22	118.20
60	1A	4098	ERY	O2-C1-C2	3.10	118.15	111.53
60	1A	4098	ERY	C32-C6-C5	3.05	115.33	110.13
60	1A	4098	ERY	C15-C16-C17	2.99	112.76	107.64
60	1A	4098	ERY	O7-C5-C6	2.83	109.78	106.40
60	1A	4098	ERY	O4-C18-C17	2.82	114.90	110.04
60	1A	4098	ERY	O5-C16-C15	-2.71	108.78	112.95
60	1A	4098	ERY	C2-C3-C4	-2.55	105.57	112.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	1A	4098	ERY	O7-C5-C4	-2.50	107.97	111.58
60	2A	3688	ERY	C20-O5-C16	2.41	122.42	117.51
60	2A	3688	ERY	O2-C1-O1	-2.33	119.75	123.95
60	1A	4098	ERY	O2-C1-O1	-2.30	119.79	123.95
60	2A	3688	ERY	C6-C7-C8	-2.23	111.16	115.61
60	2A	3688	ERY	C2-C3-C4	-2.16	106.71	112.91
60	2A	3688	ERY	C31-C4-C3	-2.14	107.63	111.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

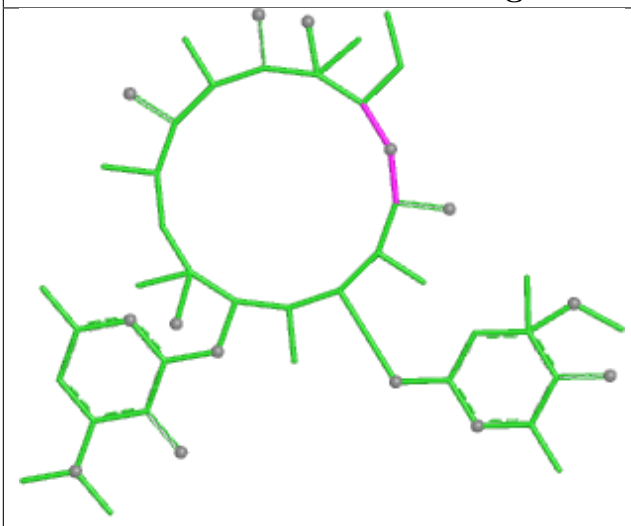
Mol	Chain	Res	Type	Atoms
60	2A	3688	ERY	C15-C16-O5-C20
60	2A	3688	ERY	C17-C16-O5-C20
60	2A	3688	ERY	C19-C16-O5-C20
60	1A	4098	ERY	C32-C6-C7-C8
60	2A	3688	ERY	C32-C6-C7-C8
60	2A	3688	ERY	C30-C2-C3-C4

There are no ring outliers.

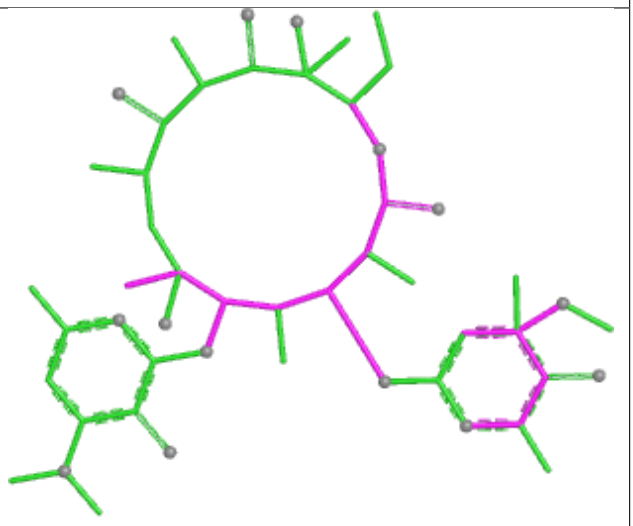
No monomer is involved in short contacts.

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

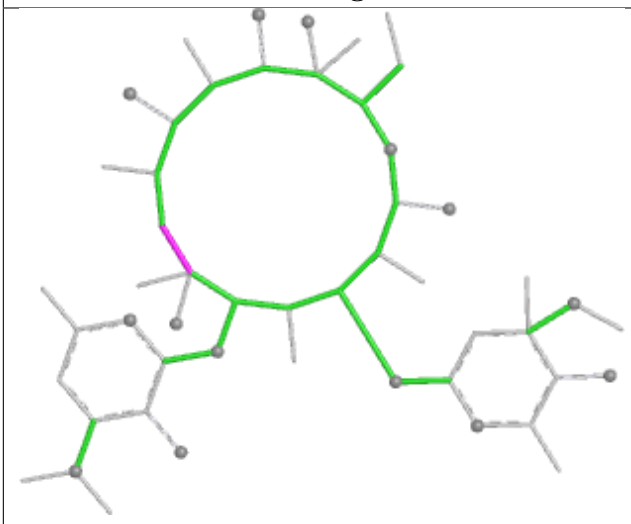
Ligand ERY 1A 4098



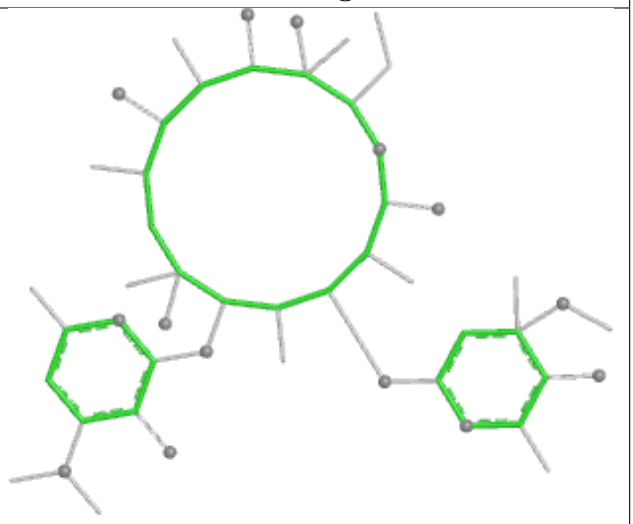
Bond lengths



Bond angles

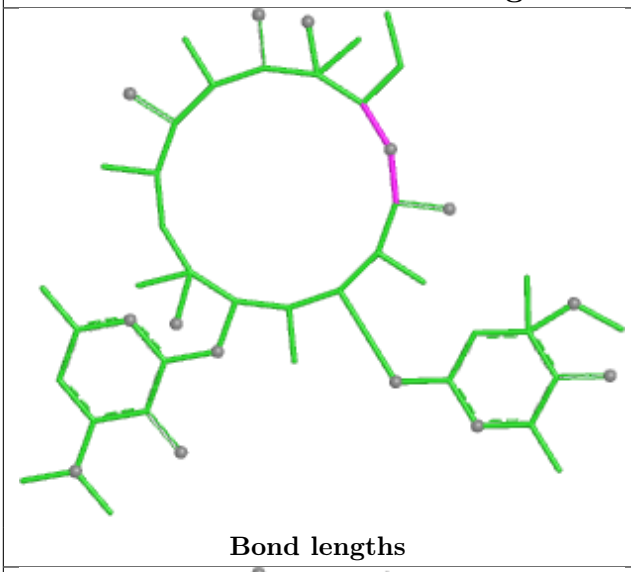


Torsions

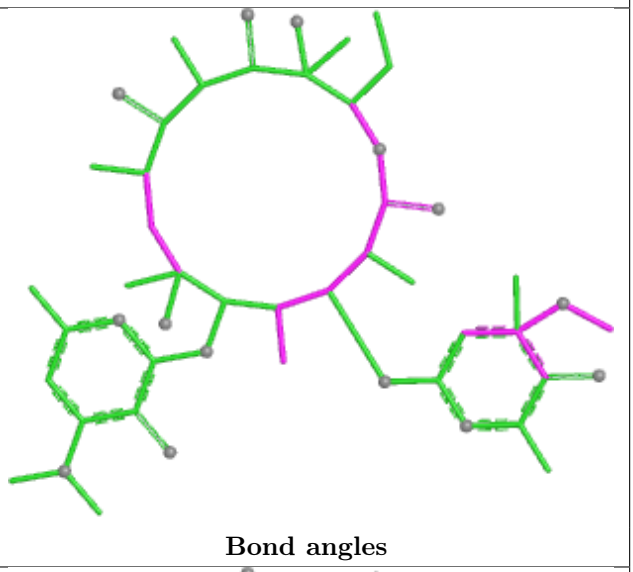


Rings

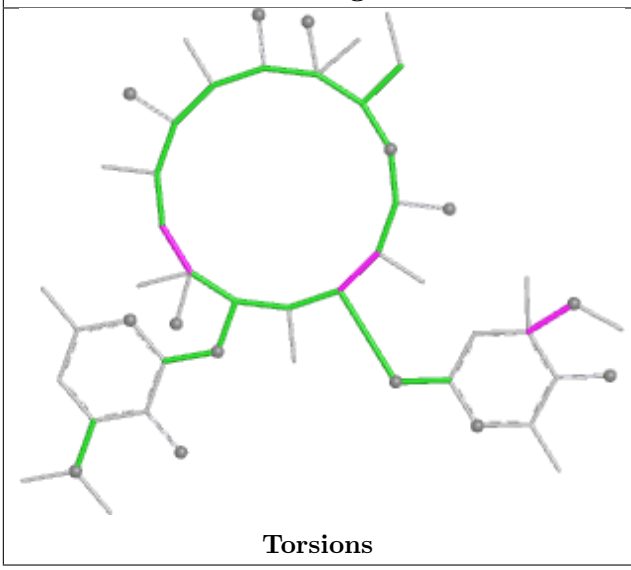
Ligand ERY 2A 3688



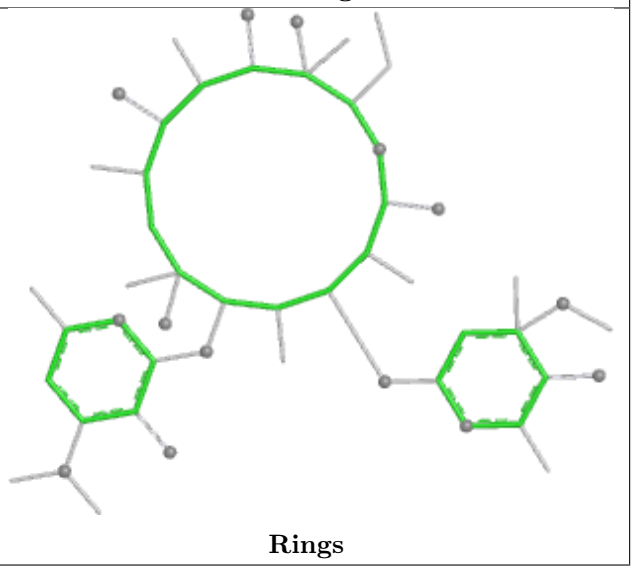
Bond lengths



Bond angles



Torsions



Rings

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1A	2860/2915 (98%)	-0.42	128 (4%) 39 37	19, 38, 99, 111	0
1	2A	2789/2915 (95%)	0.02	108 (3%) 44 42	33, 59, 95, 113	0
2	1B	120/121 (99%)	-0.35	0 100 100	31, 52, 66, 91	0
2	2B	120/121 (99%)	1.08	10 (8%) 19 17	64, 82, 90, 97	0
3	1D	275/276 (99%)	-0.25	2 (0%) 84 83	21, 38, 52, 80	0
3	2D	275/276 (99%)	0.14	2 (0%) 84 83	32, 51, 65, 79	0
4	1E	204/206 (99%)	-0.21	0 100 100	20, 44, 63, 72	0
4	2E	204/206 (99%)	0.16	2 (0%) 79 79	36, 60, 74, 84	0
5	1F	203/210 (96%)	-0.17	0 100 100	19, 44, 67, 85	0
5	2F	203/210 (96%)	0.33	5 (2%) 58 57	36, 71, 83, 88	0
6	1G	181/182 (99%)	0.42	7 (3%) 44 42	41, 61, 77, 86	0
6	2G	181/182 (99%)	1.44	41 (22%) 3 3	70, 82, 89, 96	0
7	1H	174/180 (96%)	0.19	2 (1%) 77 77	41, 56, 68, 71	0
7	2H	174/180 (96%)	0.99	12 (6%) 24 22	70, 83, 90, 93	0
8	1I	146/148 (98%)	0.50	1 (0%) 84 83	44, 75, 84, 88	0
8	2I	146/148 (98%)	0.78	9 (6%) 28 26	60, 75, 87, 90	0
9	1N	140/140 (100%)	-0.05	1 (0%) 84 83	28, 44, 62, 81	0
9	2N	140/140 (100%)	0.69	7 (5%) 35 33	45, 66, 78, 88	0
10	1O	122/122 (100%)	-0.04	1 (0%) 82 82	29, 42, 58, 69	0
10	2O	122/122 (100%)	0.22	0 100 100	46, 59, 71, 79	0
11	1P	149/150 (99%)	-0.13	0 100 100	21, 45, 68, 77	0
11	2P	149/150 (99%)	0.48	3 (2%) 64 64	36, 69, 83, 89	0
12	1Q	141/141 (100%)	-0.19	0 100 100	27, 43, 59, 73	0
12	2Q	141/141 (100%)	0.77	7 (4%) 35 33	50, 69, 79, 83	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%)	-0.21	0 100 100	28, 39, 53, 64	0
13	2R	118/118 (100%)	0.09	2 (1%) 69 68	40, 54, 65, 73	0
14	1S	110/112 (98%)	0.05	0 100 100	38, 51, 63, 71	0
14	2S	110/112 (98%)	1.28	16 (14%) 7 6	65, 75, 84, 87	0
15	1T	131/146 (89%)	0.15	4 (3%) 51 49	34, 46, 71, 78	0
15	2T	131/146 (89%)	0.35	2 (1%) 71 71	50, 62, 76, 80	0
16	1U	116/118 (98%)	-0.28	0 100 100	26, 36, 55, 67	0
16	2U	116/118 (98%)	0.50	1 (0%) 81 80	46, 63, 78, 83	0
17	1V	101/101 (100%)	-0.04	1 (0%) 79 79	25, 48, 64, 72	0
17	2V	101/101 (100%)	0.59	3 (2%) 52 50	45, 73, 81, 86	0
18	1W	112/113 (99%)	-0.18	2 (1%) 67 67	26, 37, 55, 82	0
18	2W	112/113 (99%)	0.41	4 (3%) 46 45	40, 52, 70, 96	0
19	1X	95/96 (98%)	-0.12	2 (2%) 63 63	26, 40, 62, 77	0
19	2X	95/96 (98%)	0.50	2 (2%) 63 63	44, 62, 77, 82	0
20	1Y	107/110 (97%)	0.32	1 (0%) 81 80	35, 52, 71, 80	0
20	2Y	107/110 (97%)	1.12	15 (14%) 7 7	62, 74, 85, 89	0
21	1Z	154/206 (74%)	0.67	11 (7%) 23 21	46, 68, 90, 100	0
21	2Z	160/206 (77%)	1.40	31 (19%) 4 4	68, 83, 94, 99	0
22	10	83/85 (97%)	0.01	6 (7%) 23 21	29, 40, 60, 70	0
22	20	83/85 (97%)	1.14	10 (12%) 10 9	45, 67, 76, 81	0
23	11	97/98 (98%)	0.13	2 (2%) 63 63	27, 47, 71, 78	0
23	21	97/98 (98%)	0.39	1 (1%) 79 79	41, 58, 79, 80	0
24	12	70/72 (97%)	0.09	1 (1%) 73 73	35, 51, 63, 71	0
24	22	70/72 (97%)	0.72	1 (1%) 73 73	59, 73, 81, 85	0
25	13	59/60 (98%)	-0.11	1 (1%) 69 68	29, 43, 65, 75	0
25	23	59/60 (98%)	0.69	3 (5%) 34 32	56, 68, 79, 92	0
26	14	69/71 (97%)	0.81	8 (11%) 11 10	55, 77, 89, 94	0
26	24	69/71 (97%)	1.42	18 (26%) 2 2	81, 89, 97, 100	0
27	15	59/60 (98%)	-0.03	2 (3%) 48 46	24, 39, 69, 78	0
27	25	59/60 (98%)	0.13	0 100 100	39, 53, 71, 86	0
28	16	53/54 (98%)	-0.18	1 (1%) 66 65	31, 42, 57, 60	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.73	2 (3%) 44 42	54, 64, 71, 75	0
29	17	48/49 (97%)	-0.31	2 (4%) 41 39	22, 28, 55, 63	0
29	27	48/49 (97%)	-0.03	2 (4%) 41 39	32, 41, 64, 76	0
30	18	64/65 (98%)	-0.30	0 100 100	28, 35, 43, 55	0
30	28	64/65 (98%)	0.48	0 100 100	47, 58, 66, 74	0
31	19	37/37 (100%)	-0.28	0 100 100	32, 43, 59, 67	0
31	29	37/37 (100%)	0.88	2 (5%) 32 30	64, 69, 80, 86	0
32	1a	1488/1521 (97%)	0.19	42 (2%) 55 53	36, 67, 94, 112	0
32	2a	1491/1521 (98%)	0.72	105 (7%) 24 22	52, 80, 98, 112	0
33	1b	231/256 (90%)	0.81	24 (10%) 13 12	66, 81, 89, 94	0
33	2b	231/256 (90%)	1.27	41 (17%) 4 5	75, 88, 93, 99	0
34	1c	206/239 (86%)	0.65	5 (2%) 59 58	61, 73, 82, 89	0
34	2c	206/239 (86%)	1.47	57 (27%) 2 2	75, 88, 93, 97	0
35	1d	208/209 (99%)	0.74	11 (5%) 33 31	58, 70, 81, 87	0
35	2d	208/209 (99%)	0.93	21 (10%) 14 13	62, 75, 85, 92	0
36	1e	148/162 (91%)	0.47	2 (1%) 73 73	51, 64, 75, 83	0
36	2e	148/162 (91%)	1.15	19 (12%) 9 8	69, 80, 87, 90	0
37	1f	100/101 (99%)	0.31	1 (1%) 79 79	58, 67, 77, 81	0
37	2f	100/101 (99%)	0.52	2 (2%) 64 64	64, 73, 80, 86	0
38	1g	155/156 (99%)	0.53	11 (7%) 23 21	61, 72, 89, 93	0
38	2g	155/156 (99%)	1.06	21 (13%) 8 7	74, 84, 91, 94	0
39	1h	137/138 (99%)	0.60	3 (2%) 62 61	58, 68, 76, 82	0
39	2h	137/138 (99%)	1.09	13 (9%) 15 14	71, 79, 85, 88	0
40	1i	127/128 (99%)	0.93	9 (7%) 23 21	56, 77, 85, 88	0
40	2i	127/128 (99%)	1.62	39 (30%) 1 2	76, 87, 93, 95	0
41	1j	97/105 (92%)	1.21	21 (21%) 3 3	59, 79, 87, 93	0
41	2j	96/105 (91%)	1.84	34 (35%) 1 1	75, 88, 94, 95	0
42	1k	114/129 (88%)	0.54	7 (6%) 28 26	45, 70, 81, 86	0
42	2k	114/129 (88%)	0.86	7 (6%) 28 26	60, 76, 85, 88	0
43	1l	121/132 (91%)	0.35	3 (2%) 58 57	41, 57, 68, 78	0
43	2l	121/132 (91%)	0.97	9 (7%) 22 20	57, 71, 80, 86	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.83	7 (5%) 30 28	57, 72, 82, 97	0
44	2m	122/126 (96%)	1.84	40 (32%) 1 1	73, 86, 92, 95	0
45	1n	60/61 (98%)	0.59	2 (3%) 49 47	60, 68, 76, 77	0
45	2n	60/61 (98%)	2.27	31 (51%) 0 1	78, 88, 92, 95	0
46	1o	88/89 (98%)	0.55	2 (2%) 61 60	52, 65, 75, 81	0
46	2o	88/89 (98%)	0.77	6 (6%) 25 23	63, 76, 84, 91	0
47	1p	82/88 (93%)	1.23	18 (21%) 3 3	59, 71, 79, 89	0
47	2p	82/88 (93%)	0.79	6 (7%) 22 20	59, 71, 82, 86	0
48	1q	99/105 (94%)	0.59	3 (3%) 52 50	57, 68, 78, 82	0
48	2q	99/105 (94%)	0.96	11 (11%) 12 11	65, 74, 83, 87	0
49	1r	68/88 (77%)	0.30	1 (1%) 71 71	56, 67, 78, 81	0
49	2r	68/88 (77%)	0.54	1 (1%) 71 71	66, 75, 84, 87	0
50	1s	83/93 (89%)	0.52	3 (3%) 46 45	65, 74, 83, 86	0
50	2s	83/93 (89%)	1.78	29 (34%) 1 1	81, 89, 94, 98	0
51	1t	96/106 (90%)	0.76	11 (11%) 11 10	60, 72, 82, 86	0
51	2t	96/106 (90%)	0.62	4 (4%) 41 39	60, 72, 81, 87	0
52	1u	23/27 (85%)	0.68	1 (4%) 40 39	60, 67, 73, 79	0
52	2u	23/27 (85%)	1.94	10 (43%) 1 1	78, 83, 87, 88	0
53	1v	13/24 (54%)	1.09	3 (23%) 2 3	46, 72, 98, 103	0
53	2v	11/24 (45%)	1.42	3 (27%) 2 2	69, 83, 94, 96	0
54	1w	67/76 (88%)	1.38	20 (29%) 1 2	49, 93, 103, 108	0
54	2w	67/76 (88%)	1.54	17 (25%) 2 2	66, 100, 108, 110	0
55	1x	72/77 (93%)	0.62	4 (5%) 31 29	31, 67, 84, 89	0
55	2x	72/77 (93%)	0.84	3 (4%) 41 39	47, 84, 93, 96	0
56	1z	2/3 (66%)	0.41	0 100 100	37, 37, 37, 38	0
56	2z	2/3 (66%)	0.97	0 100 100	52, 52, 52, 56	0
57	1y	68/76 (89%)	1.90	25 (36%) 1 1	59, 104, 108, 109	0
57	2y	68/76 (89%)	2.07	36 (52%) 0 1	69, 106, 110, 111	0
All	All	20882/21754 (95%)	0.36	1311 (6%) 27 25	19, 66, 93, 113	0

All (1311) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	13.2
44	2m	123	ALA	10.0
44	2m	102	ARG	9.3
44	1m	124	PRO	9.2
1	1A	2113	U	8.4
44	1m	122	LYS	8.3
44	2m	122	LYS	8.1
1	1A	2115	G	8.0
1	1A	2112	G	7.3
1	1A	2145	C	7.2
1	2A	2145	C	7.0
1	2A	2112	G	6.4
44	1m	123	ALA	6.3
1	1A	2114	A	6.2
45	2n	2	ALA	6.2
32	2a	1032	G	6.0
1	2A	2146	C	5.9
44	2m	121	LYS	5.9
45	1n	2	ALA	5.4
33	2b	165	VAL	5.3
7	1H	2	SER	5.2
1	1A	2121	G	5.2
1	2A	2113	U	5.2
44	1m	2	ALA	5.1
1	2A	2111	C	5.0
21	1Z	141	VAL	5.0
32	2a	1031	G	5.0
32	2a	973	G	5.0
32	2a	1030(B)	C	4.9
1	1A	2117	A	4.9
44	1m	121	LYS	4.8
1	1A	2159	G	4.8
32	2a	1033	G	4.8
45	2n	39	LEU	4.8
38	2g	84	ASN	4.8
41	2j	47	PHE	4.8
50	1s	84	GLY	4.7
40	2i	102	LEU	4.7
1	1A	2147	G	4.7
38	2g	83	ALA	4.7
1	1A	2146	C	4.6
32	2a	1027	C	4.6
53	1v	13	A	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	2n	34	TYR	4.6
26	24	51	ASP	4.6
1	2A	2166	G	4.6
38	1g	81	GLY	4.6
45	2n	25	VAL	4.6
1	2A	2125	G	4.6
32	2a	1532	U	4.6
1	2A	2133	G	4.6
1	2A	2155	G	4.6
1	2A	2174	C	4.5
38	2g	82	GLY	4.5
40	2i	14	VAL	4.5
1	1A	2136	C	4.5
1	1A	2178	C	4.5
1	2A	2123	G	4.4
32	2a	1034	G	4.4
32	2a	1116	C	4.4
32	1a	1257	U	4.4
32	2a	1149	C	4.4
18	2W	112	GLY	4.4
1	1A	2103	C	4.4
1	2A	2167	U	4.4
23	11	2	SER	4.4
54	1w	49	G	4.3
1	2A	2175	C	4.3
32	2a	972	C	4.3
40	1i	126	SER	4.3
33	2b	237	ALA	4.3
1	2A	2165	G	4.3
50	2s	9	VAL	4.3
22	20	7	LEU	4.2
45	2n	33	VAL	4.2
1	1A	2111	C	4.2
1	2A	2115	G	4.2
43	2l	64	TYR	4.2
50	2s	2	PRO	4.2
32	2a	1251	A	4.2
51	1t	13	LEU	4.2
1	1A	2141	G	4.2
1	2A	2168	G	4.2
32	2a	1030(A)	G	4.2
33	2b	7	VAL	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	2n	21	TYR	4.1
35	1d	157	LEU	4.1
1	2A	2147	G	4.1
27	15	60	VAL	4.1
1	2A	2169	A	4.1
15	1T	131	ALA	4.1
1	1A	2143	C	4.1
20	2Y	1	MET	4.0
25	23	60	GLU	4.0
32	2a	1036	G	4.0
1	1A	1096	A	4.0
32	2a	1224	G	4.0
23	21	2	SER	4.0
1	1A	2174	C	4.0
3	1D	276	LYS	4.0
1	1A	2119	A	4.0
1	1A	2180	U	4.0
1	2A	2144	U	4.0
6	2G	50	ALA	3.9
32	1a	1533	C	3.9
34	2c	189	ALA	3.9
1	2A	2110	G	3.9
31	29	37	GLY	3.9
38	1g	80	VAL	3.9
1	1A	1081	U	3.9
32	2a	1219	U	3.9
1	1A	2179	C	3.9
1	2A	2114	A	3.9
34	2c	188	LEU	3.9
51	1t	10	LEU	3.9
6	2G	52	ILE	3.8
1	1A	1057	A	3.8
33	1b	237	ALA	3.8
44	2m	90	LEU	3.8
6	2G	77	ILE	3.8
1	1A	2142	C	3.8
26	14	56	VAL	3.8
44	2m	6	GLY	3.8
1	1A	2160	G	3.8
1	1A	2166	G	3.8
34	2c	87	LEU	3.8
33	2b	21	ARG	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	10	ARG	3.8
21	1Z	146	ILE	3.8
21	2Z	121	HIS	3.8
1	2A	1536	C	3.7
1	2A	2126	A	3.7
1	1A	2110	G	3.7
32	2a	1002	G	3.7
20	1Y	1	MET	3.7
1	1A	548	A	3.7
32	2a	1030(D)	A	3.7
8	2I	146	ALA	3.7
1	1A	2104	G	3.7
32	2a	1202	G	3.7
40	2i	11	LYS	3.7
57	1y	5	C	3.7
1	1A	2135	A	3.7
45	2n	13	THR	3.7
8	2I	1	MET	3.7
21	2Z	144	LEU	3.6
22	20	84	LEU	3.6
57	2y	33	U	3.6
57	2y	5	C	3.6
1	1A	2169	A	3.6
1	1A	2122	U	3.6
1	1A	2130	U	3.6
1	1A	2144	U	3.6
1	1A	2167	U	3.6
41	2j	55	LYS	3.6
38	2g	80	VAL	3.6
32	2a	1358	U	3.6
21	1Z	150	LEU	3.6
1	1A	2133	G	3.6
1	2A	2117	A	3.6
1	2A	2170	A	3.6
57	1y	75	C	3.6
41	2j	75	ILE	3.6
41	2j	40	LEU	3.5
1	1A	1094	U	3.5
1	1A	2189	U	3.5
1	1A	2161	C	3.5
32	2a	974	A	3.5
38	2g	85	TYR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
46	2o	75	PRO	3.5
6	1G	146	TYR	3.5
1	1A	1095	A	3.5
1	1A	2170	A	3.5
53	1v	12	A	3.5
1	2A	2143	C	3.5
1	2A	2127	G	3.5
32	1a	1030(A)	G	3.5
21	2Z	146	ILE	3.5
1	1A	1078	U	3.5
32	2a	965	A	3.5
1	1A	886	C	3.5
1	2A	2164	C	3.5
12	2Q	121	ALA	3.5
1	1A	2116	G	3.5
1	2A	2100	G	3.5
32	1a	1036	G	3.5
32	2a	1061	G	3.5
43	2l	32	PHE	3.5
33	2b	236	TYR	3.5
38	1g	85	TYR	3.5
55	2x	47	U	3.5
19	1X	95	LEU	3.5
52	2u	14	TRP	3.5
40	2i	105	ASP	3.4
45	2n	29	ARG	3.4
2	2B	4	C	3.4
32	2a	1030	C	3.4
32	2a	1220	G	3.4
57	1y	35	U	3.4
21	1Z	171	ILE	3.4
26	24	49	PHE	3.4
1	2A	2139	C	3.4
1	2A	2116	G	3.4
32	2a	1117	G	3.4
1	1A	1026	U	3.4
41	1j	32	ALA	3.4
22	20	69	PHE	3.4
38	2g	16	LEU	3.4
33	2b	86	GLU	3.4
32	2a	1035	A	3.4
1	1A	1059	G	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	963	G	3.4
40	2i	126	SER	3.4
41	2j	79	ARG	3.4
45	2n	14	PRO	3.3
1	1A	889	C	3.3
34	2c	2	GLY	3.3
54	1w	50	C	3.3
44	2m	104	ARG	3.3
1	1A	614(B)	G	3.3
1	1A	1058	G	3.3
1	1A	1068	G	3.3
1	2A	2162	G	3.3
32	2a	1353	G	3.3
32	2a	978	A	3.3
38	2g	81	GLY	3.3
52	2u	2	GLY	3.3
44	2m	65	LYS	3.3
21	1Z	166	SER	3.3
1	1A	2108	C	3.3
1	1A	2129	C	3.3
32	2a	1114	C	3.3
33	1b	134	GLU	3.3
34	2c	124	ILE	3.3
1	1A	2165	G	3.3
34	2c	195	VAL	3.3
50	2s	58	VAL	3.3
57	1y	15	G	3.3
45	2n	31	ARG	3.3
40	1i	2	GLU	3.3
1	2A	2189	U	3.3
44	2m	60	VAL	3.3
3	2D	276	LYS	3.3
6	2G	182	LYS	3.3
1	1A	2120	G	3.3
32	2a	1026	G	3.3
22	10	3	HIS	3.2
40	2i	36	TYR	3.2
44	2m	7	VAL	3.2
44	2m	101	GLN	3.2
1	1A	2140	C	3.2
1	1A	2181	G	3.2
1	2A	1533	G	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2148	G	3.2
54	1w	19	G	3.2
57	2y	6	G	3.2
41	1j	4	ILE	3.2
6	1G	50	ALA	3.2
34	2c	137	ALA	3.2
33	2b	213	LEU	3.2
41	2j	8	LEU	3.2
41	2j	65	LEU	3.2
32	2a	1250	A	3.2
1	1A	1082	U	3.2
57	2y	20	U	3.2
1	1A	2138	C	3.2
54	1w	56	C	3.2
1	2A	2160	G	3.2
45	2n	3	ARG	3.2
6	2G	49	ASP	3.2
53	2v	14	A	3.2
1	1A	154(A)	C	3.2
1	1A	1064	C	3.2
33	2b	120	ALA	3.2
6	2G	15	VAL	3.2
7	2H	35	VAL	3.2
39	2h	30	ARG	3.2
45	2n	40	CYS	3.2
57	2y	45	G	3.1
34	2c	157	ILE	3.1
36	2e	21	ALA	3.1
40	2i	96	LEU	3.1
42	1k	14	VAL	3.1
1	2A	2128	C	3.1
32	1a	1027	C	3.1
38	2g	154	TYR	3.1
6	1G	48	GLU	3.1
6	2G	53	LEU	3.1
1	2A	1171	G	3.1
32	2a	1030(C)	G	3.1
32	2a	1257	U	3.1
20	2Y	34	LYS	3.1
44	2m	69	GLU	3.1
57	1y	70	C	3.1
6	1G	52	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	38	ILE	3.1
34	2c	52	LEU	3.1
1	2A	2122	U	3.1
32	2a	950	U	3.1
38	1g	82	GLY	3.1
57	1y	33	U	3.1
1	1A	1087	G	3.1
1	2A	883	G	3.1
1	2A	2157	G	3.1
1	2A	2173	A	3.1
32	1a	1447	A	3.1
22	20	68	GLU	3.1
34	2c	33	LEU	3.1
35	2d	154	ASN	3.1
36	2e	12	LEU	3.1
39	1h	2	LEU	3.1
40	2i	66	ARG	3.1
45	2n	20	ALA	3.1
47	2p	82	GLN	3.1
36	2e	74	GLY	3.1
44	2m	100	GLY	3.1
40	1i	114	TYR	3.1
57	2y	36	U	3.0
44	2m	58	GLU	3.0
32	2a	1289	A	3.0
22	10	7	LEU	3.0
45	2n	42	ILE	3.0
50	2s	79	THR	3.0
1	2A	2182	G	3.0
32	2a	980	C	3.0
32	2a	1223	C	3.0
40	2i	95	LYS	3.0
45	2n	4	LYS	3.0
47	2p	38	TYR	3.0
6	2G	147	ASP	3.0
1	2A	2119	A	3.0
32	1a	1030(D)	A	3.0
41	1j	76	ASN	3.0
34	2c	73	PRO	3.0
20	2Y	55	TYR	3.0
42	1k	25	TYR	3.0
33	2b	200	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	2n	6	LEU	3.0
41	2j	48	THR	3.0
38	1g	79	ARG	3.0
41	1j	60	ARG	3.0
32	2a	1364	U	3.0
34	2c	55	VAL	3.0
45	2n	30	ALA	3.0
34	2c	4	LYS	3.0
32	1a	1531	A	3.0
32	2a	532	A	3.0
35	2d	2	GLY	3.0
33	2b	131	PRO	3.0
1	2A	2104	G	3.0
26	14	57	GLU	3.0
21	2Z	57	ILE	3.0
21	2Z	171	ILE	3.0
8	2I	20	ASP	3.0
1	1A	2164	C	3.0
15	1T	130	ALA	3.0
34	2c	160	ALA	3.0
57	2y	13	C	3.0
41	2j	63	PHE	3.0
14	2S	92	TYR	2.9
46	2o	88	ARG	2.9
42	2k	31	THR	2.9
1	2A	2154	G	2.9
1	2A	2156	G	2.9
21	2Z	174	VAL	2.9
1	2A	2188	C	2.9
32	2a	1249	C	2.9
32	2a	1354	C	2.9
40	2i	99	LEU	2.9
1	2A	2171	A	2.9
22	20	43	THR	2.9
32	1a	149	A	2.9
32	2a	1357	A	2.9
44	2m	120	LYS	2.9
26	24	65	ASP	2.9
41	2j	32	ALA	2.9
41	2j	76	ASN	2.9
45	2n	16	PHE	2.9
11	2P	28	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
22	10	6	GLY	2.9
44	2m	119	GLY	2.9
32	2a	630	G	2.9
1	2A	2137	C	2.9
1	1A	2109	U	2.9
32	1a	1532	U	2.9
38	1g	154	TYR	2.9
40	2i	7	THR	2.9
36	2e	20	GLN	2.9
14	2S	29	PHE	2.9
41	2j	78	ASN	2.9
6	2G	19	LEU	2.9
41	2j	74	ILE	2.9
47	1p	19	ILE	2.9
38	2g	32	ARG	2.9
54	1w	18	G	2.9
1	1A	1060	U	2.9
1	2A	2109	U	2.9
2	2B	6	C	2.9
6	2G	161	THR	2.9
6	2G	160	VAL	2.9
14	2S	46	VAL	2.9
34	2c	153	VAL	2.9
33	1b	188	ALA	2.9
38	1g	84	ASN	2.9
1	1A	529	A	2.9
53	2v	24	A	2.9
6	1G	51	ARG	2.8
44	2m	118	ALA	2.8
1	1A	1056	G	2.8
1	1A	2123	G	2.8
1	2A	2101	G	2.8
20	2Y	107	ASP	2.8
32	1a	380	G	2.8
32	1a	1031	G	2.8
32	2a	1235	U	2.8
57	1y	4	U	2.8
1	1A	885	C	2.8
1	1A	2137	C	2.8
1	2A	2138	C	2.8
32	2a	1039	C	2.8
41	2j	93	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	1w	13	C	2.8
54	1w	67	C	2.8
57	2y	70	C	2.8
6	2G	175	LEU	2.8
39	2h	112	LEU	2.8
20	2Y	54	LYS	2.8
48	1q	100	LYS	2.8
6	2G	76	SER	2.8
32	2a	1248	A	2.8
26	24	50	VAL	2.8
33	1b	34	ALA	2.8
34	2c	181	ASN	2.8
57	2y	4	U	2.8
23	11	26	ARG	2.8
40	2i	63	ILE	2.8
1	1A	2125	G	2.8
1	1A	2162	G	2.8
2	2B	119	G	2.8
32	1a	1001(A)	G	2.8
1	1A	2175	C	2.8
32	1a	1030(B)	C	2.8
57	1y	74	C	2.8
57	2y	74	C	2.8
40	2i	27	THR	2.8
50	2s	41	VAL	2.8
1	1A	887	A	2.8
2	2B	120	A	2.8
57	1y	69	A	2.8
21	1Z	104	PHE	2.8
33	2b	234	PRO	2.8
38	2g	12	LEU	2.8
45	2n	38	GLY	2.8
24	12	69	ARG	2.8
38	2g	77	SER	2.8
1	1A	888	C	2.8
32	1a	1028	C	2.8
32	2a	1038	C	2.8
57	1y	71	C	2.8
21	2Z	172	ALA	2.8
41	1j	33	GLN	2.8
4	2E	10	GLY	2.8
26	24	54	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	2w	59	A	2.8
57	2y	69	A	2.8
26	24	5	ILE	2.7
34	2c	77	ILE	2.7
41	1j	74	ILE	2.7
36	2e	130	ASN	2.7
1	2A	2132	U	2.7
32	1a	1025	U	2.7
54	1w	47	U	2.7
21	2Z	139	VAL	2.7
34	2c	207	VAL	2.7
45	2n	18	VAL	2.7
48	2q	99	SER	2.7
6	2G	81	LYS	2.7
49	1r	78	LEU	2.7
1	1A	34	C	2.7
1	2A	2185	C	2.7
40	2i	62	TYR	2.7
55	2x	1	C	2.7
52	1u	24	ARG	2.7
32	1a	1286	A	2.7
32	2a	1447	A	2.7
33	2b	93	VAL	2.7
1	2A	2130	U	2.7
7	1H	175	LYS	2.7
12	2Q	22	LYS	2.7
38	1g	156	TRP	2.7
45	2n	36	PHE	2.7
21	2Z	150	LEU	2.7
47	1p	81	ARG	2.7
1	1A	2128	C	2.7
1	2A	2163	C	2.7
54	2w	50	C	2.7
1	1A	1099	G	2.7
1	1A	2154	G	2.7
1	1A	2182	G	2.7
1	2A	882	G	2.7
2	2B	23	G	2.7
32	1a	1034	G	2.7
39	2h	9	MET	2.7
9	2N	9	VAL	2.7
34	2c	199	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
43	2l	13	LYS	2.7
22	20	2	ALA	2.7
34	2c	24	ALA	2.7
21	2Z	170	THR	2.7
39	1h	3	THR	2.7
47	1p	6	LEU	2.7
18	2W	92	ARG	2.7
26	14	58	ARG	2.7
39	2h	130	GLY	2.7
40	2i	67	GLY	2.7
57	1y	12	U	2.7
57	2y	35	U	2.7
14	2S	35	ILE	2.7
21	1Z	120	ILE	2.7
43	1l	64	TYR	2.7
20	2Y	5	MET	2.7
33	2b	112	VAL	2.7
40	2i	28	VAL	2.7
41	2j	34	VAL	2.7
21	2Z	95	PRO	2.7
33	2b	187	LEU	2.7
1	1A	2190	G	2.7
1	2A	530	G	2.7
1	2A	2318	G	2.7
1	1A	1098	A	2.7
47	1p	5	ARG	2.7
35	1d	2	GLY	2.7
45	2n	55	GLY	2.7
33	2b	208	ILE	2.7
34	2c	184	TYR	2.6
44	2m	73	GLU	2.6
9	2N	45	ASN	2.6
33	2b	48	MET	2.6
3	1D	275	LYS	2.6
6	2G	74	LYS	2.6
48	2q	100	LYS	2.6
38	1g	9	VAL	2.6
40	2i	17	VAL	2.6
33	1b	125	PRO	2.6
33	2b	149	LEU	2.6
37	2f	21	LEU	2.6
34	2c	128	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	129	ALA	2.6
34	2c	186	PHE	2.6
40	2i	13	ALA	2.6
45	2n	44	LEU	2.6
14	2S	3	ARG	2.6
40	2i	128	ARG	2.6
32	2a	979	C	2.6
50	2s	35	SER	2.6
45	2n	7	ILE	2.6
1	2A	229	A	2.6
32	2a	1286	A	2.6
32	2a	1287	A	2.6
57	2y	38	A	2.6
1	1A	2131	G	2.6
1	1A	2157	G	2.6
1	2A	2120	G	2.6
32	1a	1024	G	2.6
32	2a	1001(A)	G	2.6
32	2a	1356	G	2.6
1	1A	2118	U	2.6
21	2Z	155	LEU	2.6
33	2b	230	VAL	2.6
43	2l	39	VAL	2.6
51	1t	24	LEU	2.6
33	2b	17	PHE	2.6
41	1j	79	ARG	2.6
21	2Z	69	THR	2.6
38	1g	153	HIS	2.6
15	2T	69	GLY	2.6
33	2b	185	ILE	2.6
52	2u	13	ILE	2.6
1	2A	885	C	2.6
1	2A	894	C	2.6
1	2A	2129	C	2.6
1	2A	2136	C	2.6
1	2A	2161	C	2.6
2	2B	12	C	2.6
26	24	63	TYR	2.6
36	2e	133	TYR	2.6
50	2s	80	TYR	2.6
57	1y	32	C	2.6
32	1a	1035	A	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1001	A	2.6
38	2g	37	ASN	2.6
1	1A	2101	G	2.6
1	1A	2156	G	2.6
33	2b	71	VAL	2.6
33	2b	197	VAL	2.6
34	2c	68	VAL	2.6
40	1i	28	VAL	2.6
47	2p	6	LEU	2.6
54	1w	1	G	2.6
57	2y	3	G	2.6
57	2y	10	G	2.6
32	1a	1000	U	2.6
35	1d	111	ALA	2.6
51	2t	97	ALA	2.6
57	2y	47	U	2.6
52	2u	15	ARG	2.6
41	2j	67	THR	2.6
41	1j	31	GLY	2.6
26	14	63	TYR	2.6
40	2i	92	TYR	2.6
40	2i	125	TYR	2.6
50	2s	13	ASP	2.6
7	2H	17	VAL	2.6
35	2d	92	VAL	2.6
1	1A	2794	C	2.6
1	2A	884	C	2.6
32	1a	1029	C	2.6
6	2G	102	PHE	2.6
36	2e	84	PHE	2.6
39	2h	3	THR	2.6
1	1A	2132	U	2.6
2	2B	1	U	2.6
34	1c	39	ILE	2.6
34	2c	13	GLY	2.6
32	1a	630	G	2.6
32	2a	971	G	2.6
42	2k	25	TYR	2.5
40	2i	50	LEU	2.5
42	2k	126	ARG	2.5
18	1W	112	GLY	2.5
32	2a	1054	C	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	2w	56	C	2.5
57	2y	25	C	2.5
32	2a	1531	A	2.5
1	2A	2118	U	2.5
57	1y	36	U	2.5
1	1A	1176	G	2.5
1	2A	2159	G	2.5
1	2A	2181	G	2.5
32	2a	1003	G	2.5
57	2y	57	G	2.5
20	2Y	90	LEU	2.5
39	2h	107	LEU	2.5
33	1b	7	VAL	2.5
50	2s	76	PRO	2.5
35	2d	73	ARG	2.5
50	2s	78	ARG	2.5
7	2H	96	ALA	2.5
36	2e	101	ILE	2.5
41	1j	98	ILE	2.5
51	2t	103	GLY	2.5
33	2b	97	TRP	2.5
1	1A	652(S)	C	2.5
1	2A	34	C	2.5
32	2a	1225	A	2.5
32	2a	1285	A	2.5
54	1w	73	A	2.5
32	1a	65	U	2.5
32	1a	202	U	2.5
32	1a	204	U	2.5
57	2y	7	U	2.5
9	2N	44	PRO	2.5
9	1N	9	VAL	2.5
12	2Q	10	ARG	2.5
50	2s	11	VAL	2.5
14	2S	12	PHE	2.5
35	2d	164	ALA	2.5
38	1g	83	ALA	2.5
1	1A	275	G	2.5
32	2a	1024	G	2.5
32	2a	1222	G	2.5
54	2w	1	G	2.5
55	1x	46	G	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
57	1y	68	G	2.5
14	2S	45	GLY	2.5
19	1X	94	GLY	2.5
20	2Y	10	GLY	2.5
34	2c	155	GLY	2.5
48	1q	78	GLU	2.5
15	2T	111	ARG	2.5
29	27	47	ARG	2.5
41	2j	77	PRO	2.5
1	2A	896	A	2.5
1	2A	2158	A	2.5
32	2a	1369	C	2.5
40	2i	101	PHE	2.5
47	1p	80	PHE	2.5
50	2s	52	TYR	2.5
54	1w	61	C	2.5
54	2w	61	C	2.5
14	2S	34	HIS	2.5
3	2D	38	LYS	2.5
8	1I	146	ALA	2.5
35	2d	144	ASP	2.5
51	1t	95	ALA	2.5
34	2c	14	ILE	2.5
34	2c	182	ILE	2.5
17	1V	101	GLY	2.5
21	2Z	26	GLY	2.5
21	2Z	106	GLY	2.5
1	1A	2127	G	2.4
32	1a	1023	G	2.4
54	1w	68	G	2.4
57	2y	15	G	2.4
39	2h	2	LEU	2.4
6	2G	128	ARG	2.4
9	2N	74	ARG	2.4
18	2W	37	ARG	2.4
44	2m	88	ARG	2.4
50	2s	59	PRO	2.4
11	2P	39	LYS	2.4
50	2s	32	LYS	2.4
4	2E	204	ALA	2.4
36	2e	108	ALA	2.4
39	2h	4	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2102	U	2.4
32	2a	1372	U	2.4
1	1A	2173	A	2.4
1	2A	2135	A	2.4
26	14	52	THR	2.4
32	1a	1008	C	2.4
57	2y	66	A	2.4
25	13	2	PRO	2.4
44	2m	113	PRO	2.4
51	1t	8	ARG	2.4
50	2s	4	SER	2.4
32	1a	1009	G	2.4
32	2a	631	G	2.4
32	2a	1370	G	2.4
43	1l	28	LYS	2.4
54	2w	15	G	2.4
54	2w	18	G	2.4
19	2X	69	TYR	2.4
36	2e	94	ALA	2.4
41	2j	27	ALA	2.4
44	2m	76	ALA	2.4
33	2b	211	ILE	2.4
40	1i	105	ASP	2.4
50	2s	53	ASN	2.4
1	1A	1101	U	2.4
54	1w	7	U	2.4
54	1w	60	U	2.4
15	1T	109	GLU	2.4
20	2Y	29	GLU	2.4
6	2G	172	LEU	2.4
32	2a	1363(A)	A	2.4
33	2b	10	LEU	2.4
40	1i	56	LEU	2.4
48	2q	98	LEU	2.4
1	1A	2188	C	2.4
1	2A	2794	C	2.4
32	1a	1038	C	2.4
55	1x	1	C	2.4
57	1y	13	C	2.4
36	2e	126	ARG	2.4
46	1o	19	PRO	2.4
43	2l	126	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	165	VAL	2.4
5	2F	90	PHE	2.4
26	24	42	PHE	2.4
41	2j	54	PHE	2.4
50	2s	24	ALA	2.4
14	2S	7	TYR	2.4
6	2G	4	ASP	2.4
22	20	76	GLY	2.4
34	2c	158	GLY	2.4
40	2i	91	ASP	2.4
50	2s	68	GLY	2.4
1	1A	880	G	2.4
1	2A	2106	G	2.4
32	1a	1002	G	2.4
32	2a	947	G	2.4
54	1w	57	G	2.4
50	2s	33	THR	2.4
9	2N	112	LEU	2.4
33	2b	11	LEU	2.4
40	2i	2	GLU	2.4
1	1A	1065	U	2.4
10	1O	49	ARG	2.4
32	2a	1205	U	2.4
32	2a	1232	U	2.4
52	2u	24	ARG	2.4
43	2l	28	LYS	2.4
1	1A	2134	A	2.4
22	20	3	HIS	2.4
33	1b	165	VAL	2.4
34	1c	207	VAL	2.4
36	2e	100	VAL	2.4
53	2v	15	A	2.4
1	1A	1075	C	2.4
1	2A	645	C	2.4
32	1a	136	C	2.4
32	2a	1192	C	2.4
35	1d	110	PHE	2.4
54	2w	32	C	2.4
40	1i	106	ALA	2.4
41	2j	23	ILE	2.4
47	1p	7	ALA	2.4
5	2F	16	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	74	GLY	2.4
42	2k	90	GLY	2.4
51	1t	69	GLY	2.4
41	1j	78	ASN	2.4
21	2Z	41	LEU	2.3
33	1b	9	GLU	2.3
33	2b	134	GLU	2.3
35	1d	179	GLU	2.3
40	1i	19	LEU	2.3
44	2m	96	LEU	2.3
45	2n	53	LEU	2.3
50	2s	71	LEU	2.3
35	2d	122	ARG	2.3
38	2g	5	ARG	2.3
41	2j	28	ARG	2.3
45	1n	3	ARG	2.3
1	2A	11	G	2.3
1	2A	2131	G	2.3
2	2B	118	G	2.3
32	2a	951	G	2.3
57	1y	10	G	2.3
57	2y	1	G	2.3
34	2c	75	VAL	2.3
41	1j	34	VAL	2.3
47	1p	21	VAL	2.3
6	2G	20	ILE	2.3
21	2Z	173	ALA	2.3
33	1b	127	ILE	2.3
34	2c	84	ILE	2.3
44	2m	22	ILE	2.3
45	2n	10	ALA	2.3
51	1t	70	SER	2.3
52	2u	11	GLY	2.3
2	2B	5	C	2.3
6	2G	146	TYR	2.3
26	14	51	ASP	2.3
34	2c	62	ASP	2.3
42	2k	117	ASN	2.3
33	2b	44	LEU	2.3
41	2j	87	THR	2.3
6	2G	35	GLU	2.3
26	24	57	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	128	GLU	2.3
29	17	48	LYS	2.3
29	27	48	LYS	2.3
52	2u	7	ARG	2.3
21	2Z	15	PRO	2.3
6	2G	70	VAL	2.3
7	2H	107	VAL	2.3
33	1b	136	VAL	2.3
1	1A	2148	G	2.3
1	2A	892	G	2.3
1	2A	2149	G	2.3
6	2G	57	ALA	2.3
32	1a	1003	G	2.3
32	2a	5	U	2.3
32	2a	953	G	2.3
48	2q	44	ALA	2.3
32	2a	1000	U	2.3
54	2w	57	G	2.3
57	2y	2	G	2.3
57	2y	22	G	2.3
57	2y	68	G	2.3
34	2c	25	GLY	2.3
42	2k	49	GLY	2.3
43	1l	63	GLY	2.3
34	2c	48	TYR	2.3
1	1A	1077	A	2.3
1	2A	2134	A	2.3
18	1W	60	ASN	2.3
21	1Z	170	THR	2.3
22	10	5	LYS	2.3
32	2a	983	A	2.3
33	2b	175	ARG	2.3
34	2c	161	GLU	2.3
34	2c	192	THR	2.3
47	1p	68	ASP	2.3
57	2y	73	A	2.3
1	1A	1079	C	2.3
1	2A	2105	C	2.3
6	2G	2	PRO	2.3
41	2j	53	PRO	2.3
34	2c	6	HIS	2.3
50	2s	14	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	24	33	VAL	2.3
33	2b	136	VAL	2.3
34	2c	130	VAL	2.3
44	2m	53	VAL	2.3
21	2Z	88	PHE	2.3
6	2G	29	TRP	2.3
39	2h	86	ILE	2.3
44	2m	78	ILE	2.3
1	1A	2102	U	2.3
1	2A	12	U	2.3
32	2a	1125	U	2.3
32	2a	1150	U	2.3
1	2A	2186	G	2.3
1	2A	2319	G	2.3
14	2S	20	ARG	2.3
17	2V	81	TYR	2.3
26	24	32	TYR	2.3
32	1a	148	G	2.3
32	2a	1221	G	2.3
34	1c	190	ARG	2.3
38	2g	4	ARG	2.3
41	1j	64	GLU	2.3
41	2j	83	GLU	2.3
57	1y	27	G	2.3
32	2a	1110	A	2.3
50	2s	83	HIS	2.3
54	1w	66	A	2.3
20	2Y	57	GLN	2.3
20	2Y	85	VAL	2.3
21	1Z	105	VAL	2.3
21	2Z	71	VAL	2.3
26	24	21	VAL	2.3
41	2j	49	VAL	2.3
47	2p	76	GLN	2.3
1	1A	1080	C	2.3
1	2A	886	C	2.3
1	2A	2107	C	2.3
7	2H	89	ILE	2.3
57	1y	25	C	2.3
40	2i	52	ALA	2.3
43	2l	56	ALA	2.3
44	2m	5	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	1e	85	GLY	2.3
22	20	5	LYS	2.2
35	2d	162	LEU	2.3
40	2i	71	SER	2.3
41	2j	88	LEU	2.3
42	1k	51	LYS	2.2
48	2q	76	LEU	2.3
21	2Z	131	ARG	2.2
41	2j	5	ARG	2.2
7	2H	36	PRO	2.2
21	2Z	154	ASP	2.2
32	1a	841	U	2.2
32	2a	1065	U	2.2
33	1b	131	PRO	2.2
41	1j	77	PRO	2.2
54	2w	33	U	2.2
54	2w	47	U	2.2
21	1Z	121	HIS	2.2
1	1A	2151	G	2.2
1	2A	2751	G	2.2
32	2a	1190	G	2.2
35	2d	178	VAL	2.2
39	2h	53	VAL	2.2
41	2j	72	VAL	2.2
47	1p	20	VAL	2.2
48	2q	35	VAL	2.2
36	2e	13	ILE	2.2
38	2g	26	PHE	2.2
1	1A	890	A	2.2
32	2a	1252	A	2.2
55	1x	72	A	2.2
57	2y	14	A	2.2
21	2Z	164	ALA	2.2
33	2b	123	ALA	2.2
44	2m	30	ALA	2.2
36	2e	85	GLY	2.2
45	2n	17	LYS	2.2
46	1o	57	LEU	2.2
51	1t	103	GLY	2.2
51	2t	74	LYS	2.2
1	2A	2108	C	2.2
54	2w	71	C	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	2F	62	ARG	2.2
6	2G	51	ARG	2.2
41	1j	45	ARG	2.2
6	2G	48	GLU	2.2
27	15	59	GLU	2.2
7	2H	83	TYR	2.2
7	2H	128	PRO	2.2
41	1j	100	THR	2.2
14	2S	36	TYR	2.2
21	2Z	29	TYR	2.2
50	2s	12	ASP	2.2
33	1b	19	HIS	2.2
7	2H	37	VAL	2.2
8	2I	15	VAL	2.2
21	2Z	74	VAL	2.2
32	2a	961	U	2.2
41	1j	24	VAL	2.2
50	1s	9	VAL	2.2
33	1b	17	PHE	2.2
51	1t	55	ILE	2.2
20	2Y	63	LYS	2.2
34	2c	163	ALA	2.2
36	1e	94	ALA	2.2
25	23	26	LEU	2.2
34	2c	167	TRP	2.2
44	2m	64	TRP	2.2
34	2c	197	GLY	2.2
40	2i	6	GLY	2.2
1	2A	2321	G	2.2
1	1A	1067	A	2.2
1	1A	1086	A	2.2
13	2R	68	ARG	2.2
57	1y	1	G	2.2
57	1y	24	G	2.2
57	1y	49	G	2.2
32	2a	969	A	2.2
32	2a	1004	A	2.2
53	1v	15	A	2.2
51	1t	11	SER	2.2
28	16	4	GLU	2.2
16	2U	2	PRO	2.2
17	2V	7	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	95	THR	2.2
41	2j	91	PRO	2.2
55	1x	16	C	2.2
18	2W	111	HIS	2.2
47	1p	16	HIS	2.2
47	1p	17	TYR	2.2
43	2l	104	VAL	2.2
20	2Y	44	ILE	2.2
35	2d	158	ILE	2.2
50	2s	31	ILE	2.2
45	2n	11	LYS	2.2
2	2B	22	U	2.2
12	2Q	103	MET	2.2
29	17	45	ALA	2.2
32	2a	982	U	2.2
42	1k	15	ALA	2.2
54	2w	60	U	2.2
19	2X	68	ARG	2.2
33	1b	203	GLY	2.2
34	2c	79	ARG	2.2
50	1s	29	ARG	2.2
52	2u	4	GLY	2.2
52	2u	6	ARG	2.2
6	1G	76	SER	2.2
14	2S	50	SER	2.2
24	22	66	GLU	2.2
33	2b	170	GLU	2.2
50	2s	38	SER	2.2
50	2s	77	THR	2.2
1	1A	1045	A	2.2
32	2a	949	A	2.2
32	2a	1503	A	2.2
40	2i	117	HIS	2.2
54	1w	69	A	2.2
1	2A	2141	G	2.2
6	2G	130	ASN	2.2
32	2a	587	G	2.2
44	2m	23	TYR	2.2
47	1p	38	TYR	2.2
54	2w	49	G	2.2
57	1y	19	G	2.2
57	2y	49	G	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	2R	69	ASP	2.2
6	2G	41	GLN	2.2
26	24	56	VAL	2.2
33	1b	214	ILE	2.2
34	2c	8	ILE	2.2
35	2d	88	VAL	2.2
35	2d	206	PHE	2.2
37	1f	88	VAL	2.2
40	2i	41	VAL	2.2
40	2i	86	VAL	2.2
40	2i	108	VAL	2.2
41	1j	84	GLN	2.2
50	2s	49	ILE	2.2
1	1A	1509	C	2.2
1	1A	2107	C	2.2
1	2A	893	C	2.2
9	2N	83	LYS	2.2
21	2Z	127	LYS	2.2
9	2N	1	MET	2.2
32	2a	962	C	2.2
32	2a	999	C	2.2
47	1p	35	LYS	2.2
6	2G	139	LEU	2.2
33	2b	13	ALA	2.2
33	2b	121	LEU	2.2
36	2e	86	ALA	2.2
35	2d	87	GLY	2.2
46	2o	68	ARG	2.2
46	2o	89	GLY	2.2
48	2q	68	ARG	2.2
33	1b	97	TRP	2.1
33	1b	167	PRO	2.1
48	2q	86	GLU	2.1
35	1d	83	SER	2.1
41	2j	59	SER	2.1
11	2P	35	HIS	2.1
45	2n	22	THR	2.1
6	2G	123	ASN	2.1
6	2G	126	ASP	2.1
26	24	25	TYR	2.1
42	2k	75	TYR	2.1
5	2F	6	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	44	VAL	2.1
26	14	49	PHE	2.1
26	24	22	ILE	2.1
33	1b	229	VAL	2.1
34	2c	5	ILE	2.1
35	1d	8	VAL	2.1
35	2d	166	LYS	2.1
38	2g	49	ILE	2.1
41	1j	55	LYS	2.1
41	2j	44	VAL	2.1
47	1p	79	VAL	2.1
1	1A	1088	A	2.1
1	1A	2158	A	2.1
1	2A	2320	A	2.1
32	1a	1503	A	2.1
57	2y	26	A	2.1
1	1A	545	G	2.1
1	1A	2149	G	2.1
1	2A	2151	G	2.1
5	2F	24	LEU	2.1
8	2I	68	LEU	2.1
38	2g	38	LEU	2.1
39	1h	112	LEU	2.1
54	2w	68	G	2.1
22	10	2	ALA	2.1
36	2e	95	ALA	2.1
40	2i	94	ALA	2.1
44	2m	94	ARG	2.1
21	2Z	143	GLY	2.1
21	2Z	147	GLY	2.1
51	1t	47	GLY	2.1
1	1A	1092	C	2.1
1	2A	888	C	2.1
55	2x	71	C	2.1
57	2y	11	C	2.1
28	26	42	TRP	2.1
26	24	7	PRO	2.1
35	1d	163	GLU	2.1
43	2l	16	GLU	2.1
6	2G	64	THR	2.1
52	2u	8	THR	2.1
48	2q	87	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	2I	3	VAL	2.1
33	1b	15	VAL	2.1
34	2c	151	VAL	2.1
35	2d	20	TYR	2.1
35	2d	68	TYR	2.1
44	2m	54	VAL	2.1
45	2n	37	PHE	2.1
49	2r	86	VAL	2.1
33	2b	145	LEU	2.1
42	1k	98	LEU	2.1
44	2m	19	LEU	2.1
44	2m	81	LEU	2.1
6	1G	46	ALA	2.1
1	1A	1103	A	2.1
34	2c	78	GLY	2.1
1	1A	892	G	2.1
1	2A	2121	G	2.1
17	2V	50	PRO	2.1
32	2a	1058	G	2.1
57	1y	6	G	2.1
57	2y	19	G	2.1
1	1A	2177	C	2.1
32	2a	91	C	2.1
32	2a	948	C	2.1
54	2w	67	C	2.1
57	2y	67	C	2.1
57	2y	71	C	2.1
34	1c	135	LYS	2.1
41	1j	59	SER	2.1
1	1A	1097	U	2.1
1	1A	2150	U	2.1
1	2A	895	U	2.1
54	1w	20	U	2.1
6	2G	92	VAL	2.1
33	2b	70	PHE	2.1
33	2b	81	VAL	2.1
33	2b	122	PHE	2.1
34	2c	138	VAL	2.1
36	2e	115	VAL	2.1
47	1p	82	GLN	2.1
21	2Z	87	ASP	2.1
31	29	24	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	2Q	17	LEU	2.1
20	2Y	31	LEU	2.1
33	2b	118	LEU	2.1
6	2G	46	ALA	2.1
8	2I	55	ALA	2.1
33	1b	13	ALA	2.1
34	2c	127	ARG	2.1
34	2c	168	ALA	2.1
34	2c	180	ALA	2.1
35	2d	209	ARG	2.1
44	1m	30	ALA	2.1
15	1T	37	GLY	2.1
35	2d	183	GLY	2.1
50	2s	46	GLY	2.1
6	2G	54	GLU	2.1
21	1Z	119	GLU	2.1
33	1b	202	PRO	2.1
35	1d	192	GLU	2.1
38	2g	112	PRO	2.1
1	1A	1073	A	2.1
1	1A	2171	A	2.1
1	2A	652(B)	A	2.1
1	2A	899	A	2.1
1	2A	1847	A	2.1
32	1a	160	A	2.1
32	2a	1005	A	2.1
32	2a	1288	A	2.1
47	2p	45	THR	2.1
21	2Z	16	SER	2.1
33	2b	214	ILE	2.1
39	2h	80	ILE	2.1
41	1j	75	ILE	2.1
1	2A	1170	G	2.1
6	2G	141	PHE	2.1
7	2H	24	VAL	2.1
8	2I	17	GLN	2.1
25	23	6	VAL	2.1
32	1a	1030(C)	G	2.1
40	2i	18	PHE	2.1
40	2i	26	VAL	2.1
44	2m	117	VAL	2.1
47	1p	62	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	2s	51	VAL	2.1
54	1w	15	G	2.1
1	1A	1076	C	2.1
1	1A	1100	C	2.1
1	2A	1509	C	2.1
22	20	62	LEU	2.1
32	1a	1037	C	2.1
32	2a	1029	C	2.1
34	1c	47	LEU	2.1
39	2h	133	LEU	2.1
44	2m	66	LEU	2.1
40	2i	4	TYR	2.1
48	2q	95	TYR	2.1
54	1w	70	C	2.1
57	2y	75	C	2.1
26	24	68	ARG	2.1
32	2a	4	U	2.1
32	2a	1148	U	2.1
38	2g	76	ARG	2.1
44	2m	99	ARG	2.1
45	2n	41	ARG	2.1
46	2o	54	ARG	2.1
47	1p	75	ARG	2.1
57	2y	12	U	2.1
40	2i	119	ALA	2.1
44	1m	118	ALA	2.1
6	2G	129	GLY	2.1
22	10	8	GLY	2.1
26	14	64	GLY	2.1
38	2g	34	GLY	2.1
8	2I	137	PRO	2.0
34	2c	7	PRO	2.0
44	2m	41	PRO	2.0
51	2t	98	PRO	2.0
35	2d	156	GLU	2.0
6	2G	47	LYS	2.0
33	1b	22	LYS	2.0
48	1q	45	HIS	2.0
14	2S	5	THR	2.0
41	2j	96	ILE	2.0
6	2G	159	VAL	2.0
12	2Q	106	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	2Y	89	PHE	2.0
28	26	48	VAL	2.0
32	2a	977	A	2.0
33	1b	122	PHE	2.0
35	2d	105	VAL	2.0
36	2e	33	VAL	2.0
40	1i	108	VAL	2.0
57	2y	51	A	2.0
7	2H	88	LEU	2.0
44	2m	56	LEU	2.0
34	2c	190	ARG	2.0
46	2o	17	ARG	2.0
26	24	67	TYR	2.0
34	2c	29	TYR	2.0
36	2e	30	ALA	2.0
1	1A	271(K)	U	2.0
1	1A	1091	G	2.0
1	2A	2124	G	2.0
32	1a	79	G	2.0
32	2a	1124	G	2.0
32	2a	1253	G	2.0
35	1d	87	GLY	2.0
44	2m	112	GLY	2.0
1	2A	2804	C	2.0
32	1a	63	C	2.0
54	2w	13	C	2.0
40	2i	49	PRO	2.0
48	2q	2	PRO	2.0
14	2S	59	LYS	2.0
42	1k	92	GLU	2.0
47	2p	16	HIS	2.0
41	1j	86	MET	2.0
39	2h	134	ILE	2.0
41	2j	82	ILE	2.0
12	2Q	104	PHE	2.0
14	2S	56	LEU	2.0
34	2c	175	LEU	2.0
37	2f	88	VAL	2.0
14	2S	13	ARG	2.0
35	1d	191	ARG	2.0
42	1k	79	SER	2.0
1	1A	1069	A	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2176	A	2.0
32	1a	1001	A	2.0
33	2b	199	TYR	2.0
35	2d	117	ALA	2.0
38	2g	151	TYR	2.0
47	1p	39	TYR	2.0
57	1y	14	A	2.0
57	1y	38	A	2.0

5.2 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	G7M	1y	46	24/25	0.35	0.17	95,104,109,118	0
57	G7M	2y	46	24/25	0.36	0.18	96,105,116,132	0
57	T6A	2y	37	22/33	0.41	0.18	89,102,113,126	0
57	U8U	1y	34	20/24	0.41	0.20	88,105,112,125	0
57	U8U	2y	34	20/24	0.42	0.23	97,108,116,129	0
57	T6A	1y	37	22/33	0.48	0.17	95,98,103,113	0
54	G7M	2w	46	24/25	0.52	0.14	91,102,116,128	0
54	PSU	2w	55	20/21	0.54	0.16	90,102,108,109	0
57	PSU	2y	55	20/21	0.55	0.15	97,107,113,117	0
54	G7M	1w	46	24/25	0.55	0.15	87,96,107,118	0
57	PSU	2y	39	20/21	0.57	0.16	93,101,106,120	0
54	PSU	1w	55	20/21	0.58	0.18	84,100,107,112	0
57	5MU	2y	54	21/22	0.58	0.14	97,105,113,122	0
57	PSU	1y	39	20/21	0.63	0.14	94,102,109,116	0
57	PSU	1y	55	20/21	0.65	0.11	99,102,112,123	0
54	5MU	2w	54	21/22	0.65	0.14	82,93,101,104	0
57	5MU	1y	54	21/22	0.66	0.12	95,101,104,119	0
54	5MU	1w	54	21/22	0.79	0.12	74,86,94,97	0
1	5MU	2A	1915	21/22	0.80	0.15	79,84,87,90	0
54	U8U	2w	34	23/24	0.80	0.20	78,89,97,100	0
32	2MG	2a	1207	24/25	0.81	0.15	81,90,101,106	0
54	PSU	2w	39	20/21	0.82	0.13	84,89,96,96	0
32	PSU	2a	516	20/21	0.83	0.14	73,85,91,92	0
54	T6A	2w	37	32/33	0.84	0.15	77,89,96,98	0
55	PSU	2x	55	20/21	0.84	0.13	79,84,89,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	4SU	2x	8	20/21	0.85	0.12	80,85,93,96	0
54	U8U	1w	34	23/24	0.86	0.14	69,76,84,87	0
55	5MU	2x	54	21/22	0.87	0.12	78,86,92,107	0
54	T6A	1w	37	32/33	0.88	0.14	60,72,81,85	0
56	FME	2z	1	10/11	0.88	0.24	51,59,66,70	0
55	PSU	1x	55	20/21	0.89	0.10	58,65,76,77	0
56	FME	1z	1	10/11	0.89	0.23	44,54,62,77	0
32	M2G	2a	966	25/26	0.89	0.16	62,72,88,91	0
32	5MC	2a	967	21/22	0.90	0.14	70,76,83,89	0
1	PSU	2A	1917	20/21	0.90	0.10	65,75,80,84	0
55	4SU	1x	8	20/21	0.91	0.12	59,65,71,77	0
55	5MU	1x	54	21/22	0.92	0.10	65,71,77,79	0
54	A1B8A	2w	76	31/32	0.92	0.12	41,56,64,65	0
43	0TD	2l	92	10/11	0.92	0.13	69,71,78,87	0
32	G7M	2a	527	24/25	0.92	0.11	59,68,74,83	0
32	5MC	2a	1404	21/22	0.93	0.11	55,62,71,74	0
1	PSU	2A	1911	20/21	0.93	0.10	57,70,78,80	0
1	5MU	1A	1915	21/22	0.93	0.10	52,59,63,68	0
54	PSU	1w	39	20/21	0.93	0.10	77,80,86,87	0
32	PSU	1a	516	20/21	0.93	0.09	62,67,70,70	0
43	0TD	1l	92	10/11	0.93	0.09	49,52,54,61	0
32	4OC	2a	1402	22/23	0.93	0.11	55,69,74,76	0
55	5MC	2x	32	21/22	0.94	0.12	71,75,82,85	0
32	5MC	2a	1407	21/22	0.94	0.11	54,60,67,69	0
54	A1B8A	1w	76	31/32	0.94	0.11	34,42,47,50	0
1	OMC	2A	1920	21/22	0.94	0.10	58,69,73,76	0
55	8AN	2x	76	22/23	0.94	0.11	42,50,56,58	0
32	5MC	2a	1400	21/22	0.94	0.14	72,77,81,84	0
1	5MC	2A	1962	21/22	0.95	0.09	39,51,58,70	0
32	MA6	1a	1519	24/25	0.95	0.10	35,45,48,51	0
32	G7M	1a	527	24/25	0.95	0.09	36,44,57,57	0
32	2MG	1a	1207	24/25	0.95	0.10	57,66,72,74	0
1	5MC	2A	1942	21/22	0.95	0.10	51,63,71,75	0
32	UR3	2a	1498	21/22	0.95	0.10	52,60,65,71	0
32	MA6	2a	1518	24/25	0.95	0.11	55,66,74,76	0
32	M2G	1a	966	25/26	0.96	0.09	51,54,62,63	0
1	OMG	2A	2251	24/25	0.96	0.09	37,43,45,48	0
1	PSU	2A	2605	20/21	0.96	0.07	31,41,44,45	0
55	5MC	1x	32	21/22	0.96	0.10	46,54,59,63	0
32	MA6	2a	1519	24/25	0.96	0.11	56,66,74,76	0
32	5MC	1a	967	21/22	0.96	0.10	50,57,64,67	0
1	5MC	1A	1942	21/22	0.96	0.10	38,42,48,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	8AN	1x	76	22/23	0.96	0.09	30,36,40,44	0
32	5MC	1a	1400	21/22	0.96	0.10	44,50,53,53	0
1	PSU	1A	1911	20/21	0.96	0.09	42,51,56,58	0
1	PSU	1A	1917	20/21	0.96	0.07	47,52,57,61	0
1	5MU	1A	1939	21/22	0.97	0.07	23,28,35,36	0
1	OMC	1A	1920	21/22	0.97	0.08	35,45,49,50	0
1	2MA	2A	2503	23/24	0.97	0.08	33,37,39,41	0
1	OMU	2A	2552	21/22	0.97	0.08	34,43,48,49	0
32	4OC	1a	1402	22/23	0.97	0.09	40,47,51,53	0
32	5MC	1a	1404	21/22	0.97	0.09	33,42,47,48	0
32	5MC	1a	1407	21/22	0.97	0.08	35,40,43,48	0
1	5MU	2A	1939	21/22	0.97	0.07	37,42,46,46	0
32	UR3	1a	1498	21/22	0.97	0.08	36,41,46,48	0
32	MA6	1a	1518	24/25	0.98	0.09	27,43,47,56	0
1	OMU	1A	2552	21/22	0.98	0.07	25,30,34,37	0
1	PSU	1A	2605	20/21	0.98	0.07	24,28,34,35	0
1	5MC	1A	1962	21/22	0.98	0.07	30,36,43,48	0
1	2MA	1A	2503	23/24	0.98	0.06	18,22,26,28	0
1	OMG	1A	2251	24/25	0.99	0.06	21,26,29,31	0

5.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1753	1/1	0.40	0.16	93,93,93,93	0
58	MG	2a	1789	1/1	0.58	0.24	88,88,88,88	0
58	MG	2A	3538	1/1	0.59	0.31	77,77,77,77	0
58	MG	1A	3813	1/1	0.60	0.23	60,60,60,60	0
58	MG	2A	3668	1/1	0.60	0.15	73,73,73,73	0
58	MG	1A	3569	1/1	0.61	0.19	64,64,64,64	0
58	MG	2a	1606	1/1	0.62	0.31	81,81,81,81	0
58	MG	1a	1680	1/1	0.63	0.33	80,80,80,80	0
58	MG	2a	1741	1/1	0.63	0.29	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1v	101	1/1	0.64	0.27	88,88,88,88	0
58	MG	2A	3107	1/1	0.64	0.26	63,63,63,63	0
58	MG	2a	1802	1/1	0.64	0.14	82,82,82,82	0
58	MG	1A	3960	1/1	0.65	0.14	64,64,64,64	0
58	MG	2a	1727	1/1	0.66	0.20	70,70,70,70	0
58	MG	2a	1762	1/1	0.66	0.15	81,81,81,81	0
58	MG	1a	1788	1/1	0.67	0.17	82,82,82,82	0
58	MG	1B	233	1/1	0.67	0.21	76,76,76,76	0
58	MG	1A	3998	1/1	0.68	0.30	83,83,83,83	0
58	MG	2A	3595	1/1	0.68	0.21	70,70,70,70	0
58	MG	1A	4094	1/1	0.68	0.21	79,79,79,79	0
58	MG	1a	1747	1/1	0.68	0.28	75,75,75,75	0
58	MG	2A	3535	1/1	0.68	0.20	79,79,79,79	0
58	MG	2A	3576	1/1	0.69	0.21	51,51,51,51	0
58	MG	2a	1708	1/1	0.69	0.15	88,88,88,88	0
58	MG	1A	4087	1/1	0.69	0.26	72,72,72,72	0
58	MG	2A	3243	1/1	0.69	0.28	83,83,83,83	0
58	MG	1a	1777	1/1	0.70	0.18	75,75,75,75	0
58	MG	1a	1812	1/1	0.70	0.20	79,79,79,79	0
58	MG	1U	212	1/1	0.71	0.44	60,60,60,60	0
58	MG	1a	1796	1/1	0.71	0.13	80,80,80,80	0
58	MG	2A	3610	1/1	0.71	0.21	89,89,89,89	0
58	MG	1A	3326	1/1	0.72	0.32	70,70,70,70	0
58	MG	2a	1644	1/1	0.72	0.12	79,79,79,79	0
58	MG	2a	1649	1/1	0.72	0.18	86,86,86,86	0
58	MG	2A	3341	1/1	0.72	0.22	73,73,73,73	0
58	MG	2A	3534	1/1	0.72	0.18	73,73,73,73	0
58	MG	1A	3512	1/1	0.73	0.17	75,75,75,75	0
58	MG	1A	3719	1/1	0.73	0.25	70,70,70,70	0
58	MG	2A	3025	1/1	0.74	0.25	61,61,61,61	0
58	MG	1B	229	1/1	0.74	0.21	71,71,71,71	0
58	MG	1a	1604	1/1	0.74	0.20	65,65,65,65	0
58	MG	2A	3553	1/1	0.74	0.18	50,50,50,50	0
58	MG	2a	1766	1/1	0.74	0.28	75,75,75,75	0
58	MG	1A	3796	1/1	0.74	0.18	80,80,80,80	0
58	MG	2A	3434	1/1	0.74	0.14	49,49,49,49	0
58	MG	2a	1808	1/1	0.74	0.28	63,63,63,63	0
58	MG	2v	101	1/1	0.74	0.18	69,69,69,69	0
58	MG	1A	3843	1/1	0.75	0.19	63,63,63,63	0
58	MG	1A	3883	1/1	0.75	0.36	76,76,76,76	0
58	MG	18	107	1/1	0.75	0.22	76,76,76,76	0
58	MG	1A	3926	1/1	0.75	0.13	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1a	1808	1/1	0.75	0.23	88,88,88,88	0
58	MG	1A	3266	1/1	0.75	0.20	68,68,68,68	0
58	MG	2l	201	1/1	0.75	0.18	69,69,69,69	0
58	MG	2l	206	1/1	0.75	0.14	77,77,77,77	0
58	MG	2A	3526	1/1	0.75	0.15	82,82,82,82	0
58	MG	2B	212	1/1	0.76	0.17	73,73,73,73	0
58	MG	2A	3342	1/1	0.76	0.13	59,59,59,59	0
58	MG	2a	1625	1/1	0.76	0.37	76,76,76,76	0
58	MG	2a	1643	1/1	0.76	0.19	66,66,66,66	0
58	MG	2A	3356	1/1	0.76	0.11	51,51,51,51	0
58	MG	1A	4021	1/1	0.76	0.20	54,54,54,54	0
58	MG	1A	3369	1/1	0.76	0.24	65,65,65,65	0
58	MG	1a	1607	1/1	0.76	0.35	71,71,71,71	0
58	MG	1a	1665	1/1	0.76	0.29	68,68,68,68	0
58	MG	2a	1783	1/1	0.77	0.17	73,73,73,73	0
58	MG	1l	201	1/1	0.77	0.20	79,79,79,79	0
58	MG	2a	1613	1/1	0.77	0.41	77,77,77,77	0
58	MG	1A	3463	1/1	0.77	0.13	53,53,53,53	0
58	MG	2A	3371	1/1	0.77	0.29	65,65,65,65	0
58	MG	2A	3406	1/1	0.77	0.16	61,61,61,61	0
58	MG	1A	4078	1/1	0.77	0.15	67,67,67,67	0
58	MG	1A	3754	1/1	0.78	0.10	33,33,33,33	0
58	MG	2A	3318	1/1	0.78	0.25	71,71,71,71	0
58	MG	2a	1745	1/1	0.78	0.22	76,76,76,76	0
58	MG	1a	1809	1/1	0.78	0.21	73,73,73,73	0
58	MG	2a	1607	1/1	0.78	0.25	75,75,75,75	0
58	MG	1a	1741	1/1	0.78	0.24	68,68,68,68	0
58	MG	2A	3544	1/1	0.78	0.30	60,60,60,60	0
58	MG	2a	1785	1/1	0.78	0.17	83,83,83,83	0
58	MG	1A	3961	1/1	0.78	0.10	24,24,24,24	0
58	MG	1A	3523	1/1	0.78	0.23	71,71,71,71	0
58	MG	2a	1804	1/1	0.78	0.21	73,73,73,73	0
58	MG	1A	3942	1/1	0.78	0.11	22,22,22,22	0
58	MG	2a	1675	1/1	0.78	0.29	78,78,78,78	0
58	MG	2a	1691	1/1	0.78	0.35	85,85,85,85	0
58	MG	1A	4069	1/1	0.78	0.22	45,45,45,45	0
58	MG	1a	1707	1/1	0.79	0.25	68,68,68,68	0
58	MG	1a	1720	1/1	0.79	0.24	75,75,75,75	0
58	MG	2A	3614	1/1	0.79	0.14	50,50,50,50	0
58	MG	1a	1722	1/1	0.79	0.13	75,75,75,75	0
58	MG	2a	1748	1/1	0.79	0.14	79,79,79,79	0
58	MG	1A	3632	1/1	0.79	0.17	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1B	230	1/1	0.79	0.19	70,70,70,70	0
58	MG	2A	3057	1/1	0.79	0.11	56,56,56,56	0
58	MG	1A	3691	1/1	0.79	0.21	65,65,65,65	0
58	MG	1I	201	1/1	0.79	0.12	72,72,72,72	0
58	MG	2a	1788	1/1	0.79	0.18	70,70,70,70	0
58	MG	2a	1634	1/1	0.79	0.22	66,66,66,66	0
58	MG	2a	1799	1/1	0.79	0.25	79,79,79,79	0
58	MG	2a	1642	1/1	0.79	0.17	78,78,78,78	0
58	MG	2A	3260	1/1	0.79	0.29	59,59,59,59	0
58	MG	2a	1807	1/1	0.79	0.25	79,79,79,79	0
58	MG	2A	3306	1/1	0.79	0.15	50,50,50,50	0
58	MG	2d	301	1/1	0.79	0.17	75,75,75,75	0
58	MG	1a	1671	1/1	0.79	0.34	74,74,74,74	0
58	MG	2A	3572	1/1	0.79	0.16	72,72,72,72	0
58	MG	1A	3588	1/1	0.79	0.13	69,69,69,69	0
58	MG	2a	1703	1/1	0.80	0.20	70,70,70,70	0
58	MG	2A	3232	1/1	0.80	0.26	63,63,63,63	0
58	MG	2a	1723	1/1	0.80	0.23	81,81,81,81	0
58	MG	1A	3840	1/1	0.80	0.14	60,60,60,60	0
58	MG	1B	202	1/1	0.80	0.30	68,68,68,68	0
58	MG	1a	1781	1/1	0.80	0.15	64,64,64,64	0
58	MG	1a	1639	1/1	0.80	0.18	76,76,76,76	0
58	MG	1A	3656	1/1	0.80	0.20	55,55,55,55	0
58	MG	1A	4015	1/1	0.80	0.20	62,62,62,62	0
58	MG	1A	3264	1/1	0.80	0.27	72,72,72,72	0
58	MG	2a	1603	1/1	0.80	0.19	71,71,71,71	0
58	MG	2A	3361	1/1	0.80	0.25	80,80,80,80	0
58	MG	2A	3366	1/1	0.80	0.17	63,63,63,63	0
58	MG	1A	3381	1/1	0.80	0.28	66,66,66,66	0
58	MG	2a	1620	1/1	0.80	0.29	87,87,87,87	0
58	MG	2a	1800	1/1	0.80	0.30	65,65,65,65	0
58	MG	1O	202	1/1	0.80	0.25	69,69,69,69	0
58	MG	1A	3815	1/1	0.80	0.12	42,42,42,42	0
58	MG	2A	3444	1/1	0.80	0.21	39,39,39,39	0
58	MG	1a	1735	1/1	0.80	0.21	67,67,67,67	0
58	MG	1a	1737	1/1	0.80	0.15	80,80,80,80	0
58	MG	2A	3070	1/1	0.80	0.17	79,79,79,79	0
58	MG	1A	3824	1/1	0.80	0.14	60,60,60,60	0
58	MG	2A	3230	1/1	0.80	0.24	77,77,77,77	0
58	MG	2A	3247	1/1	0.81	0.15	73,73,73,73	0
58	MG	1A	3753	1/1	0.81	0.20	66,66,66,66	0
58	MG	2A	3541	1/1	0.81	0.17	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1660	1/1	0.81	0.14	77,77,77,77	0
58	MG	1A	3972	1/1	0.81	0.12	66,66,66,66	0
58	MG	2A	3547	1/1	0.81	0.29	71,71,71,71	0
58	MG	1e	201	1/1	0.81	0.18	76,76,76,76	0
58	MG	1B	226	1/1	0.81	0.14	67,67,67,67	0
58	MG	2a	1709	1/1	0.81	0.26	65,65,65,65	0
58	MG	1A	3616	1/1	0.81	0.11	57,57,57,57	0
58	MG	1A	3462	1/1	0.81	0.15	75,75,75,75	0
58	MG	1A	3913	1/1	0.81	0.22	38,38,38,38	0
58	MG	2a	1743	1/1	0.81	0.40	86,86,86,86	0
58	MG	1a	1779	1/1	0.81	0.14	56,56,56,56	0
58	MG	2A	3666	1/1	0.81	0.22	73,73,73,73	0
58	MG	1A	3529	1/1	0.81	0.34	59,59,59,59	0
58	MG	2A	3682	1/1	0.81	0.18	56,56,56,56	0
58	MG	2B	201	1/1	0.81	0.29	76,76,76,76	0
58	MG	2B	208	1/1	0.81	0.27	79,79,79,79	0
58	MG	2A	3376	1/1	0.81	0.15	51,51,51,51	0
58	MG	2E	305	1/1	0.81	0.23	82,82,82,82	0
58	MG	2A	3404	1/1	0.81	0.26	71,71,71,71	0
58	MG	2A	3179	1/1	0.81	0.11	65,65,65,65	0
58	MG	2A	3198	1/1	0.81	0.30	71,71,71,71	0
58	MG	2a	1609	1/1	0.81	0.44	71,71,71,71	0
58	MG	2a	1612	1/1	0.81	0.50	80,80,80,80	0
58	MG	1a	1700	1/1	0.81	0.35	75,75,75,75	0
58	MG	2A	3466	1/1	0.81	0.10	52,52,52,52	0
58	MG	2a	1622	1/1	0.81	0.34	68,68,68,68	0
58	MG	2j	201	1/1	0.81	0.15	77,77,77,77	0
58	MG	2A	3495	1/1	0.81	0.20	67,67,67,67	0
58	MG	1A	3351	1/1	0.81	0.20	60,60,60,60	0
58	MG	1A	3401	1/1	0.81	0.24	63,63,63,63	0
58	MG	2A	3436	1/1	0.82	0.26	58,58,58,58	0
58	MG	2B	209	1/1	0.82	0.24	80,80,80,80	0
58	MG	2a	1722	1/1	0.82	0.24	81,81,81,81	0
58	MG	1A	3477	1/1	0.82	0.13	67,67,67,67	0
58	MG	2E	303	1/1	0.82	0.12	66,66,66,66	0
58	MG	2a	1737	1/1	0.82	0.46	78,78,78,78	0
58	MG	1b	301	1/1	0.82	0.14	79,79,79,79	0
58	MG	1A	3102	1/1	0.82	0.28	66,66,66,66	0
58	MG	2a	1604	1/1	0.82	0.25	80,80,80,80	0
58	MG	1A	3513	1/1	0.82	0.17	81,81,81,81	0
58	MG	1a	1669	1/1	0.82	0.34	77,77,77,77	0
58	MG	2A	3328	1/1	0.82	0.17	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3335	1/1	0.82	0.25	68,68,68,68	0
58	MG	1a	1762	1/1	0.82	0.16	65,65,65,65	0
58	MG	2a	1618	1/1	0.82	0.20	76,76,76,76	0
58	MG	1A	3806	1/1	0.82	0.10	52,52,52,52	0
58	MG	2A	3343	1/1	0.82	0.20	57,57,57,57	0
58	MG	2A	3353	1/1	0.82	0.18	67,67,67,67	0
58	MG	1A	3648	1/1	0.82	0.24	58,58,58,58	0
58	MG	2A	3360	1/1	0.82	0.19	55,55,55,55	0
58	MG	2A	3090	1/1	0.82	0.26	66,66,66,66	0
58	MG	1A	3412	1/1	0.82	0.27	74,74,74,74	0
58	MG	2A	3176	1/1	0.82	0.23	69,69,69,69	0
58	MG	2a	1812	1/1	0.82	0.32	73,73,73,73	0
58	MG	1A	4092	1/1	0.82	0.12	49,49,49,49	0
58	MG	1A	3185	1/1	0.82	0.15	68,68,68,68	0
58	MG	1A	3205	1/1	0.82	0.10	56,56,56,56	0
58	MG	2a	1701	1/1	0.82	0.29	71,71,71,71	0
58	MG	1a	1734	1/1	0.82	0.13	61,61,61,61	0
58	MG	2x	3303	1/1	0.82	0.24	79,79,79,79	0
58	MG	1a	1742	1/1	0.83	0.18	75,75,75,75	0
58	MG	1A	3362	1/1	0.83	0.36	51,51,51,51	0
58	MG	2A	3188	1/1	0.83	0.15	69,69,69,69	0
58	MG	2a	1652	1/1	0.83	0.28	71,71,71,71	0
58	MG	2a	1657	1/1	0.83	0.18	75,75,75,75	0
58	MG	1a	1758	1/1	0.83	0.18	64,64,64,64	0
58	MG	2A	3205	1/1	0.83	0.35	71,71,71,71	0
58	MG	2A	3222	1/1	0.83	0.30	80,80,80,80	0
58	MG	2A	3225	1/1	0.83	0.31	76,76,76,76	0
58	MG	1A	3767	1/1	0.83	0.11	18,18,18,18	0
58	MG	1a	1765	1/1	0.83	0.14	65,65,65,65	0
58	MG	1a	1772	1/1	0.83	0.19	78,78,78,78	0
58	MG	2a	1714	1/1	0.83	0.19	73,73,73,73	0
58	MG	1A	3422	1/1	0.83	0.23	71,71,71,71	0
58	MG	1a	1623	1/1	0.83	0.39	65,65,65,65	0
58	MG	2a	1726	1/1	0.83	0.21	73,73,73,73	0
58	MG	1A	3028	1/1	0.83	0.29	77,77,77,77	0
58	MG	1a	1652	1/1	0.83	0.20	68,68,68,68	0
58	MG	2a	1739	1/1	0.83	0.36	74,74,74,74	0
58	MG	2A	3319	1/1	0.83	0.12	68,68,68,68	0
58	MG	1A	3341	1/1	0.83	0.12	54,54,54,54	0
58	MG	1B	225	1/1	0.83	0.17	55,55,55,55	0
58	MG	2B	204	1/1	0.83	0.21	79,79,79,79	0
58	MG	1A	3473	1/1	0.83	0.10	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3821	1/1	0.83	0.16	54,54,54,54	0
58	MG	2B	210	1/1	0.83	0.28	69,69,69,69	0
58	MG	1A	3705	1/1	0.83	0.10	55,55,55,55	0
58	MG	1A	3309	1/1	0.83	0.22	63,63,63,63	0
58	MG	1a	1709	1/1	0.83	0.30	62,62,62,62	0
58	MG	20	103	1/1	0.83	0.26	58,58,58,58	0
58	MG	1n	101	1/1	0.83	0.12	51,51,51,51	0
58	MG	1t	201	1/1	0.83	0.19	65,65,65,65	0
58	MG	1A	3597	1/1	0.83	0.35	42,42,42,42	0
58	MG	1w	101	1/1	0.83	0.09	66,66,66,66	0
58	MG	1N	201	1/1	0.83	0.20	52,52,52,52	0
58	MG	2A	3028	1/1	0.83	0.22	65,65,65,65	0
58	MG	1A	3871	1/1	0.83	0.17	39,39,39,39	0
58	MG	1T	202	1/1	0.83	0.21	52,52,52,52	0
58	MG	1A	4070	1/1	0.83	0.14	61,61,61,61	0
58	MG	2A	3102	1/1	0.83	0.32	79,79,79,79	0
58	MG	2A	3458	1/1	0.83	0.15	53,53,53,53	0
58	MG	2t	201	1/1	0.83	0.17	54,54,54,54	0
58	MG	1W	201	1/1	0.83	0.22	52,52,52,52	0
58	MG	2A	3119	1/1	0.83	0.18	72,72,72,72	0
58	MG	1A	3979	1/1	0.84	0.15	65,65,65,65	0
58	MG	2a	1640	1/1	0.84	0.16	59,59,59,59	0
58	MG	1a	1663	1/1	0.84	0.12	58,58,58,58	0
58	MG	2A	3531	1/1	0.84	0.16	76,76,76,76	0
58	MG	2A	3237	1/1	0.84	0.33	56,56,56,56	0
58	MG	1a	1759	1/1	0.84	0.13	60,60,60,60	0
58	MG	2A	3246	1/1	0.84	0.15	61,61,61,61	0
58	MG	2a	1654	1/1	0.84	0.13	79,79,79,79	0
58	MG	2A	3539	1/1	0.84	0.26	70,70,70,70	0
58	MG	1w	106	1/1	0.84	0.12	76,76,76,76	0
58	MG	1x	104	1/1	0.84	0.22	62,62,62,62	0
58	MG	2A	3267	1/1	0.84	0.35	66,66,66,66	0
58	MG	2A	3268	1/1	0.84	0.26	72,72,72,72	0
58	MG	2A	3557	1/1	0.84	0.20	66,66,66,66	0
58	MG	2A	3566	1/1	0.84	0.14	58,58,58,58	0
58	MG	2A	3273	1/1	0.84	0.24	62,62,62,62	0
58	MG	2A	3278	1/1	0.84	0.17	72,72,72,72	0
58	MG	2A	3582	1/1	0.84	0.18	63,63,63,63	0
58	MG	1x	109	1/1	0.84	0.32	67,67,67,67	0
58	MG	2A	3606	1/1	0.84	0.11	72,72,72,72	0
58	MG	2A	3307	1/1	0.84	0.28	70,70,70,70	0
58	MG	2A	3612	1/1	0.84	0.13	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3270	1/1	0.84	0.14	54,54,54,54	0
58	MG	1P	202	1/1	0.84	0.20	46,46,46,46	0
58	MG	2A	3056	1/1	0.84	0.13	63,63,63,63	0
58	MG	2A	3330	1/1	0.84	0.35	70,70,70,70	0
58	MG	2A	3333	1/1	0.84	0.23	62,62,62,62	0
58	MG	1A	3251	1/1	0.84	0.15	56,56,56,56	0
58	MG	2a	1756	1/1	0.84	0.30	66,66,66,66	0
58	MG	2B	205	1/1	0.84	0.24	73,73,73,73	0
58	MG	1A	3578	1/1	0.84	0.10	32,32,32,32	0
58	MG	2A	3089	1/1	0.84	0.24	69,69,69,69	0
58	MG	1a	1696	1/1	0.84	0.27	62,62,62,62	0
58	MG	1A	4042	1/1	0.84	0.17	57,57,57,57	0
58	MG	1Y	203	1/1	0.84	0.13	71,71,71,71	0
58	MG	2a	1795	1/1	0.84	0.22	64,64,64,64	0
58	MG	1A	3263	1/1	0.84	0.27	70,70,70,70	0
58	MG	2A	3127	1/1	0.84	0.10	71,71,71,71	0
58	MG	2A	3128	1/1	0.84	0.24	61,61,61,61	0
58	MG	1A	3870	1/1	0.84	0.20	46,46,46,46	0
58	MG	2a	1806	1/1	0.84	0.22	73,73,73,73	0
58	MG	1A	3593	1/1	0.84	0.29	60,60,60,60	0
58	MG	2A	3378	1/1	0.84	0.34	64,64,64,64	0
58	MG	2A	3180	1/1	0.84	0.22	59,59,59,59	0
58	MG	2a	1817	1/1	0.84	0.28	67,67,67,67	0
58	MG	2a	1820	1/1	0.84	0.33	75,75,75,75	0
58	MG	2a	1610	1/1	0.84	0.26	72,72,72,72	0
58	MG	1G	203	1/1	0.84	0.13	61,61,61,61	0
58	MG	1a	1630	1/1	0.84	0.34	59,59,59,59	0
58	MG	2l	204	1/1	0.84	0.28	73,73,73,73	0
58	MG	2A	3203	1/1	0.84	0.33	65,65,65,65	0
58	MG	1A	3878	1/1	0.84	0.27	63,63,63,63	0
58	MG	1a	1641	1/1	0.84	0.18	73,73,73,73	0
58	MG	1a	1647	1/1	0.84	0.25	70,70,70,70	0
58	MG	2A	3139	1/1	0.85	0.14	68,68,68,68	0
58	MG	1A	3603	1/1	0.85	0.30	71,71,71,71	0
58	MG	1A	3349	1/1	0.85	0.15	65,65,65,65	0
58	MG	1A	3896	1/1	0.85	0.28	81,81,81,81	0
58	MG	2A	3355	1/1	0.85	0.20	67,67,67,67	0
58	MG	1A	3033	1/1	0.85	0.18	38,38,38,38	0
58	MG	2A	3623	1/1	0.85	0.13	58,58,58,58	0
58	MG	2A	3628	1/1	0.85	0.11	35,35,35,35	0
58	MG	1d	301	1/1	0.85	0.39	61,61,61,61	0
58	MG	1a	1708	1/1	0.85	0.21	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3671	1/1	0.85	0.17	67,67,67,67	0
58	MG	2A	3674	1/1	0.85	0.11	58,58,58,58	0
58	MG	2A	3678	1/1	0.85	0.13	60,60,60,60	0
58	MG	2A	3680	1/1	0.85	0.21	65,65,65,65	0
58	MG	2a	1729	1/1	0.85	0.23	57,57,57,57	0
58	MG	1A	3920	1/1	0.85	0.14	47,47,47,47	0
58	MG	2A	3221	1/1	0.85	0.14	73,73,73,73	0
58	MG	2A	3373	1/1	0.85	0.19	64,64,64,64	0
58	MG	15	104	1/1	0.85	0.11	59,59,59,59	0
58	MG	1A	3441	1/1	0.85	0.12	52,52,52,52	0
58	MG	2A	3379	1/1	0.85	0.18	64,64,64,64	0
58	MG	2A	3400	1/1	0.85	0.22	64,64,64,64	0
58	MG	1A	3538	1/1	0.85	0.14	62,62,62,62	0
58	MG	1A	3954	1/1	0.85	0.16	65,65,65,65	0
58	MG	1w	104	1/1	0.85	0.09	83,83,83,83	0
58	MG	2V	201	1/1	0.85	0.16	62,62,62,62	0
58	MG	1a	1614	1/1	0.85	0.12	66,66,66,66	0
58	MG	28	101	1/1	0.85	0.19	64,64,64,64	0
58	MG	2A	3244	1/1	0.85	0.15	67,67,67,67	0
58	MG	1a	1619	1/1	0.85	0.18	61,61,61,61	0
58	MG	1A	3816	1/1	0.85	0.13	39,39,39,39	0
58	MG	2A	3005	1/1	0.85	0.20	66,66,66,66	0
58	MG	2A	3263	1/1	0.85	0.20	58,58,58,58	0
58	MG	2A	3528	1/1	0.85	0.15	62,62,62,62	0
58	MG	1A	3189	1/1	0.85	0.25	61,61,61,61	0
58	MG	1A	3193	1/1	0.85	0.14	54,54,54,54	0
58	MG	1A	3149	1/1	0.85	0.14	40,40,40,40	0
58	MG	1a	1644	1/1	0.85	0.18	65,65,65,65	0
58	MG	2a	1813	1/1	0.85	0.19	61,61,61,61	0
58	MG	1A	3346	1/1	0.85	0.12	52,52,52,52	0
58	MG	1a	1767	1/1	0.85	0.12	63,63,63,63	0
58	MG	1E	311	1/1	0.85	0.21	57,57,57,57	0
58	MG	2g	201	1/1	0.85	0.15	78,78,78,78	0
58	MG	1A	3404	1/1	0.85	0.10	55,55,55,55	0
58	MG	2A	3324	1/1	0.85	0.34	63,63,63,63	0
58	MG	1A	3758	1/1	0.85	0.17	56,56,56,56	0
58	MG	1A	4028	1/1	0.85	0.14	56,56,56,56	0
58	MG	2q	202	1/1	0.85	0.15	83,83,83,83	0
58	MG	2a	1645	1/1	0.85	0.19	77,77,77,77	0
58	MG	1A	4036	1/1	0.85	0.11	25,25,25,25	0
58	MG	1a	1678	1/1	0.85	0.19	68,68,68,68	0
58	MG	2A	3096	1/1	0.86	0.20	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3514	1/1	0.86	0.16	75,75,75,75	0
58	MG	1A	3405	1/1	0.86	0.11	68,68,68,68	0
58	MG	2a	1674	1/1	0.86	0.28	69,69,69,69	0
58	MG	1A	4072	1/1	0.86	0.25	58,58,58,58	0
58	MG	2a	1689	1/1	0.86	0.22	71,71,71,71	0
58	MG	2A	3122	1/1	0.86	0.19	70,70,70,70	0
58	MG	2a	1700	1/1	0.86	0.16	72,72,72,72	0
58	MG	1A	3526	1/1	0.86	0.28	58,58,58,58	0
58	MG	2A	3638	1/1	0.86	0.11	45,45,45,45	0
58	MG	1A	3880	1/1	0.86	0.14	59,59,59,59	0
58	MG	1A	3350	1/1	0.86	0.13	53,53,53,53	0
58	MG	2A	3175	1/1	0.86	0.26	63,63,63,63	0
58	MG	1A	3166	1/1	0.86	0.37	63,63,63,63	0
58	MG	1A	3548	1/1	0.86	0.41	41,41,41,41	0
58	MG	1a	1648	1/1	0.86	0.26	60,60,60,60	0
58	MG	2A	3181	1/1	0.86	0.26	56,56,56,56	0
58	MG	1a	1802	1/1	0.86	0.10	60,60,60,60	0
58	MG	2a	1732	1/1	0.86	0.42	84,84,84,84	0
58	MG	1B	216	1/1	0.86	0.13	70,70,70,70	0
58	MG	1A	3756	1/1	0.86	0.11	64,64,64,64	0
58	MG	1A	3325	1/1	0.86	0.20	54,54,54,54	0
58	MG	1A	3937	1/1	0.86	0.12	61,61,61,61	0
58	MG	1A	3455	1/1	0.86	0.17	39,39,39,39	0
58	MG	1A	3584	1/1	0.86	0.19	71,71,71,71	0
58	MG	2a	1751	1/1	0.86	0.23	72,72,72,72	0
58	MG	1A	3025	1/1	0.86	0.18	52,52,52,52	0
58	MG	1A	3104	1/1	0.86	0.11	63,63,63,63	0
58	MG	1A	3967	1/1	0.86	0.15	53,53,53,53	0
58	MG	20	102	1/1	0.86	0.09	62,62,62,62	0
58	MG	1A	3814	1/1	0.86	0.15	38,38,38,38	0
58	MG	2A	3482	1/1	0.86	0.19	68,68,68,68	0
58	MG	2a	1787	1/1	0.86	0.24	68,68,68,68	0
58	MG	1A	3390	1/1	0.86	0.13	55,55,55,55	0
58	MG	1A	3994	1/1	0.86	0.11	34,34,34,34	0
58	MG	2a	1792	1/1	0.86	0.16	71,71,71,71	0
58	MG	1R	206	1/1	0.86	0.12	41,41,41,41	0
58	MG	1A	3997	1/1	0.86	0.20	83,83,83,83	0
58	MG	1A	3393	1/1	0.86	0.35	39,39,39,39	0
58	MG	2A	3264	1/1	0.86	0.19	54,54,54,54	0
58	MG	1x	111	1/1	0.86	0.33	69,69,69,69	0
58	MG	1A	3604	1/1	0.86	0.24	75,75,75,75	0
58	MG	2a	1617	1/1	0.86	0.17	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3271	1/1	0.86	0.34	70,70,70,70	0
58	MG	2A	3023	1/1	0.86	0.21	54,54,54,54	0
58	MG	1A	3502	1/1	0.86	0.16	56,56,56,56	0
58	MG	10	104	1/1	0.86	0.24	51,51,51,51	0
58	MG	2a	1628	1/1	0.86	0.23	78,78,78,78	0
58	MG	1A	3107	1/1	0.86	0.15	52,52,52,52	0
58	MG	2a	1639	1/1	0.86	0.14	79,79,79,79	0
58	MG	2A	3560	1/1	0.86	0.18	47,47,47,47	0
58	MG	1a	1746	1/1	0.86	0.14	56,56,56,56	0
58	MG	2l	203	1/1	0.86	0.17	70,70,70,70	0
58	MG	1A	3090	1/1	0.86	0.12	53,53,53,53	0
58	MG	2A	3083	1/1	0.86	0.17	66,66,66,66	0
58	MG	1A	4040	1/1	0.86	0.16	56,56,56,56	0
58	MG	2r	101	1/1	0.86	0.24	74,74,74,74	0
58	MG	2A	3587	1/1	0.86	0.11	62,62,62,62	0
58	MG	1A	3856	1/1	0.86	0.14	48,48,48,48	0
58	MG	2a	1653	1/1	0.86	0.34	74,74,74,74	0
58	MG	2A	3655	1/1	0.87	0.12	60,60,60,60	0
58	MG	2a	1694	1/1	0.87	0.20	57,57,57,57	0
58	MG	2a	1699	1/1	0.87	0.13	78,78,78,78	0
58	MG	2A	3217	1/1	0.87	0.23	59,59,59,59	0
58	MG	1A	3912	1/1	0.87	0.21	44,44,44,44	0
58	MG	1a	1716	1/1	0.87	0.19	63,63,63,63	0
58	MG	1A	3027	1/1	0.87	0.19	69,69,69,69	0
58	MG	1A	3728	1/1	0.87	0.14	65,65,65,65	0
58	MG	1Z	301	1/1	0.87	0.07	55,55,55,55	0
58	MG	2a	1719	1/1	0.87	0.16	69,69,69,69	0
58	MG	1A	3924	1/1	0.87	0.14	64,64,64,64	0
58	MG	2A	3419	1/1	0.87	0.16	33,33,33,33	0
58	MG	2a	1725	1/1	0.87	0.38	52,52,52,52	0
58	MG	2A	3242	1/1	0.87	0.29	60,60,60,60	0
58	MG	1A	3491	1/1	0.87	0.20	72,72,72,72	0
58	MG	1A	4074	1/1	0.87	0.16	65,65,65,65	0
58	MG	2A	3006	1/1	0.87	0.26	56,56,56,56	0
58	MG	2a	1733	1/1	0.87	0.22	74,74,74,74	0
58	MG	1A	3831	1/1	0.87	0.12	56,56,56,56	0
58	MG	2A	3470	1/1	0.87	0.13	53,53,53,53	0
58	MG	2D	306	1/1	0.87	0.18	67,67,67,67	0
58	MG	1A	3605	1/1	0.87	0.14	49,49,49,49	0
58	MG	2A	3483	1/1	0.87	0.16	66,66,66,66	0
58	MG	2a	1747	1/1	0.87	0.34	79,79,79,79	0
58	MG	2A	3487	1/1	0.87	0.13	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3943	1/1	0.87	0.14	38,38,38,38	0
58	MG	2A	3499	1/1	0.87	0.17	61,61,61,61	0
58	MG	2a	1754	1/1	0.87	0.22	70,70,70,70	0
58	MG	1A	3842	1/1	0.87	0.12	58,58,58,58	0
58	MG	1A	3501	1/1	0.87	0.38	53,53,53,53	0
58	MG	1a	1627	1/1	0.87	0.12	49,49,49,49	0
58	MG	2a	1776	1/1	0.87	0.22	61,61,61,61	0
58	MG	1A	3854	1/1	0.87	0.13	47,47,47,47	0
58	MG	1A	3580	1/1	0.87	0.12	48,48,48,48	0
58	MG	2A	3277	1/1	0.87	0.21	55,55,55,55	0
58	MG	1A	3644	1/1	0.87	0.12	52,52,52,52	0
58	MG	1A	3343	1/1	0.87	0.20	55,55,55,55	0
58	MG	2A	3542	1/1	0.87	0.10	64,64,64,64	0
58	MG	1a	1778	1/1	0.87	0.14	36,36,36,36	0
58	MG	1A	3505	1/1	0.87	0.23	46,46,46,46	0
58	MG	1A	3530	1/1	0.87	0.27	71,71,71,71	0
58	MG	2a	1621	1/1	0.87	0.19	67,67,67,67	0
58	MG	1A	3881	1/1	0.87	0.10	29,29,29,29	0
58	MG	1A	4012	1/1	0.87	0.14	74,74,74,74	0
58	MG	2A	3562	1/1	0.87	0.12	51,51,51,51	0
58	MG	1a	1797	1/1	0.87	0.21	62,62,62,62	0
58	MG	1G	204	1/1	0.87	0.14	64,64,64,64	0
58	MG	2A	3573	1/1	0.87	0.14	53,53,53,53	0
58	MG	1A	3320	1/1	0.87	0.14	45,45,45,45	0
58	MG	1A	4017	1/1	0.87	0.21	63,63,63,63	0
58	MG	1N	204	1/1	0.87	0.13	57,57,57,57	0
58	MG	2d	302	1/1	0.87	0.24	53,53,53,53	0
58	MG	2f	202	1/1	0.87	0.15	72,72,72,72	0
58	MG	2A	3590	1/1	0.87	0.12	55,55,55,55	0
58	MG	2a	1647	1/1	0.87	0.23	63,63,63,63	0
58	MG	1A	3884	1/1	0.87	0.13	30,30,30,30	0
58	MG	2A	3602	1/1	0.87	0.25	75,75,75,75	0
58	MG	1A	3888	1/1	0.87	0.16	51,51,51,51	0
58	MG	2A	3186	1/1	0.87	0.15	63,63,63,63	0
58	MG	1A	4033	1/1	0.87	0.17	55,55,55,55	0
58	MG	1a	1705	1/1	0.87	0.26	73,73,73,73	0
58	MG	1A	3714	1/1	0.87	0.13	45,45,45,45	0
58	MG	1U	203	1/1	0.87	0.21	68,68,68,68	0
58	MG	2A	3215	1/1	0.87	0.12	66,66,66,66	0
58	MG	1A	3002	1/1	0.88	0.23	57,57,57,57	0
58	MG	2A	3386	1/1	0.88	0.23	65,65,65,65	0
58	MG	2A	3395	1/1	0.88	0.23	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3704	1/1	0.88	0.11	32,32,32,32	0
58	MG	2A	3402	1/1	0.88	0.25	63,63,63,63	0
58	MG	1a	1712	1/1	0.88	0.11	62,62,62,62	0
58	MG	1A	3154	1/1	0.88	0.13	36,36,36,36	0
58	MG	1A	3370	1/1	0.88	0.20	45,45,45,45	0
58	MG	2a	1614	1/1	0.88	0.20	60,60,60,60	0
58	MG	1A	3718	1/1	0.88	0.10	52,52,52,52	0
58	MG	1E	308	1/1	0.88	0.12	30,30,30,30	0
58	MG	1A	3097	1/1	0.88	0.10	59,59,59,59	0
58	MG	2A	3447	1/1	0.88	0.17	47,47,47,47	0
58	MG	2A	3151	1/1	0.88	0.27	71,71,71,71	0
58	MG	2A	3459	1/1	0.88	0.11	48,48,48,48	0
58	MG	1A	3271	1/1	0.88	0.10	45,45,45,45	0
58	MG	2a	1633	1/1	0.88	0.26	76,76,76,76	0
58	MG	1A	3730	1/1	0.88	0.20	55,55,55,55	0
58	MG	2a	1635	1/1	0.88	0.26	75,75,75,75	0
58	MG	2a	1637	1/1	0.88	0.14	55,55,55,55	0
58	MG	2A	3472	1/1	0.88	0.27	62,62,62,62	0
58	MG	2A	3474	1/1	0.88	0.20	46,46,46,46	0
58	MG	2A	3481	1/1	0.88	0.18	57,57,57,57	0
58	MG	1A	3731	1/1	0.88	0.16	62,62,62,62	0
58	MG	1A	3739	1/1	0.88	0.15	51,51,51,51	0
58	MG	1A	3747	1/1	0.88	0.10	19,19,19,19	0
58	MG	2a	1646	1/1	0.88	0.09	65,65,65,65	0
58	MG	1A	3949	1/1	0.88	0.19	72,72,72,72	0
58	MG	1A	3041	1/1	0.88	0.14	52,52,52,52	0
58	MG	2A	3503	1/1	0.88	0.11	65,65,65,65	0
58	MG	2A	3509	1/1	0.88	0.29	43,43,43,43	0
58	MG	2A	3513	1/1	0.88	0.16	40,40,40,40	0
58	MG	2a	1655	1/1	0.88	0.30	81,81,81,81	0
58	MG	2A	3522	1/1	0.88	0.19	52,52,52,52	0
58	MG	1A	3054	1/1	0.88	0.11	52,52,52,52	0
58	MG	2A	3200	1/1	0.88	0.28	63,63,63,63	0
58	MG	1a	1764	1/1	0.88	0.11	70,70,70,70	0
58	MG	2a	1678	1/1	0.88	0.14	70,70,70,70	0
58	MG	1A	3190	1/1	0.88	0.20	42,42,42,42	0
58	MG	2a	1690	1/1	0.88	0.15	80,80,80,80	0
58	MG	1A	3063	1/1	0.88	0.17	61,61,61,61	0
58	MG	1A	3334	1/1	0.88	0.20	52,52,52,52	0
58	MG	1A	3773	1/1	0.88	0.14	44,44,44,44	0
58	MG	1A	3980	1/1	0.88	0.13	64,64,64,64	0
58	MG	1A	3336	1/1	0.88	0.09	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3803	1/1	0.88	0.10	21,21,21,21	0
58	MG	2A	3546	1/1	0.88	0.15	49,49,49,49	0
58	MG	1A	3435	1/1	0.88	0.34	54,54,54,54	0
58	MG	2a	1710	1/1	0.88	0.28	77,77,77,77	0
58	MG	1A	3338	1/1	0.88	0.16	62,62,62,62	0
58	MG	1A	3453	1/1	0.88	0.10	61,61,61,61	0
58	MG	1A	3340	1/1	0.88	0.17	39,39,39,39	0
58	MG	1A	3118	1/1	0.88	0.28	52,52,52,52	0
58	MG	1A	3594	1/1	0.88	0.10	59,59,59,59	0
58	MG	2A	3567	1/1	0.88	0.13	64,64,64,64	0
58	MG	2A	3569	1/1	0.88	0.14	54,54,54,54	0
58	MG	1A	4032	1/1	0.88	0.12	55,55,55,55	0
58	MG	2A	3257	1/1	0.88	0.23	41,41,41,41	0
58	MG	2A	3574	1/1	0.88	0.11	78,78,78,78	0
58	MG	2a	1734	1/1	0.88	0.28	65,65,65,65	0
58	MG	2a	1735	1/1	0.88	0.20	65,65,65,65	0
58	MG	1A	3130	1/1	0.88	0.18	62,62,62,62	0
58	MG	2A	3577	1/1	0.88	0.15	61,61,61,61	0
58	MG	1A	3471	1/1	0.88	0.17	49,49,49,49	0
58	MG	1a	1631	1/1	0.88	0.16	61,61,61,61	0
58	MG	1A	3253	1/1	0.88	0.15	76,76,76,76	0
58	MG	1A	3258	1/1	0.88	0.15	64,64,64,64	0
58	MG	1p	101	1/1	0.88	0.23	64,64,64,64	0
58	MG	2A	3605	1/1	0.88	0.12	54,54,54,54	0
58	MG	1a	1643	1/1	0.88	0.20	59,59,59,59	0
58	MG	1A	4046	1/1	0.88	0.14	59,59,59,59	0
58	MG	2A	3611	1/1	0.88	0.10	62,62,62,62	0
58	MG	2a	1761	1/1	0.88	0.15	65,65,65,65	0
58	MG	1A	3486	1/1	0.88	0.12	61,61,61,61	0
58	MG	2A	3302	1/1	0.88	0.37	78,78,78,78	0
58	MG	2A	3615	1/1	0.88	0.11	62,62,62,62	0
58	MG	1A	3617	1/1	0.88	0.10	26,26,26,26	0
58	MG	1w	105	1/1	0.88	0.23	79,79,79,79	0
58	MG	2A	3633	1/1	0.88	0.11	54,54,54,54	0
58	MG	2A	3315	1/1	0.88	0.16	63,63,63,63	0
58	MG	2A	3645	1/1	0.88	0.11	71,71,71,71	0
58	MG	1A	3260	1/1	0.88	0.12	51,51,51,51	0
58	MG	2A	3664	1/1	0.88	0.17	77,77,77,77	0
58	MG	2a	1798	1/1	0.88	0.22	67,67,67,67	0
58	MG	2A	3665	1/1	0.88	0.10	63,63,63,63	0
58	MG	1A	3493	1/1	0.88	0.12	51,51,51,51	0
58	MG	2a	1801	1/1	0.88	0.17	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1x	107	1/1	0.88	0.29	71,71,71,71	0
58	MG	1A	3139	1/1	0.88	0.36	36,36,36,36	0
58	MG	1x	110	1/1	0.88	0.30	65,65,65,65	0
58	MG	2A	3675	1/1	0.88	0.18	74,74,74,74	0
58	MG	2A	3332	1/1	0.88	0.28	58,58,58,58	0
58	MG	1A	4081	1/1	0.88	0.12	47,47,47,47	0
58	MG	1A	4084	1/1	0.88	0.12	54,54,54,54	0
58	MG	1a	1672	1/1	0.88	0.15	62,62,62,62	0
58	MG	1A	3875	1/1	0.88	0.25	44,44,44,44	0
58	MG	1A	4088	1/1	0.88	0.22	63,63,63,63	0
58	MG	1a	1681	1/1	0.88	0.17	76,76,76,76	0
58	MG	2A	3041	1/1	0.88	0.14	68,68,68,68	0
58	MG	1a	1691	1/1	0.88	0.23	61,61,61,61	0
58	MG	1A	3361	1/1	0.88	0.18	43,43,43,43	0
58	MG	2A	3063	1/1	0.88	0.13	54,54,54,54	0
58	MG	1A	3663	1/1	0.88	0.16	52,52,52,52	0
58	MG	2A	3367	1/1	0.88	0.08	62,62,62,62	0
58	MG	2F	303	1/1	0.88	0.20	52,52,52,52	0
58	MG	2A	3075	1/1	0.88	0.10	70,70,70,70	0
58	MG	1a	1704	1/1	0.88	0.16	64,64,64,64	0
58	MG	1A	3685	1/1	0.88	0.13	46,46,46,46	0
58	MG	1A	3689	1/1	0.88	0.10	47,47,47,47	0
58	MG	2a	1602	1/1	0.88	0.14	74,74,74,74	0
58	MG	2x	3304	1/1	0.88	0.16	67,67,67,67	0
58	MG	1B	212	1/1	0.89	0.17	62,62,62,62	0
58	MG	1a	1684	1/1	0.89	0.14	55,55,55,55	0
58	MG	1a	1689	1/1	0.89	0.32	64,64,64,64	0
58	MG	1A	3269	1/1	0.89	0.19	59,59,59,59	0
58	MG	2a	1608	1/1	0.89	0.53	72,72,72,72	0
58	MG	2A	3078	1/1	0.89	0.19	66,66,66,66	0
58	MG	1a	1692	1/1	0.89	0.31	55,55,55,55	0
58	MG	1A	3928	1/1	0.89	0.11	47,47,47,47	0
58	MG	2A	3407	1/1	0.89	0.17	43,43,43,43	0
58	MG	1A	3113	1/1	0.89	0.19	42,42,42,42	0
58	MG	2a	1616	1/1	0.89	0.10	72,72,72,72	0
58	MG	2A	3433	1/1	0.89	0.13	48,48,48,48	0
58	MG	1A	3776	1/1	0.89	0.12	27,27,27,27	0
58	MG	2A	3435	1/1	0.89	0.16	44,44,44,44	0
58	MG	2A	3099	1/1	0.89	0.12	58,58,58,58	0
58	MG	1A	3608	1/1	0.89	0.12	46,46,46,46	0
58	MG	2A	3106	1/1	0.89	0.10	52,52,52,52	0
58	MG	1B	231	1/1	0.89	0.13	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3112	1/1	0.89	0.22	50,50,50,50	0
58	MG	1A	3945	1/1	0.89	0.15	65,65,65,65	0
58	MG	1A	3798	1/1	0.89	0.12	45,45,45,45	0
58	MG	2A	3471	1/1	0.89	0.14	54,54,54,54	0
58	MG	1A	3133	1/1	0.89	0.21	56,56,56,56	0
58	MG	1A	3291	1/1	0.89	0.15	59,59,59,59	0
58	MG	2A	3134	1/1	0.89	0.10	67,67,67,67	0
58	MG	1a	1718	1/1	0.89	0.27	69,69,69,69	0
58	MG	2A	3150	1/1	0.89	0.15	49,49,49,49	0
58	MG	1a	1719	1/1	0.89	0.27	59,59,59,59	0
58	MG	1A	3807	1/1	0.89	0.12	54,54,54,54	0
58	MG	1A	3304	1/1	0.89	0.36	62,62,62,62	0
58	MG	2A	3501	1/1	0.89	0.23	51,51,51,51	0
58	MG	2A	3177	1/1	0.89	0.43	71,71,71,71	0
58	MG	1a	1729	1/1	0.89	0.14	66,66,66,66	0
58	MG	1A	3348	1/1	0.89	0.44	44,44,44,44	0
58	MG	2A	3520	1/1	0.89	0.22	57,57,57,57	0
58	MG	1A	3974	1/1	0.89	0.16	70,70,70,70	0
58	MG	1O	201	1/1	0.89	0.09	65,65,65,65	0
58	MG	2a	1664	1/1	0.89	0.14	65,65,65,65	0
58	MG	2a	1668	1/1	0.89	0.30	59,59,59,59	0
58	MG	2a	1669	1/1	0.89	0.24	70,70,70,70	0
58	MG	1A	3416	1/1	0.89	0.08	58,58,58,58	0
58	MG	1O	205	1/1	0.89	0.18	56,56,56,56	0
58	MG	2a	1676	1/1	0.89	0.24	69,69,69,69	0
58	MG	1A	3420	1/1	0.89	0.14	52,52,52,52	0
58	MG	2a	1686	1/1	0.89	0.21	71,71,71,71	0
58	MG	2A	3201	1/1	0.89	0.20	63,63,63,63	0
58	MG	1P	206	1/1	0.89	0.24	57,57,57,57	0
58	MG	2A	3204	1/1	0.89	0.21	55,55,55,55	0
58	MG	1R	201	1/1	0.89	0.18	58,58,58,58	0
58	MG	2a	1696	1/1	0.89	0.13	76,76,76,76	0
58	MG	1A	3515	1/1	0.89	0.07	67,67,67,67	0
58	MG	1A	3995	1/1	0.89	0.12	24,24,24,24	0
58	MG	1A	3666	1/1	0.89	0.09	33,33,33,33	0
58	MG	1U	207	1/1	0.89	0.25	48,48,48,48	0
58	MG	1A	3164	1/1	0.89	0.43	35,35,35,35	0
58	MG	1a	1769	1/1	0.89	0.10	62,62,62,62	0
58	MG	1A	3053	1/1	0.89	0.24	46,46,46,46	0
58	MG	1A	4014	1/1	0.89	0.11	63,63,63,63	0
58	MG	2A	3239	1/1	0.89	0.12	61,61,61,61	0
58	MG	1A	3324	1/1	0.89	0.10	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3695	1/1	0.89	0.12	25,25,25,25	0
58	MG	14	101	1/1	0.89	0.23	78,78,78,78	0
58	MG	1A	4018	1/1	0.89	0.12	58,58,58,58	0
58	MG	1A	3851	1/1	0.89	0.14	60,60,60,60	0
58	MG	2a	1728	1/1	0.89	0.33	80,80,80,80	0
58	MG	1a	1602	1/1	0.89	0.45	74,74,74,74	0
58	MG	1A	3442	1/1	0.89	0.09	43,43,43,43	0
58	MG	2A	3578	1/1	0.89	0.19	55,55,55,55	0
58	MG	1A	3452	1/1	0.89	0.15	64,64,64,64	0
58	MG	1a	1611	1/1	0.89	0.12	71,71,71,71	0
58	MG	1a	1811	1/1	0.89	0.10	65,65,65,65	0
58	MG	2A	3593	1/1	0.89	0.14	68,68,68,68	0
58	MG	1A	3167	1/1	0.89	0.09	33,33,33,33	0
58	MG	2A	3269	1/1	0.89	0.30	56,56,56,56	0
58	MG	2A	3270	1/1	0.89	0.27	61,61,61,61	0
58	MG	1A	3566	1/1	0.89	0.14	45,45,45,45	0
58	MG	1A	3874	1/1	0.89	0.18	33,33,33,33	0
58	MG	1a	1626	1/1	0.89	0.40	64,64,64,64	0
58	MG	1A	3221	1/1	0.89	0.23	44,44,44,44	0
58	MG	2A	3281	1/1	0.89	0.30	53,53,53,53	0
58	MG	2A	3285	1/1	0.89	0.23	63,63,63,63	0
58	MG	2A	3619	1/1	0.89	0.13	53,53,53,53	0
58	MG	1A	3329	1/1	0.89	0.16	44,44,44,44	0
58	MG	2A	3304	1/1	0.89	0.30	60,60,60,60	0
58	MG	1A	4064	1/1	0.89	0.11	53,53,53,53	0
58	MG	2a	1778	1/1	0.89	0.18	55,55,55,55	0
58	MG	1a	1638	1/1	0.89	0.16	59,59,59,59	0
58	MG	1A	3265	1/1	0.89	0.12	61,61,61,61	0
58	MG	2A	3648	1/1	0.89	0.10	60,60,60,60	0
58	MG	2A	3654	1/1	0.89	0.11	36,36,36,36	0
58	MG	1A	3468	1/1	0.89	0.13	50,50,50,50	0
58	MG	1w	102	1/1	0.89	0.24	73,73,73,73	0
58	MG	2A	3321	1/1	0.89	0.18	63,63,63,63	0
58	MG	2A	3323	1/1	0.89	0.17	62,62,62,62	0
58	MG	1a	1642	1/1	0.89	0.25	78,78,78,78	0
58	MG	1A	3587	1/1	0.89	0.16	64,64,64,64	0
58	MG	1A	3740	1/1	0.89	0.17	62,62,62,62	0
58	MG	1A	4077	1/1	0.89	0.14	54,54,54,54	0
58	MG	1x	106	1/1	0.89	0.20	73,73,73,73	0
58	MG	1A	3371	1/1	0.89	0.10	46,46,46,46	0
58	MG	1A	3378	1/1	0.89	0.10	68,68,68,68	0
58	MG	1a	1659	1/1	0.89	0.24	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3897	1/1	0.89	0.08	46,46,46,46	0
58	MG	2A	3345	1/1	0.89	0.14	46,46,46,46	0
58	MG	2a	1816	1/1	0.89	0.17	64,64,64,64	0
58	MG	2A	3348	1/1	0.89	0.17	64,64,64,64	0
58	MG	1a	1664	1/1	0.89	0.15	64,64,64,64	0
58	MG	1A	3908	1/1	0.89	0.10	52,52,52,52	0
58	MG	2A	3019	1/1	0.89	0.27	65,65,65,65	0
58	MG	2f	201	1/1	0.89	0.18	61,61,61,61	0
58	MG	2B	215	1/1	0.89	0.22	75,75,75,75	0
58	MG	1A	3379	1/1	0.89	0.12	63,63,63,63	0
58	MG	1A	4090	1/1	0.89	0.17	60,60,60,60	0
58	MG	2E	304	1/1	0.89	0.09	34,34,34,34	0
58	MG	2A	3363	1/1	0.89	0.23	54,54,54,54	0
58	MG	1A	3233	1/1	0.89	0.10	48,48,48,48	0
58	MG	2P	201	1/1	0.89	0.13	50,50,50,50	0
58	MG	2A	3031	1/1	0.89	0.24	63,63,63,63	0
58	MG	2Z	301	1/1	0.89	0.23	71,71,71,71	0
58	MG	2A	3033	1/1	0.89	0.22	56,56,56,56	0
58	MG	1A	3489	1/1	0.89	0.12	61,61,61,61	0
58	MG	2w	101	1/1	0.89	0.27	68,68,68,68	0
58	MG	2A	3043	1/1	0.89	0.12	69,69,69,69	0
58	MG	1A	3764	1/1	0.89	0.13	16,16,16,16	0
58	MG	2x	3305	1/1	0.89	0.28	66,66,66,66	0
58	MG	2A	3013	1/1	0.90	0.27	49,49,49,49	0
58	MG	2B	202	1/1	0.90	0.33	71,71,71,71	0
58	MG	2A	3018	1/1	0.90	0.31	43,43,43,43	0
58	MG	1A	3018	1/1	0.90	0.19	32,32,32,32	0
58	MG	1A	3804	1/1	0.90	0.10	40,40,40,40	0
58	MG	1a	1673	1/1	0.90	0.12	58,58,58,58	0
58	MG	1a	1674	1/1	0.90	0.28	68,68,68,68	0
58	MG	2A	3339	1/1	0.90	0.28	49,49,49,49	0
58	MG	1A	3311	1/1	0.90	0.26	57,57,57,57	0
58	MG	1A	3408	1/1	0.90	0.20	61,61,61,61	0
58	MG	2E	301	1/1	0.90	0.16	70,70,70,70	0
58	MG	2A	3034	1/1	0.90	0.09	62,62,62,62	0
58	MG	2A	3036	1/1	0.90	0.13	56,56,56,56	0
58	MG	2A	3040	1/1	0.90	0.20	67,67,67,67	0
58	MG	2A	3352	1/1	0.90	0.13	45,45,45,45	0
58	MG	1A	3618	1/1	0.90	0.15	52,52,52,52	0
58	MG	1A	3411	1/1	0.90	0.09	55,55,55,55	0
58	MG	2X	101	1/1	0.90	0.09	71,71,71,71	0
58	MG	2A	3045	1/1	0.90	0.23	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3048	1/1	0.90	0.15	56,56,56,56	0
58	MG	1A	3503	1/1	0.90	0.16	70,70,70,70	0
58	MG	2A	3362	1/1	0.90	0.20	62,62,62,62	0
58	MG	2a	1601	1/1	0.90	0.16	67,67,67,67	0
58	MG	1A	3315	1/1	0.90	0.08	34,34,34,34	0
58	MG	2A	3364	1/1	0.90	0.26	63,63,63,63	0
58	MG	1A	3817	1/1	0.90	0.11	52,52,52,52	0
58	MG	2a	1605	1/1	0.90	0.32	71,71,71,71	0
58	MG	2A	3064	1/1	0.90	0.35	65,65,65,65	0
58	MG	1a	1695	1/1	0.90	0.28	72,72,72,72	0
58	MG	1A	3983	1/1	0.90	0.10	34,34,34,34	0
58	MG	1A	3655	1/1	0.90	0.11	58,58,58,58	0
58	MG	1a	1701	1/1	0.90	0.19	49,49,49,49	0
58	MG	2A	3088	1/1	0.90	0.13	59,59,59,59	0
58	MG	2A	3383	1/1	0.90	0.17	50,50,50,50	0
58	MG	1A	3211	1/1	0.90	0.14	68,68,68,68	0
58	MG	2A	3390	1/1	0.90	0.31	73,73,73,73	0
58	MG	1A	3220	1/1	0.90	0.13	54,54,54,54	0
58	MG	2A	3399	1/1	0.90	0.36	66,66,66,66	0
58	MG	2a	1619	1/1	0.90	0.10	74,74,74,74	0
58	MG	2A	3092	1/1	0.90	0.14	50,50,50,50	0
58	MG	1A	3837	1/1	0.90	0.13	63,63,63,63	0
58	MG	1A	4004	1/1	0.90	0.10	37,37,37,37	0
58	MG	1A	4007	1/1	0.90	0.07	43,43,43,43	0
58	MG	1A	3354	1/1	0.90	0.13	62,62,62,62	0
58	MG	2A	3416	1/1	0.90	0.12	47,47,47,47	0
58	MG	1a	1715	1/1	0.90	0.23	55,55,55,55	0
58	MG	2A	3426	1/1	0.90	0.17	54,54,54,54	0
58	MG	2A	3429	1/1	0.90	0.13	56,56,56,56	0
58	MG	2a	1638	1/1	0.90	0.22	64,64,64,64	0
58	MG	1A	3683	1/1	0.90	0.09	26,26,26,26	0
58	MG	1A	3424	1/1	0.90	0.12	55,55,55,55	0
58	MG	2A	3121	1/1	0.90	0.28	63,63,63,63	0
58	MG	1T	201	1/1	0.90	0.14	57,57,57,57	0
58	MG	2A	3442	1/1	0.90	0.20	41,41,41,41	0
58	MG	1A	4016	1/1	0.90	0.11	62,62,62,62	0
58	MG	1a	1721	1/1	0.90	0.29	71,71,71,71	0
58	MG	2A	3131	1/1	0.90	0.36	63,63,63,63	0
58	MG	2a	1648	1/1	0.90	0.11	81,81,81,81	0
58	MG	1A	3844	1/1	0.90	0.12	51,51,51,51	0
58	MG	2A	3135	1/1	0.90	0.20	73,73,73,73	0
58	MG	2A	3469	1/1	0.90	0.23	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3136	1/1	0.90	0.10	50,50,50,50	0
58	MG	2A	3138	1/1	0.90	0.12	51,51,51,51	0
58	MG	2a	1656	1/1	0.90	0.14	59,59,59,59	0
58	MG	1U	205	1/1	0.90	0.13	43,43,43,43	0
58	MG	2a	1658	1/1	0.90	0.30	76,76,76,76	0
58	MG	2A	3147	1/1	0.90	0.24	64,64,64,64	0
58	MG	2A	3477	1/1	0.90	0.27	64,64,64,64	0
58	MG	2a	1666	1/1	0.90	0.29	61,61,61,61	0
58	MG	2A	3479	1/1	0.90	0.17	45,45,45,45	0
58	MG	1A	3432	1/1	0.90	0.08	61,61,61,61	0
58	MG	1A	3852	1/1	0.90	0.23	44,44,44,44	0
58	MG	2A	3158	1/1	0.90	0.16	58,58,58,58	0
58	MG	2A	3486	1/1	0.90	0.14	35,35,35,35	0
58	MG	2A	3159	1/1	0.90	0.16	61,61,61,61	0
58	MG	2a	1680	1/1	0.90	0.22	64,64,64,64	0
58	MG	2a	1682	1/1	0.90	0.19	77,77,77,77	0
58	MG	2a	1684	1/1	0.90	0.28	68,68,68,68	0
58	MG	1A	4027	1/1	0.90	0.12	46,46,46,46	0
58	MG	1A	3433	1/1	0.90	0.13	49,49,49,49	0
58	MG	1A	3355	1/1	0.90	0.10	45,45,45,45	0
58	MG	10	101	1/1	0.90	0.10	42,42,42,42	0
58	MG	2A	3508	1/1	0.90	0.16	40,40,40,40	0
58	MG	1A	3075	1/1	0.90	0.20	57,57,57,57	0
58	MG	2a	1697	1/1	0.90	0.23	63,63,63,63	0
58	MG	1a	1757	1/1	0.90	0.20	68,68,68,68	0
58	MG	2A	3517	1/1	0.90	0.17	53,53,53,53	0
58	MG	10	107	1/1	0.90	0.15	61,61,61,61	0
58	MG	13	103	1/1	0.90	0.10	50,50,50,50	0
58	MG	2a	1706	1/1	0.90	0.18	75,75,75,75	0
58	MG	2A	3524	1/1	0.90	0.19	66,66,66,66	0
58	MG	2A	3525	1/1	0.90	0.26	63,63,63,63	0
58	MG	2A	3195	1/1	0.90	0.11	46,46,46,46	0
58	MG	2A	3527	1/1	0.90	0.19	64,64,64,64	0
58	MG	2a	1718	1/1	0.90	0.19	70,70,70,70	0
58	MG	1A	3534	1/1	0.90	0.30	61,61,61,61	0
58	MG	15	102	1/1	0.90	0.37	34,34,34,34	0
58	MG	2A	3533	1/1	0.90	0.09	69,69,69,69	0
58	MG	2a	1724	1/1	0.90	0.17	64,64,64,64	0
58	MG	1A	3713	1/1	0.90	0.15	42,42,42,42	0
58	MG	2A	3202	1/1	0.90	0.28	61,61,61,61	0
58	MG	1A	3056	1/1	0.90	0.13	60,60,60,60	0
58	MG	1A	4043	1/1	0.90	0.11	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1a	1770	1/1	0.90	0.11	57,57,57,57	0
58	MG	2A	3208	1/1	0.90	0.34	47,47,47,47	0
58	MG	2A	3543	1/1	0.90	0.17	72,72,72,72	0
58	MG	2A	3211	1/1	0.90	0.13	63,63,63,63	0
58	MG	1A	3234	1/1	0.90	0.09	55,55,55,55	0
58	MG	1a	1605	1/1	0.90	0.13	51,51,51,51	0
58	MG	2A	3548	1/1	0.90	0.13	64,64,64,64	0
58	MG	2A	3551	1/1	0.90	0.28	61,61,61,61	0
58	MG	1A	3551	1/1	0.90	0.19	36,36,36,36	0
58	MG	1A	3564	1/1	0.90	0.42	39,39,39,39	0
58	MG	1A	3245	1/1	0.90	0.11	60,60,60,60	0
58	MG	2A	3229	1/1	0.90	0.21	46,46,46,46	0
58	MG	1a	1617	1/1	0.90	0.10	51,51,51,51	0
58	MG	2a	1752	1/1	0.90	0.17	76,76,76,76	0
58	MG	1A	3335	1/1	0.90	0.19	53,53,53,53	0
58	MG	1a	1622	1/1	0.90	0.16	59,59,59,59	0
58	MG	2A	3238	1/1	0.90	0.36	78,78,78,78	0
58	MG	1A	3373	1/1	0.90	0.09	47,47,47,47	0
58	MG	1a	1806	1/1	0.90	0.38	73,73,73,73	0
58	MG	2a	1763	1/1	0.90	0.12	66,66,66,66	0
58	MG	2a	1764	1/1	0.90	0.20	70,70,70,70	0
58	MG	2a	1765	1/1	0.90	0.19	50,50,50,50	0
58	MG	1a	1624	1/1	0.90	0.18	60,60,60,60	0
58	MG	2a	1768	1/1	0.90	0.18	77,77,77,77	0
58	MG	2a	1771	1/1	0.90	0.18	73,73,73,73	0
58	MG	1A	4076	1/1	0.90	0.14	65,65,65,65	0
58	MG	1A	3249	1/1	0.90	0.34	67,67,67,67	0
58	MG	2a	1779	1/1	0.90	0.24	76,76,76,76	0
58	MG	2A	3579	1/1	0.90	0.15	40,40,40,40	0
58	MG	1A	3583	1/1	0.90	0.33	40,40,40,40	0
58	MG	1A	3465	1/1	0.90	0.30	54,54,54,54	0
58	MG	2A	3258	1/1	0.90	0.20	54,54,54,54	0
58	MG	2A	3591	1/1	0.90	0.16	52,52,52,52	0
58	MG	2a	1790	1/1	0.90	0.14	72,72,72,72	0
58	MG	1A	3586	1/1	0.90	0.14	44,44,44,44	0
58	MG	1A	4086	1/1	0.90	0.13	50,50,50,50	0
58	MG	2A	3597	1/1	0.90	0.12	61,61,61,61	0
58	MG	2A	3600	1/1	0.90	0.23	81,81,81,81	0
58	MG	1A	3122	1/1	0.90	0.17	40,40,40,40	0
58	MG	1A	3339	1/1	0.90	0.09	65,65,65,65	0
58	MG	1A	3760	1/1	0.90	0.08	32,32,32,32	0
58	MG	1A	3472	1/1	0.90	0.10	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1a	1645	1/1	0.90	0.18	49,49,49,49	0
58	MG	1A	3194	1/1	0.90	0.35	45,45,45,45	0
58	MG	1A	4095	1/1	0.90	0.13	55,55,55,55	0
58	MG	2a	1811	1/1	0.90	0.23	65,65,65,65	0
58	MG	1A	3295	1/1	0.90	0.14	59,59,59,59	0
58	MG	1B	210	1/1	0.90	0.15	53,53,53,53	0
58	MG	2A	3620	1/1	0.90	0.12	76,76,76,76	0
58	MG	1a	1660	1/1	0.90	0.13	65,65,65,65	0
58	MG	2a	1818	1/1	0.90	0.14	74,74,74,74	0
58	MG	2a	1819	1/1	0.90	0.20	60,60,60,60	0
58	MG	1w	107	1/1	0.90	0.15	71,71,71,71	0
58	MG	2a	1821	1/1	0.90	0.27	70,70,70,70	0
58	MG	2A	3287	1/1	0.90	0.15	58,58,58,58	0
58	MG	2A	3296	1/1	0.90	0.20	54,54,54,54	0
58	MG	2A	3299	1/1	0.90	0.13	59,59,59,59	0
58	MG	1a	1661	1/1	0.90	0.20	66,66,66,66	0
58	MG	2A	3652	1/1	0.90	0.16	50,50,50,50	0
58	MG	1x	105	1/1	0.90	0.28	67,67,67,67	0
58	MG	2A	3305	1/1	0.90	0.11	55,55,55,55	0
58	MG	1a	1662	1/1	0.90	0.12	64,64,64,64	0
58	MG	1A	3479	1/1	0.90	0.16	61,61,61,61	0
58	MG	2A	3309	1/1	0.90	0.17	69,69,69,69	0
58	MG	2A	3311	1/1	0.90	0.07	52,52,52,52	0
58	MG	2A	3313	1/1	0.90	0.37	55,55,55,55	0
58	MG	1B	215	1/1	0.90	0.17	60,60,60,60	0
58	MG	1A	3394	1/1	0.90	0.16	46,46,46,46	0
58	MG	1a	1666	1/1	0.90	0.26	64,64,64,64	0
58	MG	2x	3302	1/1	0.90	0.20	66,66,66,66	0
58	MG	1a	1667	1/1	0.90	0.22	63,63,63,63	0
58	MG	1A	3255	1/1	0.90	0.21	61,61,61,61	0
58	MG	2A	3685	1/1	0.90	0.12	65,65,65,65	0
58	MG	1A	3459	1/1	0.91	0.09	54,54,54,54	0
58	MG	2A	3493	1/1	0.91	0.14	77,77,77,77	0
58	MG	1x	102	1/1	0.91	0.16	68,68,68,68	0
58	MG	2A	3234	1/1	0.91	0.16	58,58,58,58	0
58	MG	2a	1624	1/1	0.91	0.12	66,66,66,66	0
58	MG	1A	3552	1/1	0.91	0.07	49,49,49,49	0
58	MG	2a	1626	1/1	0.91	0.25	63,63,63,63	0
58	MG	1A	3999	1/1	0.91	0.18	60,60,60,60	0
58	MG	1A	3183	1/1	0.91	0.21	49,49,49,49	0
58	MG	1A	4006	1/1	0.91	0.12	39,39,39,39	0
58	MG	1A	3845	1/1	0.91	0.23	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3514	1/1	0.91	0.23	52,52,52,52	0
58	MG	1A	4008	1/1	0.91	0.08	42,42,42,42	0
58	MG	2A	3518	1/1	0.91	0.25	66,66,66,66	0
58	MG	1O	204	1/1	0.91	0.11	60,60,60,60	0
58	MG	2a	1641	1/1	0.91	0.09	61,61,61,61	0
58	MG	1A	3847	1/1	0.91	0.08	65,65,65,65	0
58	MG	2A	3523	1/1	0.91	0.15	66,66,66,66	0
58	MG	2A	3248	1/1	0.91	0.16	67,67,67,67	0
58	MG	1a	1682	1/1	0.91	0.21	64,64,64,64	0
58	MG	1A	3386	1/1	0.91	0.27	43,43,43,43	0
58	MG	2A	3259	1/1	0.91	0.29	53,53,53,53	0
58	MG	1a	1688	1/1	0.91	0.31	46,46,46,46	0
58	MG	1A	3388	1/1	0.91	0.14	52,52,52,52	0
58	MG	2A	3022	1/1	0.91	0.18	51,51,51,51	0
58	MG	1A	3274	1/1	0.91	0.11	51,51,51,51	0
58	MG	1A	3579	1/1	0.91	0.15	37,37,37,37	0
58	MG	1S	202	1/1	0.91	0.10	73,73,73,73	0
58	MG	1A	3862	1/1	0.91	0.15	59,59,59,59	0
58	MG	2A	3540	1/1	0.91	0.19	66,66,66,66	0
58	MG	2A	3032	1/1	0.91	0.13	57,57,57,57	0
58	MG	1a	1698	1/1	0.91	0.12	60,60,60,60	0
58	MG	1A	3280	1/1	0.91	0.31	48,48,48,48	0
58	MG	1A	3083	1/1	0.91	0.13	40,40,40,40	0
58	MG	1A	3293	1/1	0.91	0.07	38,38,38,38	0
58	MG	2A	3284	1/1	0.91	0.23	55,55,55,55	0
58	MG	1A	3402	1/1	0.91	0.15	49,49,49,49	0
58	MG	2A	3549	1/1	0.91	0.16	64,64,64,64	0
58	MG	1A	3067	1/1	0.91	0.22	66,66,66,66	0
58	MG	2a	1677	1/1	0.91	0.21	64,64,64,64	0
58	MG	2A	3552	1/1	0.91	0.11	54,54,54,54	0
58	MG	2a	1679	1/1	0.91	0.25	62,62,62,62	0
58	MG	2A	3294	1/1	0.91	0.15	62,62,62,62	0
58	MG	1A	4035	1/1	0.91	0.16	29,29,29,29	0
58	MG	2A	3559	1/1	0.91	0.11	61,61,61,61	0
58	MG	1W	202	1/1	0.91	0.14	49,49,49,49	0
58	MG	2A	3054	1/1	0.91	0.08	43,43,43,43	0
58	MG	1A	3745	1/1	0.91	0.10	59,59,59,59	0
58	MG	1A	3480	1/1	0.91	0.18	52,52,52,52	0
58	MG	2a	1692	1/1	0.91	0.19	57,57,57,57	0
58	MG	1A	3297	1/1	0.91	0.12	49,49,49,49	0
58	MG	1A	3300	1/1	0.91	0.18	44,44,44,44	0
58	MG	1O	105	1/1	0.91	0.27	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1698	1/1	0.91	0.12	78,78,78,78	0
58	MG	2A	3073	1/1	0.91	0.28	50,50,50,50	0
58	MG	1A	3093	1/1	0.91	0.28	53,53,53,53	0
58	MG	10	108	1/1	0.91	0.17	62,62,62,62	0
58	MG	2A	3079	1/1	0.91	0.22	64,64,64,64	0
58	MG	2A	3081	1/1	0.91	0.19	56,56,56,56	0
58	MG	11	101	1/1	0.91	0.42	44,44,44,44	0
58	MG	2A	3086	1/1	0.91	0.24	53,53,53,53	0
58	MG	11	103	1/1	0.91	0.10	71,71,71,71	0
58	MG	13	102	1/1	0.91	0.15	59,59,59,59	0
58	MG	2a	1716	1/1	0.91	0.40	75,75,75,75	0
58	MG	1A	4047	1/1	0.91	0.19	46,46,46,46	0
58	MG	2A	3091	1/1	0.91	0.14	48,48,48,48	0
58	MG	1A	4050	1/1	0.91	0.10	47,47,47,47	0
58	MG	1A	3146	1/1	0.91	0.12	56,56,56,56	0
58	MG	2A	3601	1/1	0.91	0.15	59,59,59,59	0
58	MG	1A	3494	1/1	0.91	0.13	57,57,57,57	0
58	MG	2A	3340	1/1	0.91	0.16	58,58,58,58	0
58	MG	1A	3415	1/1	0.91	0.13	49,49,49,49	0
58	MG	2A	3105	1/1	0.91	0.13	50,50,50,50	0
58	MG	1a	1601	1/1	0.91	0.19	59,59,59,59	0
58	MG	1a	1751	1/1	0.91	0.12	53,53,53,53	0
58	MG	2A	3613	1/1	0.91	0.12	78,78,78,78	0
58	MG	1A	3116	1/1	0.91	0.07	50,50,50,50	0
58	MG	2A	3115	1/1	0.91	0.26	66,66,66,66	0
58	MG	1A	3198	1/1	0.91	0.31	52,52,52,52	0
58	MG	1A	3152	1/1	0.91	0.27	44,44,44,44	0
58	MG	1A	3921	1/1	0.91	0.09	60,60,60,60	0
58	MG	2A	3627	1/1	0.91	0.12	34,34,34,34	0
58	MG	2A	3358	1/1	0.91	0.12	70,70,70,70	0
58	MG	2a	1746	1/1	0.91	0.12	58,58,58,58	0
58	MG	1A	3507	1/1	0.91	0.14	56,56,56,56	0
58	MG	1A	4079	1/1	0.91	0.10	55,55,55,55	0
58	MG	1a	1615	1/1	0.91	0.14	55,55,55,55	0
58	MG	1A	3925	1/1	0.91	0.13	61,61,61,61	0
58	MG	1A	3423	1/1	0.91	0.23	75,75,75,75	0
58	MG	1A	3322	1/1	0.91	0.11	51,51,51,51	0
58	MG	1a	1773	1/1	0.91	0.23	62,62,62,62	0
58	MG	2A	3657	1/1	0.91	0.15	59,59,59,59	0
58	MG	2A	3661	1/1	0.91	0.09	55,55,55,55	0
58	MG	2A	3370	1/1	0.91	0.16	58,58,58,58	0
58	MG	1A	3117	1/1	0.91	0.18	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3805	1/1	0.91	0.10	47,47,47,47	0
58	MG	1A	4089	1/1	0.91	0.12	54,54,54,54	0
58	MG	1a	1780	1/1	0.91	0.17	62,62,62,62	0
58	MG	2a	1770	1/1	0.91	0.16	76,76,76,76	0
58	MG	2A	3152	1/1	0.91	0.14	58,58,58,58	0
58	MG	2a	1775	1/1	0.91	0.16	60,60,60,60	0
58	MG	2A	3381	1/1	0.91	0.25	48,48,48,48	0
58	MG	2a	1777	1/1	0.91	0.15	51,51,51,51	0
58	MG	2A	3153	1/1	0.91	0.22	63,63,63,63	0
58	MG	2A	3157	1/1	0.91	0.13	62,62,62,62	0
58	MG	2a	1780	1/1	0.91	0.11	62,62,62,62	0
58	MG	2A	3387	1/1	0.91	0.26	66,66,66,66	0
58	MG	2A	3389	1/1	0.91	0.29	63,63,63,63	0
58	MG	1A	3649	1/1	0.91	0.13	60,60,60,60	0
58	MG	1A	3650	1/1	0.91	0.18	34,34,34,34	0
58	MG	2A	3161	1/1	0.91	0.19	55,55,55,55	0
58	MG	2A	3168	1/1	0.91	0.15	45,45,45,45	0
58	MG	2B	206	1/1	0.91	0.15	57,57,57,57	0
58	MG	2B	207	1/1	0.91	0.15	72,72,72,72	0
58	MG	2a	1796	1/1	0.91	0.16	60,60,60,60	0
58	MG	1A	3948	1/1	0.91	0.26	66,66,66,66	0
58	MG	1a	1634	1/1	0.91	0.28	70,70,70,70	0
58	MG	1a	1636	1/1	0.91	0.15	61,61,61,61	0
58	MG	1a	1803	1/1	0.91	0.10	67,67,67,67	0
58	MG	1A	3812	1/1	0.91	0.45	36,36,36,36	0
58	MG	1A	3952	1/1	0.91	0.10	61,61,61,61	0
58	MG	2A	3185	1/1	0.91	0.18	68,68,68,68	0
58	MG	1A	3363	1/1	0.91	0.15	54,54,54,54	0
58	MG	1B	211	1/1	0.91	0.17	63,63,63,63	0
58	MG	2A	3191	1/1	0.91	0.20	68,68,68,68	0
58	MG	2F	301	1/1	0.91	0.09	54,54,54,54	0
58	MG	2F	302	1/1	0.91	0.11	63,63,63,63	0
58	MG	2a	1815	1/1	0.91	0.27	65,65,65,65	0
58	MG	1A	3006	1/1	0.91	0.15	64,64,64,64	0
58	MG	1a	1813	1/1	0.91	0.31	77,77,77,77	0
58	MG	2A	3199	1/1	0.91	0.17	63,63,63,63	0
58	MG	1B	213	1/1	0.91	0.12	44,44,44,44	0
58	MG	1A	3121	1/1	0.91	0.13	37,37,37,37	0
58	MG	2A	3449	1/1	0.91	0.29	58,58,58,58	0
58	MG	2A	3454	1/1	0.91	0.14	44,44,44,44	0
58	MG	23	101	1/1	0.91	0.31	70,70,70,70	0
58	MG	1A	3231	1/1	0.91	0.14	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1B	222	1/1	0.91	0.09	58,58,58,58	0
58	MG	2A	3462	1/1	0.91	0.11	37,37,37,37	0
58	MG	2A	3464	1/1	0.91	0.21	57,57,57,57	0
58	MG	1A	3669	1/1	0.91	0.12	58,58,58,58	0
58	MG	1A	3681	1/1	0.91	0.11	22,22,22,22	0
58	MG	1A	3977	1/1	0.91	0.11	65,65,65,65	0
58	MG	1A	3445	1/1	0.91	0.20	53,53,53,53	0
58	MG	2A	3214	1/1	0.91	0.13	61,61,61,61	0
58	MG	1A	3331	1/1	0.91	0.24	62,62,62,62	0
58	MG	1A	3832	1/1	0.91	0.14	47,47,47,47	0
58	MG	1w	103	1/1	0.91	0.10	65,65,65,65	0
58	MG	2v	102	1/1	0.91	0.17	74,74,74,74	0
58	MG	1A	3232	1/1	0.91	0.23	34,34,34,34	0
58	MG	1A	3081	1/1	0.91	0.12	65,65,65,65	0
58	MG	2A	3228	1/1	0.91	0.18	66,66,66,66	0
58	MG	2A	3484	1/1	0.91	0.17	54,54,54,54	0
58	MG	1F	310	1/1	0.91	0.09	58,58,58,58	0
58	MG	2A	3155	1/1	0.92	0.06	51,51,51,51	0
58	MG	1A	3464	1/1	0.92	0.08	51,51,51,51	0
58	MG	1W	206	1/1	0.92	0.11	44,44,44,44	0
58	MG	1X	101	1/1	0.92	0.47	41,41,41,41	0
58	MG	2A	3160	1/1	0.92	0.15	48,48,48,48	0
58	MG	1A	3134	1/1	0.92	0.15	31,31,31,31	0
58	MG	1Y	204	1/1	0.92	0.20	51,51,51,51	0
58	MG	2A	3171	1/1	0.92	0.15	63,63,63,63	0
58	MG	2A	3172	1/1	0.92	0.14	40,40,40,40	0
58	MG	1A	3103	1/1	0.92	0.17	38,38,38,38	0
58	MG	2A	3453	1/1	0.92	0.17	34,34,34,34	0
58	MG	1A	3591	1/1	0.92	0.14	54,54,54,54	0
58	MG	2A	3455	1/1	0.92	0.16	45,45,45,45	0
58	MG	2A	3456	1/1	0.92	0.12	45,45,45,45	0
58	MG	1A	3169	1/1	0.92	0.08	31,31,31,31	0
58	MG	2A	3178	1/1	0.92	0.20	73,73,73,73	0
58	MG	1A	3170	1/1	0.92	0.14	40,40,40,40	0
58	MG	2A	3463	1/1	0.92	0.14	47,47,47,47	0
58	MG	1A	3144	1/1	0.92	0.15	53,53,53,53	0
58	MG	1a	1774	1/1	0.92	0.15	77,77,77,77	0
58	MG	1A	3406	1/1	0.92	0.12	56,56,56,56	0
58	MG	2a	1623	1/1	0.92	0.18	65,65,65,65	0
58	MG	1A	3819	1/1	0.92	0.15	70,70,70,70	0
58	MG	1A	3319	1/1	0.92	0.35	36,36,36,36	0
58	MG	2A	3189	1/1	0.92	0.17	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3225	1/1	0.92	0.19	44,44,44,44	0
58	MG	2A	3475	1/1	0.92	0.23	65,65,65,65	0
58	MG	1A	4025	1/1	0.92	0.10	54,54,54,54	0
58	MG	1a	1784	1/1	0.92	0.18	71,71,71,71	0
58	MG	1A	3827	1/1	0.92	0.17	30,30,30,30	0
58	MG	1a	1790	1/1	0.92	0.09	73,73,73,73	0
58	MG	1A	3830	1/1	0.92	0.09	41,41,41,41	0
58	MG	1A	3483	1/1	0.92	0.09	55,55,55,55	0
58	MG	1A	3609	1/1	0.92	0.08	41,41,41,41	0
58	MG	19	101	1/1	0.92	0.16	53,53,53,53	0
58	MG	1a	1804	1/1	0.92	0.15	60,60,60,60	0
58	MG	2A	3207	1/1	0.92	0.11	57,57,57,57	0
58	MG	2A	3496	1/1	0.92	0.15	41,41,41,41	0
58	MG	1A	3834	1/1	0.92	0.23	62,62,62,62	0
58	MG	2A	3209	1/1	0.92	0.09	54,54,54,54	0
58	MG	1A	3227	1/1	0.92	0.14	58,58,58,58	0
58	MG	2A	3506	1/1	0.92	0.13	43,43,43,43	0
58	MG	1a	1603	1/1	0.92	0.20	71,71,71,71	0
58	MG	1A	3323	1/1	0.92	0.13	47,47,47,47	0
58	MG	1A	3490	1/1	0.92	0.17	45,45,45,45	0
58	MG	2A	3219	1/1	0.92	0.08	45,45,45,45	0
58	MG	1A	3619	1/1	0.92	0.21	38,38,38,38	0
58	MG	1A	3626	1/1	0.92	0.12	35,35,35,35	0
58	MG	1a	1613	1/1	0.92	0.21	47,47,47,47	0
58	MG	2A	3521	1/1	0.92	0.22	70,70,70,70	0
58	MG	2a	1662	1/1	0.92	0.28	63,63,63,63	0
58	MG	1A	3357	1/1	0.92	0.16	57,57,57,57	0
58	MG	1f	202	1/1	0.92	0.20	66,66,66,66	0
58	MG	1A	4048	1/1	0.92	0.13	49,49,49,49	0
58	MG	1A	3492	1/1	0.92	0.08	44,44,44,44	0
58	MG	2a	1671	1/1	0.92	0.23	59,59,59,59	0
58	MG	1A	4053	1/1	0.92	0.11	53,53,53,53	0
58	MG	2A	3236	1/1	0.92	0.20	48,48,48,48	0
58	MG	1A	4061	1/1	0.92	0.09	43,43,43,43	0
58	MG	1A	4063	1/1	0.92	0.09	54,54,54,54	0
58	MG	1A	3645	1/1	0.92	0.18	60,60,60,60	0
58	MG	1A	3417	1/1	0.92	0.26	47,47,47,47	0
58	MG	1A	3045	1/1	0.92	0.13	38,38,38,38	0
58	MG	1a	1629	1/1	0.92	0.28	61,61,61,61	0
58	MG	1A	3421	1/1	0.92	0.20	50,50,50,50	0
58	MG	1A	3858	1/1	0.92	0.09	52,52,52,52	0
58	MG	1A	4075	1/1	0.92	0.23	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1x	101	1/1	0.92	0.35	70,70,70,70	0
58	MG	1A	3096	1/1	0.92	0.21	53,53,53,53	0
58	MG	1A	3088	1/1	0.92	0.19	33,33,33,33	0
58	MG	2A	3545	1/1	0.92	0.20	61,61,61,61	0
58	MG	1A	3659	1/1	0.92	0.11	40,40,40,40	0
58	MG	1A	3504	1/1	0.92	0.38	33,33,33,33	0
58	MG	1A	3327	1/1	0.92	0.23	59,59,59,59	0
58	MG	2A	3266	1/1	0.92	0.28	64,64,64,64	0
58	MG	1A	3426	1/1	0.92	0.13	58,58,58,58	0
58	MG	1A	3672	1/1	0.92	0.11	27,27,27,27	0
58	MG	1A	3510	1/1	0.92	0.11	47,47,47,47	0
58	MG	1A	3430	1/1	0.92	0.30	56,56,56,56	0
58	MG	1A	3431	1/1	0.92	0.11	53,53,53,53	0
58	MG	1A	3328	1/1	0.92	0.14	55,55,55,55	0
58	MG	1a	1656	1/1	0.92	0.15	63,63,63,63	0
58	MG	2a	1711	1/1	0.92	0.15	71,71,71,71	0
58	MG	2a	1713	1/1	0.92	0.22	63,63,63,63	0
58	MG	1a	1658	1/1	0.92	0.12	59,59,59,59	0
58	MG	1A	3191	1/1	0.92	0.18	34,34,34,34	0
58	MG	1A	4093	1/1	0.92	0.11	74,74,74,74	0
58	MG	2A	3571	1/1	0.92	0.21	53,53,53,53	0
58	MG	1A	3517	1/1	0.92	0.10	52,52,52,52	0
58	MG	1A	3905	1/1	0.92	0.14	46,46,46,46	0
58	MG	2A	3288	1/1	0.92	0.25	43,43,43,43	0
58	MG	2A	3289	1/1	0.92	0.23	53,53,53,53	0
58	MG	1B	201	1/1	0.92	0.19	62,62,62,62	0
58	MG	2A	3295	1/1	0.92	0.21	70,70,70,70	0
58	MG	1A	3907	1/1	0.92	0.11	64,64,64,64	0
58	MG	2A	3581	1/1	0.92	0.08	52,52,52,52	0
58	MG	1B	204	1/1	0.92	0.28	67,67,67,67	0
58	MG	1B	207	1/1	0.92	0.15	69,69,69,69	0
58	MG	1A	3519	1/1	0.92	0.35	56,56,56,56	0
58	MG	1A	3521	1/1	0.92	0.48	49,49,49,49	0
58	MG	2A	3592	1/1	0.92	0.14	61,61,61,61	0
58	MG	1A	3114	1/1	0.92	0.16	34,34,34,34	0
58	MG	1A	3917	1/1	0.92	0.09	42,42,42,42	0
58	MG	2A	3308	1/1	0.92	0.09	51,51,51,51	0
58	MG	1A	3437	1/1	0.92	0.28	38,38,38,38	0
58	MG	2A	3046	1/1	0.92	0.18	61,61,61,61	0
58	MG	1A	3715	1/1	0.92	0.08	53,53,53,53	0
58	MG	2A	3050	1/1	0.92	0.17	52,52,52,52	0
58	MG	2A	3316	1/1	0.92	0.17	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3527	1/1	0.92	0.18	41,41,41,41	0
58	MG	1B	223	1/1	0.92	0.20	63,63,63,63	0
58	MG	1A	3439	1/1	0.92	0.24	39,39,39,39	0
58	MG	2A	3062	1/1	0.92	0.15	34,34,34,34	0
58	MG	2a	1758	1/1	0.92	0.07	50,50,50,50	0
58	MG	1A	3374	1/1	0.92	0.14	56,56,56,56	0
58	MG	1A	3333	1/1	0.92	0.26	52,52,52,52	0
58	MG	2A	3065	1/1	0.92	0.12	58,58,58,58	0
58	MG	2A	3067	1/1	0.92	0.12	52,52,52,52	0
58	MG	1a	1687	1/1	0.92	0.21	47,47,47,47	0
58	MG	1A	3929	1/1	0.92	0.09	47,47,47,47	0
58	MG	2A	3338	1/1	0.92	0.27	65,65,65,65	0
58	MG	2a	1769	1/1	0.92	0.10	76,76,76,76	0
58	MG	1A	3281	1/1	0.92	0.28	32,32,32,32	0
58	MG	1A	3738	1/1	0.92	0.14	65,65,65,65	0
58	MG	2A	3644	1/1	0.92	0.10	69,69,69,69	0
58	MG	1E	302	1/1	0.92	0.23	35,35,35,35	0
58	MG	1A	3543	1/1	0.92	0.23	38,38,38,38	0
58	MG	1A	3446	1/1	0.92	0.13	51,51,51,51	0
58	MG	1F	307	1/1	0.92	0.10	52,52,52,52	0
58	MG	2A	3347	1/1	0.92	0.11	53,53,53,53	0
58	MG	1a	1699	1/1	0.92	0.22	52,52,52,52	0
58	MG	2A	3659	1/1	0.92	0.10	56,56,56,56	0
58	MG	1A	3550	1/1	0.92	0.29	44,44,44,44	0
58	MG	1A	3285	1/1	0.92	0.15	45,45,45,45	0
58	MG	1A	3750	1/1	0.92	0.08	22,22,22,22	0
58	MG	1A	3247	1/1	0.92	0.17	54,54,54,54	0
58	MG	1A	3555	1/1	0.92	0.10	46,46,46,46	0
58	MG	2a	1793	1/1	0.92	0.14	76,76,76,76	0
58	MG	2A	3670	1/1	0.92	0.14	54,54,54,54	0
58	MG	1A	3556	1/1	0.92	0.10	52,52,52,52	0
58	MG	1A	3966	1/1	0.92	0.11	41,41,41,41	0
58	MG	1A	3454	1/1	0.92	0.21	59,59,59,59	0
58	MG	2A	3676	1/1	0.92	0.13	66,66,66,66	0
58	MG	1A	3971	1/1	0.92	0.08	65,65,65,65	0
58	MG	1A	3387	1/1	0.92	0.12	65,65,65,65	0
58	MG	1A	3761	1/1	0.92	0.10	53,53,53,53	0
58	MG	2a	1805	1/1	0.92	0.10	62,62,62,62	0
58	MG	2A	3114	1/1	0.92	0.15	49,49,49,49	0
58	MG	2A	3686	1/1	0.92	0.20	58,58,58,58	0
58	MG	1A	3976	1/1	0.92	0.11	76,76,76,76	0
58	MG	2a	1810	1/1	0.92	0.18	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3567	1/1	0.92	0.20	46,46,46,46	0
58	MG	2B	203	1/1	0.92	0.17	59,59,59,59	0
58	MG	2A	3120	1/1	0.92	0.15	46,46,46,46	0
58	MG	2a	1814	1/1	0.92	0.13	68,68,68,68	0
58	MG	1R	205	1/1	0.92	0.11	32,32,32,32	0
58	MG	1A	3456	1/1	0.92	0.07	60,60,60,60	0
58	MG	1a	1724	1/1	0.92	0.18	59,59,59,59	0
58	MG	1A	3571	1/1	0.92	0.16	61,61,61,61	0
58	MG	2A	3129	1/1	0.92	0.12	58,58,58,58	0
58	MG	2A	3384	1/1	0.92	0.14	68,68,68,68	0
58	MG	1a	1733	1/1	0.92	0.14	59,59,59,59	0
58	MG	2A	3132	1/1	0.92	0.20	53,53,53,53	0
58	MG	2D	305	1/1	0.92	0.16	45,45,45,45	0
58	MG	1A	3982	1/1	0.92	0.10	29,29,29,29	0
58	MG	1A	3572	1/1	0.92	0.14	51,51,51,51	0
58	MG	1U	201	1/1	0.92	0.29	40,40,40,40	0
58	MG	2A	3397	1/1	0.92	0.21	45,45,45,45	0
58	MG	1A	3057	1/1	0.92	0.09	35,35,35,35	0
58	MG	1A	3460	1/1	0.92	0.17	63,63,63,63	0
58	MG	2A	3140	1/1	0.92	0.19	65,65,65,65	0
58	MG	2A	3403	1/1	0.92	0.16	60,60,60,60	0
58	MG	2O	201	1/1	0.92	0.12	61,61,61,61	0
58	MG	1a	1743	1/1	0.92	0.19	59,59,59,59	0
58	MG	1A	3461	1/1	0.92	0.25	54,54,54,54	0
58	MG	1A	3195	1/1	0.92	0.28	36,36,36,36	0
58	MG	2A	3408	1/1	0.92	0.10	52,52,52,52	0
58	MG	2A	3410	1/1	0.92	0.17	55,55,55,55	0
58	MG	1V	204	1/1	0.92	0.26	52,52,52,52	0
58	MG	1A	3197	1/1	0.92	0.36	34,34,34,34	0
58	MG	25	102	1/1	0.92	0.17	61,61,61,61	0
58	MG	27	102	1/1	0.92	0.08	49,49,49,49	0
58	MG	2A	3385	1/1	0.93	0.26	51,51,51,51	0
58	MG	1A	3962	1/1	0.93	0.09	44,44,44,44	0
58	MG	1A	3795	1/1	0.93	0.06	24,24,24,24	0
58	MG	1A	3089	1/1	0.93	0.26	41,41,41,41	0
58	MG	1A	3969	1/1	0.93	0.09	63,63,63,63	0
58	MG	1O	203	1/1	0.93	0.27	69,69,69,69	0
58	MG	2A	3396	1/1	0.93	0.19	55,55,55,55	0
58	MG	1A	3970	1/1	0.93	0.13	59,59,59,59	0
58	MG	2A	3398	1/1	0.93	0.26	63,63,63,63	0
58	MG	1A	3052	1/1	0.93	0.13	26,26,26,26	0
58	MG	2N	201	1/1	0.93	0.06	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3802	1/1	0.93	0.11	24,24,24,24	0
58	MG	2A	3401	1/1	0.93	0.17	49,49,49,49	0
58	MG	1a	1725	1/1	0.93	0.13	55,55,55,55	0
58	MG	1A	3625	1/1	0.93	0.20	39,39,39,39	0
58	MG	2X	102	1/1	0.93	0.21	54,54,54,54	0
58	MG	2A	3146	1/1	0.93	0.10	59,59,59,59	0
58	MG	1A	3236	1/1	0.93	0.20	44,44,44,44	0
58	MG	1A	3389	1/1	0.93	0.39	71,71,71,71	0
58	MG	1A	3640	1/1	0.93	0.10	57,57,57,57	0
58	MG	1S	201	1/1	0.93	0.10	56,56,56,56	0
58	MG	25	104	1/1	0.93	0.15	59,59,59,59	0
58	MG	1A	3643	1/1	0.93	0.08	47,47,47,47	0
58	MG	2A	3418	1/1	0.93	0.15	59,59,59,59	0
58	MG	1A	3287	1/1	0.93	0.07	51,51,51,51	0
58	MG	2A	3423	1/1	0.93	0.21	58,58,58,58	0
58	MG	1A	3055	1/1	0.93	0.10	56,56,56,56	0
58	MG	1A	3990	1/1	0.93	0.10	59,59,59,59	0
58	MG	1A	3992	1/1	0.93	0.07	46,46,46,46	0
58	MG	1a	1749	1/1	0.93	0.19	44,44,44,44	0
58	MG	1a	1750	1/1	0.93	0.17	55,55,55,55	0
58	MG	1A	3246	1/1	0.93	0.10	48,48,48,48	0
58	MG	1a	1756	1/1	0.93	0.15	54,54,54,54	0
58	MG	1U	206	1/1	0.93	0.28	42,42,42,42	0
58	MG	1A	3400	1/1	0.93	0.12	56,56,56,56	0
58	MG	2A	3448	1/1	0.93	0.16	57,57,57,57	0
58	MG	1A	3125	1/1	0.93	0.16	47,47,47,47	0
58	MG	2a	1615	1/1	0.93	0.16	63,63,63,63	0
58	MG	2A	3450	1/1	0.93	0.10	47,47,47,47	0
58	MG	1a	1760	1/1	0.93	0.07	56,56,56,56	0
58	MG	1a	1761	1/1	0.93	0.13	66,66,66,66	0
58	MG	1A	3533	1/1	0.93	0.16	58,58,58,58	0
58	MG	1A	3818	1/1	0.93	0.10	50,50,50,50	0
58	MG	1A	4003	1/1	0.93	0.07	31,31,31,31	0
58	MG	2A	3183	1/1	0.93	0.10	57,57,57,57	0
58	MG	2A	3461	1/1	0.93	0.23	40,40,40,40	0
58	MG	1W	205	1/1	0.93	0.17	31,31,31,31	0
58	MG	1A	3153	1/1	0.93	0.35	30,30,30,30	0
58	MG	1A	3403	1/1	0.93	0.16	56,56,56,56	0
58	MG	1Y	201	1/1	0.93	0.10	54,54,54,54	0
58	MG	2a	1629	1/1	0.93	0.28	69,69,69,69	0
58	MG	2A	3190	1/1	0.93	0.07	63,63,63,63	0
58	MG	1A	3540	1/1	0.93	0.07	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3192	1/1	0.93	0.14	59,59,59,59	0
58	MG	2a	1636	1/1	0.93	0.32	71,71,71,71	0
58	MG	2A	3193	1/1	0.93	0.13	62,62,62,62	0
58	MG	1A	3299	1/1	0.93	0.38	62,62,62,62	0
58	MG	1A	4011	1/1	0.93	0.12	57,57,57,57	0
58	MG	1A	3829	1/1	0.93	0.09	33,33,33,33	0
58	MG	1A	3196	1/1	0.93	0.17	32,32,32,32	0
58	MG	1A	3670	1/1	0.93	0.07	37,37,37,37	0
58	MG	10	106	1/1	0.93	0.10	48,48,48,48	0
58	MG	1A	3302	1/1	0.93	0.18	35,35,35,35	0
58	MG	1a	1787	1/1	0.93	0.11	58,58,58,58	0
58	MG	1A	3676	1/1	0.93	0.08	37,37,37,37	0
58	MG	1A	3467	1/1	0.93	0.23	56,56,56,56	0
58	MG	2A	3488	1/1	0.93	0.13	54,54,54,54	0
58	MG	2A	3489	1/1	0.93	0.15	54,54,54,54	0
58	MG	2a	1651	1/1	0.93	0.18	76,76,76,76	0
58	MG	2A	3490	1/1	0.93	0.20	44,44,44,44	0
58	MG	2A	3492	1/1	0.93	0.17	41,41,41,41	0
58	MG	11	102	1/1	0.93	0.20	51,51,51,51	0
58	MG	1A	3838	1/1	0.93	0.19	45,45,45,45	0
58	MG	1A	3303	1/1	0.93	0.17	40,40,40,40	0
58	MG	2A	3497	1/1	0.93	0.10	44,44,44,44	0
58	MG	1A	4026	1/1	0.93	0.07	43,43,43,43	0
58	MG	1A	3553	1/1	0.93	0.17	53,53,53,53	0
58	MG	1A	3470	1/1	0.93	0.18	41,41,41,41	0
58	MG	1A	4031	1/1	0.93	0.09	34,34,34,34	0
58	MG	2a	1665	1/1	0.93	0.13	62,62,62,62	0
58	MG	2A	3220	1/1	0.93	0.25	62,62,62,62	0
58	MG	1A	3410	1/1	0.93	0.13	51,51,51,51	0
58	MG	1A	3128	1/1	0.93	0.18	37,37,37,37	0
58	MG	2a	1670	1/1	0.93	0.13	60,60,60,60	0
58	MG	1A	3696	1/1	0.93	0.13	21,21,21,21	0
58	MG	2a	1672	1/1	0.93	0.08	75,75,75,75	0
58	MG	2A	3515	1/1	0.93	0.11	56,56,56,56	0
58	MG	2A	3227	1/1	0.93	0.23	61,61,61,61	0
58	MG	1A	3849	1/1	0.93	0.16	45,45,45,45	0
58	MG	1A	4037	1/1	0.93	0.17	39,39,39,39	0
58	MG	1A	4039	1/1	0.93	0.12	43,43,43,43	0
58	MG	2A	3231	1/1	0.93	0.23	54,54,54,54	0
58	MG	1A	3699	1/1	0.93	0.10	26,26,26,26	0
58	MG	2a	1681	1/1	0.93	0.29	63,63,63,63	0
58	MG	1a	1606	1/1	0.93	0.06	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3701	1/1	0.93	0.09	32,32,32,32	0
58	MG	1A	3307	1/1	0.93	0.22	56,56,56,56	0
58	MG	2a	1687	1/1	0.93	0.21	42,42,42,42	0
58	MG	1n	102	1/1	0.93	0.21	54,54,54,54	0
58	MG	1A	3476	1/1	0.93	0.08	42,42,42,42	0
58	MG	2A	3240	1/1	0.93	0.14	60,60,60,60	0
58	MG	1A	3857	1/1	0.93	0.13	63,63,63,63	0
58	MG	1A	3712	1/1	0.93	0.10	49,49,49,49	0
58	MG	1a	1616	1/1	0.93	0.08	57,57,57,57	0
58	MG	1A	3859	1/1	0.93	0.08	32,32,32,32	0
58	MG	1A	3051	1/1	0.93	0.09	42,42,42,42	0
58	MG	1a	1620	1/1	0.93	0.06	45,45,45,45	0
58	MG	2A	3252	1/1	0.93	0.23	41,41,41,41	0
58	MG	2A	3253	1/1	0.93	0.20	45,45,45,45	0
58	MG	2A	3254	1/1	0.93	0.24	52,52,52,52	0
58	MG	2a	1704	1/1	0.93	0.22	63,63,63,63	0
58	MG	2A	3255	1/1	0.93	0.21	52,52,52,52	0
58	MG	2a	1707	1/1	0.93	0.11	75,75,75,75	0
58	MG	1A	3863	1/1	0.93	0.08	48,48,48,48	0
58	MG	1A	4062	1/1	0.93	0.16	70,70,70,70	0
58	MG	1A	3867	1/1	0.93	0.08	25,25,25,25	0
58	MG	1A	3570	1/1	0.93	0.14	43,43,43,43	0
58	MG	1A	3131	1/1	0.93	0.15	39,39,39,39	0
58	MG	1A	3259	1/1	0.93	0.23	40,40,40,40	0
58	MG	2a	1715	1/1	0.93	0.18	62,62,62,62	0
58	MG	1A	3482	1/1	0.93	0.13	52,52,52,52	0
58	MG	2a	1717	1/1	0.93	0.42	60,60,60,60	0
58	MG	1A	3721	1/1	0.93	0.10	57,57,57,57	0
58	MG	2A	3554	1/1	0.93	0.13	27,27,27,27	0
58	MG	2a	1720	1/1	0.93	0.24	51,51,51,51	0
58	MG	2a	1721	1/1	0.93	0.28	63,63,63,63	0
58	MG	2A	3556	1/1	0.93	0.12	38,38,38,38	0
58	MG	1A	3879	1/1	0.93	0.15	36,36,36,36	0
58	MG	1A	3132	1/1	0.93	0.09	64,64,64,64	0
58	MG	1A	3215	1/1	0.93	0.18	53,53,53,53	0
58	MG	1A	3218	1/1	0.93	0.24	49,49,49,49	0
58	MG	2A	3564	1/1	0.93	0.08	32,32,32,32	0
58	MG	1A	3732	1/1	0.93	0.18	58,58,58,58	0
58	MG	2A	3275	1/1	0.93	0.22	59,59,59,59	0
58	MG	2A	3568	1/1	0.93	0.10	63,63,63,63	0
58	MG	2A	3276	1/1	0.93	0.28	50,50,50,50	0
58	MG	1A	3733	1/1	0.93	0.16	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3007	1/1	0.93	0.17	53,53,53,53	0
58	MG	2A	3279	1/1	0.93	0.20	54,54,54,54	0
58	MG	1A	3894	1/1	0.93	0.07	33,33,33,33	0
58	MG	2A	3282	1/1	0.93	0.21	58,58,58,58	0
58	MG	2A	3283	1/1	0.93	0.16	50,50,50,50	0
58	MG	2A	3014	1/1	0.93	0.15	48,48,48,48	0
58	MG	1A	3895	1/1	0.93	0.11	26,26,26,26	0
58	MG	1A	3364	1/1	0.93	0.24	47,47,47,47	0
58	MG	1A	3585	1/1	0.93	0.20	59,59,59,59	0
58	MG	2A	3585	1/1	0.93	0.17	41,41,41,41	0
58	MG	1A	3898	1/1	0.93	0.17	41,41,41,41	0
58	MG	2A	3589	1/1	0.93	0.17	47,47,47,47	0
58	MG	1a	1650	1/1	0.93	0.19	46,46,46,46	0
58	MG	1A	3902	1/1	0.93	0.15	63,63,63,63	0
58	MG	1a	1653	1/1	0.93	0.11	51,51,51,51	0
58	MG	1a	1655	1/1	0.93	0.22	59,59,59,59	0
58	MG	1A	4091	1/1	0.93	0.24	57,57,57,57	0
58	MG	1a	1657	1/1	0.93	0.09	63,63,63,63	0
58	MG	2A	3599	1/1	0.93	0.16	57,57,57,57	0
58	MG	1A	3903	1/1	0.93	0.12	53,53,53,53	0
58	MG	1A	3365	1/1	0.93	0.14	49,49,49,49	0
58	MG	1A	3906	1/1	0.93	0.35	31,31,31,31	0
58	MG	1A	3741	1/1	0.93	0.07	53,53,53,53	0
58	MG	1A	3742	1/1	0.93	0.08	43,43,43,43	0
58	MG	2A	3607	1/1	0.93	0.07	58,58,58,58	0
58	MG	2A	3609	1/1	0.93	0.12	79,79,79,79	0
58	MG	1A	3910	1/1	0.93	0.10	55,55,55,55	0
58	MG	1A	3911	1/1	0.93	0.13	46,46,46,46	0
58	MG	2A	3314	1/1	0.93	0.27	58,58,58,58	0
58	MG	1A	3743	1/1	0.93	0.09	43,43,43,43	0
58	MG	1B	209	1/1	0.93	0.09	56,56,56,56	0
58	MG	2a	1782	1/1	0.93	0.14	67,67,67,67	0
58	MG	2A	3317	1/1	0.93	0.42	75,75,75,75	0
58	MG	2a	1784	1/1	0.93	0.14	73,73,73,73	0
58	MG	2A	3055	1/1	0.93	0.10	56,56,56,56	0
58	MG	1A	3425	1/1	0.93	0.12	59,59,59,59	0
58	MG	2A	3621	1/1	0.93	0.12	52,52,52,52	0
58	MG	1a	1668	1/1	0.93	0.15	62,62,62,62	0
58	MG	2A	3058	1/1	0.93	0.16	61,61,61,61	0
58	MG	2A	3059	1/1	0.93	0.10	46,46,46,46	0
58	MG	1A	3746	1/1	0.93	0.10	52,52,52,52	0
58	MG	1a	1670	1/1	0.93	0.17	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3640	1/1	0.93	0.13	46,46,46,46	0
58	MG	1A	3087	1/1	0.93	0.18	32,32,32,32	0
58	MG	1A	3429	1/1	0.93	0.29	55,55,55,55	0
58	MG	2A	3646	1/1	0.93	0.08	62,62,62,62	0
58	MG	2A	3334	1/1	0.93	0.23	72,72,72,72	0
58	MG	2A	3650	1/1	0.93	0.07	74,74,74,74	0
58	MG	2A	3651	1/1	0.93	0.10	51,51,51,51	0
58	MG	1A	3099	1/1	0.93	0.08	39,39,39,39	0
58	MG	1A	3181	1/1	0.93	0.19	35,35,35,35	0
58	MG	1a	1675	1/1	0.93	0.18	46,46,46,46	0
58	MG	1B	219	1/1	0.93	0.06	43,43,43,43	0
58	MG	2a	1809	1/1	0.93	0.28	64,64,64,64	0
58	MG	1B	220	1/1	0.93	0.09	37,37,37,37	0
58	MG	1A	3136	1/1	0.93	0.14	38,38,38,38	0
58	MG	2A	3080	1/1	0.93	0.10	34,34,34,34	0
58	MG	1A	3137	1/1	0.93	0.09	39,39,39,39	0
58	MG	1a	1683	1/1	0.93	0.23	68,68,68,68	0
58	MG	1A	3272	1/1	0.93	0.13	54,54,54,54	0
58	MG	1A	3273	1/1	0.93	0.15	37,37,37,37	0
58	MG	1B	227	1/1	0.93	0.15	59,59,59,59	0
58	MG	1A	3380	1/1	0.93	0.10	48,48,48,48	0
58	MG	1a	1690	1/1	0.93	0.33	50,50,50,50	0
58	MG	1A	3440	1/1	0.93	0.09	40,40,40,40	0
58	MG	2A	3093	1/1	0.93	0.17	56,56,56,56	0
58	MG	1A	3944	1/1	0.93	0.07	53,53,53,53	0
58	MG	2A	3097	1/1	0.93	0.12	66,66,66,66	0
58	MG	2A	3683	1/1	0.93	0.12	67,67,67,67	0
58	MG	1A	3772	1/1	0.93	0.11	26,26,26,26	0
58	MG	1D	306	1/1	0.93	0.15	43,43,43,43	0
58	MG	2A	3687	1/1	0.93	0.13	62,62,62,62	0
58	MG	1D	309	1/1	0.93	0.13	51,51,51,51	0
58	MG	2l	202	1/1	0.93	0.12	67,67,67,67	0
58	MG	1A	3070	1/1	0.93	0.10	57,57,57,57	0
58	MG	1A	3385	1/1	0.93	0.11	63,63,63,63	0
58	MG	1A	3785	1/1	0.93	0.10	33,33,33,33	0
58	MG	2q	201	1/1	0.93	0.10	75,75,75,75	0
58	MG	1A	3791	1/1	0.93	0.06	30,30,30,30	0
58	MG	1A	3958	1/1	0.93	0.09	37,37,37,37	0
58	MG	1a	1706	1/1	0.93	0.15	45,45,45,45	0
58	MG	1F	312	1/1	0.93	0.07	49,49,49,49	0
58	MG	1A	3959	1/1	0.93	0.10	55,55,55,55	0
58	MG	1A	3792	1/1	0.93	0.06	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2B	211	1/1	0.93	0.18	66,66,66,66	0
58	MG	1A	3794	1/1	0.93	0.07	45,45,45,45	0
58	MG	2B	213	1/1	0.93	0.21	59,59,59,59	0
58	MG	2B	214	1/1	0.93	0.12	60,60,60,60	0
58	MG	2x	3306	1/1	0.93	0.17	71,71,71,71	0
58	MG	1A	3040	1/1	0.94	0.19	31,31,31,31	0
58	MG	1A	4044	1/1	0.94	0.08	18,18,18,18	0
58	MG	1A	4045	1/1	0.94	0.15	50,50,50,50	0
58	MG	1A	3565	1/1	0.94	0.10	41,41,41,41	0
58	MG	23	102	1/1	0.94	0.08	63,63,63,63	0
58	MG	1a	1771	1/1	0.94	0.18	65,65,65,65	0
58	MG	2A	3445	1/1	0.94	0.19	43,43,43,43	0
58	MG	1A	3727	1/1	0.94	0.09	22,22,22,22	0
58	MG	1A	3174	1/1	0.94	0.16	43,43,43,43	0
58	MG	2A	3182	1/1	0.94	0.10	50,50,50,50	0
58	MG	1A	3073	1/1	0.94	0.23	32,32,32,32	0
58	MG	17	104	1/1	0.94	0.15	31,31,31,31	0
58	MG	18	101	1/1	0.94	0.25	52,52,52,52	0
58	MG	2A	3187	1/1	0.94	0.09	50,50,50,50	0
58	MG	18	102	1/1	0.94	0.25	38,38,38,38	0
58	MG	18	105	1/1	0.94	0.14	45,45,45,45	0
58	MG	1A	4051	1/1	0.94	0.15	53,53,53,53	0
58	MG	1A	3138	1/1	0.94	0.21	26,26,26,26	0
58	MG	1A	4057	1/1	0.94	0.06	25,25,25,25	0
58	MG	2a	1611	1/1	0.94	0.28	72,72,72,72	0
58	MG	1A	3885	1/1	0.94	0.07	28,28,28,28	0
58	MG	2A	3194	1/1	0.94	0.21	59,59,59,59	0
58	MG	1A	3886	1/1	0.94	0.09	35,35,35,35	0
58	MG	2A	3196	1/1	0.94	0.09	49,49,49,49	0
58	MG	1a	1795	1/1	0.94	0.07	77,77,77,77	0
58	MG	1A	3887	1/1	0.94	0.12	28,28,28,28	0
58	MG	1A	3474	1/1	0.94	0.22	55,55,55,55	0
58	MG	1A	4068	1/1	0.94	0.10	43,43,43,43	0
58	MG	1A	3475	1/1	0.94	0.07	49,49,49,49	0
58	MG	1a	1609	1/1	0.94	0.13	59,59,59,59	0
58	MG	1A	3094	1/1	0.94	0.09	46,46,46,46	0
58	MG	1A	3574	1/1	0.94	0.07	53,53,53,53	0
58	MG	2A	3206	1/1	0.94	0.18	58,58,58,58	0
58	MG	1A	3576	1/1	0.94	0.08	41,41,41,41	0
58	MG	1A	3241	1/1	0.94	0.12	40,40,40,40	0
58	MG	1A	3901	1/1	0.94	0.08	59,59,59,59	0
58	MG	2A	3210	1/1	0.94	0.09	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3478	1/1	0.94	0.17	62,62,62,62	0
58	MG	2A	3212	1/1	0.94	0.07	52,52,52,52	0
58	MG	1A	3187	1/1	0.94	0.07	45,45,45,45	0
58	MG	1A	3744	1/1	0.94	0.08	46,46,46,46	0
58	MG	1A	4080	1/1	0.94	0.19	46,46,46,46	0
58	MG	2A	3218	1/1	0.94	0.22	52,52,52,52	0
58	MG	1e	202	1/1	0.94	0.19	60,60,60,60	0
58	MG	1f	201	1/1	0.94	0.13	51,51,51,51	0
58	MG	1A	3582	1/1	0.94	0.18	53,53,53,53	0
58	MG	2A	3500	1/1	0.94	0.09	36,36,36,36	0
58	MG	1k	201	1/1	0.94	0.19	58,58,58,58	0
58	MG	2A	3223	1/1	0.94	0.11	61,61,61,61	0
58	MG	2A	3224	1/1	0.94	0.17	58,58,58,58	0
58	MG	1A	3140	1/1	0.94	0.10	48,48,48,48	0
58	MG	2A	3226	1/1	0.94	0.09	44,44,44,44	0
58	MG	1a	1625	1/1	0.94	0.20	56,56,56,56	0
58	MG	1A	3481	1/1	0.94	0.15	47,47,47,47	0
58	MG	2a	1650	1/1	0.94	0.07	83,83,83,83	0
58	MG	1A	3748	1/1	0.94	0.12	31,31,31,31	0
58	MG	1A	3749	1/1	0.94	0.07	40,40,40,40	0
58	MG	1A	3353	1/1	0.94	0.17	36,36,36,36	0
58	MG	1A	3141	1/1	0.94	0.18	37,37,37,37	0
58	MG	1a	1633	1/1	0.94	0.23	57,57,57,57	0
58	MG	1A	3916	1/1	0.94	0.09	26,26,26,26	0
58	MG	1A	3026	1/1	0.94	0.13	40,40,40,40	0
58	MG	1a	1637	1/1	0.94	0.21	51,51,51,51	0
58	MG	2a	1659	1/1	0.94	0.13	47,47,47,47	0
58	MG	1A	3918	1/1	0.94	0.14	51,51,51,51	0
58	MG	2a	1661	1/1	0.94	0.09	62,62,62,62	0
58	MG	1A	3755	1/1	0.94	0.10	45,45,45,45	0
58	MG	1A	3356	1/1	0.94	0.09	49,49,49,49	0
58	MG	1A	3590	1/1	0.94	0.12	42,42,42,42	0
58	MG	1A	3145	1/1	0.94	0.14	62,62,62,62	0
58	MG	2A	3532	1/1	0.94	0.18	57,57,57,57	0
58	MG	2A	3245	1/1	0.94	0.15	64,64,64,64	0
58	MG	1A	3308	1/1	0.94	0.29	45,45,45,45	0
58	MG	1A	3252	1/1	0.94	0.25	36,36,36,36	0
58	MG	2A	3537	1/1	0.94	0.12	55,55,55,55	0
58	MG	2a	1673	1/1	0.94	0.13	67,67,67,67	0
58	MG	1A	3765	1/1	0.94	0.10	50,50,50,50	0
58	MG	1A	3080	1/1	0.94	0.10	38,38,38,38	0
58	MG	1A	3313	1/1	0.94	0.14	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3497	1/1	0.94	0.10	49,49,49,49	0
58	MG	2A	3002	1/1	0.94	0.15	59,59,59,59	0
58	MG	2A	3003	1/1	0.94	0.23	53,53,53,53	0
58	MG	1A	3498	1/1	0.94	0.06	39,39,39,39	0
58	MG	1B	214	1/1	0.94	0.15	57,57,57,57	0
58	MG	1A	3428	1/1	0.94	0.08	47,47,47,47	0
58	MG	2A	3009	1/1	0.94	0.08	48,48,48,48	0
58	MG	2a	1685	1/1	0.94	0.24	74,74,74,74	0
58	MG	1A	3788	1/1	0.94	0.08	19,19,19,19	0
58	MG	1A	3314	1/1	0.94	0.16	47,47,47,47	0
58	MG	2a	1688	1/1	0.94	0.33	57,57,57,57	0
58	MG	1A	3613	1/1	0.94	0.10	24,24,24,24	0
58	MG	1A	3004	1/1	0.94	0.04	24,24,24,24	0
58	MG	1A	3957	1/1	0.94	0.12	54,54,54,54	0
58	MG	1A	3318	1/1	0.94	0.10	44,44,44,44	0
58	MG	1A	3257	1/1	0.94	0.07	56,56,56,56	0
58	MG	2A	3272	1/1	0.94	0.35	55,55,55,55	0
58	MG	1A	3150	1/1	0.94	0.11	42,42,42,42	0
58	MG	2A	3030	1/1	0.94	0.09	31,31,31,31	0
58	MG	1A	3624	1/1	0.94	0.13	15,15,15,15	0
58	MG	1A	3321	1/1	0.94	0.22	35,35,35,35	0
58	MG	1A	3963	1/1	0.94	0.08	62,62,62,62	0
58	MG	1B	232	1/1	0.94	0.09	53,53,53,53	0
58	MG	2A	3280	1/1	0.94	0.15	50,50,50,50	0
58	MG	2a	1705	1/1	0.94	0.09	81,81,81,81	0
58	MG	1A	3964	1/1	0.94	0.12	47,47,47,47	0
58	MG	2A	3038	1/1	0.94	0.13	45,45,45,45	0
58	MG	2A	3039	1/1	0.94	0.25	70,70,70,70	0
58	MG	1D	301	1/1	0.94	0.31	34,34,34,34	0
58	MG	1A	3377	1/1	0.94	0.34	46,46,46,46	0
58	MG	1A	3630	1/1	0.94	0.11	42,42,42,42	0
58	MG	2A	3044	1/1	0.94	0.13	53,53,53,53	0
58	MG	1D	310	1/1	0.94	0.07	40,40,40,40	0
58	MG	2A	3290	1/1	0.94	0.16	47,47,47,47	0
58	MG	2A	3580	1/1	0.94	0.12	59,59,59,59	0
58	MG	2A	3291	1/1	0.94	0.11	50,50,50,50	0
58	MG	1A	3631	1/1	0.94	0.11	49,49,49,49	0
58	MG	2A	3047	1/1	0.94	0.17	58,58,58,58	0
58	MG	1E	307	1/1	0.94	0.08	54,54,54,54	0
58	MG	1a	1676	1/1	0.94	0.20	65,65,65,65	0
58	MG	2A	3301	1/1	0.94	0.08	46,46,46,46	0
58	MG	1a	1677	1/1	0.94	0.19	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3438	1/1	0.94	0.12	42,42,42,42	0
58	MG	1A	3635	1/1	0.94	0.05	26,26,26,26	0
58	MG	1F	301	1/1	0.94	0.10	33,33,33,33	0
58	MG	1F	305	1/1	0.94	0.17	34,34,34,34	0
58	MG	2A	3598	1/1	0.94	0.14	73,73,73,73	0
58	MG	1A	3020	1/1	0.94	0.09	39,39,39,39	0
58	MG	2a	1730	1/1	0.94	0.30	68,68,68,68	0
58	MG	2a	1731	1/1	0.94	0.26	69,69,69,69	0
58	MG	1A	3642	1/1	0.94	0.06	26,26,26,26	0
58	MG	1a	1685	1/1	0.94	0.05	62,62,62,62	0
58	MG	1A	3084	1/1	0.94	0.27	38,38,38,38	0
58	MG	2A	3604	1/1	0.94	0.08	49,49,49,49	0
58	MG	1A	3030	1/1	0.94	0.07	41,41,41,41	0
58	MG	1A	3518	1/1	0.94	0.11	43,43,43,43	0
58	MG	1A	3208	1/1	0.94	0.14	55,55,55,55	0
58	MG	2A	3608	1/1	0.94	0.12	59,59,59,59	0
58	MG	1A	3444	1/1	0.94	0.14	65,65,65,65	0
58	MG	1A	3382	1/1	0.94	0.21	56,56,56,56	0
58	MG	2A	3077	1/1	0.94	0.07	51,51,51,51	0
58	MG	1A	3987	1/1	0.94	0.11	36,36,36,36	0
58	MG	1A	3989	1/1	0.94	0.09	55,55,55,55	0
58	MG	1A	3524	1/1	0.94	0.23	40,40,40,40	0
58	MG	1A	3826	1/1	0.94	0.06	29,29,29,29	0
58	MG	2A	3617	1/1	0.94	0.06	48,48,48,48	0
58	MG	2a	1755	1/1	0.94	0.15	66,66,66,66	0
58	MG	2A	3082	1/1	0.94	0.14	64,64,64,64	0
58	MG	2a	1757	1/1	0.94	0.18	67,67,67,67	0
58	MG	1A	3158	1/1	0.94	0.23	45,45,45,45	0
58	MG	2A	3084	1/1	0.94	0.17	55,55,55,55	0
58	MG	1A	3213	1/1	0.94	0.15	45,45,45,45	0
58	MG	1A	3160	1/1	0.94	0.13	55,55,55,55	0
58	MG	1Q	202	1/1	0.94	0.19	38,38,38,38	0
58	MG	1Q	206	1/1	0.94	0.07	45,45,45,45	0
58	MG	2A	3635	1/1	0.94	0.10	52,52,52,52	0
58	MG	2A	3637	1/1	0.94	0.09	57,57,57,57	0
58	MG	1Q	207	1/1	0.94	0.09	36,36,36,36	0
58	MG	1A	3105	1/1	0.94	0.17	38,38,38,38	0
58	MG	2A	3642	1/1	0.94	0.11	43,43,43,43	0
58	MG	2a	1773	1/1	0.94	0.12	60,60,60,60	0
58	MG	2a	1774	1/1	0.94	0.10	60,60,60,60	0
58	MG	1A	3668	1/1	0.94	0.07	28,28,28,28	0
58	MG	1a	1710	1/1	0.94	0.16	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1a	1711	1/1	0.94	0.37	66,66,66,66	0
58	MG	1A	3532	1/1	0.94	0.21	45,45,45,45	0
58	MG	2A	3100	1/1	0.94	0.09	69,69,69,69	0
58	MG	2A	3349	1/1	0.94	0.10	41,41,41,41	0
58	MG	2A	3101	1/1	0.94	0.19	49,49,49,49	0
58	MG	1a	1713	1/1	0.94	0.06	47,47,47,47	0
58	MG	2A	3354	1/1	0.94	0.17	62,62,62,62	0
58	MG	2A	3103	1/1	0.94	0.11	61,61,61,61	0
58	MG	2a	1786	1/1	0.94	0.24	60,60,60,60	0
58	MG	1A	3165	1/1	0.94	0.19	49,49,49,49	0
58	MG	1A	4005	1/1	0.94	0.08	19,19,19,19	0
58	MG	2A	3662	1/1	0.94	0.12	57,57,57,57	0
58	MG	1A	3064	1/1	0.94	0.10	42,42,42,42	0
58	MG	2a	1791	1/1	0.94	0.15	60,60,60,60	0
58	MG	1A	3536	1/1	0.94	0.19	58,58,58,58	0
58	MG	1A	3457	1/1	0.94	0.20	47,47,47,47	0
58	MG	2a	1794	1/1	0.94	0.10	58,58,58,58	0
58	MG	1A	3391	1/1	0.94	0.19	43,43,43,43	0
58	MG	2A	3117	1/1	0.94	0.23	47,47,47,47	0
58	MG	1A	3541	1/1	0.94	0.26	54,54,54,54	0
58	MG	1A	3542	1/1	0.94	0.28	36,36,36,36	0
58	MG	1A	3223	1/1	0.94	0.13	51,51,51,51	0
58	MG	1a	1728	1/1	0.94	0.07	58,58,58,58	0
58	MG	2A	3677	1/1	0.94	0.13	69,69,69,69	0
58	MG	2A	3372	1/1	0.94	0.12	40,40,40,40	0
58	MG	1A	3224	1/1	0.94	0.09	53,53,53,53	0
58	MG	2A	3681	1/1	0.94	0.13	53,53,53,53	0
58	MG	1V	201	1/1	0.94	0.41	29,29,29,29	0
58	MG	1A	3549	1/1	0.94	0.16	35,35,35,35	0
58	MG	2A	3684	1/1	0.94	0.18	50,50,50,50	0
58	MG	1A	3397	1/1	0.94	0.09	53,53,53,53	0
58	MG	1a	1736	1/1	0.94	0.09	46,46,46,46	0
58	MG	2A	3133	1/1	0.94	0.19	38,38,38,38	0
58	MG	1A	3398	1/1	0.94	0.06	48,48,48,48	0
58	MG	1a	1738	1/1	0.94	0.15	54,54,54,54	0
58	MG	1A	4024	1/1	0.94	0.10	48,48,48,48	0
58	MG	1A	3703	1/1	0.94	0.14	35,35,35,35	0
58	MG	1W	207	1/1	0.94	0.12	55,55,55,55	0
58	MG	1a	1744	1/1	0.94	0.10	54,54,54,54	0
58	MG	2A	3142	1/1	0.94	0.16	55,55,55,55	0
58	MG	2A	3145	1/1	0.94	0.17	61,61,61,61	0
58	MG	1a	1745	1/1	0.94	0.17	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3108	1/1	0.94	0.13	33,33,33,33	0
58	MG	1X	102	1/1	0.94	0.11	35,35,35,35	0
58	MG	2e	201	1/1	0.94	0.06	74,74,74,74	0
58	MG	1A	3337	1/1	0.94	0.08	49,49,49,49	0
58	MG	1A	3709	1/1	0.94	0.08	44,44,44,44	0
58	MG	1A	3711	1/1	0.94	0.13	40,40,40,40	0
58	MG	1a	1752	1/1	0.94	0.28	66,66,66,66	0
58	MG	1A	3001	1/1	0.94	0.08	37,37,37,37	0
58	MG	1A	3229	1/1	0.94	0.09	52,52,52,52	0
58	MG	1A	3868	1/1	0.94	0.20	54,54,54,54	0
58	MG	1A	3560	1/1	0.94	0.08	53,53,53,53	0
58	MG	1A	3562	1/1	0.94	0.10	45,45,45,45	0
58	MG	2A	3411	1/1	0.94	0.13	24,24,24,24	0
58	MG	2A	3412	1/1	0.94	0.27	56,56,56,56	0
58	MG	2A	3163	1/1	0.94	0.20	42,42,42,42	0
58	MG	2A	3164	1/1	0.94	0.09	50,50,50,50	0
58	MG	1A	3872	1/1	0.94	0.18	37,37,37,37	0
58	MG	2A	3170	1/1	0.94	0.13	55,55,55,55	0
58	MG	1A	3717	1/1	0.94	0.12	51,51,51,51	0
58	MG	2Q	202	1/1	0.94	0.11	49,49,49,49	0
58	MG	2R	201	1/1	0.94	0.17	32,32,32,32	0
58	MG	1A	3563	1/1	0.94	0.21	43,43,43,43	0
58	MG	2A	3431	1/1	0.94	0.16	56,56,56,56	0
58	MG	2A	3173	1/1	0.94	0.10	60,60,60,60	0
59	K	2x	3301	1/1	0.94	0.08	59,59,59,59	0
61	ZN	14	102	1/1	0.94	0.11	121,121,121,121	0
61	ZN	24	501	1/1	0.94	0.12	136,136,136,136	0
58	MG	1a	1608	1/1	0.95	0.09	49,49,49,49	0
58	MG	1A	3932	1/1	0.95	0.06	53,53,53,53	0
58	MG	2F	304	1/1	0.95	0.11	55,55,55,55	0
58	MG	2A	3420	1/1	0.95	0.07	45,45,45,45	0
58	MG	2A	3421	1/1	0.95	0.10	36,36,36,36	0
58	MG	2A	3422	1/1	0.95	0.12	63,63,63,63	0
58	MG	2Q	201	1/1	0.95	0.10	64,64,64,64	0
58	MG	1a	1798	1/1	0.95	0.09	59,59,59,59	0
58	MG	2A	3425	1/1	0.95	0.11	46,46,46,46	0
58	MG	2T	201	1/1	0.95	0.11	60,60,60,60	0
58	MG	2T	202	1/1	0.95	0.13	60,60,60,60	0
58	MG	1A	3936	1/1	0.95	0.06	39,39,39,39	0
58	MG	1A	3161	1/1	0.95	0.09	32,32,32,32	0
58	MG	2A	3430	1/1	0.95	0.09	34,34,34,34	0
58	MG	1A	3939	1/1	0.95	0.12	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3162	1/1	0.95	0.23	38,38,38,38	0
58	MG	1a	1807	1/1	0.95	0.23	64,64,64,64	0
58	MG	1A	3100	1/1	0.95	0.12	25,25,25,25	0
58	MG	1A	3043	1/1	0.95	0.21	34,34,34,34	0
58	MG	25	101	1/1	0.95	0.38	49,49,49,49	0
58	MG	2A	3437	1/1	0.95	0.13	38,38,38,38	0
58	MG	1a	1618	1/1	0.95	0.06	52,52,52,52	0
58	MG	27	101	1/1	0.95	0.16	49,49,49,49	0
58	MG	2A	3443	1/1	0.95	0.13	47,47,47,47	0
58	MG	1A	3495	1/1	0.95	0.06	51,51,51,51	0
58	MG	1A	3496	1/1	0.95	0.19	47,47,47,47	0
58	MG	1A	3678	1/1	0.95	0.10	24,24,24,24	0
58	MG	1A	4096	1/1	0.95	0.14	46,46,46,46	0
58	MG	1d	302	1/1	0.95	0.18	50,50,50,50	0
58	MG	1A	3680	1/1	0.95	0.10	23,23,23,23	0
58	MG	2A	3451	1/1	0.95	0.25	58,58,58,58	0
58	MG	1A	3124	1/1	0.95	0.17	43,43,43,43	0
58	MG	1B	203	1/1	0.95	0.13	49,49,49,49	0
58	MG	1A	3202	1/1	0.95	0.14	26,26,26,26	0
58	MG	1a	1628	1/1	0.95	0.20	56,56,56,56	0
58	MG	2A	3197	1/1	0.95	0.24	58,58,58,58	0
58	MG	1B	205	1/1	0.95	0.06	51,51,51,51	0
58	MG	1B	206	1/1	0.95	0.17	46,46,46,46	0
58	MG	1A	3500	1/1	0.95	0.07	48,48,48,48	0
58	MG	1A	3687	1/1	0.95	0.05	32,32,32,32	0
58	MG	1A	3143	1/1	0.95	0.17	16,16,16,16	0
58	MG	1a	1635	1/1	0.95	0.07	43,43,43,43	0
58	MG	1A	3690	1/1	0.95	0.06	33,33,33,33	0
58	MG	1A	3575	1/1	0.95	0.07	52,52,52,52	0
58	MG	1A	3694	1/1	0.95	0.06	33,33,33,33	0
58	MG	1A	3206	1/1	0.95	0.13	27,27,27,27	0
58	MG	1A	3344	1/1	0.95	0.30	46,46,46,46	0
58	MG	1A	3447	1/1	0.95	0.07	53,53,53,53	0
58	MG	1A	3345	1/1	0.95	0.20	40,40,40,40	0
58	MG	2A	3478	1/1	0.95	0.13	60,60,60,60	0
58	MG	1A	3702	1/1	0.95	0.06	29,29,29,29	0
58	MG	2A	3480	1/1	0.95	0.12	50,50,50,50	0
58	MG	1B	221	1/1	0.95	0.07	39,39,39,39	0
58	MG	2a	1630	1/1	0.95	0.20	49,49,49,49	0
58	MG	2a	1631	1/1	0.95	0.30	54,54,54,54	0
58	MG	2a	1632	1/1	0.95	0.31	55,55,55,55	0
58	MG	2A	3213	1/1	0.95	0.08	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1x	103	1/1	0.95	0.23	63,63,63,63	0
58	MG	1a	1646	1/1	0.95	0.13	49,49,49,49	0
58	MG	1A	3581	1/1	0.95	0.20	28,28,28,28	0
58	MG	1A	3015	1/1	0.95	0.09	40,40,40,40	0
58	MG	1B	224	1/1	0.95	0.09	47,47,47,47	0
58	MG	1x	108	1/1	0.95	0.10	27,27,27,27	0
58	MG	1A	3209	1/1	0.95	0.14	43,43,43,43	0
58	MG	1A	3210	1/1	0.95	0.08	56,56,56,56	0
58	MG	1a	1654	1/1	0.95	0.17	47,47,47,47	0
58	MG	2A	3001	1/1	0.95	0.17	51,51,51,51	0
58	MG	1A	3841	1/1	0.95	0.24	66,66,66,66	0
58	MG	1A	3254	1/1	0.95	0.07	48,48,48,48	0
58	MG	2A	3498	1/1	0.95	0.07	39,39,39,39	0
58	MG	2A	3004	1/1	0.95	0.29	57,57,57,57	0
58	MG	1A	3068	1/1	0.95	0.10	38,38,38,38	0
58	MG	1A	3981	1/1	0.95	0.05	54,54,54,54	0
58	MG	1A	3171	1/1	0.95	0.18	58,58,58,58	0
58	MG	1A	3516	1/1	0.95	0.09	74,74,74,74	0
58	MG	2A	3011	1/1	0.95	0.07	44,44,44,44	0
58	MG	2A	3233	1/1	0.95	0.16	40,40,40,40	0
58	MG	2A	3510	1/1	0.95	0.09	37,37,37,37	0
58	MG	2A	3511	1/1	0.95	0.10	61,61,61,61	0
58	MG	1A	3986	1/1	0.95	0.10	34,34,34,34	0
58	MG	1D	304	1/1	0.95	0.17	33,33,33,33	0
58	MG	1A	3173	1/1	0.95	0.07	45,45,45,45	0
58	MG	1A	3988	1/1	0.95	0.08	47,47,47,47	0
58	MG	2A	3020	1/1	0.95	0.22	44,44,44,44	0
58	MG	2A	3519	1/1	0.95	0.26	62,62,62,62	0
58	MG	1A	3848	1/1	0.95	0.12	51,51,51,51	0
58	MG	1A	3407	1/1	0.95	0.17	49,49,49,49	0
58	MG	2A	3024	1/1	0.95	0.08	51,51,51,51	0
58	MG	1A	3991	1/1	0.95	0.16	38,38,38,38	0
58	MG	1A	3850	1/1	0.95	0.10	50,50,50,50	0
58	MG	1A	3312	1/1	0.95	0.13	41,41,41,41	0
58	MG	1E	313	1/1	0.95	0.15	44,44,44,44	0
58	MG	1A	3409	1/1	0.95	0.08	48,48,48,48	0
58	MG	2A	3251	1/1	0.95	0.19	68,68,68,68	0
58	MG	2A	3529	1/1	0.95	0.07	37,37,37,37	0
58	MG	2A	3530	1/1	0.95	0.09	54,54,54,54	0
58	MG	1F	304	1/1	0.95	0.05	42,42,42,42	0
58	MG	1A	3853	1/1	0.95	0.09	52,52,52,52	0
58	MG	2A	3035	1/1	0.95	0.16	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3216	1/1	0.95	0.06	47,47,47,47	0
58	MG	1F	309	1/1	0.95	0.09	47,47,47,47	0
58	MG	2A	3536	1/1	0.95	0.10	49,49,49,49	0
58	MG	1A	3855	1/1	0.95	0.07	17,17,17,17	0
58	MG	1F	311	1/1	0.95	0.13	28,28,28,28	0
58	MG	2a	1683	1/1	0.95	0.17	60,60,60,60	0
58	MG	1A	4002	1/1	0.95	0.06	32,32,32,32	0
58	MG	2A	3262	1/1	0.95	0.09	40,40,40,40	0
58	MG	2A	3042	1/1	0.95	0.16	69,69,69,69	0
58	MG	1a	1679	1/1	0.95	0.18	69,69,69,69	0
58	MG	1G	201	1/1	0.95	0.12	42,42,42,42	0
58	MG	1A	3722	1/1	0.95	0.09	44,44,44,44	0
58	MG	1A	3598	1/1	0.95	0.12	39,39,39,39	0
58	MG	1A	3019	1/1	0.95	0.17	42,42,42,42	0
58	MG	1A	3525	1/1	0.95	0.16	40,40,40,40	0
58	MG	2A	3049	1/1	0.95	0.06	44,44,44,44	0
58	MG	1A	3466	1/1	0.95	0.11	60,60,60,60	0
58	MG	2A	3051	1/1	0.95	0.18	55,55,55,55	0
58	MG	2A	3274	1/1	0.95	0.19	55,55,55,55	0
58	MG	2A	3052	1/1	0.95	0.16	50,50,50,50	0
58	MG	1A	3606	1/1	0.95	0.13	28,28,28,28	0
58	MG	1A	4010	1/1	0.95	0.12	40,40,40,40	0
58	MG	2a	1702	1/1	0.95	0.16	55,55,55,55	0
58	MG	1A	3607	1/1	0.95	0.17	48,48,48,48	0
58	MG	1A	3358	1/1	0.95	0.16	49,49,49,49	0
58	MG	1A	4013	1/1	0.95	0.08	46,46,46,46	0
58	MG	2A	3561	1/1	0.95	0.13	61,61,61,61	0
58	MG	1P	201	1/1	0.95	0.21	31,31,31,31	0
58	MG	1A	3262	1/1	0.95	0.18	60,60,60,60	0
58	MG	1P	203	1/1	0.95	0.15	35,35,35,35	0
58	MG	1P	204	1/1	0.95	0.24	35,35,35,35	0
58	MG	1A	3612	1/1	0.95	0.08	48,48,48,48	0
58	MG	2a	1712	1/1	0.95	0.16	58,58,58,58	0
58	MG	2A	3286	1/1	0.95	0.17	48,48,48,48	0
58	MG	2A	3066	1/1	0.95	0.10	46,46,46,46	0
58	MG	1A	3219	1/1	0.95	0.29	43,43,43,43	0
58	MG	1Q	205	1/1	0.95	0.10	53,53,53,53	0
58	MG	2A	3072	1/1	0.95	0.07	43,43,43,43	0
58	MG	2A	3575	1/1	0.95	0.11	56,56,56,56	0
58	MG	1a	1702	1/1	0.95	0.07	51,51,51,51	0
58	MG	1A	3873	1/1	0.95	0.10	36,36,36,36	0
58	MG	2A	3076	1/1	0.95	0.12	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3615	1/1	0.95	0.10	24,24,24,24	0
58	MG	2A	3297	1/1	0.95	0.13	51,51,51,51	0
58	MG	1A	4019	1/1	0.95	0.16	45,45,45,45	0
58	MG	1A	4020	1/1	0.95	0.08	41,41,41,41	0
58	MG	2A	3583	1/1	0.95	0.19	51,51,51,51	0
58	MG	1A	3531	1/1	0.95	0.12	34,34,34,34	0
58	MG	1A	4023	1/1	0.95	0.16	24,24,24,24	0
58	MG	2A	3588	1/1	0.95	0.18	60,60,60,60	0
58	MG	1A	3017	1/1	0.95	0.12	65,65,65,65	0
58	MG	1A	3182	1/1	0.95	0.24	54,54,54,54	0
58	MG	1A	3222	1/1	0.95	0.09	47,47,47,47	0
58	MG	1A	3620	1/1	0.95	0.14	47,47,47,47	0
58	MG	2A	3087	1/1	0.95	0.15	49,49,49,49	0
58	MG	2A	3594	1/1	0.95	0.07	66,66,66,66	0
58	MG	2a	1736	1/1	0.95	0.24	54,54,54,54	0
58	MG	2A	3310	1/1	0.95	0.20	54,54,54,54	0
58	MG	2a	1738	1/1	0.95	0.16	60,60,60,60	0
58	MG	1A	3882	1/1	0.95	0.09	58,58,58,58	0
58	MG	1A	3267	1/1	0.95	0.17	44,44,44,44	0
58	MG	1A	3268	1/1	0.95	0.15	45,45,45,45	0
58	MG	1A	3091	1/1	0.95	0.12	38,38,38,38	0
58	MG	1U	209	1/1	0.95	0.42	42,42,42,42	0
58	MG	1U	211	1/1	0.95	0.27	40,40,40,40	0
58	MG	2A	3094	1/1	0.95	0.11	43,43,43,43	0
58	MG	1A	3752	1/1	0.95	0.06	47,47,47,47	0
58	MG	1A	3060	1/1	0.95	0.11	41,41,41,41	0
58	MG	2A	3098	1/1	0.95	0.14	58,58,58,58	0
58	MG	1A	3078	1/1	0.95	0.23	45,45,45,45	0
58	MG	1V	206	1/1	0.95	0.14	63,63,63,63	0
58	MG	2A	3329	1/1	0.95	0.25	57,57,57,57	0
58	MG	1A	3891	1/1	0.95	0.11	25,25,25,25	0
58	MG	1A	3893	1/1	0.95	0.09	23,23,23,23	0
58	MG	1A	4041	1/1	0.95	0.09	25,25,25,25	0
58	MG	2A	3104	1/1	0.95	0.07	44,44,44,44	0
58	MG	1A	3226	1/1	0.95	0.12	40,40,40,40	0
58	MG	2A	3616	1/1	0.95	0.09	49,49,49,49	0
58	MG	1A	3544	1/1	0.95	0.28	50,50,50,50	0
58	MG	2A	3618	1/1	0.95	0.12	54,54,54,54	0
58	MG	1A	3636	1/1	0.95	0.11	29,29,29,29	0
58	MG	2A	3110	1/1	0.95	0.17	36,36,36,36	0
58	MG	1A	3759	1/1	0.95	0.15	30,30,30,30	0
58	MG	1X	105	1/1	0.95	0.09	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1772	1/1	0.95	0.22	64,64,64,64	0
58	MG	2A	3625	1/1	0.95	0.06	39,39,39,39	0
58	MG	1A	3061	1/1	0.95	0.15	51,51,51,51	0
58	MG	2A	3344	1/1	0.95	0.27	61,61,61,61	0
58	MG	2A	3629	1/1	0.95	0.13	50,50,50,50	0
58	MG	2A	3631	1/1	0.95	0.11	49,49,49,49	0
58	MG	1A	3062	1/1	0.95	0.06	42,42,42,42	0
58	MG	2A	3346	1/1	0.95	0.08	45,45,45,45	0
58	MG	2A	3636	1/1	0.95	0.05	50,50,50,50	0
58	MG	2A	3118	1/1	0.95	0.06	36,36,36,36	0
58	MG	1A	3762	1/1	0.95	0.12	47,47,47,47	0
58	MG	1A	3279	1/1	0.95	0.28	37,37,37,37	0
58	MG	2A	3641	1/1	0.95	0.12	61,61,61,61	0
58	MG	1A	3332	1/1	0.95	0.15	51,51,51,51	0
58	MG	10	103	1/1	0.95	0.07	40,40,40,40	0
58	MG	2A	3123	1/1	0.95	0.13	52,52,52,52	0
58	MG	2A	3124	1/1	0.95	0.06	57,57,57,57	0
58	MG	2A	3125	1/1	0.95	0.11	45,45,45,45	0
58	MG	1a	1748	1/1	0.95	0.20	48,48,48,48	0
58	MG	1A	3484	1/1	0.95	0.08	47,47,47,47	0
58	MG	1A	4054	1/1	0.95	0.13	14,14,14,14	0
58	MG	2A	3653	1/1	0.95	0.08	37,37,37,37	0
58	MG	2A	3130	1/1	0.95	0.08	46,46,46,46	0
58	MG	1A	4056	1/1	0.95	0.13	51,51,51,51	0
58	MG	2a	1797	1/1	0.95	0.24	56,56,56,56	0
58	MG	1A	3768	1/1	0.95	0.10	40,40,40,40	0
58	MG	2A	3365	1/1	0.95	0.14	63,63,63,63	0
58	MG	1A	3646	1/1	0.95	0.07	21,21,21,21	0
58	MG	1A	3647	1/1	0.95	0.08	19,19,19,19	0
58	MG	2A	3368	1/1	0.95	0.17	51,51,51,51	0
58	MG	1A	3774	1/1	0.95	0.09	31,31,31,31	0
58	MG	1A	3485	1/1	0.95	0.26	68,68,68,68	0
58	MG	2A	3667	1/1	0.95	0.09	67,67,67,67	0
58	MG	12	101	1/1	0.95	0.14	48,48,48,48	0
58	MG	1A	4065	1/1	0.95	0.12	37,37,37,37	0
58	MG	2A	3374	1/1	0.95	0.27	65,65,65,65	0
58	MG	2A	3672	1/1	0.95	0.07	54,54,54,54	0
58	MG	2A	3375	1/1	0.95	0.17	46,46,46,46	0
58	MG	1A	4066	1/1	0.95	0.10	53,53,53,53	0
58	MG	2A	3141	1/1	0.95	0.09	54,54,54,54	0
58	MG	1a	1763	1/1	0.95	0.09	53,53,53,53	0
58	MG	2A	3380	1/1	0.95	0.07	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3143	1/1	0.95	0.10	54,54,54,54	0
58	MG	1A	3778	1/1	0.95	0.12	34,34,34,34	0
58	MG	15	101	1/1	0.95	0.20	42,42,42,42	0
58	MG	1a	1766	1/1	0.95	0.06	52,52,52,52	0
58	MG	1A	3782	1/1	0.95	0.09	39,39,39,39	0
58	MG	1A	3159	1/1	0.95	0.10	39,39,39,39	0
58	MG	2a	1822	1/1	0.95	0.09	56,56,56,56	0
58	MG	2A	3388	1/1	0.95	0.13	56,56,56,56	0
58	MG	1A	3487	1/1	0.95	0.31	42,42,42,42	0
58	MG	1A	3652	1/1	0.95	0.09	37,37,37,37	0
58	MG	2A	3393	1/1	0.95	0.28	51,51,51,51	0
58	MG	2A	3394	1/1	0.95	0.07	44,44,44,44	0
58	MG	1A	3654	1/1	0.95	0.07	37,37,37,37	0
58	MG	2A	3156	1/1	0.95	0.10	49,49,49,49	0
58	MG	18	104	1/1	0.95	0.10	61,61,61,61	0
58	MG	1A	3923	1/1	0.95	0.08	44,44,44,44	0
58	MG	18	106	1/1	0.95	0.11	49,49,49,49	0
58	MG	1A	3558	1/1	0.95	0.15	33,33,33,33	0
58	MG	1A	3434	1/1	0.95	0.31	36,36,36,36	0
58	MG	2A	3162	1/1	0.95	0.23	59,59,59,59	0
58	MG	1A	3561	1/1	0.95	0.33	35,35,35,35	0
58	MG	1A	3927	1/1	0.95	0.09	34,34,34,34	0
58	MG	2A	3405	1/1	0.95	0.12	47,47,47,47	0
58	MG	2A	3166	1/1	0.95	0.12	43,43,43,43	0
58	MG	2D	302	1/1	0.95	0.17	43,43,43,43	0
58	MG	2D	304	1/1	0.95	0.22	41,41,41,41	0
58	MG	2A	3167	1/1	0.95	0.31	64,64,64,64	0
58	MG	1A	3661	1/1	0.95	0.07	36,36,36,36	0
58	MG	1A	4082	1/1	0.95	0.13	58,58,58,58	0
58	MG	1A	4083	1/1	0.95	0.12	61,61,61,61	0
58	MG	1A	3022	1/1	0.95	0.06	37,37,37,37	0
59	K	1A	3554	1/1	0.95	0.08	55,55,55,55	0
58	MG	2A	3415	1/1	0.95	0.14	51,51,51,51	0
58	MG	2E	306	1/1	0.95	0.13	52,52,52,52	0
58	MG	1A	4085	1/1	0.95	0.21	54,54,54,54	0
61	ZN	2n	501	1/1	0.95	0.07	103,103,103,103	0
58	MG	1V	207	1/1	0.96	0.09	66,66,66,66	0
58	MG	1A	3781	1/1	0.96	0.11	63,63,63,63	0
58	MG	1A	3660	1/1	0.96	0.07	34,34,34,34	0
58	MG	1a	1717	1/1	0.96	0.14	44,44,44,44	0
58	MG	2A	3069	1/1	0.96	0.07	49,49,49,49	0
58	MG	2A	3512	1/1	0.96	0.07	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3568	1/1	0.96	0.14	45,45,45,45	0
58	MG	2A	3071	1/1	0.96	0.10	48,48,48,48	0
58	MG	1A	3787	1/1	0.96	0.14	55,55,55,55	0
58	MG	1A	3919	1/1	0.96	0.19	61,61,61,61	0
58	MG	1A	3276	1/1	0.96	0.07	45,45,45,45	0
58	MG	1A	3790	1/1	0.96	0.09	46,46,46,46	0
58	MG	1A	3922	1/1	0.96	0.09	42,42,42,42	0
58	MG	1A	3664	1/1	0.96	0.09	35,35,35,35	0
58	MG	1a	1726	1/1	0.96	0.14	57,57,57,57	0
58	MG	1Y	202	1/1	0.96	0.16	46,46,46,46	0
58	MG	2a	1627	1/1	0.96	0.06	71,71,71,71	0
58	MG	1A	3277	1/1	0.96	0.09	37,37,37,37	0
58	MG	1a	1730	1/1	0.96	0.07	40,40,40,40	0
58	MG	1a	1731	1/1	0.96	0.10	30,30,30,30	0
58	MG	1A	3793	1/1	0.96	0.10	43,43,43,43	0
58	MG	1A	3278	1/1	0.96	0.21	23,23,23,23	0
58	MG	1Z	302	1/1	0.96	0.13	54,54,54,54	0
58	MG	1A	3032	1/1	0.96	0.29	28,28,28,28	0
58	MG	1A	3443	1/1	0.96	0.10	39,39,39,39	0
58	MG	1A	3238	1/1	0.96	0.34	35,35,35,35	0
58	MG	1A	3799	1/1	0.96	0.15	53,53,53,53	0
58	MG	1A	3800	1/1	0.96	0.10	25,25,25,25	0
58	MG	1A	3673	1/1	0.96	0.05	23,23,23,23	0
58	MG	1A	3675	1/1	0.96	0.12	27,27,27,27	0
58	MG	2A	3095	1/1	0.96	0.13	50,50,50,50	0
58	MG	2A	3298	1/1	0.96	0.27	44,44,44,44	0
58	MG	10	109	1/1	0.96	0.04	49,49,49,49	0
58	MG	2A	3300	1/1	0.96	0.12	46,46,46,46	0
58	MG	1A	3239	1/1	0.96	0.17	30,30,30,30	0
58	MG	1A	3577	1/1	0.96	0.12	46,46,46,46	0
58	MG	2A	3303	1/1	0.96	0.17	55,55,55,55	0
58	MG	1A	3098	1/1	0.96	0.19	37,37,37,37	0
58	MG	11	104	1/1	0.96	0.07	47,47,47,47	0
58	MG	1A	3392	1/1	0.96	0.12	36,36,36,36	0
58	MG	13	101	1/1	0.96	0.08	38,38,38,38	0
58	MG	1A	3946	1/1	0.96	0.10	57,57,57,57	0
58	MG	1a	1755	1/1	0.96	0.08	44,44,44,44	0
58	MG	1A	3509	1/1	0.96	0.09	47,47,47,47	0
58	MG	1A	3684	1/1	0.96	0.06	29,29,29,29	0
58	MG	1A	3950	1/1	0.96	0.11	61,61,61,61	0
58	MG	2A	3109	1/1	0.96	0.14	62,62,62,62	0
58	MG	2A	3555	1/1	0.96	0.10	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3448	1/1	0.96	0.07	45,45,45,45	0
58	MG	2A	3111	1/1	0.96	0.12	54,54,54,54	0
58	MG	2A	3558	1/1	0.96	0.17	59,59,59,59	0
58	MG	1A	3953	1/1	0.96	0.12	58,58,58,58	0
58	MG	2a	1663	1/1	0.96	0.17	58,58,58,58	0
58	MG	1A	3511	1/1	0.96	0.09	48,48,48,48	0
58	MG	17	105	1/1	0.96	0.06	44,44,44,44	0
58	MG	1A	3955	1/1	0.96	0.07	50,50,50,50	0
58	MG	2a	1667	1/1	0.96	0.13	54,54,54,54	0
58	MG	1A	3688	1/1	0.96	0.12	25,25,25,25	0
58	MG	2A	3565	1/1	0.96	0.10	33,33,33,33	0
58	MG	18	103	1/1	0.96	0.19	46,46,46,46	0
58	MG	2A	3326	1/1	0.96	0.20	49,49,49,49	0
58	MG	2A	3327	1/1	0.96	0.30	63,63,63,63	0
58	MG	1A	3451	1/1	0.96	0.19	48,48,48,48	0
58	MG	1A	3244	1/1	0.96	0.15	41,41,41,41	0
58	MG	1a	1768	1/1	0.96	0.12	57,57,57,57	0
58	MG	1A	4097	1/1	0.96	0.16	45,45,45,45	0
58	MG	1A	3288	1/1	0.96	0.17	52,52,52,52	0
58	MG	1A	3692	1/1	0.96	0.06	35,35,35,35	0
58	MG	1A	3396	1/1	0.96	0.05	47,47,47,47	0
58	MG	2A	3336	1/1	0.96	0.08	44,44,44,44	0
58	MG	2A	3337	1/1	0.96	0.22	58,58,58,58	0
58	MG	1A	3289	1/1	0.96	0.09	50,50,50,50	0
58	MG	1A	3290	1/1	0.96	0.11	47,47,47,47	0
58	MG	1a	1776	1/1	0.96	0.08	71,71,71,71	0
58	MG	1A	3697	1/1	0.96	0.06	28,28,28,28	0
58	MG	1A	3698	1/1	0.96	0.09	62,62,62,62	0
58	MG	1A	3968	1/1	0.96	0.09	54,54,54,54	0
58	MG	1A	3399	1/1	0.96	0.10	54,54,54,54	0
58	MG	1A	3342	1/1	0.96	0.05	55,55,55,55	0
58	MG	1a	1782	1/1	0.96	0.15	55,55,55,55	0
58	MG	1a	1783	1/1	0.96	0.08	56,56,56,56	0
58	MG	1A	3833	1/1	0.96	0.16	43,43,43,43	0
58	MG	1a	1610	1/1	0.96	0.12	27,27,27,27	0
58	MG	1A	3050	1/1	0.96	0.06	25,25,25,25	0
58	MG	1a	1789	1/1	0.96	0.10	55,55,55,55	0
58	MG	1a	1612	1/1	0.96	0.08	70,70,70,70	0
58	MG	2A	3144	1/1	0.96	0.10	43,43,43,43	0
58	MG	1a	1791	1/1	0.96	0.14	48,48,48,48	0
58	MG	2A	3357	1/1	0.96	0.12	53,53,53,53	0
58	MG	1A	3835	1/1	0.96	0.09	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3359	1/1	0.96	0.12	34,34,34,34	0
58	MG	1A	3204	1/1	0.96	0.14	37,37,37,37	0
58	MG	2A	3149	1/1	0.96	0.17	59,59,59,59	0
58	MG	1A	3142	1/1	0.96	0.14	38,38,38,38	0
58	MG	1B	218	1/1	0.96	0.09	46,46,46,46	0
58	MG	1a	1799	1/1	0.96	0.11	61,61,61,61	0
58	MG	1a	1801	1/1	0.96	0.07	58,58,58,58	0
58	MG	1A	3839	1/1	0.96	0.07	36,36,36,36	0
58	MG	1A	3086	1/1	0.96	0.17	33,33,33,33	0
58	MG	1A	3706	1/1	0.96	0.09	28,28,28,28	0
58	MG	1A	3707	1/1	0.96	0.06	19,19,19,19	0
58	MG	1a	1621	1/1	0.96	0.18	51,51,51,51	0
58	MG	1A	3599	1/1	0.96	0.17	56,56,56,56	0
58	MG	1A	3985	1/1	0.96	0.08	23,23,23,23	0
58	MG	1a	1810	1/1	0.96	0.10	64,64,64,64	0
58	MG	1A	3600	1/1	0.96	0.11	43,43,43,43	0
58	MG	1A	3347	1/1	0.96	0.07	45,45,45,45	0
58	MG	2A	3377	1/1	0.96	0.22	50,50,50,50	0
58	MG	2A	3165	1/1	0.96	0.07	62,62,62,62	0
58	MG	1A	3846	1/1	0.96	0.09	40,40,40,40	0
58	MG	1A	3250	1/1	0.96	0.24	41,41,41,41	0
58	MG	1A	3528	1/1	0.96	0.19	39,39,39,39	0
58	MG	2A	3626	1/1	0.96	0.11	59,59,59,59	0
58	MG	2A	3382	1/1	0.96	0.14	45,45,45,45	0
58	MG	1A	3101	1/1	0.96	0.06	38,38,38,38	0
58	MG	1A	3123	1/1	0.96	0.28	37,37,37,37	0
58	MG	2A	3630	1/1	0.96	0.06	47,47,47,47	0
58	MG	1A	3172	1/1	0.96	0.09	34,34,34,34	0
58	MG	1B	234	1/1	0.96	0.09	50,50,50,50	0
58	MG	2A	3174	1/1	0.96	0.14	46,46,46,46	0
58	MG	1A	3469	1/1	0.96	0.12	43,43,43,43	0
58	MG	1D	302	1/1	0.96	0.06	34,34,34,34	0
58	MG	1D	303	1/1	0.96	0.16	40,40,40,40	0
58	MG	2A	3391	1/1	0.96	0.32	52,52,52,52	0
58	MG	1l	202	1/1	0.96	0.13	61,61,61,61	0
58	MG	1A	3720	1/1	0.96	0.04	17,17,17,17	0
58	MG	2A	3643	1/1	0.96	0.10	32,32,32,32	0
58	MG	2a	1740	1/1	0.96	0.30	62,62,62,62	0
58	MG	1A	3610	1/1	0.96	0.06	22,22,22,22	0
58	MG	2a	1742	1/1	0.96	0.21	63,63,63,63	0
58	MG	1A	3611	1/1	0.96	0.08	42,42,42,42	0
58	MG	2a	1744	1/1	0.96	0.06	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	4000	1/1	0.96	0.19	44,44,44,44	0
58	MG	1A	4001	1/1	0.96	0.08	29,29,29,29	0
58	MG	2A	3649	1/1	0.96	0.08	26,26,26,26	0
58	MG	2A	3184	1/1	0.96	0.24	52,52,52,52	0
58	MG	2a	1749	1/1	0.96	0.09	64,64,64,64	0
58	MG	1E	304	1/1	0.96	0.16	34,34,34,34	0
58	MG	1E	305	1/1	0.96	0.09	47,47,47,47	0
58	MG	1A	3723	1/1	0.96	0.07	59,59,59,59	0
58	MG	1A	3726	1/1	0.96	0.12	34,34,34,34	0
58	MG	1E	309	1/1	0.96	0.12	23,23,23,23	0
58	MG	2A	3656	1/1	0.96	0.07	48,48,48,48	0
58	MG	1A	3352	1/1	0.96	0.11	63,63,63,63	0
58	MG	1A	3014	1/1	0.96	0.10	28,28,28,28	0
58	MG	1a	1651	1/1	0.96	0.12	54,54,54,54	0
58	MG	1A	3861	1/1	0.96	0.11	51,51,51,51	0
58	MG	1A	3535	1/1	0.96	0.09	58,58,58,58	0
58	MG	1A	3016	1/1	0.96	0.27	56,56,56,56	0
58	MG	1A	4009	1/1	0.96	0.07	31,31,31,31	0
58	MG	2A	3414	1/1	0.96	0.13	74,74,74,74	0
58	MG	1F	308	1/1	0.96	0.07	47,47,47,47	0
58	MG	2A	3669	1/1	0.96	0.11	49,49,49,49	0
58	MG	1A	3413	1/1	0.96	0.20	48,48,48,48	0
58	MG	2A	3417	1/1	0.96	0.11	32,32,32,32	0
58	MG	1A	3539	1/1	0.96	0.05	56,56,56,56	0
58	MG	1A	3735	1/1	0.96	0.07	38,38,38,38	0
58	MG	1A	3414	1/1	0.96	0.10	51,51,51,51	0
58	MG	1A	3256	1/1	0.96	0.07	57,57,57,57	0
58	MG	1A	3621	1/1	0.96	0.09	46,46,46,46	0
58	MG	1A	3177	1/1	0.96	0.09	34,34,34,34	0
58	MG	2A	3424	1/1	0.96	0.14	52,52,52,52	0
58	MG	1H	201	1/1	0.96	0.17	44,44,44,44	0
58	MG	1A	3180	1/1	0.96	0.05	33,33,33,33	0
58	MG	2a	1781	1/1	0.96	0.17	58,58,58,58	0
58	MG	1A	3419	1/1	0.96	0.07	45,45,45,45	0
58	MG	1N	202	1/1	0.96	0.05	44,44,44,44	0
58	MG	1N	203	1/1	0.96	0.06	51,51,51,51	0
58	MG	2A	3008	1/1	0.96	0.05	45,45,45,45	0
58	MG	1A	3627	1/1	0.96	0.06	59,59,59,59	0
58	MG	2A	3010	1/1	0.96	0.12	48,48,48,48	0
58	MG	1A	3628	1/1	0.96	0.06	27,27,27,27	0
58	MG	1A	3545	1/1	0.96	0.14	39,39,39,39	0
58	MG	2A	3441	1/1	0.96	0.21	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	4022	1/1	0.96	0.08	43,43,43,43	0
58	MG	2A	3015	1/1	0.96	0.11	56,56,56,56	0
58	MG	1A	3546	1/1	0.96	0.18	37,37,37,37	0
58	MG	1A	3021	1/1	0.96	0.07	24,24,24,24	0
58	MG	1A	3151	1/1	0.96	0.22	28,28,28,28	0
58	MG	1A	3077	1/1	0.96	0.06	31,31,31,31	0
58	MG	1A	3751	1/1	0.96	0.25	61,61,61,61	0
58	MG	1A	3637	1/1	0.96	0.05	20,20,20,20	0
58	MG	1A	4029	1/1	0.96	0.08	44,44,44,44	0
58	MG	2A	3452	1/1	0.96	0.09	35,35,35,35	0
58	MG	1P	208	1/1	0.96	0.09	64,64,64,64	0
58	MG	2D	301	1/1	0.96	0.07	41,41,41,41	0
58	MG	2a	1803	1/1	0.96	0.20	61,61,61,61	0
58	MG	1Q	201	1/1	0.96	0.13	42,42,42,42	0
58	MG	1A	3184	1/1	0.96	0.04	49,49,49,49	0
58	MG	1Q	204	1/1	0.96	0.11	60,60,60,60	0
58	MG	2A	3457	1/1	0.96	0.18	53,53,53,53	0
58	MG	1A	3890	1/1	0.96	0.07	43,43,43,43	0
58	MG	1A	3641	1/1	0.96	0.10	28,28,28,28	0
58	MG	1A	3042	1/1	0.96	0.06	31,31,31,31	0
58	MG	1A	3031	1/1	0.96	0.33	36,36,36,36	0
58	MG	2A	3037	1/1	0.96	0.14	39,39,39,39	0
58	MG	2E	307	1/1	0.96	0.10	49,49,49,49	0
58	MG	1R	204	1/1	0.96	0.29	43,43,43,43	0
58	MG	2A	3465	1/1	0.96	0.07	27,27,27,27	0
58	MG	2A	3235	1/1	0.96	0.07	51,51,51,51	0
58	MG	1A	3188	1/1	0.96	0.15	37,37,37,37	0
58	MG	1A	3157	1/1	0.96	0.14	45,45,45,45	0
58	MG	1A	3557	1/1	0.96	0.20	33,33,33,33	0
58	MG	1a	1693	1/1	0.96	0.27	50,50,50,50	0
58	MG	2A	3473	1/1	0.96	0.11	40,40,40,40	0
58	MG	1a	1694	1/1	0.96	0.30	57,57,57,57	0
58	MG	2A	3241	1/1	0.96	0.14	56,56,56,56	0
58	MG	2R	202	1/1	0.96	0.20	60,60,60,60	0
58	MG	1A	3109	1/1	0.96	0.05	31,31,31,31	0
58	MG	1A	3900	1/1	0.96	0.13	42,42,42,42	0
58	MG	1a	1697	1/1	0.96	0.30	62,62,62,62	0
58	MG	1A	3112	1/1	0.96	0.08	42,42,42,42	0
58	MG	1A	3192	1/1	0.96	0.29	32,32,32,32	0
58	MG	1A	3065	1/1	0.96	0.35	50,50,50,50	0
58	MG	1U	204	1/1	0.96	0.18	40,40,40,40	0
58	MG	1A	3904	1/1	0.96	0.08	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3651	1/1	0.96	0.07	29,29,29,29	0
58	MG	2A	3053	1/1	0.96	0.08	51,51,51,51	0
58	MG	23	103	1/1	0.96	0.25	54,54,54,54	0
58	MG	1A	3082	1/1	0.96	0.15	42,42,42,42	0
58	MG	1A	4049	1/1	0.96	0.05	30,30,30,30	0
58	MG	2A	3256	1/1	0.96	0.22	50,50,50,50	0
58	MG	1U	210	1/1	0.96	0.17	39,39,39,39	0
58	MG	1A	3115	1/1	0.96	0.09	36,36,36,36	0
58	MG	1A	3163	1/1	0.96	0.07	30,30,30,30	0
58	MG	1A	3275	1/1	0.96	0.18	47,47,47,47	0
58	MG	2A	3261	1/1	0.96	0.33	58,58,58,58	0
58	MG	2A	3060	1/1	0.96	0.14	45,45,45,45	0
58	MG	2A	3061	1/1	0.96	0.06	48,48,48,48	0
58	MG	1A	3658	1/1	0.96	0.06	45,45,45,45	0
58	MG	2A	3265	1/1	0.96	0.32	54,54,54,54	0
58	MG	2A	3502	1/1	0.96	0.16	45,45,45,45	0
60	ERY	1A	4098	51/51	0.96	0.09	19,32,41,45	0
60	ERY	2A	3688	51/51	0.96	0.10	35,47,57,68	0
58	MG	1A	3330	1/1	0.96	0.18	49,49,49,49	0
61	ZN	2Y	501	1/1	0.96	0.06	104,104,104,104	0
58	MG	2A	3504	1/1	0.96	0.12	55,55,55,55	0
58	MG	2A	3505	1/1	0.96	0.09	34,34,34,34	0
58	MG	2A	3126	1/1	0.97	0.17	53,53,53,53	0
58	MG	1A	3499	1/1	0.97	0.07	37,37,37,37	0
58	MG	1A	3126	1/1	0.97	0.13	33,33,33,33	0
58	MG	1m	3001	1/1	0.97	0.09	53,53,53,53	0
58	MG	1A	3186	1/1	0.97	0.04	36,36,36,36	0
58	MG	1U	208	1/1	0.97	0.15	28,28,28,28	0
58	MG	1A	3127	1/1	0.97	0.36	32,32,32,32	0
58	MG	1A	3036	1/1	0.97	0.06	34,34,34,34	0
58	MG	1A	3066	1/1	0.97	0.06	35,35,35,35	0
58	MG	1A	3384	1/1	0.97	0.28	32,32,32,32	0
58	MG	2A	3639	1/1	0.97	0.11	43,43,43,43	0
58	MG	1A	3573	1/1	0.97	0.05	52,52,52,52	0
58	MG	1V	202	1/1	0.97	0.16	35,35,35,35	0
58	MG	1A	3506	1/1	0.97	0.33	39,39,39,39	0
58	MG	2A	3292	1/1	0.97	0.06	50,50,50,50	0
58	MG	1V	205	1/1	0.97	0.08	43,43,43,43	0
58	MG	1A	3653	1/1	0.97	0.08	41,41,41,41	0
58	MG	1A	3973	1/1	0.97	0.05	48,48,48,48	0
58	MG	2A	3647	1/1	0.97	0.11	70,70,70,70	0
58	MG	1A	3039	1/1	0.97	0.15	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3467	1/1	0.97	0.18	55,55,55,55	0
58	MG	2A	3468	1/1	0.97	0.09	44,44,44,44	0
58	MG	1a	1686	1/1	0.97	0.13	46,46,46,46	0
58	MG	1A	3975	1/1	0.97	0.12	31,31,31,31	0
58	MG	1W	203	1/1	0.97	0.11	39,39,39,39	0
58	MG	2a	1693	1/1	0.97	0.20	64,64,64,64	0
58	MG	1W	204	1/1	0.97	0.15	43,43,43,43	0
58	MG	2a	1695	1/1	0.97	0.10	74,74,74,74	0
58	MG	2A	3148	1/1	0.97	0.18	54,54,54,54	0
58	MG	1A	3228	1/1	0.97	0.10	45,45,45,45	0
58	MG	1A	3005	1/1	0.97	0.06	40,40,40,40	0
58	MG	2A	3658	1/1	0.97	0.18	55,55,55,55	0
58	MG	1A	3230	1/1	0.97	0.12	31,31,31,31	0
58	MG	2A	3660	1/1	0.97	0.10	60,60,60,60	0
58	MG	1A	3860	1/1	0.97	0.09	35,35,35,35	0
58	MG	1A	3024	1/1	0.97	0.17	40,40,40,40	0
58	MG	2A	3663	1/1	0.97	0.07	46,46,46,46	0
58	MG	2A	3154	1/1	0.97	0.14	61,61,61,61	0
58	MG	1X	103	1/1	0.97	0.10	42,42,42,42	0
58	MG	1A	3072	1/1	0.97	0.09	19,19,19,19	0
58	MG	1A	3135	1/1	0.97	0.06	41,41,41,41	0
58	MG	1A	3984	1/1	0.97	0.15	30,30,30,30	0
58	MG	2A	3485	1/1	0.97	0.11	56,56,56,56	0
58	MG	1A	3864	1/1	0.97	0.06	41,41,41,41	0
58	MG	1A	3865	1/1	0.97	0.06	50,50,50,50	0
58	MG	1A	3662	1/1	0.97	0.06	35,35,35,35	0
58	MG	1A	3111	1/1	0.97	0.23	37,37,37,37	0
58	MG	1A	3007	1/1	0.97	0.06	37,37,37,37	0
58	MG	2A	3491	1/1	0.97	0.10	35,35,35,35	0
58	MG	1A	3665	1/1	0.97	0.05	27,27,27,27	0
58	MG	1A	3237	1/1	0.97	0.06	70,70,70,70	0
58	MG	2A	3494	1/1	0.97	0.07	40,40,40,40	0
58	MG	2A	3322	1/1	0.97	0.18	46,46,46,46	0
58	MG	1A	3667	1/1	0.97	0.04	19,19,19,19	0
58	MG	1A	3993	1/1	0.97	0.06	44,44,44,44	0
58	MG	2A	3325	1/1	0.97	0.11	30,30,30,30	0
58	MG	1A	3092	1/1	0.97	0.08	53,53,53,53	0
58	MG	1A	3282	1/1	0.97	0.27	35,35,35,35	0
58	MG	2A	3016	1/1	0.97	0.04	40,40,40,40	0
58	MG	1A	3996	1/1	0.97	0.09	44,44,44,44	0
58	MG	1A	3876	1/1	0.97	0.25	38,38,38,38	0
58	MG	2A	3331	1/1	0.97	0.22	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3877	1/1	0.97	0.24	32,32,32,32	0
58	MG	1a	1714	1/1	0.97	0.14	37,37,37,37	0
58	MG	1A	3763	1/1	0.97	0.07	46,46,46,46	0
58	MG	1A	3520	1/1	0.97	0.11	39,39,39,39	0
58	MG	1A	3458	1/1	0.97	0.13	32,32,32,32	0
58	MG	2A	3026	1/1	0.97	0.05	44,44,44,44	0
58	MG	12	102	1/1	0.97	0.06	41,41,41,41	0
58	MG	1A	3589	1/1	0.97	0.10	41,41,41,41	0
58	MG	1A	3674	1/1	0.97	0.04	19,19,19,19	0
58	MG	1A	3769	1/1	0.97	0.08	34,34,34,34	0
58	MG	2A	3516	1/1	0.97	0.12	40,40,40,40	0
58	MG	1A	3771	1/1	0.97	0.05	26,26,26,26	0
58	MG	1B	228	1/1	0.97	0.07	42,42,42,42	0
58	MG	1A	3522	1/1	0.97	0.24	44,44,44,44	0
58	MG	2D	303	1/1	0.97	0.04	30,30,30,30	0
58	MG	15	103	1/1	0.97	0.11	33,33,33,33	0
58	MG	1A	3074	1/1	0.97	0.04	13,13,13,13	0
58	MG	16	101	1/1	0.97	0.07	60,60,60,60	0
58	MG	17	103	1/1	0.97	0.08	28,28,28,28	0
58	MG	1A	3677	1/1	0.97	0.08	32,32,32,32	0
58	MG	2a	1750	1/1	0.97	0.11	71,71,71,71	0
58	MG	2A	3350	1/1	0.97	0.24	42,42,42,42	0
58	MG	1A	3592	1/1	0.97	0.09	34,34,34,34	0
58	MG	1A	3240	1/1	0.97	0.19	32,32,32,32	0
58	MG	1A	3200	1/1	0.97	0.19	37,37,37,37	0
58	MG	1A	3595	1/1	0.97	0.05	31,31,31,31	0
58	MG	1A	3201	1/1	0.97	0.07	41,41,41,41	0
58	MG	1A	3168	1/1	0.97	0.08	41,41,41,41	0
58	MG	1A	3686	1/1	0.97	0.07	54,54,54,54	0
58	MG	2a	1760	1/1	0.97	0.08	53,53,53,53	0
58	MG	1A	3009	1/1	0.97	0.04	34,34,34,34	0
58	MG	1D	308	1/1	0.97	0.15	41,41,41,41	0
58	MG	1A	3292	1/1	0.97	0.20	28,28,28,28	0
58	MG	1A	3095	1/1	0.97	0.07	19,19,19,19	0
58	MG	1D	311	1/1	0.97	0.14	36,36,36,36	0
58	MG	1A	3294	1/1	0.97	0.10	51,51,51,51	0
58	MG	2a	1767	1/1	0.97	0.04	82,82,82,82	0
58	MG	1A	3248	1/1	0.97	0.07	53,53,53,53	0
58	MG	2R	203	1/1	0.97	0.06	48,48,48,48	0
58	MG	1A	3296	1/1	0.97	0.07	48,48,48,48	0
58	MG	1E	306	1/1	0.97	0.07	52,52,52,52	0
58	MG	1A	3059	1/1	0.97	0.04	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3369	1/1	0.97	0.05	40,40,40,40	0
58	MG	1A	3797	1/1	0.97	0.09	54,54,54,54	0
58	MG	1a	1753	1/1	0.97	0.08	62,62,62,62	0
58	MG	1A	3207	1/1	0.97	0.07	31,31,31,31	0
58	MG	1E	310	1/1	0.97	0.06	51,51,51,51	0
58	MG	1A	3044	1/1	0.97	0.28	32,32,32,32	0
58	MG	1E	312	1/1	0.97	0.10	46,46,46,46	0
58	MG	2A	3550	1/1	0.97	0.08	19,19,19,19	0
58	MG	1A	3301	1/1	0.97	0.10	29,29,29,29	0
58	MG	1A	3119	1/1	0.97	0.13	29,29,29,29	0
58	MG	25	103	1/1	0.97	0.07	52,52,52,52	0
58	MG	1F	302	1/1	0.97	0.21	28,28,28,28	0
58	MG	1F	303	1/1	0.97	0.11	44,44,44,44	0
58	MG	2A	3068	1/1	0.97	0.06	44,44,44,44	0
58	MG	1A	3120	1/1	0.97	0.08	35,35,35,35	0
58	MG	1A	3700	1/1	0.97	0.11	38,38,38,38	0
58	MG	1A	4030	1/1	0.97	0.10	38,38,38,38	0
58	MG	1A	3175	1/1	0.97	0.42	37,37,37,37	0
58	MG	1A	3614	1/1	0.97	0.13	48,48,48,48	0
58	MG	2A	3074	1/1	0.97	0.07	39,39,39,39	0
58	MG	1A	3306	1/1	0.97	0.06	35,35,35,35	0
58	MG	2A	3563	1/1	0.97	0.15	36,36,36,36	0
58	MG	1A	3212	1/1	0.97	0.07	34,34,34,34	0
58	MG	1A	3418	1/1	0.97	0.07	44,44,44,44	0
58	MG	1A	3079	1/1	0.97	0.14	38,38,38,38	0
58	MG	1G	202	1/1	0.97	0.19	51,51,51,51	0
58	MG	1A	4038	1/1	0.97	0.11	36,36,36,36	0
58	MG	1A	3359	1/1	0.97	0.13	45,45,45,45	0
58	MG	2A	3570	1/1	0.97	0.14	58,58,58,58	0
58	MG	1A	3214	1/1	0.97	0.31	37,37,37,37	0
58	MG	1A	3179	1/1	0.97	0.08	19,19,19,19	0
58	MG	1A	3147	1/1	0.97	0.26	32,32,32,32	0
58	MG	2A	3085	1/1	0.97	0.18	50,50,50,50	0
58	MG	1A	3217	1/1	0.97	0.07	38,38,38,38	0
58	MG	1A	3820	1/1	0.97	0.05	24,24,24,24	0
58	MG	1A	3261	1/1	0.97	0.24	44,44,44,44	0
58	MG	1N	205	1/1	0.97	0.12	45,45,45,45	0
58	MG	1A	3822	1/1	0.97	0.27	25,25,25,25	0
58	MG	1A	3823	1/1	0.97	0.06	33,33,33,33	0
58	MG	1a	1785	1/1	0.97	0.12	62,62,62,62	0
58	MG	1A	3366	1/1	0.97	0.17	33,33,33,33	0
58	MG	1A	3933	1/1	0.97	0.06	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3584	1/1	0.97	0.15	54,54,54,54	0
58	MG	1A	3825	1/1	0.97	0.07	23,23,23,23	0
58	MG	2A	3586	1/1	0.97	0.12	38,38,38,38	0
58	MG	2A	3409	1/1	0.97	0.13	32,32,32,32	0
58	MG	1A	3716	1/1	0.97	0.04	47,47,47,47	0
58	MG	2A	3249	1/1	0.97	0.10	55,55,55,55	0
58	MG	1A	3367	1/1	0.97	0.08	60,60,60,60	0
58	MG	1A	3940	1/1	0.97	0.08	55,55,55,55	0
58	MG	1A	3629	1/1	0.97	0.10	24,24,24,24	0
58	MG	1P	205	1/1	0.97	0.29	32,32,32,32	0
58	MG	1a	1649	1/1	0.97	0.07	51,51,51,51	0
58	MG	1A	3368	1/1	0.97	0.09	53,53,53,53	0
58	MG	1A	3010	1/1	0.97	0.08	40,40,40,40	0
58	MG	1A	3316	1/1	0.97	0.10	48,48,48,48	0
58	MG	1A	3633	1/1	0.97	0.06	20,20,20,20	0
58	MG	1A	3559	1/1	0.97	0.18	37,37,37,37	0
58	MG	1A	3724	1/1	0.97	0.15	40,40,40,40	0
58	MG	2A	3108	1/1	0.97	0.08	44,44,44,44	0
58	MG	1A	3836	1/1	0.97	0.17	61,61,61,61	0
58	MG	2l	205	1/1	0.97	0.06	67,67,67,67	0
58	MG	1A	3951	1/1	0.97	0.11	46,46,46,46	0
58	MG	2A	3427	1/1	0.97	0.09	60,60,60,60	0
58	MG	1A	3725	1/1	0.97	0.14	50,50,50,50	0
58	MG	1R	202	1/1	0.97	0.10	38,38,38,38	0
58	MG	2A	3113	1/1	0.97	0.11	41,41,41,41	0
58	MG	2A	3432	1/1	0.97	0.09	41,41,41,41	0
58	MG	1R	203	1/1	0.97	0.10	50,50,50,50	0
58	MG	1A	3317	1/1	0.97	0.11	50,50,50,50	0
58	MG	1A	4071	1/1	0.97	0.13	42,42,42,42	0
58	MG	1A	3047	1/1	0.97	0.06	35,35,35,35	0
58	MG	1A	3639	1/1	0.97	0.04	21,21,21,21	0
58	MG	2A	3438	1/1	0.97	0.09	44,44,44,44	0
58	MG	2A	3440	1/1	0.97	0.14	41,41,41,41	0
58	MG	1A	3956	1/1	0.97	0.05	42,42,42,42	0
58	MG	1A	3729	1/1	0.97	0.05	40,40,40,40	0
58	MG	1A	3034	1/1	0.97	0.31	27,27,27,27	0
58	MG	1A	3375	1/1	0.97	0.07	42,42,42,42	0
58	MG	2A	3622	1/1	0.97	0.10	39,39,39,39	0
58	MG	1A	3436	1/1	0.97	0.16	36,36,36,36	0
58	MG	2A	3446	1/1	0.97	0.09	27,27,27,27	0
58	MG	1A	3035	1/1	0.97	0.27	35,35,35,35	0
58	MG	2A	3507	1/1	0.98	0.12	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3243	1/1	0.98	0.11	28,28,28,28	0
58	MG	1A	3203	1/1	0.98	0.06	33,33,33,33	0
58	MG	1a	1800	1/1	0.98	0.08	48,48,48,48	0
58	MG	1A	4034	1/1	0.98	0.13	39,39,39,39	0
58	MG	2A	3634	1/1	0.98	0.08	45,45,45,45	0
58	MG	2A	3392	1/1	0.98	0.25	42,42,42,42	0
58	MG	1A	3376	1/1	0.98	0.06	26,26,26,26	0
58	MG	2A	3169	1/1	0.98	0.14	39,39,39,39	0
58	MG	1A	3708	1/1	0.98	0.11	20,20,20,20	0
58	MG	1A	3058	1/1	0.98	0.17	39,39,39,39	0
58	MG	1a	1805	1/1	0.98	0.04	57,57,57,57	0
58	MG	1A	3085	1/1	0.98	0.04	39,39,39,39	0
58	MG	1A	3889	1/1	0.98	0.07	50,50,50,50	0
58	MG	1A	3965	1/1	0.98	0.10	20,20,20,20	0
58	MG	1A	3508	1/1	0.98	0.14	33,33,33,33	0
58	MG	1U	202	1/1	0.98	0.13	36,36,36,36	0
58	MG	1A	3828	1/1	0.98	0.03	34,34,34,34	0
58	MG	1A	3892	1/1	0.98	0.06	26,26,26,26	0
58	MG	1A	3011	1/1	0.98	0.07	33,33,33,33	0
58	MG	1A	3110	1/1	0.98	0.25	38,38,38,38	0
58	MG	1A	3622	1/1	0.98	0.10	19,19,19,19	0
58	MG	1A	3623	1/1	0.98	0.09	43,43,43,43	0
58	MG	1A	3076	1/1	0.98	0.05	32,32,32,32	0
58	MG	1B	235	1/1	0.98	0.07	30,30,30,30	0
58	MG	1A	3770	1/1	0.98	0.06	34,34,34,34	0
58	MG	1A	3899	1/1	0.98	0.07	48,48,48,48	0
58	MG	1A	3547	1/1	0.98	0.14	35,35,35,35	0
58	MG	2a	1759	1/1	0.98	0.21	50,50,50,50	0
58	MG	1A	4052	1/1	0.98	0.08	42,42,42,42	0
58	MG	1V	203	1/1	0.98	0.24	34,34,34,34	0
58	MG	1A	3012	1/1	0.98	0.04	26,26,26,26	0
58	MG	1D	307	1/1	0.98	0.07	35,35,35,35	0
58	MG	1a	1723	1/1	0.98	0.12	54,54,54,54	0
58	MG	1a	1632	1/1	0.98	0.10	28,28,28,28	0
58	MG	1A	3383	1/1	0.98	0.20	32,32,32,32	0
58	MG	1A	3155	1/1	0.98	0.10	30,30,30,30	0
58	MG	1a	1727	1/1	0.98	0.08	49,49,49,49	0
58	MG	1A	3775	1/1	0.98	0.06	24,24,24,24	0
58	MG	1A	3156	1/1	0.98	0.07	43,43,43,43	0
58	MG	1E	301	1/1	0.98	0.19	36,36,36,36	0
58	MG	2A	3312	1/1	0.98	0.06	53,53,53,53	0
58	MG	1A	3777	1/1	0.98	0.05	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3013	1/1	0.98	0.16	23,23,23,23	0
58	MG	1a	1640	1/1	0.98	0.23	53,53,53,53	0
58	MG	2A	3673	1/1	0.98	0.06	28,28,28,28	0
58	MG	1A	3780	1/1	0.98	0.04	39,39,39,39	0
58	MG	1A	3909	1/1	0.98	0.10	42,42,42,42	0
58	MG	1A	3449	1/1	0.98	0.10	44,44,44,44	0
58	MG	1A	3450	1/1	0.98	0.06	39,39,39,39	0
58	MG	2A	3320	1/1	0.98	0.14	46,46,46,46	0
58	MG	2A	3679	1/1	0.98	0.07	34,34,34,34	0
58	MG	1a	1739	1/1	0.98	0.05	39,39,39,39	0
58	MG	1a	1740	1/1	0.98	0.10	33,33,33,33	0
58	MG	2A	3439	1/1	0.98	0.11	38,38,38,38	0
58	MG	1A	3069	1/1	0.98	0.04	29,29,29,29	0
58	MG	1X	104	1/1	0.98	0.05	38,38,38,38	0
58	MG	1A	3786	1/1	0.98	0.05	49,49,49,49	0
58	MG	1A	3679	1/1	0.98	0.08	31,31,31,31	0
58	MG	1A	3048	1/1	0.98	0.10	35,35,35,35	0
58	MG	1A	4073	1/1	0.98	0.10	41,41,41,41	0
58	MG	2A	3216	1/1	0.98	0.07	48,48,48,48	0
58	MG	1A	3789	1/1	0.98	0.04	61,61,61,61	0
58	MG	1A	3129	1/1	0.98	0.23	39,39,39,39	0
58	MG	1A	3682	1/1	0.98	0.04	25,25,25,25	0
58	MG	1A	3305	1/1	0.98	0.05	35,35,35,35	0
58	MG	10	102	1/1	0.98	0.09	42,42,42,42	0
58	MG	1A	3638	1/1	0.98	0.05	38,38,38,38	0
58	MG	1A	3596	1/1	0.98	0.12	28,28,28,28	0
58	MG	1a	1754	1/1	0.98	0.07	54,54,54,54	0
58	MG	2A	3116	1/1	0.98	0.25	49,49,49,49	0
58	MG	1A	3734	1/1	0.98	0.04	31,31,31,31	0
58	MG	1A	3235	1/1	0.98	0.06	47,47,47,47	0
58	MG	2A	3012	1/1	0.98	0.06	43,43,43,43	0
58	MG	1A	3737	1/1	0.98	0.04	29,29,29,29	0
58	MG	2A	3460	1/1	0.98	0.12	42,42,42,42	0
58	MG	1A	3071	1/1	0.98	0.09	33,33,33,33	0
58	MG	1A	3037	1/1	0.98	0.06	36,36,36,36	0
58	MG	1A	3199	1/1	0.98	0.05	43,43,43,43	0
58	MG	2A	3017	1/1	0.98	0.05	37,37,37,37	0
58	MG	1A	3930	1/1	0.98	0.07	45,45,45,45	0
58	MG	1A	3931	1/1	0.98	0.03	20,20,20,20	0
58	MG	2E	302	1/1	0.98	0.06	45,45,45,45	0
58	MG	1A	3601	1/1	0.98	0.12	26,26,26,26	0
58	MG	2A	3021	1/1	0.98	0.04	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3351	1/1	0.98	0.08	52,52,52,52	0
58	MG	1A	3602	1/1	0.98	0.03	22,22,22,22	0
58	MG	1A	3935	1/1	0.98	0.04	29,29,29,29	0
58	MG	1A	3310	1/1	0.98	0.05	50,50,50,50	0
58	MG	1A	3693	1/1	0.98	0.05	22,22,22,22	0
58	MG	1A	3938	1/1	0.98	0.09	38,38,38,38	0
58	MG	1A	3866	1/1	0.98	0.06	49,49,49,49	0
58	MG	2A	3476	1/1	0.98	0.05	42,42,42,42	0
58	MG	2A	3029	1/1	0.98	0.14	44,44,44,44	0
58	MG	2A	3596	1/1	0.98	0.04	37,37,37,37	0
58	MG	1A	3427	1/1	0.98	0.08	43,43,43,43	0
58	MG	2A	3137	1/1	0.98	0.14	37,37,37,37	0
58	MG	1A	3941	1/1	0.98	0.06	46,46,46,46	0
58	MG	1A	3283	1/1	0.98	0.27	28,28,28,28	0
58	MG	1A	3869	1/1	0.98	0.04	32,32,32,32	0
58	MG	2A	3250	1/1	0.98	0.13	35,35,35,35	0
58	MG	1A	3808	1/1	0.98	0.11	28,28,28,28	0
58	MG	1a	1775	1/1	0.98	0.05	40,40,40,40	0
58	MG	17	101	1/1	0.98	0.04	33,33,33,33	0
58	MG	17	102	1/1	0.98	0.17	33,33,33,33	0
58	MG	1A	3809	1/1	0.98	0.06	25,25,25,25	0
58	MG	20	101	1/1	0.98	0.09	53,53,53,53	0
58	MG	1A	3810	1/1	0.98	0.06	40,40,40,40	0
58	MG	1A	3947	1/1	0.98	0.10	44,44,44,44	0
58	MG	1A	3811	1/1	0.98	0.07	24,24,24,24	0
58	MG	1A	3284	1/1	0.98	0.12	43,43,43,43	0
58	MG	1B	208	1/1	0.98	0.07	52,52,52,52	0
58	MG	1A	3038	1/1	0.98	0.07	24,24,24,24	0
58	MG	1A	3286	1/1	0.98	0.10	38,38,38,38	0
58	MG	1a	1786	1/1	0.98	0.06	53,53,53,53	0
58	MG	1A	3106	1/1	0.98	0.12	29,29,29,29	0
58	MG	1A	3148	1/1	0.98	0.19	31,31,31,31	0
58	MG	1Q	203	1/1	0.98	0.06	44,44,44,44	0
58	MG	1A	3372	1/1	0.98	0.07	42,42,42,42	0
58	MG	1A	3242	1/1	0.98	0.17	34,34,34,34	0
58	MG	1a	1792	1/1	0.98	0.04	46,46,46,46	0
58	MG	1a	1793	1/1	0.98	0.06	61,61,61,61	0
58	MG	1A	3537	1/1	0.98	0.08	58,58,58,58	0
58	MG	1A	3657	1/1	0.98	0.06	41,41,41,41	0
58	MG	1B	217	1/1	0.98	0.05	50,50,50,50	0
62	SF4	2d	303	8/8	0.98	0.05	71,78,88,104	0
58	MG	1A	3671	1/1	0.99	0.04	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3978	1/1	0.99	0.06	53,53,53,53	0
58	MG	1A	3008	1/1	0.99	0.06	27,27,27,27	0
58	MG	1D	305	1/1	0.99	0.03	24,24,24,24	0
58	MG	1A	3298	1/1	0.99	0.04	31,31,31,31	0
58	MG	1A	3934	1/1	0.99	0.04	23,23,23,23	0
58	MG	1A	3757	1/1	0.99	0.04	41,41,41,41	0
58	MG	2A	3293	1/1	0.99	0.16	27,27,27,27	0
58	MG	1A	3029	1/1	0.99	0.15	30,30,30,30	0
58	MG	1A	3914	1/1	0.99	0.03	22,22,22,22	0
58	MG	1A	4058	1/1	0.99	0.04	44,44,44,44	0
58	MG	2A	3603	1/1	0.99	0.13	42,42,42,42	0
58	MG	1A	4059	1/1	0.99	0.07	52,52,52,52	0
58	MG	1A	4060	1/1	0.99	0.05	25,25,25,25	0
58	MG	1E	303	1/1	0.99	0.12	33,33,33,33	0
58	MG	1A	3915	1/1	0.99	0.02	22,22,22,22	0
58	MG	1A	3046	1/1	0.99	0.03	34,34,34,34	0
58	MG	2A	3413	1/1	0.99	0.08	36,36,36,36	0
58	MG	1A	3023	1/1	0.99	0.03	18,18,18,18	0
58	MG	1A	3003	1/1	0.99	0.07	25,25,25,25	0
58	MG	1A	3395	1/1	0.99	0.21	39,39,39,39	0
58	MG	1A	3779	1/1	0.99	0.04	17,17,17,17	0
58	MG	1a	1794	1/1	0.99	0.04	57,57,57,57	0
58	MG	1A	4067	1/1	0.99	0.13	39,39,39,39	0
58	MG	1A	3049	1/1	0.99	0.17	32,32,32,32	0
58	MG	1A	3360	1/1	0.99	0.04	51,51,51,51	0
58	MG	1A	3801	1/1	0.99	0.07	24,24,24,24	0
58	MG	1A	3488	1/1	0.99	0.18	34,34,34,34	0
58	MG	1A	3783	1/1	0.99	0.04	20,20,20,20	0
58	MG	1a	1732	1/1	0.99	0.12	40,40,40,40	0
58	MG	1A	3784	1/1	0.99	0.03	24,24,24,24	0
58	MG	1P	207	1/1	0.99	0.04	32,32,32,32	0
58	MG	2A	3624	1/1	0.99	0.10	42,42,42,42	0
58	MG	2A	3428	1/1	0.99	0.05	40,40,40,40	0
58	MG	2A	3027	1/1	0.99	0.16	40,40,40,40	0
58	MG	1A	3766	1/1	0.99	0.09	40,40,40,40	0
61	ZN	1Y	205	1/1	0.99	0.02	66,66,66,66	0
58	MG	1A	3176	1/1	0.99	0.16	32,32,32,32	0
61	ZN	15	105	1/1	0.99	0.04	67,67,67,67	0
61	ZN	19	102	1/1	0.99	0.04	44,44,44,44	0
61	ZN	1n	103	1/1	0.99	0.03	67,67,67,67	0
58	MG	1a	1703	1/1	0.99	0.05	49,49,49,49	0
58	MG	1F	306	1/1	0.99	0.20	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
61	ZN	25	105	1/1	0.99	0.05	91,91,91,91	0
61	ZN	26	501	1/1	0.99	0.06	71,71,71,71	0
61	ZN	29	501	1/1	0.99	0.03	70,70,70,70	0
58	MG	1A	3634	1/1	0.99	0.04	52,52,52,52	0
62	SF4	1d	303	8/8	0.99	0.06	59,66,69,71	0
58	MG	1A	3710	1/1	0.99	0.05	31,31,31,31	0
58	MG	1A	4055	1/1	1.00	0.03	17,17,17,17	0
58	MG	1A	3178	1/1	1.00	0.06	19,19,19,19	0
58	MG	1A	3736	1/1	1.00	0.02	27,27,27,27	0
58	MG	2A	3632	1/1	1.00	0.06	28,28,28,28	0
61	ZN	16	102	1/1	1.00	0.05	46,46,46,46	0

5.5 Other polymers (i)

There are no such residues in this entry.