Full wwPDB X-ray Structure Validation Report (i)

Feb 25, 2024 – 03:04 PM EST

PDB ID	:	5HAU
Title	:	Crystal structure of antimicrobial peptide Bac7(1-19) bound to the Thermus thermophilus 70S ribosome
Authors	:	Gagnon, M.G.; Roy, R.N.; Lomakin, I.B.; Florin, T.; Mankin, A.S.; Steitz, T.A.
Deposited on	:	2015-12-30
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

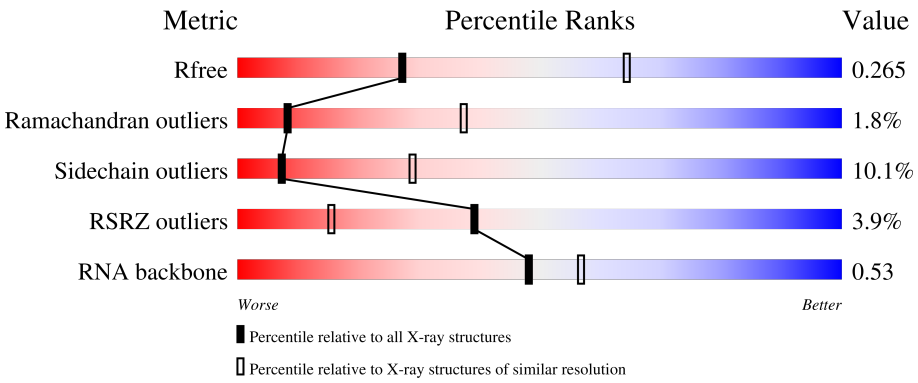
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	3% 82% 16% ••
1	2A	2915	3% 80% 18% ••
2	1B	121	91% 8% •
2	2B	121	84% 15% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	1C	229	45% 51% 7% 41%
3	2C	229	48% 51% 7% 41%
4	1D	276	91% 8%
4	2D	276	92% 7%
5	1E	206	92% 7%
5	2E	206	91% 8%
6	1F	210	87% 10%
6	2F	210	89% 8%
7	1G	182	% 88% 12%
7	2G	182	86% 13%
8	1H	180	% 92% 5%
8	2H	180	% 87% 10%
9	1J	173	7% 64% 12% 25%
9	2J	173	12% 62% 13% 25%
10	1K	147	14% 37% 8% 54%
10	2K	147	26% 35% 10% 55%
11	1L	140	93% 7%
11	2L	140	91% 9%
12	1M	122	95% 5%
12	2M	122	91% 9%
13	1N	150	90% 9%
13	2N	150	% 91% 8%
14	1O	141	94% 6%
14	2O	141	92% 7%
15	1P	118	85% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	2P	118	86% 14%
16	1Q	112	90% 8%
16	2Q	112	88% 10%
17	1R	146	81% 8% 10%
17	2R	146	82% 8% 10%
18	1S	118	90% 8%
18	2S	118	93% 5%
19	1T	101	90% 9%
19	2T	101	92% 7%
20	1U	113	93% 6%
20	2U	113	93% 6%
21	1V	96	92% 6%
21	2V	96	96%
22	1W	110	92% 5%
22	2W	110	89% 8%
23	1X	206	81% 10% 10%
23	2X	206	81% 10% 10%
24	1Y	85	82% 7% 11%
24	2Y	85	85% 5% 11%
25	1Z	98	91% 8%
25	2Z	98	90% 9%
26	10	72	89% 8%
26	20	72	85% 12%
27	11	60	90% 8%
27	21	60	90% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	12	71	4% 76% 20%
28	22	71	7% 76% 18%
29	13	60	90% 8%
29	23	60	88% 10%
30	14	54	89% 9%
30	24	54	89% 9%
31	15	49	94%
31	25	49	90% 8%
32	16	65	91% 8%
32	26	65	91% 8%
33	17	37	100%
33	27	37	3% 97%
34	1a	1521	2% 80% 18%
34	2a	1521	2% 81% 17%
35	1b	256	% 79% 10% 10%
35	2b	256	5% 81% 9% 10%
36	1c	239	82% 5% 14%
36	2c	239	2% 79% 8% 14%
37	1d	209	91% 8%
37	2d	209	92% 7%
38	1e	162	84% 7% 9%
38	2e	162	86% 6% 9%
39	1f	101	90% 9%
39	2f	101	92% 7%
40	1g	156	6% 93% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	2g	156	9% 90% 9%
41	1h	138	88% 11%
41	2h	138	86% 13%
42	1i	128	90% 9%
42	2i	128	6% 87% 12%
43	1j	105	2% 83% 10% 8%
43	2j	105	10% 87% 5% 9%
44	1k	129	83% 5% 12%
44	2k	129	85% 12%
45	1l	132	87% 5% 8%
45	2l	132	86% 7% 8%
46	1m	126	6% 88% 9%
46	2m	126	7% 88% 9%
47	1n	61	2% 87% 11%
47	2n	61	3% 87% 11%
48	1o	89	91% 8%
48	2o	89	88% 11%
49	1p	88	% 85% 8% 7%
49	2p	88	83% 10% 7%
50	1q	105	90% 5% 6%
50	2q	105	% 88% 7% 6%
51	1r	88	3% 72% 6% 23%
51	2r	88	% 73% 23%
52	1s	93	3% 81% 10% 10%
52	2s	93	6% 81% 9% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	1t	106	%, 79%, 11%, 9%
53	2t	106	83%, 8%, 9%
54	1u	27	81%, 15%
54	2u	27	7%, 78%, 7%, 15%
55	1z	758	11%, 84%, 11%
55	2z	758	14%, 84%, 12%
56	1y	24	25%, 75%
56	2y	24	4%, 21%, 79%
57	1w	77	66%, 30%
57	2w	77	66%, 32%
58	1x	35	49%, 46%
58	2x	35	43%, 9%, 46%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	1A	3018	-	-	-	X
59	MG	1A	3023	-	-	-	X
59	MG	1A	3104	-	-	-	X
59	MG	1A	3207	-	-	-	X
59	MG	1A	3223	-	-	-	X
59	MG	1A	3636	-	-	-	X
59	MG	1a	1622	-	-	-	X
59	MG	1a	1771	-	-	-	X
59	MG	2A	3220	-	-	-	X
59	MG	2A	3238	-	-	-	X
59	MG	2a	1603	-	-	-	X
59	MG	2a	1657	-	-	-	X
59	MG	2a	1754	-	-	-	X
60	ZN	13	103	-	-	-	X

2 Entry composition (i)

There are 63 unique types of molecules in this entry. The entry contains 306384 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1A	2872	61861	27532	11574	19884	2871	0	0	0
1	2A	2868	61771	27492	11554	19858	2867	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	1B	120	2573	1146	476	832	119	0	0	0
2	2B	120	2573	1146	476	832	119	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	1C	135	1020	641	190	188	1	3	0	0
3	2C	135	1020	641	190	188	1	3	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	1D	275	2136	1349	423	361	3	0	0	0
4	2D	275	2142	1352	426	361	3	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	1E	204	1559	985	298	270	6	0	0	0
5	2E	204	1559	985	298	270	6	0	0	0

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	1F	203	1584	1009	298	275	2	0	0	1
6	2F	203	1580	1007	297	274	2	0	0	1

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	1G	181	1425	914	256	251	4	0	0	0
7	2G	181	1424	911	258	251	4	0	0	0

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	1H	174	1330	845	248	236	1	0	0	0
8	2H	174	1330	845	248	236	1	0	0	0

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	1J	130	641	381	130	130	0	0	0
9	2J	130	641	381	130	130	0	0	0

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	1K	67	499	310	94	92	3	0	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	2K	66	498	310	93	92	3	0	0	0

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	1L	140	1117	719	207	187	4	0	0	0
			Total	C	N	O	S			
11	2L	140	1117	719	207	187	4	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	1M	122	933	588	171	170	4	0	0	0
			Total	C	N	O	S			
12	2M	122	933	588	171	170	4	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	1N	149	1139	709	231	196	3	0	0	0
			Total	C	N	O	S			
13	2N	149	1135	706	230	196	3	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	1O	141	1122	715	212	188	7	0	0	0
			Total	C	N	O	S			
14	2O	141	1122	715	212	188	7	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	1P	118	968	604	203	160	1	0	0	0
			Total	C	N	O	S			
15	2P	118	968	604	203	160	1	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
16	1Q	110	877	553	175	149	0	0	0
16	2Q	110	870	549	173	148	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	1R	131	1091	680	225	185	1	0	0	0
17	2R	131	1083	675	224	183	1	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	1S	116	959	608	201	149	1	0	0	0
18	2S	116	959	608	201	149	1	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	1T	101	771	495	140	135	1	0	0	0
19	2T	101	771	495	140	135	1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	1U	112	886	557	174	153	2	0	0	0
20	2U	112	886	557	174	153	2	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	1V	95	750	488	135	126	1	0	0	0
21	2V	95	750	488	135	126	1	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	1W	107	806	517	152	131	6	0	0	0
22	2W	107	806	517	152	131	6	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	1X	186	1460	932	259	267	2	0	0	0
23	2X	186	1454	929	256	267	2	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	1Y	76	604	373	128	102	1	0	0	0
24	2Y	76	602	372	128	101	1	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	1Z	97	755	475	148	131	1	0	0	0
25	2Z	97	755	475	148	131	1	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	10	70	588	365	118	103	2	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	20	70	588	365	118	103	2	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
27	11	59	469	298	90	81	0	0	0
27	21	59	464	296	90	78	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	12	69	558	352	102	99	5	0	0	0
28	22	69	532	339	97	91	5	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	13	59	455	285	89	76	5	0	0	0
29	23	59	455	285	89	76	5	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	14	53	453	281	91	77	4	0	0	0
30	24	53	449	279	91	75	4	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	15	48	418	257	104	55	2	0	0	0
31	25	48	418	257	104	55	2	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	16	64	517	331	102	82	2	0	0	0
32	26	64	517	331	102	82	2	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	17	37	307	188	68	47	4	0	0	0
33	27	37	307	188	68	47	4	0	0	0

- Molecule 34 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
34	1a	1495	32141	14304	5958	10384	1495	0	0	0
34	2a	1501	32268	14361	5980	10426	1501	0	0	0

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	1b	231	1846	1179	331	331	5	0	0	0
35	2b	231	1825	1167	326	327	5	0	0	0

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	1c	206	1552	976	302	273	1	0	0	0
36	2c	206	1544	970	300	273	1	0	0	0

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	1d	208	1659	1040	326	286	7	0	0	0
37	2d	208	1678	1052	333	286	7	0	0	0

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	1e	148	1129	714	213	198	4	0	0	0
38	2e	148	1133	716	214	199	4	0	0	0

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	1f	100	812	514	146	149	3	0	0	0
39	2f	100	820	518	147	152	3	0	0	0

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	1g	155	1231	766	243	216	6	0	0	0
40	2g	155	1235	769	244	216	6	0	0	0

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	1h	137	1088	689	206	191	2	0	0	0
41	2h	137	1088	689	206	191	2	0	0	0

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
42	1i	127	986	626	193	167	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
42	2i	127	978	619	190	169	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
43	1j	97	709	440	138	131	0	0	0
43	2j	96	714	445	138	131	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	1k	114	833	519	156	155	3	0	0	0
44	2k	114	833	519	156	155	3	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	1l	122	930	585	185	159	1	0	0	0
45	2l	122	930	585	185	159	1	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	1m	123	966	598	200	166	2	0	0	0
46	2m	122	950	586	197	165	2	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	1n	60	492	312	104	72	4	0	0	0
47	2n	60	492	312	104	72	4	0	0	0

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	1o	88	728	456	144	126	2	0	0	0
48	2o	88	728	456	144	126	2	0	0	0

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	1p	82	681	433	134	113	1	0	0	0
49	2p	82	677	430	133	113	1	0	0	0

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	1q	99	823	528	151	142	2	0	0	0
50	2q	99	823	528	151	142	2	0	0	0

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
51	1r	68	555	355	108	92	0	0	0
51	2r	68	555	355	108	92	0	0	0

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	1s	84	661	423	122	114	2	0	0	0
52	2s	83	646	412	119	113	2	0	0	0

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	1t	96	728	446	156	124	2	0	0	0
53	2t	96	731	449	156	124	2	0	0	0

- Molecule 54 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
54	1u	23	199	122	48	29	0	0	0
54	2u	23	199	122	48	29	0	0	0

- Molecule 55 is a protein called Chimera protein of 50S ribosomal protein L9 and Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	1z	730	5690	3616	980	1075	19	0	0	0
55	2z	730	5690	3616	980	1075	19	0	0	0

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
56	1y	6	129	58	24	41	6	0	0	0
56	2y	5	109	49	22	33	5	0	0	0

- Molecule 57 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
57	1w	76	1625	725	294	529	76	1	0	0	0
57	2w	76	1625	725	294	529	76	1	0	0	0

- Molecule 58 is a protein called Cathelicidin-3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
58	1x	19	168	106	43	19	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
58	2x	19	168	106	43	19	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
59	1A	780	780	780	0	0
59	1B	24	24	24	0	0
59	1D	4	4	4	0	0
59	1E	6	6	6	0	0
59	1F	7	7	7	0	0
59	1G	2	2	2	0	0
59	1H	1	1	1	0	0
59	1L	2	2	2	0	0
59	1M	1	1	1	0	0
59	1N	2	2	2	0	0
59	1O	2	2	2	0	0
59	1P	2	2	2	0	0
59	1S	4	4	4	0	0
59	1T	1	1	1	0	0
59	1U	3	3	3	0	0
59	1W	1	1	1	0	0
59	1X	2	2	2	0	0
59	1Y	5	5	5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
59	10	2	2	2	0	0
59	11	1	1	1	0	0
59	13	3	3	3	0	0
59	14	1	1	1	0	0
59	15	2	2	2	0	0
59	16	2	2	2	0	0
59	17	2	2	2	0	0
59	1a	204	204	204	0	0
59	1b	1	1	1	0	0
59	1d	2	2	2	0	0
59	1f	1	1	1	0	0
59	1l	3	3	3	0	0
59	1t	1	1	1	0	0
59	1z	1	1	1	0	0
59	1w	6	6	6	0	0
59	2A	620	620	620	0	0
59	2B	13	13	13	0	0
59	2D	4	4	4	0	0
59	2E	4	4	4	0	0
59	2F	3	3	3	0	0
59	2G	1	1	1	0	0

Continued on next page...

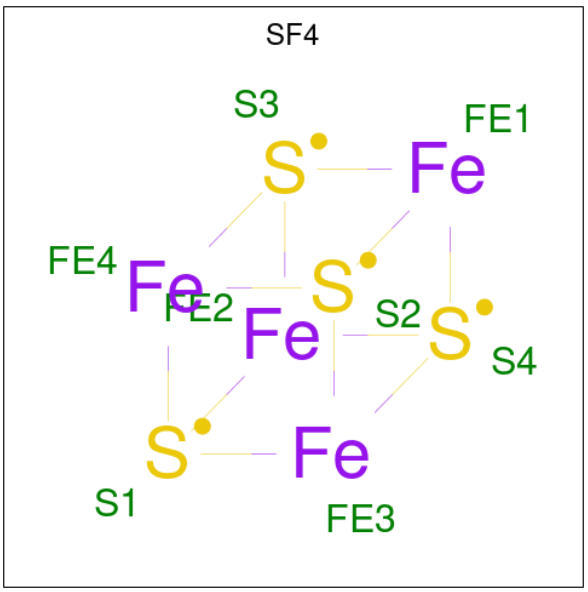
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
59	2M	2	2	2	0	0
59	2N	1	1	1	0	0
59	2O	2	2	2	0	0
59	2P	1	1	1	0	0
59	2R	1	1	1	0	0
59	2S	2	2	2	0	0
59	2W	1	1	1	0	0
59	2Y	1	1	1	0	0
59	23	1	1	1	0	0
59	26	2	2	2	0	0
59	2a	173	173	173	0	0
59	2d	1	1	1	0	0
59	2f	2	2	2	0	0
59	2j	1	1	1	0	0
59	2l	1	1	1	0	0
59	2n	1	1	1	0	0
59	2q	1	1	1	0	0
59	2t	1	1	1	0	0
59	2z	4	4	4	0	0
59	2w	4	4	4	0	0

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

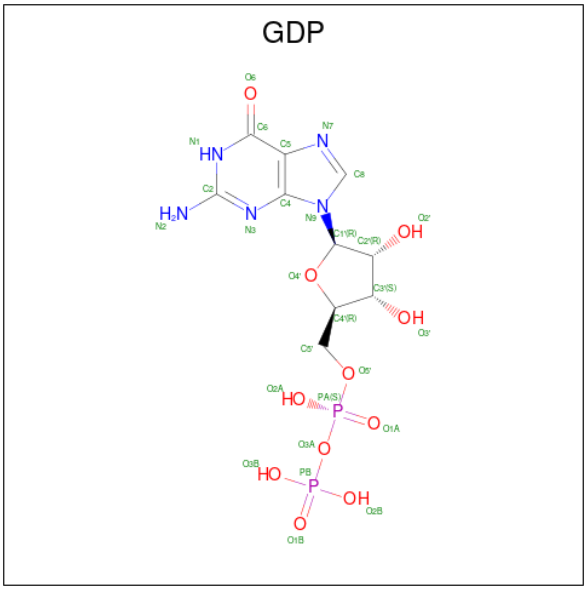
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1W	1	Total Zn 1 1	0	0
60	12	1	Total Zn 1 1	0	0
60	13	1	Total Zn 1 1	0	0
60	14	1	Total Zn 1 1	0	0
60	17	1	Total Zn 1 1	0	0
60	1n	1	Total Zn 1 1	0	0
60	2W	1	Total Zn 1 1	0	0
60	22	1	Total Zn 1 1	0	0
60	23	1	Total Zn 1 1	0	0
60	24	1	Total Zn 1 1	0	0
60	27	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
62	1z	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
62	2z	1	28	10	5	11	2	0	0

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
63	1A	1299	1299	1299	0	0
			Total	O		
63	1B	39	39	39	0	0
			Total	O		
63	1D	15	15	15	0	0
			Total	O		
63	1E	19	19	19	0	0
			Total	O		
63	1F	12	12	12	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	1	Total O 1 1	0	0
63	1M	2	Total O 2 2	0	0
63	1N	12	Total O 12 12	0	0
63	1O	2	Total O 2 2	0	0
63	1P	4	Total O 4 4	0	0
63	1Q	1	Total O 1 1	0	0
63	1R	2	Total O 2 2	0	0
63	1S	4	Total O 4 4	0	0
63	1T	1	Total O 1 1	0	0
63	1U	2	Total O 2 2	0	0
63	1V	3	Total O 3 3	0	0
63	1X	2	Total O 2 2	0	0
63	1Y	4	Total O 4 4	0	0
63	1Z	1	Total O 1 1	0	0
63	11	2	Total O 2 2	0	0
63	15	2	Total O 2 2	0	0
63	16	10	Total O 10 10	0	0
63	17	1	Total O 1 1	0	0
63	1a	155	Total O 155 155	0	0
63	1d	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1j	1	Total O 1 1	0	0
63	1l	2	Total O 2 2	0	0
63	1o	1	Total O 1 1	0	0
63	1p	2	Total O 2 2	0	0
63	1z	5	Total O 5 5	0	0
63	1w	4	Total O 4 4	0	0
63	1x	1	Total O 1 1	0	0
63	2A	650	Total O 650 650	0	0
63	2B	11	Total O 11 11	0	0
63	2D	8	Total O 8 8	0	0
63	2E	7	Total O 7 7	0	0
63	2F	5	Total O 5 5	0	0
63	2L	1	Total O 1 1	0	0
63	2M	2	Total O 2 2	0	0
63	2N	6	Total O 6 6	0	0
63	2O	3	Total O 3 3	0	0
63	2P	1	Total O 1 1	0	0
63	2R	2	Total O 2 2	0	0
63	2S	2	Total O 2 2	0	0
63	2U	1	Total O 1 1	0	0
63	2V	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

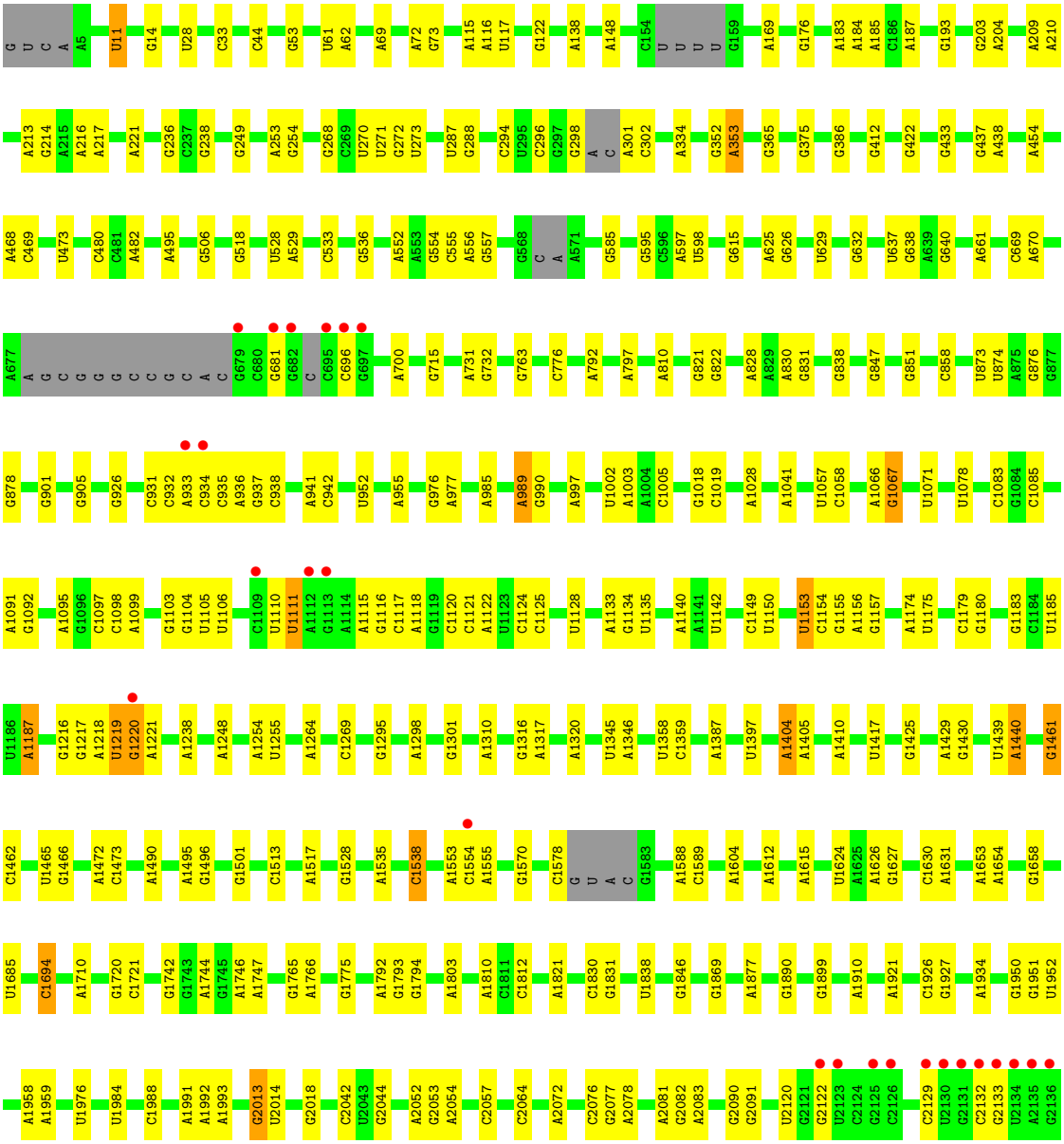
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	2W	1	Total O 1 1	0	0
63	2Y	5	Total O 5 5	0	0
63	2Z	2	Total O 2 2	0	0
63	21	2	Total O 2 2	0	0
63	24	1	Total O 1 1	0	0
63	26	3	Total O 3 3	0	0
63	2a	122	Total O 122 122	0	0
63	2f	1	Total O 1 1	0	0
63	2h	1	Total O 1 1	0	0
63	2j	1	Total O 1 1	0	0
63	2n	1	Total O 1 1	0	0
63	2t	1	Total O 1 1	0	0
63	2z	1	Total O 1 1	0	0
63	2y	1	Total O 1 1	0	0
63	2w	2	Total O 2 2	0	0

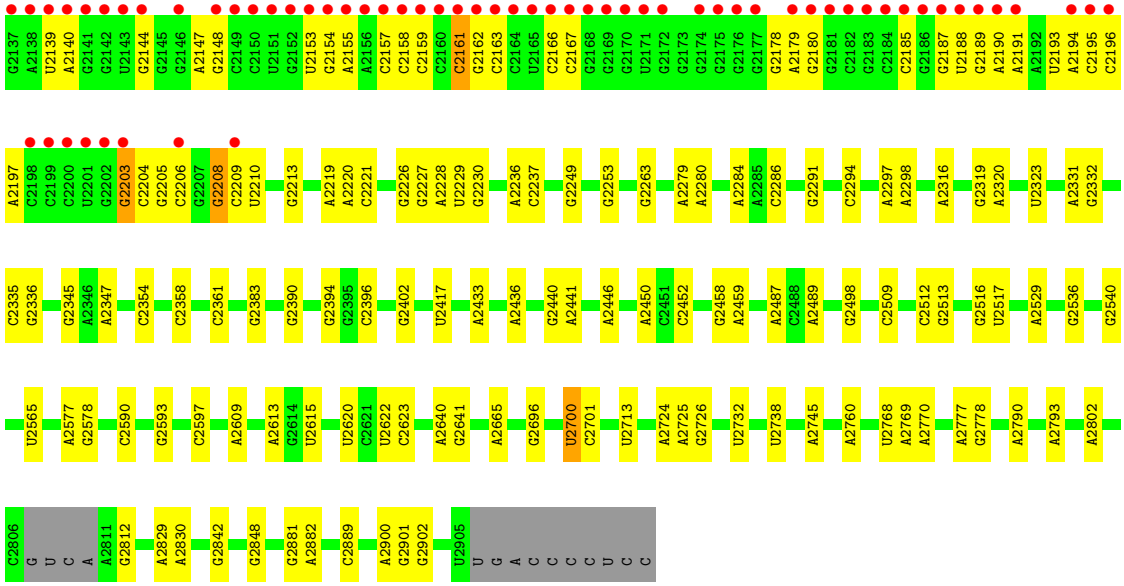
3 Residue-property plots (i)

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

- Molecule 1: 23S Ribosomal RNA

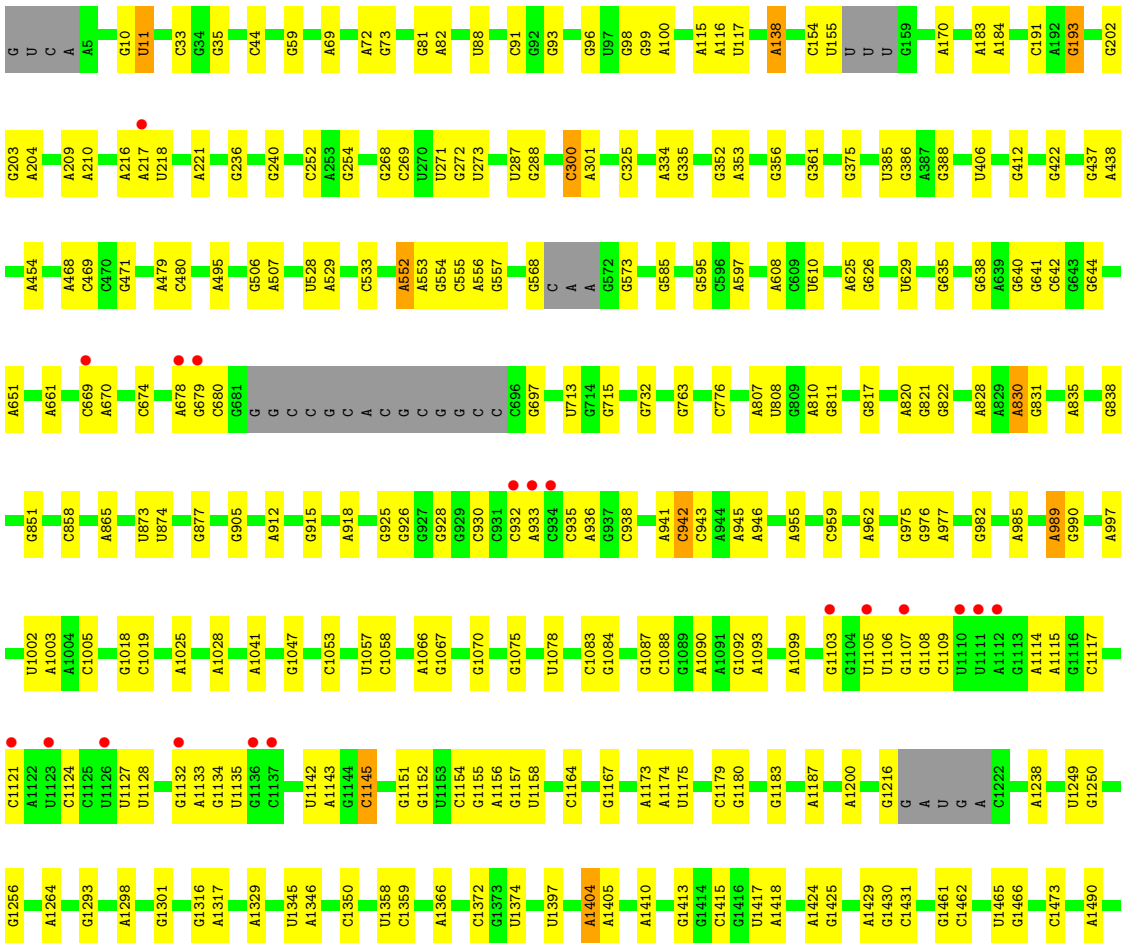
Chain 1A:

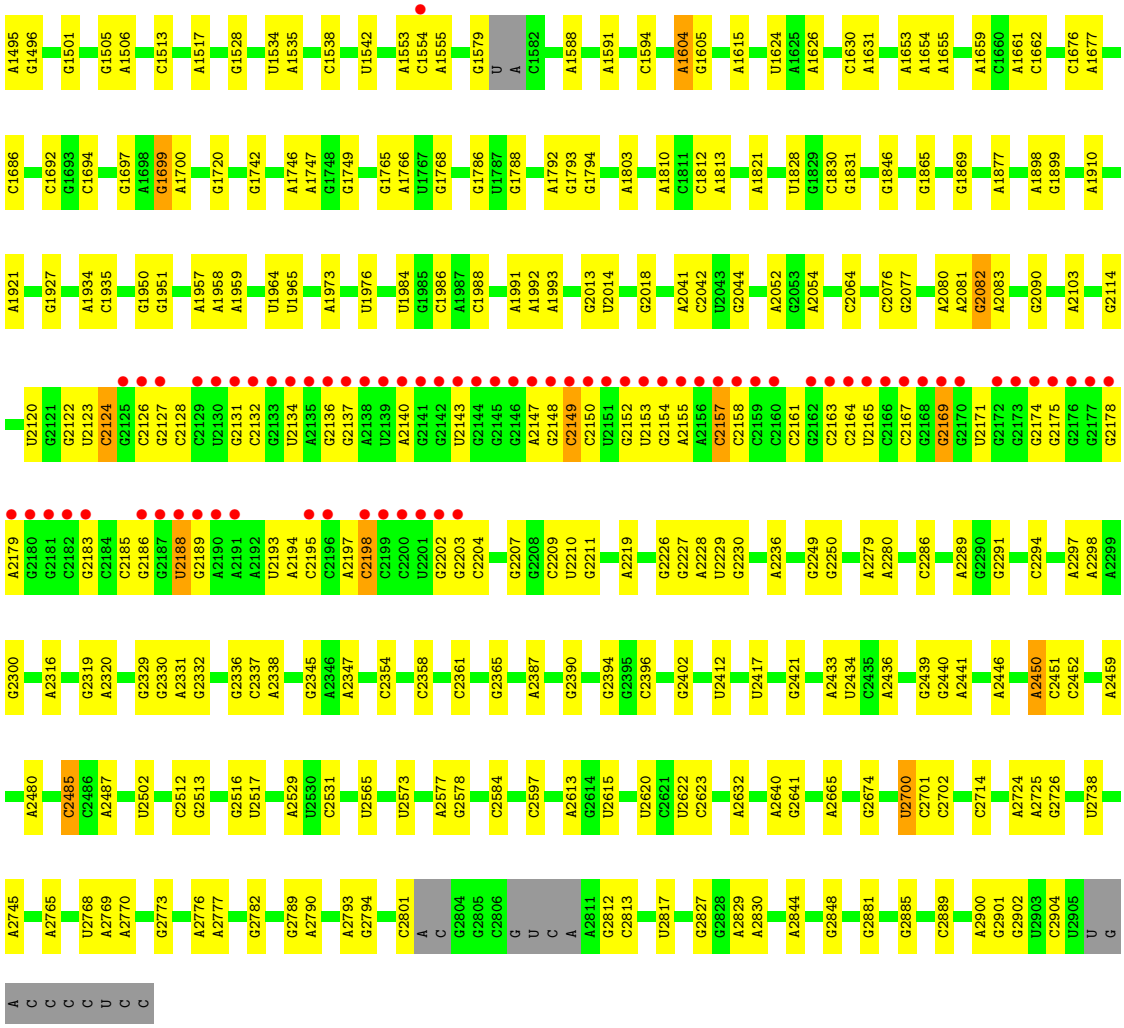




- Molecule 1: 23S Ribosomal RNA

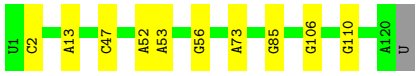
Chain 2A:





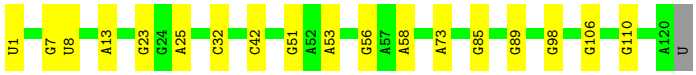
- Molecule 2: 5S Ribosomal RNA

Chain 1B:



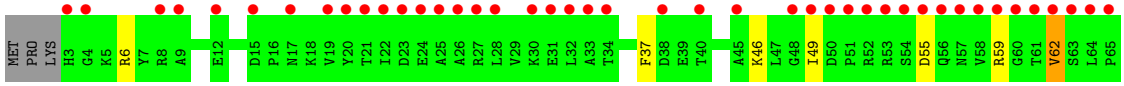
- Molecule 2: 5S Ribosomal RNA

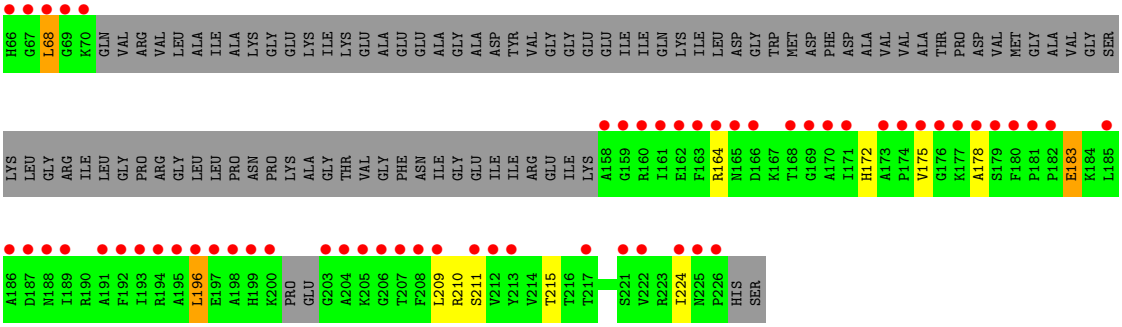
Chain 2B:



- Molecule 3: 50S ribosomal protein L1

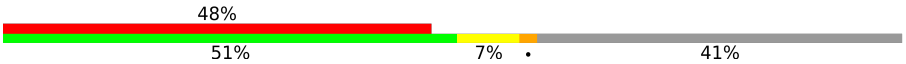
Chain 1C:

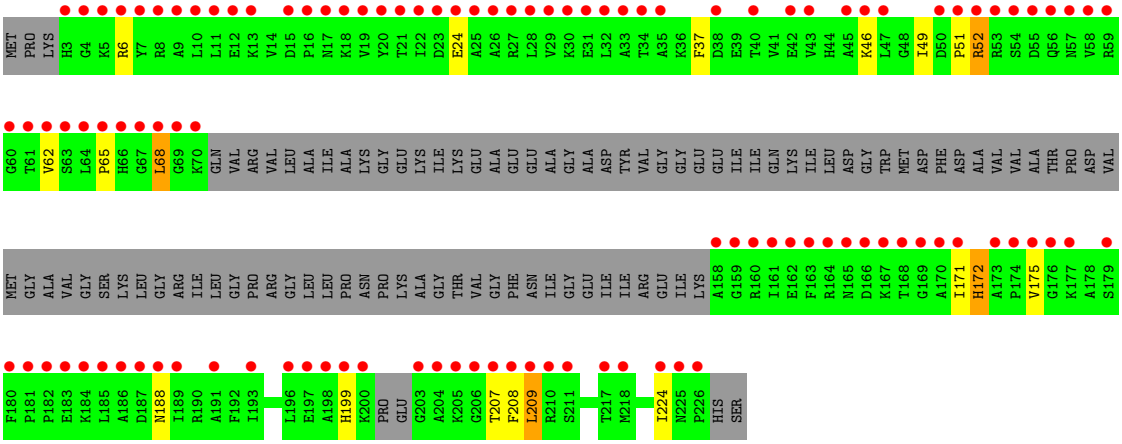




- Molecule 3: 50S ribosomal protein L1

Chain 2C:



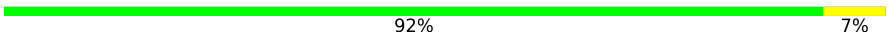


- Molecule 4: 50S ribosomal protein L2

Chain 1D:

- Molecule 4: 50S ribosomal protein L2

Chain 2D:



- Molecule 5: 50S ribosomal protein L3

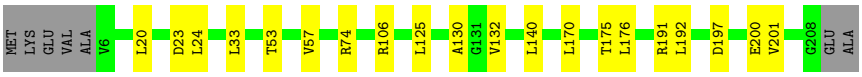
Chain 1E:

- Molecule 5: 50S ribosomal protein L3

Chain 2E:

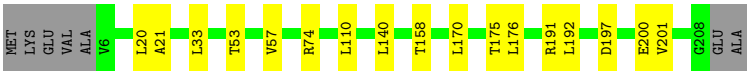
• Molecule 6: 50S ribosomal protein L4

Chain 1F:



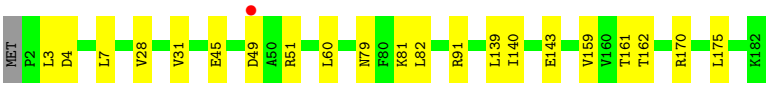
• Molecule 6: 50S ribosomal protein L4

Chain 2F:



• Molecule 7: 50S ribosomal protein L5

Chain 1G:

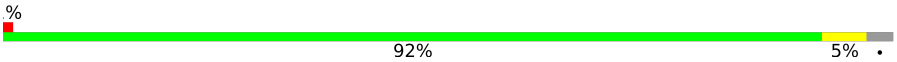


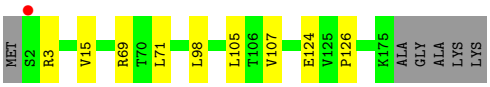
• Molecule 7: 50S ribosomal protein L5

Chain 2G:

• Molecule 8: 50S ribosomal protein L6

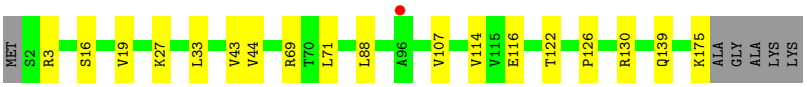
Chain 1H:





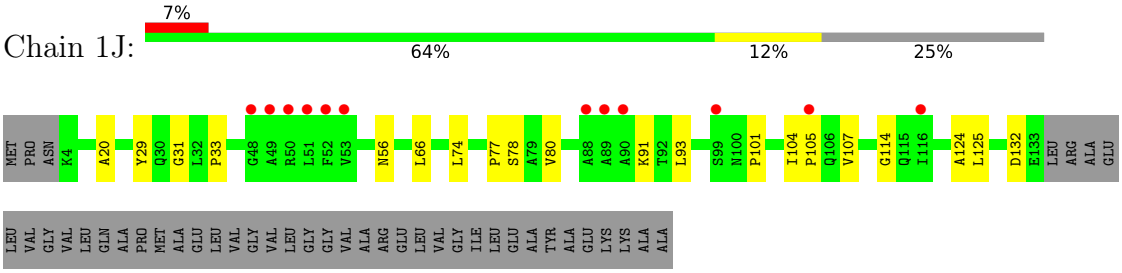
• Molecule 8: 50S ribosomal protein L6

Chain 2H:



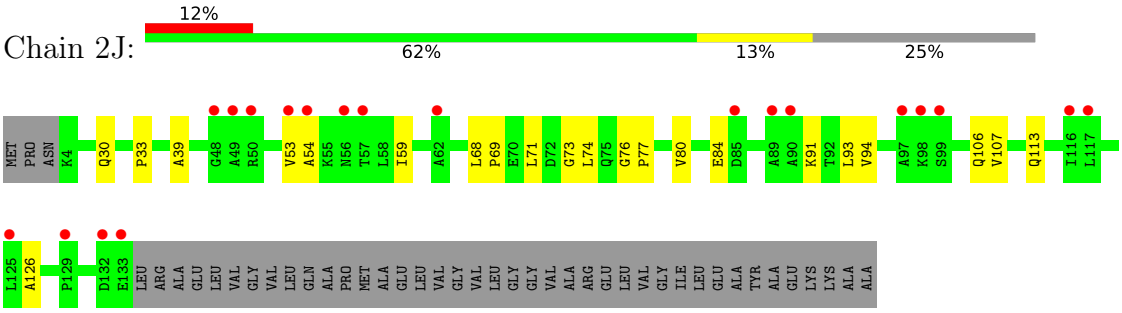
• Molecule 9: 50S ribosomal protein L10

Chain 1J:



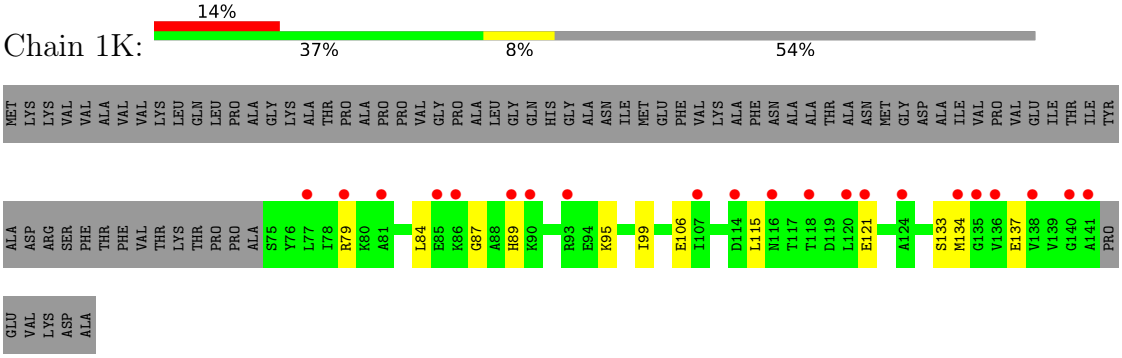
• Molecule 9: 50S ribosomal protein L10

Chain 2J:



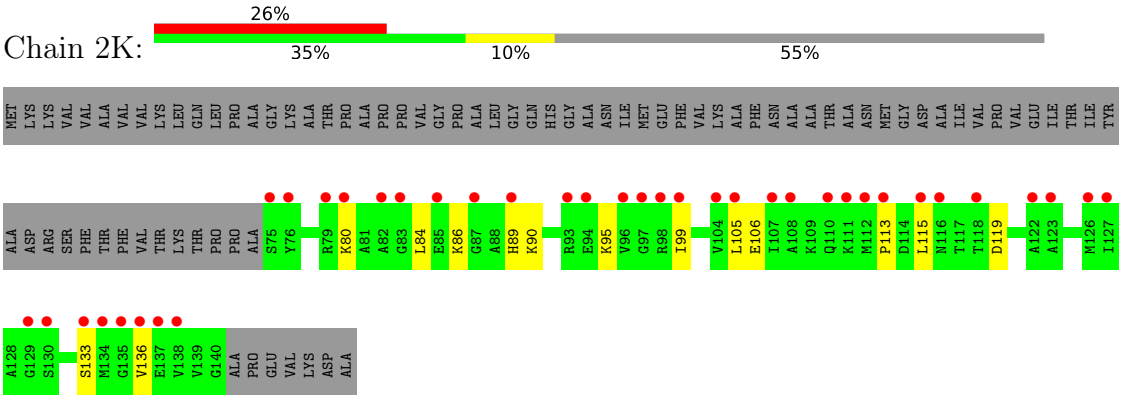
• Molecule 10: 50S ribosomal protein L11

Chain 1K:



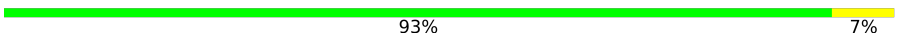
• Molecule 10: 50S ribosomal protein L11

Chain 2K:



• Molecule 11: 50S ribosomal protein L13

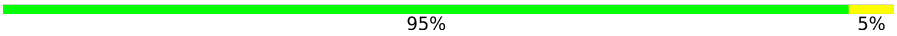
Chain 1L:



• Molecule 11: 50S ribosomal protein L13

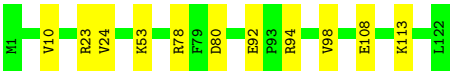
Chain 2L:

• Molecule 12: 50S ribosomal protein L14

Chain 1M: 

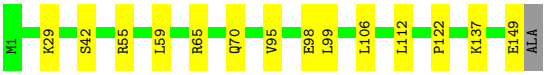
• Molecule 12: 50S ribosomal protein L14

Chain 2M:

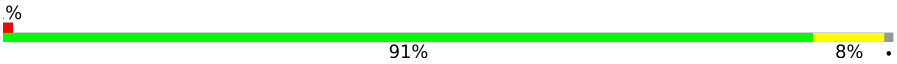


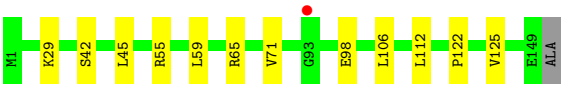
• Molecule 13: 50S ribosomal protein L15

Chain 1N:

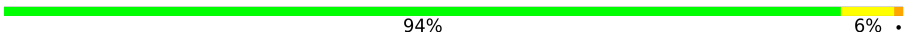


• Molecule 13: 50S ribosomal protein L15

Chain 2N: 

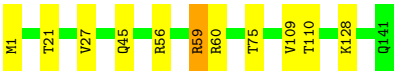


• Molecule 14: 50S ribosomal protein L16

Chain 1O: 

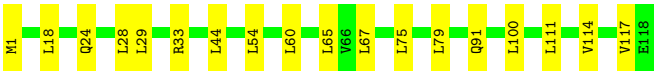
• Molecule 14: 50S ribosomal protein L16

Chain 2O:



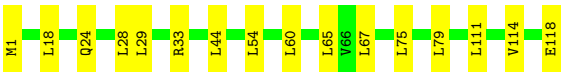
• Molecule 15: 50S ribosomal protein L17

Chain 1P:



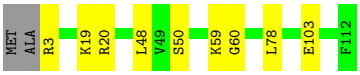
• Molecule 15: 50S ribosomal protein L17

Chain 2P:



• Molecule 16: 50S ribosomal protein L18

Chain 1Q:



• Molecule 16: 50S ribosomal protein L18

Chain 2Q:

• Molecule 17: 50S ribosomal protein L19

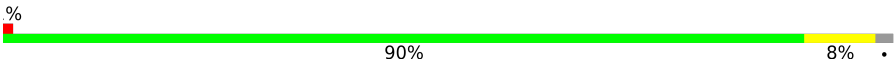
Chain 1R:

• Molecule 17: 50S ribosomal protein L19

Chain 2R:

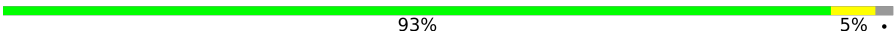
• Molecule 18: 50S ribosomal protein L20

Chain 1S:



• Molecule 18: 50S ribosomal protein L20

Chain 2S:

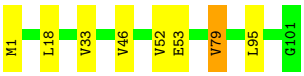


• Molecule 19: 50S ribosomal protein L21

Chain 1T:

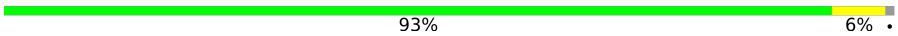
• Molecule 19: 50S ribosomal protein L21

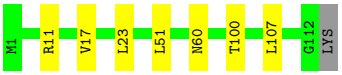
Chain 2T:



• Molecule 20: 50S ribosomal protein L22

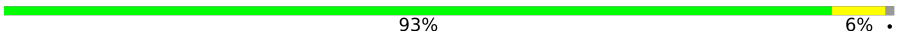
Chain 1U:

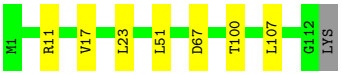




• Molecule 20: 50S ribosomal protein L22

Chain 2U:



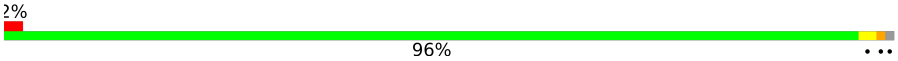


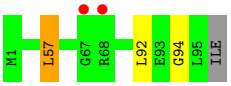
• Molecule 21: 50S ribosomal protein L23

Chain 1V:

• Molecule 21: 50S ribosomal protein L23

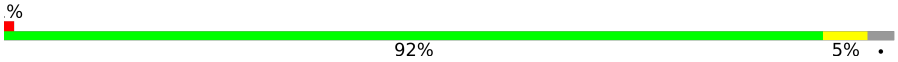
Chain 2V:





• Molecule 22: 50S ribosomal protein L24

Chain 1W:



• Molecule 22: 50S ribosomal protein L24

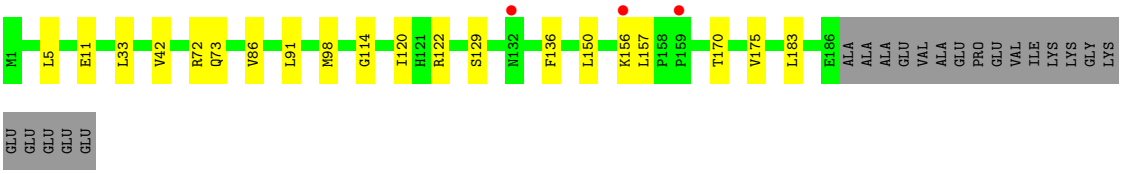
Chain 2W:

• Molecule 23: 50S ribosomal protein L25

Chain 1X:

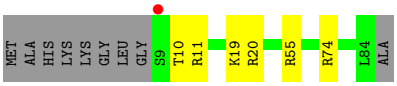
• Molecule 23: 50S ribosomal protein L25

Chain 2X:



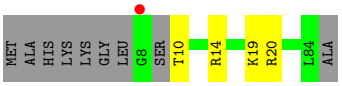
• Molecule 24: 50S ribosomal protein L27

Chain 1Y:



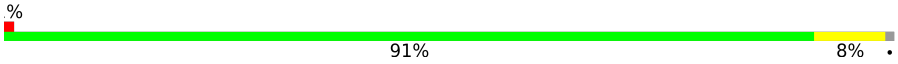
• Molecule 24: 50S ribosomal protein L27

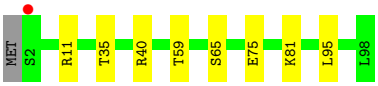
Chain 2Y:



• Molecule 25: 50S ribosomal protein L28

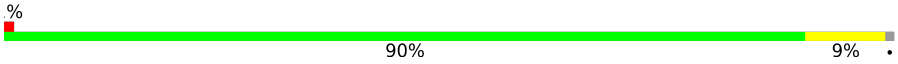
Chain 1Z:

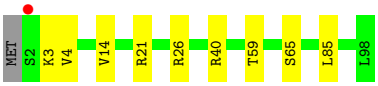




• Molecule 25: 50S ribosomal protein L28

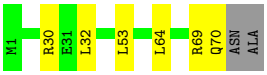
Chain 2Z:





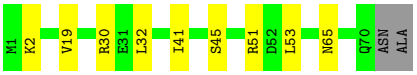
• Molecule 26: 50S ribosomal protein L29

Chain 10:



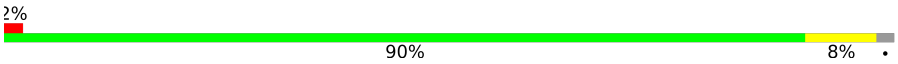
• Molecule 26: 50S ribosomal protein L29

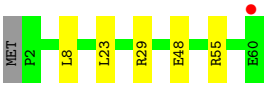
Chain 20:



• Molecule 27: 50S ribosomal protein L30

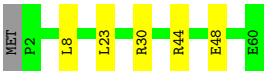
Chain 11:





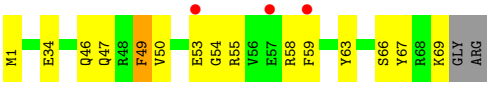
• Molecule 27: 50S ribosomal protein L30

Chain 21:



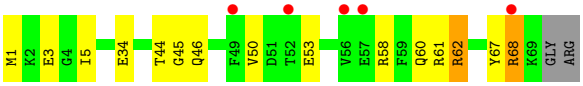
• Molecule 28: 50S ribosomal protein L31

Chain 12:



• Molecule 28: 50S ribosomal protein L31

Chain 22:

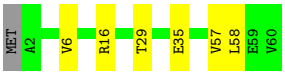


• Molecule 29: 50S ribosomal protein L32

Chain 13:

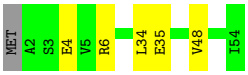
• Molecule 29: 50S ribosomal protein L32

Chain 23:



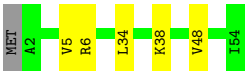
• Molecule 30: 50S ribosomal protein L33

Chain 14:



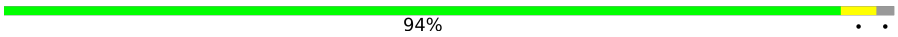
• Molecule 30: 50S ribosomal protein L33

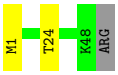
Chain 24:



• Molecule 31: 50S ribosomal protein L34

Chain 15:



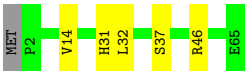


• Molecule 31: 50S ribosomal protein L34

Chain 25:

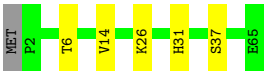
• Molecule 32: 50S ribosomal protein L35

Chain 16:



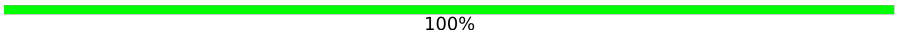
• Molecule 32: 50S ribosomal protein L35

Chain 26:



• Molecule 33: 50S ribosomal protein L36

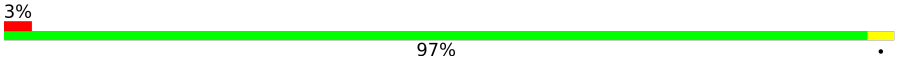
Chain 17:



There are no outlier residues recorded for this chain.

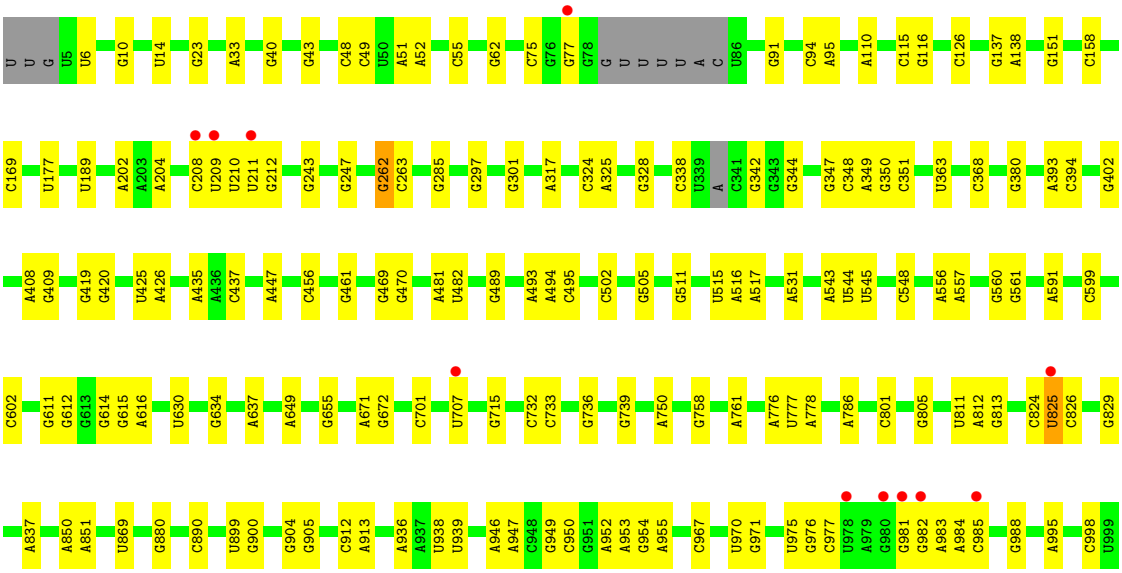
• Molecule 33: 50S ribosomal protein L36

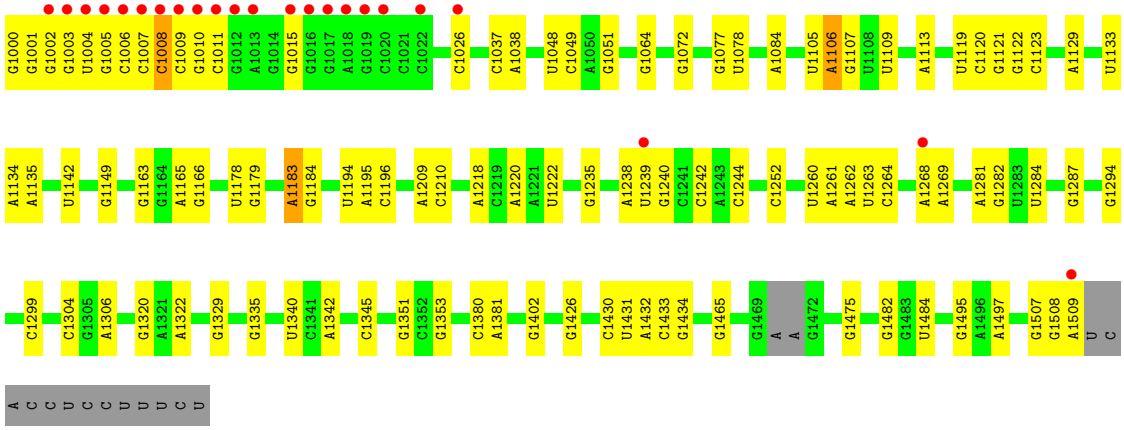
Chain 27:



• Molecule 34: 16S Ribosomal RNA

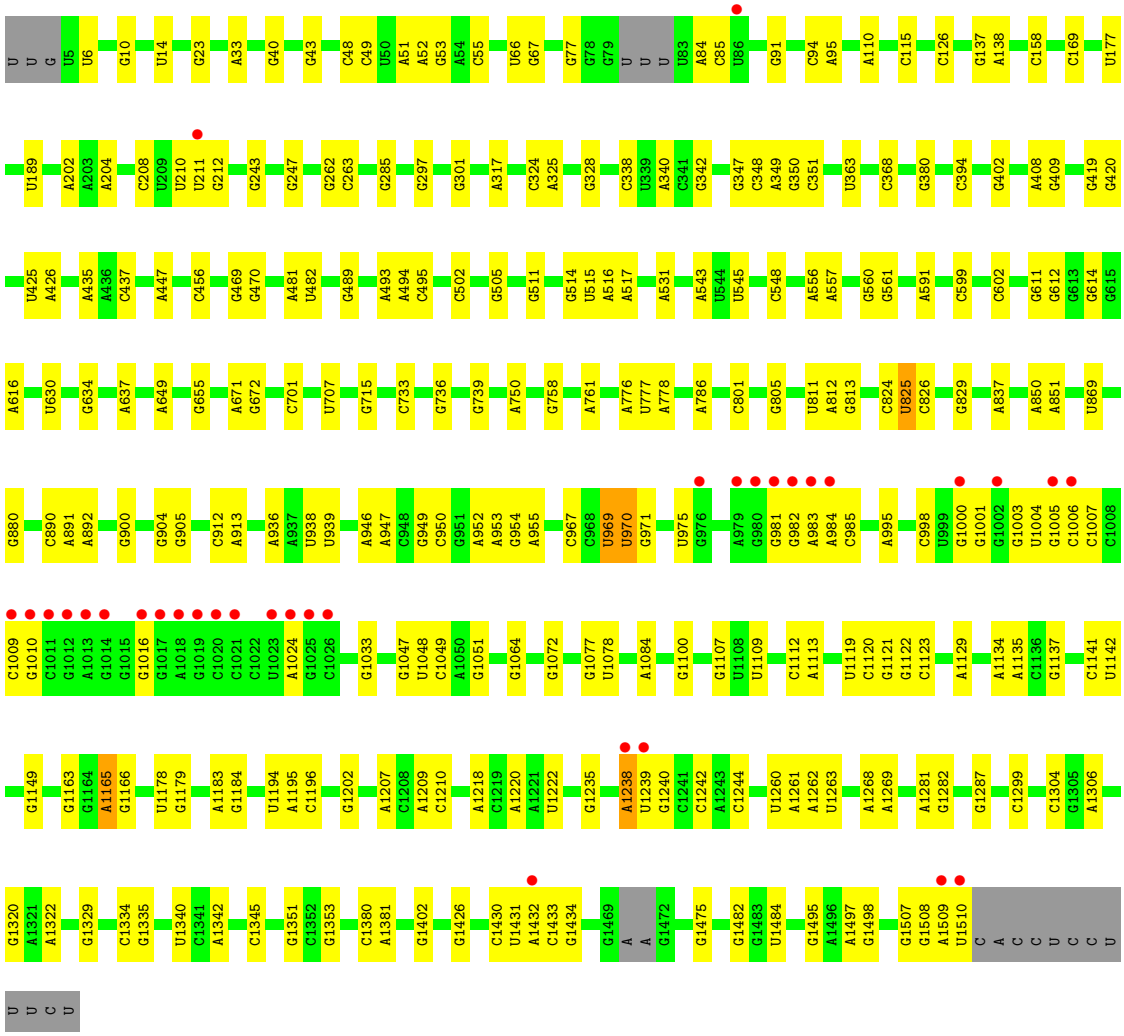
Chain 1a:





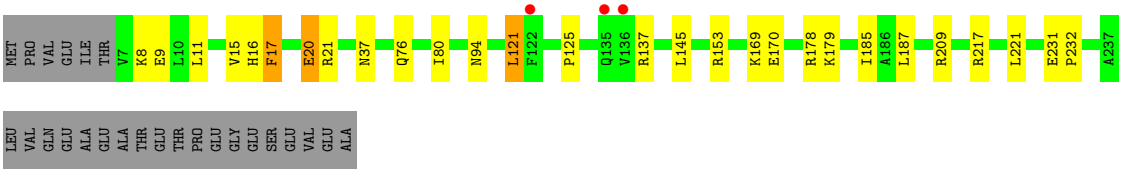
• Molecule 34: 16S Ribosomal RNA

Chain 2a:



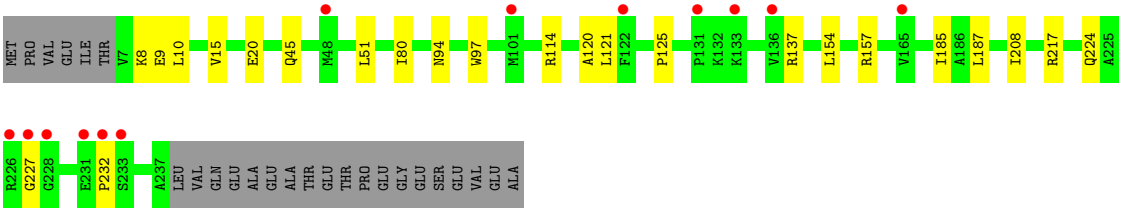
• Molecule 35: 30S ribosomal protein S2

Chain 1b:



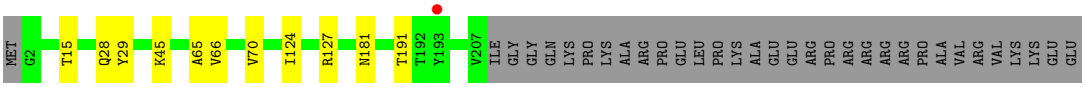
• Molecule 35: 30S ribosomal protein S2

Chain 2b:



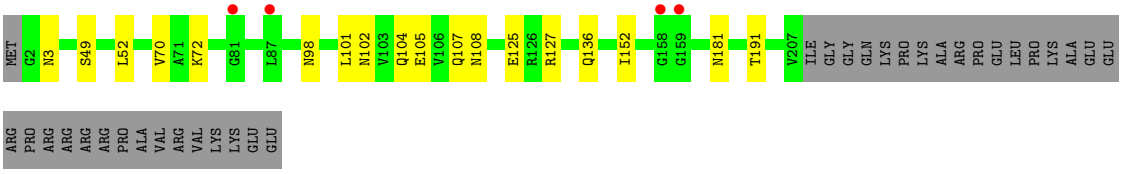
• Molecule 36: 30S ribosomal protein S3

Chain 1c:



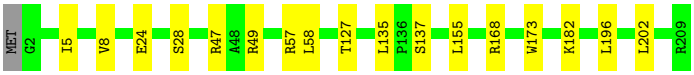
• Molecule 36: 30S ribosomal protein S3

Chain 2c:



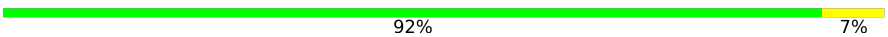
• Molecule 37: 30S ribosomal protein S4

Chain 1d:



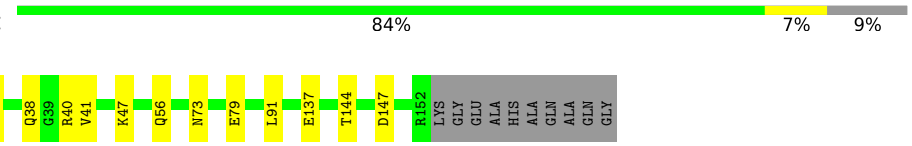
• Molecule 37: 30S ribosomal protein S4

Chain 2d:



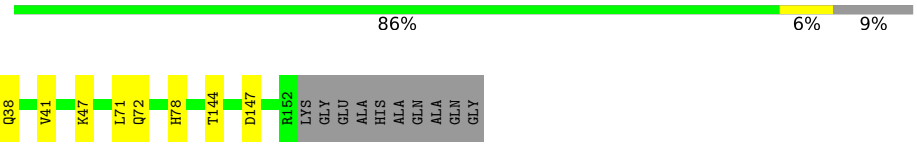
• Molecule 38: 30S ribosomal protein S5

Chain 1e:



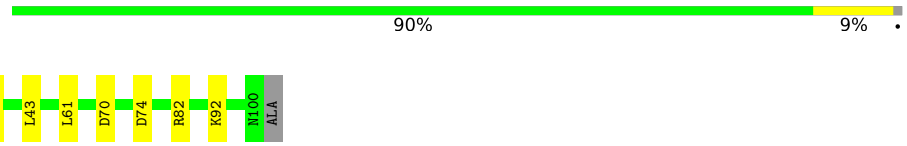
• Molecule 38: 30S ribosomal protein S5

Chain 2e:



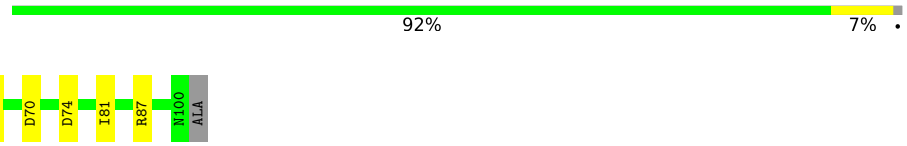
• Molecule 39: 30S ribosomal protein S6

Chain 1f:



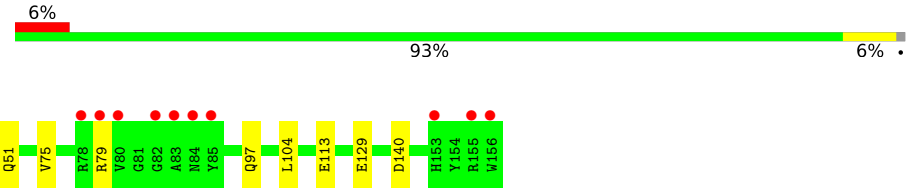
• Molecule 39: 30S ribosomal protein S6

Chain 2f:



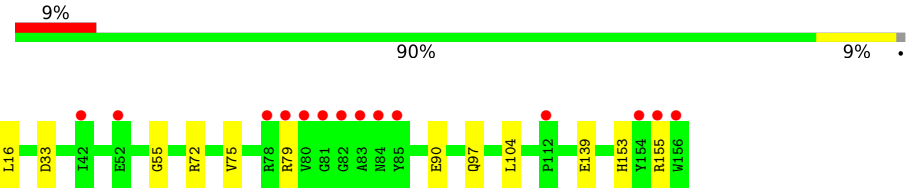
• Molecule 40: 30S ribosomal protein S7

Chain 1g:



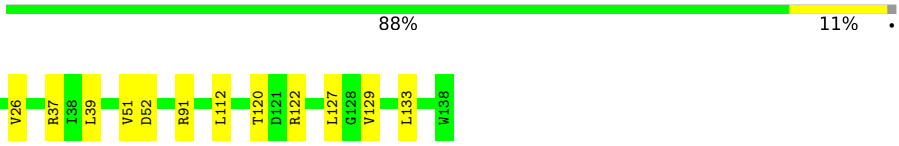
• Molecule 40: 30S ribosomal protein S7

Chain 2g:



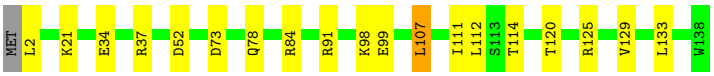
• Molecule 41: 30S ribosomal protein S8

Chain 1h:



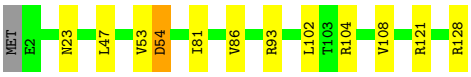
• Molecule 41: 30S ribosomal protein S8

Chain 2h:



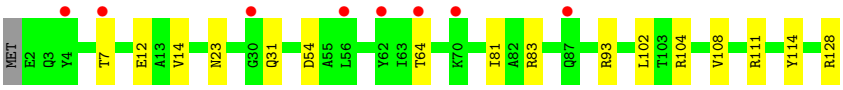
• Molecule 42: 30S ribosomal protein S9

Chain 1i:



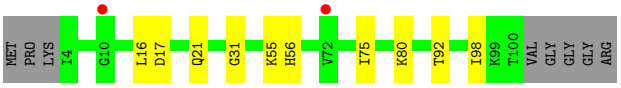
• Molecule 42: 30S ribosomal protein S9

Chain 2i:



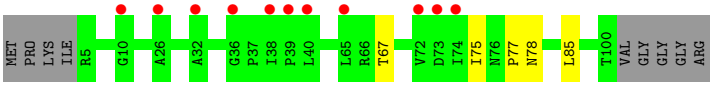
• Molecule 43: 30S ribosomal protein S10

Chain 1j:



• Molecule 43: 30S ribosomal protein S10

Chain 2j:

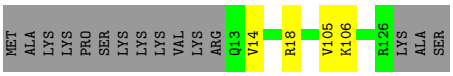


• Molecule 44: 30S ribosomal protein S11

Chain 1k:

• Molecule 44: 30S ribosomal protein S11

Chain 2k:

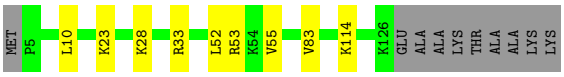


• Molecule 45: 30S ribosomal protein S12

Chain 1l:

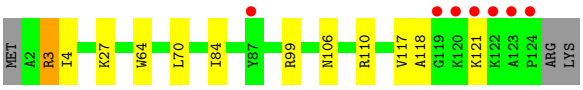
• Molecule 45: 30S ribosomal protein S12

Chain 2l:



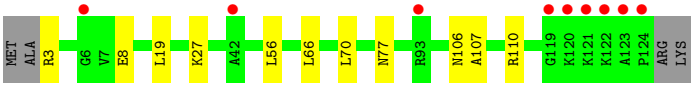
• Molecule 46: 30S ribosomal protein S13

Chain 1m:



• Molecule 46: 30S ribosomal protein S13

Chain 2m:

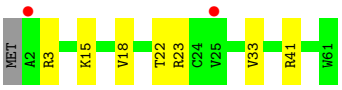


• Molecule 47: 30S ribosomal protein S14 type Z

Chain 1n:

• Molecule 47: 30S ribosomal protein S14 type Z

Chain 2n:



• Molecule 48: 30S ribosomal protein S15

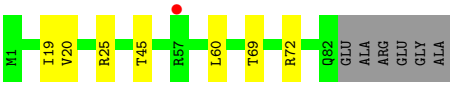
Chain 1o:

• Molecule 48: 30S ribosomal protein S15

Chain 2o:

• Molecule 49: 30S ribosomal protein S16

Chain 1p:

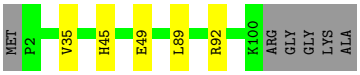


• Molecule 49: 30S ribosomal protein S16

Chain 2p:

• Molecule 50: 30S ribosomal protein S17

Chain 1q:

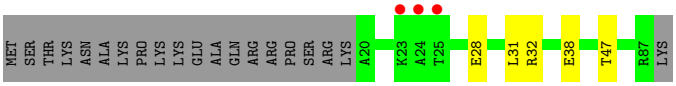


• Molecule 50: 30S ribosomal protein S17

Chain 2q:

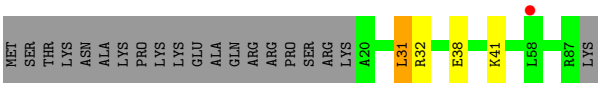
• Molecule 51: 30S ribosomal protein S18

Chain 1r:



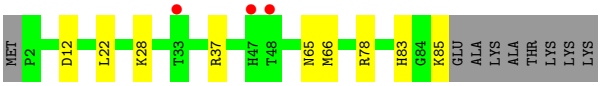
• Molecule 51: 30S ribosomal protein S18

Chain 2r:



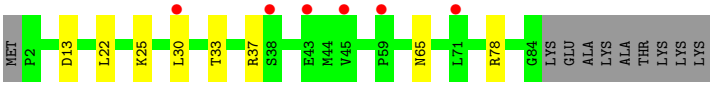
• Molecule 52: 30S ribosomal protein S19

Chain 1s:



• Molecule 52: 30S ribosomal protein S19

Chain 2s:



• Molecule 53: 30S ribosomal protein S20

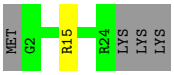
Chain 1t:

• Molecule 53: 30S ribosomal protein S20

Chain 2t:

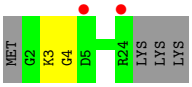
• Molecule 54: 30S ribosomal protein Thx

Chain 1u:



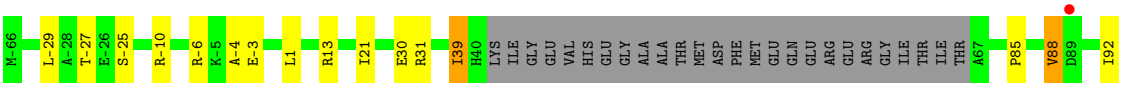
• Molecule 54: 30S ribosomal protein Thx

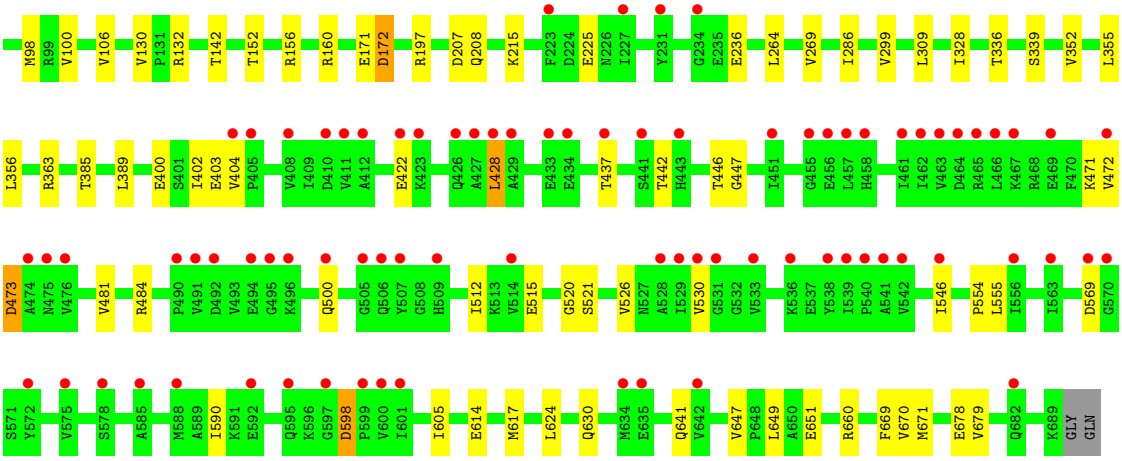
Chain 2u:



• Molecule 55: Chimera protein of 50S ribosomal protein L9 and Elongation factor G

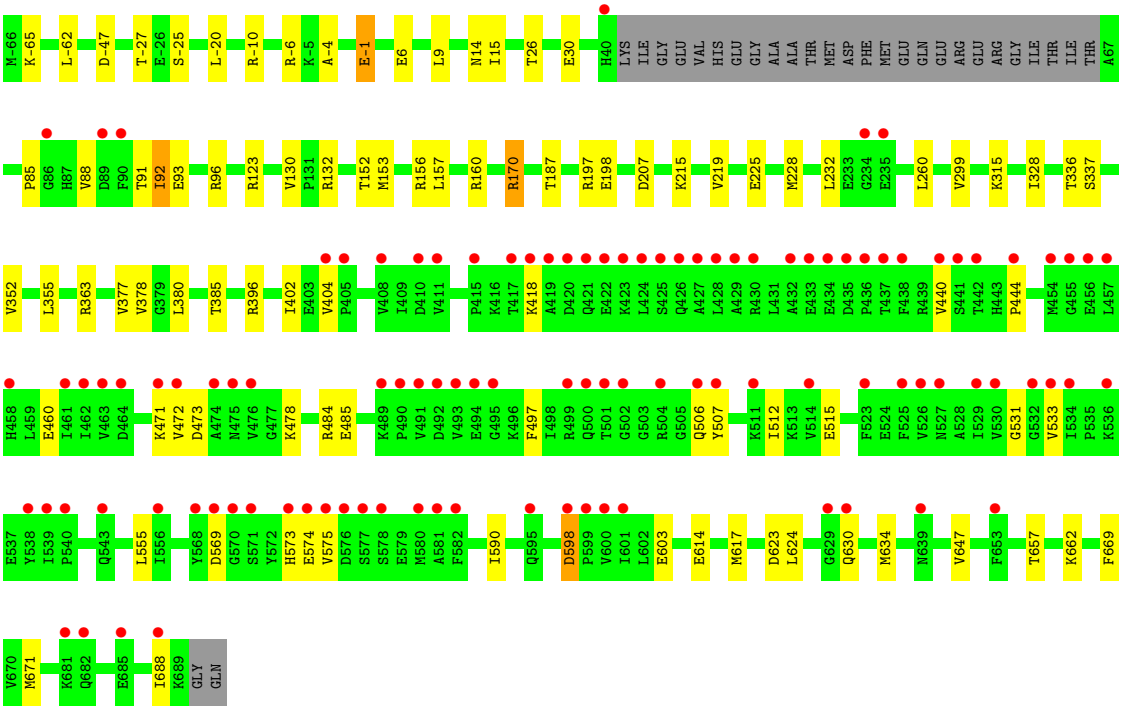
Chain 1z:





• Molecule 55: Chimera protein of 50S ribosomal protein L9 and Elongation factor G

Chain 2z:

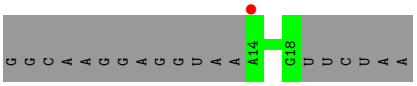


• Molecule 56: mRNA

Chain 1y:

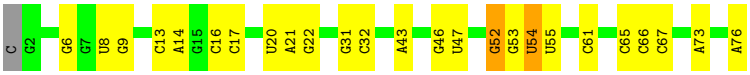
• Molecule 56: mRNA

Chain 2y:



• Molecule 57: P-site tRNA

Chain 1w:



• Molecule 57: P-site tRNA

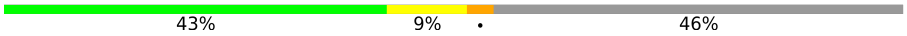
Chain 2w:

• Molecule 58: Cathelicidin-3

Chain 1x:

• Molecule 58: Cathelicidin-3

Chain 2x:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	208.78Å 449.03Å 619.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.48 – 3.00 49.48 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.48-3.00) 99.1 (49.48-3.00)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.208 , 0.265 0.208 , 0.265	Depositor DCC
R_{free} test set	57205 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	55.7	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 66.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	306384	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 4SU, 5MC, SF4, PSU, 5MU, GDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	1A	0.58	4/69281 (0.0%)	0.95	75/108144 (0.1%)
1	2A	0.45	2/69179 (0.0%)	0.92	59/107984 (0.1%)
2	1B	0.47	0/2878	0.93	0/4490
2	2B	0.43	0/2878	0.92	1/4490 (0.0%)
3	1C	0.48	0/1038	0.70	2/1403 (0.1%)
3	2C	0.45	0/1038	0.68	1/1403 (0.1%)
4	1D	0.42	0/2186	0.57	0/2944
4	2D	0.36	0/2192	0.57	0/2951
5	1E	0.42	0/1592	0.56	0/2149
5	2E	0.35	0/1592	0.55	0/2149
6	1F	0.38	0/1619	0.54	0/2193
6	2F	0.34	0/1615	0.55	0/2188
7	1G	0.31	0/1450	0.53	0/1959
7	2G	0.32	0/1449	0.56	0/1958
8	1H	0.34	0/1356	0.53	0/1834
8	2H	0.33	0/1356	0.56	0/1834
9	1J	0.28	0/640	0.59	0/889
9	2J	0.29	0/640	0.55	1/889 (0.1%)
10	1K	0.35	0/504	0.58	0/675
10	2K	0.46	0/503	0.66	0/673
11	1L	0.38	0/1144	0.53	0/1543
11	2L	0.31	0/1144	0.53	0/1543
12	1M	0.40	0/943	0.57	0/1269
12	2M	0.37	0/943	0.54	0/1269
13	1N	0.37	0/1156	0.57	0/1537
13	2N	0.34	0/1152	0.57	0/1533
14	1O	0.41	0/1143	0.52	0/1527
14	2O	0.35	0/1143	0.54	0/1527
15	1P	0.38	0/982	0.59	0/1312
15	2P	0.33	0/982	0.55	0/1312
16	1Q	0.35	0/887	0.57	0/1180
16	2Q	0.33	0/880	0.58	1/1172 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	1R	0.37	0/1105	0.53	0/1477
17	2R	0.33	0/1097	0.54	0/1468
18	1S	0.42	0/977	0.55	0/1301
18	2S	0.32	0/977	0.48	0/1301
19	1T	0.38	0/782	0.54	0/1049
19	2T	0.32	0/782	0.53	0/1049
20	1U	0.39	0/897	0.53	0/1205
20	2U	0.35	0/897	0.52	0/1205
21	1V	0.38	0/764	0.58	1/1025 (0.1%)
21	2V	0.33	0/764	0.55	1/1025 (0.1%)
22	1W	0.39	0/819	0.58	0/1095
22	2W	0.34	0/819	0.56	0/1095
23	1X	0.34	0/1492	0.55	0/2029
23	2X	0.34	0/1486	0.57	0/2022
24	1Y	0.38	0/612	0.57	0/816
24	2Y	0.33	0/609	0.51	0/810
25	1Z	0.37	0/762	0.51	0/1014
25	2Z	0.33	0/762	0.53	0/1014
26	10	0.33	0/590	0.54	0/781
26	20	0.33	0/590	0.51	0/781
27	11	0.41	0/474	0.54	0/635
27	21	0.33	0/469	0.56	0/630
28	12	0.34	0/571	0.64	0/768
28	22	0.37	0/545	0.58	0/737
29	13	0.42	0/469	0.58	0/635
29	23	0.36	0/469	0.53	0/635
30	14	0.46	0/460	0.52	0/613
30	24	0.41	0/456	0.52	0/608
31	15	0.38	0/426	0.54	0/561
31	25	0.34	0/426	0.58	0/561
32	16	0.40	0/525	0.58	0/691
32	26	0.33	0/525	0.52	0/691
33	17	0.43	0/310	0.54	0/407
33	27	0.33	0/310	0.48	0/407
34	1a	0.40	0/35976	0.89	14/56145 (0.0%)
34	2a	0.39	0/36119	0.89	18/56370 (0.0%)
35	1b	0.33	0/1881	0.59	0/2542
35	2b	0.34	0/1860	0.56	0/2518
36	1c	0.29	0/1576	0.50	0/2130
36	2c	0.33	0/1568	0.53	0/2122
37	1d	0.31	0/1689	0.52	0/2267
37	2d	0.30	0/1708	0.54	1/2289 (0.0%)
38	1e	0.32	0/1145	0.52	0/1543

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	2e	0.31	0/1149	0.56	0/1548
39	1f	0.32	0/825	0.53	0/1118
39	2f	0.32	0/833	0.49	0/1128
40	1g	0.29	0/1250	0.48	0/1679
40	2g	0.31	0/1254	0.52	0/1683
41	1h	0.30	0/1108	0.52	0/1494
41	2h	0.29	0/1108	0.55	1/1494 (0.1%)
42	1i	0.30	0/1005	0.51	0/1350
42	2i	0.33	0/997	0.55	0/1343
43	1j	0.29	0/722	0.59	0/982
43	2j	0.33	0/727	0.52	0/988
44	1k	0.33	0/848	0.52	0/1149
44	2k	0.29	0/848	0.52	0/1149
45	1l	0.32	0/946	0.50	0/1274
45	2l	0.33	0/946	0.58	0/1274
46	1m	0.30	0/977	0.55	0/1310
46	2m	0.30	0/961	0.54	0/1291
47	1n	0.31	0/501	0.56	0/664
47	2n	0.31	0/501	0.55	0/664
48	1o	0.32	0/739	0.53	0/985
48	2o	0.31	0/739	0.52	0/985
49	1p	0.30	0/697	0.51	0/939
49	2p	0.30	0/693	0.50	0/935
50	1q	0.33	0/836	0.50	0/1117
50	2q	0.31	0/836	0.50	0/1117
51	1r	0.29	0/560	0.55	1/746 (0.1%)
51	2r	0.31	0/560	0.55	1/746 (0.1%)
52	1s	0.29	0/676	0.53	0/911
52	2s	0.32	0/661	0.60	0/893
53	1t	0.31	0/730	0.54	0/965
53	2t	0.28	0/733	0.49	0/969
54	1u	0.29	0/203	0.54	0/266
54	2u	0.30	0/203	0.48	0/266
55	1z	0.35	0/5792	0.59	1/7844 (0.0%)
55	2z	0.36	0/5792	0.58	0/7844
56	1y	0.47	0/144	0.96	0/222
56	2y	0.59	0/122	1.17	0/188
57	1w	0.57	2/1725 (0.1%)	1.15	22/2689 (0.8%)
57	2w	0.53	0/1725	1.17	20/2689 (0.7%)
58	1x	0.40	0/175	0.68	0/238
58	2x	0.38	0/175	0.98	1/238 (0.4%)
All	All	0.44	8/327047 (0.0%)	0.83	222/487364 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
28	12	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1187	A	N9-C4	-10.39	1.31	1.37
1	1A	1066	A	N9-C4	-6.00	1.34	1.37
57	1w	22	G	N7-C5	5.90	1.42	1.39
1	1A	353	A	N9-C4	-5.88	1.34	1.37
57	1w	46	G	C6-N1	5.85	1.43	1.39
1	2A	552	A	N9-C4	-5.83	1.34	1.37
1	1A	552	A	N9-C4	-5.61	1.34	1.37
1	2A	1187	A	N9-C4	-5.33	1.34	1.37

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	1w	46	G	C6-N1-C2	-11.71	118.07	125.10
57	2w	46	G	C6-N1-C2	-10.97	118.52	125.10
1	1A	1149	C	OP1-P-O3'	-10.93	81.15	105.20
57	1w	22	G	C5-N7-C8	-10.78	98.91	104.30
57	2w	22	G	C5-N7-C8	-10.15	99.22	104.30
1	1A	1066	A	C2-N3-C4	-9.37	105.92	110.60
1	1A	1187	A	C2-N3-C4	-9.16	106.02	110.60
1	1A	1149	C	OP2-P-O3'	-9.00	85.40	105.20
1	1A	2161	C	N1-C2-O2	8.95	124.27	118.90
1	1A	353	A	C2-N3-C4	-8.94	106.13	110.60
1	1A	552	A	C2-N3-C4	-8.91	106.14	110.60
1	2A	552	A	C2-N3-C4	-8.88	106.16	110.60
1	1A	2161	C	N3-C2-O2	-8.67	115.83	121.90
57	2w	14	A	C5-N7-C8	8.64	108.22	103.90
1	1A	1187	A	N3-C4-C5	8.49	132.74	126.80
57	2w	46	G	N3-C2-N2	-8.34	114.06	119.90
1	2A	2164	C	C2-N3-C4	8.33	124.07	119.90
1	1A	2161	C	C2-N1-C1'	8.27	127.90	118.80
1	1A	847	G	O5'-P-OP2	-8.17	98.34	105.70
57	1w	22	G	N7-C8-N9	8.07	117.14	113.10
1	1A	1066	A	N1-C2-N3	8.05	133.32	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	989	A	N1-C6-N6	8.00	123.40	118.60
34	2a	825	U	C5-C6-N1	7.96	126.68	122.70
34	2a	1238	A	N1-C6-N6	7.92	123.35	118.60
57	2w	14	A	C4-C5-C6	7.90	120.95	117.00
1	1A	989	A	N1-C6-N6	7.89	123.34	118.60
57	2w	46	G	N9-C4-C5	7.86	108.55	105.40
1	1A	1153	U	C5-C6-N1	7.80	126.60	122.70
1	1A	138	A	N7-C8-N9	7.79	117.69	113.80
57	1w	46	G	C5-C6-N1	7.76	115.38	111.50
57	2w	22	G	N7-C8-N9	7.75	116.97	113.10
1	2A	11	U	C2-N1-C1'	7.62	126.85	117.70
57	1w	22	G	C4-C5-C6	-7.59	114.25	118.80
1	2A	2124	C	C2-N3-C4	7.58	123.69	119.90
1	2A	11	U	N1-C2-O2	7.52	128.07	122.80
1	1A	1310	A	O5'-P-OP2	-7.51	98.94	105.70
1	1A	2161	C	C6-N1-C2	-7.50	117.30	120.30
1	2A	2188	U	N3-C2-O2	-7.46	116.98	122.20
1	1A	1694	C	O5'-P-OP1	-7.33	99.10	105.70
57	1w	46	G	C5-C6-O6	-7.30	124.22	128.60
1	1A	1187	A	N3-C4-N9	-7.29	121.56	127.40
1	1A	2609	A	O5'-P-OP1	-7.25	99.17	105.70
3	2C	209	LEU	CA-CB-CG	7.19	131.84	115.30
1	2A	2188	U	N1-C2-O2	7.15	127.81	122.80
34	2a	1137	G	C5-C6-O6	7.13	132.88	128.60
1	2A	11	U	N3-C2-O2	-7.11	117.22	122.20
55	1z	428	LEU	CA-CB-CG	6.97	131.33	115.30
57	1w	22	G	N1-C6-O6	-6.93	115.74	119.90
1	2A	2157	C	N1-C2-O2	6.89	123.03	118.90
34	2a	1238	A	N9-C4-C5	-6.88	103.05	105.80
1	1A	1358	U	C2-N1-C1'	6.87	125.95	117.70
57	1w	14	A	C4-C5-C6	6.87	120.44	117.00
1	1A	536	G	O4'-C1'-N9	6.86	113.69	108.20
34	1a	1011	C	C2-N1-C1'	6.82	126.31	118.80
1	1A	138	A	C8-N9-C4	-6.81	103.08	105.80
1	2A	989	A	C4-C5-N7	6.80	114.10	110.70
57	1w	14	A	C5-N7-C8	6.79	107.29	103.90
1	1A	1538	C	N1-C2-O2	6.78	122.97	118.90
34	1a	975	U	C5-C4-O4	6.78	129.97	125.90
1	2A	138	A	C8-N9-C4	-6.77	103.09	105.80
1	1A	989	A	C6-C5-N7	-6.72	127.60	132.30
57	2w	46	G	C4-C5-N7	-6.70	108.12	110.80
1	1A	1111	U	N3-C2-O2	-6.69	117.52	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1359	C	C2-N1-C1'	6.69	126.16	118.80
1	2A	989	A	O4'-C1'-N9	6.65	113.52	108.20
1	2A	2197	A	N1-C6-N6	-6.65	114.61	118.60
1	1A	1150	U	OP1-P-OP2	6.61	129.51	119.60
1	2A	1187	A	C2-N3-C4	-6.57	107.31	110.60
1	1A	1111	U	N1-C2-O2	6.54	127.38	122.80
57	2w	22	G	C4-C5-C6	-6.51	114.89	118.80
1	1A	1067	G	N3-C4-N9	-6.51	122.09	126.00
1	2A	2188	U	C2-N1-C1'	6.50	125.50	117.70
34	1a	1133	U	C2-N3-C4	6.48	130.89	127.00
34	2a	1238	A	C5-C6-N6	-6.47	118.53	123.70
1	2A	2197	A	C5-C6-N6	6.43	128.85	123.70
1	2A	138	A	N7-C8-N9	6.40	117.00	113.80
1	2A	989	A	C5-N7-C8	-6.33	100.73	103.90
34	2a	1141	C	C2-N1-C1'	6.32	125.75	118.80
34	1a	1106	A	C6-N1-C2	6.24	122.35	118.60
1	2A	989	A	C6-C5-N7	-6.24	127.93	132.30
57	2w	22	G	C4-C5-N7	6.24	113.30	110.80
57	2w	22	G	C5-C6-N1	6.23	114.62	111.50
1	1A	138	A	C5-N7-C8	-6.18	100.81	103.90
34	1a	1011	C	C6-N1-C2	-6.12	117.85	120.30
34	2a	983	A	O4'-C1'-N9	6.11	113.09	108.20
16	2Q	78	LEU	CA-CB-CG	6.10	129.34	115.30
1	2A	2512	C	C2-N1-C1'	-6.09	112.10	118.80
1	1A	2013	G	P-O3'-C3'	6.09	127.01	119.70
1	2A	138	A	O4'-C1'-N9	6.08	113.07	108.20
57	2w	46	G	C5-C6-N1	6.08	114.54	111.50
1	1A	1066	A	C5-N7-C8	-6.07	100.86	103.90
1	2A	2164	C	C5-C6-N1	6.05	124.03	121.00
1	1A	2700	U	N3-C2-O2	-6.03	117.98	122.20
57	2w	46	G	N1-C2-N3	6.02	127.51	123.90
1	2A	2485	C	C2-N1-C1'	6.02	125.42	118.80
1	1A	1066	A	N7-C8-N9	5.99	116.80	113.80
3	1C	62	VAL	CB-CA-C	5.97	122.75	111.40
1	1A	1538	C	N3-C2-O2	-5.97	117.72	121.90
1	1A	11	U	C2-N1-C1'	5.95	124.84	117.70
57	1w	22	G	N3-C4-N9	-5.93	122.44	126.00
1	1A	1153	U	C2-N1-C1'	5.91	124.80	117.70
1	1A	989	A	N9-C4-C5	-5.90	103.44	105.80
1	1A	2696	G	N1-C6-O6	-5.90	116.36	119.90
34	2a	66	U	P-O3'-C3'	5.90	126.78	119.70
34	2a	1238	A	O4'-C1'-N9	-5.90	103.48	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1248	A	O4'-C1'-N9	5.89	112.92	108.20
57	1w	22	G	C5-C6-N1	5.87	114.44	111.50
1	1A	977	A	C5-N7-C8	-5.86	100.97	103.90
1	2A	2169	G	C6-N1-C2	5.83	128.59	125.10
34	1a	1015	G	C5-C6-O6	5.82	132.09	128.60
1	1A	214	G	O4'-C1'-N9	5.81	112.85	108.20
34	1a	1026	C	C2-N1-C1'	5.78	125.16	118.80
1	2A	552	A	N1-C2-N3	5.78	132.19	129.30
34	1a	981	G	N3-C4-N9	5.76	129.46	126.00
57	2w	14	A	C5-C6-N1	-5.76	114.82	117.70
1	1A	2297	A	N7-C8-N9	5.73	116.66	113.80
34	2a	1141	C	N1-C2-O2	5.72	122.33	118.90
57	1w	22	G	C4-C5-N7	5.71	113.08	110.80
2	2B	1	U	C2-N1-C1'	5.71	124.55	117.70
34	2a	891	A	P-O3'-C3'	5.69	126.53	119.70
21	1V	57	LEU	CA-CB-CG	5.67	128.33	115.30
1	1A	2057	C	O5'-P-OP1	-5.64	100.62	105.70
1	1A	552	A	N3-C4-N9	-5.64	122.89	127.40
1	1A	1439	U	O5'-P-OP1	-5.62	100.64	105.70
57	2w	22	G	C8-N9-C1'	5.61	134.30	127.00
1	2A	300	C	C2-N1-C1'	5.61	124.97	118.80
1	2A	989	A	N9-C4-C5	-5.60	103.56	105.80
1	1A	598	U	O5'-P-OP1	-5.59	100.67	105.70
1	1A	989	A	C2-N3-C4	-5.59	107.80	110.60
1	1A	1404	A	N1-C2-N3	-5.59	126.50	129.30
58	2x	10	LEU	CA-CB-CG	5.59	128.15	115.30
1	1A	989	A	C4-C5-N7	5.57	113.48	110.70
1	1A	1066	A	C8-N9-C4	-5.57	103.57	105.80
9	2J	76	GLY	C-N-CA	5.57	145.37	122.00
1	2A	2485	C	N1-C2-O2	5.55	122.23	118.90
1	1A	2402	G	O4'-C1'-N9	5.54	112.64	108.20
34	2a	1047	G	P-O3'-C3'	5.54	126.35	119.70
1	2A	1358	U	C2-N1-C1'	5.54	124.35	117.70
1	1A	2512	C	C2-N1-C1'	-5.53	112.72	118.80
34	2a	514	G	C4-N9-C1'	5.52	133.67	126.50
1	1A	1219	U	P-O3'-C3'	5.49	126.29	119.70
1	1A	2263	G	N3-C4-N9	-5.49	122.70	126.00
1	2A	2450	A	O4'-C1'-N9	-5.48	103.82	108.20
1	1A	1067	G	N9-C4-C5	5.46	107.58	105.40
57	1w	46	G	N1-C2-N3	5.46	127.17	123.90
1	2A	552	A	N3-C4-C5	5.46	130.62	126.80
1	2A	1604	A	P-O3'-C3'	5.46	126.25	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	1w	46	G	N3-C2-N2	-5.45	116.08	119.90
1	1A	2203	G	C5-C6-O6	5.44	131.87	128.60
1	1A	1417	U	C5-C4-O4	-5.44	122.64	125.90
1	1A	353	A	N1-C2-N3	5.43	132.02	129.30
1	1A	1440	A	O4'-C1'-N9	5.43	112.55	108.20
57	1w	14	A	C5-C6-N1	-5.43	114.99	117.70
1	2A	2204	C	C2-N3-C4	5.42	122.61	119.90
37	2d	194	LEU	CA-CB-CG	5.41	127.74	115.30
1	2A	2485	C	C6-N1-C1'	-5.40	114.32	120.80
34	2a	970	U	P-O3'-C3'	5.40	126.18	119.70
21	2V	57	LEU	CA-CB-CG	5.40	127.71	115.30
1	2A	942	C	N1-C2-O2	5.39	122.13	118.90
34	1a	732	C	P-O3'-C3'	5.38	126.16	119.70
34	1a	1008	C	C5-C4-N4	5.37	123.96	120.20
57	1w	14	A	C4-C5-N7	-5.36	108.02	110.70
57	1w	46	G	N9-C4-C5	5.36	107.55	105.40
1	1A	1067	G	N3-C2-N2	-5.36	116.15	119.90
57	2w	22	G	C8-N9-C4	-5.36	104.26	106.40
1	2A	2700	U	P-O3'-C3'	5.35	126.12	119.70
34	2a	969	U	P-O3'-C3'	5.35	126.12	119.70
41	2h	107	LEU	CA-CB-CG	5.35	127.61	115.30
1	2A	1066	A	C2-N3-C4	-5.34	107.93	110.60
1	2A	1659	A	O5'-P-OP1	-5.32	100.91	105.70
1	1A	2297	A	C5-N7-C8	-5.32	101.24	103.90
57	2w	14	A	C4-C5-N7	-5.32	108.04	110.70
1	1A	1461	G	O4'-C1'-N9	5.30	112.44	108.20
1	2A	2082	G	O5'-P-OP2	-5.29	100.94	105.70
57	2w	14	A	C4-N9-C1'	5.29	135.81	126.30
1	2A	11	U	C6-N1-C1'	-5.28	113.81	121.20
1	1A	989	A	C5-C6-N6	-5.27	119.49	123.70
34	1a	262	G	P-O3'-C3'	5.26	126.01	119.70
34	2a	1334	C	N1-C2-O2	-5.26	115.75	118.90
1	2A	1958	A	O4'-C1'-N9	5.25	112.40	108.20
1	2A	977	A	C5-N7-C8	-5.25	101.28	103.90
34	1a	1183	A	P-O3'-C3'	5.25	126.00	119.70
57	2w	14	A	C8-N9-C1'	-5.25	118.25	127.70
1	2A	2149	C	N1-C2-O2	5.24	122.05	118.90
57	1w	14	A	C4-N9-C1'	5.24	135.73	126.30
57	1w	22	G	C8-N9-C1'	5.24	133.81	127.00
1	2A	2080	A	O4'-C1'-N9	5.24	112.39	108.20
1	1A	2208	G	C5-C6-O6	5.23	131.74	128.60
1	2A	1145	C	C2-N1-C1'	5.23	124.55	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	11	U	O4'-C1'-N1	-5.22	104.03	108.20
1	1A	1744	A	O4'-C1'-N9	5.21	112.37	108.20
1	1A	1122	A	O4'-C1'-N9	5.21	112.37	108.20
1	2A	191	C	N1-C2-O2	-5.21	115.77	118.90
34	1a	899	U	C2-N3-C4	5.21	130.12	127.00
1	1A	253	A	O4'-C1'-N9	5.20	112.36	108.20
1	2A	989	A	C5-C6-N6	-5.20	119.54	123.70
1	2A	193	G	C8-N9-C4	5.20	108.48	106.40
1	2A	977	A	N7-C8-N9	5.19	116.40	113.80
34	1a	825	U	C5-C6-N1	5.19	125.29	122.70
57	1w	52	G	N3-C4-C5	-5.18	126.01	128.60
1	2A	2198	C	C6-N1-C2	-5.15	118.24	120.30
3	1C	62	VAL	CA-C-N	5.15	128.53	117.20
57	1w	14	A	C8-N9-C1'	-5.13	118.47	127.70
1	1A	2197	A	N1-C6-N6	-5.12	115.53	118.60
1	2A	138	A	C5-N7-C8	-5.12	101.34	103.90
51	2r	31	LEU	CA-CB-CG	5.12	127.08	115.30
1	1A	552	A	N1-C2-N3	5.12	131.86	129.30
51	1r	31	LEU	CA-CB-CG	5.11	127.06	115.30
1	2A	1699	G	P-O3'-C3'	5.10	125.81	119.70
34	2a	1165	A	P-O3'-C3'	5.09	125.81	119.70
1	2A	830	A	O4'-C1'-N9	5.09	112.27	108.20
1	1A	2161	C	C6-N1-C1'	-5.08	114.71	120.80
34	2a	975	U	C5-C4-O4	5.06	128.94	125.90
1	2A	2169	G	C5-C6-O6	5.06	131.64	128.60
57	1w	22	G	C8-N9-C4	-5.06	104.38	106.40
1	2A	1404	A	N1-C2-N3	-5.06	126.77	129.30
57	2w	46	G	C8-N9-C4	-5.05	104.38	106.40
1	1A	1220	G	P-O3'-C3'	5.04	125.75	119.70
1	2A	2122	G	N3-C4-C5	-5.03	126.08	128.60
1	2A	2904	C	N1-C2-O2	5.03	121.92	118.90
1	1A	353	A	N3-C4-C5	5.02	130.31	126.80
1	2A	2207	G	C6-N1-C2	5.01	128.11	125.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	12	59	PHE	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	1C	129/229 (56%)	96 (74%)	25 (19%)	8 (6%)	1 8
3	2C	129/229 (56%)	96 (74%)	26 (20%)	7 (5%)	2 11
4	1D	273/276 (99%)	258 (94%)	12 (4%)	3 (1%)	14 50
4	2D	273/276 (99%)	253 (93%)	16 (6%)	4 (2%)	10 42
5	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29 68
5	2E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	29 68
6	1F	201/210 (96%)	192 (96%)	8 (4%)	1 (0%)	29 68
6	2F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	29 68
7	1G	179/182 (98%)	162 (90%)	16 (9%)	1 (1%)	25 64
7	2G	179/182 (98%)	160 (89%)	16 (9%)	3 (2%)	9 39
8	1H	172/180 (96%)	159 (92%)	12 (7%)	1 (1%)	25 64
8	2H	172/180 (96%)	159 (92%)	12 (7%)	1 (1%)	25 64
9	1J	128/173 (74%)	71 (56%)	37 (29%)	20 (16%)	0 1
9	2J	128/173 (74%)	81 (63%)	26 (20%)	21 (16%)	0 1
10	1K	65/147 (44%)	52 (80%)	11 (17%)	2 (3%)	4 23
10	2K	64/147 (44%)	45 (70%)	17 (27%)	2 (3%)	4 23
11	1L	138/140 (99%)	135 (98%)	3 (2%)	0	100 100
11	2L	138/140 (99%)	134 (97%)	3 (2%)	1 (1%)	22 60
12	1M	120/122 (98%)	114 (95%)	6 (5%)	0	100 100
12	2M	120/122 (98%)	113 (94%)	7 (6%)	0	100 100
13	1N	147/150 (98%)	139 (95%)	6 (4%)	2 (1%)	11 43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	2N	147/150 (98%)	139 (95%)	5 (3%)	3 (2%)	7	34
14	1O	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	22	60
14	2O	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	11	43
15	1P	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
15	2P	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
16	1Q	108/112 (96%)	97 (90%)	9 (8%)	2 (2%)	8	36
16	2Q	108/112 (96%)	98 (91%)	8 (7%)	2 (2%)	8	36
17	1R	129/146 (88%)	118 (92%)	9 (7%)	2 (2%)	9	40
17	2R	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
18	1S	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
18	2S	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
19	1T	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	53
19	2T	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	7	34
20	1U	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
20	2U	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
21	1V	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	14	50
21	2V	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	14	50
22	1W	105/110 (96%)	92 (88%)	12 (11%)	1 (1%)	15	53
22	2W	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
23	1X	184/206 (89%)	164 (89%)	17 (9%)	3 (2%)	9	40
23	2X	184/206 (89%)	161 (88%)	20 (11%)	3 (2%)	9	40
24	1Y	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
24	2Y	73/85 (86%)	70 (96%)	3 (4%)	0	100	100
25	1Z	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	14	50
25	2Z	95/98 (97%)	89 (94%)	5 (5%)	1 (1%)	14	50
26	10	68/72 (94%)	64 (94%)	3 (4%)	1 (2%)	10	42
26	20	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
27	11	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
27	21	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	12	67/71 (94%)	51 (76%)	13 (19%)	3 (4%)	2	14
28	22	67/71 (94%)	49 (73%)	12 (18%)	6 (9%)	1	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
29	23	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
30	14	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
30	24	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
31	15	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
31	25	46/49 (94%)	44 (96%)	0	2 (4%)	2	15
32	16	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
32	26	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
33	17	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	27	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
35	1b	229/256 (90%)	193 (84%)	27 (12%)	9 (4%)	3	17
35	2b	229/256 (90%)	193 (84%)	28 (12%)	8 (4%)	3	20
36	1c	204/239 (85%)	181 (89%)	20 (10%)	3 (2%)	10	42
36	2c	204/239 (85%)	185 (91%)	14 (7%)	5 (2%)	5	28
37	1d	206/209 (99%)	184 (89%)	22 (11%)	0	100	100
37	2d	206/209 (99%)	182 (88%)	24 (12%)	0	100	100
38	1e	146/162 (90%)	133 (91%)	13 (9%)	0	100	100
38	2e	146/162 (90%)	134 (92%)	11 (8%)	1 (1%)	22	60
39	1f	98/101 (97%)	92 (94%)	5 (5%)	1 (1%)	15	53
39	2f	98/101 (97%)	92 (94%)	5 (5%)	1 (1%)	15	53
40	1g	153/156 (98%)	139 (91%)	13 (8%)	1 (1%)	22	60
40	2g	153/156 (98%)	140 (92%)	9 (6%)	4 (3%)	5	27
41	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
41	2h	135/138 (98%)	126 (93%)	8 (6%)	1 (1%)	22	60
42	1i	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	19	57
42	2i	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	19	57
43	1j	95/105 (90%)	81 (85%)	9 (10%)	5 (5%)	2	11
43	2j	94/105 (90%)	83 (88%)	8 (8%)	3 (3%)	4	22
44	1k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	17	55
44	2k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	17	55
45	1l	120/132 (91%)	114 (95%)	6 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	2l	120/132 (91%)	112 (93%)	7 (6%)	1 (1%)	19	57
46	1m	121/126 (96%)	107 (88%)	12 (10%)	2 (2%)	9	39
46	2m	120/126 (95%)	106 (88%)	13 (11%)	1 (1%)	19	57
47	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
47	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
48	1o	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	6	30
48	2o	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	6	30
49	1p	80/88 (91%)	75 (94%)	5 (6%)	0	100	100
49	2p	80/88 (91%)	75 (94%)	5 (6%)	0	100	100
50	1q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
50	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
51	1r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
51	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
52	1s	82/93 (88%)	70 (85%)	12 (15%)	0	100	100
52	2s	81/93 (87%)	70 (86%)	8 (10%)	3 (4%)	3	19
53	1t	94/106 (89%)	85 (90%)	5 (5%)	4 (4%)	2	15
53	2t	94/106 (89%)	87 (93%)	5 (5%)	2 (2%)	7	33
54	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
54	2u	21/27 (78%)	17 (81%)	2 (10%)	2 (10%)	0	3
55	1z	726/758 (96%)	610 (84%)	92 (13%)	24 (3%)	4	21
55	2z	726/758 (96%)	609 (84%)	95 (13%)	22 (3%)	4	24
58	1x	17/35 (49%)	16 (94%)	0	1 (6%)	1	9
58	2x	17/35 (49%)	13 (76%)	1 (6%)	3 (18%)	0	0
All	All	13263/14516 (91%)	11963 (90%)	1067 (8%)	233 (2%)	8	37

All (233) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	1C	175	VAL
3	1C	224	ILE
6	1F	130	ALA
7	1G	51	ARG
8	1H	126	PRO
9	1J	29	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	1J	74	LEU
9	1J	77	PRO
9	1J	80	VAL
9	1J	104	ILE
9	1J	105	PRO
9	1J	125	LEU
10	1K	87	GLY
10	1K	89	HIS
16	1Q	59	LYS
28	12	49	PHE
28	12	53	GLU
35	1b	9	GLU
35	1b	16	HIS
35	1b	17	PHE
35	1b	125	PRO
35	1b	231	GLU
35	1b	232	PRO
42	1i	54	ASP
43	1j	55	LYS
43	1j	56	HIS
46	1m	3	ARG
55	1z	-25	SER
55	1z	172	ASP
55	1z	400	GLU
55	1z	402	ILE
55	1z	404	VAL
55	1z	472	VAL
55	1z	473	ASP
55	1z	617	MET
3	2C	51	PRO
3	2C	52	ARG
3	2C	224	ILE
4	2D	275	LYS
6	2F	21	ALA
7	2G	51	ARG
7	2G	81	LYS
7	2G	181	ARG
8	2H	126	PRO
9	2J	33	PRO
9	2J	39	ALA
9	2J	53	VAL
9	2J	71	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	2J	74	LEU
9	2J	77	PRO
9	2J	106	GLN
10	2K	89	HIS
28	22	46	GLN
28	22	62	ARG
31	25	46	VAL
35	2b	121	LEU
35	2b	125	PRO
36	2c	101	LEU
40	2g	4	ARG
40	2g	33	ASP
40	2g	79	ARG
42	2i	54	ASP
44	2k	106	LYS
46	2m	107	ALA
52	2s	30	LEU
54	2u	3	LYS
55	2z	92	ILE
55	2z	153	MET
55	2z	402	ILE
55	2z	472	VAL
55	2z	617	MET
3	1C	196	LEU
9	1J	20	ALA
9	1J	31	GLY
9	1J	33	PRO
9	1J	66	LEU
9	1J	78	SER
9	1J	91	LYS
9	1J	93	LEU
9	1J	101	PRO
9	1J	107	VAL
9	1J	132	ASP
14	1O	59	ARG
21	1V	94	GLY
23	1X	152	ALA
23	1X	172	ALA
35	1b	37	ASN
39	1f	40	VAL
40	1g	79	ARG
43	1j	31	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	1j	75	ILE
43	1j	80	LYS
46	1m	118	ALA
53	1t	47	GLY
53	1t	96	GLY
53	1t	100	ILE
55	1z	88	VAL
55	1z	269	VAL
55	1z	446	THR
55	1z	447	GLY
55	1z	555	LEU
3	2C	68	LEU
4	2D	3	VAL
4	2D	239	ARG
9	2J	69	PRO
9	2J	80	VAL
9	2J	84	GLU
9	2J	93	LEU
9	2J	94	VAL
9	2J	107	VAL
9	2J	113	GLN
19	2T	79	VAL
21	2V	94	GLY
23	2X	175	VAL
28	22	45	GLY
35	2b	9	GLU
35	2b	10	LEU
36	2c	107	GLN
36	2c	181	ASN
43	2j	78	ASN
45	2l	28	LYS
48	2o	19	PRO
53	2t	47	GLY
55	2z	-25	SER
55	2z	88	VAL
55	2z	93	GLU
55	2z	380	LEU
55	2z	671	MET
58	2x	14	ARG
3	1C	68	LEU
3	1C	172	HIS
3	1C	183	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	1J	56	ASN
13	1N	122	PRO
36	1c	65	ALA
48	1o	19	PRO
55	1z	-4	ALA
55	1z	39	ILE
55	1z	85	PRO
55	1z	171	GLU
55	1z	554	PRO
55	1z	671	MET
9	2J	91	LYS
9	2J	126	ALA
10	2K	113	PRO
13	2N	29	LYS
16	2Q	84	GLN
19	2T	53	GLU
23	2X	114	GLY
25	2Z	3	LYS
28	22	60	GLN
31	25	45	ALA
38	2e	37	ARG
43	2j	75	ILE
48	2o	23	GLY
54	2u	4	GLY
55	2z	-1	GLU
55	2z	85	PRO
55	2z	170	ARG
55	2z	404	VAL
4	1D	275	LYS
5	1E	52	LEU
9	1J	124	ALA
13	1N	29	LYS
17	1R	128	GLU
19	1T	79	VAL
23	1X	157	LEU
48	1o	23	GLY
53	1t	102	GLY
55	1z	521	SER
58	1x	18	LEU
3	2C	172	HIS
5	2E	52	LEU
9	2J	30	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	2N	122	PRO
14	2O	27	VAL
14	2O	59	ARG
35	2b	20	GLU
36	2c	70	VAL
36	2c	108	ASN
52	2s	25	LYS
55	2z	-65	LYS
55	2z	460	GLU
58	2x	4	ARG
3	1C	178	ALA
9	1J	114	GLY
16	1Q	60	GLY
22	1W	54	LYS
26	10	69	ARG
35	1b	121	LEU
36	1c	66	VAL
55	1z	403	GLU
55	1z	471	LYS
9	2J	54	ALA
9	2J	68	LEU
11	2L	2	LYS
13	2N	45	LEU
23	2X	157	LEU
28	22	44	THR
28	22	68	ARG
35	2b	120	ALA
39	2f	40	VAL
41	2h	73	ASP
52	2s	13	ASP
55	2z	-4	ALA
3	1C	62	VAL
4	1D	125	ILE
4	1D	156	ALA
17	1R	129	ARG
25	1Z	81	LYS
35	1b	20	GLU
55	1z	520	GLY
55	1z	598	ASP
35	2b	232	PRO
53	2t	100	ILE
55	2z	506	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	2z	531	GLY
44	1k	105	VAL
3	2C	171	ILE
4	2D	125	ILE
9	2J	59	ILE
35	2b	227	GLY
55	2z	533	VAL
16	2Q	85	VAL
9	2J	73	GLY
55	2z	444	PRO
55	2z	598	ASP
58	2x	10	LEU
28	12	54	GLY
36	1c	70	VAL
40	2g	55	GLY
43	2j	77	PRO
3	2C	65	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1C	103/181 (57%)	89 (86%)	14 (14%)	3 17
3	2C	103/181 (57%)	88 (85%)	15 (15%)	3 15
4	1D	215/218 (99%)	195 (91%)	20 (9%)	9 33
4	2D	216/218 (99%)	200 (93%)	16 (7%)	13 44
5	1E	164/166 (99%)	151 (92%)	13 (8%)	12 41
5	2E	164/166 (99%)	147 (90%)	17 (10%)	7 27
6	1F	160/166 (96%)	141 (88%)	19 (12%)	5 22
6	2F	159/166 (96%)	143 (90%)	16 (10%)	7 29
7	1G	143/156 (92%)	123 (86%)	20 (14%)	3 16
7	2G	142/156 (91%)	119 (84%)	23 (16%)	2 12
8	1H	144/148 (97%)	136 (94%)	8 (6%)	21 56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	2H	144/148 (97%)	127 (88%)	17 (12%)	5	22
10	1K	50/111 (45%)	40 (80%)	10 (20%)	1	7
10	2K	50/111 (45%)	38 (76%)	12 (24%)	0	3
11	1L	118/119 (99%)	108 (92%)	10 (8%)	10	38
11	2L	118/119 (99%)	107 (91%)	11 (9%)	9	33
12	1M	100/100 (100%)	94 (94%)	6 (6%)	19	53
12	2M	100/100 (100%)	89 (89%)	11 (11%)	6	25
13	1N	116/116 (100%)	104 (90%)	12 (10%)	7	28
13	2N	115/116 (99%)	106 (92%)	9 (8%)	12	42
14	1O	111/111 (100%)	102 (92%)	9 (8%)	11	40
14	2O	111/111 (100%)	101 (91%)	10 (9%)	9	35
15	1P	101/101 (100%)	83 (82%)	18 (18%)	2	9
15	2P	101/101 (100%)	85 (84%)	16 (16%)	2	12
16	1Q	87/88 (99%)	80 (92%)	7 (8%)	12	40
16	2Q	85/88 (97%)	75 (88%)	10 (12%)	5	22
17	1R	115/127 (91%)	103 (90%)	12 (10%)	7	27
17	2R	113/127 (89%)	102 (90%)	11 (10%)	8	31
18	1S	93/94 (99%)	83 (89%)	10 (11%)	6	26
18	2S	93/94 (99%)	87 (94%)	6 (6%)	17	50
19	1T	80/82 (98%)	70 (88%)	10 (12%)	4	20
19	2T	80/82 (98%)	73 (91%)	7 (9%)	10	36
20	1U	90/92 (98%)	83 (92%)	7 (8%)	12	42
20	2U	90/92 (98%)	83 (92%)	7 (8%)	12	42
21	1V	77/78 (99%)	71 (92%)	6 (8%)	12	42
21	2V	77/78 (99%)	75 (97%)	2 (3%)	46	78
22	1W	85/91 (93%)	80 (94%)	5 (6%)	19	54
22	2W	85/91 (93%)	76 (89%)	9 (11%)	6	26
23	1X	157/179 (88%)	140 (89%)	17 (11%)	6	26
23	2X	156/179 (87%)	139 (89%)	17 (11%)	6	25
24	1Y	61/67 (91%)	55 (90%)	6 (10%)	8	30
24	2Y	60/67 (90%)	56 (93%)	4 (7%)	16	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	1Z	80/83 (96%)	73 (91%)	7 (9%)	10	36
25	2Z	80/83 (96%)	72 (90%)	8 (10%)	7	29
26	10	65/67 (97%)	60 (92%)	5 (8%)	13	42
26	20	65/67 (97%)	56 (86%)	9 (14%)	3	17
27	11	51/52 (98%)	46 (90%)	5 (10%)	8	30
27	21	50/52 (96%)	45 (90%)	5 (10%)	7	29
28	12	60/63 (95%)	48 (80%)	12 (20%)	1	7
28	22	53/63 (84%)	42 (79%)	11 (21%)	1	5
29	13	50/52 (96%)	45 (90%)	5 (10%)	7	29
29	23	50/52 (96%)	44 (88%)	6 (12%)	5	22
30	14	51/52 (98%)	46 (90%)	5 (10%)	8	30
30	24	50/52 (96%)	45 (90%)	5 (10%)	7	29
31	15	41/42 (98%)	39 (95%)	2 (5%)	25	61
31	25	41/42 (98%)	39 (95%)	2 (5%)	25	61
32	16	54/55 (98%)	49 (91%)	5 (9%)	9	33
32	26	54/55 (98%)	49 (91%)	5 (9%)	9	33
33	17	34/34 (100%)	34 (100%)	0	100	100
33	27	34/34 (100%)	33 (97%)	1 (3%)	42	76
35	1b	192/220 (87%)	170 (88%)	22 (12%)	5	24
35	2b	187/220 (85%)	171 (91%)	16 (9%)	10	37
36	1c	143/188 (76%)	135 (94%)	8 (6%)	21	56
36	2c	141/188 (75%)	128 (91%)	13 (9%)	9	34
37	1d	170/181 (94%)	153 (90%)	17 (10%)	7	29
37	2d	174/181 (96%)	158 (91%)	16 (9%)	9	34
38	1e	113/123 (92%)	101 (89%)	12 (11%)	6	26
38	2e	114/123 (93%)	106 (93%)	8 (7%)	15	47
39	1f	84/90 (93%)	76 (90%)	8 (10%)	8	32
39	2f	86/90 (96%)	80 (93%)	6 (7%)	15	47
40	1g	119/127 (94%)	110 (92%)	9 (8%)	13	43
40	2g	120/127 (94%)	110 (92%)	10 (8%)	11	39
41	1h	114/119 (96%)	99 (87%)	15 (13%)	4	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	2h	114/119 (96%)	96 (84%)	18 (16%)	2	12
42	1i	91/99 (92%)	79 (87%)	12 (13%)	4	18
42	2i	89/99 (90%)	74 (83%)	15 (17%)	2	11
43	1j	66/92 (72%)	61 (92%)	5 (8%)	13	43
43	2j	69/92 (75%)	67 (97%)	2 (3%)	42	76
44	1k	83/99 (84%)	77 (93%)	6 (7%)	14	45
44	2k	83/99 (84%)	80 (96%)	3 (4%)	35	70
45	1l	97/109 (89%)	90 (93%)	7 (7%)	14	45
45	2l	97/109 (89%)	89 (92%)	8 (8%)	11	39
46	1m	95/101 (94%)	84 (88%)	11 (12%)	5	23
46	2m	92/101 (91%)	82 (89%)	10 (11%)	6	25
47	1n	49/50 (98%)	42 (86%)	7 (14%)	3	15
47	2n	49/50 (98%)	42 (86%)	7 (14%)	3	15
48	1o	78/80 (98%)	73 (94%)	5 (6%)	17	51
48	2o	78/80 (98%)	70 (90%)	8 (10%)	7	28
49	1p	69/74 (93%)	62 (90%)	7 (10%)	7	29
49	2p	68/74 (92%)	59 (87%)	9 (13%)	4	18
50	1q	94/97 (97%)	89 (95%)	5 (5%)	22	58
50	2q	94/97 (97%)	87 (93%)	7 (7%)	13	44
51	1r	59/77 (77%)	55 (93%)	4 (7%)	16	48
51	2r	59/77 (77%)	55 (93%)	4 (7%)	16	48
52	1s	70/80 (88%)	61 (87%)	9 (13%)	4	19
52	2s	67/80 (84%)	62 (92%)	5 (8%)	13	43
53	1t	70/82 (85%)	62 (89%)	8 (11%)	5	24
53	2t	71/82 (87%)	65 (92%)	6 (8%)	10	38
54	1u	18/22 (82%)	17 (94%)	1 (6%)	21	56
54	2u	18/22 (82%)	18 (100%)	0	100	100
55	1z	609/636 (96%)	538 (88%)	71 (12%)	5	22
55	2z	609/636 (96%)	534 (88%)	75 (12%)	4	21
58	1x	19/34 (56%)	17 (90%)	2 (10%)	7	27
58	2x	19/34 (56%)	18 (95%)	1 (5%)	22	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	10695/11742 (91%)	9614 (90%)	1081 (10%)	7 29

All (1081) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1C	6	ARG
3	1C	37	PHE
3	1C	46	LYS
3	1C	49	ILE
3	1C	55	ASP
3	1C	59	ARG
3	1C	68	LEU
3	1C	164	ARG
3	1C	183	GLU
3	1C	196	LEU
3	1C	209	LEU
3	1C	210	ARG
3	1C	211	SER
3	1C	215	THR
4	1D	27	THR
4	1D	61	LEU
4	1D	94	LEU
4	1D	103	ARG
4	1D	111	LEU
4	1D	113	VAL
4	1D	122	ASP
4	1D	126	GLN
4	1D	134	ARG
4	1D	142	VAL
4	1D	157	ARG
4	1D	200	ASP
4	1D	211	ARG
4	1D	221	VAL
4	1D	229	VAL
4	1D	242	ARG
4	1D	257	LEU
4	1D	259	THR
4	1D	260	ARG
4	1D	273	ARG
5	1E	21	VAL
5	1E	34	VAL
5	1E	64	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1E	75	VAL
5	1E	82	ARG
5	1E	116	VAL
5	1E	119	ARG
5	1E	144	ARG
5	1E	154	LYS
5	1E	163	GLU
5	1E	170	LEU
5	1E	175	VAL
5	1E	181	LEU
6	1F	20	LEU
6	1F	23	ASP
6	1F	24	LEU
6	1F	33	LEU
6	1F	53	THR
6	1F	57	VAL
6	1F	74	ARG
6	1F	106	ARG
6	1F	125	LEU
6	1F	132	VAL
6	1F	140	LEU
6	1F	170	LEU
6	1F	175	THR
6	1F	176	LEU
6	1F	191	ARG
6	1F	192	LEU
6	1F	197	ASP
6	1F	200	GLU
6	1F	201	VAL
7	1G	3	LEU
7	1G	4	ASP
7	1G	7	LEU
7	1G	28	VAL
7	1G	31	VAL
7	1G	45	GLU
7	1G	49	ASP
7	1G	60	LEU
7	1G	79	ASN
7	1G	81	LYS
7	1G	82	LEU
7	1G	91	ARG
7	1G	139	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	1G	140	ILE
7	1G	143	GLU
7	1G	159	VAL
7	1G	161	THR
7	1G	162	THR
7	1G	170	ARG
7	1G	175	LEU
8	1H	3	ARG
8	1H	15	VAL
8	1H	69	ARG
8	1H	71	LEU
8	1H	98	LEU
8	1H	105	LEU
8	1H	107	VAL
8	1H	124	GLU
10	1K	79	ARG
10	1K	84	LEU
10	1K	95	LYS
10	1K	99	ILE
10	1K	106	GLU
10	1K	115	LEU
10	1K	121	GLU
10	1K	133	SER
10	1K	134	MET
10	1K	137	GLU
11	1L	28	THR
11	1L	33	LEU
11	1L	34	LEU
11	1L	48	MET
11	1L	61	ARG
11	1L	73	THR
11	1L	84	LYS
11	1L	87	LEU
11	1L	120	LEU
11	1L	133	GLN
12	1M	23	ARG
12	1M	24	VAL
12	1M	94	ARG
12	1M	98	VAL
12	1M	105	GLU
12	1M	113	LYS
13	1N	42	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	1N	55	ARG
13	1N	59	LEU
13	1N	65	ARG
13	1N	70	GLN
13	1N	95	VAL
13	1N	98	GLU
13	1N	99	LEU
13	1N	106	LEU
13	1N	112	LEU
13	1N	137	LYS
13	1N	149	GLU
14	1O	1	MET
14	1O	21	THR
14	1O	35	VAL
14	1O	45	GLN
14	1O	55	VAL
14	1O	56	ARG
14	1O	59	ARG
14	1O	75	THR
14	1O	98	LYS
15	1P	1	MET
15	1P	18	LEU
15	1P	24	GLN
15	1P	28	LEU
15	1P	29	LEU
15	1P	33	ARG
15	1P	44	LEU
15	1P	54	LEU
15	1P	60	LEU
15	1P	65	LEU
15	1P	67	LEU
15	1P	75	LEU
15	1P	79	LEU
15	1P	91	GLN
15	1P	100	LEU
15	1P	111	LEU
15	1P	114	VAL
15	1P	117	VAL
16	1Q	3	ARG
16	1Q	19	LYS
16	1Q	20	ARG
16	1Q	48	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	1Q	50	SER
16	1Q	78	LEU
16	1Q	103	GLU
17	1R	16	ARG
17	1R	28	VAL
17	1R	42	ILE
17	1R	49	VAL
17	1R	65	LYS
17	1R	74	ARG
17	1R	78	LEU
17	1R	89	VAL
17	1R	96	ARG
17	1R	109	GLU
17	1R	118	ARG
17	1R	128	GLU
18	1S	8	VAL
18	1S	36	ARG
18	1S	60	LEU
18	1S	74	LEU
18	1S	84	LYS
18	1S	92	ARG
18	1S	95	LEU
18	1S	104	GLN
18	1S	108	GLU
18	1S	111	GLU
19	1T	1	MET
19	1T	18	LEU
19	1T	21	ARG
19	1T	43	GLU
19	1T	46	VAL
19	1T	52	VAL
19	1T	61	VAL
19	1T	62	LEU
19	1T	79	VAL
19	1T	95	LEU
20	1U	11	ARG
20	1U	17	VAL
20	1U	23	LEU
20	1U	51	LEU
20	1U	60	ASN
20	1U	100	THR
20	1U	107	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	1V	33	LYS
21	1V	35	THR
21	1V	52	VAL
21	1V	57	LEU
21	1V	66	LEU
21	1V	88	LYS
22	1W	7	VAL
22	1W	23	ARG
22	1W	43	ASN
22	1W	90	LEU
22	1W	91	GLU
23	1X	5	LEU
23	1X	11	GLU
23	1X	18	LEU
23	1X	19	ARG
23	1X	31	ARG
23	1X	33	LEU
23	1X	58	VAL
23	1X	72	ARG
23	1X	73	GLN
23	1X	76	LEU
23	1X	86	VAL
23	1X	87	ASP
23	1X	91	LEU
23	1X	107	THR
23	1X	126	VAL
23	1X	136	PHE
23	1X	150	LEU
24	1Y	10	THR
24	1Y	11	ARG
24	1Y	19	LYS
24	1Y	20	ARG
24	1Y	55	ARG
24	1Y	74	ARG
25	1Z	11	ARG
25	1Z	35	THR
25	1Z	40	ARG
25	1Z	59	THR
25	1Z	65	SER
25	1Z	75	GLU
25	1Z	95	LEU
26	10	30	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	10	32	LEU
26	10	53	LEU
26	10	64	LEU
26	10	70	GLN
27	11	8	LEU
27	11	23	LEU
27	11	29	ARG
27	11	48	GLU
27	11	55	ARG
28	12	1	MET
28	12	34	GLU
28	12	46	GLN
28	12	47	GLN
28	12	49	PHE
28	12	50	VAL
28	12	55	ARG
28	12	58	ARG
28	12	63	TYR
28	12	66	SER
28	12	67	TYR
28	12	69	LYS
29	13	6	VAL
29	13	16	ARG
29	13	26	THR
29	13	40	LYS
29	13	58	LEU
30	14	4	GLU
30	14	6	ARG
30	14	34	LEU
30	14	35	GLU
30	14	48	VAL
31	15	1	MET
31	15	24	THR
32	16	14	VAL
32	16	31	HIS
32	16	32	LEU
32	16	37	SER
32	16	46	ARG
35	1b	8	LYS
35	1b	11	LEU
35	1b	15	VAL
35	1b	17	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	1b	20	GLU
35	1b	21	ARG
35	1b	76	GLN
35	1b	80	ILE
35	1b	94	ASN
35	1b	121	LEU
35	1b	137	ARG
35	1b	145	LEU
35	1b	153	ARG
35	1b	169	LYS
35	1b	170	GLU
35	1b	178	ARG
35	1b	179	LYS
35	1b	185	ILE
35	1b	187	LEU
35	1b	209	ARG
35	1b	217	ARG
35	1b	221	LEU
36	1c	15	THR
36	1c	28	GLN
36	1c	29	TYR
36	1c	45	LYS
36	1c	124	ILE
36	1c	127	ARG
36	1c	181	ASN
36	1c	191	THR
37	1d	5	ILE
37	1d	8	VAL
37	1d	24	GLU
37	1d	28	SER
37	1d	47	ARG
37	1d	49	ARG
37	1d	57	ARG
37	1d	58	LEU
37	1d	127	THR
37	1d	135	LEU
37	1d	137	SER
37	1d	155	LEU
37	1d	168	ARG
37	1d	173	TRP
37	1d	182	LYS
37	1d	196	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	1d	202	LEU
38	1e	13	ILE
38	1e	38	GLN
38	1e	40	ARG
38	1e	41	VAL
38	1e	47	LYS
38	1e	56	GLN
38	1e	73	ASN
38	1e	79	GLU
38	1e	91	LEU
38	1e	137	GLU
38	1e	144	THR
38	1e	147	ASP
39	1f	25	ILE
39	1f	28	ARG
39	1f	43	LEU
39	1f	61	LEU
39	1f	70	ASP
39	1f	74	ASP
39	1f	82	ARG
39	1f	92	LYS
40	1g	8	GLU
40	1g	16	LEU
40	1g	51	GLN
40	1g	75	VAL
40	1g	97	GLN
40	1g	104	LEU
40	1g	113	GLU
40	1g	129	GLU
40	1g	140	ASP
41	1h	3	THR
41	1h	18	ARG
41	1h	21	LYS
41	1h	26	VAL
41	1h	37	ARG
41	1h	39	LEU
41	1h	51	VAL
41	1h	52	ASP
41	1h	91	ARG
41	1h	112	LEU
41	1h	120	THR
41	1h	122	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1h	127	LEU
41	1h	129	VAL
41	1h	133	LEU
42	1i	23	ASN
42	1i	47	LEU
42	1i	53	VAL
42	1i	54	ASP
42	1i	81	ILE
42	1i	86	VAL
42	1i	93	ARG
42	1i	102	LEU
42	1i	104	ARG
42	1i	108	VAL
42	1i	121	ARG
42	1i	128	ARG
43	1j	16	LEU
43	1j	17	ASP
43	1j	21	GLN
43	1j	92	THR
43	1j	98	ILE
44	1k	14	VAL
44	1k	48	ILE
44	1k	77	MET
44	1k	79	SER
44	1k	106	LYS
44	1k	114	VAL
45	1l	23	LYS
45	1l	27	LEU
45	1l	36	VAL
45	1l	55	VAL
45	1l	67	THR
45	1l	83	VAL
45	1l	116	SER
46	1m	3	ARG
46	1m	4	ILE
46	1m	27	LYS
46	1m	64	TRP
46	1m	70	LEU
46	1m	84	ILE
46	1m	99	ARG
46	1m	106	ASN
46	1m	110	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	1m	117	VAL
46	1m	121	LYS
47	1n	18	VAL
47	1n	22	THR
47	1n	23	ARG
47	1n	31	ARG
47	1n	33	VAL
47	1n	41	ARG
47	1n	57	ARG
48	1o	5	LYS
48	1o	26	GLU
48	1o	39	LEU
48	1o	57	LEU
48	1o	66	LEU
49	1p	19	ILE
49	1p	20	VAL
49	1p	25	ARG
49	1p	45	THR
49	1p	60	LEU
49	1p	69	THR
49	1p	72	ARG
50	1q	35	VAL
50	1q	45	HIS
50	1q	49	GLU
50	1q	89	LEU
50	1q	92	ARG
51	1r	28	GLU
51	1r	32	ARG
51	1r	38	GLU
51	1r	47	THR
52	1s	12	ASP
52	1s	22	LEU
52	1s	28	LYS
52	1s	37	ARG
52	1s	65	ASN
52	1s	66	MET
52	1s	78	ARG
52	1s	83	HIS
52	1s	85	LYS
53	1t	9	ASN
53	1t	10	LEU
53	1t	13	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	1t	24	LEU
53	1t	56	MET
53	1t	62	LEU
53	1t	75	ASN
53	1t	84	LEU
54	1u	15	ARG
55	1z	-29	LEU
55	1z	-27	THR
55	1z	-10	ARG
55	1z	-6	ARG
55	1z	-3	GLU
55	1z	1	LEU
55	1z	13	ARG
55	1z	21	ILE
55	1z	30	GLU
55	1z	31	ARG
55	1z	39	ILE
55	1z	88	VAL
55	1z	92	ILE
55	1z	98	MET
55	1z	100	VAL
55	1z	106	VAL
55	1z	130	VAL
55	1z	132	ARG
55	1z	142	THR
55	1z	152	THR
55	1z	156	ARG
55	1z	160	ARG
55	1z	172	ASP
55	1z	197	ARG
55	1z	207	ASP
55	1z	208	GLN
55	1z	215	LYS
55	1z	225	GLU
55	1z	236	GLU
55	1z	264	LEU
55	1z	286	ILE
55	1z	299	VAL
55	1z	309	LEU
55	1z	328	ILE
55	1z	336	THR
55	1z	339	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	1z	352	VAL
55	1z	355	LEU
55	1z	356	LEU
55	1z	363	ARG
55	1z	385	THR
55	1z	389	LEU
55	1z	422	GLU
55	1z	428	LEU
55	1z	437	THR
55	1z	442	THR
55	1z	473	ASP
55	1z	481	VAL
55	1z	484	ARG
55	1z	500	GLN
55	1z	512	ILE
55	1z	515	GLU
55	1z	526	VAL
55	1z	530	VAL
55	1z	546	ILE
55	1z	569	ASP
55	1z	590	ILE
55	1z	598	ASP
55	1z	605	ILE
55	1z	614	GLU
55	1z	624	LEU
55	1z	630	GLN
55	1z	641	GLN
55	1z	647	VAL
55	1z	649	LEU
55	1z	651	GLU
55	1z	660	ARG
55	1z	669	PHE
55	1z	670	VAL
55	1z	678	GLU
55	1z	679	VAL
58	1x	9	ARG
58	1x	18	LEU
3	2C	6	ARG
3	2C	24	GLU
3	2C	37	PHE
3	2C	46	LYS
3	2C	49	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2C	52	ARG
3	2C	62	VAL
3	2C	68	LEU
3	2C	172	HIS
3	2C	175	VAL
3	2C	188	ASN
3	2C	199	HIS
3	2C	207	THR
3	2C	208	PHE
3	2C	209	LEU
4	2D	54	ARG
4	2D	61	LEU
4	2D	94	LEU
4	2D	99	ASP
4	2D	103	ARG
4	2D	134	ARG
4	2D	142	VAL
4	2D	157	ARG
4	2D	211	ARG
4	2D	221	VAL
4	2D	229	VAL
4	2D	242	ARG
4	2D	257	LEU
4	2D	259	THR
4	2D	260	ARG
4	2D	276	LYS
5	2E	21	VAL
5	2E	38	THR
5	2E	40	GLU
5	2E	52	LEU
5	2E	58	ARG
5	2E	75	VAL
5	2E	76	ARG
5	2E	79	ARG
5	2E	82	ARG
5	2E	119	ARG
5	2E	144	ARG
5	2E	154	LYS
5	2E	167	VAL
5	2E	175	VAL
5	2E	181	LEU
5	2E	195	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	2E	202	LYS
6	2F	20	LEU
6	2F	33	LEU
6	2F	53	THR
6	2F	57	VAL
6	2F	74	ARG
6	2F	110	LEU
6	2F	140	LEU
6	2F	158	THR
6	2F	170	LEU
6	2F	175	THR
6	2F	176	LEU
6	2F	191	ARG
6	2F	192	LEU
6	2F	197	ASP
6	2F	200	GLU
6	2F	201	VAL
7	2G	3	LEU
7	2G	4	ASP
7	2G	16	ARG
7	2G	21	ARG
7	2G	45	GLU
7	2G	49	ASP
7	2G	51	ARG
7	2G	60	LEU
7	2G	79	ASN
7	2G	91	ARG
7	2G	96	ARG
7	2G	98	ARG
7	2G	113	ARG
7	2G	115	ARG
7	2G	136	ARG
7	2G	139	LEU
7	2G	140	ILE
7	2G	143	GLU
7	2G	148	MET
7	2G	152	LEU
7	2G	159	VAL
7	2G	162	THR
7	2G	170	ARG
8	2H	3	ARG
8	2H	16	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	2H	19	VAL
8	2H	27	LYS
8	2H	33	LEU
8	2H	43	VAL
8	2H	44	VAL
8	2H	69	ARG
8	2H	71	LEU
8	2H	88	LEU
8	2H	107	VAL
8	2H	114	VAL
8	2H	116	GLU
8	2H	122	THR
8	2H	130	ARG
8	2H	139	GLN
8	2H	175	LYS
10	2K	80	LYS
10	2K	84	LEU
10	2K	86	LYS
10	2K	90	LYS
10	2K	95	LYS
10	2K	99	ILE
10	2K	105	LEU
10	2K	106	GLU
10	2K	115	LEU
10	2K	119	ASP
10	2K	133	SER
10	2K	136	VAL
11	2L	10	GLU
11	2L	33	LEU
11	2L	34	LEU
11	2L	38	HIS
11	2L	48	MET
11	2L	87	LEU
11	2L	115	ARG
11	2L	120	LEU
11	2L	121	LYS
11	2L	133	GLN
11	2L	138	LEU
12	2M	10	VAL
12	2M	23	ARG
12	2M	24	VAL
12	2M	53	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	2M	78	ARG
12	2M	80	ASP
12	2M	92	GLU
12	2M	94	ARG
12	2M	98	VAL
12	2M	108	GLU
12	2M	113	LYS
13	2N	42	SER
13	2N	55	ARG
13	2N	59	LEU
13	2N	65	ARG
13	2N	71	VAL
13	2N	98	GLU
13	2N	106	LEU
13	2N	112	LEU
13	2N	125	VAL
14	2O	1	MET
14	2O	21	THR
14	2O	45	GLN
14	2O	56	ARG
14	2O	59	ARG
14	2O	60	ARG
14	2O	75	THR
14	2O	109	VAL
14	2O	110	THR
14	2O	128	LYS
15	2P	1	MET
15	2P	18	LEU
15	2P	24	GLN
15	2P	28	LEU
15	2P	29	LEU
15	2P	33	ARG
15	2P	44	LEU
15	2P	54	LEU
15	2P	60	LEU
15	2P	65	LEU
15	2P	67	LEU
15	2P	75	LEU
15	2P	79	LEU
15	2P	111	LEU
15	2P	114	VAL
15	2P	118	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	2Q	19	LYS
16	2Q	20	ARG
16	2Q	44	LYS
16	2Q	48	LEU
16	2Q	50	SER
16	2Q	58	LEU
16	2Q	67	ARG
16	2Q	78	LEU
16	2Q	83	LYS
16	2Q	103	GLU
17	2R	9	LEU
17	2R	17	THR
17	2R	28	VAL
17	2R	42	ILE
17	2R	53	ARG
17	2R	78	LEU
17	2R	85	LYS
17	2R	87	ASP
17	2R	96	ARG
17	2R	118	ARG
17	2R	123	GLN
18	2S	52	ARG
18	2S	60	LEU
18	2S	74	LEU
18	2S	92	ARG
18	2S	95	LEU
18	2S	104	GLN
19	2T	1	MET
19	2T	18	LEU
19	2T	33	VAL
19	2T	46	VAL
19	2T	52	VAL
19	2T	79	VAL
19	2T	95	LEU
20	2U	11	ARG
20	2U	17	VAL
20	2U	23	LEU
20	2U	51	LEU
20	2U	67	ASP
20	2U	100	THR
20	2U	107	LEU
21	2V	57	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	2V	92	LEU
22	2W	6	HIS
22	2W	7	VAL
22	2W	23	ARG
22	2W	43	ASN
22	2W	49	VAL
22	2W	70	SER
22	2W	72	VAL
22	2W	94	LYS
22	2W	107	ASP
23	2X	5	LEU
23	2X	11	GLU
23	2X	33	LEU
23	2X	42	VAL
23	2X	72	ARG
23	2X	73	GLN
23	2X	86	VAL
23	2X	91	LEU
23	2X	98	MET
23	2X	120	ILE
23	2X	122	ARG
23	2X	129	SER
23	2X	136	PHE
23	2X	150	LEU
23	2X	156	LYS
23	2X	170	THR
23	2X	183	LEU
24	2Y	10	THR
24	2Y	14	ARG
24	2Y	19	LYS
24	2Y	20	ARG
25	2Z	4	VAL
25	2Z	14	VAL
25	2Z	21	ARG
25	2Z	26	ARG
25	2Z	40	ARG
25	2Z	59	THR
25	2Z	65	SER
25	2Z	85	LEU
26	20	2	LYS
26	20	19	VAL
26	20	30	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	20	32	LEU
26	20	41	ILE
26	20	45	SER
26	20	51	ARG
26	20	53	LEU
26	20	65	ASN
27	21	8	LEU
27	21	23	LEU
27	21	30	ARG
27	21	44	ARG
27	21	48	GLU
28	22	1	MET
28	22	3	GLU
28	22	5	ILE
28	22	34	GLU
28	22	50	VAL
28	22	53	GLU
28	22	58	ARG
28	22	61	ARG
28	22	62	ARG
28	22	67	TYR
28	22	68	ARG
29	23	6	VAL
29	23	16	ARG
29	23	29	THR
29	23	35	GLU
29	23	57	VAL
29	23	58	LEU
30	24	5	VAL
30	24	6	ARG
30	24	34	LEU
30	24	38	LYS
30	24	48	VAL
31	25	1	MET
31	25	32	LYS
32	26	6	THR
32	26	14	VAL
32	26	26	LYS
32	26	31	HIS
32	26	37	SER
33	27	8	LYS
35	2b	8	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2b	15	VAL
35	2b	45	GLN
35	2b	51	LEU
35	2b	80	ILE
35	2b	94	ASN
35	2b	97	TRP
35	2b	114	ARG
35	2b	137	ARG
35	2b	154	LEU
35	2b	157	ARG
35	2b	185	ILE
35	2b	187	LEU
35	2b	208	ILE
35	2b	217	ARG
35	2b	224	GLN
36	2c	3	ASN
36	2c	49	SER
36	2c	52	LEU
36	2c	72	LYS
36	2c	98	ASN
36	2c	102	ASN
36	2c	104	GLN
36	2c	105	GLU
36	2c	125	GLU
36	2c	127	ARG
36	2c	136	GLN
36	2c	152	ILE
36	2c	191	THR
37	2d	3	ARG
37	2d	8	VAL
37	2d	34	GLU
37	2d	47	ARG
37	2d	61	LYS
37	2d	65	ARG
37	2d	73	ARG
37	2d	127	THR
37	2d	135	LEU
37	2d	141	ARG
37	2d	150	GLU
37	2d	155	LEU
37	2d	157	LEU
37	2d	187	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	2d	194	LEU
37	2d	196	LEU
38	2e	38	GLN
38	2e	41	VAL
38	2e	47	LYS
38	2e	71	LEU
38	2e	72	GLN
38	2e	78	HIS
38	2e	144	THR
38	2e	147	ASP
39	2f	61	LEU
39	2f	63	TYR
39	2f	70	ASP
39	2f	74	ASP
39	2f	81	ILE
39	2f	87	ARG
40	2g	12	LEU
40	2g	16	LEU
40	2g	72	ARG
40	2g	75	VAL
40	2g	90	GLU
40	2g	97	GLN
40	2g	104	LEU
40	2g	139	GLU
40	2g	153	HIS
40	2g	155	ARG
41	2h	2	LEU
41	2h	21	LYS
41	2h	34	GLU
41	2h	37	ARG
41	2h	52	ASP
41	2h	78	GLN
41	2h	84	ARG
41	2h	91	ARG
41	2h	98	LYS
41	2h	99	GLU
41	2h	107	LEU
41	2h	111	ILE
41	2h	112	LEU
41	2h	114	THR
41	2h	120	THR
41	2h	125	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	2h	129	VAL
41	2h	133	LEU
42	2i	7	THR
42	2i	12	GLU
42	2i	14	VAL
42	2i	23	ASN
42	2i	31	GLN
42	2i	64	THR
42	2i	81	ILE
42	2i	83	ARG
42	2i	93	ARG
42	2i	102	LEU
42	2i	104	ARG
42	2i	108	VAL
42	2i	111	ARG
42	2i	114	TYR
42	2i	128	ARG
43	2j	67	THR
43	2j	85	LEU
44	2k	14	VAL
44	2k	18	ARG
44	2k	105	VAL
45	2l	10	LEU
45	2l	23	LYS
45	2l	33	ARG
45	2l	52	LEU
45	2l	53	ARG
45	2l	55	VAL
45	2l	83	VAL
45	2l	114	LYS
46	2m	3	ARG
46	2m	8	GLU
46	2m	19	LEU
46	2m	27	LYS
46	2m	56	LEU
46	2m	66	LEU
46	2m	70	LEU
46	2m	77	ASN
46	2m	106	ASN
46	2m	110	ARG
47	2n	3	ARG
47	2n	15	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	2n	18	VAL
47	2n	22	THR
47	2n	23	ARG
47	2n	33	VAL
47	2n	41	ARG
48	2o	3	ILE
48	2o	4	THR
48	2o	38	ARG
48	2o	39	LEU
48	2o	48	LYS
48	2o	66	LEU
48	2o	68	ARG
48	2o	83	GLU
49	2p	6	LEU
49	2p	20	VAL
49	2p	28	ARG
49	2p	45	THR
49	2p	57	ARG
49	2p	60	LEU
49	2p	62	VAL
49	2p	67	THR
49	2p	74	LEU
50	2q	4	LYS
50	2q	6	LEU
50	2q	14	LYS
50	2q	49	GLU
50	2q	63	ARG
50	2q	76	LEU
50	2q	91	ARG
51	2r	31	LEU
51	2r	32	ARG
51	2r	38	GLU
51	2r	41	LYS
52	2s	22	LEU
52	2s	33	THR
52	2s	37	ARG
52	2s	65	ASN
52	2s	78	ARG
53	2t	24	LEU
53	2t	45	GLN
53	2t	56	MET
53	2t	62	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	2t	75	ASN
53	2t	84	LEU
55	2z	-62	LEU
55	2z	-47	ASP
55	2z	-27	THR
55	2z	-20	LEU
55	2z	-10	ARG
55	2z	-6	ARG
55	2z	-1	GLU
55	2z	6	GLU
55	2z	9	LEU
55	2z	14	ASN
55	2z	15	ILE
55	2z	26	THR
55	2z	30	GLU
55	2z	91	THR
55	2z	92	ILE
55	2z	96	ARG
55	2z	123	ARG
55	2z	130	VAL
55	2z	132	ARG
55	2z	152	THR
55	2z	156	ARG
55	2z	157	LEU
55	2z	160	ARG
55	2z	170	ARG
55	2z	187	THR
55	2z	197	ARG
55	2z	198	GLU
55	2z	207	ASP
55	2z	215	LYS
55	2z	219	VAL
55	2z	225	GLU
55	2z	228	MET
55	2z	232	LEU
55	2z	260	LEU
55	2z	299	VAL
55	2z	315	LYS
55	2z	328	ILE
55	2z	336	THR
55	2z	337	SER
55	2z	352	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	2z	355	LEU
55	2z	363	ARG
55	2z	377	VAL
55	2z	378	VAL
55	2z	385	THR
55	2z	396	ARG
55	2z	418	LYS
55	2z	440	VAL
55	2z	471	LYS
55	2z	473	ASP
55	2z	478	LYS
55	2z	484	ARG
55	2z	485	GLU
55	2z	497	PHE
55	2z	507	TYR
55	2z	512	ILE
55	2z	515	GLU
55	2z	555	LEU
55	2z	569	ASP
55	2z	573	HIS
55	2z	574	GLU
55	2z	575	VAL
55	2z	590	ILE
55	2z	598	ASP
55	2z	603	GLU
55	2z	614	GLU
55	2z	623	ASP
55	2z	624	LEU
55	2z	630	GLN
55	2z	634	MET
55	2z	647	VAL
55	2z	657	THR
55	2z	662	LYS
55	2z	669	PHE
55	2z	688	ILE
58	2x	18	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (160) such sidechains are listed below:

Mol	Chain	Res	Type
4	1D	87	ASN
4	1D	201	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	1D	253	GLN
6	1F	169	ASN
6	1F	203	GLN
7	1G	40	ASN
10	1K	103	GLN
11	1L	69	GLN
11	1L	133	GLN
13	1N	27	HIS
13	1N	38	GLN
14	1O	57	HIS
14	1O	123	HIS
17	1R	58	ASN
17	1R	123	GLN
18	1S	94	ASN
18	1S	104	GLN
18	1S	117	GLN
21	1V	31	HIS
21	1V	82	GLN
22	1W	6	HIS
22	1W	43	ASN
23	1X	55	HIS
23	1X	73	GLN
23	1X	151	HIS
26	10	9	GLN
26	10	70	GLN
28	12	46	GLN
29	13	23	HIS
32	16	35	GLN
33	17	36	GLN
35	1b	94	ASN
35	1b	95	GLN
36	1c	28	GLN
36	1c	123	GLN
36	1c	136	GLN
36	1c	162	GLN
36	1c	181	ASN
37	1d	45	GLN
37	1d	123	HIS
38	1e	38	GLN
38	1e	56	GLN
38	1e	73	ASN
38	1e	141	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	1f	7	ASN
40	1g	28	ASN
40	1g	64	GLN
40	1g	96	GLN
40	1g	97	GLN
42	1i	23	ASN
42	1i	31	GLN
42	1i	34	ASN
42	1i	73	GLN
42	1i	89	ASN
42	1i	124	GLN
43	1j	56	HIS
44	1k	104	GLN
45	1l	78	GLN
48	1o	28	GLN
50	1q	16	GLN
50	1q	94	ASN
52	1s	65	ASN
52	1s	69	HIS
52	1s	83	HIS
53	1t	26	ASN
53	1t	45	GLN
55	1z	-50	GLN
55	1z	-13	GLN
55	1z	7	ASN
55	1z	77	HIS
55	1z	124	GLN
55	1z	154	GLN
55	1z	165	GLN
55	1z	359	HIS
55	1z	426	GLN
55	1z	458	HIS
55	1z	500	GLN
55	1z	543	GLN
55	1z	573	HIS
55	1z	641	GLN
55	1z	664	GLN
55	1z	675	HIS
55	1z	677	GLN
4	2D	253	GLN
6	2F	75	HIS
6	2F	169	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	2F	203	GLN
7	2G	40	ASN
7	2G	132	ASN
8	2H	147	ASN
10	2K	89	HIS
10	2K	103	GLN
10	2K	116	ASN
11	2L	8	GLN
11	2L	69	GLN
11	2L	133	GLN
13	2N	35	HIS
13	2N	38	GLN
14	2O	57	HIS
16	2Q	68	GLN
17	2R	58	ASN
18	2S	104	GLN
20	2U	60	ASN
21	2V	31	HIS
21	2V	82	GLN
22	2W	43	ASN
23	2X	121	HIS
23	2X	151	HIS
29	23	23	HIS
32	26	35	GLN
33	27	20	HIS
33	27	36	GLN
35	2b	16	HIS
35	2b	40	HIS
35	2b	45	GLN
35	2b	94	ASN
35	2b	95	GLN
35	2b	104	ASN
35	2b	224	GLN
36	2c	3	ASN
36	2c	6	HIS
36	2c	37	GLN
36	2c	123	GLN
36	2c	162	GLN
37	2d	45	GLN
37	2d	123	HIS
37	2d	129	ASN
37	2d	160	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	2d	161	ASN
38	2e	72	GLN
38	2e	130	ASN
39	2f	7	ASN
39	2f	27	GLN
39	2f	94	GLN
40	2g	28	ASN
40	2g	97	GLN
40	2g	110	GLN
42	2i	31	GLN
42	2i	73	GLN
43	2j	62	HIS
43	2j	68	HIS
45	2l	49	ASN
45	2l	75	HIS
45	2l	78	GLN
45	2l	99	HIS
48	2o	28	GLN
50	2q	16	GLN
52	2s	83	HIS
55	2z	-50	GLN
55	2z	14	ASN
55	2z	77	HIS
55	2z	165	GLN
55	2z	426	GLN
55	2z	509	HIS
55	2z	543	GLN
55	2z	573	HIS
55	2z	595	GLN
55	2z	641	GLN
55	2z	675	HIS
55	2z	677	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	434 (15%)	24 (0%)
1	2A	2860/2915 (98%)	515 (18%)	22 (0%)
2	1B	119/121 (98%)	10 (8%)	1 (0%)
2	2B	119/121 (98%)	17 (14%)	0
34	1a	1491/1521 (98%)	266 (17%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	2a	1498/1521 (98%)	258 (17%)	0
56	1y	5/24 (20%)	0	0
56	2y	4/24 (16%)	0	0
57	1w	75/77 (97%)	19 (25%)	0
57	2w	75/77 (97%)	18 (24%)	0
All	All	9111/9316 (97%)	1537 (16%)	47 (0%)

All (1537) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	U
1	1A	14	G
1	1A	28	U
1	1A	33	C
1	1A	44	C
1	1A	53	G
1	1A	61	U
1	1A	62	A
1	1A	69	A
1	1A	72	A
1	1A	73	G
1	1A	115	A
1	1A	116	A
1	1A	117	U
1	1A	122	G
1	1A	148	A
1	1A	169	A
1	1A	176	G
1	1A	184	A
1	1A	185	A
1	1A	187	A
1	1A	193	G
1	1A	203	G
1	1A	204	A
1	1A	209	A
1	1A	210	A
1	1A	213	A
1	1A	216	A
1	1A	217	A
1	1A	221	A
1	1A	236	G
1	1A	238	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	249	G
1	1A	254	G
1	1A	268	G
1	1A	270	U
1	1A	271	U
1	1A	272	G
1	1A	273	U
1	1A	287	U
1	1A	288	G
1	1A	294	C
1	1A	296	C
1	1A	298	G
1	1A	302	C
1	1A	334	A
1	1A	352	G
1	1A	353	A
1	1A	365	G
1	1A	375	G
1	1A	386	G
1	1A	412	G
1	1A	422	G
1	1A	433	G
1	1A	437	G
1	1A	438	A
1	1A	454	A
1	1A	468	A
1	1A	469	C
1	1A	473	U
1	1A	480	C
1	1A	482	A
1	1A	495	A
1	1A	506	G
1	1A	518	G
1	1A	528	U
1	1A	529	A
1	1A	533	C
1	1A	554	G
1	1A	555	C
1	1A	556	A
1	1A	557	G
1	1A	585	G
1	1A	595	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	597	A
1	1A	615	G
1	1A	625	A
1	1A	626	G
1	1A	629	U
1	1A	632	G
1	1A	637	U
1	1A	638	G
1	1A	640	G
1	1A	661	A
1	1A	669	C
1	1A	670	A
1	1A	681	G
1	1A	696	C
1	1A	700	A
1	1A	715	G
1	1A	731	A
1	1A	732	G
1	1A	763	G
1	1A	776	C
1	1A	797	A
1	1A	810	A
1	1A	821	G
1	1A	822	G
1	1A	828	A
1	1A	830	A
1	1A	831	G
1	1A	838	G
1	1A	851	G
1	1A	858	C
1	1A	873	U
1	1A	874	U
1	1A	876	G
1	1A	878	G
1	1A	901	G
1	1A	905	G
1	1A	926	G
1	1A	931	C
1	1A	932	C
1	1A	933	A
1	1A	934	C
1	1A	935	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	936	A
1	1A	937	G
1	1A	938	C
1	1A	941	A
1	1A	942	C
1	1A	952	U
1	1A	955	A
1	1A	976	G
1	1A	985	A
1	1A	989	A
1	1A	990	G
1	1A	997	A
1	1A	1002	U
1	1A	1003	A
1	1A	1005	C
1	1A	1018	G
1	1A	1019	C
1	1A	1028	A
1	1A	1041	A
1	1A	1057	U
1	1A	1058	C
1	1A	1067	G
1	1A	1071	U
1	1A	1078	U
1	1A	1083	C
1	1A	1085	C
1	1A	1091	A
1	1A	1092	G
1	1A	1095	A
1	1A	1098	C
1	1A	1099	A
1	1A	1103	G
1	1A	1104	G
1	1A	1105	U
1	1A	1106	U
1	1A	1110	U
1	1A	1111	U
1	1A	1115	A
1	1A	1116	G
1	1A	1117	C
1	1A	1118	A
1	1A	1120	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1121	C
1	1A	1124	C
1	1A	1125	C
1	1A	1128	U
1	1A	1133	A
1	1A	1135	U
1	1A	1140	A
1	1A	1142	U
1	1A	1153	U
1	1A	1154	C
1	1A	1155	G
1	1A	1156	A
1	1A	1157	G
1	1A	1174	A
1	1A	1175	U
1	1A	1179	C
1	1A	1180	G
1	1A	1183	G
1	1A	1185	U
1	1A	1216	G
1	1A	1217	G
1	1A	1218	A
1	1A	1219	U
1	1A	1220	G
1	1A	1221	A
1	1A	1254	A
1	1A	1255	U
1	1A	1264	A
1	1A	1269	C
1	1A	1295	G
1	1A	1298	A
1	1A	1301	G
1	1A	1316	G
1	1A	1317	A
1	1A	1320	A
1	1A	1345	U
1	1A	1346	A
1	1A	1387	A
1	1A	1397	U
1	1A	1404	A
1	1A	1405	A
1	1A	1410	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1425	G
1	1A	1429	A
1	1A	1430	G
1	1A	1440	A
1	1A	1461	G
1	1A	1462	C
1	1A	1465	U
1	1A	1466	G
1	1A	1472	A
1	1A	1473	C
1	1A	1490	A
1	1A	1495	A
1	1A	1496	G
1	1A	1501	G
1	1A	1513	C
1	1A	1517	A
1	1A	1528	G
1	1A	1535	A
1	1A	1538	C
1	1A	1553	A
1	1A	1554	C
1	1A	1555	A
1	1A	1570	G
1	1A	1578	C
1	1A	1588	A
1	1A	1589	C
1	1A	1604	A
1	1A	1612	A
1	1A	1615	A
1	1A	1624	U
1	1A	1626	A
1	1A	1627	G
1	1A	1630	C
1	1A	1631	A
1	1A	1653	A
1	1A	1654	A
1	1A	1658	G
1	1A	1685	U
1	1A	1694	C
1	1A	1710	A
1	1A	1720	G
1	1A	1721	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1742	G
1	1A	1746	A
1	1A	1747	A
1	1A	1765	G
1	1A	1766	A
1	1A	1775	G
1	1A	1792	A
1	1A	1793	G
1	1A	1794	G
1	1A	1803	A
1	1A	1810	A
1	1A	1812	C
1	1A	1821	A
1	1A	1830	C
1	1A	1831	G
1	1A	1838	U
1	1A	1846	G
1	1A	1869	G
1	1A	1877	A
1	1A	1890	G
1	1A	1899	G
1	1A	1910	A
1	1A	1921	A
1	1A	1926	C
1	1A	1927	G
1	1A	1934	A
1	1A	1950	G
1	1A	1951	G
1	1A	1952	U
1	1A	1958	A
1	1A	1959	A
1	1A	1976	U
1	1A	1984	U
1	1A	1988	C
1	1A	1991	A
1	1A	1992	A
1	1A	1993	A
1	1A	2014	U
1	1A	2018	G
1	1A	2042	C
1	1A	2044	G
1	1A	2052	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2053	G
1	1A	2054	A
1	1A	2064	C
1	1A	2072	A
1	1A	2076	C
1	1A	2077	G
1	1A	2078	A
1	1A	2081	A
1	1A	2082	G
1	1A	2083	A
1	1A	2090	G
1	1A	2091	G
1	1A	2120	U
1	1A	2122	G
1	1A	2129	C
1	1A	2132	C
1	1A	2133	G
1	1A	2139	U
1	1A	2140	A
1	1A	2144	G
1	1A	2147	A
1	1A	2148	G
1	1A	2153	U
1	1A	2154	G
1	1A	2155	A
1	1A	2157	C
1	1A	2158	C
1	1A	2159	C
1	1A	2161	C
1	1A	2162	G
1	1A	2163	C
1	1A	2166	C
1	1A	2167	C
1	1A	2178	G
1	1A	2179	A
1	1A	2180	G
1	1A	2185	C
1	1A	2187	G
1	1A	2188	U
1	1A	2189	G
1	1A	2190	A
1	1A	2191	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2193	U
1	1A	2194	A
1	1A	2195	C
1	1A	2196	C
1	1A	2203	G
1	1A	2204	C
1	1A	2205	G
1	1A	2206	C
1	1A	2209	C
1	1A	2210	U
1	1A	2213	G
1	1A	2219	A
1	1A	2220	A
1	1A	2221	C
1	1A	2226	G
1	1A	2227	G
1	1A	2228	A
1	1A	2229	U
1	1A	2230	G
1	1A	2236	A
1	1A	2237	C
1	1A	2249	G
1	1A	2253	G
1	1A	2279	A
1	1A	2280	A
1	1A	2284	A
1	1A	2286	C
1	1A	2291	G
1	1A	2294	C
1	1A	2298	A
1	1A	2316	A
1	1A	2319	G
1	1A	2320	A
1	1A	2323	U
1	1A	2331	A
1	1A	2332	G
1	1A	2335	C
1	1A	2336	G
1	1A	2345	G
1	1A	2347	A
1	1A	2354	C
1	1A	2358	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2361	C
1	1A	2383	G
1	1A	2390	G
1	1A	2394	G
1	1A	2396	C
1	1A	2417	U
1	1A	2433	A
1	1A	2436	A
1	1A	2440	G
1	1A	2441	A
1	1A	2446	A
1	1A	2450	A
1	1A	2452	C
1	1A	2458	G
1	1A	2459	A
1	1A	2487	A
1	1A	2489	A
1	1A	2498	G
1	1A	2509	C
1	1A	2513	G
1	1A	2516	G
1	1A	2517	U
1	1A	2529	A
1	1A	2536	G
1	1A	2540	G
1	1A	2565	U
1	1A	2577	A
1	1A	2578	G
1	1A	2590	C
1	1A	2593	G
1	1A	2597	C
1	1A	2613	A
1	1A	2615	U
1	1A	2620	U
1	1A	2622	U
1	1A	2623	C
1	1A	2640	A
1	1A	2641	G
1	1A	2665	A
1	1A	2700	U
1	1A	2701	C
1	1A	2713	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2724	A
1	1A	2725	A
1	1A	2726	G
1	1A	2732	U
1	1A	2738	U
1	1A	2745	A
1	1A	2760	A
1	1A	2769	A
1	1A	2770	A
1	1A	2777	A
1	1A	2778	G
1	1A	2790	A
1	1A	2793	A
1	1A	2802	A
1	1A	2812	G
1	1A	2829	A
1	1A	2830	A
1	1A	2842	G
1	1A	2848	G
1	1A	2881	G
1	1A	2882	A
1	1A	2889	C
1	1A	2900	A
1	1A	2902	G
2	1B	2	C
2	1B	13	A
2	1B	47	C
2	1B	52	A
2	1B	53	A
2	1B	56	G
2	1B	73	A
2	1B	85	G
2	1B	106	G
2	1B	110	G
34	1a	6	U
34	1a	10	G
34	1a	14	U
34	1a	23	G
34	1a	33	A
34	1a	40	G
34	1a	43	G
34	1a	48	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1a	49	C
34	1a	51	A
34	1a	52	A
34	1a	55	C
34	1a	62	G
34	1a	75	C
34	1a	77	G
34	1a	91	G
34	1a	94	C
34	1a	95	A
34	1a	110	A
34	1a	115	C
34	1a	116	G
34	1a	126	C
34	1a	137	G
34	1a	138	A
34	1a	151	G
34	1a	158	C
34	1a	169	C
34	1a	177	U
34	1a	189	U
34	1a	202	A
34	1a	204	A
34	1a	208	C
34	1a	209	U
34	1a	210	U
34	1a	211	U
34	1a	212	G
34	1a	243	G
34	1a	247	G
34	1a	262	G
34	1a	263	C
34	1a	285	G
34	1a	297	G
34	1a	301	G
34	1a	317	A
34	1a	324	C
34	1a	325	A
34	1a	328	G
34	1a	338	C
34	1a	342	G
34	1a	344	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1a	347	G
34	1a	348	C
34	1a	349	A
34	1a	350	G
34	1a	351	C
34	1a	363	U
34	1a	368	C
34	1a	380	G
34	1a	393	A
34	1a	394	C
34	1a	402	G
34	1a	408	A
34	1a	409	G
34	1a	419	G
34	1a	420	G
34	1a	425	U
34	1a	426	A
34	1a	435	A
34	1a	437	C
34	1a	447	A
34	1a	456	C
34	1a	461	G
34	1a	469	G
34	1a	470	G
34	1a	481	A
34	1a	482	U
34	1a	489	G
34	1a	493	A
34	1a	494	A
34	1a	495	C
34	1a	502	C
34	1a	505	G
34	1a	511	G
34	1a	515	U
34	1a	516	A
34	1a	517	A
34	1a	531	A
34	1a	543	A
34	1a	544	U
34	1a	545	U
34	1a	548	C
34	1a	556	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1a	557	A
34	1a	560	G
34	1a	561	G
34	1a	591	A
34	1a	599	C
34	1a	602	C
34	1a	611	G
34	1a	612	G
34	1a	614	G
34	1a	615	G
34	1a	616	A
34	1a	630	U
34	1a	634	G
34	1a	637	A
34	1a	649	A
34	1a	655	G
34	1a	671	A
34	1a	672	G
34	1a	701	C
34	1a	707	U
34	1a	715	G
34	1a	733	C
34	1a	736	G
34	1a	739	G
34	1a	750	A
34	1a	758	G
34	1a	761	A
34	1a	776	A
34	1a	777	U
34	1a	778	A
34	1a	786	A
34	1a	801	C
34	1a	805	G
34	1a	811	U
34	1a	812	A
34	1a	813	G
34	1a	824	C
34	1a	825	U
34	1a	826	C
34	1a	829	G
34	1a	837	A
34	1a	850	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1a	851	A
34	1a	869	U
34	1a	880	G
34	1a	890	C
34	1a	900	G
34	1a	904	G
34	1a	905	G
34	1a	912	C
34	1a	913	A
34	1a	936	A
34	1a	938	U
34	1a	939	U
34	1a	946	A
34	1a	947	A
34	1a	949	G
34	1a	950	C
34	1a	952	A
34	1a	953	A
34	1a	954	G
34	1a	955	A
34	1a	967	C
34	1a	970	U
34	1a	971	G
34	1a	976	G
34	1a	977	C
34	1a	982	G
34	1a	983	A
34	1a	984	A
34	1a	985	C
34	1a	988	G
34	1a	995	A
34	1a	998	C
34	1a	1000	G
34	1a	1001	G
34	1a	1002	G
34	1a	1003	G
34	1a	1004	U
34	1a	1005	G
34	1a	1006	C
34	1a	1007	C
34	1a	1008	C
34	1a	1009	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1a	1010	G
34	1a	1037	C
34	1a	1038	A
34	1a	1048	U
34	1a	1049	C
34	1a	1051	G
34	1a	1064	G
34	1a	1072	G
34	1a	1077	G
34	1a	1078	U
34	1a	1084	A
34	1a	1105	U
34	1a	1106	A
34	1a	1107	G
34	1a	1109	U
34	1a	1113	A
34	1a	1119	U
34	1a	1120	C
34	1a	1121	G
34	1a	1122	G
34	1a	1123	C
34	1a	1129	A
34	1a	1134	A
34	1a	1135	A
34	1a	1142	U
34	1a	1149	G
34	1a	1163	G
34	1a	1165	A
34	1a	1166	G
34	1a	1178	U
34	1a	1179	G
34	1a	1183	A
34	1a	1184	G
34	1a	1194	U
34	1a	1195	A
34	1a	1196	C
34	1a	1209	A
34	1a	1210	C
34	1a	1218	A
34	1a	1220	A
34	1a	1222	U
34	1a	1235	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1a	1238	A
34	1a	1239	U
34	1a	1240	G
34	1a	1242	C
34	1a	1244	C
34	1a	1252	C
34	1a	1260	U
34	1a	1261	A
34	1a	1262	A
34	1a	1263	U
34	1a	1264	C
34	1a	1268	A
34	1a	1269	A
34	1a	1281	A
34	1a	1282	G
34	1a	1284	U
34	1a	1287	G
34	1a	1294	G
34	1a	1299	C
34	1a	1304	C
34	1a	1306	A
34	1a	1320	G
34	1a	1322	A
34	1a	1329	G
34	1a	1335	G
34	1a	1340	U
34	1a	1342	A
34	1a	1345	C
34	1a	1351	G
34	1a	1353	G
34	1a	1380	C
34	1a	1381	A
34	1a	1402	G
34	1a	1426	G
34	1a	1430	C
34	1a	1431	U
34	1a	1432	A
34	1a	1433	C
34	1a	1434	G
34	1a	1465	G
34	1a	1475	G
34	1a	1482	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1a	1484	U
34	1a	1495	G
34	1a	1497	A
34	1a	1507	G
34	1a	1508	G
34	1a	1509	A
57	1w	6	G
57	1w	9	G
57	1w	13	C
57	1w	16	C
57	1w	17	C
57	1w	20	U
57	1w	21	A
57	1w	31	G
57	1w	43	A
57	1w	47	U
57	1w	52	G
57	1w	53	G
57	1w	54	5MU
57	1w	61	C
57	1w	65	C
57	1w	66	C
57	1w	67	C
57	1w	73	A
57	1w	76	A
1	2A	10	G
1	2A	11	U
1	2A	33	C
1	2A	35	G
1	2A	44	C
1	2A	59	G
1	2A	69	A
1	2A	72	A
1	2A	73	G
1	2A	81	G
1	2A	82	A
1	2A	88	U
1	2A	91	C
1	2A	93	G
1	2A	96	G
1	2A	98	G
1	2A	99	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	100	A
1	2A	115	A
1	2A	116	A
1	2A	117	U
1	2A	138	A
1	2A	154	C
1	2A	155	U
1	2A	170	A
1	2A	184	A
1	2A	193	G
1	2A	202	G
1	2A	203	G
1	2A	204	A
1	2A	209	A
1	2A	210	A
1	2A	216	A
1	2A	217	A
1	2A	218	U
1	2A	221	A
1	2A	236	G
1	2A	240	G
1	2A	252	C
1	2A	254	G
1	2A	268	G
1	2A	269	C
1	2A	271	U
1	2A	272	G
1	2A	273	U
1	2A	287	U
1	2A	288	G
1	2A	300	C
1	2A	301	A
1	2A	325	C
1	2A	334	A
1	2A	335	G
1	2A	352	G
1	2A	353	A
1	2A	356	G
1	2A	361	G
1	2A	375	G
1	2A	385	U
1	2A	386	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	388	G
1	2A	406	U
1	2A	412	G
1	2A	422	G
1	2A	437	G
1	2A	438	A
1	2A	454	A
1	2A	468	A
1	2A	469	C
1	2A	471	G
1	2A	479	A
1	2A	480	C
1	2A	495	A
1	2A	506	G
1	2A	507	A
1	2A	528	U
1	2A	529	A
1	2A	533	C
1	2A	552	A
1	2A	553	A
1	2A	554	G
1	2A	555	C
1	2A	556	A
1	2A	557	G
1	2A	568	G
1	2A	573	G
1	2A	585	G
1	2A	595	G
1	2A	597	A
1	2A	608	A
1	2A	610	U
1	2A	625	A
1	2A	626	G
1	2A	629	U
1	2A	635	G
1	2A	638	G
1	2A	640	G
1	2A	641	G
1	2A	642	C
1	2A	644	G
1	2A	651	A
1	2A	661	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	669	C
1	2A	670	A
1	2A	674	C
1	2A	678	A
1	2A	679	G
1	2A	680	C
1	2A	697	G
1	2A	713	U
1	2A	715	G
1	2A	732	G
1	2A	763	G
1	2A	776	C
1	2A	807	A
1	2A	808	U
1	2A	810	A
1	2A	811	G
1	2A	817	G
1	2A	820	A
1	2A	821	G
1	2A	822	G
1	2A	828	A
1	2A	830	A
1	2A	831	G
1	2A	835	A
1	2A	838	G
1	2A	851	G
1	2A	858	C
1	2A	865	A
1	2A	873	U
1	2A	874	U
1	2A	877	G
1	2A	905	G
1	2A	912	A
1	2A	915	G
1	2A	918	A
1	2A	925	G
1	2A	926	G
1	2A	928	G
1	2A	930	C
1	2A	932	C
1	2A	933	A
1	2A	935	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	936	A
1	2A	938	C
1	2A	941	A
1	2A	942	C
1	2A	943	C
1	2A	945	A
1	2A	946	A
1	2A	955	A
1	2A	959	C
1	2A	962	A
1	2A	975	G
1	2A	976	G
1	2A	982	G
1	2A	985	A
1	2A	989	A
1	2A	990	G
1	2A	997	A
1	2A	1002	U
1	2A	1003	A
1	2A	1005	C
1	2A	1018	G
1	2A	1019	C
1	2A	1025	A
1	2A	1028	A
1	2A	1041	A
1	2A	1053	C
1	2A	1057	U
1	2A	1058	C
1	2A	1067	G
1	2A	1070	G
1	2A	1075	G
1	2A	1078	U
1	2A	1083	C
1	2A	1084	G
1	2A	1087	G
1	2A	1088	C
1	2A	1090	A
1	2A	1092	G
1	2A	1093	A
1	2A	1099	A
1	2A	1103	G
1	2A	1105	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1106	U
1	2A	1107	G
1	2A	1108	G
1	2A	1109	C
1	2A	1114	A
1	2A	1115	A
1	2A	1117	C
1	2A	1121	C
1	2A	1124	C
1	2A	1127	U
1	2A	1128	U
1	2A	1132	G
1	2A	1133	A
1	2A	1134	G
1	2A	1135	U
1	2A	1142	U
1	2A	1143	A
1	2A	1145	C
1	2A	1151	G
1	2A	1152	G
1	2A	1154	C
1	2A	1155	G
1	2A	1156	A
1	2A	1157	G
1	2A	1158	U
1	2A	1164	C
1	2A	1167	G
1	2A	1173	A
1	2A	1174	A
1	2A	1175	U
1	2A	1179	C
1	2A	1180	G
1	2A	1183	G
1	2A	1200	A
1	2A	1216	G
1	2A	1249	U
1	2A	1250	G
1	2A	1256	G
1	2A	1264	A
1	2A	1293	G
1	2A	1298	A
1	2A	1301	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1316	G
1	2A	1317	A
1	2A	1329	A
1	2A	1345	U
1	2A	1346	A
1	2A	1350	C
1	2A	1359	C
1	2A	1366	A
1	2A	1372	C
1	2A	1374	U
1	2A	1397	U
1	2A	1404	A
1	2A	1405	A
1	2A	1410	A
1	2A	1413	G
1	2A	1415	C
1	2A	1417	U
1	2A	1418	A
1	2A	1425	G
1	2A	1429	A
1	2A	1430	G
1	2A	1431	C
1	2A	1461	G
1	2A	1462	C
1	2A	1465	U
1	2A	1466	G
1	2A	1473	C
1	2A	1490	A
1	2A	1495	A
1	2A	1496	G
1	2A	1501	G
1	2A	1505	G
1	2A	1506	A
1	2A	1513	C
1	2A	1517	A
1	2A	1528	G
1	2A	1534	U
1	2A	1535	A
1	2A	1538	C
1	2A	1542	U
1	2A	1553	A
1	2A	1554	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1555	A
1	2A	1579	G
1	2A	1588	A
1	2A	1591	A
1	2A	1594	C
1	2A	1604	A
1	2A	1605	G
1	2A	1615	A
1	2A	1624	U
1	2A	1626	A
1	2A	1630	C
1	2A	1631	A
1	2A	1653	A
1	2A	1654	A
1	2A	1655	A
1	2A	1661	A
1	2A	1662	C
1	2A	1676	C
1	2A	1677	A
1	2A	1686	C
1	2A	1692	C
1	2A	1694	C
1	2A	1697	G
1	2A	1700	A
1	2A	1720	G
1	2A	1742	G
1	2A	1746	A
1	2A	1747	A
1	2A	1749	G
1	2A	1765	G
1	2A	1766	A
1	2A	1768	G
1	2A	1786	G
1	2A	1788	G
1	2A	1792	A
1	2A	1793	G
1	2A	1794	G
1	2A	1803	A
1	2A	1810	A
1	2A	1812	C
1	2A	1813	A
1	2A	1821	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1828	U
1	2A	1830	C
1	2A	1831	G
1	2A	1846	G
1	2A	1865	G
1	2A	1869	G
1	2A	1877	A
1	2A	1898	A
1	2A	1899	G
1	2A	1910	A
1	2A	1921	A
1	2A	1927	G
1	2A	1934	A
1	2A	1935	C
1	2A	1950	G
1	2A	1951	G
1	2A	1957	A
1	2A	1959	A
1	2A	1965	U
1	2A	1973	A
1	2A	1976	U
1	2A	1984	U
1	2A	1986	C
1	2A	1988	C
1	2A	1991	A
1	2A	1992	A
1	2A	1993	A
1	2A	2013	G
1	2A	2014	U
1	2A	2018	G
1	2A	2041	A
1	2A	2042	C
1	2A	2044	G
1	2A	2052	A
1	2A	2054	A
1	2A	2064	C
1	2A	2076	C
1	2A	2077	G
1	2A	2081	A
1	2A	2082	G
1	2A	2083	A
1	2A	2090	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2103	A
1	2A	2114	G
1	2A	2120	U
1	2A	2123	U
1	2A	2124	C
1	2A	2126	C
1	2A	2127	G
1	2A	2128	C
1	2A	2131	G
1	2A	2132	C
1	2A	2134	U
1	2A	2136	G
1	2A	2137	G
1	2A	2140	A
1	2A	2143	U
1	2A	2147	A
1	2A	2148	G
1	2A	2149	C
1	2A	2150	C
1	2A	2152	G
1	2A	2153	U
1	2A	2154	G
1	2A	2155	A
1	2A	2157	C
1	2A	2158	C
1	2A	2161	C
1	2A	2163	C
1	2A	2165	U
1	2A	2167	C
1	2A	2169	G
1	2A	2171	U
1	2A	2174	G
1	2A	2175	G
1	2A	2178	G
1	2A	2179	A
1	2A	2183	G
1	2A	2185	C
1	2A	2186	G
1	2A	2188	U
1	2A	2189	G
1	2A	2193	U
1	2A	2194	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2195	C
1	2A	2198	C
1	2A	2202	G
1	2A	2203	G
1	2A	2209	C
1	2A	2210	U
1	2A	2211	G
1	2A	2219	A
1	2A	2226	G
1	2A	2227	G
1	2A	2228	A
1	2A	2229	U
1	2A	2230	G
1	2A	2236	A
1	2A	2249	G
1	2A	2250	G
1	2A	2279	A
1	2A	2280	A
1	2A	2286	C
1	2A	2289	A
1	2A	2291	G
1	2A	2294	C
1	2A	2297	A
1	2A	2298	A
1	2A	2300	G
1	2A	2316	A
1	2A	2319	G
1	2A	2320	A
1	2A	2329	G
1	2A	2330	G
1	2A	2331	A
1	2A	2332	G
1	2A	2336	G
1	2A	2337	C
1	2A	2338	A
1	2A	2345	G
1	2A	2347	A
1	2A	2354	C
1	2A	2358	C
1	2A	2361	C
1	2A	2365	G
1	2A	2387	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2390	G
1	2A	2394	G
1	2A	2396	C
1	2A	2402	G
1	2A	2412	U
1	2A	2417	U
1	2A	2421	G
1	2A	2433	A
1	2A	2434	U
1	2A	2436	A
1	2A	2439	G
1	2A	2440	G
1	2A	2441	A
1	2A	2446	A
1	2A	2450	A
1	2A	2451	C
1	2A	2452	C
1	2A	2459	A
1	2A	2480	A
1	2A	2485	C
1	2A	2487	A
1	2A	2502	U
1	2A	2513	G
1	2A	2516	G
1	2A	2517	U
1	2A	2529	A
1	2A	2531	C
1	2A	2565	U
1	2A	2573	U
1	2A	2577	A
1	2A	2578	G
1	2A	2584	C
1	2A	2597	C
1	2A	2613	A
1	2A	2615	U
1	2A	2620	U
1	2A	2622	U
1	2A	2623	C
1	2A	2632	A
1	2A	2640	A
1	2A	2641	G
1	2A	2665	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2674	G
1	2A	2700	U
1	2A	2701	C
1	2A	2702	C
1	2A	2714	C
1	2A	2724	A
1	2A	2725	A
1	2A	2726	G
1	2A	2738	U
1	2A	2745	A
1	2A	2765	A
1	2A	2769	A
1	2A	2770	A
1	2A	2773	G
1	2A	2776	A
1	2A	2777	A
1	2A	2782	G
1	2A	2789	G
1	2A	2790	A
1	2A	2793	A
1	2A	2794	G
1	2A	2801	C
1	2A	2812	G
1	2A	2813	C
1	2A	2817	U
1	2A	2827	G
1	2A	2829	A
1	2A	2830	A
1	2A	2844	A
1	2A	2848	G
1	2A	2881	G
1	2A	2885	G
1	2A	2889	C
1	2A	2900	A
1	2A	2901	G
1	2A	2902	G
2	2B	7	G
2	2B	8	U
2	2B	13	A
2	2B	23	G
2	2B	25	A
2	2B	32	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2B	42	C
2	2B	51	G
2	2B	53	A
2	2B	56	G
2	2B	58	A
2	2B	73	A
2	2B	85	G
2	2B	89	G
2	2B	98	G
2	2B	106	G
2	2B	110	G
34	2a	6	U
34	2a	10	G
34	2a	14	U
34	2a	23	G
34	2a	33	A
34	2a	40	G
34	2a	43	G
34	2a	48	C
34	2a	49	C
34	2a	51	A
34	2a	52	A
34	2a	53	G
34	2a	55	C
34	2a	67	G
34	2a	77	G
34	2a	84	A
34	2a	85	C
34	2a	91	G
34	2a	94	C
34	2a	95	A
34	2a	110	A
34	2a	115	C
34	2a	126	C
34	2a	137	G
34	2a	138	A
34	2a	158	C
34	2a	169	C
34	2a	177	U
34	2a	189	U
34	2a	202	A
34	2a	204	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2a	208	C
34	2a	210	U
34	2a	211	U
34	2a	212	G
34	2a	243	G
34	2a	247	G
34	2a	262	G
34	2a	263	C
34	2a	285	G
34	2a	297	G
34	2a	301	G
34	2a	317	A
34	2a	324	C
34	2a	325	A
34	2a	328	G
34	2a	338	C
34	2a	340	A
34	2a	342	G
34	2a	347	G
34	2a	348	C
34	2a	349	A
34	2a	350	G
34	2a	351	C
34	2a	363	U
34	2a	368	C
34	2a	380	G
34	2a	394	C
34	2a	402	G
34	2a	408	A
34	2a	409	G
34	2a	419	G
34	2a	420	G
34	2a	425	U
34	2a	426	A
34	2a	435	A
34	2a	437	C
34	2a	447	A
34	2a	456	C
34	2a	469	G
34	2a	470	G
34	2a	481	A
34	2a	482	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2a	489	G
34	2a	493	A
34	2a	494	A
34	2a	495	C
34	2a	502	C
34	2a	505	G
34	2a	511	G
34	2a	515	U
34	2a	516	A
34	2a	517	A
34	2a	531	A
34	2a	543	A
34	2a	545	U
34	2a	548	C
34	2a	556	A
34	2a	557	A
34	2a	560	G
34	2a	561	G
34	2a	591	A
34	2a	599	C
34	2a	602	C
34	2a	611	G
34	2a	612	G
34	2a	614	G
34	2a	616	A
34	2a	630	U
34	2a	634	G
34	2a	637	A
34	2a	649	A
34	2a	655	G
34	2a	671	A
34	2a	672	G
34	2a	701	C
34	2a	707	U
34	2a	715	G
34	2a	733	C
34	2a	736	G
34	2a	739	G
34	2a	750	A
34	2a	758	G
34	2a	761	A
34	2a	776	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2a	777	U
34	2a	778	A
34	2a	786	A
34	2a	801	C
34	2a	805	G
34	2a	811	U
34	2a	812	A
34	2a	813	G
34	2a	824	C
34	2a	825	U
34	2a	826	C
34	2a	829	G
34	2a	837	A
34	2a	850	A
34	2a	851	A
34	2a	869	U
34	2a	880	G
34	2a	890	C
34	2a	892	A
34	2a	900	G
34	2a	904	G
34	2a	905	G
34	2a	912	C
34	2a	913	A
34	2a	936	A
34	2a	938	U
34	2a	939	U
34	2a	946	A
34	2a	947	A
34	2a	949	G
34	2a	950	C
34	2a	952	A
34	2a	953	A
34	2a	954	G
34	2a	955	A
34	2a	967	C
34	2a	969	U
34	2a	970	U
34	2a	971	G
34	2a	981	G
34	2a	982	G
34	2a	984	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2a	985	C
34	2a	995	A
34	2a	998	C
34	2a	1000	G
34	2a	1001	G
34	2a	1003	G
34	2a	1004	U
34	2a	1005	G
34	2a	1006	C
34	2a	1007	C
34	2a	1009	C
34	2a	1010	G
34	2a	1016	G
34	2a	1024	A
34	2a	1033	G
34	2a	1048	U
34	2a	1049	C
34	2a	1051	G
34	2a	1064	G
34	2a	1072	G
34	2a	1077	G
34	2a	1078	U
34	2a	1084	A
34	2a	1100	G
34	2a	1107	G
34	2a	1109	U
34	2a	1112	C
34	2a	1113	A
34	2a	1119	U
34	2a	1120	C
34	2a	1121	G
34	2a	1122	G
34	2a	1123	C
34	2a	1129	A
34	2a	1134	A
34	2a	1135	A
34	2a	1142	U
34	2a	1149	G
34	2a	1163	G
34	2a	1165	A
34	2a	1166	G
34	2a	1178	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2a	1179	G
34	2a	1183	A
34	2a	1184	G
34	2a	1194	U
34	2a	1195	A
34	2a	1196	C
34	2a	1202	G
34	2a	1207	A
34	2a	1209	A
34	2a	1210	C
34	2a	1218	A
34	2a	1220	A
34	2a	1222	U
34	2a	1235	G
34	2a	1238	A
34	2a	1239	U
34	2a	1240	G
34	2a	1242	C
34	2a	1244	C
34	2a	1260	U
34	2a	1261	A
34	2a	1262	A
34	2a	1263	U
34	2a	1268	A
34	2a	1269	A
34	2a	1281	A
34	2a	1282	G
34	2a	1287	G
34	2a	1299	C
34	2a	1304	C
34	2a	1306	A
34	2a	1320	G
34	2a	1322	A
34	2a	1329	G
34	2a	1335	G
34	2a	1340	U
34	2a	1342	A
34	2a	1345	C
34	2a	1351	G
34	2a	1353	G
34	2a	1380	C
34	2a	1381	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2a	1402	G
34	2a	1426	G
34	2a	1430	C
34	2a	1431	U
34	2a	1432	A
34	2a	1433	C
34	2a	1434	G
34	2a	1475	G
34	2a	1482	G
34	2a	1484	U
34	2a	1495	G
34	2a	1497	A
34	2a	1498	G
34	2a	1507	G
34	2a	1508	G
34	2a	1509	A
34	2a	1510	U
57	2w	6	G
57	2w	9	G
57	2w	13	C
57	2w	16	C
57	2w	17	C
57	2w	20	U
57	2w	21	A
57	2w	31	G
57	2w	43	A
57	2w	47	U
57	2w	50	U
57	2w	52	G
57	2w	61	C
57	2w	65	C
57	2w	66	C
57	2w	67	C
57	2w	73	A
57	2w	76	A

All (47) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	183	A
1	1A	184	A
1	1A	270	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	301	A
1	1A	792	A
1	1A	1097	C
1	1A	1134	G
1	1A	1153	U
1	1A	1187	A
1	1A	1218	A
1	1A	1219	U
1	1A	1220	G
1	1A	1238	A
1	1A	1254	A
1	1A	1425	G
1	1A	1653	A
1	1A	2013	G
1	1A	2204	C
1	1A	2208	G
1	1A	2433	A
1	1A	2450	A
1	1A	2700	U
1	1A	2768	U
1	1A	2901	G
2	1B	52	A
1	2A	183	A
1	2A	272	G
1	2A	300	C
1	2A	552	A
1	2A	810	A
1	2A	945	A
1	2A	1047	G
1	2A	1087	G
1	2A	1238	A
1	2A	1424	A
1	2A	1425	G
1	2A	1604	A
1	2A	1699	G
1	2A	1934	A
1	2A	1964	U
1	2A	2013	G
1	2A	2131	G
1	2A	2329	G
1	2A	2417	U
1	2A	2433	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2700	U
1	2A	2768	U

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

8 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	$\#\|Z\| > 2$
57	5MU	2w	54	57	19,22,23	1.40	4 (21%)	28,32,35	2.16	6 (21%)
57	4SU	1w	8	57	18,21,22	2.03	4 (22%)	26,30,33	1.42	5 (19%)
57	PSU	1w	55	57	18,21,22	1.31	2 (11%)	22,30,33	1.83	4 (18%)
57	4SU	2w	8	57	18,21,22	1.96	4 (22%)	26,30,33	1.21	3 (11%)
57	5MU	1w	54	57	19,22,23	1.46	5 (26%)	28,32,35	1.86	6 (21%)
57	5MC	2w	32	57	18,22,23	1.02	2 (11%)	26,32,35	1.27	3 (11%)
57	5MC	1w	32	57	18,22,23	1.02	2 (11%)	26,32,35	1.17	2 (7%)
57	PSU	2w	55	57	18,21,22	1.41	2 (11%)	22,30,33	2.01	4 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	5MU	2w	54	57	-	0/7/25/26	0/2/2/2
57	4SU	1w	8	57	-	0/7/25/26	0/2/2/2
57	PSU	1w	55	57	-	0/7/25/26	0/2/2/2
57	4SU	2w	8	57	-	0/7/25/26	0/2/2/2
57	5MU	1w	54	57	-	2/7/25/26	0/2/2/2
57	5MC	2w	32	57	-	0/7/25/26	0/2/2/2
57	5MC	1w	32	57	-	0/7/25/26	0/2/2/2
57	PSU	2w	55	57	-	0/7/25/26	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2w	8	4SU	C4-N3	-4.91	1.32	1.37
57	1w	8	4SU	C4-N3	-4.82	1.32	1.37
57	1w	8	4SU	C4-S4	-4.06	1.60	1.68
57	2w	8	4SU	C4-S4	-3.84	1.61	1.68
57	1w	8	4SU	C2-N3	-3.65	1.31	1.38
57	2w	55	PSU	C6-C5	3.46	1.39	1.35
57	1w	55	PSU	C6-C5	3.30	1.39	1.35
57	1w	8	4SU	C5-C4	-3.18	1.38	1.42
57	2w	8	4SU	C2-N3	-3.12	1.32	1.38
57	2w	32	5MC	C6-C5	3.03	1.39	1.34
57	2w	54	5MU	C6-C5	3.01	1.39	1.34
57	2w	8	4SU	C5-C4	-2.93	1.38	1.42
57	1w	54	5MU	C6-C5	2.85	1.39	1.34
57	1w	32	5MC	C6-C5	2.84	1.39	1.34
57	1w	54	5MU	C4-N3	-2.73	1.33	1.38
57	2w	55	PSU	C4-N3	-2.66	1.33	1.38
57	1w	55	PSU	C4-N3	-2.59	1.34	1.38
57	2w	54	5MU	C4-N3	-2.57	1.34	1.38
57	2w	54	5MU	C4-C5	2.51	1.48	1.44
57	1w	54	5MU	C2-N1	2.47	1.42	1.38
57	1w	32	5MC	C6-N1	-2.40	1.34	1.38
57	1w	54	5MU	C4-C5	2.33	1.48	1.44
57	2w	54	5MU	C6-N1	-2.16	1.34	1.38
57	1w	54	5MU	C6-N1	-2.10	1.34	1.38
57	2w	32	5MC	C6-N1	-2.06	1.34	1.38

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	2w	55	PSU	N1-C2-N3	6.38	122.35	115.13
57	1w	55	PSU	N1-C2-N3	5.53	121.40	115.13
57	2w	54	5MU	C4-N3-C2	-5.49	120.24	127.35
57	2w	54	5MU	N3-C2-N1	5.11	121.67	114.89
57	2w	54	5MU	C5-C4-N3	4.70	119.32	115.31
57	1w	54	5MU	N3-C2-N1	4.63	121.03	114.89
57	1w	54	5MU	C4-N3-C2	-4.34	121.73	127.35
57	2w	55	PSU	C4-N3-C2	-4.15	120.36	126.34
57	2w	54	5MU	C5-C6-N1	-4.13	119.09	123.34
57	1w	55	PSU	C4-N3-C2	-3.90	120.72	126.34
57	2w	54	5MU	O4-C4-C5	-3.85	120.44	124.90
57	1w	8	4SU	C6-C5-C4	-3.77	116.69	119.95
57	1w	32	5MC	C5-C6-N1	-3.77	119.46	123.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	2w	32	5MC	C5-C6-N1	-3.75	119.48	123.34
57	2w	54	5MU	O2-C2-N1	-3.65	117.94	122.79
57	1w	54	5MU	C5-C4-N3	3.51	118.30	115.31
57	1w	54	5MU	C5-C6-N1	-3.34	119.90	123.34
57	1w	54	5MU	O4-C4-C5	-3.32	121.06	124.90
57	1w	8	4SU	C5-C4-N3	3.14	117.60	114.69
57	2w	8	4SU	C6-C5-C4	-3.05	117.31	119.95
57	2w	55	PSU	O2-C2-N1	-2.96	119.54	122.79
57	2w	32	5MC	O2-C2-N3	-2.94	117.55	122.33
57	1w	32	5MC	C5-C4-N3	-2.87	118.58	121.67
57	1w	55	PSU	O2-C2-N1	-2.66	119.86	122.79
57	2w	32	5MC	C5-C4-N3	-2.64	118.82	121.67
57	2w	55	PSU	C5-C6-N1	-2.60	118.21	122.11
57	1w	8	4SU	O2-C2-N1	2.59	126.23	122.79
57	2w	8	4SU	C5-C4-N3	2.57	117.07	114.69
57	2w	8	4SU	C1'-N1-C2	2.56	122.20	117.57
57	1w	8	4SU	C1'-N1-C2	2.52	122.13	117.57
57	1w	55	PSU	C5-C6-N1	-2.32	118.63	122.11
57	1w	54	5MU	C1'-N1-C2	2.06	121.30	117.57
57	1w	8	4SU	O2-C2-N3	-2.00	117.77	121.50

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	1w	54	5MU	O4'-C4'-C5'-O5'
57	1w	54	5MU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1945 ligands modelled in this entry, 1941 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	GDP	2z	702	59	24,30,30	0.94	1 (4%)	30,47,47	1.25	3 (10%)
61	SF4	1d	501	37	0,12,12	-	-	-		
61	SF4	2d	501	37	0,12,12	-	-	-		
62	GDP	1z	701	59	24,30,30	0.92	1 (4%)	30,47,47	1.43	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	SF4	1d	501	37	-	-	0/6/5/5
62	GDP	2z	702	59	-	4/12/32/32	0/3/3/3
61	SF4	2d	501	37	-	-	0/6/5/5
62	GDP	1z	701	59	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	1z	701	GDP	C6-N1	-2.48	1.34	1.37
62	2z	702	GDP	C6-N1	-2.27	1.34	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	1z	701	GDP	PA-O3A-PB	-5.01	115.63	132.83
62	2z	702	GDP	PA-O3A-PB	-4.03	118.98	132.83
62	1z	701	GDP	C8-N7-C5	2.39	107.54	102.99
62	2z	702	GDP	O4'-C1'-C2'	-2.38	103.45	106.93
62	1z	701	GDP	C5-C6-N1	2.34	118.08	113.95
62	2z	702	GDP	C8-N7-C5	2.32	107.41	102.99

There are no chirality outliers.

All (4) torsion outliers are listed below:

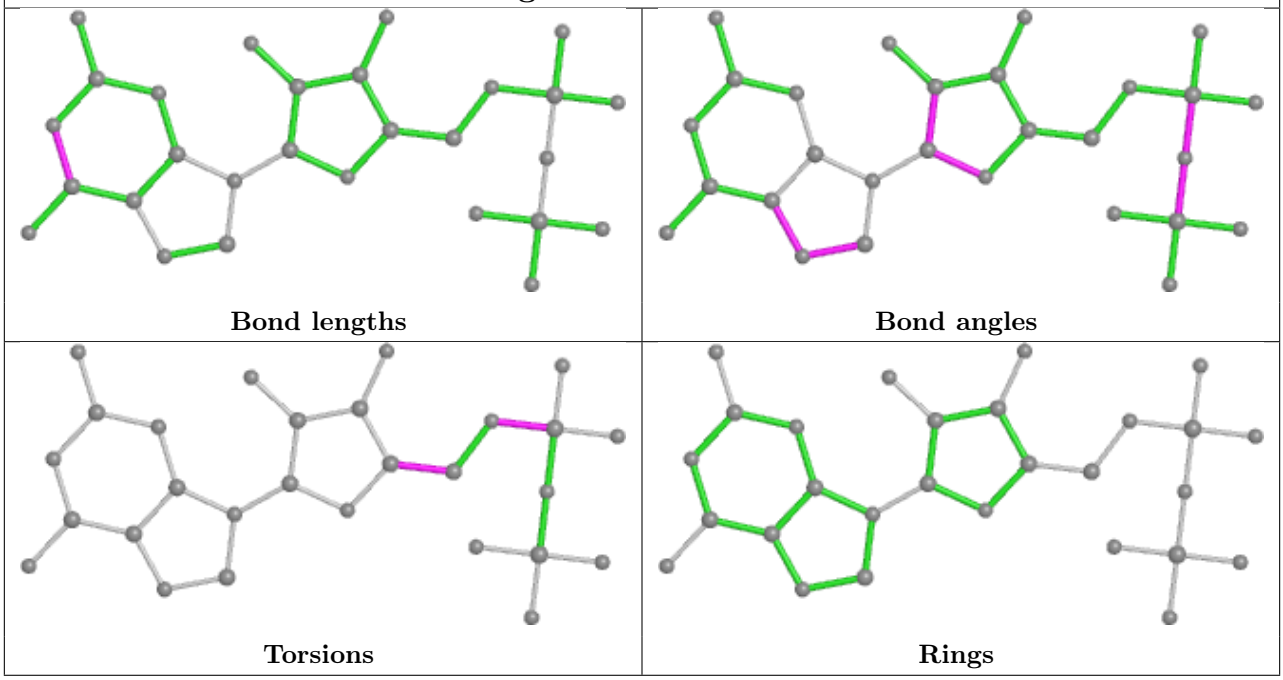
Mol	Chain	Res	Type	Atoms
62	2z	702	GDP	O4'-C4'-C5'-O5'
62	2z	702	GDP	C3'-C4'-C5'-O5'
62	2z	702	GDP	C5'-O5'-PA-O3A
62	2z	702	GDP	C5'-O5'-PA-O2A

There are no ring outliers.

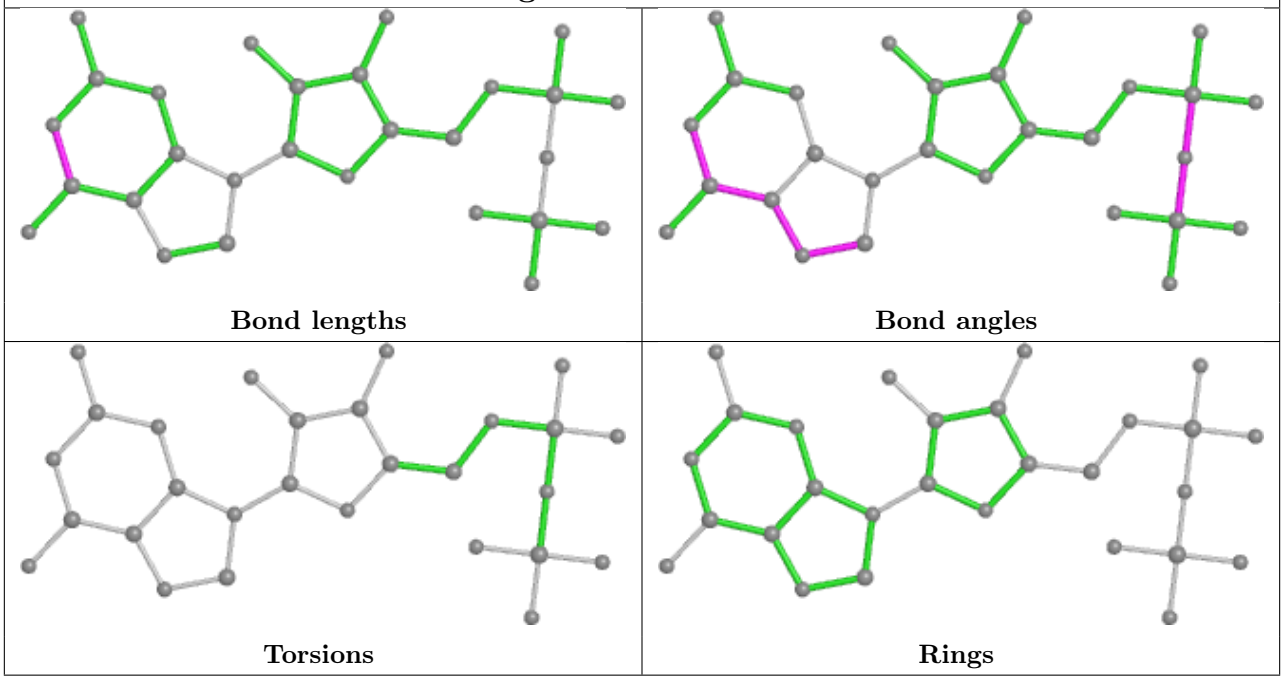
No monomer is involved in short contacts.

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 GDP 2z 702



Ligand GDP 1z 701



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	1A	2872/2915 (98%)	-0.12	87 (3%)	50	22	20, 43, 93, 111	0
1	2A	2868/2915 (98%)	-0.29	90 (3%)	49	21	22, 46, 97, 112	0
2	1B	120/121 (99%)	-0.37	0	100	100	37, 57, 71, 82	0
2	2B	120/121 (99%)	-0.41	0	100	100	43, 62, 74, 83	0
3	1C	135/229 (58%)	3.52	102 (75%)	0	0	82, 99, 105, 108	2 (1%)
3	2C	135/229 (58%)	3.83	111 (82%)	0	0	82, 100, 104, 108	2 (1%)
4	1D	275/276 (99%)	-0.50	0	100	100	23, 41, 57, 85	0
4	2D	275/276 (99%)	-0.58	0	100	100	24, 42, 58, 84	0
5	1E	204/206 (99%)	-0.44	0	100	100	23, 44, 63, 75	0
5	2E	204/206 (99%)	-0.48	0	100	100	22, 48, 65, 77	0
6	1F	203/210 (96%)	-0.39	0	100	100	22, 51, 72, 89	0
6	2F	203/210 (96%)	-0.42	0	100	100	25, 54, 73, 88	0
7	1G	181/182 (99%)	-0.40	1 (0%)	89	72	50, 66, 81, 88	0
7	2G	181/182 (99%)	-0.19	0	100	100	55, 69, 82, 90	0
8	1H	174/180 (96%)	-0.33	1 (0%)	89	72	45, 62, 75, 81	0
8	2H	174/180 (96%)	0.27	1 (0%)	89	72	50, 66, 78, 83	0
9	1J	130/173 (75%)	0.45	12 (9%)	9	3	65, 82, 95, 100	0
9	2J	130/173 (75%)	1.04	20 (15%)	2	1	70, 88, 100, 104	0
10	1K	67/147 (45%)	1.68	21 (31%)	0	0	79, 94, 100, 102	0
10	2K	66/147 (44%)	2.51	38 (57%)	0	0	87, 95, 101, 104	0
11	1L	140/140 (100%)	-0.43	0	100	100	31, 44, 65, 82	0
11	2L	140/140 (100%)	-0.37	0	100	100	33, 49, 67, 81	0
12	1M	122/122 (100%)	-0.43	0	100	100	27, 46, 64, 71	0
12	2M	122/122 (100%)	-0.50	0	100	100	30, 47, 66, 73	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1N	149/150 (99%)	-0.32	0 100 100	24, 53, 76, 84	0
13	2N	149/150 (99%)	-0.13	1 (0%) 87 69	27, 56, 77, 88	0
14	1O	141/141 (100%)	-0.37	0 100 100	32, 48, 61, 74	0
14	2O	141/141 (100%)	-0.60	0 100 100	35, 51, 65, 76	0
15	1P	118/118 (100%)	-0.41	0 100 100	27, 40, 54, 66	0
15	2P	118/118 (100%)	-0.45	0 100 100	29, 43, 58, 68	0
16	1Q	110/112 (98%)	-0.32	0 100 100	44, 56, 71, 76	0
16	2Q	110/112 (98%)	-0.17	0 100 100	47, 60, 73, 78	0
17	1R	131/146 (89%)	-0.41	1 (0%) 86 65	33, 50, 72, 84	0
17	2R	131/146 (89%)	-0.53	0 100 100	34, 52, 73, 82	0
18	1S	116/118 (98%)	-0.65	1 (0%) 84 63	15, 31, 47, 71	0
18	2S	116/118 (98%)	-0.43	0 100 100	37, 56, 70, 74	0
19	1T	101/101 (100%)	-0.58	0 100 100	21, 35, 57, 72	0
19	2T	101/101 (100%)	-0.26	0 100 100	33, 65, 78, 83	0
20	1U	112/113 (99%)	-0.58	0 100 100	19, 32, 54, 85	0
20	2U	112/113 (99%)	-0.39	0 100 100	35, 49, 65, 82	0
21	1V	95/96 (98%)	-0.52	0 100 100	23, 39, 60, 84	0
21	2V	95/96 (98%)	-0.21	2 (2%) 63 34	40, 59, 76, 84	0
22	1W	107/110 (97%)	-0.28	1 (0%) 84 63	39, 57, 74, 81	0
22	2W	107/110 (97%)	0.23	2 (1%) 66 37	44, 61, 76, 85	0
23	1X	186/206 (90%)	-0.40	0 100 100	44, 65, 77, 85	0
23	2X	186/206 (90%)	-0.01	3 (1%) 72 44	50, 68, 80, 88	0
24	1Y	76/85 (89%)	-0.51	1 (1%) 77 51	20, 36, 58, 67	0
24	2Y	76/85 (89%)	-0.12	1 (1%) 77 51	38, 56, 69, 79	0
25	1Z	97/98 (98%)	-0.31	1 (1%) 82 59	24, 44, 67, 75	0
25	2Z	97/98 (98%)	-0.25	1 (1%) 82 59	31, 56, 77, 81	0
26	10	70/72 (97%)	-0.31	0 100 100	44, 57, 69, 81	0
26	20	70/72 (97%)	-0.34	0 100 100	46, 60, 70, 81	0
27	11	59/60 (98%)	-0.23	1 (1%) 70 41	30, 45, 63, 76	0
27	21	59/60 (98%)	0.05	0 100 100	34, 49, 68, 79	0
28	12	69/71 (97%)	0.12	3 (4%) 35 13	61, 81, 93, 98	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	22	69/71 (97%)	0.18	5 (7%) 15 4	66, 82, 95, 99	0
29	13	59/60 (98%)	-0.47	0 100 100	24, 40, 57, 63	0
29	23	59/60 (98%)	-0.52	0 100 100	27, 42, 62, 68	0
30	14	53/54 (98%)	-0.40	0 100 100	37, 47, 59, 64	0
30	24	53/54 (98%)	-0.38	0 100 100	40, 49, 61, 65	0
31	15	48/49 (97%)	-0.33	0 100 100	23, 29, 58, 72	0
31	25	48/49 (97%)	-0.38	0 100 100	30, 40, 66, 78	0
32	16	64/65 (98%)	-0.56	0 100 100	20, 33, 44, 61	0
32	26	64/65 (98%)	-0.34	0 100 100	37, 50, 60, 72	0
33	17	37/37 (100%)	-0.05	0 100 100	36, 49, 59, 65	0
33	27	37/37 (100%)	-0.19	1 (2%) 54 26	39, 53, 63, 68	0
34	1a	1495/1521 (98%)	-0.12	34 (2%) 60 31	40, 72, 96, 109	0
34	2a	1501/1521 (98%)	-0.12	34 (2%) 60 31	42, 73, 96, 109	0
35	1b	231/256 (90%)	0.01	3 (1%) 77 51	67, 82, 91, 100	0
35	2b	231/256 (90%)	0.17	13 (5%) 24 8	68, 83, 93, 103	0
36	1c	206/239 (86%)	0.05	1 (0%) 91 75	68, 80, 90, 95	0
36	2c	206/239 (86%)	0.24	4 (1%) 66 37	71, 81, 90, 95	0
37	1d	208/209 (99%)	-0.24	0 100 100	56, 73, 83, 92	0
37	2d	208/209 (99%)	-0.25	0 100 100	58, 73, 82, 92	0
38	1e	148/162 (91%)	-0.33	0 100 100	54, 68, 77, 83	0
38	2e	148/162 (91%)	-0.19	0 100 100	56, 70, 78, 85	0
39	1f	100/101 (99%)	-0.43	0 100 100	54, 70, 79, 85	0
39	2f	100/101 (99%)	-0.23	0 100 100	56, 71, 81, 84	0
40	1g	155/156 (99%)	0.11	10 (6%) 18 5	70, 78, 89, 94	0
40	2g	155/156 (99%)	0.35	14 (9%) 9 3	69, 79, 91, 96	0
41	1h	137/138 (99%)	-0.19	0 100 100	58, 70, 79, 85	0
41	2h	137/138 (99%)	-0.17	0 100 100	60, 71, 78, 85	0
42	1i	127/128 (99%)	0.16	0 100 100	62, 82, 89, 94	0
42	2i	127/128 (99%)	0.63	8 (6%) 20 6	66, 83, 90, 94	0
43	1j	97/105 (92%)	0.28	2 (2%) 63 34	66, 84, 92, 94	0
43	2j	96/105 (91%)	0.77	11 (11%) 4 1	68, 85, 93, 96	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	1k	114/129 (88%)	-0.25	0	100	100	53, 69, 80, 84	0
44	2k	114/129 (88%)	-0.05	0	100	100	54, 71, 82, 85	0
45	1l	122/132 (92%)	-0.34	0	100	100	50, 60, 70, 75	0
45	2l	122/132 (92%)	-0.31	0	100	100	49, 61, 70, 75	0
46	1m	123/126 (97%)	0.27	7 (5%)	23	8	65, 78, 90, 105	0
46	2m	122/126 (96%)	0.57	9 (7%)	14	4	70, 83, 94, 105	0
47	1n	60/61 (98%)	-0.07	1 (1%)	70	41	69, 79, 84, 86	0
47	2n	60/61 (98%)	0.35	2 (3%)	46	20	70, 81, 85, 89	0
48	1o	88/89 (98%)	-0.16	0	100	100	52, 67, 79, 87	0
48	2o	88/89 (98%)	-0.05	0	100	100	51, 68, 78, 87	0
49	1p	82/88 (93%)	0.01	1 (1%)	79	54	54, 69, 79, 85	0
49	2p	82/88 (93%)	0.03	0	100	100	54, 69, 79, 84	0
50	1q	99/105 (94%)	-0.21	0	100	100	54, 67, 76, 83	0
50	2q	99/105 (94%)	-0.04	1 (1%)	82	59	55, 67, 77, 85	0
51	1r	68/88 (77%)	0.19	3 (4%)	34	13	57, 69, 82, 90	0
51	2r	68/88 (77%)	0.14	1 (1%)	73	46	60, 70, 81, 90	0
52	1s	84/93 (90%)	0.65	3 (3%)	42	17	76, 84, 92, 95	0
52	2s	83/93 (89%)	0.84	6 (7%)	15	4	75, 85, 92, 94	0
53	1t	96/106 (90%)	0.05	1 (1%)	82	59	60, 70, 80, 85	0
53	2t	96/106 (90%)	-0.04	0	100	100	59, 70, 81, 84	0
54	1u	23/27 (85%)	0.50	0	100	100	70, 77, 81, 82	0
54	2u	23/27 (85%)	1.00	2 (8%)	10	3	70, 78, 82, 84	0
55	1z	730/758 (96%)	0.38	82 (11%)	5	1	52, 79, 96, 105	0
55	2z	730/758 (96%)	0.56	108 (14%)	2	1	47, 81, 99, 108	0
56	1y	6/24 (25%)	0.58	0	100	100	61, 67, 93, 95	0
56	2y	5/24 (20%)	0.86	1 (20%)	1	0	64, 66, 89, 96	0
57	1w	72/77 (93%)	-0.20	0	100	100	32, 64, 78, 97	0
57	2w	72/77 (93%)	-0.09	0	100	100	33, 66, 79, 98	0
58	1x	19/35 (54%)	-0.31	0	100	100	35, 42, 64, 65	0
58	2x	19/35 (54%)	-0.14	0	100	100	36, 45, 65, 65	0
All	All	22619/23832 (94%)	-0.07	871 (3%)	39	15	15, 63, 94, 112	4 (0%)

All (871) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
46	2m	124	PRO	13.7
3	2C	165	ASN	11.9
46	1m	123	ALA	11.7
3	1C	165	ASN	11.3
3	1C	56	GLN	10.9
3	1C	170	ALA	10.9
46	2m	123	ALA	10.7
3	2C	174	PRO	10.5
46	2m	122	LYS	10.5
3	1C	166	ASP	10.1
3	2C	63	SER	9.9
46	2m	119	GLY	9.7
3	1C	58	VAL	9.7
55	2z	576	ASP	9.4
46	2m	121	LYS	9.3
3	2C	57	ASN	9.1
3	1C	225	ASN	8.8
3	2C	4	GLY	8.8
3	1C	158	ALA	8.6
3	1C	65	PRO	8.3
3	2C	58	VAL	8.2
3	2C	179	SER	8.1
55	2z	575	VAL	8.0
1	2A	2144	G	7.8
3	1C	24	GLU	7.8
1	1A	2166	C	7.7
1	1A	2136	G	7.7
3	2C	186	ALA	7.6
3	2C	170	ALA	7.5
1	1A	2200	C	7.5
3	2C	34	THR	7.4
3	2C	51	PRO	7.3
1	2A	2145	G	7.3
1	2A	1110	U	7.3
3	1C	176	GLY	7.3
1	2A	2167	C	7.2
10	2K	107	ILE	7.2
3	2C	203	GLY	7.1
3	1C	163	PHE	7.1
3	2C	180	PHE	7.0
1	2A	2136	G	6.8
3	2C	188	ASN	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	1C	168	THR	6.7
1	1A	2187	G	6.7
55	2z	425	SER	6.6
10	2K	123	ALA	6.6
3	2C	164	ARG	6.5
1	1A	2164	C	6.5
46	2m	120	LYS	6.5
55	2z	569	ASP	6.4
3	1C	51	PRO	6.4
3	2C	166	ASP	6.4
46	1m	119	GLY	6.4
3	1C	171	ILE	6.4
3	2C	226	PRO	6.4
55	2z	463	VAL	6.3
3	2C	175	VAL	6.3
3	2C	211	SER	6.3
1	2A	2180	G	6.3
3	2C	21	THR	6.3
3	1C	63	SER	6.3
1	2A	2195	C	6.3
55	2z	507	TYR	6.2
1	2A	1111	U	6.2
3	2C	56	GLN	6.1
3	2C	26	ALA	6.1
1	2A	2132	C	6.1
9	1J	88	ALA	6.1
1	1A	2167	C	6.0
55	1z	89	ASP	6.0
1	1A	2165	U	6.0
1	1A	2138	A	6.0
1	2A	2131	G	6.0
3	1C	57	ASN	6.0
3	1C	196	LEU	6.0
46	1m	120	LYS	5.9
1	2A	2133	G	5.9
1	1A	2133	G	5.9
1	2A	2200	C	5.9
1	1A	2202	G	5.9
1	1A	2181	G	5.8
3	2C	67	GLY	5.8
3	1C	164	ARG	5.8
1	2A	2166	C	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	2C	187	ASP	5.8
46	1m	124	PRO	5.8
55	2z	89	ASP	5.8
55	2z	532	GLY	5.8
1	1A	2162	G	5.7
55	2z	423	LYS	5.7
34	2a	1239	U	5.7
24	2Y	8	GLY	5.7
55	2z	574	GLU	5.7
3	1C	21	THR	5.7
1	1A	2134	U	5.7
10	2K	99	ILE	5.6
46	2m	6	GLY	5.6
1	1A	2199	C	5.6
3	2C	181	PRO	5.6
1	1A	2150	C	5.6
3	2C	183	GLU	5.6
1	2A	2181	G	5.6
55	1z	492	ASP	5.5
3	2C	25	ALA	5.5
9	2J	125	LEU	5.5
40	2g	83	ALA	5.5
55	2z	436	PRO	5.5
3	2C	59	ARG	5.5
55	2z	435	ASP	5.5
55	2z	419	ALA	5.5
1	2A	2165	U	5.5
3	1C	162	GLU	5.5
3	2C	185	LEU	5.5
1	1A	1113	G	5.5
55	2z	506	GLN	5.5
1	2A	2141	G	5.4
55	2z	422	GLU	5.4
9	2J	85	ASP	5.4
3	1C	66	HIS	5.4
1	1A	2151	U	5.4
3	2C	182	PRO	5.4
3	1C	197	GLU	5.4
1	2A	2154	G	5.4
3	1C	179	SER	5.3
10	2K	97	GLY	5.3
3	2C	60	GLY	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
55	2z	410	ASP	5.3
55	2z	461	ILE	5.3
1	2A	2149	C	5.3
1	1A	2189	G	5.3
46	1m	121	LYS	5.2
1	2A	2135	A	5.2
9	1J	89	ALA	5.2
3	1C	50	ASP	5.2
40	1g	156	TRP	5.2
55	1z	411	VAL	5.2
3	2C	69	GLY	5.2
3	2C	208	PHE	5.1
3	1C	34	THR	5.1
46	1m	122	LYS	5.1
34	2a	981	G	5.1
1	2A	2163	C	5.1
3	1C	55	ASP	5.1
1	1A	2188	U	5.1
3	2C	173	ALA	5.1
3	1C	62	VAL	5.0
40	2g	80	VAL	5.0
9	1J	53	VAL	5.0
1	2A	2142	G	5.0
34	1a	1011	C	5.0
1	1A	2142	G	5.0
1	1A	2180	G	5.0
9	2J	49	ALA	5.0
55	2z	437	THR	5.0
1	2A	2190	A	5.0
3	1C	20	TYR	4.9
1	1A	2131	G	4.9
1	1A	2168	G	4.9
1	2A	2138	A	4.9
55	2z	418	LYS	4.9
1	2A	2199	C	4.9
34	2a	1011	C	4.9
3	1C	67	GLY	4.9
1	1A	2141	G	4.9
10	2K	85	GLU	4.9
40	2g	78	ARG	4.8
3	2C	66	HIS	4.8
10	2K	108	ALA	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	2C	17	ASN	4.8
35	2b	233	SER	4.8
55	2z	573	HIS	4.8
1	2A	2201	U	4.8
34	2a	979	A	4.8
1	2A	1123	U	4.8
10	2K	98	ARG	4.8
55	2z	462	ILE	4.8
3	1C	188	ASN	4.8
1	2A	2175	G	4.8
1	1A	2153	U	4.8
1	2A	2164	C	4.7
1	1A	2130	U	4.7
1	2A	2143	U	4.7
1	1A	2137	G	4.7
55	2z	420	ASP	4.7
1	1A	2135	A	4.7
1	1A	2132	C	4.7
1	2A	2168	G	4.7
3	1C	68	LEU	4.6
3	2C	28	LEU	4.6
55	2z	530	VAL	4.6
1	1A	2175	G	4.6
3	2C	193	ILE	4.6
40	2g	82	GLY	4.6
34	2a	980	G	4.6
3	1C	198	ALA	4.6
1	1A	2157	C	4.6
55	2z	492	ASP	4.6
3	1C	25	ALA	4.6
3	2C	68	LEU	4.6
3	2C	22	ILE	4.6
9	1J	49	ALA	4.6
55	1z	461	ILE	4.5
1	2A	2130	U	4.5
3	1C	187	ASP	4.5
3	2C	65	PRO	4.5
10	2K	127	ILE	4.5
40	1g	85	TYR	4.5
3	2C	161	ILE	4.5
1	2A	2159	C	4.5
34	1a	981	G	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	2C	35	ALA	4.5
9	2J	133	GLU	4.4
3	1C	193	ILE	4.4
3	1C	49	ILE	4.4
3	1C	161	ILE	4.4
34	2a	1010	G	4.4
1	1A	1112	A	4.4
3	2C	55	ASP	4.4
3	1C	199	HIS	4.4
1	2A	2137	G	4.4
55	1z	427	ALA	4.4
55	2z	472	VAL	4.4
34	2a	1012	G	4.4
10	1K	135	GLY	4.4
3	1C	4	GLY	4.4
10	2K	105	LEU	4.3
55	2z	494	GLU	4.3
10	2K	76	TYR	4.3
3	2C	9	ALA	4.3
55	1z	458	HIS	4.3
55	2z	421	GLN	4.3
55	2z	570	GLY	4.3
1	2A	2150	C	4.3
34	1a	982	G	4.3
34	1a	1019	G	4.3
3	1C	173	ALA	4.3
3	1C	178	ALA	4.3
1	2A	2179	A	4.3
3	2C	30	LYS	4.3
55	1z	466	LEU	4.3
1	2A	2146	G	4.3
10	1K	136	VAL	4.3
10	2K	129	GLY	4.2
1	1A	1220	G	4.2
1	1A	2170	G	4.2
3	1C	64	LEU	4.2
10	2K	136	VAL	4.2
3	1C	195	ALA	4.2
3	2C	11	LEU	4.2
9	1J	50	ARG	4.2
55	2z	415	PRO	4.2
1	1A	2144	G	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2189	G	4.2
55	2z	601	ILE	4.2
9	2J	50	ARG	4.1
1	2A	2169	G	4.1
1	2A	2176	G	4.1
3	2C	46	LYS	4.1
55	2z	441	SER	4.1
1	1A	2152	G	4.1
1	1A	2195	C	4.1
55	2z	527	ASN	4.1
3	2C	33	ALA	4.1
10	2K	138	VAL	4.1
3	2C	27	ARG	4.1
34	1a	980	G	4.1
3	1C	9	ALA	4.1
3	2C	204	ALA	4.1
10	2K	130	SER	4.1
34	2a	1016	G	4.1
1	1A	2163	C	4.1
55	2z	490	PRO	4.1
1	1A	2201	U	4.1
3	2C	163	PHE	4.0
1	2A	2187	G	4.0
3	2C	31	GLU	4.0
55	2z	491	VAL	4.0
40	2g	154	TYR	4.0
3	2C	184	LYS	4.0
3	1C	60	GLY	4.0
1	1A	2182	C	4.0
3	1C	182	PRO	4.0
10	2K	137	GLU	4.0
3	2C	167	LYS	4.0
3	2C	168	THR	4.0
55	2z	538	TYR	4.0
55	2z	475	ASN	4.0
3	2C	54	SER	4.0
1	1A	2143	U	4.0
55	1z	570	GLY	4.0
3	1C	59	ARG	4.0
1	1A	2190	A	3.9
55	1z	457	LEU	3.9
1	2A	2198	C	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2183	G	3.9
55	1z	433	GLU	3.9
55	2z	411	VAL	3.9
3	1C	191	ALA	3.9
3	1C	159	GLY	3.9
1	2A	2178	G	3.9
3	2C	189	ILE	3.9
10	2K	83	GLY	3.9
3	2C	198	ALA	3.9
36	2c	87	LEU	3.9
1	2A	2160	C	3.9
3	1C	169	GLY	3.9
3	2C	43	VAL	3.9
1	2A	1112	A	3.9
1	2A	2202	G	3.9
3	2C	162	GLU	3.9
1	2A	2134	U	3.9
55	2z	427	ALA	3.9
1	2A	934	C	3.8
3	2C	171	ILE	3.8
55	2z	408	VAL	3.8
55	2z	432	ALA	3.8
3	2C	10	LEU	3.8
3	2C	199	HIS	3.8
10	2K	104	VAL	3.8
55	1z	463	VAL	3.8
55	2z	501	THR	3.8
3	1C	204	ALA	3.8
3	2C	3	HIS	3.8
55	1z	530	VAL	3.8
3	2C	24	GLU	3.8
3	1C	175	VAL	3.8
55	1z	528	ALA	3.8
1	1A	2129	C	3.8
1	1A	2125	G	3.7
22	2W	1	MET	3.7
1	1A	2169	G	3.7
55	2z	581	ALA	3.7
34	2a	1509	A	3.7
1	1A	2172	G	3.7
3	2C	16	PRO	3.7
34	2a	1019	G	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	2K	135	GLY	3.7
55	1z	456	GLU	3.7
9	2J	89	ALA	3.7
55	2z	514	VAL	3.7
55	2z	234	GLY	3.7
3	2C	191	ALA	3.7
10	1K	134	MET	3.7
3	2C	207	THR	3.7
10	1K	124	ALA	3.7
55	1z	462	ILE	3.7
3	1C	26	ALA	3.7
1	1A	2186	G	3.7
34	2a	1510	U	3.6
55	1z	476	VAL	3.6
3	2C	177	LYS	3.6
10	2K	113	PRO	3.6
3	2C	47	LEU	3.6
1	1A	2176	G	3.6
55	1z	437	THR	3.6
34	1a	1010	G	3.6
1	1A	2161	C	3.6
1	2A	2188	U	3.6
10	2K	122	ALA	3.6
3	2C	169	GLY	3.6
42	2i	30	GLY	3.6
3	2C	29	VAL	3.6
10	2K	94	GLU	3.6
3	1C	33	ALA	3.6
55	1z	464	ASP	3.6
54	2u	24	ARG	3.5
3	1C	200	LYS	3.5
3	2C	197	GLU	3.5
55	2z	457	LEU	3.5
55	1z	451	ILE	3.5
55	1z	514	VAL	3.5
55	1z	642	VAL	3.5
55	2z	599	PRO	3.5
10	1K	118	THR	3.5
55	1z	546	ILE	3.5
1	1A	1554	C	3.5
55	2z	474	ALA	3.5
34	1a	1013	A	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
55	1z	563	ILE	3.5
55	2z	539	ILE	3.5
3	2C	176	GLY	3.5
3	2C	52	ARG	3.5
34	1a	1008	C	3.5
3	2C	206	GLY	3.5
1	2A	2127	G	3.5
55	2z	434	GLU	3.4
34	2a	1000	G	3.4
3	1C	22	ILE	3.4
1	1A	2159	C	3.4
9	2J	116	ILE	3.4
34	1a	1003	G	3.4
1	2A	1554	C	3.4
10	2K	79	ARG	3.4
34	1a	1018	A	3.4
1	2A	2157	C	3.4
3	1C	180	PHE	3.4
3	2C	210	ARG	3.4
9	1J	52	PHE	3.4
55	2z	424	LEU	3.4
1	2A	2153	U	3.4
43	2j	10	GLY	3.4
40	1g	84	ASN	3.4
3	1C	40	THR	3.4
55	1z	509	HIS	3.4
1	2A	1121	C	3.4
10	1K	90	LYS	3.4
1	2A	2148	G	3.4
10	1K	86	LYS	3.4
9	1J	51	LEU	3.3
3	1C	189	ILE	3.3
55	2z	464	ASP	3.3
55	1z	422	GLU	3.3
55	2z	629	GLY	3.3
3	1C	61	THR	3.3
1	1A	697	G	3.3
9	2J	62	ALA	3.3
1	1A	2154	G	3.3
55	2z	499	ARG	3.3
3	1C	226	PRO	3.3
1	1A	2191	A	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	1C	69	GLY	3.3
10	1K	120	LEU	3.3
1	1A	934	C	3.3
3	1C	192	PHE	3.3
10	2K	80	LYS	3.3
10	2K	96	VAL	3.3
1	2A	2186	G	3.2
55	2z	444	PRO	3.2
13	2N	93	GLY	3.2
43	2j	26	ALA	3.2
9	2J	97	ALA	3.2
55	1z	541	ALA	3.2
1	2A	2191	A	3.2
1	2A	2203	G	3.2
10	1K	89	HIS	3.2
9	1J	99	SER	3.2
10	2K	133	SER	3.2
1	1A	2148	G	3.2
28	12	53	GLU	3.2
3	1C	27	ARG	3.2
55	2z	525	PHE	3.2
1	2A	217	A	3.2
1	2A	2155	A	3.2
34	2a	1013	A	3.2
1	2A	2126	C	3.2
34	2a	1020	C	3.2
3	2C	61	THR	3.2
3	1C	19	VAL	3.2
40	2g	156	TRP	3.2
55	2z	429	ALA	3.2
55	2z	500	GLN	3.2
55	1z	405	PRO	3.2
43	1j	10	GLY	3.2
55	2z	493	VAL	3.2
34	1a	1009	C	3.1
3	2C	38	ASP	3.1
1	1A	2203	G	3.1
34	1a	1005	G	3.1
34	2a	1017	G	3.1
55	2z	454	MET	3.1
55	2z	455	GLY	3.1
40	1g	83	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2g	155	ARG	3.1
34	2a	1023	U	3.1
3	2C	50	ASP	3.1
1	1A	2198	C	3.1
55	2z	417	THR	3.1
40	2g	79	ARG	3.1
55	1z	472	VAL	3.1
34	1a	1509	A	3.1
36	2c	81	GLY	3.1
55	1z	408	VAL	3.1
10	2K	93	ARG	3.1
55	1z	426	GLN	3.1
3	2C	18	LYS	3.1
3	1C	28	LEU	3.1
55	1z	599	PRO	3.1
34	2a	1025	G	3.1
1	1A	2179	A	3.1
3	2C	70	LYS	3.0
3	1C	207	THR	3.0
3	1C	3	HIS	3.0
3	1C	70	LYS	3.0
43	2j	36	GLY	3.0
1	1A	2140	A	3.0
3	1C	208	PHE	3.0
55	1z	531	GLY	3.0
1	1A	2149	C	3.0
8	1H	2	SER	3.0
1	2A	2162	G	3.0
35	2b	232	PRO	3.0
43	2j	73	ASP	3.0
3	1C	177	LYS	3.0
24	1Y	9	SER	3.0
55	2z	540	PRO	3.0
3	1C	23	ASP	3.0
55	2z	577	SER	3.0
28	22	68	ARG	3.0
1	1A	2185	C	3.0
40	2g	81	GLY	3.0
1	1A	2155	A	3.0
3	2C	64	LEU	3.0
1	1A	682	G	3.0
55	1z	500	GLN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	2C	19	VAL	3.0
40	1g	78	ARG	3.0
46	2m	93	ARG	3.0
55	2z	476	VAL	3.0
9	2J	56	ASN	3.0
3	1C	209	LEU	2.9
40	1g	79	ARG	2.9
55	2z	40	HIS	2.9
1	2A	2156	A	2.9
40	1g	82	GLY	2.9
55	2z	433	GLU	2.9
1	2A	1136	G	2.9
42	2i	87	GLN	2.9
1	1A	695	C	2.9
1	1A	1109	C	2.9
1	2A	2196	C	2.9
34	1a	1020	C	2.9
3	2C	209	LEU	2.9
10	2K	89	HIS	2.9
3	2C	160	ARG	2.9
3	1C	52	ARG	2.9
28	12	57	GLU	2.9
55	2z	430	ARG	2.9
40	2g	84	ASN	2.9
1	2A	2158	C	2.9
3	2C	23	ASP	2.9
1	2A	2170	G	2.9
9	2J	129	PRO	2.9
10	2K	116	ASN	2.9
52	2s	59	PRO	2.9
55	1z	467	LYS	2.9
1	1A	2126	C	2.9
1	1A	2158	C	2.9
3	1C	181	PRO	2.9
34	1a	209	U	2.9
55	1z	404	VAL	2.9
55	2z	582	PHE	2.9
1	2A	2177	G	2.9
3	1C	194	ARG	2.9
34	2a	976	G	2.9
55	1z	496	LYS	2.9
9	1J	90	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2a	982	G	2.8
10	1K	107	ILE	2.8
34	2a	211	U	2.8
3	1C	15	ASP	2.8
34	2a	1018	A	2.8
28	22	49	PHE	2.8
1	2A	2182	C	2.8
3	2C	12	GLU	2.8
3	1C	53	ARG	2.8
1	1A	2156	A	2.8
55	1z	495	GLY	2.8
34	1a	1015	G	2.8
34	2a	1002	G	2.8
55	1z	529	ILE	2.8
3	1C	186	ALA	2.8
51	1r	23	LYS	2.8
10	1K	85	GLU	2.8
1	1A	2160	C	2.8
3	1C	17	ASN	2.8
55	2z	456	GLU	2.8
55	1z	634	MET	2.8
3	1C	160	ARG	2.8
55	1z	428	LEU	2.8
51	1r	24	ALA	2.8
55	1z	507	TYR	2.8
55	1z	575	VAL	2.8
55	1z	465	ARG	2.7
55	2z	600	VAL	2.7
51	2r	58	LEU	2.7
1	2A	2152	G	2.7
25	2Z	2	SER	2.7
55	2z	571	SER	2.7
55	1z	538	TYR	2.7
34	1a	1004	U	2.7
55	1z	410	ASP	2.7
1	2A	2125	G	2.7
10	1K	138	VAL	2.7
55	2z	533	VAL	2.7
34	1a	707	U	2.7
3	2C	15	ASP	2.7
10	2K	82	ALA	2.7
47	1n	2	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1a	211	U	2.7
55	1z	539	ILE	2.7
55	2z	568	TYR	2.7
55	2z	681	LYS	2.7
1	2A	2151	U	2.7
55	1z	572	TYR	2.7
28	22	52	THR	2.7
35	1b	136	VAL	2.7
1	2A	678	A	2.7
3	2C	217	THR	2.7
55	2z	543	GLN	2.7
55	2z	682	GLN	2.7
1	2A	679	G	2.7
3	2C	62	VAL	2.7
40	1g	80	VAL	2.7
34	2a	1026	C	2.6
55	2z	578	SER	2.6
3	1C	45	ALA	2.6
9	2J	48	GLY	2.6
27	11	60	GLU	2.6
35	2b	226	ARG	2.6
55	2z	595	GLN	2.6
1	2A	1126	U	2.6
1	2A	1137	C	2.6
55	1z	569	ASP	2.6
1	1A	2123	U	2.6
1	2A	2174	G	2.6
9	2J	99	SER	2.6
55	2z	511	LYS	2.6
55	2z	534	ILE	2.6
55	2z	688	ILE	2.6
3	2C	13	LYS	2.6
55	1z	412	ALA	2.6
53	1t	9	ASN	2.6
55	2z	440	VAL	2.6
3	1C	48	GLY	2.6
47	2n	25	VAL	2.6
55	1z	506	GLN	2.6
10	1K	141	ALA	2.6
43	1j	72	VAL	2.6
55	2z	405	PRO	2.6
1	1A	696	C	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1a	985	C	2.5
3	1C	32	LEU	2.5
55	1z	536	LYS	2.5
55	2z	630	GLN	2.5
34	2a	983	A	2.5
1	1A	2122	G	2.5
3	2C	5	LYS	2.5
9	2J	53	VAL	2.5
9	2J	98	LYS	2.5
3	1C	224	ILE	2.5
3	1C	38	ASP	2.5
1	2A	2139	U	2.5
34	1a	1017	G	2.5
3	1C	185	LEU	2.5
43	2j	40	LEU	2.5
55	1z	423	LYS	2.5
34	1a	1002	G	2.5
1	2A	933	A	2.5
1	2A	2140	A	2.5
10	1K	79	ARG	2.5
9	2J	57	THR	2.5
34	1a	1239	U	2.5
55	2z	438	PHE	2.5
43	2j	38	ILE	2.5
56	2y	14	A	2.4
55	2z	653	PHE	2.4
10	1K	121	GLU	2.4
3	1C	211	SER	2.4
1	1A	2177	G	2.4
1	2A	1107	G	2.4
9	1J	48	GLY	2.4
34	1a	77	G	2.4
34	1a	1012	G	2.4
9	2J	132	ASP	2.4
3	2C	6	ARG	2.4
42	2i	70	LYS	2.4
1	1A	2146	G	2.4
3	1C	203	GLY	2.4
34	2a	1014	G	2.4
55	1z	592	GLU	2.4
34	2a	1009	C	2.4
34	2a	1005	G	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	1C	174	PRO	2.4
40	1g	153	HIS	2.4
3	1C	12	GLU	2.4
28	22	57	GLU	2.4
55	1z	601	ILE	2.4
1	1A	2194	A	2.4
1	2A	2147	A	2.4
55	1z	234	GLY	2.4
9	2J	54	ALA	2.4
55	2z	639	ASN	2.4
40	2g	85	TYR	2.4
34	1a	1016	G	2.4
55	2z	442	THR	2.4
3	2C	159	GLY	2.3
10	1K	140	GLY	2.3
34	1a	825	U	2.3
52	2s	43	GLU	2.3
1	1A	681	G	2.3
3	2C	7	TYR	2.3
3	2C	224	ILE	2.3
43	2j	39	PRO	2.3
55	2z	556	ILE	2.3
42	2i	7	THR	2.3
55	1z	455	GLY	2.3
55	2z	86	GLY	2.3
23	2X	156	LYS	2.3
35	1b	122	PHE	2.3
55	2z	526	VAL	2.3
3	1C	30	LYS	2.3
1	1A	933	A	2.3
36	1c	193	TYR	2.3
55	1z	505	GLY	2.3
1	1A	2174	G	2.3
21	2V	68	ARG	2.3
3	2C	196	LEU	2.3
10	1K	81	ALA	2.3
52	2s	71	LEU	2.3
55	2z	529	ILE	2.3
9	1J	105	PRO	2.3
52	2s	45	VAL	2.3
1	1A	2139	U	2.3
10	2K	87	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
55	1z	491	VAL	2.3
3	1C	217	THR	2.3
55	1z	429	ALA	2.3
17	1R	37	GLY	2.3
1	2A	932	C	2.3
34	1a	208	C	2.3
3	1C	213	TYR	2.3
3	2C	20	TYR	2.3
46	2m	42	ALA	2.3
55	2z	90	PHE	2.3
35	2b	227	GLY	2.3
10	1K	77	LEU	2.3
3	2C	225	ASN	2.3
3	1C	206	GLY	2.3
10	1K	114	ASP	2.3
55	2z	426	GLN	2.3
28	12	59	PHE	2.3
35	2b	122	PHE	2.3
7	1G	49	ASP	2.3
55	1z	635	GLU	2.3
35	2b	101	MET	2.3
21	2V	67	GLY	2.2
34	1a	1268	A	2.3
55	1z	443	HIS	2.3
55	2z	404	VAL	2.3
1	2A	2172	G	2.2
10	2K	110	GLN	2.2
34	1a	1022	C	2.2
55	1z	585	ALA	2.2
52	1s	48	THR	2.2
3	1C	31	GLU	2.2
1	1A	2209	C	2.2
55	1z	540	PRO	2.2
3	2C	32	LEU	2.2
10	2K	126	MET	2.2
34	2a	1021	C	2.2
35	2b	48	MET	2.2
52	2s	38	SER	2.2
43	2j	72	VAL	2.2
55	1z	533	VAL	2.2
42	2i	64	THR	2.2
55	1z	231	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
55	1z	475	ASN	2.2
9	1J	116	ILE	2.2
1	2A	2183	G	2.2
3	2C	40	THR	2.2
55	2z	428	LEU	2.2
55	1z	434	GLU	2.2
55	1z	469	GLU	2.2
1	1A	2196	C	2.2
9	2J	117	LEU	2.2
34	1a	1007	C	2.2
1	2A	669	C	2.2
35	2b	136	VAL	2.2
35	2b	165	VAL	2.2
55	1z	542	VAL	2.2
55	2z	235	GLU	2.2
55	2z	458	HIS	2.2
1	1A	2171	U	2.2
47	2n	2	ALA	2.2
55	1z	441	SER	2.2
3	2C	42	GLU	2.2
10	2K	118	THR	2.2
10	2K	134	MET	2.2
22	2W	91	GLU	2.2
28	22	56	VAL	2.2
40	1g	155	ARG	2.2
3	1C	222	VAL	2.2
35	2b	231	GLU	2.2
3	1C	205	LYS	2.2
52	1s	33	THR	2.2
52	1s	47	HIS	2.2
55	1z	597	GLY	2.2
34	1a	1006	C	2.1
35	1b	135	GLN	2.1
55	1z	223	PHE	2.1
22	1W	1	MET	2.1
55	2z	536	LYS	2.1
46	1m	87	TYR	2.1
3	1C	54	SER	2.1
23	2X	159	PRO	2.1
43	2j	74	ILE	2.1
34	2a	86	U	2.1
54	2u	5	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	2C	45	ALA	2.1
9	2J	90	ALA	2.1
42	2i	62	TYR	2.1
1	2A	1103	G	2.1
1	2A	2173	G	2.1
34	2a	1238	A	2.1
25	1Z	2	SER	2.1
34	1a	1026	C	2.1
55	2z	502	GLY	2.1
42	2i	56	LEU	2.1
51	1r	25	THR	2.1
55	1z	490	PRO	2.1
1	2A	2129	C	2.1
8	2H	96	ALA	2.1
34	1a	978	U	2.1
55	2z	685	GLU	2.1
10	2K	115	LEU	2.1
35	2b	228	GLY	2.1
55	1z	227	ILE	2.1
55	1z	600	VAL	2.1
43	2j	65	LEU	2.1
55	2z	580	MET	2.1
55	2z	523	PHE	2.1
3	2C	218	MET	2.1
36	2c	158	GLY	2.1
36	2c	159	GLY	2.1
55	2z	489	LYS	2.1
3	2C	158	ALA	2.1
55	1z	474	ALA	2.1
55	1z	578	SER	2.1
3	2C	205	LYS	2.1
49	1p	57	ARG	2.1
55	2z	471	LYS	2.1
55	2z	495	GLY	2.1
3	1C	212	VAL	2.1
3	2C	53	ARG	2.1
3	1C	221	SER	2.1
10	2K	75	SER	2.1
40	2g	42	ILE	2.1
55	2z	598	ASP	2.1
18	1S	117	GLN	2.1
34	2a	1006	C	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	2K	111	LYS	2.0
40	2g	52	GLU	2.0
55	1z	494	GLU	2.0
55	2z	504	ARG	2.0
1	2A	1105	U	2.0
23	2X	132	ASN	2.0
50	2q	8	GLY	2.0
34	2a	984	A	2.0
34	2a	1432	A	2.0
1	1A	2184	C	2.0
1	1A	2206	C	2.0
40	2g	112	PRO	2.0
3	2C	200	LYS	2.0
34	2a	1024	A	2.0
43	2j	32	ALA	2.0
10	1K	116	ASN	2.0
35	2b	131	PRO	2.0
10	2K	112	MET	2.0
55	1z	588	MET	2.0
1	2A	1132	G	2.0
55	1z	595	GLN	2.0
33	27	37	GLY	2.0
10	1K	93	ARG	2.0
55	1z	556	ILE	2.0
1	1A	679	G	2.0
35	2b	133	LYS	2.0
55	1z	682	GLN	2.0
3	1C	8	ARG	2.0
3	2C	8	ARG	2.0
42	2i	4	TYR	2.0
52	2s	30	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	PSU	1w	55	20/21	0.93	0.16	53,63,72,82	0
57	PSU	2w	55	20/21	0.93	0.12	53,63,80,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	4SU	2w	8	20/21	0.94	0.16	51,68,81,83	0
57	5MU	2w	54	21/22	0.94	0.17	61,67,79,97	0
57	5MC	2w	32	21/22	0.95	0.22	52,75,83,85	0
57	4SU	1w	8	20/21	0.95	0.14	43,61,72,73	0
57	5MU	1w	54	21/22	0.96	0.13	22,55,66,75	0
57	5MC	1w	32	21/22	0.96	0.20	48,64,75,79	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1a	1771	1/1	0.33	0.79	94,94,94,94	0
59	MG	2B	206	1/1	0.41	0.27	67,67,67,67	0
60	ZN	13	103	1/1	0.48	0.52	278,278,278,278	0
59	MG	1A	3104	1/1	0.53	0.48	52,52,52,52	0
59	MG	1B	205	1/1	0.54	0.37	72,72,72,72	0
59	MG	2A	3238	1/1	0.54	0.42	60,60,60,60	0
59	MG	2a	1657	1/1	0.57	0.44	66,66,66,66	0
59	MG	2A	3263	1/1	0.60	0.38	69,69,69,69	0
59	MG	1A	3636	1/1	0.62	0.52	56,56,56,56	0
59	MG	1A	3509	1/1	0.63	0.15	50,50,50,50	0
59	MG	2a	1765	1/1	0.64	0.34	79,79,79,79	0
59	MG	1A	3576	1/1	0.65	0.30	51,51,51,51	0
59	MG	2a	1762	1/1	0.65	0.26	65,65,65,65	0
59	MG	2w	3003	1/1	0.66	0.20	80,80,80,80	0
59	MG	1A	3515	1/1	0.69	0.12	48,48,48,48	0
59	MG	2a	1754	1/1	0.69	0.63	61,61,61,61	0
59	MG	2A	3252	1/1	0.70	0.23	55,55,55,55	0
59	MG	1a	1622	1/1	0.70	0.40	64,64,64,64	0
59	MG	1a	1630	1/1	0.70	0.23	69,69,69,69	0
59	MG	2F	301	1/1	0.71	0.30	58,58,58,58	0
59	MG	1F	306	1/1	0.71	0.34	46,46,46,46	0
59	MG	2a	1662	1/1	0.71	0.38	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
59	MG	1A	3483	1/1	0.71	0.20	40,40,40,40	0
59	MG	2A	3326	1/1	0.72	0.27	49,49,49,49	0
59	MG	1A	3710	1/1	0.72	0.37	60,60,60,60	0
59	MG	2a	1661	1/1	0.72	0.15	67,67,67,67	0
59	MG	1a	1643	1/1	0.73	0.12	50,50,50,50	0
59	MG	1A	3226	1/1	0.74	0.28	50,50,50,50	0
59	MG	1A	3023	1/1	0.74	0.79	37,37,37,37	0
59	MG	1A	3638	1/1	0.74	0.23	89,89,89,89	0
59	MG	1A	3771	1/1	0.75	0.37	68,68,68,68	0
59	MG	2A	3330	1/1	0.75	0.19	28,28,28,28	0
59	MG	1A	3497	1/1	0.75	0.25	30,30,30,30	0
59	MG	1A	3673	1/1	0.76	0.20	70,70,70,70	0
59	MG	2B	201	1/1	0.76	0.32	62,62,62,62	0
59	MG	1A	3737	1/1	0.77	0.12	65,65,65,65	0
59	MG	1a	1686	1/1	0.77	0.31	75,75,75,75	0
59	MG	1A	3259	1/1	0.77	0.14	45,45,45,45	0
59	MG	2A	3122	1/1	0.77	0.24	42,42,42,42	0
59	MG	2A	3228	1/1	0.78	0.31	46,46,46,46	0
59	MG	2a	1603	1/1	0.78	0.74	65,65,65,65	0
59	MG	1A	3211	1/1	0.78	0.40	59,59,59,59	0
59	MG	1a	1604	1/1	0.78	0.12	51,51,51,51	0
59	MG	1a	1701	1/1	0.78	0.24	65,65,65,65	0
59	MG	2A	3311	1/1	0.78	0.31	63,63,63,63	0
59	MG	1A	3301	1/1	0.78	0.19	65,65,65,65	0
59	MG	1A	3321	1/1	0.78	0.17	74,74,74,74	0
59	MG	2A	3145	1/1	0.78	0.23	55,55,55,55	0
59	MG	2A	3180	1/1	0.78	0.15	56,56,56,56	0
59	MG	1A	3196	1/1	0.79	0.33	49,49,49,49	0
59	MG	2A	3220	1/1	0.79	0.46	60,60,60,60	0
59	MG	1A	3002	1/1	0.79	0.22	44,44,44,44	0
59	MG	2a	1621	1/1	0.79	0.29	66,66,66,66	0
59	MG	1A	3223	1/1	0.79	0.41	59,59,59,59	0
59	MG	1a	1799	1/1	0.79	0.29	80,80,80,80	0
59	MG	2A	3032	1/1	0.79	0.33	57,57,57,57	0
59	MG	2a	1687	1/1	0.79	0.35	48,48,48,48	0
59	MG	2a	1689	1/1	0.79	0.16	69,69,69,69	0
59	MG	2A	3273	1/1	0.79	0.18	63,63,63,63	0
59	MG	2A	3035	1/1	0.79	0.25	45,45,45,45	0
59	MG	1A	3114	1/1	0.79	0.11	43,43,43,43	0
59	MG	2A	3136	1/1	0.79	0.32	52,52,52,52	0
59	MG	1a	1684	1/1	0.79	0.17	78,78,78,78	0
59	MG	1A	3018	1/1	0.80	0.44	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1a	1666	1/1	0.80	0.16	49,49,49,49	0
59	MG	1a	1681	1/1	0.80	0.18	60,60,60,60	0
59	MG	2A	3432	1/1	0.80	0.08	55,55,55,55	0
59	MG	2A	3500	1/1	0.80	0.25	56,56,56,56	0
59	MG	1A	3207	1/1	0.80	0.47	45,45,45,45	0
59	MG	2A	3088	1/1	0.80	0.19	41,41,41,41	0
59	MG	2A	3094	1/1	0.80	0.26	53,53,53,53	0
59	MG	1A	3040	1/1	0.80	0.31	31,31,31,31	0
59	MG	1A	3141	1/1	0.80	0.14	46,46,46,46	0
59	MG	2A	3236	1/1	0.81	0.38	48,48,48,48	0
59	MG	1A	3072	1/1	0.81	0.39	61,61,61,61	0
59	MG	2A	3063	1/1	0.81	0.27	52,52,52,52	0
59	MG	2a	1616	1/1	0.81	0.25	57,57,57,57	0
59	MG	1A	3017	1/1	0.81	0.09	50,50,50,50	0
59	MG	2a	1640	1/1	0.81	0.11	65,65,65,65	0
59	MG	2a	1649	1/1	0.81	0.22	69,69,69,69	0
59	MG	1B	221	1/1	0.81	0.12	42,42,42,42	0
59	MG	1A	3305	1/1	0.81	0.12	42,42,42,42	0
59	MG	1A	3055	1/1	0.81	0.25	49,49,49,49	0
59	MG	1A	3403	1/1	0.81	0.19	57,57,57,57	0
59	MG	2A	3349	1/1	0.81	0.28	56,56,56,56	0
59	MG	2a	1711	1/1	0.81	0.24	76,76,76,76	0
59	MG	2A	3393	1/1	0.81	0.23	45,45,45,45	0
59	MG	1A	3760	1/1	0.81	0.39	44,44,44,44	0
59	MG	2A	3002	1/1	0.81	0.20	40,40,40,40	0
59	MG	2A	3516	1/1	0.81	0.07	78,78,78,78	0
59	MG	1A	3764	1/1	0.81	0.29	33,33,33,33	0
59	MG	2a	1617	1/1	0.82	0.12	65,65,65,65	0
59	MG	1A	3505	1/1	0.82	0.18	55,55,55,55	0
59	MG	1a	1713	1/1	0.82	0.16	62,62,62,62	0
59	MG	1a	1720	1/1	0.82	0.32	54,54,54,54	0
59	MG	2A	3352	1/1	0.82	0.12	31,31,31,31	0
59	MG	2a	1658	1/1	0.82	0.23	58,58,58,58	0
59	MG	1a	1639	1/1	0.82	0.18	67,67,67,67	0
59	MG	1A	3568	1/1	0.82	0.36	54,54,54,54	0
59	MG	1A	3013	1/1	0.82	0.28	35,35,35,35	0
59	MG	2A	3507	1/1	0.82	0.20	39,39,39,39	0
59	MG	2A	3009	1/1	0.82	0.16	50,50,50,50	0
59	MG	1a	1667	1/1	0.82	0.10	67,67,67,67	0
59	MG	1A	3682	1/1	0.82	0.14	97,97,97,97	0
59	MG	1a	1610	1/1	0.82	0.17	50,50,50,50	0
59	MG	1A	3691	1/1	0.82	0.15	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
59	MG	1a	1695	1/1	0.82	0.28	49,49,49,49	0
59	MG	1A	3146	1/1	0.83	0.17	56,56,56,56	0
59	MG	1A	3118	1/1	0.83	0.30	42,42,42,42	0
59	MG	1U	202	1/1	0.83	0.27	37,37,37,37	0
59	MG	1A	3389	1/1	0.83	0.20	37,37,37,37	0
59	MG	2A	3179	1/1	0.83	0.39	50,50,50,50	0
59	MG	1a	1608	1/1	0.83	0.19	65,65,65,65	0
59	MG	2A	3186	1/1	0.83	0.22	38,38,38,38	0
59	MG	2S	202	1/1	0.83	0.18	58,58,58,58	0
59	MG	1A	3234	1/1	0.83	0.23	50,50,50,50	0
59	MG	1a	1612	1/1	0.83	0.18	41,41,41,41	0
59	MG	2A	3231	1/1	0.83	0.21	56,56,56,56	0
59	MG	1A	3717	1/1	0.83	0.35	89,89,89,89	0
59	MG	1A	3461	1/1	0.83	0.17	31,31,31,31	0
59	MG	1t	3001	1/1	0.83	0.32	54,54,54,54	0
59	MG	2a	1651	1/1	0.83	0.18	67,67,67,67	0
59	MG	1A	3580	1/1	0.83	0.32	54,54,54,54	0
59	MG	2A	3272	1/1	0.83	0.25	51,51,51,51	0
59	MG	1A	3611	1/1	0.83	0.14	46,46,46,46	0
59	MG	2A	3300	1/1	0.83	0.18	48,48,48,48	0
59	MG	2a	1673	1/1	0.83	0.33	55,55,55,55	0
59	MG	1a	1654	1/1	0.83	0.14	42,42,42,42	0
59	MG	1a	1660	1/1	0.83	0.37	59,59,59,59	0
59	MG	2A	3038	1/1	0.83	0.21	43,43,43,43	0
59	MG	2a	1742	1/1	0.83	0.34	82,82,82,82	0
59	MG	1A	3139	1/1	0.83	0.15	67,67,67,67	0
59	MG	2a	1760	1/1	0.83	0.19	44,44,44,44	0
59	MG	2A	3076	1/1	0.83	0.18	45,45,45,45	0
59	MG	1A	3115	1/1	0.83	0.29	36,36,36,36	0
59	MG	2A	3419	1/1	0.83	0.20	30,30,30,30	0
59	MG	2A	3422	1/1	0.83	0.15	37,37,37,37	0
59	MG	2A	3274	1/1	0.84	0.21	56,56,56,56	0
59	MG	2A	3101	1/1	0.84	0.21	50,50,50,50	0
59	MG	2A	3301	1/1	0.84	0.12	30,30,30,30	0
59	MG	2a	1625	1/1	0.84	0.42	60,60,60,60	0
59	MG	2a	1626	1/1	0.84	0.34	57,57,57,57	0
59	MG	1G	3002	1/1	0.84	0.09	64,64,64,64	0
59	MG	1b	3001	1/1	0.84	0.16	70,70,70,70	0
59	MG	2A	3144	1/1	0.84	0.47	50,50,50,50	0
59	MG	1a	1688	1/1	0.84	0.14	60,60,60,60	0
59	MG	1A	3122	1/1	0.84	0.18	60,60,60,60	0
59	MG	2a	1659	1/1	0.84	0.22	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
59	MG	1A	3127	1/1	0.84	0.28	31,31,31,31	0
59	MG	1a	1636	1/1	0.84	0.26	62,62,62,62	0
59	MG	1A	3222	1/1	0.84	0.23	49,49,49,49	0
59	MG	1a	1741	1/1	0.84	0.26	71,71,71,71	0
59	MG	2A	3039	1/1	0.84	0.57	43,43,43,43	0
59	MG	2a	1691	1/1	0.84	0.51	64,64,64,64	0
59	MG	2A	3055	1/1	0.84	0.17	41,41,41,41	0
59	MG	2A	3237	1/1	0.84	0.14	54,54,54,54	0
59	MG	2A	3592	1/1	0.84	0.17	63,63,63,63	0
59	MG	2a	1757	1/1	0.84	0.11	64,64,64,64	0
59	MG	1a	1749	1/1	0.84	0.12	68,68,68,68	0
59	MG	1a	1757	1/1	0.84	0.12	56,56,56,56	0
59	MG	1A	3027	1/1	0.84	0.52	34,34,34,34	0
59	MG	2j	8001	1/1	0.84	0.22	65,65,65,65	0
59	MG	2w	3001	1/1	0.84	0.15	64,64,64,64	0
59	MG	2A	3091	1/1	0.84	0.31	60,60,60,60	0
59	MG	1a	1778	1/1	0.84	0.07	81,81,81,81	0
60	ZN	17	102	1/1	0.84	0.32	120,120,120,120	0
59	MG	1a	1634	1/1	0.85	0.12	48,48,48,48	0
59	MG	2a	1620	1/1	0.85	0.24	63,63,63,63	0
59	MG	2A	3280	1/1	0.85	0.29	68,68,68,68	0
59	MG	1a	1693	1/1	0.85	0.11	57,57,57,57	0
59	MG	1A	3603	1/1	0.85	0.22	65,65,65,65	0
59	MG	2a	1630	1/1	0.85	0.41	55,55,55,55	0
59	MG	1A	3212	1/1	0.85	0.20	40,40,40,40	0
59	MG	1a	1706	1/1	0.85	0.28	57,57,57,57	0
59	MG	1a	1707	1/1	0.85	0.20	60,60,60,60	0
59	MG	2A	3337	1/1	0.85	0.20	41,41,41,41	0
59	MG	1A	3635	1/1	0.85	0.18	72,72,72,72	0
59	MG	2A	3351	1/1	0.85	0.13	43,43,43,43	0
59	MG	2A	3210	1/1	0.85	0.08	45,45,45,45	0
59	MG	2A	3354	1/1	0.85	0.23	33,33,33,33	0
59	MG	1A	3770	1/1	0.85	0.13	68,68,68,68	0
59	MG	2A	3224	1/1	0.85	0.31	62,62,62,62	0
59	MG	1a	1739	1/1	0.85	0.20	44,44,44,44	0
59	MG	1A	3704	1/1	0.85	0.38	71,71,71,71	0
59	MG	2a	1695	1/1	0.85	0.23	61,61,61,61	0
59	MG	2A	3460	1/1	0.85	0.18	59,59,59,59	0
59	MG	2A	3068	1/1	0.85	0.29	43,43,43,43	0
59	MG	2a	1744	1/1	0.85	0.28	65,65,65,65	0
59	MG	1A	3215	1/1	0.85	0.43	37,37,37,37	0
59	MG	2A	3081	1/1	0.85	0.13	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
59	MG	2A	3241	1/1	0.85	0.13	52,52,52,52	0
59	MG	1a	1613	1/1	0.85	0.14	66,66,66,66	0
59	MG	2A	3259	1/1	0.85	0.90	72,72,72,72	0
59	MG	1a	1616	1/1	0.85	0.37	55,55,55,55	0
59	MG	2l	201	1/1	0.85	0.16	64,64,64,64	0
59	MG	2z	704	1/1	0.85	0.23	55,55,55,55	0
59	MG	2A	3265	1/1	0.85	0.56	62,62,62,62	0
59	MG	1A	3535	1/1	0.85	0.26	54,54,54,54	0
59	MG	2a	1614	1/1	0.85	0.20	49,49,49,49	0
59	MG	1A	3729	1/1	0.85	0.33	54,54,54,54	0
59	MG	1A	3019	1/1	0.86	0.24	50,50,50,50	0
59	MG	1A	3311	1/1	0.86	0.16	40,40,40,40	0
59	MG	2a	1604	1/1	0.86	0.15	51,51,51,51	0
59	MG	1a	1629	1/1	0.86	0.41	45,45,45,45	0
59	MG	1A	3506	1/1	0.86	0.26	33,33,33,33	0
59	MG	1A	3162	1/1	0.86	0.34	46,46,46,46	0
59	MG	1A	3170	1/1	0.86	0.10	61,61,61,61	0
59	MG	1B	204	1/1	0.86	0.15	51,51,51,51	0
59	MG	1a	1642	1/1	0.86	0.42	43,43,43,43	0
59	MG	1A	3180	1/1	0.86	0.23	50,50,50,50	0
59	MG	1a	1764	1/1	0.86	0.11	67,67,67,67	0
59	MG	1a	1647	1/1	0.86	0.20	73,73,73,73	0
59	MG	2A	3331	1/1	0.86	0.20	39,39,39,39	0
59	MG	2A	3170	1/1	0.86	0.30	54,54,54,54	0
59	MG	2A	3176	1/1	0.86	0.15	38,38,38,38	0
59	MG	2A	3350	1/1	0.86	0.19	71,71,71,71	0
59	MG	1A	3680	1/1	0.86	0.30	46,46,46,46	0
59	MG	1A	3551	1/1	0.86	0.16	48,48,48,48	0
59	MG	1a	1800	1/1	0.86	0.44	68,68,68,68	0
59	MG	2a	1668	1/1	0.86	0.18	43,43,43,43	0
59	MG	2A	3357	1/1	0.86	0.17	27,27,27,27	0
59	MG	2a	1680	1/1	0.86	0.27	52,52,52,52	0
59	MG	1A	3437	1/1	0.86	0.09	49,49,49,49	0
59	MG	2A	3403	1/1	0.86	0.20	28,28,28,28	0
59	MG	2A	3414	1/1	0.86	0.12	42,42,42,42	0
59	MG	1H	3001	1/1	0.86	0.15	51,51,51,51	0
59	MG	2a	1703	1/1	0.86	0.15	50,50,50,50	0
59	MG	2a	1705	1/1	0.86	0.17	52,52,52,52	0
59	MG	1w	3004	1/1	0.86	0.24	49,49,49,49	0
59	MG	1A	3694	1/1	0.86	0.17	47,47,47,47	0
59	MG	1a	1683	1/1	0.86	0.15	75,75,75,75	0
59	MG	2a	1751	1/1	0.86	0.36	104,104,104,104	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3465	1/1	0.86	0.17	22,22,22,22	0
59	MG	2A	3485	1/1	0.86	0.15	38,38,38,38	0
59	MG	2a	1759	1/1	0.86	0.32	62,62,62,62	0
59	MG	1A	3010	1/1	0.86	0.29	45,45,45,45	0
59	MG	1A	3303	1/1	0.86	0.24	48,48,48,48	0
59	MG	1a	1687	1/1	0.86	0.22	55,55,55,55	0
59	MG	2A	3581	1/1	0.86	0.19	71,71,71,71	0
59	MG	1A	3594	1/1	0.86	0.11	22,22,22,22	0
59	MG	2A	3611	1/1	0.86	0.17	59,59,59,59	0
59	MG	2z	705	1/1	0.86	0.30	67,67,67,67	0
59	MG	2A	3246	1/1	0.86	0.22	47,47,47,47	0
59	MG	1A	3596	1/1	0.86	0.14	52,52,52,52	0
59	MG	2B	210	1/1	0.86	0.15	55,55,55,55	0
59	MG	1A	3732	1/1	0.86	0.29	75,75,75,75	0
59	MG	1a	1606	1/1	0.87	0.12	63,63,63,63	0
59	MG	2A	3036	1/1	0.87	0.14	53,53,53,53	0
59	MG	2D	301	1/1	0.87	0.29	48,48,48,48	0
59	MG	1A	3036	1/1	0.87	0.28	38,38,38,38	0
59	MG	1A	3068	1/1	0.87	0.42	33,33,33,33	0
59	MG	2A	3052	1/1	0.87	0.17	47,47,47,47	0
59	MG	2A	3268	1/1	0.87	0.37	56,56,56,56	0
59	MG	2a	1607	1/1	0.87	0.12	68,68,68,68	0
59	MG	1a	1611	1/1	0.87	0.26	84,84,84,84	0
59	MG	2A	3062	1/1	0.87	0.11	41,41,41,41	0
59	MG	1A	3050	1/1	0.87	0.21	42,42,42,42	0
59	MG	2A	3277	1/1	0.87	0.14	69,69,69,69	0
59	MG	1A	3758	1/1	0.87	0.21	34,34,34,34	0
59	MG	2A	3292	1/1	0.87	0.14	46,46,46,46	0
59	MG	2A	3072	1/1	0.87	0.09	65,65,65,65	0
59	MG	1A	3759	1/1	0.87	0.41	46,46,46,46	0
59	MG	2A	3306	1/1	0.87	0.15	45,45,45,45	0
59	MG	1A	3076	1/1	0.87	0.09	50,50,50,50	0
59	MG	2A	3316	1/1	0.87	0.15	65,65,65,65	0
59	MG	1A	3763	1/1	0.87	0.35	38,38,38,38	0
59	MG	1a	1716	1/1	0.87	0.39	63,63,63,63	0
59	MG	1A	3357	1/1	0.87	0.14	22,22,22,22	0
59	MG	1A	3371	1/1	0.87	0.16	30,30,30,30	0
59	MG	1A	3546	1/1	0.87	0.12	54,54,54,54	0
59	MG	2A	3126	1/1	0.87	0.10	45,45,45,45	0
59	MG	1a	1744	1/1	0.87	0.24	64,64,64,64	0
59	MG	1A	3121	1/1	0.87	0.65	49,49,49,49	0
59	MG	1A	3081	1/1	0.87	0.20	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
59	MG	1a	1760	1/1	0.87	0.17	65,65,65,65	0
59	MG	2A	3359	1/1	0.87	0.12	33,33,33,33	0
59	MG	2A	3174	1/1	0.87	0.18	34,34,34,34	0
59	MG	2A	3396	1/1	0.87	0.22	24,24,24,24	0
59	MG	1B	218	1/1	0.87	0.17	65,65,65,65	0
59	MG	1a	1766	1/1	0.87	0.37	67,67,67,67	0
59	MG	2a	1725	1/1	0.87	0.12	64,64,64,64	0
59	MG	1A	3093	1/1	0.87	0.24	41,41,41,41	0
59	MG	2A	3185	1/1	0.87	0.35	33,33,33,33	0
59	MG	1a	1653	1/1	0.87	0.30	60,60,60,60	0
59	MG	2A	3441	1/1	0.87	0.38	45,45,45,45	0
59	MG	2a	1755	1/1	0.87	0.33	77,77,77,77	0
59	MG	2A	3193	1/1	0.87	0.25	51,51,51,51	0
59	MG	1a	1798	1/1	0.87	0.34	55,55,55,55	0
59	MG	1D	304	1/1	0.87	0.34	40,40,40,40	0
59	MG	1a	1659	1/1	0.87	0.22	63,63,63,63	0
59	MG	1A	3298	1/1	0.87	0.23	43,43,43,43	0
59	MG	1A	3464	1/1	0.87	0.14	43,43,43,43	0
59	MG	2A	3517	1/1	0.87	0.12	50,50,50,50	0
59	MG	2A	3538	1/1	0.87	0.30	28,28,28,28	0
59	MG	2A	3572	1/1	0.87	0.19	61,61,61,61	0
59	MG	1A	3712	1/1	0.87	0.24	80,80,80,80	0
59	MG	1A	3098	1/1	0.87	0.28	49,49,49,49	0
59	MG	1Y	104	1/1	0.87	0.20	50,50,50,50	0
59	MG	1A	3724	1/1	0.87	0.19	47,47,47,47	0
59	MG	2A	3142	1/1	0.88	0.20	48,48,48,48	0
59	MG	1A	3332	1/1	0.88	0.11	44,44,44,44	0
59	MG	2E	303	1/1	0.88	0.28	31,31,31,31	0
59	MG	2E	304	1/1	0.88	0.46	56,56,56,56	0
59	MG	1a	1702	1/1	0.88	0.15	51,51,51,51	0
59	MG	2F	302	1/1	0.88	0.16	46,46,46,46	0
59	MG	2A	3169	1/1	0.88	0.35	54,54,54,54	0
59	MG	1A	3544	1/1	0.88	0.22	43,43,43,43	0
59	MG	1A	3082	1/1	0.88	0.21	39,39,39,39	0
59	MG	2A	3013	1/1	0.88	0.22	55,55,55,55	0
59	MG	2a	1612	1/1	0.88	0.24	48,48,48,48	0
59	MG	2A	3022	1/1	0.88	0.09	54,54,54,54	0
59	MG	1A	3745	1/1	0.88	0.17	87,87,87,87	0
59	MG	1A	3756	1/1	0.88	0.22	30,30,30,30	0
59	MG	2A	3339	1/1	0.88	0.14	46,46,46,46	0
59	MG	1A	3670	1/1	0.88	0.16	60,60,60,60	0
59	MG	2a	1624	1/1	0.88	0.14	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
59	MG	2A	3188	1/1	0.88	0.21	41,41,41,41	0
59	MG	2A	3192	1/1	0.88	0.19	47,47,47,47	0
59	MG	2a	1627	1/1	0.88	0.38	44,44,44,44	0
59	MG	1a	1729	1/1	0.88	0.41	83,83,83,83	0
59	MG	2A	3195	1/1	0.88	0.22	53,53,53,53	0
59	MG	1A	3467	1/1	0.88	0.21	27,27,27,27	0
59	MG	2A	3211	1/1	0.88	0.29	48,48,48,48	0
59	MG	2A	3363	1/1	0.88	0.12	53,53,53,53	0
59	MG	2A	3368	1/1	0.88	0.16	56,56,56,56	0
59	MG	2A	3213	1/1	0.88	0.20	48,48,48,48	0
59	MG	2A	3218	1/1	0.88	0.18	50,50,50,50	0
59	MG	2A	3046	1/1	0.88	0.25	51,51,51,51	0
59	MG	2a	1667	1/1	0.88	0.11	65,65,65,65	0
59	MG	2A	3404	1/1	0.88	0.22	30,30,30,30	0
59	MG	1A	3475	1/1	0.88	0.15	50,50,50,50	0
59	MG	2a	1677	1/1	0.88	0.68	52,52,52,52	0
59	MG	2a	1678	1/1	0.88	0.11	51,51,51,51	0
59	MG	1a	1607	1/1	0.88	0.32	69,69,69,69	0
59	MG	2a	1686	1/1	0.88	0.16	40,40,40,40	0
59	MG	2A	3061	1/1	0.88	0.23	31,31,31,31	0
59	MG	2A	3429	1/1	0.88	0.12	56,56,56,56	0
59	MG	1A	3174	1/1	0.88	0.18	38,38,38,38	0
59	MG	1A	3157	1/1	0.88	0.18	34,34,34,34	0
59	MG	2A	3066	1/1	0.88	0.23	45,45,45,45	0
59	MG	1a	1759	1/1	0.88	0.18	65,65,65,65	0
59	MG	1A	3401	1/1	0.88	0.08	44,44,44,44	0
59	MG	1a	1763	1/1	0.88	0.27	55,55,55,55	0
59	MG	2a	1732	1/1	0.88	0.25	55,55,55,55	0
59	MG	1A	3193	1/1	0.88	0.17	47,47,47,47	0
59	MG	2a	1743	1/1	0.88	0.15	68,68,68,68	0
59	MG	1A	3779	1/1	0.88	0.41	39,39,39,39	0
59	MG	2A	3264	1/1	0.88	0.24	49,49,49,49	0
59	MG	2A	3520	1/1	0.88	0.17	54,54,54,54	0
59	MG	1a	1615	1/1	0.88	0.31	54,54,54,54	0
59	MG	2A	3544	1/1	0.88	0.33	53,53,53,53	0
59	MG	2A	3546	1/1	0.88	0.38	56,56,56,56	0
59	MG	2A	3550	1/1	0.88	0.23	50,50,50,50	0
59	MG	1A	3433	1/1	0.88	0.24	34,34,34,34	0
59	MG	1a	1619	1/1	0.88	0.10	51,51,51,51	0
59	MG	2A	3110	1/1	0.88	0.23	38,38,38,38	0
59	MG	2A	3593	1/1	0.88	0.10	73,73,73,73	0
59	MG	2A	3602	1/1	0.88	0.26	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
59	MG	2A	3606	1/1	0.88	0.17	29,29,29,29	0
59	MG	1A	3606	1/1	0.88	0.34	60,60,60,60	0
59	MG	2A	3618	1/1	0.88	0.22	43,43,43,43	0
59	MG	1A	3128	1/1	0.88	0.19	28,28,28,28	0
59	MG	1A	3621	1/1	0.88	0.15	21,21,21,21	0
59	MG	1A	3360	1/1	0.89	0.31	36,36,36,36	0
59	MG	2B	202	1/1	0.89	0.19	56,56,56,56	0
59	MG	1A	3362	1/1	0.89	0.26	40,40,40,40	0
59	MG	1A	3637	1/1	0.89	0.14	59,59,59,59	0
59	MG	1A	3290	1/1	0.89	0.21	34,34,34,34	0
59	MG	1A	3669	1/1	0.89	0.25	52,52,52,52	0
59	MG	2A	3276	1/1	0.89	0.17	61,61,61,61	0
59	MG	2A	3082	1/1	0.89	0.26	45,45,45,45	0
59	MG	1a	1742	1/1	0.89	0.16	43,43,43,43	0
59	MG	2N	201	1/1	0.89	0.21	42,42,42,42	0
59	MG	1A	3508	1/1	0.89	0.19	47,47,47,47	0
59	MG	2A	3092	1/1	0.89	0.20	40,40,40,40	0
59	MG	1A	3377	1/1	0.89	0.13	27,27,27,27	0
59	MG	1a	1756	1/1	0.89	0.34	67,67,67,67	0
59	MG	1A	3133	1/1	0.89	0.27	44,44,44,44	0
59	MG	2A	3115	1/1	0.89	0.31	42,42,42,42	0
59	MG	1A	3527	1/1	0.89	0.15	38,38,38,38	0
59	MG	1D	301	1/1	0.89	0.39	32,32,32,32	0
59	MG	1a	1652	1/1	0.89	0.11	48,48,48,48	0
59	MG	2A	3334	1/1	0.89	0.19	54,54,54,54	0
59	MG	1A	3390	1/1	0.89	0.20	53,53,53,53	0
59	MG	1A	3046	1/1	0.89	0.27	57,57,57,57	0
59	MG	1a	1655	1/1	0.89	0.25	53,53,53,53	0
59	MG	2A	3166	1/1	0.89	0.12	43,43,43,43	0
59	MG	1a	1656	1/1	0.89	0.54	51,51,51,51	0
59	MG	1a	1657	1/1	0.89	0.28	48,48,48,48	0
59	MG	2a	1641	1/1	0.89	0.13	51,51,51,51	0
59	MG	2a	1647	1/1	0.89	0.14	61,61,61,61	0
59	MG	1A	3167	1/1	0.89	0.62	50,50,50,50	0
59	MG	1A	3412	1/1	0.89	0.17	54,54,54,54	0
59	MG	1A	3563	1/1	0.89	0.23	53,53,53,53	0
59	MG	1Y	101	1/1	0.89	0.16	51,51,51,51	0
59	MG	2A	3365	1/1	0.89	0.13	22,22,22,22	0
59	MG	2A	3367	1/1	0.89	0.15	45,45,45,45	0
59	MG	2A	3182	1/1	0.89	0.17	41,41,41,41	0
59	MG	1w	3003	1/1	0.89	0.12	54,54,54,54	0
59	MG	1A	3716	1/1	0.89	0.16	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
59	MG	2A	3397	1/1	0.89	0.15	46,46,46,46	0
59	MG	2A	3402	1/1	0.89	0.17	45,45,45,45	0
59	MG	2A	3187	1/1	0.89	0.21	55,55,55,55	0
59	MG	1a	1682	1/1	0.89	0.23	55,55,55,55	0
59	MG	2A	3007	1/1	0.89	0.14	28,28,28,28	0
59	MG	13	104	1/1	0.89	0.42	48,48,48,48	0
59	MG	1A	3213	1/1	0.89	0.16	47,47,47,47	0
59	MG	1A	3235	1/1	0.89	0.15	49,49,49,49	0
59	MG	2A	3023	1/1	0.89	0.30	34,34,34,34	0
59	MG	2A	3438	1/1	0.89	0.23	54,54,54,54	0
59	MG	2A	3212	1/1	0.89	0.23	46,46,46,46	0
59	MG	2A	3447	1/1	0.89	0.20	41,41,41,41	0
59	MG	1A	3152	1/1	0.89	0.14	24,24,24,24	0
59	MG	2A	3215	1/1	0.89	0.13	51,51,51,51	0
59	MG	2a	1735	1/1	0.89	0.13	50,50,50,50	0
59	MG	2a	1736	1/1	0.89	0.11	42,42,42,42	0
59	MG	2A	3033	1/1	0.89	0.13	50,50,50,50	0
59	MG	1A	3587	1/1	0.89	0.18	18,18,18,18	0
59	MG	2A	3221	1/1	0.89	0.22	41,41,41,41	0
59	MG	1A	3266	1/1	0.89	0.13	28,28,28,28	0
59	MG	1A	3466	1/1	0.89	0.23	26,26,26,26	0
59	MG	1a	1696	1/1	0.89	0.06	54,54,54,54	0
59	MG	2A	3042	1/1	0.89	0.12	39,39,39,39	0
59	MG	2a	1758	1/1	0.89	0.24	65,65,65,65	0
59	MG	2A	3045	1/1	0.89	0.28	56,56,56,56	0
59	MG	1A	3344	1/1	0.89	0.10	42,42,42,42	0
59	MG	1A	3347	1/1	0.89	0.15	27,27,27,27	0
59	MG	2A	3054	1/1	0.89	0.28	48,48,48,48	0
59	MG	1a	1705	1/1	0.89	0.24	64,64,64,64	0
59	MG	2A	3256	1/1	0.89	0.23	48,48,48,48	0
59	MG	2A	3258	1/1	0.89	0.39	55,55,55,55	0
59	MG	2A	3595	1/1	0.89	0.17	51,51,51,51	0
59	MG	1A	3482	1/1	0.89	0.15	27,27,27,27	0
59	MG	2A	3262	1/1	0.89	0.23	51,51,51,51	0
59	MG	1A	3286	1/1	0.89	0.23	71,71,71,71	0
59	MG	1a	1618	1/1	0.89	0.29	42,42,42,42	0
59	MG	2A	3070	1/1	0.90	0.26	36,36,36,36	0
59	MG	1a	1710	1/1	0.90	0.41	42,42,42,42	0
59	MG	1A	3538	1/1	0.90	0.13	63,63,63,63	0
59	MG	2A	3078	1/1	0.90	0.19	47,47,47,47	0
59	MG	2A	3269	1/1	0.90	0.28	48,48,48,48	0
59	MG	2A	3270	1/1	0.90	0.18	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
59	MG	1A	3045	1/1	0.90	0.31	44,44,44,44	0
59	MG	1A	3696	1/1	0.90	0.13	70,70,70,70	0
59	MG	2A	3087	1/1	0.90	0.14	56,56,56,56	0
59	MG	1a	1722	1/1	0.90	0.26	78,78,78,78	0
59	MG	2M	202	1/1	0.90	0.17	55,55,55,55	0
59	MG	1A	3199	1/1	0.90	0.17	34,34,34,34	0
59	MG	2O	3002	1/1	0.90	0.26	59,59,59,59	0
59	MG	1A	3548	1/1	0.90	0.09	61,61,61,61	0
59	MG	2a	1601	1/1	0.90	0.08	68,68,68,68	0
59	MG	2A	3282	1/1	0.90	0.12	26,26,26,26	0
59	MG	2A	3291	1/1	0.90	0.09	34,34,34,34	0
59	MG	1A	3435	1/1	0.90	0.21	45,45,45,45	0
59	MG	1A	3552	1/1	0.90	0.24	47,47,47,47	0
59	MG	1A	3553	1/1	0.90	0.12	47,47,47,47	0
59	MG	1a	1748	1/1	0.90	0.44	82,82,82,82	0
59	MG	2A	3121	1/1	0.90	0.14	57,57,57,57	0
59	MG	1A	3719	1/1	0.90	0.12	68,68,68,68	0
59	MG	1A	3328	1/1	0.90	0.24	50,50,50,50	0
59	MG	2a	1623	1/1	0.90	0.12	37,37,37,37	0
59	MG	2A	3132	1/1	0.90	0.10	46,46,46,46	0
59	MG	2A	3135	1/1	0.90	0.16	45,45,45,45	0
59	MG	1A	3204	1/1	0.90	0.25	42,42,42,42	0
59	MG	1A	3255	1/1	0.90	0.23	63,63,63,63	0
59	MG	1a	1626	1/1	0.90	0.31	54,54,54,54	0
59	MG	1A	3083	1/1	0.90	0.38	55,55,55,55	0
59	MG	2A	3153	1/1	0.90	0.10	43,43,43,43	0
59	MG	2A	3165	1/1	0.90	0.36	44,44,44,44	0
59	MG	1A	3586	1/1	0.90	0.11	56,56,56,56	0
59	MG	1A	3746	1/1	0.90	0.24	53,53,53,53	0
59	MG	2a	1653	1/1	0.90	0.21	43,43,43,43	0
59	MG	1A	3749	1/1	0.90	0.25	54,54,54,54	0
59	MG	2A	3171	1/1	0.90	0.23	54,54,54,54	0
59	MG	1A	3263	1/1	0.90	0.19	33,33,33,33	0
59	MG	2A	3175	1/1	0.90	0.15	44,44,44,44	0
59	MG	1A	3589	1/1	0.90	0.15	29,29,29,29	0
59	MG	1A	3468	1/1	0.90	0.20	37,37,37,37	0
59	MG	2A	3373	1/1	0.90	0.17	47,47,47,47	0
59	MG	1A	3470	1/1	0.90	0.25	28,28,28,28	0
59	MG	2A	3181	1/1	0.90	0.20	37,37,37,37	0
59	MG	1a	1802	1/1	0.90	0.16	45,45,45,45	0
59	MG	2A	3399	1/1	0.90	0.25	39,39,39,39	0
59	MG	1A	3762	1/1	0.90	0.35	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3113	1/1	0.90	0.28	27,27,27,27	0
59	MG	1A	3605	1/1	0.90	0.18	67,67,67,67	0
59	MG	2a	1690	1/1	0.90	0.22	63,63,63,63	0
59	MG	1A	3476	1/1	0.90	0.19	29,29,29,29	0
59	MG	1A	3479	1/1	0.90	0.17	50,50,50,50	0
59	MG	1A	3776	1/1	0.90	0.30	46,46,46,46	0
59	MG	1a	1658	1/1	0.90	0.11	64,64,64,64	0
59	MG	2A	3205	1/1	0.90	0.32	58,58,58,58	0
59	MG	1A	3620	1/1	0.90	0.17	26,26,26,26	0
59	MG	2A	3439	1/1	0.90	0.18	52,52,52,52	0
59	MG	1A	3004	1/1	0.90	0.16	30,30,30,30	0
59	MG	1A	3630	1/1	0.90	0.11	51,51,51,51	0
59	MG	1B	208	1/1	0.90	0.22	38,38,38,38	0
59	MG	1A	3366	1/1	0.90	0.12	51,51,51,51	0
59	MG	1B	219	1/1	0.90	0.21	71,71,71,71	0
59	MG	1A	3179	1/1	0.90	0.20	51,51,51,51	0
59	MG	1A	3294	1/1	0.90	0.18	18,18,18,18	0
59	MG	1A	3381	1/1	0.90	0.09	23,23,23,23	0
59	MG	1A	3646	1/1	0.90	0.18	48,48,48,48	0
59	MG	1A	3653	1/1	0.90	0.17	62,62,62,62	0
59	MG	2A	3235	1/1	0.90	0.24	39,39,39,39	0
59	MG	1A	3097	1/1	0.90	0.17	55,55,55,55	0
59	MG	2A	3047	1/1	0.90	0.23	48,48,48,48	0
59	MG	1A	3217	1/1	0.90	0.24	45,45,45,45	0
59	MG	1A	3393	1/1	0.90	0.15	28,28,28,28	0
59	MG	1Y	103	1/1	0.90	0.83	73,73,73,73	0
59	MG	2n	502	1/1	0.90	0.65	76,76,76,76	0
59	MG	1A	3674	1/1	0.90	0.14	48,48,48,48	0
59	MG	2A	3253	1/1	0.90	0.27	53,53,53,53	0
59	MG	10	102	1/1	0.90	0.19	44,44,44,44	0
59	MG	1A	3192	1/1	0.90	0.23	47,47,47,47	0
59	MG	1A	3131	1/1	0.90	0.17	47,47,47,47	0
59	MG	1a	1709	1/1	0.90	0.49	50,50,50,50	0
60	ZN	22	501	1/1	0.90	0.04	118,118,118,118	0
59	MG	2A	3111	1/1	0.91	0.36	47,47,47,47	0
59	MG	2A	3612	1/1	0.91	0.21	46,46,46,46	0
59	MG	1a	1635	1/1	0.91	0.24	55,55,55,55	0
59	MG	2A	3119	1/1	0.91	0.21	39,39,39,39	0
59	MG	1A	3775	1/1	0.91	0.17	41,41,41,41	0
59	MG	1a	1762	1/1	0.91	0.32	62,62,62,62	0
59	MG	1A	3386	1/1	0.91	0.20	32,32,32,32	0
59	MG	1A	3665	1/1	0.91	0.10	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
59	MG	1B	202	1/1	0.91	0.27	59,59,59,59	0
59	MG	1A	3293	1/1	0.91	0.08	41,41,41,41	0
59	MG	1A	3187	1/1	0.91	0.15	48,48,48,48	0
59	MG	1A	3005	1/1	0.91	0.22	52,52,52,52	0
59	MG	2A	3303	1/1	0.91	0.10	43,43,43,43	0
59	MG	1B	209	1/1	0.91	0.14	45,45,45,45	0
59	MG	1B	213	1/1	0.91	0.14	39,39,39,39	0
59	MG	1A	3060	1/1	0.91	0.19	45,45,45,45	0
59	MG	2A	3323	1/1	0.91	0.15	50,50,50,50	0
59	MG	2a	1602	1/1	0.91	0.12	47,47,47,47	0
59	MG	1A	3124	1/1	0.91	0.21	46,46,46,46	0
59	MG	1A	3161	1/1	0.91	0.27	54,54,54,54	0
59	MG	1A	3425	1/1	0.91	0.14	68,68,68,68	0
59	MG	1A	3306	1/1	0.91	0.21	23,23,23,23	0
59	MG	1a	1663	1/1	0.91	0.20	79,79,79,79	0
59	MG	1F	304	1/1	0.91	0.13	33,33,33,33	0
59	MG	1A	3695	1/1	0.91	0.18	38,38,38,38	0
59	MG	2A	3178	1/1	0.91	0.21	50,50,50,50	0
59	MG	1a	1680	1/1	0.91	0.22	65,65,65,65	0
59	MG	1A	3561	1/1	0.91	0.10	35,35,35,35	0
59	MG	1A	3064	1/1	0.91	0.18	52,52,52,52	0
59	MG	2A	3356	1/1	0.91	0.09	58,58,58,58	0
59	MG	2A	3024	1/1	0.91	0.22	45,45,45,45	0
59	MG	2A	3030	1/1	0.91	0.17	37,37,37,37	0
59	MG	2a	1629	1/1	0.91	0.09	57,57,57,57	0
59	MG	2A	3031	1/1	0.91	0.44	52,52,52,52	0
59	MG	2a	1635	1/1	0.91	0.20	40,40,40,40	0
59	MG	2a	1639	1/1	0.91	0.26	43,43,43,43	0
59	MG	1U	201	1/1	0.91	0.14	48,48,48,48	0
59	MG	1A	3237	1/1	0.91	0.14	55,55,55,55	0
59	MG	2a	1645	1/1	0.91	0.18	58,58,58,58	0
59	MG	1a	1685	1/1	0.91	0.29	51,51,51,51	0
59	MG	1A	3452	1/1	0.91	0.27	46,46,46,46	0
59	MG	1A	3246	1/1	0.91	0.15	39,39,39,39	0
59	MG	2A	3197	1/1	0.91	0.53	55,55,55,55	0
59	MG	2a	1655	1/1	0.91	0.22	63,63,63,63	0
59	MG	2a	1656	1/1	0.91	0.24	61,61,61,61	0
59	MG	1A	3331	1/1	0.91	0.26	53,53,53,53	0
59	MG	2A	3207	1/1	0.91	0.24	51,51,51,51	0
59	MG	2A	3040	1/1	0.91	0.23	45,45,45,45	0
59	MG	10	101	1/1	0.91	0.18	38,38,38,38	0
59	MG	1A	3205	1/1	0.91	0.39	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
59	MG	2a	1664	1/1	0.91	0.32	59,59,59,59	0
59	MG	2A	3410	1/1	0.91	0.15	27,27,27,27	0
59	MG	1A	3257	1/1	0.91	0.25	34,34,34,34	0
59	MG	1a	1699	1/1	0.91	0.23	60,60,60,60	0
59	MG	1a	1602	1/1	0.91	0.13	49,49,49,49	0
59	MG	2A	3426	1/1	0.91	0.29	58,58,58,58	0
59	MG	2a	1679	1/1	0.91	0.13	50,50,50,50	0
59	MG	1a	1603	1/1	0.91	0.24	69,69,69,69	0
59	MG	2a	1683	1/1	0.91	0.35	59,59,59,59	0
59	MG	1A	3112	1/1	0.91	0.12	44,44,44,44	0
59	MG	1a	1605	1/1	0.91	0.11	40,40,40,40	0
59	MG	1A	3595	1/1	0.91	0.12	49,49,49,49	0
59	MG	1A	3349	1/1	0.91	0.24	18,18,18,18	0
59	MG	1A	3744	1/1	0.91	0.15	45,45,45,45	0
59	MG	1A	3353	1/1	0.91	0.20	26,26,26,26	0
59	MG	2A	3069	1/1	0.91	0.14	50,50,50,50	0
59	MG	2A	3471	1/1	0.91	0.15	56,56,56,56	0
59	MG	2a	1708	1/1	0.91	0.13	64,64,64,64	0
59	MG	2A	3478	1/1	0.91	0.34	58,58,58,58	0
59	MG	2a	1720	1/1	0.91	0.13	63,63,63,63	0
59	MG	2A	3482	1/1	0.91	0.10	53,53,53,53	0
59	MG	1A	3260	1/1	0.91	0.17	48,48,48,48	0
59	MG	2A	3492	1/1	0.91	0.29	48,48,48,48	0
59	MG	1A	3359	1/1	0.91	0.13	22,22,22,22	0
59	MG	2A	3075	1/1	0.91	0.09	46,46,46,46	0
59	MG	2A	3510	1/1	0.91	0.18	35,35,35,35	0
59	MG	2A	3515	1/1	0.91	0.23	48,48,48,48	0
59	MG	2A	3249	1/1	0.91	0.19	39,39,39,39	0
59	MG	1A	3751	1/1	0.91	0.13	43,43,43,43	0
59	MG	1a	1726	1/1	0.91	0.16	60,60,60,60	0
59	MG	2A	3528	1/1	0.91	0.25	30,30,30,30	0
59	MG	2A	3537	1/1	0.91	0.29	38,38,38,38	0
59	MG	1A	3048	1/1	0.91	0.27	32,32,32,32	0
59	MG	1A	3265	1/1	0.91	0.13	36,36,36,36	0
59	MG	2A	3083	1/1	0.91	0.24	55,55,55,55	0
59	MG	1A	3091	1/1	0.91	0.16	54,54,54,54	0
59	MG	2a	1768	1/1	0.91	0.14	64,64,64,64	0
59	MG	2A	3564	1/1	0.91	0.33	72,72,72,72	0
59	MG	1A	3274	1/1	0.91	0.18	25,25,25,25	0
59	MG	2A	3576	1/1	0.91	0.15	40,40,40,40	0
59	MG	1A	3008	1/1	0.91	0.15	31,31,31,31	0
59	MG	1A	3380	1/1	0.91	0.18	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
59	MG	2A	3266	1/1	0.91	0.18	38,38,38,38	0
59	MG	1A	3095	1/1	0.91	0.55	40,40,40,40	0
59	MG	1A	3514	1/1	0.91	0.07	43,43,43,43	0
59	MG	1A	3383	1/1	0.91	0.17	47,47,47,47	0
59	MG	2A	3609	1/1	0.91	0.12	51,51,51,51	0
59	MG	2A	3095	1/1	0.92	0.16	37,37,37,37	0
59	MG	2A	3096	1/1	0.92	0.26	55,55,55,55	0
59	MG	1A	3164	1/1	0.92	0.15	46,46,46,46	0
59	MG	2A	3104	1/1	0.92	0.15	53,53,53,53	0
59	MG	1A	3130	1/1	0.92	0.25	34,34,34,34	0
59	MG	2A	3617	1/1	0.92	0.26	62,62,62,62	0
59	MG	1a	1650	1/1	0.92	0.16	48,48,48,48	0
59	MG	1A	3453	1/1	0.92	0.19	36,36,36,36	0
59	MG	1a	1770	1/1	0.92	0.11	67,67,67,67	0
59	MG	1A	3198	1/1	0.92	0.09	60,60,60,60	0
59	MG	1A	3555	1/1	0.92	0.11	56,56,56,56	0
59	MG	2B	213	1/1	0.92	0.13	64,64,64,64	0
59	MG	1a	1781	1/1	0.92	0.13	48,48,48,48	0
59	MG	1A	3463	1/1	0.92	0.20	26,26,26,26	0
59	MG	2A	3134	1/1	0.92	0.12	36,36,36,36	0
59	MG	1A	3099	1/1	0.92	0.18	63,63,63,63	0
59	MG	1A	3230	1/1	0.92	0.23	56,56,56,56	0
59	MG	2G	3001	1/1	0.92	0.17	34,34,34,34	0
59	MG	2A	3140	1/1	0.92	0.27	39,39,39,39	0
59	MG	1A	3292	1/1	0.92	0.10	39,39,39,39	0
59	MG	1E	303	1/1	0.92	0.32	41,41,41,41	0
59	MG	2A	3318	1/1	0.92	0.14	42,42,42,42	0
59	MG	1d	503	1/1	0.92	0.09	80,80,80,80	0
59	MG	2A	3146	1/1	0.92	0.37	60,60,60,60	0
59	MG	2A	3148	1/1	0.92	0.18	40,40,40,40	0
59	MG	1A	3231	1/1	0.92	0.69	45,45,45,45	0
59	MG	2A	3161	1/1	0.92	0.30	47,47,47,47	0
59	MG	2a	1609	1/1	0.92	0.27	53,53,53,53	0
59	MG	2A	3163	1/1	0.92	0.21	47,47,47,47	0
59	MG	1a	1661	1/1	0.92	0.17	47,47,47,47	0
59	MG	1A	3584	1/1	0.92	0.12	62,62,62,62	0
59	MG	2A	3167	1/1	0.92	0.12	52,52,52,52	0
59	MG	2a	1618	1/1	0.92	0.13	47,47,47,47	0
59	MG	1G	3001	1/1	0.92	0.11	31,31,31,31	0
59	MG	1A	3585	1/1	0.92	0.12	52,52,52,52	0
59	MG	1a	1671	1/1	0.92	0.14	53,53,53,53	0
59	MG	2A	3173	1/1	0.92	0.12	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
59	MG	1A	3363	1/1	0.92	0.11	45,45,45,45	0
59	MG	1N	201	1/1	0.92	0.17	40,40,40,40	0
59	MG	1A	3232	1/1	0.92	0.17	47,47,47,47	0
59	MG	1A	3203	1/1	0.92	0.27	36,36,36,36	0
59	MG	2A	3026	1/1	0.92	0.21	44,44,44,44	0
59	MG	1X	3001	1/1	0.92	0.29	55,55,55,55	0
59	MG	1A	3591	1/1	0.92	0.12	47,47,47,47	0
59	MG	2A	3377	1/1	0.92	0.22	44,44,44,44	0
59	MG	1A	3726	1/1	0.92	0.28	34,34,34,34	0
59	MG	2A	3395	1/1	0.92	0.09	53,53,53,53	0
59	MG	1A	3300	1/1	0.92	0.17	47,47,47,47	0
59	MG	2A	3034	1/1	0.92	0.18	47,47,47,47	0
59	MG	1A	3153	1/1	0.92	0.33	33,33,33,33	0
59	MG	2a	1652	1/1	0.92	0.16	36,36,36,36	0
59	MG	1a	1689	1/1	0.92	0.21	22,22,22,22	0
59	MG	1A	3735	1/1	0.92	0.29	32,32,32,32	0
59	MG	1A	3176	1/1	0.92	0.16	33,33,33,33	0
59	MG	1A	3739	1/1	0.92	0.22	50,50,50,50	0
59	MG	1A	3741	1/1	0.92	0.16	50,50,50,50	0
59	MG	2A	3416	1/1	0.92	0.15	50,50,50,50	0
59	MG	2A	3417	1/1	0.92	0.15	53,53,53,53	0
59	MG	2A	3202	1/1	0.92	0.24	35,35,35,35	0
59	MG	1A	3600	1/1	0.92	0.10	33,33,33,33	0
59	MG	2a	1665	1/1	0.92	0.24	65,65,65,65	0
59	MG	1A	3245	1/1	0.92	0.46	31,31,31,31	0
59	MG	1A	3155	1/1	0.92	0.12	31,31,31,31	0
59	MG	2a	1670	1/1	0.92	0.15	51,51,51,51	0
59	MG	2a	1671	1/1	0.92	0.14	38,38,38,38	0
59	MG	1A	3748	1/1	0.92	0.35	67,67,67,67	0
59	MG	2A	3436	1/1	0.92	0.12	50,50,50,50	0
59	MG	1A	3308	1/1	0.92	0.13	52,52,52,52	0
59	MG	1A	3750	1/1	0.92	0.21	53,53,53,53	0
59	MG	2A	3060	1/1	0.92	0.10	36,36,36,36	0
59	MG	2A	3217	1/1	0.92	0.12	45,45,45,45	0
59	MG	2A	3456	1/1	0.92	0.07	65,65,65,65	0
59	MG	2A	3458	1/1	0.92	0.15	52,52,52,52	0
59	MG	1A	3250	1/1	0.92	0.18	51,51,51,51	0
59	MG	1a	1712	1/1	0.92	0.20	69,69,69,69	0
59	MG	2A	3469	1/1	0.92	0.17	60,60,60,60	0
59	MG	2a	1692	1/1	0.92	0.31	45,45,45,45	0
59	MG	1A	3069	1/1	0.92	0.24	39,39,39,39	0
59	MG	2A	3473	1/1	0.92	0.29	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
59	MG	2a	1704	1/1	0.92	0.15	39,39,39,39	0
59	MG	1A	3513	1/1	0.92	0.18	43,43,43,43	0
59	MG	2a	1707	1/1	0.92	0.20	49,49,49,49	0
59	MG	2A	3227	1/1	0.92	0.21	49,49,49,49	0
59	MG	1A	3181	1/1	0.92	0.27	52,52,52,52	0
59	MG	2a	1717	1/1	0.92	0.21	52,52,52,52	0
59	MG	1A	3052	1/1	0.92	0.27	40,40,40,40	0
59	MG	2a	1721	1/1	0.92	0.38	62,62,62,62	0
59	MG	2A	3232	1/1	0.92	0.10	52,52,52,52	0
59	MG	2a	1730	1/1	0.92	0.11	47,47,47,47	0
59	MG	1A	3518	1/1	0.92	0.17	59,59,59,59	0
59	MG	1A	3520	1/1	0.92	0.20	70,70,70,70	0
59	MG	1A	3405	1/1	0.92	0.14	55,55,55,55	0
59	MG	2a	1739	1/1	0.92	0.11	51,51,51,51	0
59	MG	1A	3768	1/1	0.92	0.25	50,50,50,50	0
59	MG	1A	3075	1/1	0.92	0.20	44,44,44,44	0
59	MG	2A	3079	1/1	0.92	0.08	33,33,33,33	0
59	MG	2A	3080	1/1	0.92	0.33	36,36,36,36	0
59	MG	2A	3530	1/1	0.92	0.17	40,40,40,40	0
59	MG	2A	3250	1/1	0.92	0.21	45,45,45,45	0
59	MG	2A	3251	1/1	0.92	0.26	28,28,28,28	0
59	MG	1A	3650	1/1	0.92	0.17	49,49,49,49	0
59	MG	1a	1632	1/1	0.92	0.17	63,63,63,63	0
59	MG	1A	3652	1/1	0.92	0.27	39,39,39,39	0
59	MG	1a	1752	1/1	0.92	0.27	75,75,75,75	0
59	MG	2A	3568	1/1	0.92	0.14	72,72,72,72	0
59	MG	1A	3333	1/1	0.92	0.15	45,45,45,45	0
59	MG	2A	3089	1/1	0.92	0.14	51,51,51,51	0
59	MG	2A	3577	1/1	0.92	0.18	56,56,56,56	0
59	MG	2A	3578	1/1	0.92	0.12	46,46,46,46	0
59	MG	2q	201	1/1	0.92	0.17	52,52,52,52	0
59	MG	2A	3090	1/1	0.92	0.18	40,40,40,40	0
59	MG	2A	3586	1/1	0.92	0.23	45,45,45,45	0
59	MG	1A	3335	1/1	0.92	0.12	46,46,46,46	0
59	MG	1A	3668	1/1	0.92	0.11	48,48,48,48	0
59	MG	2A	3594	1/1	0.92	0.14	56,56,56,56	0
59	MG	1A	3216	1/1	0.92	0.30	47,47,47,47	0
59	MG	2A	3600	1/1	0.92	0.25	47,47,47,47	0
60	ZN	2n	501	1/1	0.92	0.10	102,102,102,102	0
59	MG	2A	3604	1/1	0.93	0.16	40,40,40,40	0
59	MG	2A	3275	1/1	0.93	0.09	58,58,58,58	0
59	MG	2A	3607	1/1	0.93	0.20	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
59	MG	1A	3247	1/1	0.93	0.41	35,35,35,35	0
59	MG	1A	3686	1/1	0.93	0.12	62,62,62,62	0
59	MG	1a	1777	1/1	0.93	0.18	53,53,53,53	0
59	MG	1A	3688	1/1	0.93	0.09	89,89,89,89	0
59	MG	2A	3130	1/1	0.93	0.21	34,34,34,34	0
59	MG	2A	3620	1/1	0.93	0.14	58,58,58,58	0
59	MG	1A	3689	1/1	0.93	0.26	57,57,57,57	0
59	MG	2A	3293	1/1	0.93	0.30	44,44,44,44	0
59	MG	2A	3294	1/1	0.93	0.11	21,21,21,21	0
59	MG	2B	207	1/1	0.93	0.26	40,40,40,40	0
59	MG	1a	1786	1/1	0.93	0.27	48,48,48,48	0
59	MG	1a	1795	1/1	0.93	0.07	45,45,45,45	0
59	MG	1B	210	1/1	0.93	0.23	49,49,49,49	0
59	MG	2D	302	1/1	0.93	0.27	62,62,62,62	0
59	MG	2D	304	1/1	0.93	0.24	51,51,51,51	0
59	MG	1B	212	1/1	0.93	0.06	49,49,49,49	0
59	MG	2A	3310	1/1	0.93	0.16	55,55,55,55	0
59	MG	1A	3582	1/1	0.93	0.19	17,17,17,17	0
59	MG	1A	3041	1/1	0.93	0.18	52,52,52,52	0
59	MG	1A	3338	1/1	0.93	0.20	38,38,38,38	0
59	MG	2A	3320	1/1	0.93	0.19	40,40,40,40	0
59	MG	2A	3322	1/1	0.93	0.23	28,28,28,28	0
59	MG	1B	220	1/1	0.93	0.09	38,38,38,38	0
59	MG	1l	201	1/1	0.93	0.15	50,50,50,50	0
59	MG	23	502	1/1	0.93	0.48	49,49,49,49	0
59	MG	2A	3150	1/1	0.93	0.12	37,37,37,37	0
59	MG	1l	202	1/1	0.93	0.16	47,47,47,47	0
59	MG	2A	3156	1/1	0.93	0.11	53,53,53,53	0
59	MG	2A	3160	1/1	0.93	0.21	41,41,41,41	0
59	MG	1A	3486	1/1	0.93	0.07	65,65,65,65	0
59	MG	1w	3002	1/1	0.93	0.07	51,51,51,51	0
59	MG	2a	1610	1/1	0.93	0.36	52,52,52,52	0
59	MG	2A	3164	1/1	0.93	0.18	48,48,48,48	0
59	MG	2a	1613	1/1	0.93	0.08	43,43,43,43	0
59	MG	1A	3698	1/1	0.93	0.16	33,33,33,33	0
59	MG	1D	302	1/1	0.93	0.42	39,39,39,39	0
59	MG	1A	3703	1/1	0.93	0.34	42,42,42,42	0
59	MG	1A	3006	1/1	0.93	0.15	33,33,33,33	0
59	MG	1F	302	1/1	0.93	0.49	40,40,40,40	0
59	MG	2A	3358	1/1	0.93	0.10	56,56,56,56	0
59	MG	1A	3705	1/1	0.93	0.68	56,56,56,56	0
59	MG	1A	3706	1/1	0.93	0.14	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
59	MG	1a	1679	1/1	0.93	0.42	60,60,60,60	0
59	MG	1A	3501	1/1	0.93	0.08	49,49,49,49	0
59	MG	2A	3025	1/1	0.93	0.12	42,42,42,42	0
59	MG	2a	1628	1/1	0.93	0.32	62,62,62,62	0
59	MG	1A	3502	1/1	0.93	0.19	20,20,20,20	0
59	MG	1A	3714	1/1	0.93	0.12	72,72,72,72	0
59	MG	2A	3386	1/1	0.93	0.27	43,43,43,43	0
59	MG	2A	3388	1/1	0.93	0.10	55,55,55,55	0
59	MG	1A	3346	1/1	0.93	0.20	26,26,26,26	0
59	MG	1S	3001	1/1	0.93	0.44	40,40,40,40	0
59	MG	2a	1643	1/1	0.93	0.29	39,39,39,39	0
59	MG	1T	201	1/1	0.93	0.27	40,40,40,40	0
59	MG	1A	3037	1/1	0.93	0.21	41,41,41,41	0
59	MG	2A	3398	1/1	0.93	0.15	32,32,32,32	0
59	MG	2a	1650	1/1	0.93	0.18	43,43,43,43	0
59	MG	1A	3408	1/1	0.93	0.12	55,55,55,55	0
59	MG	1A	3599	1/1	0.93	0.21	51,51,51,51	0
59	MG	2A	3037	1/1	0.93	0.15	37,37,37,37	0
59	MG	2a	1654	1/1	0.93	0.22	29,29,29,29	0
59	MG	2A	3190	1/1	0.93	0.39	34,34,34,34	0
59	MG	2A	3406	1/1	0.93	0.16	43,43,43,43	0
59	MG	1A	3134	1/1	0.93	0.15	54,54,54,54	0
59	MG	1a	1691	1/1	0.93	0.30	54,54,54,54	0
59	MG	2A	3194	1/1	0.93	0.27	35,35,35,35	0
59	MG	1A	3137	1/1	0.93	0.08	55,55,55,55	0
59	MG	1A	3125	1/1	0.93	0.67	39,39,39,39	0
59	MG	2A	3044	1/1	0.93	0.15	47,47,47,47	0
59	MG	1A	3733	1/1	0.93	0.32	59,59,59,59	0
59	MG	2a	1666	1/1	0.93	0.36	48,48,48,48	0
59	MG	1A	3434	1/1	0.93	0.23	48,48,48,48	0
59	MG	2A	3208	1/1	0.93	0.31	47,47,47,47	0
59	MG	2A	3209	1/1	0.93	0.23	46,46,46,46	0
59	MG	1A	3736	1/1	0.93	0.16	69,69,69,69	0
59	MG	2A	3049	1/1	0.93	0.19	38,38,38,38	0
59	MG	1a	1601	1/1	0.93	0.12	30,30,30,30	0
59	MG	2A	3444	1/1	0.93	0.15	45,45,45,45	0
59	MG	2A	3445	1/1	0.93	0.12	52,52,52,52	0
59	MG	1a	1704	1/1	0.93	0.38	54,54,54,54	0
59	MG	2a	1681	1/1	0.93	0.55	58,58,58,58	0
59	MG	2A	3448	1/1	0.93	0.14	37,37,37,37	0
59	MG	1A	3608	1/1	0.93	0.20	59,59,59,59	0
59	MG	1A	3035	1/1	0.93	0.10	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
59	MG	2a	1688	1/1	0.93	0.14	35,35,35,35	0
59	MG	1A	3612	1/1	0.93	0.25	48,48,48,48	0
59	MG	1A	3142	1/1	0.93	0.26	55,55,55,55	0
59	MG	1A	3526	1/1	0.93	0.17	47,47,47,47	0
59	MG	2A	3222	1/1	0.93	0.18	40,40,40,40	0
59	MG	1a	1711	1/1	0.93	0.19	52,52,52,52	0
59	MG	2A	3474	1/1	0.93	0.20	41,41,41,41	0
59	MG	2A	3225	1/1	0.93	0.12	45,45,45,45	0
59	MG	1A	3440	1/1	0.93	0.32	50,50,50,50	0
59	MG	1A	3269	1/1	0.93	0.13	21,21,21,21	0
59	MG	2A	3230	1/1	0.93	0.08	54,54,54,54	0
59	MG	2a	1709	1/1	0.93	0.24	68,68,68,68	0
59	MG	1A	3271	1/1	0.93	0.25	40,40,40,40	0
59	MG	2A	3501	1/1	0.93	0.20	50,50,50,50	0
59	MG	1A	3457	1/1	0.93	0.20	47,47,47,47	0
59	MG	1A	3459	1/1	0.93	0.16	30,30,30,30	0
59	MG	2A	3514	1/1	0.93	0.22	58,58,58,58	0
59	MG	2a	1727	1/1	0.93	0.10	63,63,63,63	0
59	MG	2a	1728	1/1	0.93	0.15	60,60,60,60	0
59	MG	1A	3645	1/1	0.93	0.41	40,40,40,40	0
59	MG	1a	1727	1/1	0.93	0.15	39,39,39,39	0
59	MG	1a	1614	1/1	0.93	0.09	53,53,53,53	0
59	MG	2A	3240	1/1	0.93	0.19	42,42,42,42	0
59	MG	2a	1738	1/1	0.93	0.26	52,52,52,52	0
59	MG	2A	3521	1/1	0.93	0.19	69,69,69,69	0
59	MG	2A	3524	1/1	0.93	0.22	78,78,78,78	0
59	MG	1A	3319	1/1	0.93	0.20	42,42,42,42	0
59	MG	1A	3368	1/1	0.93	0.18	26,26,26,26	0
59	MG	2a	1750	1/1	0.93	0.19	49,49,49,49	0
59	MG	1a	1617	1/1	0.93	0.18	72,72,72,72	0
59	MG	1A	3651	1/1	0.93	0.11	28,28,28,28	0
59	MG	1A	3145	1/1	0.93	0.16	47,47,47,47	0
59	MG	1A	3322	1/1	0.93	0.26	42,42,42,42	0
59	MG	1a	1623	1/1	0.93	0.64	65,65,65,65	0
59	MG	1a	1753	1/1	0.93	0.12	65,65,65,65	0
59	MG	1A	3106	1/1	0.93	0.21	48,48,48,48	0
59	MG	2A	3569	1/1	0.93	0.12	60,60,60,60	0
59	MG	2a	1763	1/1	0.93	0.32	71,71,71,71	0
59	MG	2A	3570	1/1	0.93	0.34	48,48,48,48	0
59	MG	1A	3667	1/1	0.93	0.19	52,52,52,52	0
59	MG	2A	3093	1/1	0.93	0.17	28,28,28,28	0
59	MG	1a	1758	1/1	0.93	0.11	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3560	1/1	0.93	0.14	56,56,56,56	0
59	MG	1A	3330	1/1	0.93	0.11	41,41,41,41	0
59	MG	1A	3287	1/1	0.93	0.19	22,22,22,22	0
59	MG	2A	3103	1/1	0.93	0.23	46,46,46,46	0
59	MG	1A	3565	1/1	0.93	0.12	46,46,46,46	0
59	MG	2A	3108	1/1	0.93	0.21	44,44,44,44	0
59	MG	1A	3384	1/1	0.93	0.10	25,25,25,25	0
59	MG	2A	3596	1/1	0.93	0.13	64,64,64,64	0
59	MG	1A	3219	1/1	0.93	0.32	55,55,55,55	0
59	MG	1a	1767	1/1	0.93	0.22	60,60,60,60	0
59	MG	1a	1796	1/1	0.94	0.22	55,55,55,55	0
59	MG	1A	3533	1/1	0.94	0.17	53,53,53,53	0
59	MG	1A	3178	1/1	0.94	0.31	46,46,46,46	0
59	MG	2A	3522	1/1	0.94	0.11	38,38,38,38	0
59	MG	1A	3391	1/1	0.94	0.22	55,55,55,55	0
59	MG	2A	3527	1/1	0.94	0.26	32,32,32,32	0
59	MG	1A	3392	1/1	0.94	0.14	31,31,31,31	0
59	MG	1A	3227	1/1	0.94	0.32	45,45,45,45	0
59	MG	1A	3397	1/1	0.94	0.20	49,49,49,49	0
59	MG	1A	3107	1/1	0.94	0.20	37,37,37,37	0
59	MG	1A	3718	1/1	0.94	0.22	53,53,53,53	0
59	MG	1A	3402	1/1	0.94	0.12	22,22,22,22	0
59	MG	1A	3108	1/1	0.94	0.36	38,38,38,38	0
59	MG	2A	3551	1/1	0.94	0.13	58,58,58,58	0
59	MG	2A	3560	1/1	0.94	0.35	32,32,32,32	0
59	MG	2A	3561	1/1	0.94	0.25	46,46,46,46	0
59	MG	1A	3725	1/1	0.94	0.12	43,43,43,43	0
59	MG	2A	3565	1/1	0.94	0.32	25,25,25,25	0
59	MG	1A	3554	1/1	0.94	0.14	43,43,43,43	0
59	MG	2A	3001	1/1	0.94	0.29	29,29,29,29	0
59	MG	1A	3727	1/1	0.94	0.18	38,38,38,38	0
59	MG	2A	3006	1/1	0.94	0.19	29,29,29,29	0
59	MG	1A	3053	1/1	0.94	0.21	46,46,46,46	0
59	MG	1A	3730	1/1	0.94	0.27	25,25,25,25	0
59	MG	2A	3011	1/1	0.94	0.15	40,40,40,40	0
59	MG	1a	1627	1/1	0.94	0.20	50,50,50,50	0
59	MG	2A	3582	1/1	0.94	0.13	62,62,62,62	0
59	MG	2A	3583	1/1	0.94	0.12	38,38,38,38	0
59	MG	2A	3229	1/1	0.94	0.19	44,44,44,44	0
59	MG	2A	3589	1/1	0.94	0.29	50,50,50,50	0
59	MG	2A	3018	1/1	0.94	0.18	39,39,39,39	0
59	MG	1A	3313	1/1	0.94	0.07	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3184	1/1	0.94	0.19	39,39,39,39	0
59	MG	2A	3233	1/1	0.94	0.13	41,41,41,41	0
59	MG	1A	3416	1/1	0.94	0.08	49,49,49,49	0
59	MG	1a	1633	1/1	0.94	0.10	46,46,46,46	0
59	MG	1A	3185	1/1	0.94	0.19	60,60,60,60	0
59	MG	1A	3567	1/1	0.94	0.09	63,63,63,63	0
59	MG	1A	3014	1/1	0.94	0.11	41,41,41,41	0
59	MG	1a	1638	1/1	0.94	0.20	46,46,46,46	0
59	MG	2A	3242	1/1	0.94	0.20	38,38,38,38	0
59	MG	2A	3243	1/1	0.94	0.26	39,39,39,39	0
59	MG	2A	3245	1/1	0.94	0.20	51,51,51,51	0
59	MG	1A	3243	1/1	0.94	0.12	51,51,51,51	0
59	MG	2A	3247	1/1	0.94	0.20	45,45,45,45	0
59	MG	2A	3248	1/1	0.94	0.17	49,49,49,49	0
59	MG	1a	1640	1/1	0.94	0.11	44,44,44,44	0
59	MG	1A	3742	1/1	0.94	0.28	47,47,47,47	0
59	MG	1A	3577	1/1	0.94	0.14	60,60,60,60	0
59	MG	1a	1645	1/1	0.94	0.21	45,45,45,45	0
59	MG	2B	208	1/1	0.94	0.24	58,58,58,58	0
59	MG	1A	3329	1/1	0.94	0.25	33,33,33,33	0
59	MG	2B	211	1/1	0.94	0.23	56,56,56,56	0
59	MG	2B	212	1/1	0.94	0.14	47,47,47,47	0
59	MG	2A	3254	1/1	0.94	0.25	35,35,35,35	0
59	MG	1A	3188	1/1	0.94	0.28	56,56,56,56	0
59	MG	1A	3190	1/1	0.94	0.21	28,28,28,28	0
59	MG	1A	3447	1/1	0.94	0.04	30,30,30,30	0
59	MG	1A	3448	1/1	0.94	0.08	41,41,41,41	0
59	MG	1A	3450	1/1	0.94	0.14	53,53,53,53	0
59	MG	1A	3030	1/1	0.94	0.22	50,50,50,50	0
59	MG	1A	3757	1/1	0.94	0.15	26,26,26,26	0
59	MG	1A	3086	1/1	0.94	0.11	31,31,31,31	0
59	MG	1A	3455	1/1	0.94	0.17	50,50,50,50	0
59	MG	1A	3456	1/1	0.94	0.21	32,32,32,32	0
59	MG	1A	3148	1/1	0.94	0.19	30,30,30,30	0
59	MG	2S	201	1/1	0.94	0.25	52,52,52,52	0
59	MG	1a	1662	1/1	0.94	0.20	58,58,58,58	0
59	MG	2W	502	1/1	0.94	0.12	45,45,45,45	0
59	MG	1A	3336	1/1	0.94	0.19	20,20,20,20	0
59	MG	26	101	1/1	0.94	0.27	33,33,33,33	0
59	MG	1a	1664	1/1	0.94	0.11	48,48,48,48	0
59	MG	1a	1665	1/1	0.94	0.20	41,41,41,41	0
59	MG	1A	3460	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
59	MG	1A	3765	1/1	0.94	0.15	58,58,58,58	0
59	MG	2A	3278	1/1	0.94	0.25	44,44,44,44	0
59	MG	1A	3337	1/1	0.94	0.22	30,30,30,30	0
59	MG	2A	3281	1/1	0.94	0.22	43,43,43,43	0
59	MG	2a	1611	1/1	0.94	0.43	70,70,70,70	0
59	MG	1a	1673	1/1	0.94	0.12	43,43,43,43	0
59	MG	2A	3285	1/1	0.94	0.09	53,53,53,53	0
59	MG	1a	1674	1/1	0.94	0.12	54,54,54,54	0
59	MG	2A	3073	1/1	0.94	0.18	28,28,28,28	0
59	MG	1a	1675	1/1	0.94	0.17	38,38,38,38	0
59	MG	1A	3090	1/1	0.94	0.22	35,35,35,35	0
59	MG	1A	3342	1/1	0.94	0.10	48,48,48,48	0
59	MG	1A	3034	1/1	0.94	0.10	50,50,50,50	0
59	MG	2a	1622	1/1	0.94	0.23	33,33,33,33	0
59	MG	1A	3200	1/1	0.94	0.15	40,40,40,40	0
59	MG	2A	3304	1/1	0.94	0.17	38,38,38,38	0
59	MG	1A	3777	1/1	0.94	0.11	45,45,45,45	0
59	MG	1A	3154	1/1	0.94	0.09	64,64,64,64	0
59	MG	1A	3024	1/1	0.94	0.07	47,47,47,47	0
59	MG	2A	3085	1/1	0.94	0.54	58,58,58,58	0
59	MG	1B	203	1/1	0.94	0.17	43,43,43,43	0
59	MG	1A	3156	1/1	0.94	0.15	54,54,54,54	0
59	MG	2a	1634	1/1	0.94	0.28	52,52,52,52	0
59	MG	2A	3321	1/1	0.94	0.09	31,31,31,31	0
59	MG	2a	1636	1/1	0.94	0.16	42,42,42,42	0
59	MG	1A	3624	1/1	0.94	0.20	48,48,48,48	0
59	MG	1A	3628	1/1	0.94	0.22	13,13,13,13	0
59	MG	2A	3325	1/1	0.94	0.18	30,30,30,30	0
59	MG	1A	3025	1/1	0.94	0.17	42,42,42,42	0
59	MG	2a	1644	1/1	0.94	0.28	50,50,50,50	0
59	MG	2A	3328	1/1	0.94	0.19	30,30,30,30	0
59	MG	1a	1692	1/1	0.94	0.28	57,57,57,57	0
59	MG	2a	1648	1/1	0.94	0.23	61,61,61,61	0
59	MG	1A	3478	1/1	0.94	0.21	28,28,28,28	0
59	MG	2A	3332	1/1	0.94	0.14	25,25,25,25	0
59	MG	1A	3159	1/1	0.94	0.34	53,53,53,53	0
59	MG	1A	3481	1/1	0.94	0.14	27,27,27,27	0
59	MG	1A	3096	1/1	0.94	0.18	47,47,47,47	0
59	MG	1A	3641	1/1	0.94	0.30	49,49,49,49	0
59	MG	2A	3102	1/1	0.94	0.05	48,48,48,48	0
59	MG	1A	3643	1/1	0.94	0.09	23,23,23,23	0
59	MG	1A	3361	1/1	0.94	0.18	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3280	1/1	0.94	0.09	40,40,40,40	0
59	MG	2A	3109	1/1	0.94	0.26	47,47,47,47	0
59	MG	1A	3488	1/1	0.94	0.09	45,45,45,45	0
59	MG	1A	3492	1/1	0.94	0.21	48,48,48,48	0
59	MG	2a	1663	1/1	0.94	0.14	51,51,51,51	0
59	MG	1E	301	1/1	0.94	0.13	18,18,18,18	0
59	MG	2A	3362	1/1	0.94	0.17	35,35,35,35	0
59	MG	2A	3116	1/1	0.94	0.12	34,34,34,34	0
59	MG	1A	3493	1/1	0.94	0.13	41,41,41,41	0
59	MG	1E	304	1/1	0.94	0.22	58,58,58,58	0
59	MG	2a	1669	1/1	0.94	0.58	55,55,55,55	0
59	MG	1E	305	1/1	0.94	0.11	30,30,30,30	0
59	MG	2A	3124	1/1	0.94	0.27	44,44,44,44	0
59	MG	2a	1672	1/1	0.94	0.12	57,57,57,57	0
59	MG	2A	3376	1/1	0.94	0.12	41,41,41,41	0
59	MG	2a	1674	1/1	0.94	0.23	60,60,60,60	0
59	MG	2a	1675	1/1	0.94	0.21	43,43,43,43	0
59	MG	1A	3281	1/1	0.94	0.15	42,42,42,42	0
59	MG	2A	3379	1/1	0.94	0.14	48,48,48,48	0
59	MG	1A	3656	1/1	0.94	0.17	45,45,45,45	0
59	MG	1a	1719	1/1	0.94	0.24	59,59,59,59	0
59	MG	2A	3133	1/1	0.94	0.14	52,52,52,52	0
59	MG	2a	1682	1/1	0.94	0.14	42,42,42,42	0
59	MG	1A	3282	1/1	0.94	0.13	21,21,21,21	0
59	MG	1A	3049	1/1	0.94	0.29	41,41,41,41	0
59	MG	1A	3369	1/1	0.94	0.18	53,53,53,53	0
59	MG	2A	3138	1/1	0.94	0.46	58,58,58,58	0
59	MG	1A	3026	1/1	0.94	0.26	42,42,42,42	0
59	MG	1a	1728	1/1	0.94	0.13	44,44,44,44	0
59	MG	1A	3039	1/1	0.94	0.18	36,36,36,36	0
59	MG	1a	1732	1/1	0.94	0.17	54,54,54,54	0
59	MG	1a	1733	1/1	0.94	0.15	61,61,61,61	0
59	MG	2a	1696	1/1	0.94	0.34	40,40,40,40	0
59	MG	2a	1697	1/1	0.94	0.24	55,55,55,55	0
59	MG	2a	1698	1/1	0.94	0.18	29,29,29,29	0
59	MG	2a	1702	1/1	0.94	0.25	53,53,53,53	0
59	MG	2A	3407	1/1	0.94	0.30	32,32,32,32	0
59	MG	1P	202	1/1	0.94	0.18	36,36,36,36	0
59	MG	1A	3378	1/1	0.94	0.19	24,24,24,24	0
59	MG	1S	3002	1/1	0.94	0.55	32,32,32,32	0
59	MG	2A	3154	1/1	0.94	0.22	59,59,59,59	0
59	MG	1A	3511	1/1	0.94	0.13	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
59	MG	2A	3420	1/1	0.94	0.19	36,36,36,36	0
59	MG	2A	3159	1/1	0.94	0.43	49,49,49,49	0
59	MG	1A	3675	1/1	0.94	0.23	32,32,32,32	0
59	MG	1A	3679	1/1	0.94	0.18	55,55,55,55	0
59	MG	2A	3430	1/1	0.94	0.34	40,40,40,40	0
59	MG	1U	203	1/1	0.94	0.38	39,39,39,39	0
59	MG	1W	201	1/1	0.94	0.20	32,32,32,32	0
59	MG	2A	3437	1/1	0.94	0.12	37,37,37,37	0
59	MG	1A	3168	1/1	0.94	0.32	60,60,60,60	0
59	MG	1A	3100	1/1	0.94	0.25	38,38,38,38	0
59	MG	2A	3440	1/1	0.94	0.14	51,51,51,51	0
59	MG	1A	3684	1/1	0.94	0.18	57,57,57,57	0
59	MG	1A	3382	1/1	0.94	0.22	46,46,46,46	0
59	MG	1A	3516	1/1	0.94	0.09	27,27,27,27	0
59	MG	1A	3220	1/1	0.94	0.11	33,33,33,33	0
59	MG	2A	3172	1/1	0.94	0.14	49,49,49,49	0
59	MG	2a	1749	1/1	0.94	0.17	59,59,59,59	0
59	MG	2A	3452	1/1	0.94	0.34	52,52,52,52	0
59	MG	13	102	1/1	0.94	0.17	34,34,34,34	0
59	MG	1A	3221	1/1	0.94	0.28	38,38,38,38	0
59	MG	15	101	1/1	0.94	0.21	54,54,54,54	0
59	MG	16	102	1/1	0.94	0.24	47,47,47,47	0
59	MG	1a	1769	1/1	0.94	0.18	68,68,68,68	0
59	MG	17	103	1/1	0.94	0.17	34,34,34,34	0
59	MG	2A	3472	1/1	0.94	0.21	21,21,21,21	0
59	MG	2a	1761	1/1	0.94	0.11	39,39,39,39	0
59	MG	1A	3078	1/1	0.94	0.30	45,45,45,45	0
59	MG	1a	1774	1/1	0.94	0.09	68,68,68,68	0
59	MG	2A	3477	1/1	0.94	0.10	54,54,54,54	0
59	MG	2a	1766	1/1	0.94	0.28	61,61,61,61	0
59	MG	1a	1776	1/1	0.94	0.18	66,66,66,66	0
59	MG	2A	3184	1/1	0.94	0.34	56,56,56,56	0
59	MG	1A	3079	1/1	0.94	0.19	22,22,22,22	0
59	MG	2A	3489	1/1	0.94	0.10	47,47,47,47	0
59	MG	1A	3529	1/1	0.94	0.14	53,53,53,53	0
59	MG	2z	701	1/1	0.94	0.19	76,76,76,76	0
59	MG	1a	1779	1/1	0.94	0.41	54,54,54,54	0
59	MG	1A	3530	1/1	0.94	0.22	34,34,34,34	0
59	MG	2A	3502	1/1	0.94	0.22	47,47,47,47	0
59	MG	2w	3002	1/1	0.94	0.07	52,52,52,52	0
59	MG	1a	1782	1/1	0.94	0.10	48,48,48,48	0
60	ZN	12	501	1/1	0.94	0.09	100,100,100,100	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3531	1/1	0.94	0.17	61,61,61,61	0
59	MG	1a	1791	1/1	0.94	0.17	52,52,52,52	0
59	MG	1a	1793	1/1	0.94	0.24	53,53,53,53	0
59	MG	1A	3532	1/1	0.94	0.10	25,25,25,25	0
59	MG	1a	1740	1/1	0.95	0.33	39,39,39,39	0
59	MG	1A	3214	1/1	0.95	0.84	61,61,61,61	0
59	MG	2A	3099	1/1	0.95	0.18	58,58,58,58	0
59	MG	2A	3580	1/1	0.95	0.07	53,53,53,53	0
59	MG	2A	3100	1/1	0.95	0.21	32,32,32,32	0
59	MG	1A	3396	1/1	0.95	0.14	51,51,51,51	0
59	MG	1A	3601	1/1	0.95	0.11	33,33,33,33	0
59	MG	1A	3734	1/1	0.95	0.24	45,45,45,45	0
59	MG	1A	3602	1/1	0.95	0.15	53,53,53,53	0
59	MG	1A	3323	1/1	0.95	0.26	33,33,33,33	0
59	MG	1A	3400	1/1	0.95	0.06	66,66,66,66	0
59	MG	2A	3284	1/1	0.95	0.15	53,53,53,53	0
59	MG	1A	3738	1/1	0.95	0.48	88,88,88,88	0
59	MG	2A	3287	1/1	0.95	0.22	55,55,55,55	0
59	MG	2A	3290	1/1	0.95	0.25	25,25,25,25	0
59	MG	1A	3183	1/1	0.95	0.23	33,33,33,33	0
59	MG	2A	3114	1/1	0.95	0.46	37,37,37,37	0
59	MG	1A	3073	1/1	0.95	0.10	35,35,35,35	0
59	MG	1A	3609	1/1	0.95	0.18	26,26,26,26	0
59	MG	2A	3608	1/1	0.95	0.22	35,35,35,35	0
59	MG	2A	3295	1/1	0.95	0.20	52,52,52,52	0
59	MG	2A	3296	1/1	0.95	0.11	45,45,45,45	0
59	MG	1A	3610	1/1	0.95	0.31	46,46,46,46	0
59	MG	2A	3614	1/1	0.95	0.13	53,53,53,53	0
59	MG	2A	3120	1/1	0.95	0.19	53,53,53,53	0
59	MG	1A	3261	1/1	0.95	0.06	34,34,34,34	0
59	MG	2A	3619	1/1	0.95	0.22	43,43,43,43	0
59	MG	1A	3262	1/1	0.95	0.10	53,53,53,53	0
59	MG	1A	3747	1/1	0.95	0.11	42,42,42,42	0
59	MG	2A	3308	1/1	0.95	0.22	29,29,29,29	0
59	MG	2B	204	1/1	0.95	0.17	45,45,45,45	0
59	MG	2B	205	1/1	0.95	0.30	56,56,56,56	0
59	MG	2A	3309	1/1	0.95	0.12	27,27,27,27	0
59	MG	1A	3614	1/1	0.95	0.47	43,43,43,43	0
59	MG	2A	3128	1/1	0.95	0.25	29,29,29,29	0
59	MG	1A	3617	1/1	0.95	0.12	25,25,25,25	0
59	MG	1A	3619	1/1	0.95	0.18	49,49,49,49	0
59	MG	1a	1625	1/1	0.95	0.09	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
59	MG	1A	3063	1/1	0.95	0.09	47,47,47,47	0
59	MG	1A	3752	1/1	0.95	0.20	42,42,42,42	0
59	MG	1A	3755	1/1	0.95	0.19	53,53,53,53	0
59	MG	2D	303	1/1	0.95	0.23	24,24,24,24	0
59	MG	1A	3409	1/1	0.95	0.11	29,29,29,29	0
59	MG	2A	3139	1/1	0.95	0.20	42,42,42,42	0
59	MG	2A	3327	1/1	0.95	0.22	59,59,59,59	0
59	MG	1A	3410	1/1	0.95	0.10	52,52,52,52	0
59	MG	2A	3329	1/1	0.95	0.17	46,46,46,46	0
59	MG	1A	3625	1/1	0.95	0.14	58,58,58,58	0
59	MG	2M	201	1/1	0.95	0.09	54,54,54,54	0
59	MG	1A	3186	1/1	0.95	0.23	45,45,45,45	0
59	MG	1A	3414	1/1	0.95	0.13	53,53,53,53	0
59	MG	2O	3001	1/1	0.95	0.24	42,42,42,42	0
59	MG	1a	1785	1/1	0.95	0.31	41,41,41,41	0
59	MG	2P	8001	1/1	0.95	0.09	30,30,30,30	0
59	MG	2A	3336	1/1	0.95	0.13	30,30,30,30	0
59	MG	1A	3633	1/1	0.95	0.14	23,23,23,23	0
59	MG	2A	3338	1/1	0.95	0.18	31,31,31,31	0
59	MG	2Y	8001	1/1	0.95	0.18	59,59,59,59	0
59	MG	1A	3087	1/1	0.95	0.56	48,48,48,48	0
59	MG	2A	3343	1/1	0.95	0.14	43,43,43,43	0
59	MG	26	102	1/1	0.95	0.25	47,47,47,47	0
59	MG	2A	3345	1/1	0.95	0.11	25,25,25,25	0
59	MG	2A	3152	1/1	0.95	0.12	27,27,27,27	0
59	MG	1A	3135	1/1	0.95	0.18	36,36,36,36	0
59	MG	1A	3521	1/1	0.95	0.09	45,45,45,45	0
59	MG	2a	1605	1/1	0.95	0.13	40,40,40,40	0
59	MG	1A	3430	1/1	0.95	0.08	63,63,63,63	0
59	MG	1A	3270	1/1	0.95	0.16	47,47,47,47	0
59	MG	1A	3642	1/1	0.95	0.22	45,45,45,45	0
59	MG	1a	1646	1/1	0.95	0.32	43,43,43,43	0
59	MG	1a	1801	1/1	0.95	0.17	55,55,55,55	0
59	MG	1A	3773	1/1	0.95	0.14	25,25,25,25	0
59	MG	2A	3361	1/1	0.95	0.10	26,26,26,26	0
59	MG	2a	1615	1/1	0.95	0.18	43,43,43,43	0
59	MG	1A	3028	1/1	0.95	0.56	40,40,40,40	0
59	MG	1d	502	1/1	0.95	0.36	39,39,39,39	0
59	MG	1A	3119	1/1	0.95	0.45	41,41,41,41	0
59	MG	2a	1619	1/1	0.95	0.50	46,46,46,46	0
59	MG	1A	3225	1/1	0.95	0.17	39,39,39,39	0
59	MG	1A	3647	1/1	0.95	0.13	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
59	MG	2A	3369	1/1	0.95	0.30	29,29,29,29	0
59	MG	1l	203	1/1	0.95	0.18	56,56,56,56	0
59	MG	1A	3439	1/1	0.95	0.29	26,26,26,26	0
59	MG	1A	3102	1/1	0.95	0.34	43,43,43,43	0
59	MG	1A	3195	1/1	0.95	0.24	21,21,21,21	0
59	MG	2A	3381	1/1	0.95	0.16	42,42,42,42	0
59	MG	2A	3385	1/1	0.95	0.10	45,45,45,45	0
59	MG	1A	3229	1/1	0.95	0.16	51,51,51,51	0
59	MG	1w	3005	1/1	0.95	0.13	78,78,78,78	0
59	MG	2a	1632	1/1	0.95	0.12	45,45,45,45	0
59	MG	2A	3389	1/1	0.95	0.19	39,39,39,39	0
59	MG	2A	3177	1/1	0.95	0.21	15,15,15,15	0
59	MG	2A	3394	1/1	0.95	0.17	34,34,34,34	0
59	MG	1w	3006	1/1	0.95	0.19	72,72,72,72	0
59	MG	1A	3541	1/1	0.95	0.10	53,53,53,53	0
59	MG	1A	3658	1/1	0.95	0.61	38,38,38,38	0
59	MG	2a	1642	1/1	0.95	0.15	29,29,29,29	0
59	MG	2A	3003	1/1	0.95	0.14	40,40,40,40	0
59	MG	1A	3660	1/1	0.95	0.19	55,55,55,55	0
59	MG	2A	3400	1/1	0.95	0.06	46,46,46,46	0
59	MG	2A	3401	1/1	0.95	0.17	25,25,25,25	0
59	MG	1B	211	1/1	0.95	0.10	32,32,32,32	0
59	MG	1A	3350	1/1	0.95	0.25	29,29,29,29	0
59	MG	1A	3065	1/1	0.95	0.09	36,36,36,36	0
59	MG	2A	3012	1/1	0.95	0.24	39,39,39,39	0
59	MG	1A	3355	1/1	0.95	0.21	27,27,27,27	0
59	MG	2A	3408	1/1	0.95	0.14	33,33,33,33	0
59	MG	1A	3550	1/1	0.95	0.12	36,36,36,36	0
59	MG	2A	3412	1/1	0.95	0.15	39,39,39,39	0
59	MG	1A	3454	1/1	0.95	0.11	52,52,52,52	0
59	MG	2A	3415	1/1	0.95	0.30	34,34,34,34	0
59	MG	1a	1670	1/1	0.95	0.19	54,54,54,54	0
59	MG	1A	3672	1/1	0.95	0.06	47,47,47,47	0
59	MG	1a	1672	1/1	0.95	0.30	43,43,43,43	0
59	MG	1A	3289	1/1	0.95	0.11	46,46,46,46	0
59	MG	2A	3421	1/1	0.95	0.11	48,48,48,48	0
59	MG	2A	3199	1/1	0.95	0.41	41,41,41,41	0
59	MG	2A	3424	1/1	0.95	0.14	23,23,23,23	0
59	MG	2A	3425	1/1	0.95	0.27	50,50,50,50	0
59	MG	2A	3201	1/1	0.95	0.34	38,38,38,38	0
59	MG	2A	3028	1/1	0.95	0.10	40,40,40,40	0
59	MG	2A	3029	1/1	0.95	0.26	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
59	MG	2A	3431	1/1	0.95	0.22	46,46,46,46	0
59	MG	2A	3206	1/1	0.95	0.32	39,39,39,39	0
59	MG	1A	3143	1/1	0.95	0.09	46,46,46,46	0
59	MG	1D	303	1/1	0.95	0.11	33,33,33,33	0
59	MG	1a	1676	1/1	0.95	0.15	42,42,42,42	0
59	MG	1A	3169	1/1	0.95	0.15	55,55,55,55	0
59	MG	1A	3123	1/1	0.95	0.23	38,38,38,38	0
59	MG	1A	3201	1/1	0.95	0.20	36,36,36,36	0
59	MG	2A	3443	1/1	0.95	0.21	52,52,52,52	0
59	MG	1A	3295	1/1	0.95	0.21	36,36,36,36	0
59	MG	1A	3683	1/1	0.95	0.16	62,62,62,62	0
59	MG	1A	3297	1/1	0.95	0.10	45,45,45,45	0
59	MG	1A	3171	1/1	0.95	0.32	50,50,50,50	0
59	MG	2a	1685	1/1	0.95	0.25	51,51,51,51	0
59	MG	1A	3299	1/1	0.95	0.12	44,44,44,44	0
59	MG	2A	3454	1/1	0.95	0.08	66,66,66,66	0
59	MG	2A	3455	1/1	0.95	0.16	47,47,47,47	0
59	MG	2A	3041	1/1	0.95	0.23	22,22,22,22	0
59	MG	1A	3238	1/1	0.95	0.23	29,29,29,29	0
59	MG	1A	3571	1/1	0.95	0.14	45,45,45,45	0
59	MG	1A	3692	1/1	0.95	0.19	45,45,45,45	0
59	MG	1M	201	1/1	0.95	0.20	48,48,48,48	0
59	MG	1A	3574	1/1	0.95	0.15	47,47,47,47	0
59	MG	1N	202	1/1	0.95	0.41	29,29,29,29	0
59	MG	1a	1694	1/1	0.95	0.14	39,39,39,39	0
59	MG	2a	1699	1/1	0.95	0.10	47,47,47,47	0
59	MG	2A	3053	1/1	0.95	0.29	44,44,44,44	0
59	MG	2A	3475	1/1	0.95	0.15	51,51,51,51	0
59	MG	1O	3002	1/1	0.95	0.21	27,27,27,27	0
59	MG	1P	201	1/1	0.95	0.30	52,52,52,52	0
59	MG	2A	3479	1/1	0.95	0.09	34,34,34,34	0
59	MG	2A	3480	1/1	0.95	0.07	59,59,59,59	0
59	MG	2A	3059	1/1	0.95	0.13	49,49,49,49	0
59	MG	1a	1698	1/1	0.95	0.16	45,45,45,45	0
59	MG	2a	1714	1/1	0.95	0.25	60,60,60,60	0
59	MG	2a	1716	1/1	0.95	0.18	62,62,62,62	0
59	MG	1A	3575	1/1	0.95	0.12	52,52,52,52	0
59	MG	2a	1718	1/1	0.95	0.10	50,50,50,50	0
59	MG	2A	3491	1/1	0.95	0.23	42,42,42,42	0
59	MG	1A	3241	1/1	0.95	0.34	40,40,40,40	0
59	MG	2A	3494	1/1	0.95	0.10	44,44,44,44	0
59	MG	2A	3495	1/1	0.95	0.07	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3498	1/1	0.95	0.15	36,36,36,36	0
59	MG	2A	3499	1/1	0.95	0.12	53,53,53,53	0
59	MG	2a	1731	1/1	0.95	0.19	48,48,48,48	0
59	MG	2A	3239	1/1	0.95	0.67	50,50,50,50	0
59	MG	1A	3302	1/1	0.95	0.20	29,29,29,29	0
59	MG	2A	3064	1/1	0.95	0.29	28,28,28,28	0
59	MG	2A	3503	1/1	0.95	0.15	32,32,32,32	0
59	MG	2A	3505	1/1	0.95	0.14	46,46,46,46	0
59	MG	2a	1740	1/1	0.95	0.31	53,53,53,53	0
59	MG	1a	1703	1/1	0.95	0.21	52,52,52,52	0
59	MG	1A	3702	1/1	0.95	0.10	51,51,51,51	0
59	MG	2A	3512	1/1	0.95	0.06	63,63,63,63	0
59	MG	1A	3579	1/1	0.95	0.12	44,44,44,44	0
59	MG	1A	3033	1/1	0.95	0.43	49,49,49,49	0
59	MG	1A	3304	1/1	0.95	0.15	39,39,39,39	0
59	MG	2a	1752	1/1	0.95	0.19	64,64,64,64	0
59	MG	2a	1753	1/1	0.95	0.09	39,39,39,39	0
59	MG	1A	3244	1/1	0.95	0.17	41,41,41,41	0
59	MG	1A	3094	1/1	0.95	0.23	43,43,43,43	0
59	MG	1A	3151	1/1	0.95	0.18	36,36,36,36	0
59	MG	1A	3057	1/1	0.95	0.10	38,38,38,38	0
59	MG	1A	3110	1/1	0.95	0.27	61,61,61,61	0
59	MG	1A	3590	1/1	0.95	0.12	44,44,44,44	0
59	MG	1a	1717	1/1	0.95	0.11	56,56,56,56	0
59	MG	2A	3255	1/1	0.95	0.18	37,37,37,37	0
59	MG	1A	3316	1/1	0.95	0.07	48,48,48,48	0
59	MG	11	8001	1/1	0.95	0.67	44,44,44,44	0
59	MG	2A	3540	1/1	0.95	0.40	31,31,31,31	0
59	MG	2a	1767	1/1	0.95	0.14	45,45,45,45	0
59	MG	2A	3541	1/1	0.95	0.14	49,49,49,49	0
59	MG	2a	1769	1/1	0.95	0.22	54,54,54,54	0
59	MG	1A	3593	1/1	0.95	0.17	53,53,53,53	0
59	MG	2A	3260	1/1	0.95	0.09	49,49,49,49	0
59	MG	2A	3261	1/1	0.95	0.16	27,27,27,27	0
59	MG	1A	3720	1/1	0.95	0.15	64,64,64,64	0
59	MG	2A	3552	1/1	0.95	0.29	39,39,39,39	0
59	MG	2z	703	1/1	0.95	0.17	41,41,41,41	0
59	MG	1A	3252	1/1	0.95	0.11	45,45,45,45	0
59	MG	15	102	1/1	0.95	0.12	40,40,40,40	0
59	MG	2A	3562	1/1	0.95	0.06	34,34,34,34	0
59	MG	1A	3490	1/1	0.95	0.09	64,64,64,64	0
59	MG	1a	1731	1/1	0.95	0.20	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
59	MG	1A	3029	1/1	0.95	0.62	40,40,40,40	0
59	MG	1A	3597	1/1	0.95	0.11	50,50,50,50	0
59	MG	1A	3598	1/1	0.95	0.21	48,48,48,48	0
59	MG	2A	3271	1/1	0.95	0.18	58,58,58,58	0
59	MG	2A	3573	1/1	0.95	0.25	43,43,43,43	0
59	MG	2A	3143	1/1	0.96	0.30	47,47,47,47	0
59	MG	2A	3597	1/1	0.96	0.21	43,43,43,43	0
59	MG	1A	3623	1/1	0.96	0.20	16,16,16,16	0
59	MG	2A	3601	1/1	0.96	0.25	53,53,53,53	0
59	MG	1a	1787	1/1	0.96	0.14	70,70,70,70	0
59	MG	1a	1789	1/1	0.96	0.22	43,43,43,43	0
59	MG	1a	1790	1/1	0.96	0.16	51,51,51,51	0
59	MG	2A	3149	1/1	0.96	0.30	46,46,46,46	0
59	MG	1A	3512	1/1	0.96	0.18	19,19,19,19	0
59	MG	1A	3158	1/1	0.96	0.26	29,29,29,29	0
59	MG	2A	3610	1/1	0.96	0.08	52,52,52,52	0
59	MG	1a	1794	1/1	0.96	0.08	71,71,71,71	0
59	MG	1A	3345	1/1	0.96	0.14	38,38,38,38	0
59	MG	2A	3340	1/1	0.96	0.17	44,44,44,44	0
59	MG	2A	3615	1/1	0.96	0.21	53,53,53,53	0
59	MG	2A	3341	1/1	0.96	0.26	24,24,24,24	0
59	MG	1A	3044	1/1	0.96	0.18	33,33,33,33	0
59	MG	2A	3344	1/1	0.96	0.13	49,49,49,49	0
59	MG	2A	3157	1/1	0.96	0.36	35,35,35,35	0
59	MG	1A	3631	1/1	0.96	0.11	48,48,48,48	0
59	MG	1A	3413	1/1	0.96	0.29	47,47,47,47	0
59	MG	1A	3517	1/1	0.96	0.26	27,27,27,27	0
59	MG	2A	3162	1/1	0.96	0.24	30,30,30,30	0
59	MG	1A	3160	1/1	0.96	0.13	36,36,36,36	0
59	MG	1A	3016	1/1	0.96	0.26	37,37,37,37	0
59	MG	1A	3766	1/1	0.96	0.09	28,28,28,28	0
59	MG	1A	3418	1/1	0.96	0.11	37,37,37,37	0
59	MG	1a	1649	1/1	0.96	0.23	52,52,52,52	0
59	MG	2A	3168	1/1	0.96	0.21	45,45,45,45	0
59	MG	1A	3522	1/1	0.96	0.12	42,42,42,42	0
59	MG	1A	3126	1/1	0.96	0.18	34,34,34,34	0
59	MG	1A	3427	1/1	0.96	0.06	30,30,30,30	0
59	MG	2A	3366	1/1	0.96	0.23	40,40,40,40	0
59	MG	1A	3774	1/1	0.96	0.40	49,49,49,49	0
59	MG	2E	301	1/1	0.96	0.25	20,20,20,20	0
59	MG	2E	302	1/1	0.96	0.14	27,27,27,27	0
59	MG	1w	3001	1/1	0.96	0.07	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
59	MG	1A	3528	1/1	0.96	0.18	49,49,49,49	0
59	MG	2A	3370	1/1	0.96	0.14	46,46,46,46	0
59	MG	2A	3372	1/1	0.96	0.09	36,36,36,36	0
59	MG	1A	3351	1/1	0.96	0.09	29,29,29,29	0
59	MG	2A	3375	1/1	0.96	0.12	28,28,28,28	0
59	MG	1A	3431	1/1	0.96	0.05	44,44,44,44	0
59	MG	1A	3352	1/1	0.96	0.14	33,33,33,33	0
59	MG	1B	201	1/1	0.96	0.16	54,54,54,54	0
59	MG	1A	3248	1/1	0.96	0.17	36,36,36,36	0
59	MG	2A	3382	1/1	0.96	0.18	34,34,34,34	0
59	MG	2A	3384	1/1	0.96	0.14	25,25,25,25	0
59	MG	1A	3354	1/1	0.96	0.18	31,31,31,31	0
59	MG	1A	3436	1/1	0.96	0.05	46,46,46,46	0
59	MG	2A	3004	1/1	0.96	0.12	53,53,53,53	0
59	MG	1A	3537	1/1	0.96	0.20	46,46,46,46	0
59	MG	2A	3391	1/1	0.96	0.13	47,47,47,47	0
59	MG	2A	3392	1/1	0.96	0.15	39,39,39,39	0
59	MG	1B	206	1/1	0.96	0.08	33,33,33,33	0
59	MG	1B	207	1/1	0.96	0.18	50,50,50,50	0
59	MG	1A	3296	1/1	0.96	0.21	17,17,17,17	0
59	MG	1A	3438	1/1	0.96	0.13	49,49,49,49	0
59	MG	2A	3189	1/1	0.96	0.37	29,29,29,29	0
59	MG	1A	3661	1/1	0.96	0.11	40,40,40,40	0
59	MG	2a	1608	1/1	0.96	0.26	56,56,56,56	0
59	MG	2A	3016	1/1	0.96	0.11	48,48,48,48	0
59	MG	1A	3663	1/1	0.96	0.13	32,32,32,32	0
59	MG	1A	3542	1/1	0.96	0.23	67,67,67,67	0
59	MG	1A	3249	1/1	0.96	0.19	40,40,40,40	0
59	MG	1A	3358	1/1	0.96	0.16	30,30,30,30	0
59	MG	1A	3547	1/1	0.96	0.10	42,42,42,42	0
59	MG	1A	3442	1/1	0.96	0.09	50,50,50,50	0
59	MG	2A	3027	1/1	0.96	0.39	44,44,44,44	0
59	MG	1a	1678	1/1	0.96	0.11	48,48,48,48	0
59	MG	2A	3409	1/1	0.96	0.06	48,48,48,48	0
59	MG	1A	3445	1/1	0.96	0.12	46,46,46,46	0
59	MG	2A	3411	1/1	0.96	0.26	43,43,43,43	0
59	MG	1B	222	1/1	0.96	0.09	41,41,41,41	0
59	MG	2A	3413	1/1	0.96	0.11	30,30,30,30	0
59	MG	1B	223	1/1	0.96	0.16	46,46,46,46	0
59	MG	1A	3446	1/1	0.96	0.05	31,31,31,31	0
59	MG	1A	3012	1/1	0.96	0.18	40,40,40,40	0
59	MG	1A	3189	1/1	0.96	0.05	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
59	MG	1A	3677	1/1	0.96	0.29	58,58,58,58	0
59	MG	1A	3253	1/1	0.96	0.12	40,40,40,40	0
59	MG	1A	3165	1/1	0.96	0.08	40,40,40,40	0
59	MG	1A	3557	1/1	0.96	0.14	44,44,44,44	0
59	MG	2a	1631	1/1	0.96	0.15	48,48,48,48	0
59	MG	2A	3423	1/1	0.96	0.24	34,34,34,34	0
59	MG	2a	1633	1/1	0.96	0.14	36,36,36,36	0
59	MG	1A	3047	1/1	0.96	0.12	37,37,37,37	0
59	MG	2A	3219	1/1	0.96	0.20	43,43,43,43	0
59	MG	1A	3364	1/1	0.96	0.17	27,27,27,27	0
59	MG	2a	1637	1/1	0.96	0.23	54,54,54,54	0
59	MG	2A	3428	1/1	0.96	0.16	28,28,28,28	0
59	MG	1A	3365	1/1	0.96	0.24	39,39,39,39	0
59	MG	1F	305	1/1	0.96	0.14	36,36,36,36	0
59	MG	2A	3043	1/1	0.96	0.12	43,43,43,43	0
59	MG	1A	3258	1/1	0.96	0.13	24,24,24,24	0
59	MG	2A	3434	1/1	0.96	0.27	54,54,54,54	0
59	MG	2A	3226	1/1	0.96	0.27	34,34,34,34	0
59	MG	2a	1646	1/1	0.96	0.08	55,55,55,55	0
59	MG	1A	3147	1/1	0.96	0.17	32,32,32,32	0
59	MG	1A	3690	1/1	0.96	0.07	56,56,56,56	0
59	MG	1A	3056	1/1	0.96	0.10	30,30,30,30	0
59	MG	1A	3150	1/1	0.96	0.21	31,31,31,31	0
59	MG	2A	3050	1/1	0.96	0.05	42,42,42,42	0
59	MG	2A	3051	1/1	0.96	0.15	35,35,35,35	0
59	MG	1a	1700	1/1	0.96	0.16	50,50,50,50	0
59	MG	2A	3234	1/1	0.96	0.52	56,56,56,56	0
59	MG	1A	3693	1/1	0.96	0.14	48,48,48,48	0
59	MG	1A	3374	1/1	0.96	0.15	35,35,35,35	0
59	MG	2A	3451	1/1	0.96	0.11	56,56,56,56	0
59	MG	1A	3375	1/1	0.96	0.16	12,12,12,12	0
59	MG	2A	3057	1/1	0.96	0.15	41,41,41,41	0
59	MG	2A	3058	1/1	0.96	0.13	48,48,48,48	0
59	MG	1A	3307	1/1	0.96	0.16	18,18,18,18	0
59	MG	1A	3085	1/1	0.96	0.44	55,55,55,55	0
59	MG	1A	3699	1/1	0.96	0.22	51,51,51,51	0
59	MG	2A	3461	1/1	0.96	0.07	54,54,54,54	0
59	MG	2A	3462	1/1	0.96	0.27	40,40,40,40	0
59	MG	2A	3463	1/1	0.96	0.10	45,45,45,45	0
59	MG	1A	3701	1/1	0.96	0.13	47,47,47,47	0
59	MG	2A	3466	1/1	0.96	0.09	51,51,51,51	0
59	MG	2A	3467	1/1	0.96	0.10	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3468	1/1	0.96	0.15	55,55,55,55	0
59	MG	1a	1708	1/1	0.96	0.21	37,37,37,37	0
59	MG	1S	3003	1/1	0.96	0.58	57,57,57,57	0
59	MG	1A	3578	1/1	0.96	0.19	40,40,40,40	0
59	MG	1A	3173	1/1	0.96	0.23	48,48,48,48	0
59	MG	2a	1676	1/1	0.96	0.48	47,47,47,47	0
59	MG	1A	3007	1/1	0.96	0.16	18,18,18,18	0
59	MG	1A	3581	1/1	0.96	0.12	61,61,61,61	0
59	MG	2A	3476	1/1	0.96	0.17	61,61,61,61	0
59	MG	1A	3059	1/1	0.96	0.06	36,36,36,36	0
59	MG	1A	3708	1/1	0.96	0.18	51,51,51,51	0
59	MG	2A	3074	1/1	0.96	0.19	39,39,39,39	0
59	MG	1A	3583	1/1	0.96	0.29	39,39,39,39	0
59	MG	2a	1684	1/1	0.96	0.45	55,55,55,55	0
59	MG	2A	3481	1/1	0.96	0.09	51,51,51,51	0
59	MG	1A	3471	1/1	0.96	0.17	23,23,23,23	0
59	MG	2A	3484	1/1	0.96	0.08	38,38,38,38	0
59	MG	1A	3713	1/1	0.96	0.63	42,42,42,42	0
59	MG	2A	3486	1/1	0.96	0.16	49,49,49,49	0
59	MG	2A	3487	1/1	0.96	0.06	41,41,41,41	0
59	MG	1A	3472	1/1	0.96	0.16	47,47,47,47	0
59	MG	1A	3715	1/1	0.96	0.27	42,42,42,42	0
59	MG	2a	1694	1/1	0.96	0.08	41,41,41,41	0
59	MG	1A	3268	1/1	0.96	0.08	48,48,48,48	0
59	MG	1A	3202	1/1	0.96	0.38	38,38,38,38	0
59	MG	1A	3588	1/1	0.96	0.11	51,51,51,51	0
59	MG	2A	3497	1/1	0.96	0.09	41,41,41,41	0
59	MG	1A	3477	1/1	0.96	0.12	18,18,18,18	0
59	MG	2a	1701	1/1	0.96	0.13	63,63,63,63	0
59	MG	1A	3385	1/1	0.96	0.14	43,43,43,43	0
59	MG	1a	1734	1/1	0.96	0.15	36,36,36,36	0
59	MG	1a	1738	1/1	0.96	0.19	66,66,66,66	0
59	MG	1A	3721	1/1	0.96	0.10	31,31,31,31	0
59	MG	2a	1706	1/1	0.96	0.18	87,87,87,87	0
59	MG	1A	3011	1/1	0.96	0.12	28,28,28,28	0
59	MG	1A	3480	1/1	0.96	0.07	26,26,26,26	0
59	MG	1A	3387	1/1	0.96	0.23	17,17,17,17	0
59	MG	2A	3509	1/1	0.96	0.11	49,49,49,49	0
59	MG	1A	3233	1/1	0.96	0.16	51,51,51,51	0
59	MG	1a	1745	1/1	0.96	0.11	47,47,47,47	0
59	MG	1a	1746	1/1	0.96	0.06	76,76,76,76	0
59	MG	2A	3097	1/1	0.96	0.08	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
59	MG	1A	3273	1/1	0.96	0.27	37,37,37,37	0
59	MG	1A	3484	1/1	0.96	0.14	42,42,42,42	0
59	MG	2A	3519	1/1	0.96	0.06	31,31,31,31	0
59	MG	1a	1751	1/1	0.96	0.42	48,48,48,48	0
59	MG	1A	3061	1/1	0.96	0.35	21,21,21,21	0
59	MG	2a	1729	1/1	0.96	0.20	54,54,54,54	0
59	MG	1A	3487	1/1	0.96	0.18	47,47,47,47	0
59	MG	1A	3276	1/1	0.96	0.23	18,18,18,18	0
59	MG	2A	3526	1/1	0.96	0.27	56,56,56,56	0
59	MG	2a	1734	1/1	0.96	0.19	70,70,70,70	0
59	MG	2A	3283	1/1	0.96	0.08	32,32,32,32	0
59	MG	2A	3105	1/1	0.96	0.09	33,33,33,33	0
59	MG	2a	1737	1/1	0.96	0.24	63,63,63,63	0
59	MG	1A	3277	1/1	0.96	0.12	36,36,36,36	0
59	MG	2A	3534	1/1	0.96	0.28	58,58,58,58	0
59	MG	2A	3535	1/1	0.96	0.06	55,55,55,55	0
59	MG	2a	1741	1/1	0.96	0.12	43,43,43,43	0
59	MG	2A	3536	1/1	0.96	0.15	50,50,50,50	0
59	MG	1A	3395	1/1	0.96	0.22	42,42,42,42	0
59	MG	2A	3289	1/1	0.96	0.15	45,45,45,45	0
59	MG	2a	1745	1/1	0.96	0.21	60,60,60,60	0
59	MG	2A	3539	1/1	0.96	0.41	41,41,41,41	0
59	MG	1A	3279	1/1	0.96	0.12	45,45,45,45	0
59	MG	1A	3604	1/1	0.96	0.15	52,52,52,52	0
59	MG	1A	3496	1/1	0.96	0.11	36,36,36,36	0
59	MG	1A	3740	1/1	0.96	0.07	45,45,45,45	0
59	MG	1A	3138	1/1	0.96	0.06	43,43,43,43	0
59	MG	1A	3499	1/1	0.96	0.21	39,39,39,39	0
59	MG	2a	1756	1/1	0.96	0.27	73,73,73,73	0
59	MG	1A	3399	1/1	0.96	0.12	55,55,55,55	0
59	MG	2A	3554	1/1	0.96	0.16	47,47,47,47	0
59	MG	2A	3298	1/1	0.96	0.19	42,42,42,42	0
59	MG	2A	3299	1/1	0.96	0.10	38,38,38,38	0
59	MG	1A	3236	1/1	0.96	0.68	52,52,52,52	0
59	MG	1A	3504	1/1	0.96	0.18	21,21,21,21	0
59	MG	1A	3077	1/1	0.96	0.22	38,38,38,38	0
59	MG	2A	3567	1/1	0.96	0.19	45,45,45,45	0
59	MG	2A	3125	1/1	0.96	0.10	30,30,30,30	0
59	MG	1a	1772	1/1	0.96	0.20	59,59,59,59	0
59	MG	2A	3127	1/1	0.96	0.20	38,38,38,38	0
59	MG	2A	3571	1/1	0.96	0.33	36,36,36,36	0
59	MG	1a	1773	1/1	0.96	0.27	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
59	MG	1a	1624	1/1	0.96	0.12	38,38,38,38	0
59	MG	1A	3283	1/1	0.96	0.13	33,33,33,33	0
59	MG	2A	3313	1/1	0.96	0.21	30,30,30,30	0
59	MG	2t	3001	1/1	0.96	0.35	45,45,45,45	0
59	MG	2A	3314	1/1	0.96	0.14	54,54,54,54	0
59	MG	1A	3507	1/1	0.96	0.20	21,21,21,21	0
59	MG	1A	3210	1/1	0.96	0.33	38,38,38,38	0
59	MG	2A	3319	1/1	0.96	0.28	29,29,29,29	0
59	MG	1a	1628	1/1	0.96	0.16	53,53,53,53	0
59	MG	2A	3584	1/1	0.96	0.16	40,40,40,40	0
59	MG	1a	1780	1/1	0.96	0.26	33,33,33,33	0
59	MG	2w	3004	1/1	0.96	0.28	52,52,52,52	0
59	MG	2A	3137	1/1	0.96	0.23	40,40,40,40	0
59	MG	1A	3339	1/1	0.96	0.10	30,30,30,30	0
59	MG	1A	3182	1/1	0.96	0.10	37,37,37,37	0
59	MG	1a	1783	1/1	0.96	0.23	44,44,44,44	0
60	ZN	24	501	1/1	0.96	0.18	72,72,72,72	0
59	MG	1A	3753	1/1	0.96	0.06	54,54,54,54	0
62	GDP	2z	702	28/28	0.96	0.14	50,62,73,81	0
59	MG	1A	3592	1/1	0.97	0.17	44,44,44,44	0
59	MG	1A	3415	1/1	0.97	0.20	42,42,42,42	0
59	MG	2B	203	1/1	0.97	0.07	62,62,62,62	0
59	MG	1a	1690	1/1	0.97	0.30	58,58,58,58	0
59	MG	1L	3001	1/1	0.97	0.13	38,38,38,38	0
59	MG	2A	3390	1/1	0.97	0.25	36,36,36,36	0
59	MG	2A	3196	1/1	0.97	0.23	51,51,51,51	0
59	MG	1L	3002	1/1	0.97	0.13	29,29,29,29	0
59	MG	1A	3503	1/1	0.97	0.23	19,19,19,19	0
59	MG	1A	3288	1/1	0.97	0.17	45,45,45,45	0
59	MG	1A	3711	1/1	0.97	0.17	41,41,41,41	0
59	MG	2A	3203	1/1	0.97	0.38	36,36,36,36	0
59	MG	1O	3001	1/1	0.97	0.26	35,35,35,35	0
59	MG	1A	3240	1/1	0.97	0.35	37,37,37,37	0
59	MG	1A	3419	1/1	0.97	0.14	46,46,46,46	0
59	MG	1A	3421	1/1	0.97	0.14	41,41,41,41	0
59	MG	1A	3038	1/1	0.97	0.09	40,40,40,40	0
59	MG	1A	3426	1/1	0.97	0.11	57,57,57,57	0
59	MG	1A	3510	1/1	0.97	0.10	42,42,42,42	0
59	MG	1S	3004	1/1	0.97	0.26	36,36,36,36	0
59	MG	1A	3242	1/1	0.97	0.72	51,51,51,51	0
59	MG	2A	3214	1/1	0.97	0.20	41,41,41,41	0
59	MG	2F	303	1/1	0.97	0.14	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
59	MG	1A	3140	1/1	0.97	0.16	42,42,42,42	0
59	MG	2A	3216	1/1	0.97	0.25	42,42,42,42	0
59	MG	1A	3088	1/1	0.97	0.37	39,39,39,39	0
59	MG	1A	3432	1/1	0.97	0.22	47,47,47,47	0
59	MG	1A	3722	1/1	0.97	0.19	27,27,27,27	0
59	MG	2A	3048	1/1	0.97	0.21	40,40,40,40	0
59	MG	1A	3356	1/1	0.97	0.17	26,26,26,26	0
59	MG	1A	3607	1/1	0.97	0.33	27,27,27,27	0
59	MG	2A	3223	1/1	0.97	0.17	39,39,39,39	0
59	MG	1Y	102	1/1	0.97	0.07	31,31,31,31	0
59	MG	1A	3089	1/1	0.97	0.10	42,42,42,42	0
59	MG	1a	1714	1/1	0.97	0.11	48,48,48,48	0
59	MG	1a	1715	1/1	0.97	0.19	28,28,28,28	0
59	MG	1A	3172	1/1	0.97	0.19	53,53,53,53	0
59	MG	2A	3056	1/1	0.97	0.13	27,27,27,27	0
59	MG	1Y	105	1/1	0.97	0.17	57,57,57,57	0
59	MG	1a	1718	1/1	0.97	0.13	39,39,39,39	0
59	MG	1A	3206	1/1	0.97	0.18	34,34,34,34	0
59	MG	2A	3427	1/1	0.97	0.20	44,44,44,44	0
59	MG	2a	1606	1/1	0.97	0.19	24,24,24,24	0
59	MG	1A	3070	1/1	0.97	0.13	37,37,37,37	0
59	MG	1A	3731	1/1	0.97	0.23	16,16,16,16	0
59	MG	13	101	1/1	0.97	0.18	38,38,38,38	0
59	MG	1A	3144	1/1	0.97	0.32	44,44,44,44	0
59	MG	1A	3175	1/1	0.97	0.34	46,46,46,46	0
59	MG	2A	3065	1/1	0.97	0.27	51,51,51,51	0
59	MG	2A	3435	1/1	0.97	0.17	38,38,38,38	0
59	MG	14	101	1/1	0.97	0.08	46,46,46,46	0
59	MG	1A	3616	1/1	0.97	0.09	63,63,63,63	0
59	MG	1A	3523	1/1	0.97	0.13	35,35,35,35	0
59	MG	1A	3525	1/1	0.97	0.57	61,61,61,61	0
59	MG	17	101	1/1	0.97	0.18	45,45,45,45	0
59	MG	1a	1735	1/1	0.97	0.11	69,69,69,69	0
59	MG	2A	3442	1/1	0.97	0.13	49,49,49,49	0
59	MG	1a	1736	1/1	0.97	0.22	32,32,32,32	0
59	MG	1a	1737	1/1	0.97	0.07	40,40,40,40	0
59	MG	1A	3001	1/1	0.97	0.11	30,30,30,30	0
59	MG	2A	3446	1/1	0.97	0.06	45,45,45,45	0
59	MG	1A	3177	1/1	0.97	0.19	21,21,21,21	0
59	MG	1A	3443	1/1	0.97	0.11	49,49,49,49	0
59	MG	1A	3444	1/1	0.97	0.09	35,35,35,35	0
59	MG	1A	3254	1/1	0.97	0.29	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1a	1743	1/1	0.97	0.14	64,64,64,64	0
59	MG	1A	3092	1/1	0.97	0.19	48,48,48,48	0
59	MG	2A	3084	1/1	0.97	0.09	33,33,33,33	0
59	MG	2A	3457	1/1	0.97	0.07	48,48,48,48	0
59	MG	1A	3743	1/1	0.97	0.09	53,53,53,53	0
59	MG	2A	3257	1/1	0.97	0.08	49,49,49,49	0
59	MG	2A	3086	1/1	0.97	0.19	25,25,25,25	0
59	MG	1A	3629	1/1	0.97	0.12	27,27,27,27	0
59	MG	1a	1747	1/1	0.97	0.15	47,47,47,47	0
59	MG	2A	3464	1/1	0.97	0.09	60,60,60,60	0
59	MG	1A	3256	1/1	0.97	0.09	49,49,49,49	0
59	MG	1a	1609	1/1	0.97	0.23	37,37,37,37	0
59	MG	1a	1750	1/1	0.97	0.12	86,86,86,86	0
59	MG	1A	3120	1/1	0.97	0.17	31,31,31,31	0
59	MG	1A	3632	1/1	0.97	0.12	14,14,14,14	0
59	MG	2A	3470	1/1	0.97	0.09	26,26,26,26	0
59	MG	1A	3534	1/1	0.97	0.08	38,38,38,38	0
59	MG	1a	1754	1/1	0.97	0.06	42,42,42,42	0
59	MG	1A	3058	1/1	0.97	0.48	34,34,34,34	0
59	MG	1A	3536	1/1	0.97	0.26	31,31,31,31	0
59	MG	2A	3098	1/1	0.97	0.28	50,50,50,50	0
59	MG	1A	3373	1/1	0.97	0.13	37,37,37,37	0
59	MG	1A	3074	1/1	0.97	0.27	28,28,28,28	0
59	MG	1A	3539	1/1	0.97	0.16	31,31,31,31	0
59	MG	1A	3540	1/1	0.97	0.20	47,47,47,47	0
59	MG	1A	3309	1/1	0.97	0.13	37,37,37,37	0
59	MG	1A	3644	1/1	0.97	0.11	26,26,26,26	0
59	MG	1A	3218	1/1	0.97	0.21	58,58,58,58	0
59	MG	2A	3483	1/1	0.97	0.10	47,47,47,47	0
59	MG	2A	3279	1/1	0.97	0.28	37,37,37,37	0
59	MG	2A	3107	1/1	0.97	0.21	38,38,38,38	0
59	MG	1A	3312	1/1	0.97	0.14	30,30,30,30	0
59	MG	1A	3015	1/1	0.97	0.21	45,45,45,45	0
59	MG	2A	3488	1/1	0.97	0.25	51,51,51,51	0
59	MG	1A	3761	1/1	0.97	0.35	27,27,27,27	0
59	MG	2A	3490	1/1	0.97	0.09	32,32,32,32	0
59	MG	1A	3458	1/1	0.97	0.09	47,47,47,47	0
59	MG	2A	3112	1/1	0.97	0.24	20,20,20,20	0
59	MG	2A	3113	1/1	0.97	0.23	33,33,33,33	0
59	MG	2A	3288	1/1	0.97	0.20	34,34,34,34	0
59	MG	1A	3009	1/1	0.97	0.09	20,20,20,20	0
59	MG	1A	3318	1/1	0.97	0.16	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3042	1/1	0.97	0.23	19,19,19,19	0
59	MG	1a	1631	1/1	0.97	0.06	41,41,41,41	0
59	MG	1A	3655	1/1	0.97	0.12	31,31,31,31	0
59	MG	1A	3767	1/1	0.97	0.05	44,44,44,44	0
59	MG	1A	3264	1/1	0.97	0.07	47,47,47,47	0
59	MG	2A	3123	1/1	0.97	0.20	39,39,39,39	0
59	MG	2A	3506	1/1	0.97	0.11	56,56,56,56	0
59	MG	2A	3297	1/1	0.97	0.09	29,29,29,29	0
59	MG	1A	3657	1/1	0.97	0.10	43,43,43,43	0
59	MG	1A	3062	1/1	0.97	0.17	17,17,17,17	0
59	MG	2A	3511	1/1	0.97	0.21	39,39,39,39	0
59	MG	1A	3772	1/1	0.97	0.17	20,20,20,20	0
59	MG	2A	3513	1/1	0.97	0.10	54,54,54,54	0
59	MG	1A	3043	1/1	0.97	0.23	23,23,23,23	0
59	MG	2A	3302	1/1	0.97	0.14	35,35,35,35	0
59	MG	1A	3326	1/1	0.97	0.14	34,34,34,34	0
59	MG	1A	3662	1/1	0.97	0.08	31,31,31,31	0
59	MG	2A	3305	1/1	0.97	0.09	46,46,46,46	0
59	MG	2A	3131	1/1	0.97	0.36	40,40,40,40	0
59	MG	2A	3307	1/1	0.97	0.11	27,27,27,27	0
59	MG	2a	1693	1/1	0.97	0.37	51,51,51,51	0
59	MG	1A	3556	1/1	0.97	0.13	57,57,57,57	0
59	MG	2A	3523	1/1	0.97	0.09	38,38,38,38	0
59	MG	1A	3327	1/1	0.97	0.14	36,36,36,36	0
59	MG	2A	3525	1/1	0.97	0.25	41,41,41,41	0
59	MG	1A	3558	1/1	0.97	0.14	42,42,42,42	0
59	MG	1A	3559	1/1	0.97	0.14	44,44,44,44	0
59	MG	2a	1700	1/1	0.97	0.15	45,45,45,45	0
59	MG	1a	1792	1/1	0.97	0.11	55,55,55,55	0
59	MG	1a	1648	1/1	0.97	0.17	60,60,60,60	0
59	MG	2A	3531	1/1	0.97	0.29	38,38,38,38	0
59	MG	2A	3315	1/1	0.97	0.16	38,38,38,38	0
59	MG	1A	3224	1/1	0.97	0.42	35,35,35,35	0
59	MG	1A	3080	1/1	0.97	0.11	43,43,43,43	0
59	MG	1a	1651	1/1	0.97	0.26	54,54,54,54	0
59	MG	2A	3141	1/1	0.97	0.44	49,49,49,49	0
59	MG	1a	1797	1/1	0.97	0.25	66,66,66,66	0
59	MG	1A	3671	1/1	0.97	0.20	36,36,36,36	0
59	MG	2a	1713	1/1	0.97	0.11	43,43,43,43	0
59	MG	1A	3129	1/1	0.97	0.13	29,29,29,29	0
59	MG	2a	1715	1/1	0.97	0.14	68,68,68,68	0
59	MG	1A	3474	1/1	0.97	0.09	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
59	MG	2A	3545	1/1	0.97	0.17	38,38,38,38	0
59	MG	1A	3566	1/1	0.97	0.13	49,49,49,49	0
59	MG	1A	3021	1/1	0.97	0.18	40,40,40,40	0
59	MG	1a	1803	1/1	0.97	0.25	53,53,53,53	0
59	MG	2a	1724	1/1	0.97	0.26	52,52,52,52	0
59	MG	1a	1804	1/1	0.97	0.10	60,60,60,60	0
59	MG	2a	1726	1/1	0.97	0.17	62,62,62,62	0
59	MG	2A	3553	1/1	0.97	0.26	40,40,40,40	0
59	MG	2A	3151	1/1	0.97	0.17	29,29,29,29	0
59	MG	2A	3556	1/1	0.97	0.12	37,37,37,37	0
59	MG	2A	3557	1/1	0.97	0.18	60,60,60,60	0
59	MG	2A	3558	1/1	0.97	0.29	30,30,30,30	0
59	MG	1A	3676	1/1	0.97	0.13	51,51,51,51	0
59	MG	1A	3394	1/1	0.97	0.21	50,50,50,50	0
59	MG	1A	3570	1/1	0.97	0.23	54,54,54,54	0
59	MG	1A	3054	1/1	0.97	0.36	43,43,43,43	0
59	MG	1A	3681	1/1	0.97	0.12	30,30,30,30	0
59	MG	2A	3158	1/1	0.97	0.14	33,33,33,33	0
59	MG	1B	215	1/1	0.97	0.10	37,37,37,37	0
59	MG	1B	216	1/1	0.97	0.07	34,34,34,34	0
59	MG	1z	702	1/1	0.97	0.33	39,39,39,39	0
59	MG	1B	217	1/1	0.97	0.11	24,24,24,24	0
59	MG	1A	3572	1/1	0.97	0.13	43,43,43,43	0
59	MG	1A	3191	1/1	0.97	0.24	31,31,31,31	0
59	MG	2A	3574	1/1	0.97	0.33	62,62,62,62	0
59	MG	2a	1747	1/1	0.97	0.21	39,39,39,39	0
59	MG	2a	1748	1/1	0.97	0.13	39,39,39,39	0
59	MG	2A	3575	1/1	0.97	0.17	36,36,36,36	0
59	MG	2A	3346	1/1	0.97	0.11	64,64,64,64	0
59	MG	2A	3347	1/1	0.97	0.08	51,51,51,51	0
59	MG	1A	3334	1/1	0.97	0.11	29,29,29,29	0
59	MG	1a	1669	1/1	0.97	0.21	44,44,44,44	0
59	MG	1A	3398	1/1	0.97	0.15	26,26,26,26	0
59	MG	1A	3275	1/1	0.97	0.18	51,51,51,51	0
59	MG	1A	3132	1/1	0.97	0.14	36,36,36,36	0
59	MG	2A	3355	1/1	0.97	0.24	27,27,27,27	0
59	MG	2A	3585	1/1	0.97	0.11	49,49,49,49	0
59	MG	1A	3066	1/1	0.97	0.63	43,43,43,43	0
59	MG	2A	3588	1/1	0.97	0.23	32,32,32,32	0
59	MG	1A	3194	1/1	0.97	0.34	43,43,43,43	0
59	MG	2A	3590	1/1	0.97	0.09	38,38,38,38	0
59	MG	1A	3084	1/1	0.97	0.24	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
59	MG	1A	3404	1/1	0.97	0.11	40,40,40,40	0
59	MG	2A	3360	1/1	0.97	0.19	34,34,34,34	0
59	MG	2A	3008	1/1	0.97	0.20	33,33,33,33	0
59	MG	1a	1677	1/1	0.97	0.17	36,36,36,36	0
59	MG	2A	3010	1/1	0.97	0.11	34,34,34,34	0
59	MG	2a	1772	1/1	0.97	0.17	64,64,64,64	0
59	MG	2d	502	1/1	0.97	0.21	35,35,35,35	0
59	MG	2A	3598	1/1	0.97	0.14	46,46,46,46	0
59	MG	2A	3364	1/1	0.97	0.13	30,30,30,30	0
59	MG	1A	3163	1/1	0.97	0.15	43,43,43,43	0
59	MG	1E	302	1/1	0.97	0.17	51,51,51,51	0
59	MG	1A	3406	1/1	0.97	0.13	56,56,56,56	0
59	MG	2A	3015	1/1	0.97	0.17	36,36,36,36	0
59	MG	1A	3067	1/1	0.97	0.12	43,43,43,43	0
59	MG	1A	3032	1/1	0.97	0.68	46,46,46,46	0
59	MG	2A	3183	1/1	0.97	0.18	45,45,45,45	0
59	MG	2A	3019	1/1	0.97	0.12	41,41,41,41	0
59	MG	2A	3020	1/1	0.97	0.33	37,37,37,37	0
59	MG	1A	3285	1/1	0.97	0.27	51,51,51,51	0
59	MG	2A	3613	1/1	0.97	0.18	21,21,21,21	0
59	MG	1A	3111	1/1	0.97	0.38	39,39,39,39	0
59	MG	1A	3498	1/1	0.97	0.11	70,70,70,70	0
59	MG	2A	3616	1/1	0.97	0.36	51,51,51,51	0
60	ZN	2W	501	1/1	0.97	0.06	79,79,79,79	0
59	MG	2A	3380	1/1	0.97	0.10	36,36,36,36	0
60	ZN	23	501	1/1	0.97	0.15	85,85,85,85	0
59	MG	1A	3348	1/1	0.97	0.19	28,28,28,28	0
60	ZN	27	101	1/1	0.97	0.11	68,68,68,68	0
59	MG	1A	3239	1/1	0.97	0.09	49,49,49,49	0
62	GDP	1z	701	28/28	0.97	0.14	30,50,64,75	0
59	MG	2A	3191	1/1	0.97	0.22	44,44,44,44	0
59	MG	2A	3543	1/1	0.98	0.24	28,28,28,28	0
59	MG	1A	3325	1/1	0.98	0.27	64,64,64,64	0
59	MG	1a	1755	1/1	0.98	0.11	42,42,42,42	0
59	MG	1A	3428	1/1	0.98	0.18	64,64,64,64	0
59	MG	2A	3548	1/1	0.98	0.23	32,32,32,32	0
59	MG	2A	3549	1/1	0.98	0.36	31,31,31,31	0
59	MG	2A	3405	1/1	0.98	0.25	45,45,45,45	0
59	MG	1A	3429	1/1	0.98	0.12	44,44,44,44	0
59	MG	1A	3388	1/1	0.98	0.15	21,21,21,21	0
59	MG	1A	3666	1/1	0.98	0.17	32,32,32,32	0
59	MG	1A	3166	1/1	0.98	0.25	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
59	MG	2A	3555	1/1	0.98	0.39	42,42,42,42	0
59	MG	1a	1761	1/1	0.98	0.18	41,41,41,41	0
59	MG	1A	3103	1/1	0.98	0.06	40,40,40,40	0
59	MG	1A	3031	1/1	0.98	0.13	28,28,28,28	0
59	MG	1A	3071	1/1	0.98	0.30	31,31,31,31	0
59	MG	1a	1765	1/1	0.98	0.07	44,44,44,44	0
59	MG	1A	3149	1/1	0.98	0.10	36,36,36,36	0
59	MG	2A	3563	1/1	0.98	0.20	41,41,41,41	0
59	MG	1A	3284	1/1	0.98	0.14	48,48,48,48	0
59	MG	1a	1768	1/1	0.98	0.16	56,56,56,56	0
59	MG	2a	1660	1/1	0.98	0.38	36,36,36,36	0
59	MG	2A	3566	1/1	0.98	0.10	54,54,54,54	0
59	MG	2A	3418	1/1	0.98	0.13	46,46,46,46	0
59	MG	1A	3485	1/1	0.98	0.12	29,29,29,29	0
59	MG	1A	3003	1/1	0.98	0.09	29,29,29,29	0
59	MG	1A	3754	1/1	0.98	0.12	28,28,28,28	0
59	MG	1A	3101	1/1	0.98	0.11	38,38,38,38	0
59	MG	1A	3267	1/1	0.98	0.19	45,45,45,45	0
59	MG	1A	3543	1/1	0.98	0.07	61,61,61,61	0
59	MG	1A	3489	1/1	0.98	0.04	48,48,48,48	0
59	MG	1A	3545	1/1	0.98	0.20	46,46,46,46	0
59	MG	1A	3251	1/1	0.98	0.22	48,48,48,48	0
59	MG	1A	3116	1/1	0.98	0.20	40,40,40,40	0
59	MG	2A	3067	1/1	0.98	0.23	42,42,42,42	0
59	MG	2A	3579	1/1	0.98	0.10	42,42,42,42	0
59	MG	1A	3208	1/1	0.98	0.32	33,33,33,33	0
59	MG	1A	3549	1/1	0.98	0.11	27,27,27,27	0
59	MG	1A	3685	1/1	0.98	0.16	60,60,60,60	0
59	MG	2A	3433	1/1	0.98	0.10	35,35,35,35	0
59	MG	2A	3071	1/1	0.98	0.05	35,35,35,35	0
59	MG	1A	3494	1/1	0.98	0.22	46,46,46,46	0
59	MG	1a	1784	1/1	0.98	0.23	37,37,37,37	0
59	MG	1A	3495	1/1	0.98	0.17	53,53,53,53	0
59	MG	1A	3291	1/1	0.98	0.20	60,60,60,60	0
59	MG	1A	3613	1/1	0.98	0.06	53,53,53,53	0
59	MG	2A	3077	1/1	0.98	0.32	40,40,40,40	0
59	MG	1a	1788	1/1	0.98	0.19	45,45,45,45	0
59	MG	1A	3769	1/1	0.98	0.14	35,35,35,35	0
59	MG	1A	3209	1/1	0.98	0.27	41,41,41,41	0
59	MG	2A	3312	1/1	0.98	0.19	60,60,60,60	0
59	MG	16	101	1/1	0.98	0.15	24,24,24,24	0
59	MG	1A	3615	1/1	0.98	0.05	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
59	MG	1A	3370	1/1	0.98	0.07	21,21,21,21	0
59	MG	1A	3340	1/1	0.98	0.14	19,19,19,19	0
59	MG	2A	3449	1/1	0.98	0.11	27,27,27,27	0
59	MG	2A	3450	1/1	0.98	0.07	45,45,45,45	0
59	MG	2A	3605	1/1	0.98	0.12	35,35,35,35	0
59	MG	2A	3198	1/1	0.98	0.40	20,20,20,20	0
59	MG	1A	3618	1/1	0.98	0.09	33,33,33,33	0
59	MG	2A	3453	1/1	0.98	0.15	21,21,21,21	0
59	MG	2A	3200	1/1	0.98	0.25	34,34,34,34	0
59	MG	1A	3500	1/1	0.98	0.12	63,63,63,63	0
59	MG	1A	3697	1/1	0.98	0.33	43,43,43,43	0
59	MG	1A	3372	1/1	0.98	0.11	19,19,19,19	0
59	MG	2A	3324	1/1	0.98	0.10	43,43,43,43	0
59	MG	2A	3459	1/1	0.98	0.08	48,48,48,48	0
59	MG	2A	3204	1/1	0.98	0.14	26,26,26,26	0
59	MG	1a	1697	1/1	0.98	0.07	61,61,61,61	0
59	MG	1A	3778	1/1	0.98	0.31	33,33,33,33	0
59	MG	1A	3449	1/1	0.98	0.15	47,47,47,47	0
59	MG	2a	1710	1/1	0.98	0.16	46,46,46,46	0
59	MG	1A	3780	1/1	0.98	0.47	31,31,31,31	0
59	MG	2a	1712	1/1	0.98	0.22	62,62,62,62	0
59	MG	1A	3700	1/1	0.98	0.06	66,66,66,66	0
59	MG	1A	3622	1/1	0.98	0.10	21,21,21,21	0
59	MG	1A	3341	1/1	0.98	0.15	29,29,29,29	0
59	MG	2A	3333	1/1	0.98	0.18	35,35,35,35	0
59	MG	1A	3451	1/1	0.98	0.27	51,51,51,51	0
59	MG	1A	3407	1/1	0.98	0.09	32,32,32,32	0
59	MG	2a	1719	1/1	0.98	0.12	56,56,56,56	0
59	MG	1f	3001	1/1	0.98	0.30	39,39,39,39	0
59	MG	1A	3626	1/1	0.98	0.16	31,31,31,31	0
59	MG	2a	1722	1/1	0.98	0.21	45,45,45,45	0
59	MG	2a	1723	1/1	0.98	0.12	65,65,65,65	0
59	MG	1A	3627	1/1	0.98	0.07	34,34,34,34	0
59	MG	1A	3707	1/1	0.98	0.12	51,51,51,51	0
59	MG	1A	3562	1/1	0.98	0.06	38,38,38,38	0
59	MG	2A	3342	1/1	0.98	0.20	48,48,48,48	0
59	MG	1A	3709	1/1	0.98	0.15	41,41,41,41	0
59	MG	1A	3314	1/1	0.98	0.13	36,36,36,36	0
59	MG	1A	3315	1/1	0.98	0.09	34,34,34,34	0
59	MG	2A	3106	1/1	0.98	0.21	39,39,39,39	0
59	MG	1a	1620	1/1	0.98	0.07	40,40,40,40	0
59	MG	2a	1733	1/1	0.98	0.12	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
59	MG	2A	3348	1/1	0.98	0.10	36,36,36,36	0
59	MG	1A	3376	1/1	0.98	0.04	45,45,45,45	0
59	MG	1A	3411	1/1	0.98	0.18	21,21,21,21	0
59	MG	1A	3109	1/1	0.98	0.10	36,36,36,36	0
59	MG	1A	3569	1/1	0.98	0.13	41,41,41,41	0
59	MG	2A	3353	1/1	0.98	0.12	44,44,44,44	0
59	MG	1A	3317	1/1	0.98	0.15	33,33,33,33	0
59	MG	1A	3379	1/1	0.98	0.16	38,38,38,38	0
59	MG	1A	3197	1/1	0.98	0.21	41,41,41,41	0
59	MG	1a	1721	1/1	0.98	0.09	46,46,46,46	0
59	MG	1A	3640	1/1	0.98	0.17	41,41,41,41	0
59	MG	2A	3493	1/1	0.98	0.15	23,23,23,23	0
59	MG	2a	1746	1/1	0.98	0.21	43,43,43,43	0
59	MG	2A	3117	1/1	0.98	0.30	35,35,35,35	0
59	MG	2A	3118	1/1	0.98	0.27	35,35,35,35	0
59	MG	2R	8001	1/1	0.98	0.05	41,41,41,41	0
59	MG	2A	3496	1/1	0.98	0.36	41,41,41,41	0
59	MG	1a	1723	1/1	0.98	0.16	43,43,43,43	0
59	MG	1a	1724	1/1	0.98	0.15	18,18,18,18	0
59	MG	1a	1725	1/1	0.98	0.15	50,50,50,50	0
59	MG	1A	3573	1/1	0.98	0.11	50,50,50,50	0
59	MG	1A	3051	1/1	0.98	0.15	35,35,35,35	0
59	MG	1B	224	1/1	0.98	0.07	56,56,56,56	0
59	MG	2A	3014	1/1	0.98	0.16	34,34,34,34	0
59	MG	1A	3417	1/1	0.98	0.06	51,51,51,51	0
59	MG	1a	1730	1/1	0.98	0.15	49,49,49,49	0
59	MG	2A	3244	1/1	0.98	0.35	49,49,49,49	0
59	MG	2A	3508	1/1	0.98	0.17	32,32,32,32	0
59	MG	2A	3017	1/1	0.98	0.12	47,47,47,47	0
59	MG	2A	3129	1/1	0.98	0.21	39,39,39,39	0
59	MG	2a	1764	1/1	0.98	0.21	61,61,61,61	0
59	MG	1A	3723	1/1	0.98	0.16	36,36,36,36	0
59	MG	1A	3320	1/1	0.98	0.12	35,35,35,35	0
59	MG	1A	3465	1/1	0.98	0.16	33,33,33,33	0
59	MG	2A	3378	1/1	0.98	0.22	35,35,35,35	0
59	MG	1a	1637	1/1	0.98	0.39	42,42,42,42	0
59	MG	2a	1770	1/1	0.98	0.10	59,59,59,59	0
59	MG	2a	1771	1/1	0.98	0.17	72,72,72,72	0
59	MG	1A	3136	1/1	0.98	0.16	41,41,41,41	0
59	MG	2a	1773	1/1	0.98	0.09	50,50,50,50	0
59	MG	1A	3519	1/1	0.98	0.14	21,21,21,21	0
59	MG	2A	3518	1/1	0.98	0.26	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
59	MG	1A	3728	1/1	0.98	0.21	35,35,35,35	0
59	MG	2A	3383	1/1	0.98	0.10	39,39,39,39	0
59	MG	1a	1641	1/1	0.98	0.08	49,49,49,49	0
59	MG	1A	3649	1/1	0.98	0.15	35,35,35,35	0
59	MG	1A	3420	1/1	0.98	0.14	38,38,38,38	0
59	MG	2A	3387	1/1	0.98	0.12	46,46,46,46	0
59	MG	1F	301	1/1	0.98	0.25	27,27,27,27	0
59	MG	1A	3228	1/1	0.98	0.15	44,44,44,44	0
59	MG	1F	303	1/1	0.98	0.12	45,45,45,45	0
59	MG	1A	3469	1/1	0.98	0.21	36,36,36,36	0
59	MG	1A	3422	1/1	0.98	0.13	21,21,21,21	0
59	MG	1A	3654	1/1	0.98	0.20	54,54,54,54	0
59	MG	2A	3532	1/1	0.98	0.37	35,35,35,35	0
59	MG	1F	307	1/1	0.98	0.10	19,19,19,19	0
59	MG	2A	3147	1/1	0.98	0.23	33,33,33,33	0
59	MG	1A	3524	1/1	0.98	0.14	30,30,30,30	0
59	MG	1A	3423	1/1	0.98	0.17	17,17,17,17	0
59	MG	1A	3278	1/1	0.98	0.10	37,37,37,37	0
59	MG	1A	3473	1/1	0.98	0.18	46,46,46,46	0
59	MG	1A	3659	1/1	0.98	0.36	31,31,31,31	0
59	MG	1A	3324	1/1	0.98	0.11	51,51,51,51	0
59	MG	2A	3542	1/1	0.98	0.31	36,36,36,36	0
59	MG	2a	1638	1/1	0.98	0.38	54,54,54,54	0
59	MG	2A	3547	1/1	0.99	0.25	42,42,42,42	0
59	MG	2A	3335	1/1	0.99	0.22	25,25,25,25	0
59	MG	2A	3155	1/1	0.99	0.21	27,27,27,27	0
59	MG	2A	3591	1/1	0.99	0.12	31,31,31,31	0
59	MG	1A	3117	1/1	0.99	0.15	38,38,38,38	0
59	MG	2A	3371	1/1	0.99	0.13	26,26,26,26	0
59	MG	1A	3639	1/1	0.99	0.10	54,54,54,54	0
59	MG	1A	3310	1/1	0.99	0.06	39,39,39,39	0
59	MG	2A	3374	1/1	0.99	0.06	26,26,26,26	0
59	MG	1A	3105	1/1	0.99	0.22	22,22,22,22	0
59	MG	1A	3020	1/1	0.99	0.20	25,25,25,25	0
59	MG	2A	3599	1/1	0.99	0.18	46,46,46,46	0
59	MG	1A	3491	1/1	0.99	0.09	41,41,41,41	0
59	MG	2A	3021	1/1	0.99	0.13	25,25,25,25	0
59	MG	2A	3559	1/1	0.99	0.32	48,48,48,48	0
59	MG	2A	3603	1/1	0.99	0.12	50,50,50,50	0
59	MG	1A	3564	1/1	0.99	0.08	30,30,30,30	0
59	MG	1A	3678	1/1	0.99	0.08	16,16,16,16	0
59	MG	1A	3343	1/1	0.99	0.16	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
59	MG	1E	306	1/1	0.99	0.16	39,39,39,39	0
59	MG	1B	214	1/1	0.99	0.15	41,41,41,41	0
59	MG	2f	3001	1/1	0.99	0.07	40,40,40,40	0
59	MG	2f	3002	1/1	0.99	0.07	69,69,69,69	0
59	MG	1A	3272	1/1	0.99	0.11	33,33,33,33	0
59	MG	2A	3317	1/1	0.99	0.28	37,37,37,37	0
59	MG	2A	3286	1/1	0.99	0.19	30,30,30,30	0
59	MG	1A	3022	1/1	0.99	0.11	36,36,36,36	0
59	MG	2A	3529	1/1	0.99	0.14	28,28,28,28	0
59	MG	1a	1668	1/1	0.99	0.13	41,41,41,41	0
59	MG	1a	1644	1/1	0.99	0.11	33,33,33,33	0
59	MG	1a	1621	1/1	0.99	0.10	66,66,66,66	0
59	MG	2A	3533	1/1	0.99	0.35	23,23,23,23	0
59	MG	1A	3664	1/1	0.99	0.17	39,39,39,39	0
59	MG	2A	3005	1/1	0.99	0.10	27,27,27,27	0
59	MG	1A	3648	1/1	0.99	0.14	40,40,40,40	0
59	MG	1A	3441	1/1	0.99	0.14	34,34,34,34	0
60	ZN	1W	202	1/1	0.99	0.12	68,68,68,68	0
59	MG	1A	3634	1/1	0.99	0.07	20,20,20,20	0
59	MG	1a	1775	1/1	0.99	0.34	46,46,46,46	0
60	ZN	14	102	1/1	0.99	0.15	48,48,48,48	0
59	MG	1A	3462	1/1	0.99	0.25	42,42,42,42	0
60	ZN	1n	501	1/1	0.99	0.13	77,77,77,77	0
59	MG	2A	3267	1/1	0.99	0.22	23,23,23,23	0
59	MG	2A	3504	1/1	0.99	0.09	33,33,33,33	0
59	MG	1X	3002	1/1	0.99	0.12	53,53,53,53	0
59	MG	1A	3687	1/1	0.99	0.17	69,69,69,69	0
59	MG	2B	209	1/1	0.99	0.18	71,71,71,71	0
59	MG	1A	3367	1/1	0.99	0.15	49,49,49,49	0
61	SF4	1d	501	8/8	0.99	0.13	61,67,75,78	0
61	SF4	2d	501	8/8	0.99	0.12	63,67,88,88	0
59	MG	1A	3424	1/1	0.99	0.19	34,34,34,34	0
59	MG	2A	3587	1/1	0.99	0.28	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.