



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 06:01 am BST

PDB ID : 6CFK  
Title : Crystal structure of the Thermus thermophilus 70S ribosome in complex with D-histidyl-CAM and bound to protein Y (YfiA) at 2.7Å resolution  
Authors : Tereshchenkov, A.G.; Dobosz-Bartoszek, M.; Osterman, I.A.; Marks, J.; Sergeeva, V.A.; Kasatsky, P.; Komarova, E.S.; Stavrianidi, A.N.; Rodin, I.A.; Konevega, A.L.; Sergiev, P.V.; Sumbatyan, N.V.; Mankin, A.S.; Bogdanov, A.A.; Polikanov, Y.S.  
Deposited on : 2018-02-15  
Resolution : 2.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

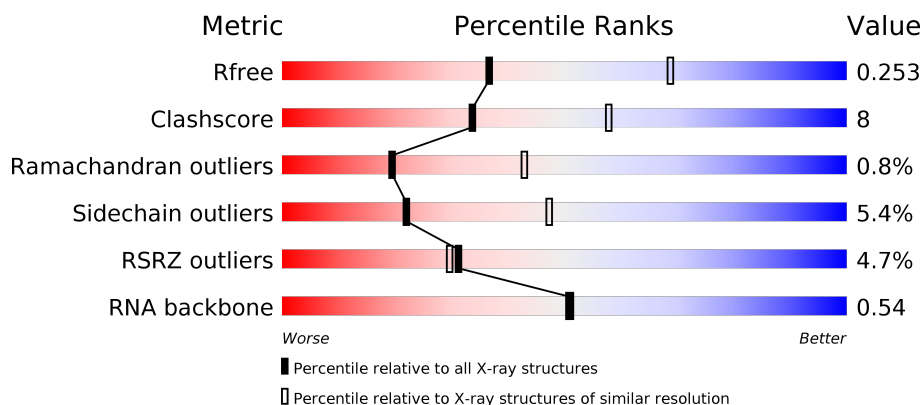
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>2%</div> <div>64%</div> <div>28%</div> <div>6%</div> <div>..</div> </div>
1	2A	2915	<div> <div>2%</div> <div>57%</div> <div>33%</div> <div>8%</div> <div>.</div> </div>
2	1B	121	<div> <div>75%</div> <div>21%</div> <div>..</div> </div>
2	2B	121	<div> <div>59%</div> <div>35%</div> <div>6%</div> <div>.</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	















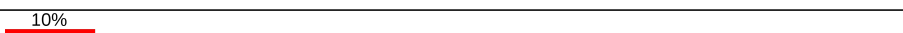
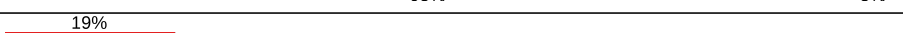
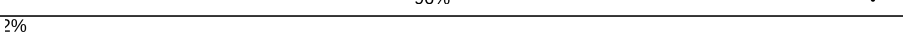


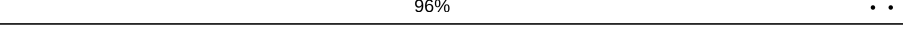
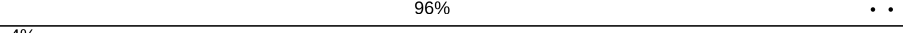
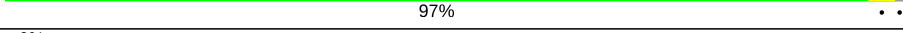
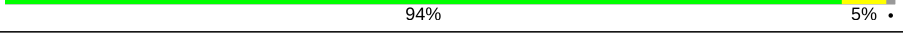
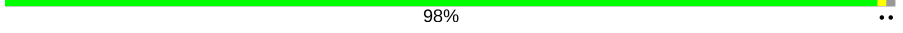
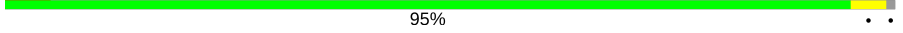
*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	2T	146	% 66% 21% 10%
16	1U	118	% 80% 17% ...
16	2U	118	8% 76% 22% .
17	1V	101	74% 24% .
17	2V	101	3% 72% 25% ..
18	1W	113	% 83% 13% ..
18	2W	113	7% 81% 15% ..
19	1X	96	% 76% 20% ..
19	2X	96	5% 79% 18% ..
20	1Y	110	% 72% 23% ..
20	2Y	110	14% 75% 22% ..
21	1Z	206	% 78% 19% ..
21	2Z	206	4% 73% 22% ..
22	10	85	% 74% 15% . 9%
22	20	85	14% 73% 16% . 9%
23	11	98	5% 79% 17% ..
23	21	98	8% 72% 23% ..
24	12	72	% 82% 14% ..
24	22	72	3% 81% 15% ..
25	13	60	75% 18% 5% .
25	23	60	23% 65% 30% ..
26	14	71	6% 63% 28% 6% .
26	24	71	8% 44% 49% . .
27	15	60	67% 28% ..
27	25	60	3% 82% 15% ..

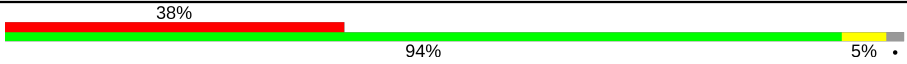
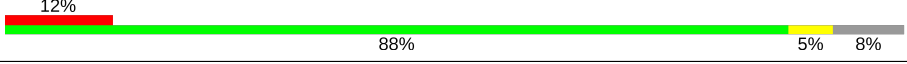



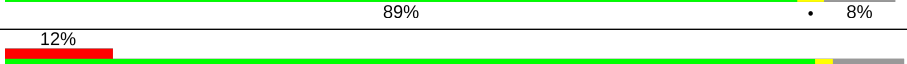
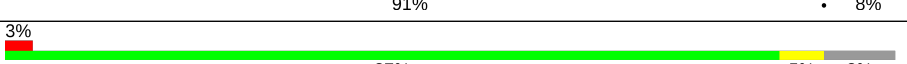
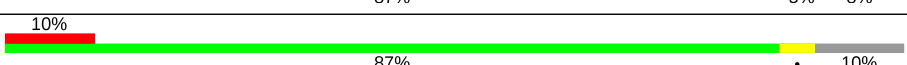
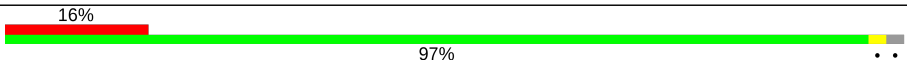
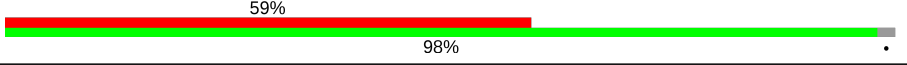
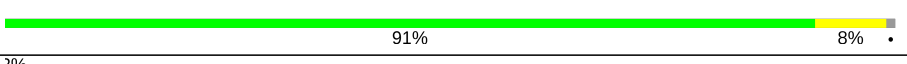
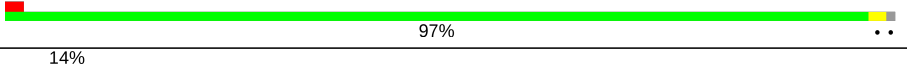

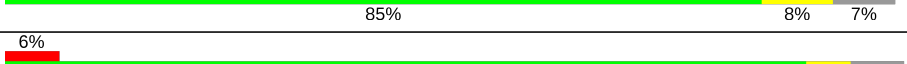
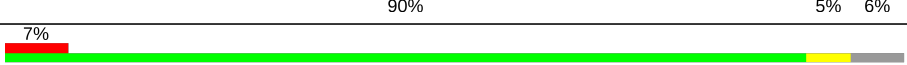
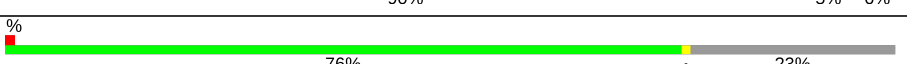









Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

Continued on next page...

Continued from previous page...

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

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
53	1y	113	
53	2y	113	

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
54	MG	1A	3189	-	-	-	X
54	MG	1A	3921	-	-	-	X
54	MG	1F	311	-	-	-	X
54	MG	1a	1767	-	-	-	X
54	MG	1a	1851	-	-	-	X
54	MG	2A	3146	-	-	-	X
54	MG	2A	3206	-	-	-	X

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 295438 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2872	Total	C	N	O	P	0	0	0
			61869	27540	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2572	1145	476	832	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

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

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

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



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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			877	553	175	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	131			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	2m	114	Total	C	N	O	S	0	0	0
			895	550	186	157	2			

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

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

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

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

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

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



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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			

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

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

- Molecule 53 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1y	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			
53	2y	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	2E	6	Total	Mg	0	0
			6	6		
54	17	2	Total	Mg	0	0
			2	2		
54	1T	3	Total	Mg	0	0
			3	3		
54	1N	3	Total	Mg	0	0
			3	3		
54	20	1	Total	Mg	0	0
			1	1		
54	18	1	Total	Mg	0	0
			1	1		
54	1o	1	Total	Mg	0	0
			1	1		
54	2W	2	Total	Mg	0	0
			2	2		
54	2I	1	Total	Mg	0	0
			1	1		
54	13	2	Total	Mg	0	0
			2	2		
54	1f	2	Total	Mg	0	0
			2	2		
54	1P	3	Total	Mg	0	0
			3	3		
54	2B	19	Total	Mg	0	0
			19	19		
54	2a	151	Total	Mg	0	0
			151	151		
54	1E	7	Total	Mg	0	0
			7	7		
54	1b	1	Total	Mg	0	0
			1	1		
54	2F	3	Total	Mg	0	0
			3	3		
54	2p	1	Total	Mg	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	28	3	Total 3	Mg 3	0	0
54	2e	1	Total 1	Mg 1	0	0
54	1W	2	Total 2	Mg 2	0	0
54	1A	1024	Total 1024	Mg 1024	0	0
54	1t	1	Total 1	Mg 1	0	0
54	1n	1	Total 1	Mg 1	0	0
54	2P	2	Total 2	Mg 2	0	0
54	1X	2	Total 2	Mg 2	0	0
54	2q	1	Total 1	Mg 1	0	0
54	1y	4	Total 4	Mg 4	0	0
54	1S	1	Total 1	Mg 1	0	0
54	25	1	Total 1	Mg 1	0	0
54	2T	4	Total 4	Mg 4	0	0
54	1D	13	Total 13	Mg 13	0	0
54	2N	1	Total 1	Mg 1	0	0
54	1e	2	Total 2	Mg 2	0	0
54	2G	3	Total 3	Mg 3	0	0
54	2f	1	Total 1	Mg 1	0	0
54	1V	3	Total 3	Mg 3	0	0
54	2X	1	Total 1	Mg 1	0	0
54	1a	255	Total 255	Mg 255	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	2Q	2	Total 2	Mg 2	0	0
54	15	3	Total 3	Mg 3	0	0
54	2j	1	Total 1	Mg 1	0	0
54	1R	3	Total 3	Mg 3	0	0
54	1G	4	Total 4	Mg 4	0	0
54	2O	1	Total 1	Mg 1	0	0
54	11	3	Total 3	Mg 3	0	0
54	1d	6	Total 6	Mg 6	0	0
54	2r	1	Total 1	Mg 1	0	0
54	1H	2	Total 2	Mg 2	0	0
54	21	1	Total 1	Mg 1	0	0
54	1i	1	Total 1	Mg 1	0	0
54	2R	1	Total 1	Mg 1	0	0
54	1Z	1	Total 1	Mg 1	0	0
54	2D	8	Total 8	Mg 8	0	0
54	14	1	Total 1	Mg 1	0	0
54	1U	2	Total 2	Mg 2	0	0
54	1O	2	Total 2	Mg 2	0	0
54	19	2	Total 2	Mg 2	0	0
54	1l	2	Total 2	Mg 2	0	0
54	2V	1	Total 1	Mg 1	0	0

*Continued on next page...*

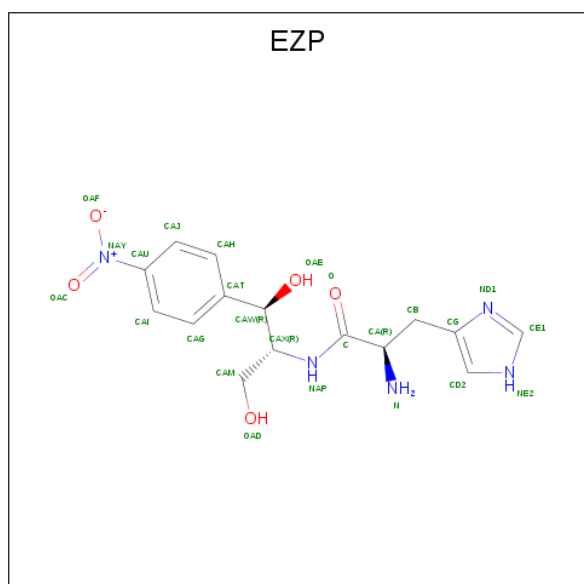
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	1F	13	Total Mg 13 13	0	0
54	10	6	Total Mg 6 6	0	0
54	1g	3	Total Mg 3 3	0	0
54	2t	1	Total Mg 1 1	0	0
54	1Q	4	Total Mg 4 4	0	0
54	2A	721	Total Mg 721 721	0	0
54	1h	2	Total Mg 2 2	0	0
54	1B	29	Total Mg 29 29	0	0

- Molecule 55 is POTASSIUM ION (three-letter code: K) (formula: K).

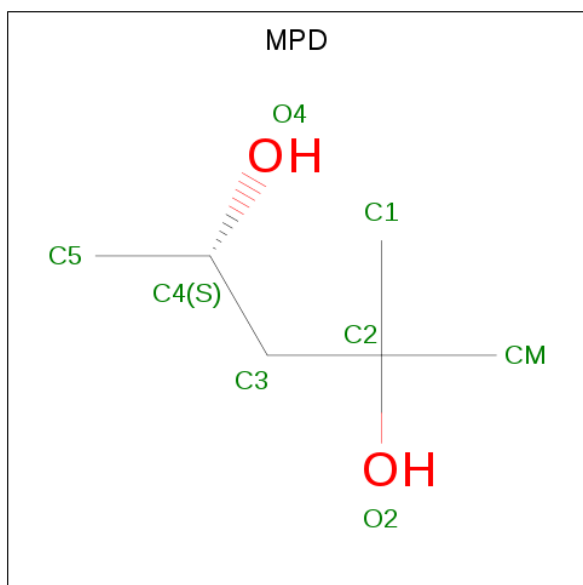
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1A	1	Total K 1 1	0	0
55	2A	1	Total K 1 1	0	0

- Molecule 56 is N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]-D-histidinamide (three-letter code: EZP) (formula: C<sub>15</sub>H<sub>19</sub>N<sub>5</sub>O<sub>5</sub>).



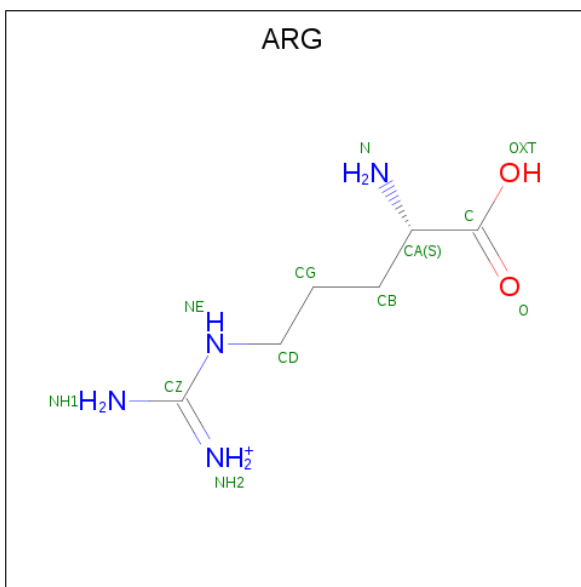
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	1A	1	Total	C	N	O	0	0
			25	15	5	5		
56	2A	1	Total	C	N	O	0	0
			25	15	5	5		

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	1A	1	Total	C	O	0	0
			8	6	2		
57	1T	1	Total	C	O	0	0
			8	6	2		
57	18	1	Total	C	O	0	0
			8	6	2		
57	1a	1	Total	C	O	0	0
			8	6	2		
57	2A	1	Total	C	O	0	0
			8	6	2		
57	2A	1	Total	C	O	0	0
			8	6	2		
57	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 58 is ARGinine (three-letter code: ARG) (formula:  $C_6H_{15}N_4O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	1B	1	Total	C	N	O	0	0
			12	6	4	2		
58	1F	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

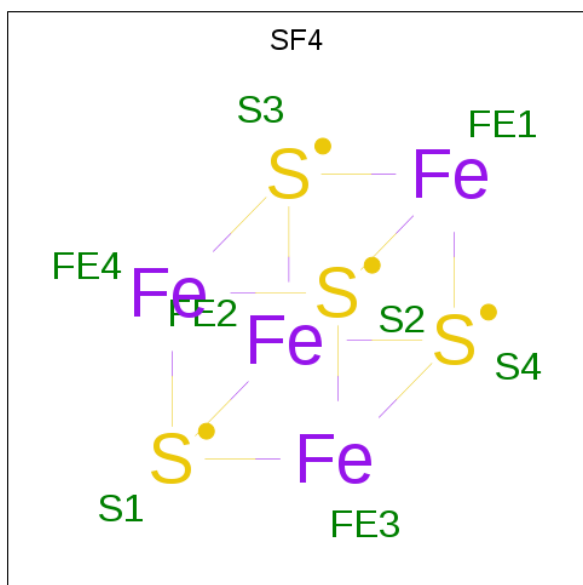
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	29	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	2n	1	Total	Zn	0	0
			1	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2Y	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	1d	1	Total	Fe	S	0	0
			8	4	4		
60	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2980	Total	O	0	0
			2980	2980		
61	1B	105	Total	O	0	0
			105	105		
61	1D	116	Total	O	0	0
			116	116		
61	1E	76	Total	O	0	0
			76	76		
61	1F	63	Total	O	0	0
			63	63		

Continued on next page...



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1G	22	Total 22	O 22	0	0
61	1H	16	Total 16	O 16	0	0
61	1I	7	Total 7	O 7	0	0
61	1N	50	Total 50	O 50	0	0
61	1O	22	Total 22	O 22	0	0
61	1P	58	Total 58	O 58	0	0
61	1Q	42	Total 42	O 42	0	0
61	1R	37	Total 37	O 37	0	0
61	1S	13	Total 13	O 13	0	0
61	1T	42	Total 42	O 42	0	0
61	1U	45	Total 45	O 45	0	0
61	1V	37	Total 37	O 37	0	0
61	1W	24	Total 24	O 24	0	0
61	1X	24	Total 24	O 24	0	0
61	1Y	15	Total 15	O 15	0	0
61	1Z	14	Total 14	O 14	0	0
61	10	22	Total 22	O 22	0	0
61	11	28	Total 28	O 28	0	0
61	12	14	Total 14	O 14	0	0
61	13	22	Total 22	O 22	0	0
61	14	2	Total 2	O 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	15	26	Total 26	O 26	0	0
61	16	17	Total 17	O 17	0	0
61	17	14	Total 14	O 14	0	0
61	18	30	Total 30	O 30	0	0
61	19	8	Total 8	O 8	0	0
61	1a	261	Total 261	O 261	0	0
61	1b	1	Total 1	O 1	0	0
61	1d	9	Total 9	O 9	0	0
61	1e	6	Total 6	O 6	0	0
61	1f	3	Total 3	O 3	0	0
61	1h	1	Total 1	O 1	0	0
61	1i	1	Total 1	O 1	0	0
61	1j	1	Total 1	O 1	0	0
61	1k	1	Total 1	O 1	0	0
61	1l	4	Total 4	O 4	0	0
61	1n	1	Total 1	O 1	0	0
61	1o	5	Total 5	O 5	0	0
61	1p	3	Total 3	O 3	0	0
61	1y	5	Total 5	O 5	0	0
61	2A	1686	Total 1686	O 1686	0	0
61	2B	65	Total 65	O 65	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2D	52	Total 52	O 52	0	0
61	2E	25	Total 25	O 25	0	0
61	2F	21	Total 21	O 21	0	0
61	2G	7	Total 7	O 7	0	0
61	2H	4	Total 4	O 4	0	0
61	2I	4	Total 4	O 4	0	0
61	2N	6	Total 6	O 6	0	0
61	2O	22	Total 22	O 22	0	0
61	2P	23	Total 23	O 23	0	0
61	2Q	30	Total 30	O 30	0	0
61	2R	21	Total 21	O 21	0	0
61	2S	8	Total 8	O 8	0	0
61	2T	10	Total 10	O 10	0	0
61	2U	14	Total 14	O 14	0	0
61	2V	9	Total 9	O 9	0	0
61	2W	21	Total 21	O 21	0	0
61	2X	9	Total 9	O 9	0	0
61	2Y	3	Total 3	O 3	0	0
61	2Z	15	Total 15	O 15	0	0
61	20	13	Total 13	O 13	0	0
61	21	24	Total 24	O 24	0	0

*Continued on next page...*

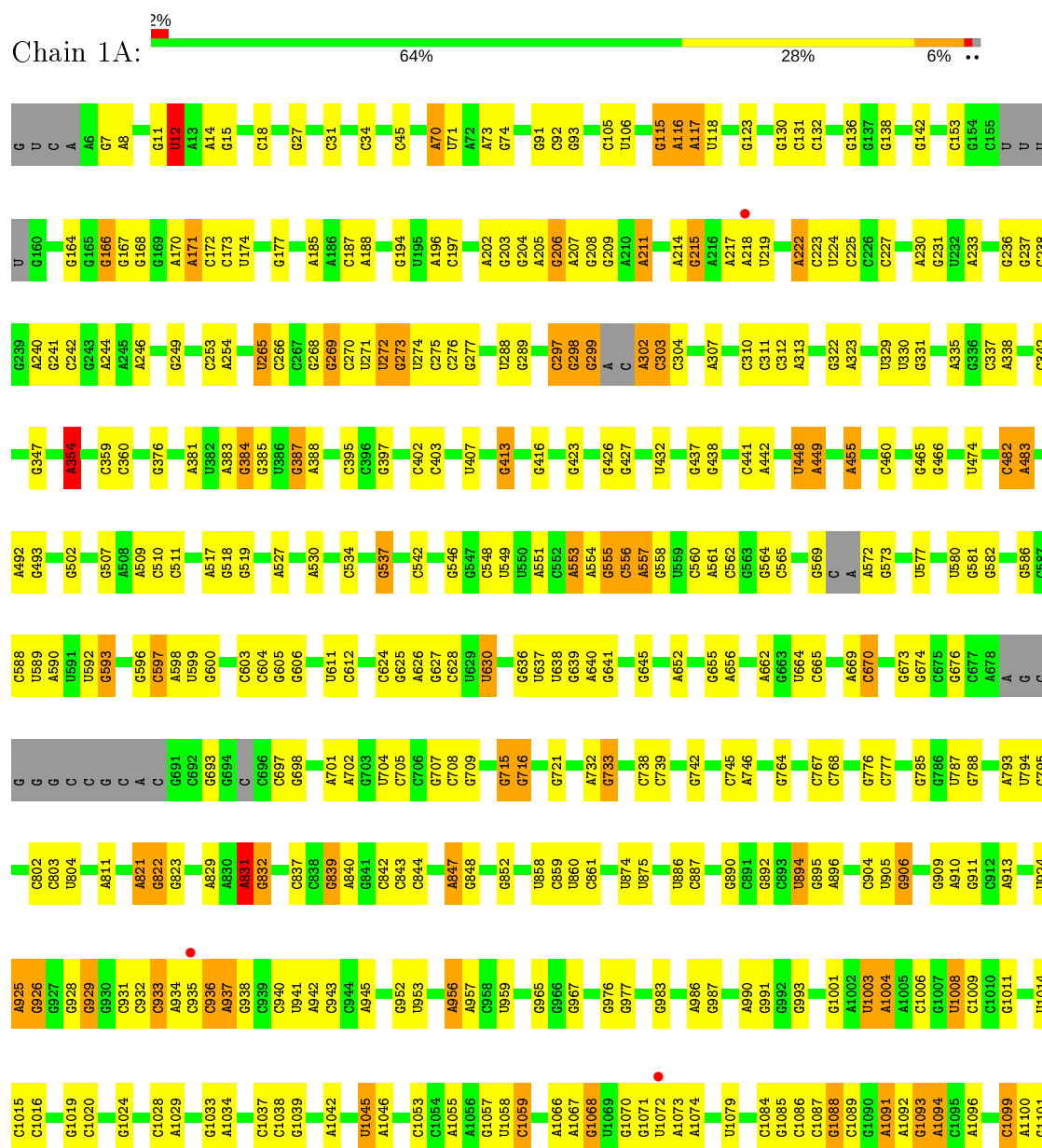
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	22	5	Total 5	O 5	0	0
61	23	3	Total 3	O 3	0	0
61	24	2	Total 2	O 2	0	0
61	25	9	Total 9	O 9	0	0
61	26	6	Total 6	O 6	0	0
61	27	7	Total 7	O 7	0	0
61	28	15	Total 15	O 15	0	0
61	29	2	Total 2	O 2	0	0
61	2a	100	Total 100	O 100	0	0
61	2d	6	Total 6	O 6	0	0
61	2e	1	Total 1	O 1	0	0
61	2f	1	Total 1	O 1	0	0
61	2j	2	Total 2	O 2	0	0
61	2l	1	Total 1	O 1	0	0
61	2m	1	Total 1	O 1	0	0
61	2o	2	Total 2	O 2	0	0
61	2p	1	Total 1	O 1	0	0
61	2q	1	Total 1	O 1	0	0
61	2r	4	Total 4	O 4	0	0
61	2y	1	Total 1	O 1	0	0

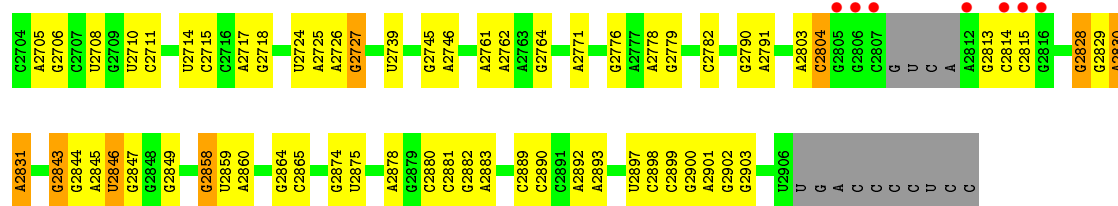
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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.

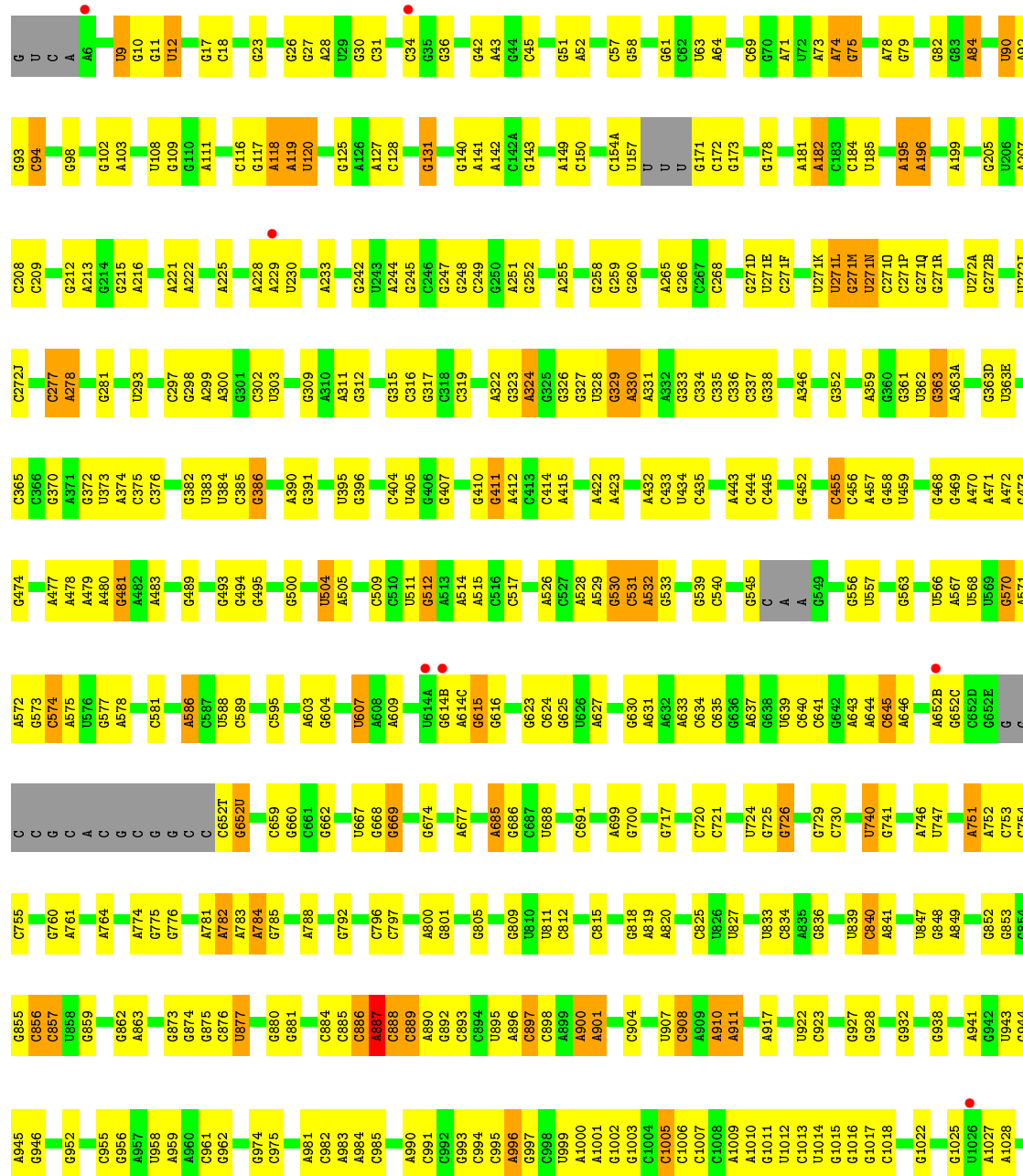
#### • Molecule 1: 23S Ribosomal RNA



U2566	C2436	G2209	U2140	A2042	A1878	C1757	G1631	C1514	A1405	G1296	A1174	G1102
U2567	A2437	C2210	A2141	C2043	U1882	G1766	A1632	C1515	A1406	G1296	A1175	A1103
A2573	A2438	U2211	U2144	U2045	U1883	A1767	A1633	A1516		A1299	U1176	G1104
G2440	G2439	G2212	G2145	G2045	G1889	U1768	C1635	A1518	G1410	G1302	C1180	U1106
G2441	G2440	G2213		U2050		U1769			G1411		G1181	U1107
A2442	G2436	G2214	A2148	G2051	U1895		G1652	G1529			G1108	
A2576	G2337	G2215	G2149	A2052	U1896		G1653		C1416	G1305	G1184	G1109
A2577	C2338	A2220	C2150	A2053	U1899	G1777	A1654	A1532	G1417		C1185	C1110
G2579	A2340	G2227	C2151	G2054	A1899	G1787	A1655	G1533	U1418	G1310	C1186	U1111
C2580	G2341	A2447	U2152	A2055	C1901	A1793	A1656	C1539	G1426	G1311	U1187	U1112
			G2153	C2058		G1794	G1674	A1541	A1425	G1312	A1188	A1113
A2584	G2346	G2228	U2154	G2059	A1911	G1795	U1675	A1542	G1427	G1313		A1114
C2585	A2347	A2229	G2155	G2060	A1911				G1428	A1314	C1196	A1115
U2596	A2348	A2237	A2157	G2065	G1921	A1804	A1679		C1429	C1316	C1199	G1117
U2597			C2158	C2065	A1922				C1430	A1315	C1199	C1118
			U2159	G2071	G1928	U1809	G1682	C1551	G1431	A1318	A1201	A1119
A2602	C2354	U2245	C2160	G2072		U1810	U1686	C1552	C1432		A1202	G1120
C2603	G2357	G2246	C2161	A2073	A1935	A1812	U1687	C1553	C1433	G1327	G1210	C1122
G2604	A2358	G2250	C2162	A2073	U1936	C1813	C1687	C1554	G1435	G1331	G1210	A1123
U2605	C2359	G2251	C2163	C2077	A1814	A1814	G1689	C1555	U1436	G1332	C1212	U1124
	U2360		C2164	G2078	A1941	A1815		A1556		A1333	G1216	C1125
A2614	G2361	U2255	U2165		C1942	A1816	G1694	A1557	A1441	A1334	G1217	U1127
G2615	C2362	U2256	C2167	A2082	G1943	A1817	G1695			C1335	G1218	U1128
			C2168	G2083					U1452	C1336	G1219	U1129
G2620	C2371	G2271	G2169	A2084	G1951	C1821	A1699	U1566	C1453	G1337	A1219	U1130
U2621	A2372	A2279	C2170	C2085	G1952	A1822	G1700	G1567	G1462	A1222	G1221	A1131
C2622	G2376	A2280	U2172	G2089	A1958	U1825	A1701	A1575	C1463	C1343	G1223	A1132
U2623	C2377	A2281	C2173	U2090	A1959	C1826			G1464		C1224	G1133
C2624	G2383	G2283	G2174	G2091	A1960	U1827	A1711	C1579	U1465	U1346	C1225	A1134
			C2175	A2093	C1964	U1828		G	U1466	A1347	C1226	U1136
C2629	A2388	G2289	G2176	G2094	U1965	U1829		U	G1467	A1349	A1227	G1137
G2639	A2389	A2290	G2177	A2104	A1974	C1830	A1715	C	A1473	G1349	G1138	
A2641	A2390	G2291	G2178			G1832	C1717		C1474	C1350	G1139	
G2642			G2179	U2108	U1977	A1833	U1718		G1475	C1351	U1140	
	C2393	C2295	A2180	G2109	U1985	C1835	U1720	A1589	C1476	C1352	A1141	
U2649	G2394	A2299	G2181			U1836	U1721	C1590	U1477		A1142	
C2658	G2395	A2299	C2182	C2119	C1989	A1841	C1730	C1594	A1485	U1355	C1246	A1144
U2659	G2396	A2300	C2183	U2120		G1842	C1731	C1595	A1491	A1358	A1355	G1145
U2662	U2402	G2301	G2186	U2121	A1992	A1843			G1495	U1359	U1256	
C2663	G2411	C2304	G2188	G2122	A1993	G1844	C1732	C1604	G1496	C1360	G1257	
A2666	G2412	G2316	G2190	U2124	A1994	G1845	G1734	A1605	G1497	C1361	A1149	
			A2193	G2125		A1846			G1498	A1367	C1263	U1151
A2674	C2416	A2317	U2194	C2129	C2010	G1847	U1740	A1613	C1498		G1264	G1152
	G2417		A2195	C2130					C1499			
G2686	U2418	A2321	U2199	U2015	U2015	G1857	A1747	A1616	A1500	G1370	G1273	C1155
U2694	G2421	A2322	A2198	C2018	C2018	A1860	G1749	A1617	U1501	U1374	G1275	G1156
	G2422	A2323		G2019	G2019	G1870	G1750	A1618	G1502	G1375	A1157	A1157
U2699		U2324	G2204	U2135	A2035	G1871	U1753	U1625	G1506	G1378	G1286	G1158
U2700	G2426	C2325	C2205	A2136	A2036				A1507		A1287	G1162
U2701	C2326	G2327	G2206	G2137	A2037	C1874	C1754	G1628	C1508	U1387	A1288	
C2702	A2434		C2207	G2138			C1755	G1629	C1509		G1171	
C2703	U2435		G2208	A2139			U1756	A1630		U1398	G1291	

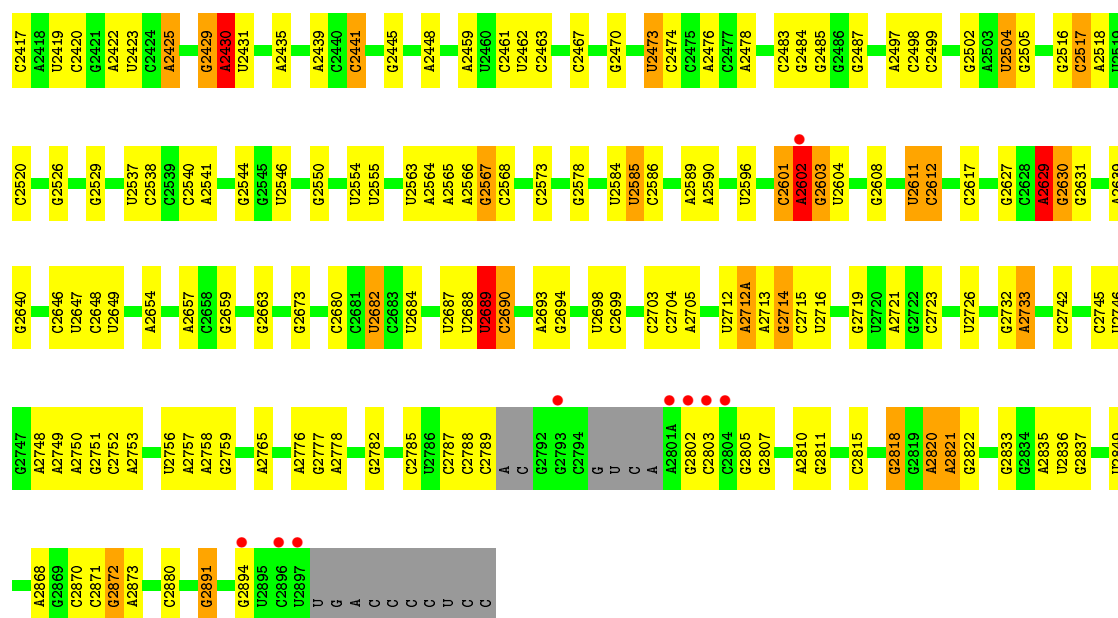


• Molecule 1: 23S Ribosomal RNA



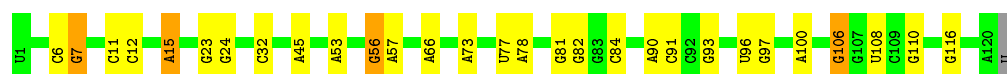
G2321	G2322	G2323	G2324	G2325	G2326	G2327	G2328	G2329	G2332	G2333	G2334	G2335	G2336	G2343	G2344	G2347	G2350	G2354	G2355	G2356	G2357	G2358	G2364	G2365	G2366	G2375	G2376	G2377	G2378	G2379	G2383	G2384	G2385	G2388	G2389	G2390	G2391	G2397	G2400	G2401	G2402	G2406	G2410	G2414																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
U2243	U2244	C2248	G2251	G2252	G2253	C2260	G2261	G2262	A2267	A2268	A2269	G2270	G2271	U2272	A2273	C2274	C2275	G2280	C2283	C2284	C2285	A2286	A2287	A2288	G2289	C2292	C2295	U2296	C2297	A2298	G2299	G2302	G2303	G2304	A2305	G2307	G2308	A2309	A2310	A2311	U2312	C2313	G2314	G2315	G2316	G2317	G2318	G2319	G2320																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	G2158	G2159	G2160	<b>G2161</b>	G2162	G2163	G2164	G2165	G2166	U2167	G2168	<b>G2169</b>	A2170	A2171	U2172	A2173	<b>G2174</b>	G2175	A2176	<b>G2177</b>	G2178	G2179	U2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	U2189	G2190	G2191	G2192	A2198	G2206	G2207	A2208	G2219	A2225	G2237	G2238	G2239																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
U2079	U2086	G2087	G2092	G2093	<b>G2094</b>	G2095	U2096	U2099	G2100	<b>G2101</b>	U2102	<b>C2103</b>	<b>G2104</b>	G2105	G2106	G2107	G2108	U2109	G2110	C2111	G2112	U2113	G2115	G2116	G2117	G2118	G2119	G2120	G2121	G2122	G2123	G2124	G2125	G2126	G2127	G2128	G2129	U2130	G2131	U2132	G2133	A2134	<b>G2135</b>	G2136	G2137	G2138	G2139	G2140	G2141	G2142	G2143	G2144	G2145	G2146																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
C1947	U1818	A1952	A1953	<b>G1954</b>	U1955	U1963	U1967	A1970	A1971	A1972	U1991	<b>G1992</b>	U1993	G1996	<b>G1997</b>	A2001	G2002	A2014	A2020	<b>C2021</b>	G2022	<b>G2023</b>	A2030	<b>A2031</b>	<b>G2032</b>	A2033	G2036	G2037	G2038	<b>G2039</b>	G2040	C2043	A2051	G2055	G2056	A2060	G2061	<b>A2062</b>	G2069	G2070	U2074	U2075	G2076	G2077	G2078	G2079	G2080	G2081	G2082	G2083	G2084	G2085	G2086	G2087	G2088	G2089	G2090	G2091	G2092	G2093	G2094	G2095	G2096	G2097	G2098	G2099	G2100	G2101	G2102	G2103	G2104	G2105	G2106	G2107	G2108	G2109	G2110	G2111	G2112	G2113	G2114	G2115	G2116	G2117	G2118	G2119	G2120	G2121	G2122	G2123	G2124	G2125	G2126	G2127	G2128	G2129	U2130	G2131	U2132	G2133	A2134	<b>G2135</b>	G2136	G2137	G2138	G2139	G2140	G2141	G2142	G2143	G2144	G2145	G2146	G2147	G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	G2158	G2159	G2160	G2161	G2162	G2163	G2164	G2165	G2166	G2167	G2168	G2169	G2170	G2171	G2172	G2173	G2174	G2175	G2176	G2177	G2178	G2179	G2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	G2189	G2190	G2191	G2192	A2198	G2206	G2207	A2208	G2219	A2225	G2237	G2238	G2239																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
U1817	U1818	G1826	G1827	<b>G1828</b>	G1829	<b>G1830</b>	G1831	G1832	G1835	G1839	G1842	A1847	<b>A1848</b>	G1858	U1864	A1876	A1877	G1878	C1881	G1882	<b>G1883</b>	G1889	A1890	G1899	A1900	A1901	G1902	G1906	G1910	U1911	<b>A1912</b>	A1913	U1914	U1915	A1916	U1917	G1921	G1929	G1930	A1937	A1938	U1939	U1946	U1947	U1948	U1949	U1950	U1951	U1952	U1953	U1954	U1955	U1956	U1957	U1958	U1959	U1960	U1961	U1962	U1963	U1964	U1965	U1966	U1967	U1968	U1969	U1970	U1971	U1972	U1973	U1974	U1975	U1976	U1977	U1978	U1979	U1980	U1981	U1982	U1983	U1984	U1985	U1986	U1987	U1988	U1989	U1990	U1991	U1992	U1993	U1994	U1995	U1996	U1997	U1998	U1999	U2000	U2001	U2002	U2003	U2004	U2005	U2006	U2007	U2008	U2009	U2010	U2011	U2012	U2013	U2014	U2015	U2016	U2017	U2018	U2019	U2020	U2021	U2022	U2023	U2024	U2025	U2026	U2027	U2028	U2029	U2030	U2031	U2032	U2033	U2034	U2035	U2036	U2037	U2038	U2039	U2040	U2041	U2042	U2043	U2044	U2045	U2046	U2047	U2048	U2049	U2050	U2051	U2052	U2053	U2054	U2055	U2056	U2057	U2058	U2059	U2060	U2061	U2062	U2063	U2064	U2065	U2066	U2067	U2068	U2069	U2070	U2071	U2072	U2073	U2074	U2075	U2076	U2077	U2078	U2079	U2080	U2081	U2082	U2083	U2084	U2085	U2086	U2087	U2088	U2089	U2090	U2091	U2092	U2093	U2094	U2095	U2096	U2097	U2098	U2099	U2100	U2101	U2102	U2103	U2104	U2105	U2106	U2107	U2108	U2109	U2110	U2111	U2112	U2113	U2114	U2115	U2116	U2117	U2118	U2119	U2120	U2121	U2122	U2123	U2124	U2125	U2126	U2127	U2128	U2129	U2130	U2131	U2132	U2133	U2134	U2135	U2136	U2137	U2138	U2139	U2140	U2141	U2142	U2143	U2144	U2145	U2146	U2147	U2148	U2149	U2150	U2151	U2152	U2153	U2154	U2155	U2156	U2157	U2158	U2159	U2160	U2161	U2162	U2163	U2164	U2165	U2166	U2167	U2168	U2169	U2170	U2171	U2172	U2173	U2174	U2175	U2176	U2177	U2178	U2179	U2180	U2181	U2182	U2183	U2184	U2185	U2186	U2187	U2188	U2189	U2190	U2191	U2192	U2193	U2194	U2195	U2196	U2197	U2198	U2199	U2200	U2201	U2202	U2203	U2204	U2205	U2206	U2207	U2208	U2209	U2210	U2211	U2212	U2213	U2214	U2215	U2216	U2217	U2218	U2219	U2220	U2221	U2222	U2223	U2224	U2225	U2226	U2227	U2228	U2229	U2230	U2231	U2232	U2233	U2234	U2235	U2236	U2237	U2238	U2239	U2240	U2241	U2242	U2243	U2244	U2245	U2246	U2247	U2248	U2249	U2250	U2251	U2252	U2253	U2254	U2255	U2256	U2257	U2258	U2259	U2260	U2261	U2262	U2263	U2264	U2265	U2266	U2267	U2268	U2269	U2270	U2271	U2272	U2273	U2274	U2275	U2276	U2277	U2278	U2279	U2280	U2281	U2282	U2283	U2284	U2285	U2286	U2287	U2288	U2289	U2290	U2291	U2292	U2293	U2294	U2295	U2296	U2297	U2298	U2299	U2300	U2301	U2302	U2303	U2304	U2305	U2306	U2307	U2308	U2309	U2310	U2311	U2312	U2313	U2314	U2315	U2316	U2317	U2318	U2319	U2320	U2321	U2322	U2323	U2324	U2325	U2326	U2327	U2328	U2329	U2330	U2331	U2332	U2333	U2334	U2335	U2336	U2337	U2338	U2339	U2340	U2341	U2342	U2343	U2344	U2345	U2346	U2347	U2348	U2349	U2350	U2351	U2352	U2353	U2354	U2355	U2356	U2357	U2358	U2359	U2360	U2361	U2362	U2363	U2364	U2365	U2366	U2367	U2368	U2369	U2370	U2371	U2372	U2373	U2374	U2375	U2376	U2377	U2378	U2379	U2380	U2381	U2382	U2383	U2384	U2385	U2386	U2387	U2388	U2389	U2390	U2391	U2392	U2393	U2394	U2395	U2396	U2397	U2398	U2399	U2400	U2401	U2402	U2403	U2404	U2405	U2406	U2407	U2408	U2409	U2410	U2411	U2412	U2413	U2414	U2415	U2416	U2417	U2418	U2419	U2420	U2421	U2422	U2423	U2424	U2425	U2426	U2427	U2428	U2429	U2430	U2431	U2432	U2433	U2434	U2435	U2436	U2437	U2438	U2439	U2440	U2441	U2442	U2443	U2444	U2445	U2446	U2447	U2448	U2449	U2450	U2451	U2452	U2453	U2454	U2455	U2456	U2457	U2458	U2459	U2460	U2461	U2462	U2463	U2464	U2465	U2466	U2467	U2468	U2469	U2470	U2471	U2472	U2473	U2474	U2475	U2476	U2477	U2478	U2479	U2480	U2481	U2482	U2483	U2484	U2485	U2486	U2487	U2488	U2489	U2490	U2491	U2492	U2493	U2494	U2495	U2496	U2497	U2498	U2499	U2500	U2501	U2502	U2503	U2504	U2505	U2506	U2507	U2508	U2509	U2510	U2511	U2512	U2513	U2514	U2515	U2516	U2517	U2518	U2519	U2520	U2521	U2522	U2523	U2524	U2525	U2526	U2527	U2528	U2529	U2530	U2531	U2532	U2533	U2534	U2535	U2536	U2537	U2538	U2539	U2540	U2541	U2542	U2543	U2544	U2545	U2546	U2547	U2548	U2549	U2550	U2551	U2552	U2553	U2554	U2555	U2556	U2557	U2558	U2559	U2560	U2561	U2562	U2563	U2564	U2565	U2566	U2567	U2568	U2569	U2570	U2571	U2572	U2573	U2574	U2575	U2576	U2577	U2578	U2579	U2580	U2581	U2582	U2583	U2584	U2585	U2586	U2587	U2588	U2589	U2590	U2591	U2592	U2593	U2594	U2595	U2596	U2597	U2598	U2599	U2600	U2601	U2602	U2603	U2604	U2605	U2606	U2607	U2608	U2609	U2610	U2611	U2612	U2613	U2614	U2615	U2616	U2617	U2618	U2619	U2620	U2621	U2622	U2623	U2624	U2625	U2626	U2627	U2628	U2629	U2630	U2631	U2632	U2633	U2634	U2635	U2636	U2637	U2638	U2639	U2640	U2641	U2642	U2643	U2644	U2645	U2646	U2647	U2648	U2649	U2650	U2651	U2652	U2653	U2654	U2655	U2656	U2657	U2658	U2659	U2660	U2661	U2662	U2663	U2664	U2665	U2666	U2667	U2668	U2669	U2670	U2671	U2672	U2673	U2674	U2675	U2676	U2677	U2678	U2679	U2680	U2681	U2682	U2683	U2684	U2685	U2686	U2687	U2688	U2689	U2690	U2691	U2692	U2693	U2694	U2695	U2696	U2697	U2698	U2699	U2700	U2701	U2702	U2703	U2704	U2705	U2706	U2707	U2708	U2709	U2710	U2711	U2712	U2713	U2714	U2715	U2716	U2717	U2718	U2719	U2720	U2721	U2722	U2723	U2724	U2725	U2726	U2727	U2728	U2729	U2730	U2731	U2732	U2733	U2734	U2735	U2736	U2737	U2738	U2739	U2740	U2741	U2742	U2743	U2744	U2745	U2746	U2747	U2748	U2749	U2750	U2751	U2752	U2753	U2754	U2755	U2756	U2757	U2758	U2759	U2760	U2761	U2762	U2763	U2764	U2765	U2766	U2767	U2768	U2769	U2770	U2771	U2772	U2773	U2774	U2775	U2776	U2777	U2778	U2779	





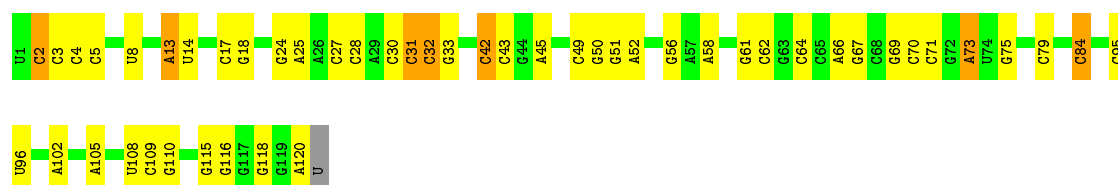
- Molecule 2: 5S Ribosomal RNA

Chain 1B: 75% 21% ..



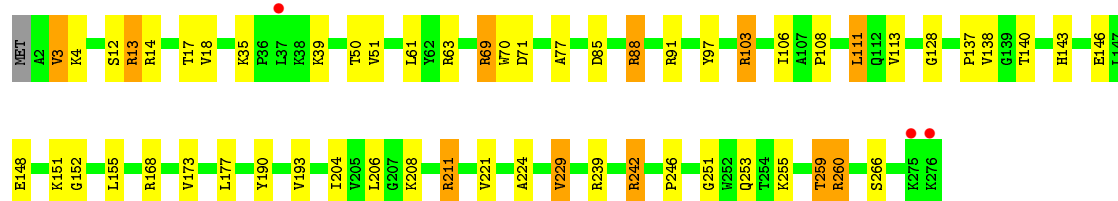
- Molecule 2: 5S Ribosomal RNA

Chain 2B: 59% 35% 6% .



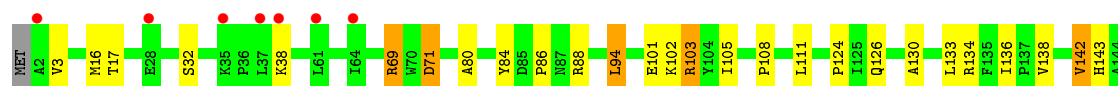
- Molecule 3: 50S ribosomal protein L2

Chain 1D: 79% 17% .

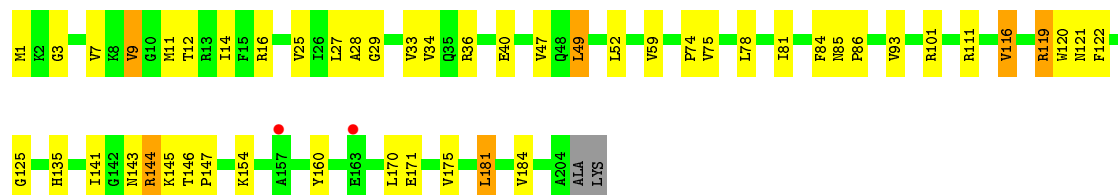
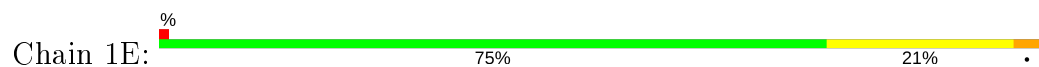


- Molecule 3: 50S ribosomal protein L2

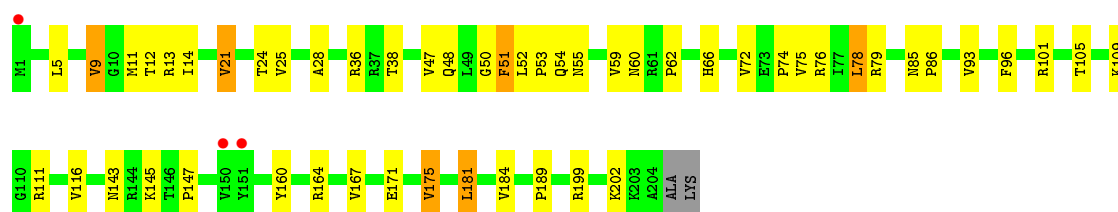
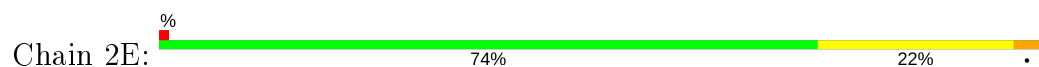
Chain 2D: 5% 82% 15% .



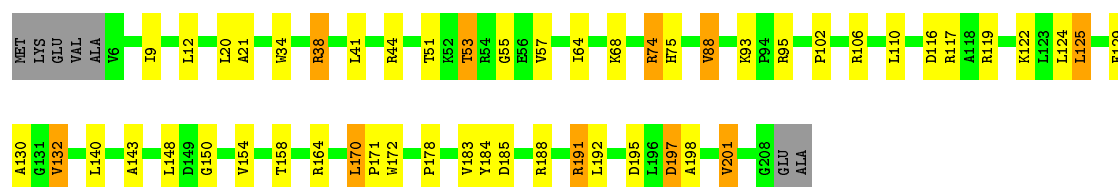
• Molecule 4: 50S ribosomal protein L3



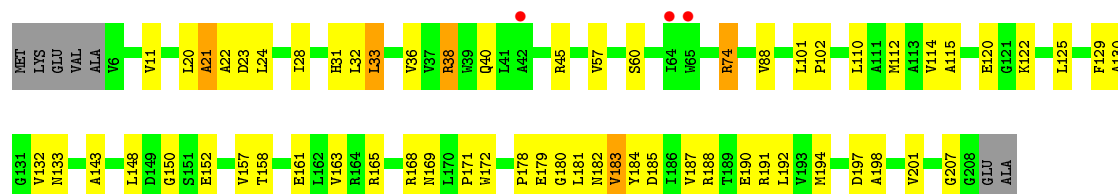
• Molecule 4: 50S ribosomal protein L3



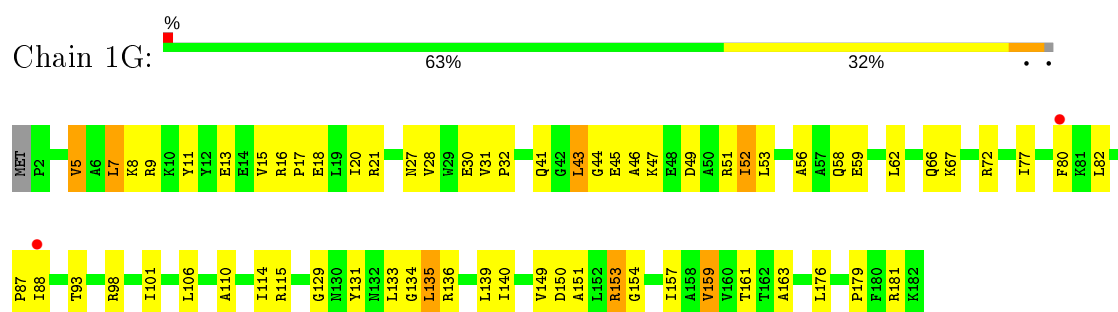
• Molecule 5: 50S ribosomal protein L4



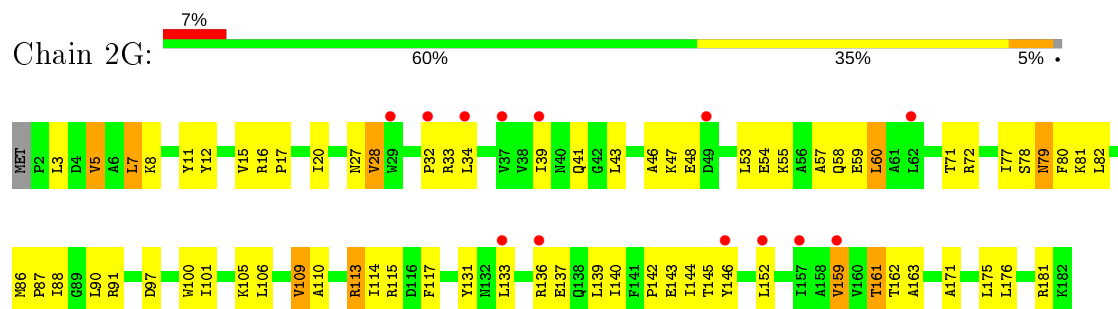
• Molecule 5: 50S ribosomal protein L4



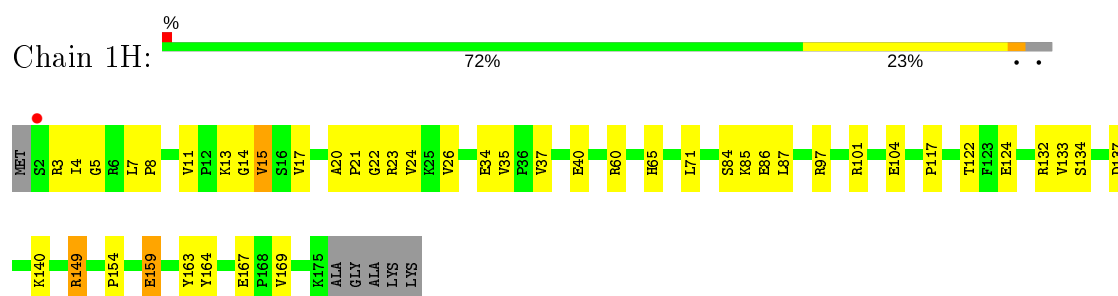
• Molecule 6: 50S ribosomal protein L5



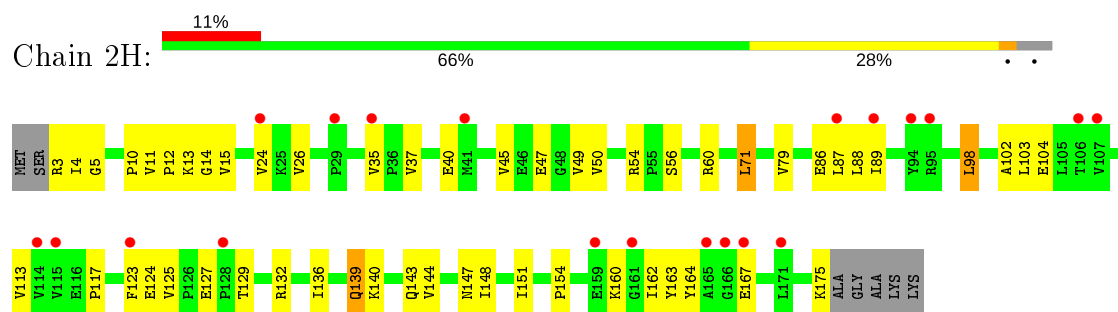
• Molecule 6: 50S ribosomal protein L5



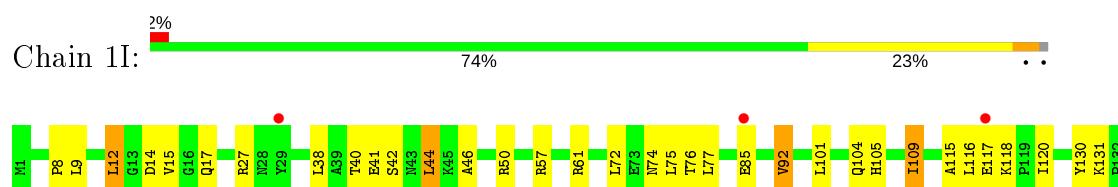
• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6

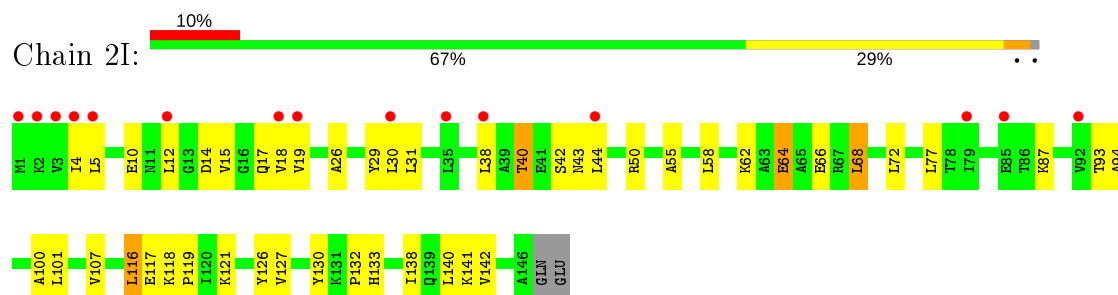


• Molecule 8: 50S ribosomal protein L9

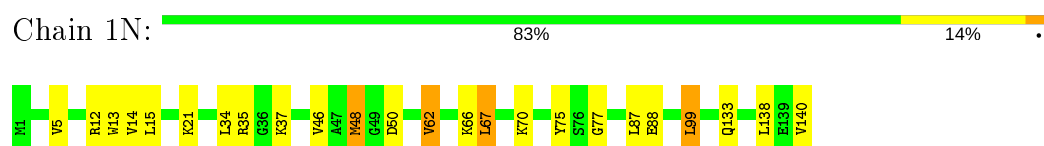




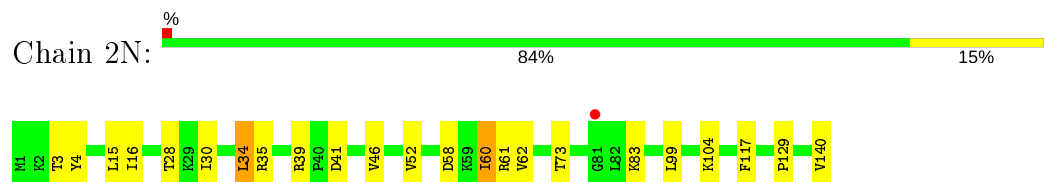
- Molecule 8: 50S ribosomal protein L9



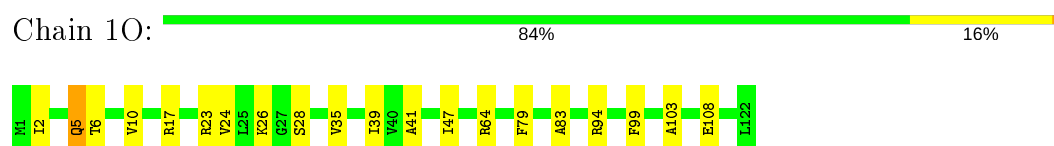
- Molecule 9: 50S ribosomal protein L13



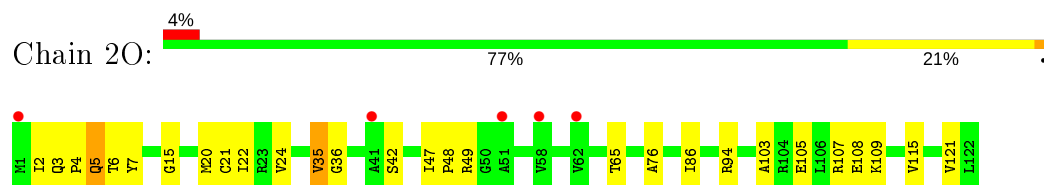
- Molecule 9: 50S ribosomal protein L13



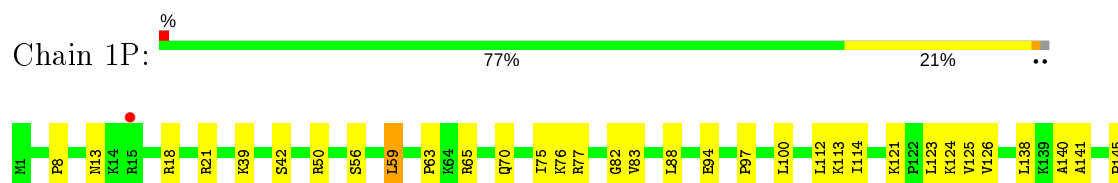
- Molecule 10: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L14

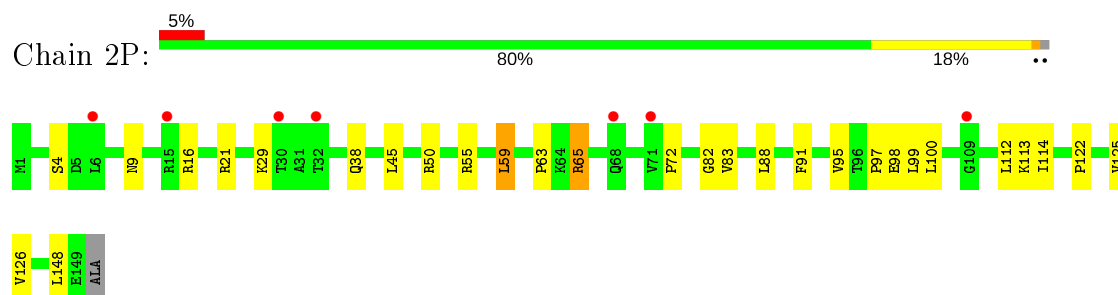


- Molecule 11: 50S ribosomal protein L15

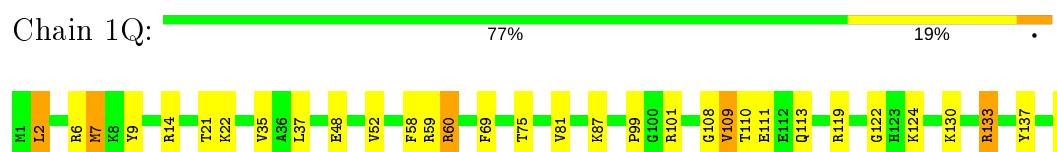




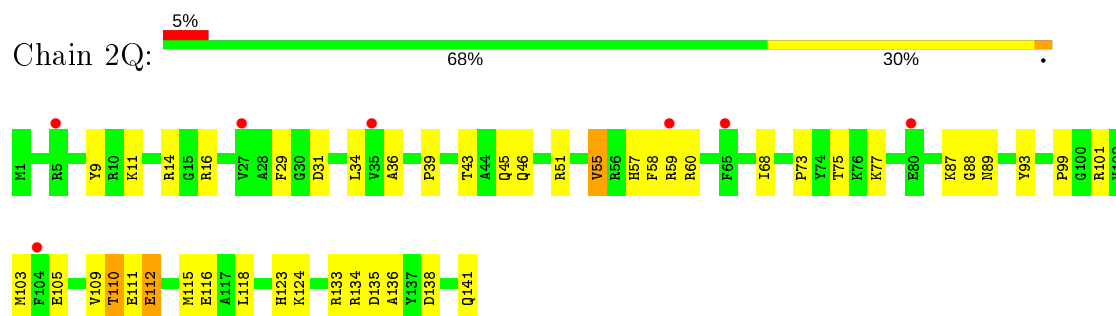
- Molecule 11: 50S ribosomal protein L15



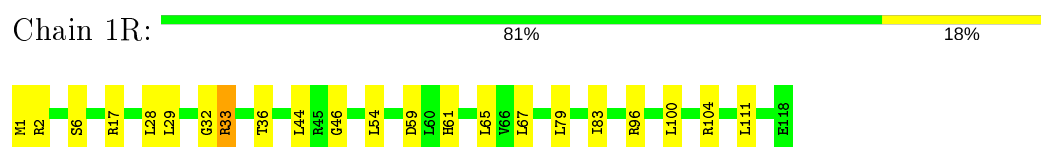
- Molecule 12: 50S ribosomal protein L16



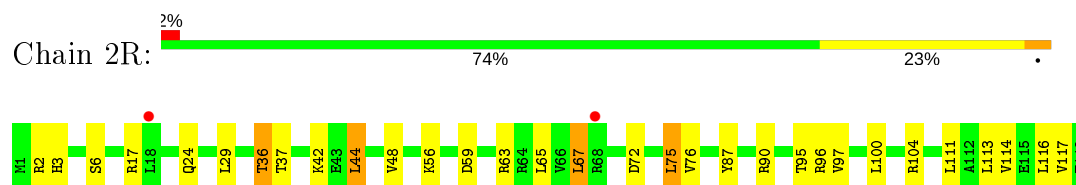
- Molecule 12: 50S ribosomal protein L16



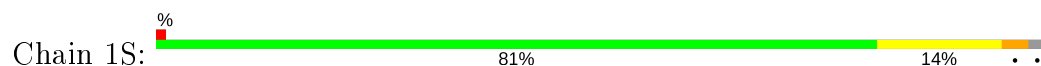
- Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17

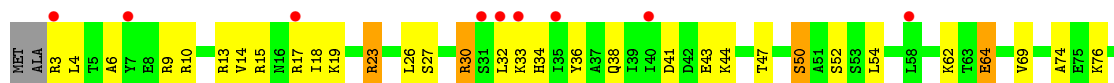


- Molecule 14: 50S ribosomal protein L18

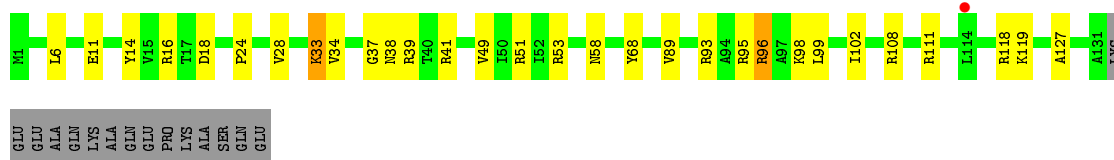




- Molecule 14: 50S ribosomal protein L18



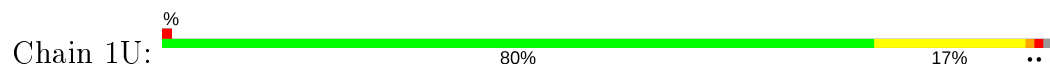
- Molecule 15: 50S ribosomal protein L19



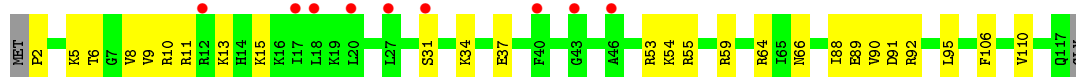
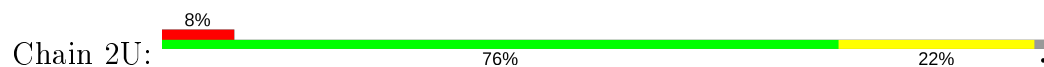
- Molecule 15: 50S ribosomal protein L19




- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20




- Molecule 17: 50S ribosomal protein L21

Chain 1V:  74% 24%




- Molecule 17: 50S ribosomal protein L21

Chain 2V:  3% 72% 25%




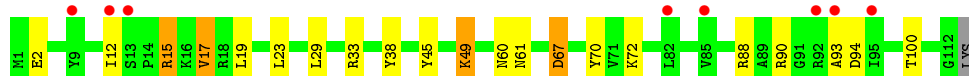
- Molecule 18: 50S ribosomal protein L22

Chain 1W:  83% 13%




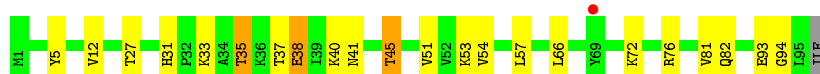
- Molecule 18: 50S ribosomal protein L22

Chain 2W:  7% 81% 15%




- Molecule 19: 50S ribosomal protein L23

Chain 1X:  76% 20%



- Molecule 19: 50S ribosomal protein L23

Chain 2X:  5% 79% 18%

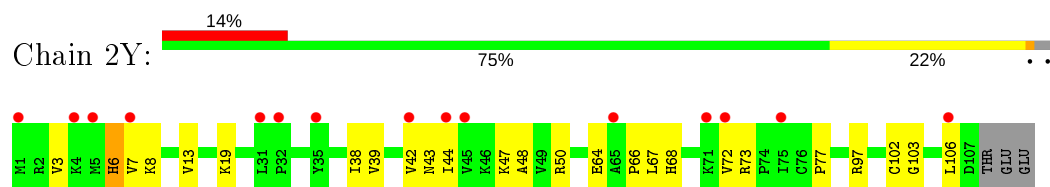


- Molecule 20: 50S ribosomal protein L24

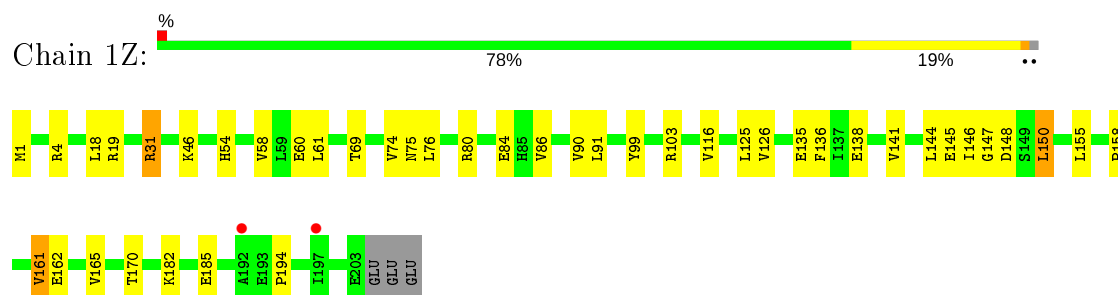
Chain 1Y:  72% 23%



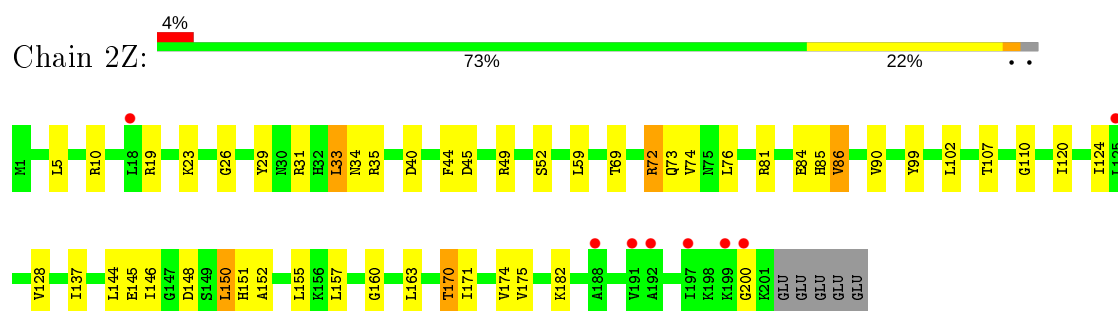
- Molecule 20: 50S ribosomal protein L24



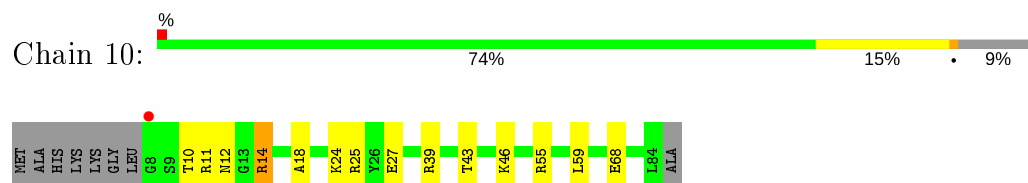
- Molecule 21: 50S ribosomal protein L25



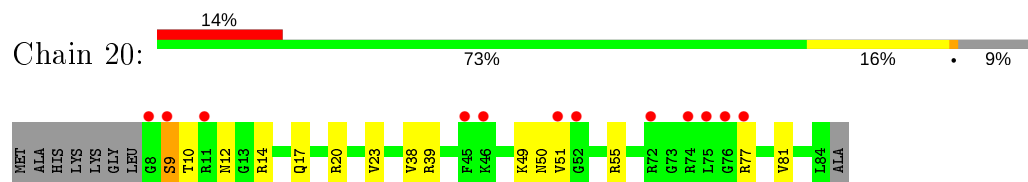
- Molecule 21: 50S ribosomal protein L25



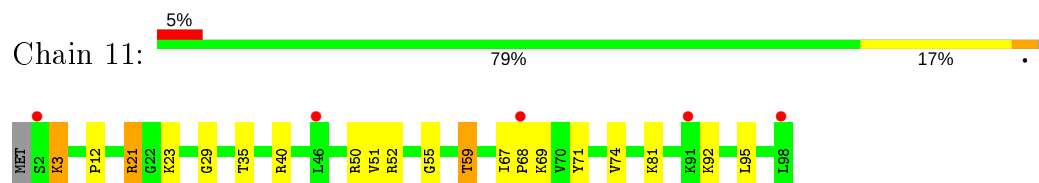
- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27

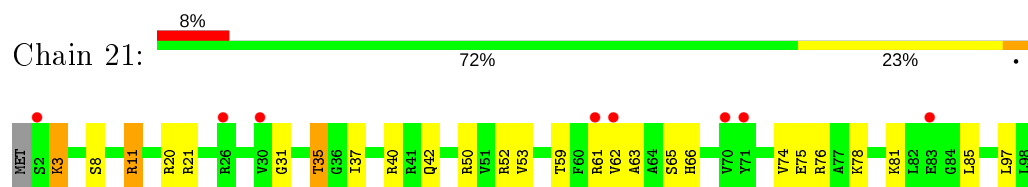


- Molecule 23: 50S ribosomal protein L28

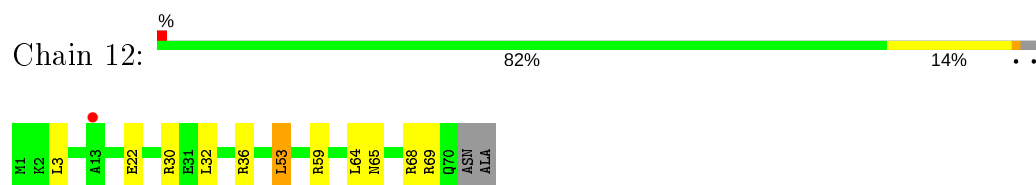




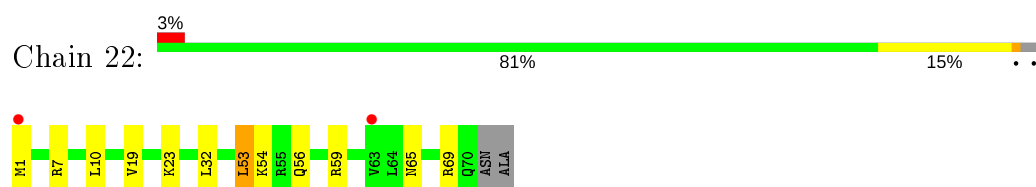
- Molecule 23: 50S ribosomal protein L28



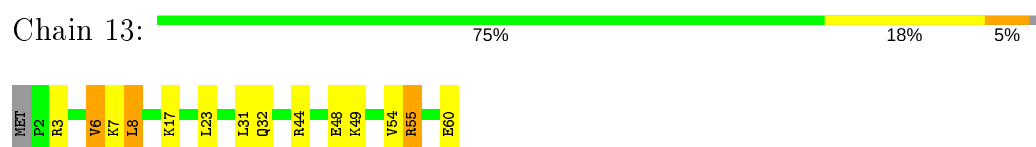
- Molecule 24: 50S ribosomal protein L29



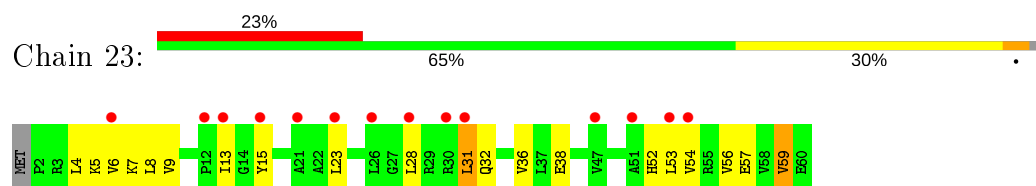
- Molecule 24: 50S ribosomal protein L29



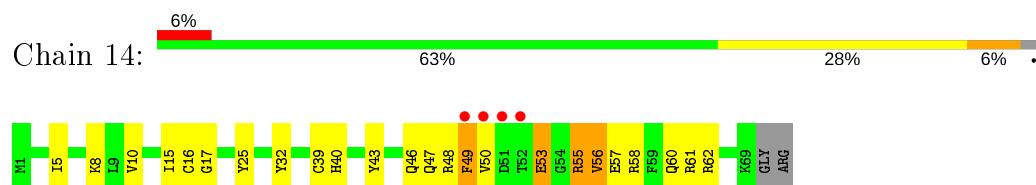
- Molecule 25: 50S ribosomal protein L30



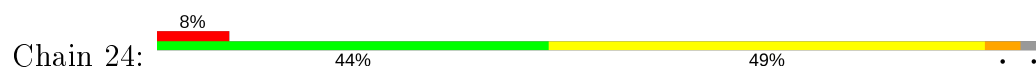
- Molecule 25: 50S ribosomal protein L30

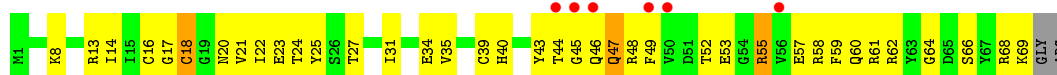


- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31

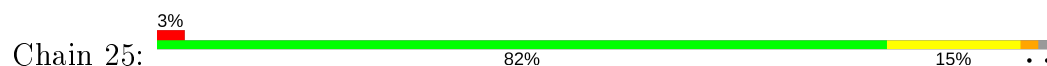




- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



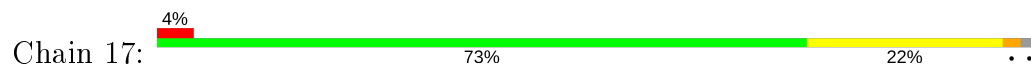
- Molecule 28: 50S ribosomal protein L33



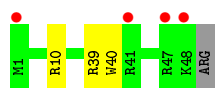
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34

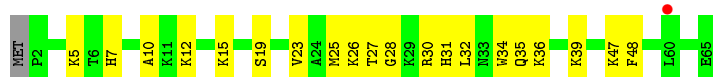


- Molecule 29: 50S ribosomal protein L34

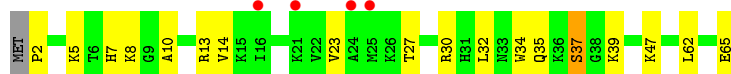


- Molecule 30: 50S ribosomal protein L35





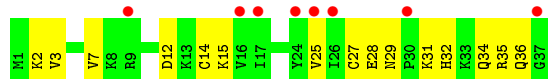
- Molecule 30: 50S ribosomal protein L35



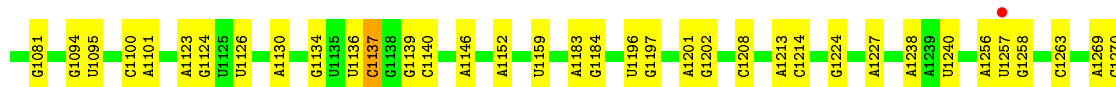
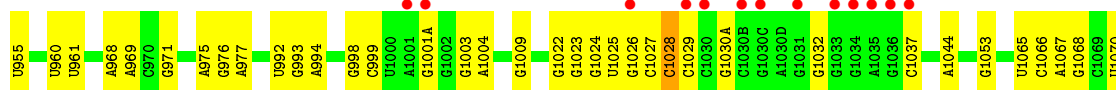
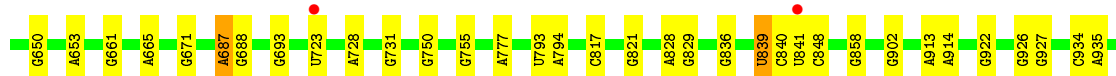
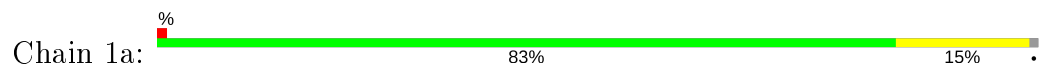
- Molecule 31: 50S ribosomal protein L36

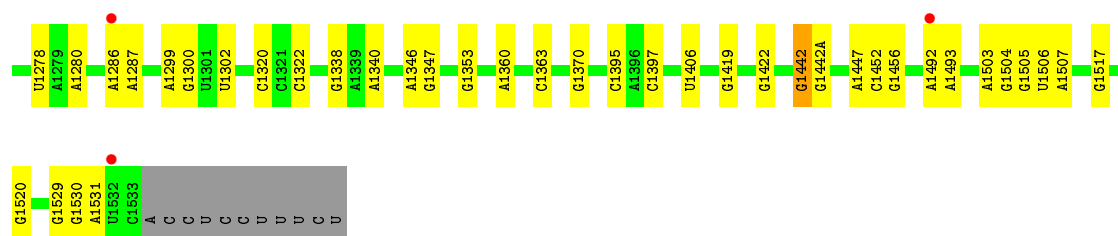


- Molecule 31: 50S ribosomal protein L36

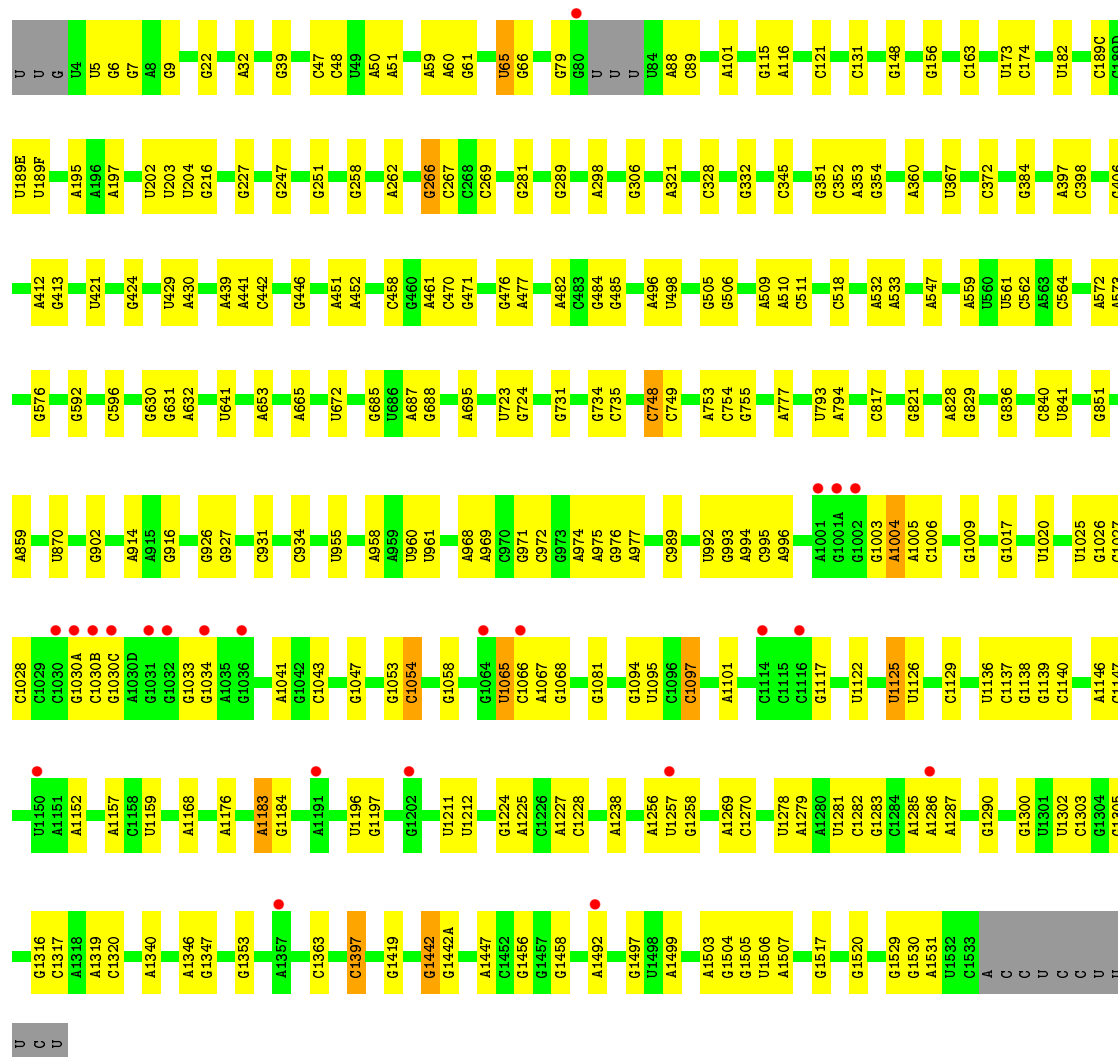
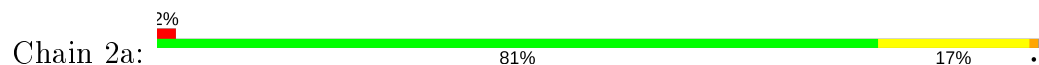


- Molecule 32: 16S Ribosomal RNA

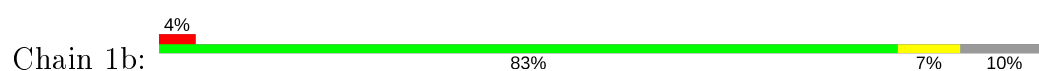




• Molecule 32: 16S Ribosomal RNA




• Molecule 33: 30S ribosomal protein S2



THR  
PRO  
GLU  
GLY  
GLU  
SER  
GLU  
VAL  
GLU  
ALA


- Molecule 33: 30S ribosomal protein S2

Chain 2b: 

MET PRO VAL GLU ILE THR V7 K8 E9 V15 H16 F17 R21 K22 R23 K27 L44 M48 F57 L69 F70 M83 Q96 R96 W97 M101 L118 E119 A120 L121 F122 A123 S124 P125 E126 I127 I128 E129 R130 P131 K132 K133 V136 R144 F152

I162 F163 V164 V165 A177 L187 A188 D189 T190 R209 I214 L215 I223 K226 G227 G228 P232 S233 A237 LEU VAL GLN GLU ALA ALA THR THR PRO GLU GLY SER VAL GLU ALA


- Molecule 34: 30S ribosomal protein S3

Chain 1c: 

MET G2 N3 I8 G9 F10 I39 L47 G80 I91 E105 V106 Q107 S112 K150 A168 I182 Y193 Y201 E206 V207 ILE GLY GLN LYS PRO LYS ALA ARG PRO GLU ALA GLU ARG PRO ARG ARG ARG VAL LYS GLU

ARG VAL LYS LYS GLU

- Molecule 34: 30S ribosomal protein S3

Chain 2c: 

MET G2 N3 K4 Y4 I5 H6 P7 I8 F10 T15 R21 Y22 Y23 L33 I39 I57 I57 A60 A65 V68 L67 V99 N108 I124 A149 I152 V153 S154 G155 R156 A160 E161 Q162 A163 E166 W167 T177 L178 Y184 G185 F186

R190 V195 L196 Y201 V207 ILE GLY GLN LYS PRO LYS ALA ARG PRO GLU LEU ARG ARG ARG ARG PRO ALA VAL VAL LYS GLU GLU

- Molecule 35: 30S ribosomal protein S4

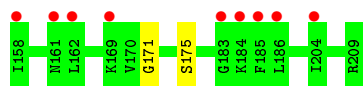
Chain 1d: 

MET G2 R3 Y4 I5 L11 L19 S28 R49 R50 L58 R59 Q62 K63 L64 I70 R73 Q74 F75 R115 G124 T127 L135 Y138 L157 L166 Q167 E179 L188 L194 V203 Y207 S208 R209

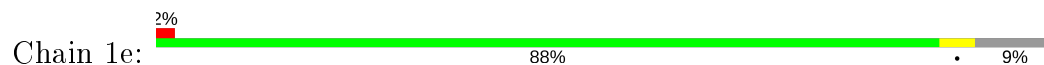
- Molecule 35: 30S ribosomal protein S4

Chain 2d: 

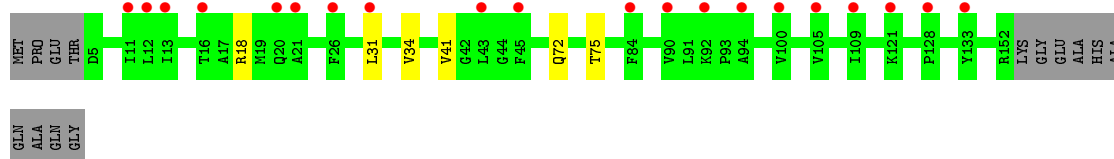
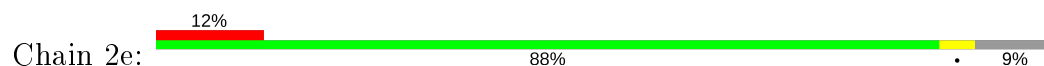
MET G2 R3 Y4 I5 V8 L11 Y20 L21 K33 E34 R35 R36 P39 Q46 R49 I67 Y68 G69 I70 R73 S83 L96 L101 V104 V105 F110 R115 R118 Q119 L120 V121 R122 L135 E145 I146 A149 S152 L157



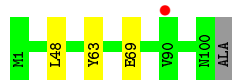
- Molecule 36: 30S ribosomal protein S5



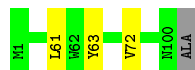
- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6



- Molecule 37: 30S ribosomal protein S6



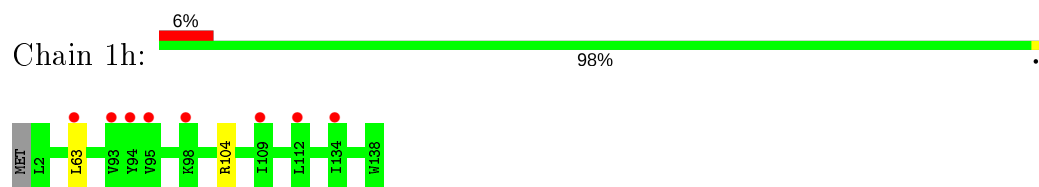
- Molecule 38: 30S ribosomal protein S7



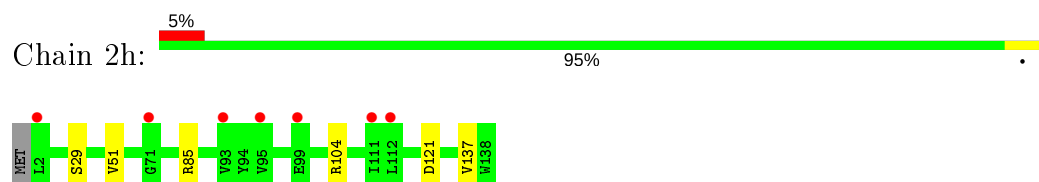
- Molecule 38: 30S ribosomal protein S7



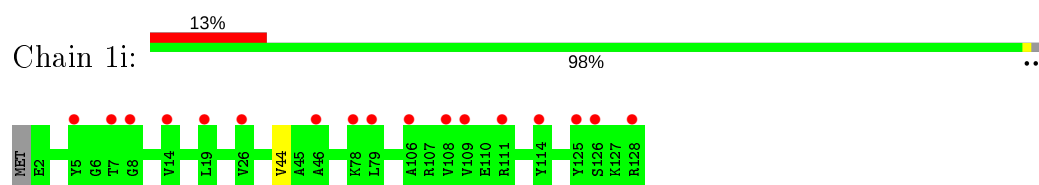
- Molecule 39: 30S ribosomal protein S8



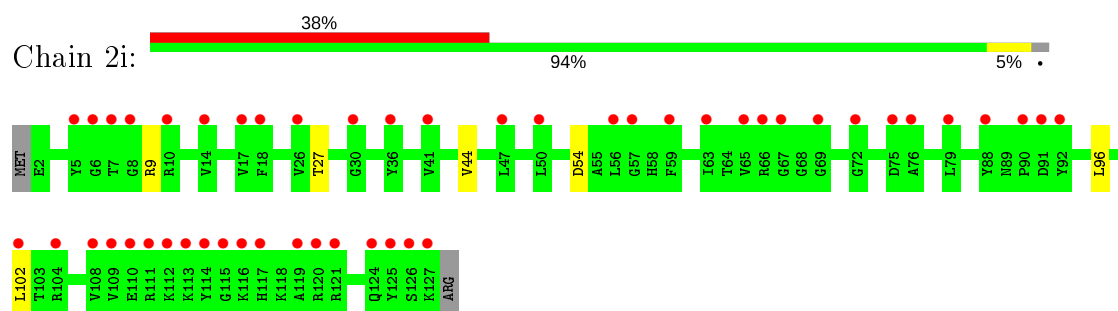
- Molecule 39: 30S ribosomal protein S8



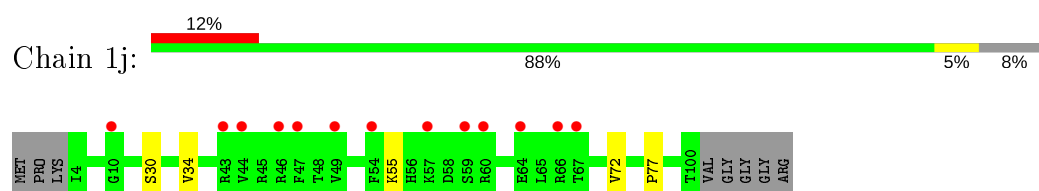
- Molecule 40: 30S ribosomal protein S9



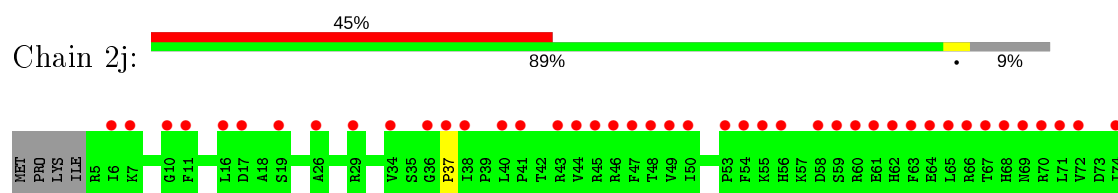
- Molecule 40: 30S ribosomal protein S9

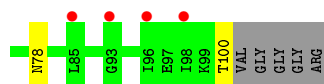


- Molecule 41: 30S ribosomal protein S10



- Molecule 41: 30S ribosomal protein S10

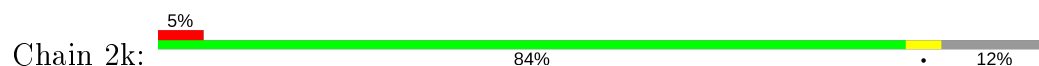




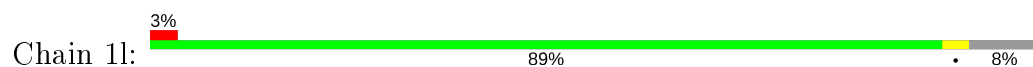
- Molecule 42: 30S ribosomal protein S11



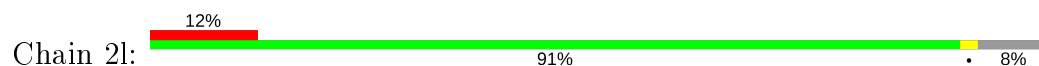
- Molecule 42: 30S ribosomal protein S11



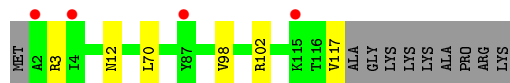
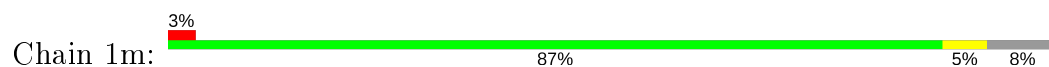
- Molecule 43: 30S ribosomal protein S12



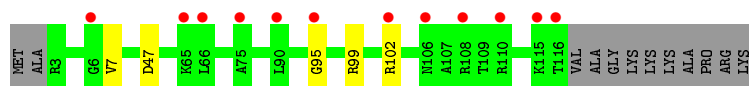
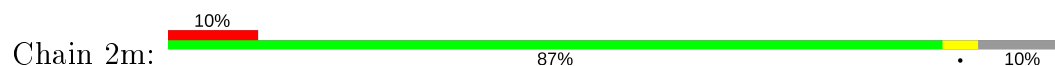
- Molecule 43: 30S ribosomal protein S12



- Molecule 44: 30S ribosomal protein S13

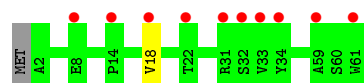


- Molecule 44: 30S ribosomal protein S13

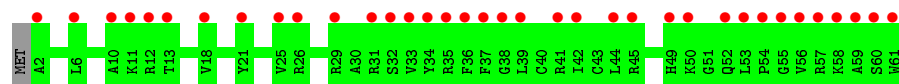


- Molecule 45: 30S ribosomal protein S14 type Z





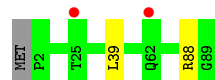
- Molecule 45: 30S ribosomal protein S14 type Z



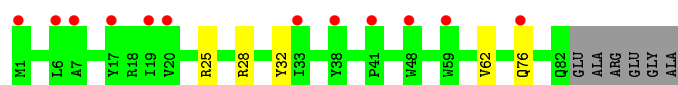
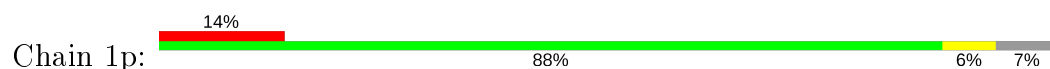
- Molecule 46: 30S ribosomal protein S15



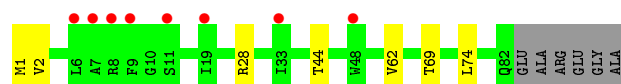
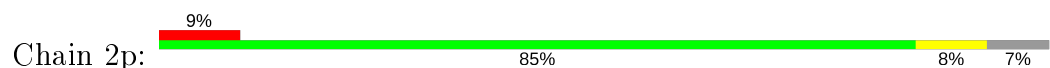
- Molecule 46: 30S ribosomal protein S15



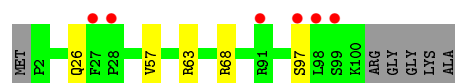
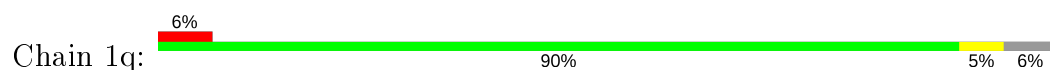
- Molecule 47: 30S ribosomal protein S16



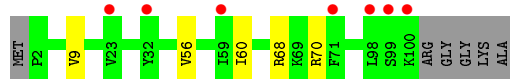
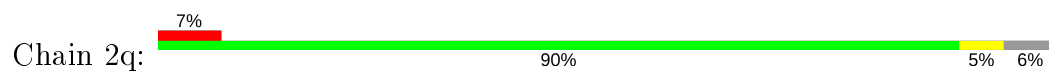
- Molecule 47: 30S ribosomal protein S16



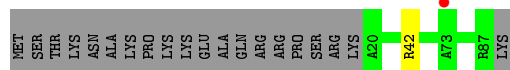
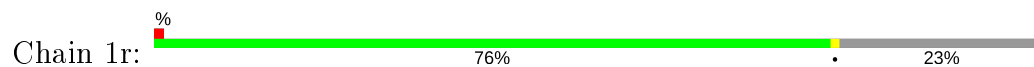
- Molecule 48: 30S ribosomal protein S17



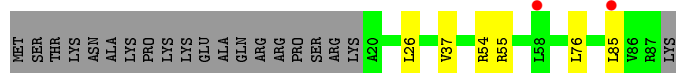
- Molecule 48: 30S ribosomal protein S17



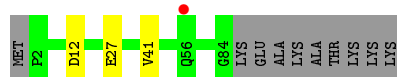
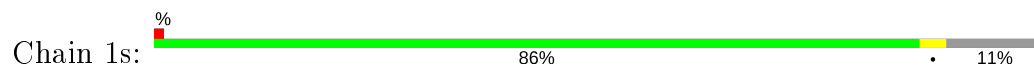
- Molecule 49: 30S ribosomal protein S18



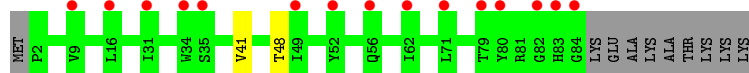
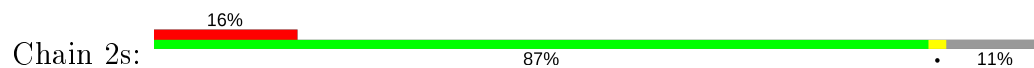
- Molecule 49: 30S ribosomal protein S18



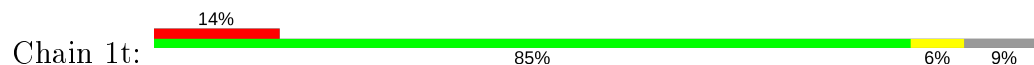
- Molecule 50: 30S ribosomal protein S19



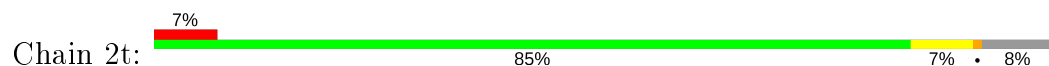
- Molecule 50: 30S ribosomal protein S19

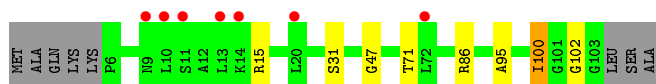


- Molecule 51: 30S ribosomal protein S20

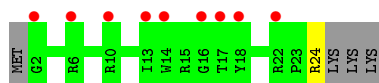
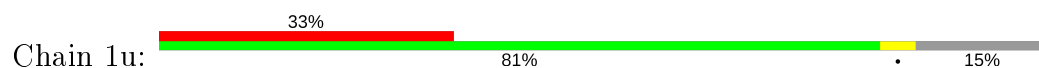


- Molecule 51: 30S ribosomal protein S20

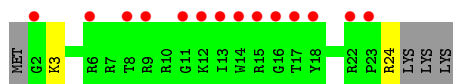
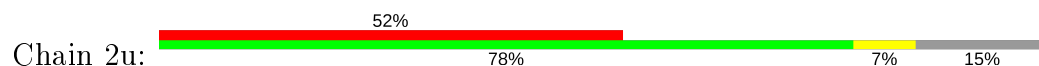




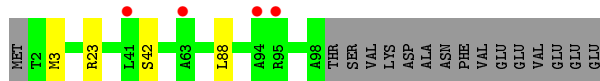
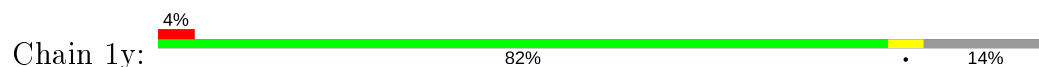
- Molecule 52: 30S ribosomal protein Thx



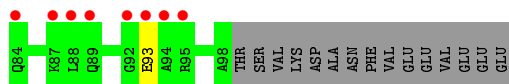
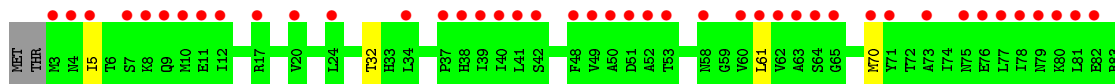
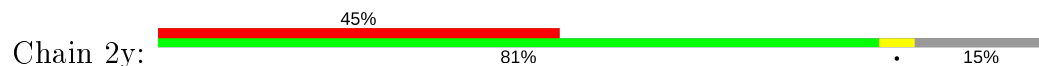
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: Ribosome-associated inhibitor A



- Molecule 53: Ribosome-associated inhibitor A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.09Å 449.12Å 621.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.92 – 2.70 364.10 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (121.92-2.70) 99.2 (364.10-2.70)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, $R_{free}$	0.206 , 0.253 0.207 , 0.253	Depositor DCC
$R_{free}$ test set	79057 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.6	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 53.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	295438	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, MPD, OMG, MA6, ZN, SF4, 0TD, EZP, MG, 2MA, 2MU, 2MG, 5MC, UR3, 4OC, M2G, 7MG, K, PSU

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	0.51	0/69029	0.96	51/107746 (0.0%)
1	2A	0.41	0/68901	0.90	41/107544 (0.0%)
2	1B	0.43	0/2876	0.90	1/4486 (0.0%)
2	2B	0.37	0/2878	0.87	0/4490
3	1D	0.37	0/2181	0.59	0/2940
3	2D	0.33	0/2186	0.55	0/2944
4	1E	0.37	0/1592	0.55	0/2149
4	2E	0.31	0/1592	0.53	0/2149
5	1F	0.34	0/1619	0.53	0/2193
5	2F	0.31	0/1615	0.52	0/2188
6	1G	0.30	0/1451	0.50	0/1961
6	2G	0.30	0/1449	0.47	0/1957
7	1H	0.33	0/1356	0.51	0/1834
7	2H	0.29	0/1350	0.47	0/1826
8	1I	0.30	0/1109	0.52	0/1512
8	2I	0.28	0/1091	0.49	0/1490
9	1N	0.36	0/1148	0.55	0/1547
9	2N	0.29	0/1144	0.48	0/1543
10	1O	0.36	0/943	0.56	0/1269
10	2O	0.33	0/943	0.54	0/1269
11	1P	0.34	0/1152	0.57	0/1533
11	2P	0.32	0/1152	0.54	0/1533
12	1Q	0.35	0/1143	0.52	0/1527
12	2Q	0.30	0/1143	0.49	0/1527
13	1R	0.34	0/982	0.58	0/1312
13	2R	0.31	0/982	0.55	1/1312 (0.1%)
14	1S	0.31	0/887	0.52	0/1180
14	2S	0.30	0/880	0.50	0/1172
15	1T	0.33	0/1105	0.54	0/1477
15	2T	0.30	0/1097	0.51	0/1468
16	1U	0.36	0/977	0.53	1/1301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.30	0/977	0.45	0/1301
17	1V	0.34	0/786	0.54	0/1053
17	2V	0.32	0/782	0.52	0/1049
18	1W	0.33	0/897	0.51	0/1205
18	2W	0.32	0/897	0.50	0/1205
19	1X	0.38	0/764	0.56	0/1025
19	2X	0.31	0/764	0.55	1/1025 (0.1%)
20	1Y	0.37	0/823	0.54	0/1099
20	2Y	0.33	0/823	0.51	0/1100
21	1Z	0.30	0/1620	0.52	0/2200
21	2Z	0.30	0/1590	0.49	0/2162
22	10	0.35	0/616	0.56	0/821
22	20	0.33	0/616	0.50	0/821
23	11	0.33	0/761	0.51	0/1013
23	21	0.32	0/766	0.50	0/1018
24	12	0.30	0/590	0.51	0/781
24	22	0.30	0/594	0.44	0/785
25	13	0.33	0/474	0.52	0/635
25	23	0.30	0/469	0.49	0/630
26	14	0.32	0/559	0.54	0/754
26	24	0.35	0/549	0.54	0/741
27	15	0.40	0/473	0.65	2/639 (0.3%)
27	25	0.33	0/469	0.53	0/635
28	16	0.33	0/460	0.56	0/613
28	26	0.32	0/456	0.49	0/608
29	17	0.38	0/426	0.58	0/561
29	27	0.31	0/426	0.50	0/561
30	18	0.36	0/525	0.56	0/691
30	28	0.31	0/525	0.52	0/691
31	19	0.37	0/310	0.53	0/407
31	29	0.31	0/310	0.52	0/407
32	1a	0.37	0/35795	0.88	18/55864 (0.0%)
32	2a	0.37	0/35890	0.89	32/56012 (0.1%)
33	1b	0.30	0/1876	0.50	0/2533
33	2b	0.33	0/1860	0.52	1/2518 (0.0%)
34	1c	0.29	0/1582	0.47	0/2137
34	2c	0.30	0/1566	0.48	0/2119
35	1d	0.30	0/1695	0.49	0/2274
35	2d	0.29	0/1698	0.46	0/2277
36	1e	0.31	0/1149	0.52	0/1548
36	2e	0.30	0/1149	0.51	0/1548
37	1f	0.32	0/827	0.51	0/1120
37	2f	0.29	0/829	0.50	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.29	0/1254	0.44	0/1683
38	2g	0.29	0/1248	0.43	0/1676
39	1h	0.28	0/1118	0.48	0/1506
39	2h	0.28	0/1108	0.47	0/1494
40	1i	0.28	0/1005	0.50	0/1351
40	2i	0.30	0/985	0.47	0/1329
41	1j	0.30	0/732	0.49	0/993
41	2j	0.28	0/723	0.48	0/984
42	1k	0.30	0/849	0.48	0/1150
42	2k	0.30	0/848	0.54	0/1149
43	1l	0.30	0/937	0.51	0/1260
43	2l	0.29	0/937	0.53	0/1260
44	1m	0.28	0/924	0.46	0/1242
44	2m	0.30	0/905	0.49	0/1217
45	1n	0.31	0/501	0.46	0/664
45	2n	0.31	0/501	0.47	0/664
46	1o	0.28	0/739	0.48	0/985
46	2o	0.28	0/739	0.46	0/985
47	1p	0.30	0/697	0.53	0/939
47	2p	0.29	0/693	0.49	0/935
48	1q	0.30	0/836	0.51	0/1117
48	2q	0.29	0/836	0.49	0/1117
49	1r	0.28	0/560	0.48	0/746
49	2r	0.28	0/560	0.47	0/746
50	1s	0.27	0/663	0.50	0/895
50	2s	0.28	0/660	0.49	0/893
51	1t	0.27	0/734	0.45	0/969
51	2t	0.27	0/736	0.41	0/976
52	1u	0.25	0/203	0.48	0/266
52	2u	0.32	0/203	0.51	0/266
53	1y	0.29	0/776	0.47	0/1048
53	2y	0.27	0/761	0.45	0/1030
All	All	0.40	0/309937	0.82	149/463223 (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
19	1X	0	1
26	24	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
33	1b	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1003	G	N3-C4-C5	-8.97	124.12	128.60
32	2a	1003	G	C8-N9-C4	-8.85	102.86	106.40
1	1A	537	G	O4'-C1'-N9	8.36	114.89	108.20
1	1A	354	A	C2-N3-C4	-8.34	106.43	110.60
32	1a	1028	C	C2-N3-C4	7.73	123.77	119.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	1X	93	GLU	Peptide
33	1b	127	ILE	Peptide
33	1b	231	GLU	Peptide
26	24	18	CYS	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61869	0	31201	614	0
1	2A	61758	0	31149	755	0
2	1B	2572	0	1305	16	0
2	2B	2573	0	1306	34	0
3	1D	2131	0	2207	49	0
3	2D	2136	0	2218	34	0
4	1E	1559	0	1618	33	0
4	2E	1559	0	1618	39	0
5	1F	1584	0	1625	32	0
5	2F	1580	0	1619	42	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	1G	1426	0	1445	42	0
6	2G	1424	0	1441	50	0
7	1H	1330	0	1407	26	0
7	2H	1324	0	1402	39	0
8	1I	1094	0	1127	32	0
8	2I	1076	0	1094	29	0
9	1N	1121	0	1195	18	0
9	2N	1117	0	1184	14	0
10	1O	933	0	996	12	0
10	2O	933	0	996	18	0
11	1P	1135	0	1212	29	0
11	2P	1135	0	1212	21	0
12	1Q	1122	0	1179	24	0
12	2Q	1122	0	1179	27	0
13	1R	968	0	1033	12	0
13	2R	968	0	1033	18	0
14	1S	877	0	938	18	0
14	2S	870	0	923	37	0
15	1T	1091	0	1151	23	0
15	2T	1083	0	1136	25	0
16	1U	959	0	1019	16	0
16	2U	959	0	1019	22	0
17	1V	775	0	841	13	0
17	2V	771	0	830	21	0
18	1W	886	0	940	10	0
18	2W	886	0	940	13	0
19	1X	750	0	814	14	0
19	2X	750	0	814	9	0
20	1Y	810	0	892	21	0
20	2Y	810	0	887	20	0
21	1Z	1587	0	1598	23	0
21	2Z	1557	0	1564	36	0
22	10	608	0	622	10	0
22	20	608	0	622	12	0
23	11	754	0	823	14	0
23	21	759	0	837	20	0
24	12	588	0	643	10	0
24	22	592	0	654	8	0
25	13	469	0	518	11	0
25	23	464	0	514	16	0
26	14	546	0	522	15	0
26	24	536	0	514	29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	15	459	0	476	11	0
27	25	455	0	465	9	0
28	16	453	0	473	11	0
28	26	449	0	469	10	0
29	17	418	0	467	10	0
29	27	418	0	467	3	0
30	18	517	0	582	16	0
30	28	517	0	582	12	0
31	19	307	0	335	9	0
31	29	307	0	335	10	0
32	1a	32246	0	16296	0	0
32	2a	32331	0	16339	0	0
33	1b	1842	0	1862	0	0
33	2b	1825	0	1828	0	0
34	1c	1558	0	1557	0	0
34	2c	1542	0	1517	0	0
35	1d	1665	0	1687	0	0
35	2d	1668	0	1703	0	0
36	1e	1133	0	1191	0	0
36	2e	1133	0	1191	0	0
37	1f	814	0	808	0	0
37	2f	816	0	808	0	0
38	1g	1235	0	1249	0	0
38	2g	1229	0	1238	0	0
39	1h	1098	0	1143	0	0
39	2h	1088	0	1126	0	0
40	1i	986	0	990	0	0
40	2i	966	0	953	0	0
41	1j	719	0	672	0	0
41	2j	710	0	661	0	0
42	1k	834	0	838	0	0
42	2k	833	0	836	0	0
43	1l	932	0	981	0	0
43	2l	932	0	981	0	0
44	1m	914	0	954	0	0
44	2m	895	0	920	0	0
45	1n	492	0	529	0	0
45	2n	492	0	529	0	0
46	1o	728	0	760	0	0
46	2o	728	0	760	0	0
47	1p	681	0	697	0	0
47	2p	677	0	686	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	1q	823	0	891	0	0
48	2q	823	0	891	0	0
49	1r	555	0	618	0	0
49	2r	555	0	618	0	0
50	1s	648	0	658	0	0
50	2s	645	0	635	0	0
51	1t	732	0	809	0	0
51	2t	733	0	795	0	0
52	1u	199	0	208	0	0
52	2u	199	0	208	0	0
53	1y	764	0	786	0	0
53	2y	749	0	757	0	0
54	10	6	0	0	0	0
54	11	3	0	0	0	0
54	13	2	0	0	0	0
54	14	1	0	0	0	0
54	15	3	0	0	0	0
54	17	2	0	0	0	0
54	18	1	0	0	0	0
54	19	2	0	0	0	0
54	1A	1024	0	0	0	0
54	1B	29	0	0	0	0
54	1D	13	0	0	0	0
54	1E	7	0	0	0	0
54	1F	13	0	0	0	0
54	1G	4	0	0	0	0
54	1H	2	0	0	0	0
54	1N	3	0	0	0	0
54	1O	2	0	0	0	0
54	1P	3	0	0	0	0
54	1Q	4	0	0	0	0
54	1R	3	0	0	0	0
54	1S	1	0	0	0	0
54	1T	3	0	0	0	0
54	1U	2	0	0	0	0
54	1V	3	0	0	0	0
54	1W	2	0	0	0	0
54	1X	2	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	255	0	0	0	0
54	1b	1	0	0	0	0
54	1d	6	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	1e	2	0	0	0	0
54	1f	2	0	0	0	0
54	1g	3	0	0	0	0
54	1h	2	0	0	0	0
54	1i	1	0	0	0	0
54	1l	2	0	0	0	0
54	1n	1	0	0	0	0
54	1o	1	0	0	0	0
54	1t	1	0	0	0	0
54	1y	4	0	0	0	0
54	20	1	0	0	0	0
54	21	1	0	0	0	0
54	25	1	0	0	0	0
54	28	3	0	0	0	0
54	2A	721	0	0	0	0
54	2B	19	0	0	0	0
54	2D	8	0	0	0	0
54	2E	6	0	0	0	0
54	2F	3	0	0	0	0
54	2G	3	0	0	0	0
54	2I	1	0	0	0	0
54	2N	1	0	0	0	0
54	2O	1	0	0	0	0
54	2P	2	0	0	0	0
54	2Q	2	0	0	0	0
54	2R	1	0	0	0	0
54	2T	4	0	0	0	0
54	2V	1	0	0	0	0
54	2W	2	0	0	0	0
54	2X	1	0	0	0	0
54	2a	151	0	0	0	0
54	2e	1	0	0	0	0
54	2f	1	0	0	0	0
54	2j	1	0	0	0	0
54	2p	1	0	0	0	0
54	2q	1	0	0	0	0
54	2r	1	0	0	0	0
54	2t	1	0	0	0	0
55	1A	1	0	0	0	0
55	2A	1	0	0	0	0
56	1A	25	0	0	0	0
56	2A	25	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	18	8	0	14	1	0
57	1A	8	0	14	0	0
57	1T	8	0	14	1	0
57	1a	8	0	14	0	0
57	2A	16	0	28	2	0
57	2B	8	0	14	0	0
58	1B	12	0	12	3	0
58	1F	12	0	12	3	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	0	0
61	10	22	0	0	0	0
61	11	28	0	0	0	0
61	12	14	0	0	2	0
61	13	22	0	0	2	0
61	14	2	0	0	0	0
61	15	26	0	0	0	0
61	16	17	0	0	1	0
61	17	14	0	0	2	0
61	18	30	0	0	0	0
61	19	8	0	0	1	0
61	1A	2980	0	0	97	0
61	1B	105	0	0	3	0
61	1D	116	0	0	6	0
61	1E	76	0	0	4	0
61	1F	63	0	0	5	0
61	1G	22	0	0	0	0
61	1H	16	0	0	0	0
61	1I	7	0	0	1	0
61	1N	50	0	0	0	0
61	1O	22	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1P	58	0	0	4	0
61	1Q	42	0	0	3	0
61	1R	37	0	0	0	0
61	1S	13	0	0	1	0
61	1T	42	0	0	3	0
61	1U	45	0	0	4	0
61	1V	37	0	0	1	0
61	1W	24	0	0	0	0
61	1X	24	0	0	1	0
61	1Y	15	0	0	1	0
61	1Z	14	0	0	0	0
61	1a	261	0	0	0	0
61	1b	1	0	0	0	0
61	1d	9	0	0	0	0
61	1e	6	0	0	0	0
61	1f	3	0	0	0	0
61	1h	1	0	0	0	0
61	1i	1	0	0	0	0
61	1j	1	0	0	0	0
61	1k	1	0	0	0	0
61	1l	4	0	0	0	0
61	1n	1	0	0	0	0
61	1o	5	0	0	0	0
61	1p	3	0	0	0	0
61	1y	5	0	0	0	0
61	20	13	0	0	2	0
61	21	24	0	0	5	0
61	22	5	0	0	0	0
61	23	3	0	0	1	0
61	24	2	0	0	0	0
61	25	9	0	0	1	0
61	26	6	0	0	1	0
61	27	7	0	0	0	0
61	28	15	0	0	1	0
61	29	2	0	0	0	0
61	2A	1686	0	0	84	0
61	2B	65	0	0	6	0
61	2D	52	0	0	2	0
61	2E	25	0	0	2	0
61	2F	21	0	0	3	0
61	2G	7	0	0	0	0
61	2H	4	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2I	4	0	0	0	0
61	2N	6	0	0	0	0
61	2O	22	0	0	0	0
61	2P	23	0	0	0	0
61	2Q	30	0	0	0	0
61	2R	21	0	0	1	0
61	2S	8	0	0	2	0
61	2T	10	0	0	0	0
61	2U	14	0	0	2	0
61	2V	9	0	0	0	0
61	2W	21	0	0	0	0
61	2X	9	0	0	0	0
61	2Y	3	0	0	0	0
61	2Z	15	0	0	3	0
61	2a	100	0	0	0	0
61	2d	6	0	0	0	0
61	2e	1	0	0	0	0
61	2f	1	0	0	0	0
61	2j	2	0	0	0	0
61	2l	1	0	0	0	0
61	2m	1	0	0	0	0
61	2o	2	0	0	0	0
61	2p	1	0	0	0	0
61	2q	1	0	0	0	0
61	2r	4	0	0	0	0
61	2y	1	0	0	0	0
All	All	295438	0	194513	2320	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 2320 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1128:U:H3	1:1A:1132:A:N6	1.36	1.23
1:1A:2159:C:N4	1:1A:2176:G:H1	1.50	1.09
1:2A:2139:C:N4	1:2A:2152:G:H1	1.56	1.01
1:1A:2331:G:H22	14:1S:3:ARG:HD3	1.23	1.01
1:1A:1128:U:O4	1:1A:1132:A:N1	1.99	0.94

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	29	54
4	2E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	29	54
5	1F	201/210 (96%)	191 (95%)	9 (4%)	1 (0%)	29	54
5	2F	201/210 (96%)	191 (95%)	7 (4%)	3 (2%)	10	26
6	1G	179/182 (98%)	163 (91%)	15 (8%)	1 (1%)	25	50
6	2G	179/182 (98%)	166 (93%)	10 (6%)	3 (2%)	9	23
7	1H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	25	50
7	2H	171/180 (95%)	152 (89%)	19 (11%)	0	100	100
8	1I	145/148 (98%)	129 (89%)	15 (10%)	1 (1%)	22	46
8	2I	144/148 (97%)	130 (90%)	12 (8%)	2 (1%)	11	28
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	130 (94%)	7 (5%)	1 (1%)	22	46
10	1O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	19	43
10	2O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	19	43
11	1P	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
11	2P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	22	46
12	1Q	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22	46
12	2Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	22	46
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
14	1S	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	17	40
14	2S	108/112 (96%)	96 (89%)	12 (11%)	0	100	100
15	1T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	19	43

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
17	1V	99/101 (98%)	97 (98%)	1 (1%)	1 (1%)	15	37
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	37
18	1W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	14	34
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14	34
20	1Y	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
20	2Y	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
21	1Z	201/206 (98%)	189 (94%)	12 (6%)	0	100	100
21	2Z	199/206 (97%)	183 (92%)	16 (8%)	0	100	100
22	10	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
22	20	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	34
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	34
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	55 (96%)	1 (2%)	1 (2%)	8	21
26	14	67/71 (94%)	52 (78%)	12 (18%)	3 (4%)	2	5
26	24	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	1
27	15	57/60 (95%)	57 (100%)	0	0	100	100
27	25	57/60 (95%)	55 (96%)	1 (2%)	1 (2%)	8	21
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	200 (87%)	20 (9%)	9 (4%)	3	6
33	2b	229/256 (90%)	200 (87%)	22 (10%)	7 (3%)	4	9
34	1c	204/239 (85%)	191 (94%)	12 (6%)	1 (0%)	29	54
34	2c	204/239 (85%)	172 (84%)	29 (14%)	3 (2%)	10	26
35	1d	206/209 (99%)	192 (93%)	13 (6%)	1 (0%)	29	54
35	2d	206/209 (99%)	189 (92%)	16 (8%)	1 (0%)	29	54
36	1e	146/162 (90%)	141 (97%)	3 (2%)	2 (1%)	11	28
36	2e	146/162 (90%)	134 (92%)	12 (8%)	0	100	100
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
37	2f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
38	1g	153/156 (98%)	145 (95%)	7 (5%)	1 (1%)	22	46
38	2g	153/156 (98%)	144 (94%)	7 (5%)	2 (1%)	12	30
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	127 (94%)	7 (5%)	1 (1%)	22	46
40	1i	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	19	43
40	2i	124/128 (97%)	111 (90%)	10 (8%)	3 (2%)	6	15
41	1j	95/105 (90%)	77 (81%)	15 (16%)	3 (3%)	4	9
41	2j	94/105 (90%)	80 (85%)	12 (13%)	2 (2%)	7	18
42	1k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	17	40
42	2k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	17	40
43	1l	119/132 (90%)	115 (97%)	4 (3%)	0	100	100
43	2l	119/132 (90%)	108 (91%)	11 (9%)	0	100	100
44	1m	114/126 (90%)	104 (91%)	8 (7%)	2 (2%)	8	21
44	2m	112/126 (89%)	98 (88%)	12 (11%)	2 (2%)	8	21
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	1 (1%)	3 (4%)	3	8
46	2o	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	13	32
47	1p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	12	30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	68 (85%)	11 (14%)	1 (1%)	12	30
48	1q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
48	2q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
49	1r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
50	1s	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	5	14
50	2s	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
51	1t	94/106 (89%)	87 (93%)	5 (5%)	2 (2%)	7	18
51	2t	96/106 (91%)	89 (93%)	3 (3%)	4 (4%)	3	5
52	1u	21/27 (78%)	21 (100%)	0	0	100	100
52	2u	21/27 (78%)	16 (76%)	4 (19%)	1 (5%)	2	4
53	1y	95/113 (84%)	90 (95%)	5 (5%)	0	100	100
53	2y	94/113 (83%)	88 (94%)	6 (6%)	0	100	100
All	All	11629/12354 (94%)	10827 (93%)	706 (6%)	96 (1%)	19	43

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	14	47	GLN
26	14	55	ARG
33	1b	21	ARG
4	2E	51	PHE
6	2G	78	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	214/218 (98%)	195 (91%)	19 (9%)	9	22
3	2D	215/218 (99%)	197 (92%)	18 (8%)	11	25
4	1E	164/166 (99%)	151 (92%)	13 (8%)	12	28

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	2E	164/166 (99%)	154 (94%)	10 (6%)	18	41
5	1F	160/166 (96%)	145 (91%)	15 (9%)	8	20
5	2F	159/166 (96%)	148 (93%)	11 (7%)	15	35
6	1G	144/156 (92%)	132 (92%)	12 (8%)	11	25
6	2G	142/156 (91%)	129 (91%)	13 (9%)	9	21
7	1H	144/148 (97%)	138 (96%)	6 (4%)	30	58
7	2H	143/148 (97%)	137 (96%)	6 (4%)	30	58
8	1I	111/124 (90%)	104 (94%)	7 (6%)	18	40
8	2I	108/124 (87%)	103 (95%)	5 (5%)	27	54
9	1N	119/119 (100%)	112 (94%)	7 (6%)	19	43
9	2N	118/119 (99%)	112 (95%)	6 (5%)	24	50
10	1O	100/100 (100%)	96 (96%)	4 (4%)	31	60
10	2O	100/100 (100%)	96 (96%)	4 (4%)	31	60
11	1P	115/116 (99%)	112 (97%)	3 (3%)	46	75
11	2P	115/116 (99%)	110 (96%)	5 (4%)	29	57
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	18	40
12	2Q	111/111 (100%)	107 (96%)	4 (4%)	35	64
13	1R	101/101 (100%)	91 (90%)	10 (10%)	8	18
13	2R	101/101 (100%)	89 (88%)	12 (12%)	5	12
14	1S	87/88 (99%)	80 (92%)	7 (8%)	12	27
14	2S	85/88 (97%)	79 (93%)	6 (7%)	14	34
15	1T	115/127 (91%)	110 (96%)	5 (4%)	29	57
15	2T	113/127 (89%)	107 (95%)	6 (5%)	22	48
16	1U	93/94 (99%)	88 (95%)	5 (5%)	22	47
16	2U	93/94 (99%)	90 (97%)	3 (3%)	39	68
17	1V	81/82 (99%)	73 (90%)	8 (10%)	8	18
17	2V	80/82 (98%)	76 (95%)	4 (5%)	24	51
18	1W	90/92 (98%)	81 (90%)	9 (10%)	7	18
18	2W	90/92 (98%)	82 (91%)	8 (9%)	9	22
19	1X	77/78 (99%)	73 (95%)	4 (5%)	23	49
19	2X	77/78 (99%)	73 (95%)	4 (5%)	23	49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	1Y	86/91 (94%)	80 (93%)	6 (7%)	15	35
20	2Y	86/91 (94%)	84 (98%)	2 (2%)	50	78
21	1Z	169/179 (94%)	154 (91%)	15 (9%)	9	22
21	2Z	165/179 (92%)	158 (96%)	7 (4%)	30	58
22	10	61/67 (91%)	57 (93%)	4 (7%)	16	38
22	20	61/67 (91%)	59 (97%)	2 (3%)	38	67
23	11	79/83 (95%)	76 (96%)	3 (4%)	33	62
23	21	81/83 (98%)	78 (96%)	3 (4%)	34	63
24	12	65/67 (97%)	64 (98%)	1 (2%)	65	86
24	22	66/67 (98%)	65 (98%)	1 (2%)	65	86
25	13	51/52 (98%)	46 (90%)	5 (10%)	8	18
25	23	50/52 (96%)	48 (96%)	2 (4%)	31	60
26	14	58/63 (92%)	55 (95%)	3 (5%)	23	49
26	24	54/63 (86%)	54 (100%)	0	100	100
27	15	51/52 (98%)	45 (88%)	6 (12%)	5	12
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	42
28	16	51/52 (98%)	46 (90%)	5 (10%)	8	18
28	26	50/52 (96%)	46 (92%)	4 (8%)	12	27
29	17	41/42 (98%)	36 (88%)	5 (12%)	5	11
29	27	41/42 (98%)	41 (100%)	0	100	100
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	32
30	28	54/55 (98%)	49 (91%)	5 (9%)	9	21
31	19	34/34 (100%)	32 (94%)	2 (6%)	19	43
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	71
33	1b	191/220 (87%)	183 (96%)	8 (4%)	30	58
33	2b	187/220 (85%)	180 (96%)	7 (4%)	34	63
34	1c	144/188 (77%)	139 (96%)	5 (4%)	36	65
34	2c	140/188 (74%)	134 (96%)	6 (4%)	29	57
35	1d	171/181 (94%)	162 (95%)	9 (5%)	22	48
35	2d	172/181 (95%)	166 (96%)	6 (4%)	36	65
36	1e	114/123 (93%)	110 (96%)	4 (4%)	36	65

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	2e	114/123 (93%)	108 (95%)	6 (5%)	22	48
37	1f	85/90 (94%)	82 (96%)	3 (4%)	36	65
37	2f	85/90 (94%)	82 (96%)	3 (4%)	36	65
38	1g	120/127 (94%)	117 (98%)	3 (2%)	47	76
38	2g	119/127 (94%)	113 (95%)	6 (5%)	24	51
39	1h	116/119 (98%)	114 (98%)	2 (2%)	60	84
39	2h	114/119 (96%)	109 (96%)	5 (4%)	28	56
40	1i	91/99 (92%)	91 (100%)	0	100	100
40	2i	88/99 (89%)	85 (97%)	3 (3%)	37	66
41	1j	68/92 (74%)	66 (97%)	2 (3%)	42	71
41	2j	68/92 (74%)	67 (98%)	1 (2%)	65	86
42	1k	83/99 (84%)	80 (96%)	3 (4%)	35	64
42	2k	83/99 (84%)	79 (95%)	4 (5%)	25	53
43	1l	96/108 (89%)	92 (96%)	4 (4%)	30	58
43	2l	96/108 (89%)	94 (98%)	2 (2%)	53	80
44	1m	90/101 (89%)	86 (96%)	4 (4%)	28	56
44	2m	87/101 (86%)	84 (97%)	3 (3%)	37	66
45	1n	49/50 (98%)	48 (98%)	1 (2%)	55	81
45	2n	49/50 (98%)	49 (100%)	0	100	100
46	1o	78/80 (98%)	74 (95%)	4 (5%)	24	50
46	2o	78/80 (98%)	77 (99%)	1 (1%)	69	87
47	1p	69/74 (93%)	65 (94%)	4 (6%)	20	43
47	2p	68/74 (92%)	62 (91%)	6 (9%)	10	23
48	1q	94/97 (97%)	89 (95%)	5 (5%)	22	48
48	2q	94/97 (97%)	89 (95%)	5 (5%)	22	48
49	1r	59/77 (77%)	58 (98%)	1 (2%)	60	84
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7	17
50	1s	68/80 (85%)	67 (98%)	1 (2%)	65	86
50	2s	67/80 (84%)	65 (97%)	2 (3%)	41	70
51	1t	71/82 (87%)	67 (94%)	4 (6%)	21	45
51	2t	70/82 (85%)	65 (93%)	5 (7%)	14	34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21	45
52	2u	18/22 (82%)	17 (94%)	1 (6%)	21	45
53	1y	82/98 (84%)	78 (95%)	4 (5%)	25	52
53	2y	79/98 (81%)	74 (94%)	5 (6%)	18	40
All	All	9524/10260 (93%)	9014 (95%)	510 (5%)	22	47

5 of 510 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	1g	104	LEU
3	2D	221	VAL
42	2k	47	VAL
42	1k	112	THR
48	1q	63	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
48	1q	16	GLN
5	2F	133	ASN
41	2j	69	ASN
50	1s	69	HIS
53	1y	38	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2862/2915 (98%)	421 (14%)	29 (1%)
1	2A	2855/2915 (97%)	492 (17%)	36 (1%)
2	1B	119/121 (98%)	11 (9%)	0
2	2B	119/121 (98%)	18 (15%)	0
32	1a	1494/1521 (98%)	233 (15%)	0
32	2a	1498/1521 (98%)	261 (17%)	0
All	All	8947/9114 (98%)	1436 (16%)	65 (0%)

5 of 1436 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	14	A
1	1A	15	G
1	1A	34	C
1	1A	45	C

5 of 65 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	9	U
1	2A	752	A
1	2A	2406	U
1	2A	195	A
1	2A	271(M)	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
32	5MC	1a	967	32	15,22,23	1.25	1 (6%)	19,32,35	1.47	3 (15%)
1	5MU	2A	1939	1	15,22,23	1.16	1 (6%)	16,32,35	1.73	2 (12%)
32	4OC	1a	1402	32	16,23,24	0.61	0	17,32,35	1.57	1 (5%)
32	5MC	1a	1404	32	15,22,23	1.37	1 (6%)	19,32,35	1.20	3 (15%)
32	MA6	1a	1518	32	19,26,27	0.96	1 (5%)	18,38,41	1.66	5 (27%)
32	M2G	2a	966	32	20,27,28	1.47	3 (15%)	22,40,43	2.11	6 (27%)
32	MA6	1a	1519	32	19,26,27	1.02	1 (5%)	18,38,41	1.54	4 (22%)
43	0TD	2l	92	43	4,9,10	3.06	1 (25%)	3,11,13	5.07	1 (33%)
32	2MG	2a	1207	32	19,26,27	1.24	2 (10%)	21,38,41	2.23	7 (33%)
1	4OC	2A	1920	1	15,22,24	0.72	0	17,31,35	1.30	2 (11%)
1	OMG	1A	2263	1,54	18,26,27	1.22	2 (11%)	20,38,41	2.21	6 (30%)
32	7MG	1a	527	32,54	22,26,27	1.77	4 (18%)	28,39,42	2.63	8 (28%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	4OC	1A	1942	1	15,22,24	0.66	0	17,31,35	1.43	2 (11%)
32	UR3	1a	1498	32	14,22,23	0.70	0	15,32,35	0.66	0
32	PSU	1a	516	32,54	17,21,22	1.49	3 (17%)	20,30,33	3.17	6 (30%)
32	2MG	1a	1207	32	19,26,27	1.33	2 (10%)	21,38,41	2.70	11 (52%)
32	5MC	1a	1400	32	15,22,23	1.42	1 (6%)	19,32,35	1.36	3 (15%)
1	2MU	2A	2552	1,54	14,22,24	0.95	1 (7%)	14,31,36	0.79	1 (7%)
1	5MU	2A	1915	1	15,22,23	1.04	1 (6%)	16,32,35	2.00	1 (6%)
1	2MU	1A	2564	1,54	14,22,24	0.88	1 (7%)	14,31,36	1.05	2 (14%)
1	PSU	1A	1939	1	17,21,22	1.43	3 (17%)	20,30,33	3.20	5 (25%)
32	M2G	1a	966	32	20,27,28	1.37	3 (15%)	22,40,43	2.20	6 (27%)
1	PSU	2A	2605	1	17,21,22	1.66	4 (23%)	20,30,33	3.23	6 (30%)
1	PSU	2A	1911	1	17,21,22	1.53	2 (11%)	20,30,33	3.04	6 (30%)
1	5MC	2A	1942	1	15,22,23	1.33	1 (6%)	19,32,35	1.37	3 (15%)
1	5MC	1A	1964	1,54	15,22,23	1.21	1 (6%)	19,32,35	1.36	3 (15%)
1	5MU	1A	1961	1,54	15,22,23	1.14	2 (13%)	16,32,35	1.88	2 (12%)
32	UR3	2a	1498	32,54	14,22,23	0.73	0	15,32,35	0.74	0
1	PSU	1A	2617	1,54	17,21,22	1.63	3 (17%)	20,30,33	3.24	6 (30%)
32	5MC	1a	1407	32	15,22,23	1.36	1 (6%)	19,32,35	1.30	2 (10%)
1	PSU	2A	1917	1	17,21,22	1.48	2 (11%)	20,30,33	3.05	5 (25%)
1	5MC	2A	1962	1,54	15,22,23	1.24	1 (6%)	19,32,35	1.33	3 (15%)
32	MA6	2a	1519	32	19,26,27	0.97	1 (5%)	18,38,41	1.84	5 (27%)
32	5MC	2a	1407	32	15,22,23	1.33	1 (6%)	19,32,35	1.38	3 (15%)
43	0TD	1l	92	43	4,9,10	3.13	1 (25%)	3,11,13	3.19	1 (33%)
1	5MC	1A	1984	1,54	15,22,23	1.30	1 (6%)	19,32,35	1.26	2 (10%)
1	5MU	1A	1937	1	15,22,23	1.06	1 (6%)	16,32,35	1.99	1 (6%)
32	7MG	2a	527	32,54	22,26,27	1.71	4 (18%)	28,39,42	2.72	8 (28%)
1	PSU	1A	1933	1	17,21,22	1.63	2 (11%)	20,30,33	3.10	7 (35%)
32	5MC	2a	1400	32	15,22,23	1.36	1 (6%)	19,32,35	1.32	3 (15%)
1	OMG	2A	2251	1,54	18,26,27	1.15	2 (11%)	20,38,41	2.21	6 (30%)
1	2MA	2A	2503	1,54	17,25,26	1.24	1 (5%)	19,37,40	2.03	3 (15%)
32	5MC	2a	967	32	15,22,23	1.55	1 (6%)	19,32,35	1.28	2 (10%)
1	2MA	1A	2515	1,54	17,25,26	1.19	1 (5%)	19,37,40	2.16	3 (15%)
32	5MC	2a	1404	32	15,22,23	1.40	1 (6%)	19,32,35	1.27	3 (15%)
32	PSU	2a	516	32,54	17,21,22	1.67	3 (17%)	20,30,33	3.13	6 (30%)
32	MA6	2a	1518	32	19,26,27	1.05	1 (5%)	18,38,41	1.67	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	4OC	2a	1402	32	16,23,24	0.66	0	17,32,35	1.42	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	967	32	-	0/5/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/5/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
32	MA6	1a	1518	32	-	3/7/29/30	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
43	0TD	2l	92	43	-	1/3/12/14	-
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
1	4OC	2A	1920	1	-	0/7/27/30	0/2/2/2
1	OMG	1A	2263	1,54	-	1/5/27/28	0/3/3/3
32	7MG	1a	527	32,54	-	0/7/37/38	0/3/3/3
1	4OC	1A	1942	1	-	1/7/27/30	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	2/5/27/28	0/3/3/3
32	5MC	1a	1400	32	-	1/5/25/26	0/2/2/2
1	2MU	2A	2552	1,54	-	0/7/27/28	0/2/2/2
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
1	2MU	1A	2564	1,54	-	0/7/27/28	0/2/2/2
1	PSU	1A	1939	1	-	1/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
1	5MC	1A	1964	1,54	-	0/5/25/26	0/2/2/2
1	5MU	1A	1961	1,54	-	0/5/25/26	0/2/2/2
32	UR3	2a	1498	32,54	-	0/5/25/26	0/2/2/2
1	PSU	1A	2617	1,54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
1	5MC	2A	1962	1,54	-	2/5/25/26	0/2/2/2
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/3/12/14	-
1	5MC	1A	1984	1,54	-	2/5/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/5/25/26	0/2/2/2
32	7MG	2a	527	32,54	-	0/7/37/38	0/3/3/3
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
1	OMG	2A	2251	1,54	-	0/5/27/28	0/3/3/3
1	2MA	2A	2503	1,54	-	1/3/25/26	0/3/3/3
32	5MC	2a	967	32	-	0/5/25/26	0/2/2/2
1	2MA	1A	2515	1,54	-	2/3/25/26	0/3/3/3
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/7/29/30	0/3/3/3
32	4OC	2a	1402	32	-	4/9/29/30	0/2/2/2

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-5.97	1.69	1.84
43	2l	92	0TD	CB-SB	-5.86	1.70	1.84
32	2a	967	5MC	C5-C4	5.60	1.50	1.41
32	1a	1400	5MC	C5-C4	5.05	1.49	1.41
32	2a	1404	5MC	C5-C4	4.99	1.49	1.41

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1939	PSU	N1-C2-N3	-9.34	121.00	128.43
32	1a	516	PSU	N1-C2-N3	-8.83	121.41	128.43
1	2A	2605	PSU	N1-C2-N3	-8.75	121.47	128.43
43	2l	92	0TD	CSB-SB-CB	-8.71	84.73	101.85
32	2a	527	7MG	N3-C4-N9	8.57	137.92	126.91

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1518	MA6	C5-C6-N6-C9
32	1a	1518	MA6	C5-C6-N6-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C10
43	2l	92	0TD	CG-CB-SB-CSB

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1939	5MU	1	0
1	1A	1942	4OC	1	0
1	2A	1915	5MU	1	0
1	1A	2564	2MU	1	0
1	2A	1911	PSU	1	0
1	1A	1964	5MC	1	0
1	2A	1917	PSU	1	0
1	2A	2251	OMG	1	0
1	1A	2515	2MA	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2389 ligands modelled in this entry, 2376 are monoatomic - leaving 13 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	$\# Z  > 2$
60	SF4	2d	501	35	0,12,12	0.00	-	-		
57	MPD	2A	3711	-	7,7,7	0.30	0	9,10,10	0.30	0
57	MPD	1A	3988	-	7,7,7	0.27	0	9,10,10	0.28	0
56	EZP	2A	3709	-	21,26,26	3.58	3 (14%)	26,35,35	0.92	1 (3%)
57	MPD	1T	204	-	7,7,7	0.32	0	9,10,10	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
57	MPD	1a	1854	-	7,7,7	0.38	0	9,10,10	0.38	0
56	EZP	1A	3987	-	21,26,26	2.81	3 (14%)	26,35,35	1.72	4 (15%)
57	MPD	2B	3020	-	7,7,7	0.30	0	9,10,10	0.30	0
57	MPD	18	102	-	7,7,7	0.27	0	9,10,10	0.38	0
60	SF4	1d	302	35	0,12,12	0.00	-	-	-	-
57	MPD	2A	3710	-	7,7,7	0.39	0	9,10,10	0.30	0

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
60	SF4	2d	501	35	-	-	0/6/5/5
57	MPD	2A	3711	-	-	3/5/5/5	-
57	MPD	1A	3988	-	-	2/5/5/5	-
56	EZP	2A	3709	-	-	7/24/26/26	0/2/2/2
57	MPD	1T	204	-	-	1/5/5/5	-
57	MPD	1a	1854	-	-	2/5/5/5	-
56	EZP	1A	3987	-	-	7/24/26/26	0/2/2/2
57	MPD	2B	3020	-	-	3/5/5/5	-
57	MPD	18	102	-	-	1/5/5/5	-
60	SF4	1d	302	35	-	-	0/6/5/5
57	MPD	2A	3710	-	-	0/5/5/5	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2A	3709	EZP	OAC-NAY	13.50	1.45	1.22
56	1A	3987	EZP	OAC-NAY	9.18	1.38	1.22
56	2A	3709	EZP	CAT-CAW	-8.10	1.39	1.51
56	1A	3987	EZP	CAT-CAW	-7.46	1.40	1.51
56	1A	3987	EZP	CAU-NAY	-4.60	1.34	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1A	3987	EZP	CAT-CAW-CAX	4.98	120.42	111.64
56	1A	3987	EZP	CAW-CAX-NAP	4.35	118.30	110.05
56	1A	3987	EZP	CAI-CAU-NAY	2.44	121.22	119.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2A	3709	EZP	CAW-CAX-NAP	2.27	114.35	110.05
56	1A	3987	EZP	CA-C-NAP	-2.26	113.01	116.15

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

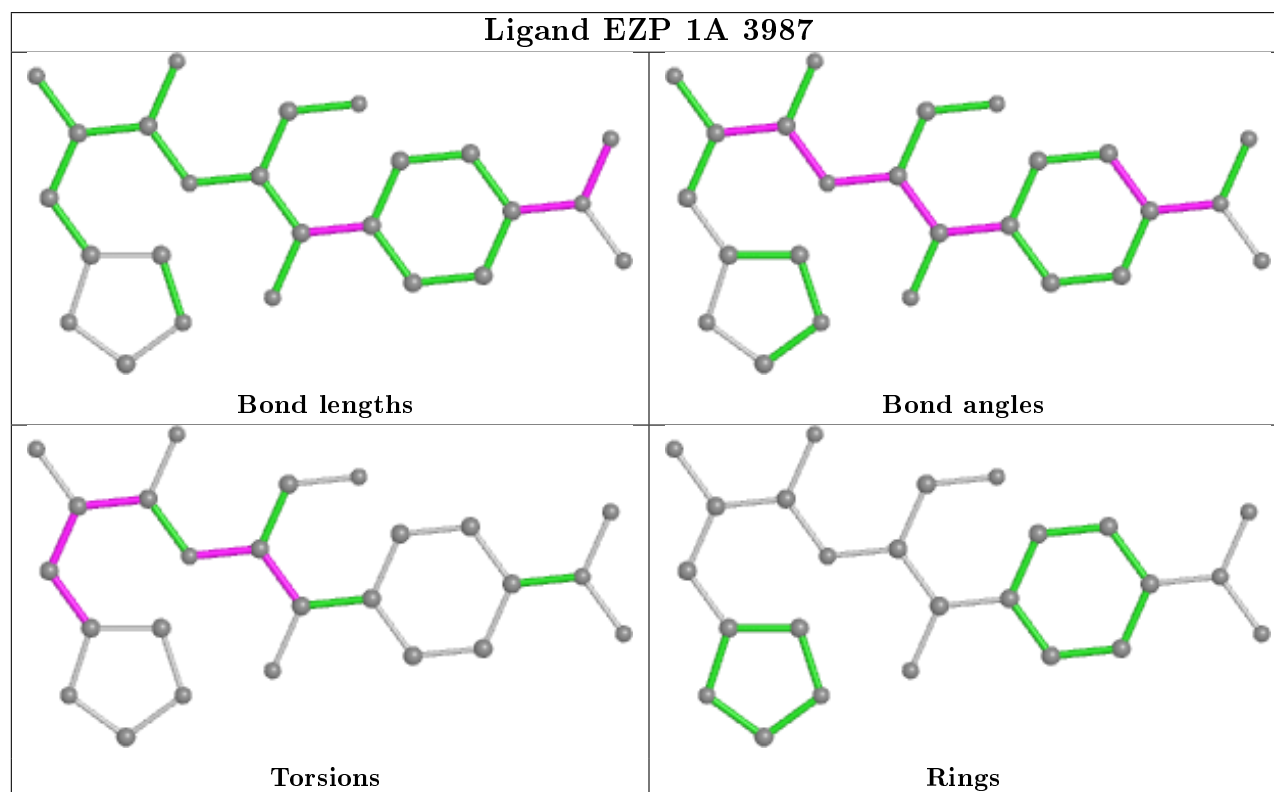
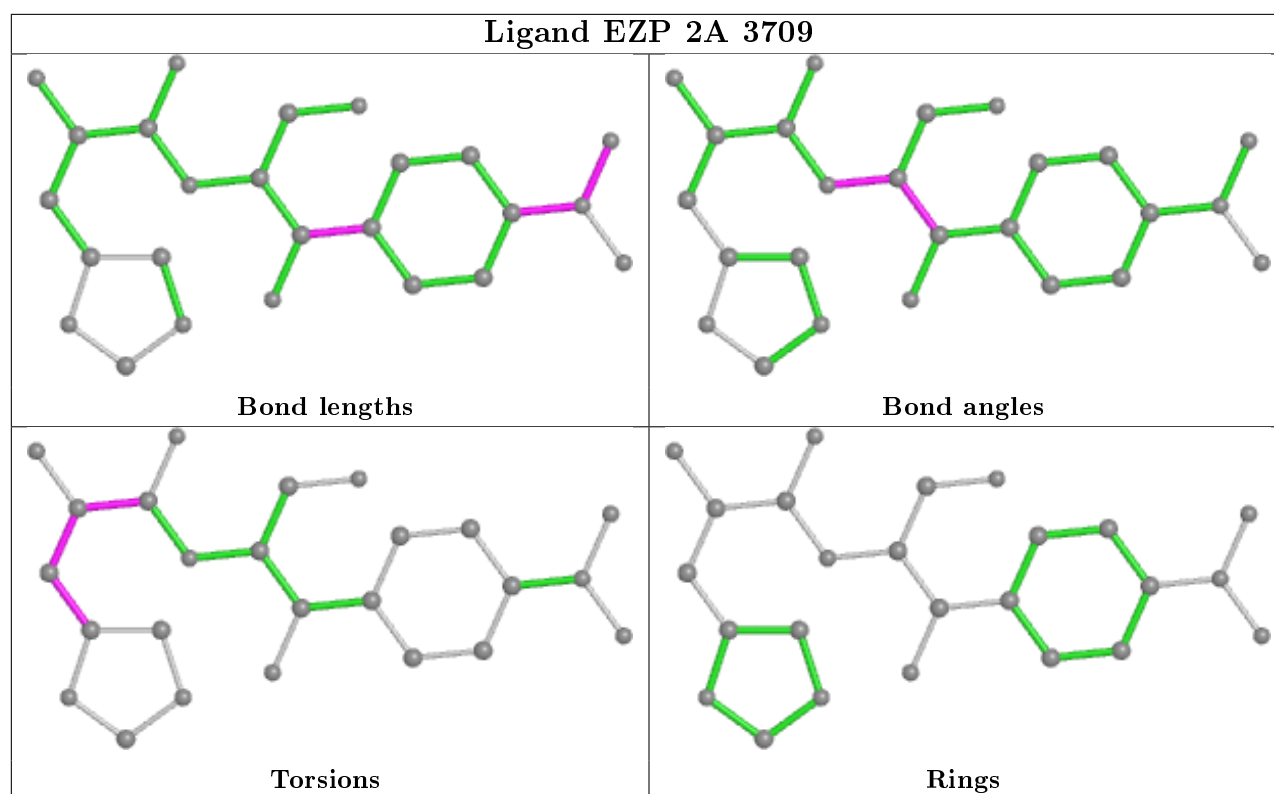
Mol	Chain	Res	Type	Atoms
56	1A	3987	EZP	NAP-C-CA-CB
56	1A	3987	EZP	O-C-CA-CB
56	1A	3987	EZP	C-CA-CB-CG
56	2A	3709	EZP	NAP-C-CA-N
56	2A	3709	EZP	NAP-C-CA-CB

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	1T	204	MPD	1	0
57	18	102	MPD	1	0
57	2A	3710	MPD	2	0

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



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1A	2861/2915 (98%)	0.42	57 (1%) 65 67	15, 31, 89, 105	0
1	2A	2856/2915 (97%)	0.28	65 (2%) 60 62	27, 50, 92, 103	0
2	1B	120/121 (99%)	0.05	0 100 100	24, 44, 58, 80	0
2	2B	120/121 (99%)	-0.06	0 100 100	52, 74, 83, 90	0
3	1D	275/276 (99%)	0.60	3 (1%) 80 82	17, 32, 46, 65	0
3	2D	275/276 (99%)	0.69	13 (4%) 31 30	26, 44, 56, 76	0
4	1E	204/206 (99%)	0.51	2 (0%) 82 83	16, 34, 55, 70	0
4	2E	204/206 (99%)	0.59	3 (1%) 73 76	29, 50, 66, 79	0
5	1F	203/210 (96%)	0.37	0 100 100	16, 35, 60, 83	0
5	2F	203/210 (96%)	0.39	3 (1%) 73 76	29, 60, 72, 85	0
6	1G	181/182 (99%)	0.16	2 (1%) 80 82	39, 56, 72, 80	0
6	2G	181/182 (99%)	0.59	13 (7%) 15 13	68, 77, 85, 89	0
7	1H	174/180 (96%)	0.29	1 (0%) 89 91	32, 46, 59, 64	0
7	2H	173/180 (96%)	0.72	20 (11%) 4 3	62, 75, 82, 86	0
8	1I	147/148 (99%)	0.15	3 (2%) 65 67	34, 66, 76, 83	0
8	2I	146/148 (98%)	0.49	15 (10%) 6 5	51, 69, 81, 84	0
9	1N	140/140 (100%)	0.41	0 100 100	22, 32, 53, 67	0
9	2N	140/140 (100%)	0.41	1 (0%) 87 89	43, 57, 71, 76	0
10	1O	122/122 (100%)	0.47	0 100 100	23, 34, 50, 58	0
10	2O	122/122 (100%)	0.58	5 (4%) 37 36	38, 51, 61, 69	0
11	1P	149/150 (99%)	0.36	1 (0%) 87 89	15, 38, 58, 71	0
11	2P	149/150 (99%)	0.66	7 (4%) 31 30	32, 59, 77, 80	0
12	1Q	141/141 (100%)	0.44	0 100 100	21, 35, 46, 62	0
12	2Q	141/141 (100%)	0.66	7 (4%) 28 27	40, 57, 67, 76	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	0.50	0 100 100	21, 29, 44, 50	0
13	2R	118/118 (100%)	0.45	2 (1%) 70 72	31, 44, 55, 65	0
14	1S	110/112 (98%)	0.31	1 (0%) 84 85	34, 45, 56, 65	0
14	2S	110/112 (98%)	0.48	9 (8%) 11 9	59, 69, 76, 81	0
15	1T	131/146 (89%)	0.30	1 (0%) 86 87	28, 38, 62, 75	0
15	2T	131/146 (89%)	0.33	1 (0%) 86 87	41, 52, 70, 76	0
16	1U	116/118 (98%)	0.63	1 (0%) 84 85	18, 25, 39, 57	0
16	2U	116/118 (98%)	0.79	9 (7%) 13 11	33, 52, 67, 74	0
17	1V	101/101 (100%)	0.36	0 100 100	15, 35, 54, 67	0
17	2V	101/101 (100%)	0.44	3 (2%) 50 51	31, 62, 72, 77	0
18	1W	112/113 (99%)	0.46	1 (0%) 84 85	19, 27, 46, 75	0
18	2W	112/113 (99%)	0.67	8 (7%) 16 14	29, 43, 59, 84	0
19	1X	95/96 (98%)	0.44	1 (1%) 80 82	23, 32, 58, 68	0
19	2X	95/96 (98%)	0.68	5 (5%) 26 25	43, 54, 69, 74	0
20	1Y	107/110 (97%)	0.39	1 (0%) 84 85	29, 42, 62, 67	0
20	2Y	107/110 (97%)	1.10	15 (14%) 2 1	49, 63, 73, 82	0
21	1Z	203/206 (98%)	0.13	2 (0%) 82 83	35, 51, 66, 76	0
21	2Z	201/206 (97%)	0.21	8 (3%) 38 37	57, 71, 79, 88	0
22	10	77/85 (90%)	0.56	1 (1%) 77 78	24, 31, 48, 54	0
22	20	77/85 (90%)	0.99	12 (15%) 2 1	43, 57, 67, 72	0
23	11	97/98 (98%)	0.83	5 (5%) 27 25	22, 39, 61, 69	0
23	21	97/98 (98%)	0.92	8 (8%) 11 9	35, 49, 71, 73	0
24	12	70/72 (97%)	0.24	1 (1%) 75 77	29, 44, 57, 78	0
24	22	70/72 (97%)	0.40	2 (2%) 51 52	53, 64, 71, 73	0
25	13	59/60 (98%)	0.44	0 100 100	20, 30, 55, 63	0
25	23	59/60 (98%)	1.13	14 (23%) 0 0	45, 55, 69, 77	0
26	14	69/71 (97%)	0.22	4 (5%) 23 22	50, 69, 86, 90	0
26	24	69/71 (97%)	0.48	6 (8%) 10 8	70, 83, 88, 91	0
27	15	59/60 (98%)	0.53	0 100 100	17, 27, 44, 54	0
27	25	59/60 (98%)	0.38	2 (3%) 45 45	29, 44, 59, 68	0
28	16	53/54 (98%)	0.15	0 100 100	28, 36, 48, 55	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	0.30	0 100 100	46, 54, 63, 68	0
29	17	48/49 (97%)	0.90	2 (4%) 36 35	17, 24, 49, 58	0
29	27	48/49 (97%)	0.85	4 (8%) 11 9	28, 36, 58, 65	0
30	18	64/65 (98%)	0.64	1 (1%) 72 74	23, 28, 34, 47	0
30	28	64/65 (98%)	0.88	4 (6%) 20 19	38, 49, 56, 63	0
31	19	37/37 (100%)	0.56	1 (2%) 54 55	22, 32, 49, 53	0
31	29	37/37 (100%)	1.34	8 (21%) 0 0	50, 60, 68, 69	0
32	1a	1488/1521 (97%)	0.11	20 (1%) 77 78	32, 62, 89, 104	0
32	2a	1492/1521 (98%)	0.13	23 (1%) 73 76	42, 71, 91, 103	0
33	1b	231/256 (90%)	0.33	9 (3%) 39 38	61, 74, 83, 88	0
33	2b	231/256 (90%)	0.72	34 (14%) 2 1	66, 80, 86, 90	0
34	1c	206/239 (86%)	0.55	11 (5%) 26 25	53, 67, 77, 81	0
34	2c	206/239 (86%)	0.92	31 (15%) 2 1	70, 79, 84, 91	0
35	1d	208/209 (99%)	0.72	20 (9%) 8 6	51, 66, 75, 81	0
35	2d	208/209 (99%)	1.14	39 (18%) 1 0	55, 68, 77, 79	0
36	1e	148/162 (91%)	0.49	4 (2%) 54 55	46, 59, 69, 80	0
36	2e	148/162 (91%)	0.82	20 (13%) 3 2	57, 68, 76, 83	0
37	1f	100/101 (99%)	0.27	1 (1%) 82 83	43, 60, 70, 74	0
37	2f	100/101 (99%)	0.02	0 100 100	52, 62, 70, 76	0
38	1g	155/156 (99%)	0.31	6 (3%) 39 38	56, 65, 76, 85	0
38	2g	155/156 (99%)	0.35	10 (6%) 18 17	68, 75, 81, 87	0
39	1h	137/138 (99%)	0.63	8 (5%) 23 22	51, 62, 71, 74	0
39	2h	137/138 (99%)	0.61	7 (5%) 28 26	58, 69, 74, 82	0
40	1i	127/128 (99%)	0.71	17 (13%) 3 2	52, 73, 79, 82	0
40	2i	126/128 (98%)	1.74	49 (38%) 0 0	67, 80, 85, 87	0
41	1j	97/105 (92%)	0.50	13 (13%) 3 2	52, 72, 83, 86	0
41	2j	96/105 (91%)	2.13	47 (48%) 0 0	71, 80, 85, 87	0
42	1k	114/129 (88%)	0.22	0 100 100	39, 58, 69, 73	0
42	2k	114/129 (88%)	0.62	7 (6%) 21 20	50, 66, 75, 81	0
43	1l	121/132 (91%)	0.46	4 (3%) 46 46	42, 54, 65, 70	0
43	2l	121/132 (91%)	0.97	16 (13%) 3 2	54, 62, 69, 77	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	116/126 (92%)	0.32	4 (3%) 45 45	52, 68, 75, 79	0
44	2m	114/126 (90%)	0.82	12 (10%) 6 4	73, 80, 85, 87	0
45	1n	60/61 (98%)	1.23	10 (16%) 1 1	57, 64, 72, 79	0
45	2n	60/61 (98%)	2.71	36 (60%) 0 0	71, 79, 85, 88	0
46	1o	88/89 (98%)	0.42	0 100 100	43, 60, 71, 77	0
46	2o	88/89 (98%)	0.61	2 (2%) 60 62	54, 67, 75, 78	0
47	1p	82/88 (93%)	1.04	12 (14%) 2 1	55, 67, 77, 80	0
47	2p	82/88 (93%)	0.80	8 (9%) 7 5	55, 65, 75, 82	0
48	1q	99/105 (94%)	0.49	6 (6%) 21 20	48, 63, 72, 73	0
48	2q	99/105 (94%)	0.55	7 (7%) 16 14	53, 63, 73, 79	0
49	1r	68/88 (77%)	0.26	1 (1%) 73 76	51, 60, 73, 76	0
49	2r	68/88 (77%)	0.35	2 (2%) 51 52	59, 67, 74, 76	0
50	1s	83/93 (89%)	0.14	1 (1%) 79 80	59, 70, 76, 79	0
50	2s	83/93 (89%)	0.98	15 (18%) 1 1	70, 82, 86, 88	0
51	1t	96/106 (90%)	0.78	15 (15%) 2 1	53, 66, 76, 82	0
51	2t	98/106 (92%)	0.45	7 (7%) 16 14	53, 64, 75, 77	0
52	1u	23/27 (85%)	1.77	9 (39%) 0 0	61, 66, 69, 72	0
52	2u	23/27 (85%)	2.31	14 (60%) 0 0	73, 76, 80, 82	0
53	1y	97/113 (85%)	0.62	4 (4%) 37 36	45, 56, 67, 71	0
53	2y	96/113 (84%)	2.26	51 (53%) 0 0	60, 72, 79, 83	0
All	All	20766/21468 (96%)	0.45	976 (4%) 31 30	15, 57, 84, 105	0

The worst 5 of 976 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1110	C	7.7
45	2n	59	ALA	7.6
1	1A	1122	C	7.4
40	2i	127	LYS	7.3
1	1A	1133	G	7.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	5MU	2A	1915	21/22	0.89	0.15	76,82,88,101	0
32	5MC	2a	967	21/22	0.90	0.25	63,68,77,88	0
43	0TD	2l	92	10/11	0.92	0.28	60,65,71,95	0
1	PSU	1A	1939	20/21	0.92	0.17	62,68,77,77	0
1	PSU	2A	1917	20/21	0.92	0.13	71,78,90,90	0
32	2MG	2a	1207	24/25	0.92	0.15	76,86,91,102	0
32	M2G	2a	966	25/26	0.93	0.22	57,67,81,92	0
1	5MU	1A	1937	21/22	0.93	0.17	67,74,83,94	0
1	PSU	2A	1911	20/21	0.93	0.13	56,70,76,78	0
1	4OC	2A	1920	21/23	0.94	0.17	61,65,72,73	0
43	0TD	1l	92	10/11	0.94	0.23	50,54,59,76	0
32	PSU	2a	516	20/21	0.94	0.16	71,76,80,84	0
32	7MG	2a	527	24/25	0.95	0.18	61,67,73,74	0
1	PSU	1A	1933	20/21	0.95	0.15	55,62,65,66	0
32	PSU	1a	516	20/21	0.95	0.17	56,60,64,65	0
32	5MC	2a	1404	21/22	0.95	0.21	51,60,63,66	0
32	2MG	1a	1207	24/25	0.95	0.17	56,66,69,71	0
32	4OC	2a	1402	22/23	0.95	0.20	53,63,68,71	0
32	5MC	2a	1407	21/22	0.96	0.18	50,60,64,68	0
32	5MC	1a	967	21/22	0.96	0.19	53,58,65,71	0
32	MA6	2a	1518	24/25	0.96	0.25	51,61,66,67	0
32	7MG	1a	527	24/25	0.96	0.22	42,51,54,59	0
1	4OC	1A	1942	21/23	0.97	0.21	39,54,59,60	0
1	5MC	2A	1942	21/22	0.97	0.17	36,48,53,54	0
32	5MC	2a	1400	21/22	0.97	0.29	65,70,73,74	0
32	UR3	2a	1498	21/22	0.97	0.20	52,58,63,66	0
32	UR3	1a	1498	21/22	0.97	0.19	43,46,52,60	0
1	5MU	2A	1939	21/22	0.97	0.19	29,36,41,43	0
32	M2G	1a	966	25/26	0.97	0.18	51,53,58,61	0
1	PSU	2A	2605	20/21	0.97	0.25	29,35,39,44	0
32	4OC	1a	1402	22/23	0.98	0.18	42,47,55,56	0
32	MA6	1a	1519	24/25	0.98	0.23	37,43,46,49	0
1	5MC	1A	1984	21/22	0.98	0.21	25,33,37,45	0
32	5MC	1a	1400	21/22	0.98	0.21	40,45,49,51	0
1	2MU	2A	2552	21/23	0.98	0.22	30,36,39,41	0
1	5MC	1A	1964	21/22	0.98	0.20	26,32,38,47	0
32	5MC	1a	1404	21/22	0.98	0.20	35,44,46,49	0
1	OMG	2A	2251	24/25	0.98	0.23	32,36,38,39	0
1	2MA	2A	2503	23/24	0.98	0.25	24,30,35,37	0
1	PSU	1A	2617	20/21	0.98	0.20	18,22,28,28	0
1	2MA	1A	2515	23/24	0.98	0.25	16,20,24,31	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	5MC	1a	1407	21/22	0.98	0.19	36,45,49,56	0
32	MA6	1a	1518	24/25	0.98	0.24	34,41,46,51	0
1	5MC	2A	1962	21/22	0.98	0.19	33,43,48,58	0
32	MA6	2a	1519	24/25	0.98	0.26	51,60,64,67	0
1	OMG	1A	2263	24/25	0.99	0.23	15,21,23,26	0
1	2MU	1A	2564	21/23	0.99	0.21	20,26,28,29	0
1	5MU	1A	1961	21/22	0.99	0.20	18,24,27,32	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3219	1/1	0.40	0.21	74,74,74,74	0
54	MG	1a	1851	1/1	0.42	0.65	94,94,94,94	0
54	MG	2A	3167	1/1	0.43	0.24	74,74,74,74	0
54	MG	2B	3007	1/1	0.47	0.27	71,71,71,71	0
54	MG	1a	1840	1/1	0.48	0.20	45,45,45,45	0
54	MG	2A	3197	1/1	0.49	0.23	73,73,73,73	0
54	MG	2A	3215	1/1	0.51	0.18	73,73,73,73	0
54	MG	1a	1828	1/1	0.54	0.18	62,62,62,62	0
54	MG	2B	3015	1/1	0.56	0.19	74,74,74,74	0
54	MG	2A	3692	1/1	0.61	0.19	63,63,63,63	0
54	MG	2A	3703	1/1	0.61	0.12	81,81,81,81	0
54	MG	2a	1684	1/1	0.62	0.13	60,60,60,60	0
54	MG	1A	3191	1/1	0.62	0.26	51,51,51,51	0
54	MG	1B	211	1/1	0.63	0.18	64,64,64,64	0
54	MG	2A	3142	1/1	0.63	0.18	68,68,68,68	0
54	MG	2a	1662	1/1	0.63	0.22	67,67,67,67	0
54	MG	1B	219	1/1	0.63	0.13	46,46,46,46	0
54	MG	2A	3318	1/1	0.64	0.19	78,78,78,78	0
54	MG	2A	3338	1/1	0.65	0.19	53,53,53,53	0
54	MG	20	101	1/1	0.66	0.21	75,75,75,75	0
54	MG	1a	1830	1/1	0.66	0.21	66,66,66,66	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3189	1/1	0.67	0.21	66,66,66,66	0
54	MG	1A	3934	1/1	0.67	0.39	50,50,50,50	0
54	MG	2A	3160	1/1	0.67	0.17	63,63,63,63	0
54	MG	1a	1766	1/1	0.68	0.28	67,67,67,67	0
54	MG	1a	1684	1/1	0.68	0.19	49,49,49,49	0
54	MG	1A	3278	1/1	0.68	0.22	38,38,38,38	0
54	MG	2a	1611	1/1	0.69	0.13	62,62,62,62	0
54	MG	1A	3327	1/1	0.69	0.19	33,33,33,33	0
54	MG	2a	1645	1/1	0.69	0.17	62,62,62,62	0
54	MG	1a	1640	1/1	0.69	0.17	59,59,59,59	0
54	MG	1a	1793	1/1	0.69	0.16	63,63,63,63	0
54	MG	1A	3982	1/1	0.69	0.08	49,49,49,49	0
54	MG	2A	3567	1/1	0.70	0.18	40,40,40,40	0
54	MG	1A	3346	1/1	0.70	0.18	48,48,48,48	0
54	MG	1a	1624	1/1	0.70	0.12	60,60,60,60	0
54	MG	2A	3173	1/1	0.70	0.20	67,67,67,67	0
54	MG	1d	307	1/1	0.70	0.14	89,89,89,89	0
54	MG	2A	3206	1/1	0.70	0.45	45,45,45,45	0
54	MG	1a	1608	1/1	0.71	0.12	63,63,63,63	0
54	MG	1B	207	1/1	0.71	0.21	41,41,41,41	0
54	MG	2A	3393	1/1	0.71	0.15	55,55,55,55	0
54	MG	1A	3986	1/1	0.71	0.34	61,61,61,61	0
54	MG	1A	3804	1/1	0.71	0.12	21,21,21,21	0
54	MG	1a	1677	1/1	0.71	0.12	64,64,64,64	0
54	MG	2I	3001	1/1	0.71	0.17	71,71,71,71	0
54	MG	2A	3635	1/1	0.71	0.10	64,64,64,64	0
54	MG	1A	3921	1/1	0.71	0.41	58,58,58,58	0
54	MG	2A	3171	1/1	0.71	0.28	58,58,58,58	0
54	MG	1A	3756	1/1	0.72	0.16	57,57,57,57	0
54	MG	1A	3422	1/1	0.72	0.13	41,41,41,41	0
54	MG	1a	1797	1/1	0.72	0.22	66,66,66,66	0
54	MG	1A	3259	1/1	0.72	0.18	62,62,62,62	0
54	MG	1A	3398	1/1	0.72	0.15	26,26,26,26	0
54	MG	1y	3002	1/1	0.73	0.25	62,62,62,62	0
54	MG	2A	3184	1/1	0.73	0.22	68,68,68,68	0
54	MG	1A	3575	1/1	0.73	0.14	65,65,65,65	0
54	MG	1A	3597	1/1	0.73	0.23	62,62,62,62	0
54	MG	2a	1673	1/1	0.73	0.15	56,56,56,56	0
54	MG	2I	101	1/1	0.73	0.13	67,67,67,67	0
54	MG	1a	1681	1/1	0.74	0.12	60,60,60,60	0
54	MG	2A	3198	1/1	0.74	0.22	60,60,60,60	0
54	MG	1A	3805	1/1	0.74	0.12	54,54,54,54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1652	1/1	0.74	0.14	61,61,61,61	0
54	MG	2A	3103	1/1	0.74	0.27	66,66,66,66	0
54	MG	1F	311	1/1	0.75	0.51	45,45,45,45	0
54	MG	1A	3957	1/1	0.75	0.32	79,79,79,79	0
54	MG	2A	3676	1/1	0.75	0.13	66,66,66,66	0
54	MG	1A	3297	1/1	0.75	0.21	37,37,37,37	0
54	MG	1A	3950	1/1	0.75	0.14	80,80,80,80	0
54	MG	2Q	3002	1/1	0.75	0.10	55,55,55,55	0
54	MG	1A	3941	1/1	0.75	0.23	68,68,68,68	0
54	MG	2A	3488	1/1	0.75	0.08	62,62,62,62	0
54	MG	1A	3894	1/1	0.76	0.38	80,80,80,80	0
54	MG	2A	3175	1/1	0.76	0.20	55,55,55,55	0
54	MG	1A	3662	1/1	0.76	0.18	62,62,62,62	0
54	MG	2a	1638	1/1	0.76	0.19	60,60,60,60	0
54	MG	2A	3685	1/1	0.76	0.13	75,75,75,75	0
54	MG	2a	1742	1/1	0.76	0.25	65,65,65,65	0
54	MG	1a	1700	1/1	0.76	0.21	65,65,65,65	0
54	MG	2a	1642	1/1	0.76	0.11	58,58,58,58	0
54	MG	1a	1752	1/1	0.76	0.17	71,71,71,71	0
54	MG	1a	1680	1/1	0.76	0.14	70,70,70,70	0
54	MG	1A	3279	1/1	0.76	0.12	61,61,61,61	0
54	MG	2A	3274	1/1	0.76	0.26	53,53,53,53	0
54	MG	1a	1834	1/1	0.76	0.29	58,58,58,58	0
54	MG	1a	1843	1/1	0.77	0.09	78,78,78,78	0
54	MG	1a	1637	1/1	0.77	0.17	67,67,67,67	0
54	MG	2B	3001	1/1	0.77	0.16	68,68,68,68	0
54	MG	1a	1606	1/1	0.77	0.14	58,58,58,58	0
54	MG	1A	3702	1/1	0.77	0.16	27,27,27,27	0
54	MG	2A	3195	1/1	0.77	0.21	54,54,54,54	0
54	MG	1a	1737	1/1	0.77	0.17	62,62,62,62	0
54	MG	2A	3098	1/1	0.77	0.19	53,53,53,53	0
54	MG	2A	3166	1/1	0.77	0.15	51,51,51,51	0
54	MG	1a	1835	1/1	0.77	0.25	67,67,67,67	0
54	MG	2B	3014	1/1	0.78	0.17	71,71,71,71	0
54	MG	2a	1630	1/1	0.78	0.12	62,62,62,62	0
54	MG	1A	3744	1/1	0.78	0.13	54,54,54,54	0
54	MG	2A	3216	1/1	0.78	0.21	54,54,54,54	0
54	MG	2W	8002	1/1	0.78	0.12	59,59,59,59	0
54	MG	1a	1748	1/1	0.78	0.13	57,57,57,57	0
54	MG	1A	3576	1/1	0.78	0.12	43,43,43,43	0
54	MG	1A	3783	1/1	0.78	0.13	48,48,48,48	0
54	MG	2A	3177	1/1	0.78	0.15	56,56,56,56	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3095	1/1	0.78	0.13	58,58,58,58	0
54	MG	2a	1604	1/1	0.78	0.23	58,58,58,58	0
54	MG	2A	3673	1/1	0.78	0.17	68,68,68,68	0
54	MG	2A	3405	1/1	0.78	0.17	66,66,66,66	0
54	MG	2A	3389	1/1	0.78	0.23	47,47,47,47	0
54	MG	1A	3794	1/1	0.78	0.14	53,53,53,53	0
54	MG	2A	3332	1/1	0.78	0.14	65,65,65,65	0
54	MG	1A	3473	1/1	0.79	0.10	63,63,63,63	0
54	MG	1a	1802	1/1	0.79	0.18	62,62,62,62	0
54	MG	1A	3100	1/1	0.79	0.26	39,39,39,39	0
54	MG	1D	309	1/1	0.79	0.13	52,52,52,52	0
54	MG	2A	3226	1/1	0.79	0.23	53,53,53,53	0
54	MG	1A	3835	1/1	0.79	0.12	50,50,50,50	0
54	MG	1A	3938	1/1	0.79	0.17	64,64,64,64	0
54	MG	1A	3011	1/1	0.79	0.18	47,47,47,47	0
54	MG	2A	3149	1/1	0.79	0.12	68,68,68,68	0
58	ARG	1F	314	12/12	0.79	0.23	47,65,78,79	0
54	MG	1A	3603	1/1	0.79	0.15	60,60,60,60	0
54	MG	2a	1737	1/1	0.79	0.18	60,60,60,60	0
54	MG	1a	1674	1/1	0.79	0.13	65,65,65,65	0
54	MG	1A	3189	1/1	0.79	0.42	41,41,41,41	0
54	MG	2A	3146	1/1	0.79	0.48	52,52,52,52	0
54	MG	2a	1689	1/1	0.79	0.24	62,62,62,62	0
54	MG	1a	1668	1/1	0.79	0.25	74,74,74,74	0
54	MG	2A	3694	1/1	0.79	0.27	69,69,69,69	0
54	MG	1A	3649	1/1	0.79	0.14	58,58,58,58	0
54	MG	1a	1782	1/1	0.79	0.22	61,61,61,61	0
54	MG	2A	3385	1/1	0.79	0.13	47,47,47,47	0
54	MG	1A	3383	1/1	0.79	0.13	24,24,24,24	0
54	MG	1a	1767	1/1	0.79	0.42	58,58,58,58	0
54	MG	1A	3782	1/1	0.80	0.11	41,41,41,41	0
54	MG	2A	3621	1/1	0.80	0.14	28,28,28,28	0
54	MG	1a	1824	1/1	0.80	0.20	55,55,55,55	0
54	MG	1A	3577	1/1	0.80	0.20	26,26,26,26	0
54	MG	2B	3018	1/1	0.80	0.27	76,76,76,76	0
54	MG	1y	3001	1/1	0.80	0.38	61,61,61,61	0
54	MG	1A	3159	1/1	0.80	0.19	38,38,38,38	0
54	MG	2A	3589	1/1	0.80	0.16	57,57,57,57	0
54	MG	2A	3608	1/1	0.80	0.11	40,40,40,40	0
54	MG	2A	3386	1/1	0.80	0.14	68,68,68,68	0
54	MG	2a	1613	1/1	0.80	0.17	51,51,51,51	0
54	MG	1d	301	1/1	0.80	0.11	68,68,68,68	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3398	1/1	0.80	0.28	55,55,55,55	0
54	MG	1a	1653	1/1	0.80	0.16	60,60,60,60	0
54	MG	2A	3304	1/1	0.80	0.10	44,44,44,44	0
54	MG	1A	3870	1/1	0.80	0.11	46,46,46,46	0
54	MG	2A	3697	1/1	0.80	0.11	53,53,53,53	0
54	MG	2A	3553	1/1	0.80	0.16	56,56,56,56	0
54	MG	1A	3594	1/1	0.80	0.17	54,54,54,54	0
54	MG	1A	3602	1/1	0.81	0.20	54,54,54,54	0
54	MG	1A	3962	1/1	0.81	0.08	55,55,55,55	0
54	MG	2A	3193	1/1	0.81	0.27	47,47,47,47	0
54	MG	1a	1754	1/1	0.81	0.23	68,68,68,68	0
54	MG	2A	3355	1/1	0.81	0.23	46,46,46,46	0
54	MG	2A	3326	1/1	0.81	0.17	61,61,61,61	0
54	MG	2X	101	1/1	0.81	0.13	59,59,59,59	0
54	MG	2a	1748	1/1	0.81	0.16	52,52,52,52	0
54	MG	1a	1720	1/1	0.81	0.13	60,60,60,60	0
54	MG	2A	3330	1/1	0.81	0.17	69,69,69,69	0
54	MG	1A	3047	1/1	0.81	0.51	38,38,38,38	0
54	MG	1A	3779	1/1	0.81	0.24	48,48,48,48	0
54	MG	1A	3858	1/1	0.81	0.14	28,28,28,28	0
54	MG	2A	3188	1/1	0.81	0.14	51,51,51,51	0
54	MG	2q	201	1/1	0.81	0.18	64,64,64,64	0
54	MG	1a	1629	1/1	0.81	0.09	45,45,45,45	0
54	MG	1R	203	1/1	0.81	0.17	34,34,34,34	0
54	MG	1A	3913	1/1	0.81	0.32	61,61,61,61	0
54	MG	2a	1605	1/1	0.81	0.13	57,57,57,57	0
54	MG	1A	3187	1/1	0.81	0.39	49,49,49,49	0
54	MG	2a	1682	1/1	0.81	0.13	60,60,60,60	0
54	MG	1A	3380	1/1	0.82	0.15	29,29,29,29	0
54	MG	2A	3165	1/1	0.82	0.28	64,64,64,64	0
54	MG	1A	3138	1/1	0.82	0.19	59,59,59,59	0
54	MG	2A	3544	1/1	0.82	0.09	56,56,56,56	0
54	MG	2A	3242	1/1	0.82	0.41	63,63,63,63	0
54	MG	10	105	1/1	0.82	0.21	59,59,59,59	0
54	MG	2a	1676	1/1	0.82	0.21	68,68,68,68	0
54	MG	2a	1648	1/1	0.82	0.11	60,60,60,60	0
54	MG	2A	3449	1/1	0.82	0.09	58,58,58,58	0
54	MG	1A	3908	1/1	0.82	0.10	52,52,52,52	0
54	MG	1a	1701	1/1	0.82	0.20	71,71,71,71	0
54	MG	1A	3151	1/1	0.82	0.47	40,40,40,40	0
54	MG	1a	1667	1/1	0.82	0.14	50,50,50,50	0
54	MG	1A	3789	1/1	0.82	0.22	31,31,31,31	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3271	1/1	0.82	0.15	49,49,49,49	0
54	MG	1A	3144	1/1	0.82	0.11	51,51,51,51	0
54	MG	2a	1709	1/1	0.82	0.32	48,48,48,48	0
54	MG	2a	1615	1/1	0.82	0.12	60,60,60,60	0
54	MG	2a	1602	1/1	0.82	0.12	52,52,52,52	0
54	MG	2A	3563	1/1	0.82	0.11	60,60,60,60	0
54	MG	1A	3330	1/1	0.82	0.17	15,15,15,15	0
54	MG	2A	3229	1/1	0.82	0.66	49,49,49,49	0
54	MG	1A	3637	1/1	0.82	0.38	47,47,47,47	0
54	MG	2A	3640	1/1	0.82	0.08	52,52,52,52	0
54	MG	1A	3445	1/1	0.82	0.10	21,21,21,21	0
54	MG	2a	1747	1/1	0.82	0.10	61,61,61,61	0
54	MG	2a	1623	1/1	0.82	0.12	64,64,64,64	0
54	MG	2A	3203	1/1	0.82	0.11	51,51,51,51	0
54	MG	2a	1669	1/1	0.83	0.19	63,63,63,63	0
54	MG	1a	1813	1/1	0.83	0.10	60,60,60,60	0
54	MG	1y	3004	1/1	0.83	0.28	76,76,76,76	0
54	MG	2A	3502	1/1	0.83	0.27	64,64,64,64	0
54	MG	1A	3735	1/1	0.83	0.12	32,32,32,32	0
54	MG	1A	3479	1/1	0.83	0.18	20,20,20,20	0
54	MG	1A	3635	1/1	0.83	0.12	62,62,62,62	0
54	MG	1d	303	1/1	0.83	0.20	68,68,68,68	0
54	MG	2A	3053	1/1	0.83	0.28	47,47,47,47	0
54	MG	1A	3927	1/1	0.83	0.09	42,42,42,42	0
54	MG	2a	1678	1/1	0.83	0.10	57,57,57,57	0
54	MG	1A	3836	1/1	0.83	0.13	51,51,51,51	0
54	MG	1a	1707	1/1	0.83	0.09	58,58,58,58	0
54	MG	1A	3961	1/1	0.83	0.14	38,38,38,38	0
54	MG	2A	3116	1/1	0.83	0.16	53,53,53,53	0
54	MG	2A	3569	1/1	0.83	0.19	51,51,51,51	0
54	MG	1a	1679	1/1	0.83	0.22	60,60,60,60	0
54	MG	1a	1783	1/1	0.83	0.20	64,64,64,64	0
54	MG	2A	3520	1/1	0.83	0.18	54,54,54,54	0
54	MG	1a	1686	1/1	0.83	0.23	61,61,61,61	0
54	MG	1A	3567	1/1	0.83	0.12	62,62,62,62	0
54	MG	2A	3112	1/1	0.83	0.19	44,44,44,44	0
54	MG	2A	3251	1/1	0.83	0.15	60,60,60,60	0
54	MG	2A	3548	1/1	0.83	0.15	54,54,54,54	0
54	MG	2A	3341	1/1	0.83	0.15	33,33,33,33	0
54	MG	2A	3060	1/1	0.83	0.16	48,48,48,48	0
54	MG	1A	3039	1/1	0.83	0.14	56,56,56,56	0
54	MG	1a	1662	1/1	0.83	0.19	56,56,56,56	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3194	1/1	0.83	0.21	54,54,54,54	0
54	MG	2A	3056	1/1	0.83	0.32	46,46,46,46	0
54	MG	1A	3899	1/1	0.83	0.14	51,51,51,51	0
54	MG	1a	1604	1/1	0.83	0.13	62,62,62,62	0
54	MG	2A	3194	1/1	0.83	0.16	60,60,60,60	0
54	MG	1A	3190	1/1	0.83	0.19	45,45,45,45	0
54	MG	2A	3691	1/1	0.83	0.12	64,64,64,64	0
54	MG	2A	3472	1/1	0.83	0.17	52,52,52,52	0
54	MG	2A	3619	1/1	0.83	0.15	66,66,66,66	0
54	MG	1A	3737	1/1	0.83	0.24	53,53,53,53	0
54	MG	2p	3001	1/1	0.83	0.15	61,61,61,61	0
54	MG	1N	202	1/1	0.83	0.18	56,56,56,56	0
54	MG	1a	1749	1/1	0.83	0.13	46,46,46,46	0
54	MG	2j	8001	1/1	0.84	0.24	82,82,82,82	0
54	MG	1a	1814	1/1	0.84	0.23	52,52,52,52	0
54	MG	1A	3177	1/1	0.84	0.12	51,51,51,51	0
54	MG	2A	3508	1/1	0.84	0.22	57,57,57,57	0
54	MG	1a	1846	1/1	0.84	0.15	74,74,74,74	0
54	MG	1a	1620	1/1	0.84	0.14	43,43,43,43	0
54	MG	1A	3825	1/1	0.84	0.12	45,45,45,45	0
54	MG	1A	3903	1/1	0.84	0.22	63,63,63,63	0
54	MG	1A	3854	1/1	0.84	0.15	19,19,19,19	0
54	MG	1B	202	1/1	0.84	0.23	36,36,36,36	0
54	MG	2a	1614	1/1	0.84	0.21	74,74,74,74	0
54	MG	1a	1833	1/1	0.84	0.29	60,60,60,60	0
54	MG	2A	3214	1/1	0.84	0.10	56,56,56,56	0
54	MG	2a	1656	1/1	0.84	0.08	63,63,63,63	0
54	MG	1A	3817	1/1	0.84	0.16	65,65,65,65	0
54	MG	2A	3587	1/1	0.84	0.48	44,44,44,44	0
54	MG	1B	206	1/1	0.84	0.12	45,45,45,45	0
54	MG	2A	3072	1/1	0.84	0.17	49,49,49,49	0
54	MG	1A	3499	1/1	0.84	0.40	50,50,50,50	0
54	MG	2A	3191	1/1	0.84	0.23	57,57,57,57	0
54	MG	2A	3658	1/1	0.84	0.15	34,34,34,34	0
54	MG	2A	3335	1/1	0.84	0.19	56,56,56,56	0
54	MG	1a	1612	1/1	0.84	0.11	72,72,72,72	0
54	MG	1a	1617	1/1	0.84	0.15	58,58,58,58	0
54	MG	1A	3214	1/1	0.84	0.30	30,30,30,30	0
54	MG	1A	4023	1/1	0.84	0.49	36,36,36,36	0
54	MG	1a	1704	1/1	0.84	0.18	77,77,77,77	0
54	MG	2A	3401	1/1	0.84	0.07	54,54,54,54	0
54	MG	2A	3308	1/1	0.84	0.15	48,48,48,48	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3014	1/1	0.84	0.15	51,51,51,51	0
54	MG	2A	3428	1/1	0.84	0.15	53,53,53,53	0
54	MG	1A	3748	1/1	0.84	0.12	68,68,68,68	0
54	MG	1A	3949	1/1	0.84	0.28	68,68,68,68	0
54	MG	1A	3951	1/1	0.84	0.13	50,50,50,50	0
54	MG	2a	1700	1/1	0.84	0.21	48,48,48,48	0
54	MG	1a	1715	1/1	0.84	0.20	58,58,58,58	0
54	MG	1a	1676	1/1	0.84	0.17	46,46,46,46	0
54	MG	1A	3373	1/1	0.84	0.15	25,25,25,25	0
54	MG	2A	3202	1/1	0.84	0.09	62,62,62,62	0
54	MG	2A	3303	1/1	0.85	0.11	40,40,40,40	0
54	MG	2A	3581	1/1	0.85	0.19	39,39,39,39	0
54	MG	2A	3096	1/1	0.85	0.12	60,60,60,60	0
54	MG	1A	3056	1/1	0.85	0.12	52,52,52,52	0
54	MG	1a	1659	1/1	0.85	0.12	64,64,64,64	0
54	MG	1A	3430	1/1	0.85	0.17	38,38,38,38	0
54	MG	2A	3447	1/1	0.85	0.14	55,55,55,55	0
54	MG	2A	3552	1/1	0.85	0.10	63,63,63,63	0
54	MG	2A	3218	1/1	0.85	0.23	57,57,57,57	0
54	MG	1a	1702	1/1	0.85	0.11	52,52,52,52	0
54	MG	2A	3667	1/1	0.85	0.14	49,49,49,49	0
54	MG	1A	3887	1/1	0.85	0.06	69,69,69,69	0
54	MG	2A	3021	1/1	0.85	0.09	47,47,47,47	0
54	MG	1a	1628	1/1	0.85	0.18	49,49,49,49	0
54	MG	1A	3303	1/1	0.85	0.12	55,55,55,55	0
54	MG	2a	1631	1/1	0.85	0.09	52,52,52,52	0
54	MG	1a	1755	1/1	0.85	0.11	68,68,68,68	0
54	MG	2A	3618	1/1	0.85	0.11	50,50,50,50	0
54	MG	1U	202	1/1	0.85	0.20	48,48,48,48	0
54	MG	1A	3798	1/1	0.85	0.18	35,35,35,35	0
54	MG	2A	3273	1/1	0.85	0.15	51,51,51,51	0
54	MG	1A	3663	1/1	0.85	0.11	43,43,43,43	0
54	MG	2A	3467	1/1	0.85	0.15	79,79,79,79	0
54	MG	2D	305	1/1	0.85	0.20	53,53,53,53	0
54	MG	2A	3476	1/1	0.85	0.10	54,54,54,54	0
54	MG	2A	3486	1/1	0.85	0.15	56,56,56,56	0
54	MG	2A	3610	1/1	0.85	0.22	51,51,51,51	0
54	MG	1A	3434	1/1	0.85	0.13	44,44,44,44	0
54	MG	2A	3314	1/1	0.85	0.13	30,30,30,30	0
54	MG	1A	3209	1/1	0.85	0.18	52,52,52,52	0
54	MG	2A	3087	1/1	0.85	0.10	52,52,52,52	0
54	MG	1A	3208	1/1	0.85	0.13	53,53,53,53	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3036	1/1	0.85	0.17	57,57,57,57	0
54	MG	2a	1729	1/1	0.85	0.12	64,64,64,64	0
54	MG	2a	1726	1/1	0.85	0.19	62,62,62,62	0
54	MG	2A	3350	1/1	0.85	0.16	31,31,31,31	0
54	MG	1A	3173	1/1	0.85	0.17	43,43,43,43	0
54	MG	2B	3013	1/1	0.85	0.16	80,80,80,80	0
54	MG	2A	3080	1/1	0.85	0.23	57,57,57,57	0
54	MG	1t	3001	1/1	0.85	0.11	52,52,52,52	0
54	MG	1A	3563	1/1	0.85	0.25	30,30,30,30	0
54	MG	1a	1810	1/1	0.85	0.16	63,63,63,63	0
54	MG	1a	1777	1/1	0.85	0.21	61,61,61,61	0
54	MG	1A	3527	1/1	0.85	0.09	51,51,51,51	0
54	MG	1A	3379	1/1	0.85	0.13	73,73,73,73	0
54	MG	2A	3170	1/1	0.85	0.28	60,60,60,60	0
54	MG	2A	3669	1/1	0.86	0.17	59,59,59,59	0
54	MG	1A	3131	1/1	0.86	0.20	48,48,48,48	0
54	MG	1a	1775	1/1	0.86	0.15	59,59,59,59	0
54	MG	1a	1817	1/1	0.86	0.15	57,57,57,57	0
54	MG	1l	3002	1/1	0.86	0.21	72,72,72,72	0
54	MG	1A	3752	1/1	0.86	0.12	55,55,55,55	0
54	MG	1A	3730	1/1	0.86	0.16	26,26,26,26	0
54	MG	2A	3430	1/1	0.86	0.12	41,41,41,41	0
54	MG	1G	3003	1/1	0.86	0.15	57,57,57,57	0
54	MG	2A	3590	1/1	0.86	0.58	58,58,58,58	0
54	MG	2A	3399	1/1	0.86	0.15	42,42,42,42	0
54	MG	1D	310	1/1	0.86	0.22	62,62,62,62	0
54	MG	1A	3488	1/1	0.86	0.09	56,56,56,56	0
54	MG	2A	3137	1/1	0.86	0.21	52,52,52,52	0
54	MG	1A	3559	1/1	0.86	0.17	55,55,55,55	0
57	MPD	2A	3710	8/8	0.86	0.40	43,49,51,57	0
54	MG	1A	3720	1/1	0.86	0.10	52,52,52,52	0
54	MG	1a	1841	1/1	0.86	0.12	57,57,57,57	0
54	MG	2A	3262	1/1	0.86	0.13	62,62,62,62	0
54	MG	1a	1855	1/1	0.86	0.07	68,68,68,68	0
54	MG	1A	3339	1/1	0.86	0.13	48,48,48,48	0
57	MPD	2B	3020	8/8	0.86	0.26	61,66,69,79	0
54	MG	2A	3147	1/1	0.86	0.68	44,44,44,44	0
54	MG	1A	3642	1/1	0.86	0.10	51,51,51,51	0
54	MG	1A	3584	1/1	0.86	0.14	51,51,51,51	0
54	MG	17	102	1/1	0.86	0.14	40,40,40,40	0
54	MG	2A	3579	1/1	0.86	0.16	65,65,65,65	0
54	MG	2a	1607	1/1	0.86	0.19	64,64,64,64	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3672	1/1	0.86	0.19	55,55,55,55	0
54	MG	1B	204	1/1	0.86	0.18	52,52,52,52	0
54	MG	1a	1641	1/1	0.86	0.22	54,54,54,54	0
54	MG	1a	1671	1/1	0.86	0.13	60,60,60,60	0
54	MG	1a	1776	1/1	0.86	0.12	69,69,69,69	0
54	MG	2A	3321	1/1	0.86	0.13	43,43,43,43	0
54	MG	2a	1685	1/1	0.86	0.16	52,52,52,52	0
54	MG	1A	3847	1/1	0.86	0.09	39,39,39,39	0
54	MG	1A	3233	1/1	0.86	0.38	48,48,48,48	0
54	MG	1A	3953	1/1	0.86	0.15	51,51,51,51	0
54	MG	2a	1618	1/1	0.86	0.22	66,66,66,66	0
54	MG	1A	3969	1/1	0.86	0.34	45,45,45,45	0
54	MG	1A	3799	1/1	0.86	0.17	46,46,46,46	0
54	MG	2a	1704	1/1	0.86	0.28	63,63,63,63	0
54	MG	1A	3082	1/1	0.86	0.14	55,55,55,55	0
54	MG	1A	3901	1/1	0.86	0.14	37,37,37,37	0
54	MG	2A	3521	1/1	0.86	0.19	51,51,51,51	0
54	MG	2A	3493	1/1	0.86	0.10	55,55,55,55	0
54	MG	2A	3675	1/1	0.86	0.11	73,73,73,73	0
54	MG	2A	3183	1/1	0.86	0.32	53,53,53,53	0
54	MG	2a	1663	1/1	0.86	0.12	48,48,48,48	0
54	MG	1a	1780	1/1	0.86	0.25	60,60,60,60	0
54	MG	1B	224	1/1	0.86	0.15	43,43,43,43	0
54	MG	1a	1794	1/1	0.86	0.10	67,67,67,67	0
54	MG	1A	3875	1/1	0.86	0.31	49,49,49,49	0
54	MG	2A	3126	1/1	0.86	0.22	42,42,42,42	0
54	MG	1A	3867	1/1	0.86	0.12	47,47,47,47	0
54	MG	2a	1627	1/1	0.86	0.09	61,61,61,61	0
54	MG	2a	1675	1/1	0.87	0.12	56,56,56,56	0
54	MG	2A	3448	1/1	0.87	0.07	47,47,47,47	0
54	MG	2A	3510	1/1	0.87	0.21	64,64,64,64	0
54	MG	2A	3651	1/1	0.87	0.11	58,58,58,58	0
54	MG	2A	3684	1/1	0.87	0.15	65,65,65,65	0
54	MG	2A	3368	1/1	0.87	0.15	30,30,30,30	0
54	MG	2a	1603	1/1	0.87	0.12	57,57,57,57	0
54	MG	28	8003	1/1	0.87	0.19	56,56,56,56	0
54	MG	1A	3670	1/1	0.87	0.18	25,25,25,25	0
54	MG	2A	3068	1/1	0.87	0.44	59,59,59,59	0
54	MG	2A	3466	1/1	0.87	0.14	68,68,68,68	0
54	MG	1A	3937	1/1	0.87	0.15	74,74,74,74	0
54	MG	1A	3280	1/1	0.87	0.17	44,44,44,44	0
54	MG	2A	3071	1/1	0.87	0.31	46,46,46,46	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3252	1/1	0.87	0.23	61,61,61,61	0
54	MG	2A	3477	1/1	0.87	0.34	59,59,59,59	0
54	MG	2A	3547	1/1	0.87	0.13	38,38,38,38	0
54	MG	1A	3906	1/1	0.87	0.19	55,55,55,55	0
54	MG	1A	3755	1/1	0.87	0.10	47,47,47,47	0
54	MG	1A	3120	1/1	0.87	0.17	44,44,44,44	0
54	MG	1G	3002	1/1	0.87	0.13	66,66,66,66	0
54	MG	1a	1658	1/1	0.87	0.15	46,46,46,46	0
54	MG	1A	3291	1/1	0.87	0.17	45,45,45,45	0
54	MG	2a	1694	1/1	0.87	0.20	60,60,60,60	0
54	MG	2a	1716	1/1	0.87	0.25	57,57,57,57	0
54	MG	2A	3397	1/1	0.87	0.35	55,55,55,55	0
54	MG	1a	1832	1/1	0.87	0.10	42,42,42,42	0
54	MG	1D	302	1/1	0.87	0.42	42,42,42,42	0
54	MG	1A	3182	1/1	0.87	0.15	43,43,43,43	0
54	MG	2P	202	1/1	0.87	0.24	59,59,59,59	0
54	MG	2A	3010	1/1	0.87	0.26	54,54,54,54	0
54	MG	2A	3659	1/1	0.87	0.41	49,49,49,49	0
54	MG	1A	3866	1/1	0.87	0.10	35,35,35,35	0
54	MG	1A	3031	1/1	0.87	0.25	39,39,39,39	0
54	MG	2A	3629	1/1	0.87	0.11	51,51,51,51	0
54	MG	2A	3370	1/1	0.87	0.10	70,70,70,70	0
54	MG	2A	3305	1/1	0.87	0.16	26,26,26,26	0
54	MG	1a	1773	1/1	0.87	0.24	61,61,61,61	0
54	MG	1A	3440	1/1	0.87	0.17	18,18,18,18	0
54	MG	1A	3252	1/1	0.87	0.12	52,52,52,52	0
54	MG	2a	1681	1/1	0.87	0.19	57,57,57,57	0
54	MG	2a	1683	1/1	0.87	0.18	57,57,57,57	0
54	MG	1A	3832	1/1	0.87	0.13	57,57,57,57	0
54	MG	2a	1651	1/1	0.87	0.19	58,58,58,58	0
54	MG	1A	3354	1/1	0.87	0.14	20,20,20,20	0
54	MG	28	8002	1/1	0.87	0.09	45,45,45,45	0
54	MG	1a	1633	1/1	0.87	0.16	37,37,37,37	0
54	MG	1H	8001	1/1	0.87	0.16	67,67,67,67	0
54	MG	2A	3285	1/1	0.87	0.16	65,65,65,65	0
54	MG	1E	305	1/1	0.87	0.15	50,50,50,50	0
54	MG	2A	3231	1/1	0.87	0.10	42,42,42,42	0
54	MG	1A	3943	1/1	0.87	0.20	52,52,52,52	0
54	MG	2A	3078	1/1	0.87	0.08	63,63,63,63	0
54	MG	2a	1639	1/1	0.87	0.28	54,54,54,54	0
54	MG	2A	3599	1/1	0.87	0.15	45,45,45,45	0
54	MG	2a	1749	1/1	0.87	0.27	64,64,64,64	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3148	1/1	0.87	0.74	57,57,57,57	0
54	MG	1A	3361	1/1	0.87	0.19	27,27,27,27	0
54	MG	1A	3757	1/1	0.87	0.11	48,48,48,48	0
54	MG	1A	3675	1/1	0.87	0.16	54,54,54,54	0
54	MG	1a	1649	1/1	0.87	0.43	41,41,41,41	0
54	MG	1A	4017	1/1	0.87	0.20	34,34,34,34	0
54	MG	1A	3158	1/1	0.87	0.23	41,41,41,41	0
54	MG	2A	3172	1/1	0.87	0.22	56,56,56,56	0
54	MG	1A	3043	1/1	0.87	0.25	52,52,52,52	0
54	MG	2A	3545	1/1	0.87	0.12	53,53,53,53	0
54	MG	1a	1650	1/1	0.87	0.22	62,62,62,62	0
54	MG	1a	1805	1/1	0.87	0.11	52,52,52,52	0
54	MG	2A	3421	1/1	0.87	0.11	62,62,62,62	0
54	MG	1A	3665	1/1	0.87	0.09	32,32,32,32	0
54	MG	1A	3342	1/1	0.87	0.10	48,48,48,48	0
54	MG	1A	3519	1/1	0.87	0.10	38,38,38,38	0
54	MG	1A	3095	1/1	0.87	0.19	49,49,49,49	0
54	MG	2A	3683	1/1	0.87	0.09	73,73,73,73	0
54	MG	1f	3002	1/1	0.87	0.14	53,53,53,53	0
54	MG	2A	3721	1/1	0.88	0.09	42,42,42,42	0
54	MG	1A	3550	1/1	0.88	0.19	53,53,53,53	0
54	MG	1A	3672	1/1	0.88	0.10	40,40,40,40	0
54	MG	2A	3562	1/1	0.88	0.09	63,63,63,63	0
54	MG	2A	3134	1/1	0.88	0.14	36,36,36,36	0
54	MG	1X	101	1/1	0.88	0.19	52,52,52,52	0
54	MG	1A	3324	1/1	0.88	0.20	39,39,39,39	0
54	MG	1A	3242	1/1	0.88	0.16	53,53,53,53	0
54	MG	2A	3124	1/1	0.88	0.27	54,54,54,54	0
54	MG	2a	1695	1/1	0.88	0.16	62,62,62,62	0
54	MG	2a	1641	1/1	0.88	0.25	66,66,66,66	0
54	MG	2A	3029	1/1	0.88	0.19	55,55,55,55	0
54	MG	2G	3003	1/1	0.88	0.17	79,79,79,79	0
54	MG	1a	1816	1/1	0.88	0.17	52,52,52,52	0
54	MG	2A	3423	1/1	0.88	0.13	45,45,45,45	0
54	MG	2A	3192	1/1	0.88	0.19	52,52,52,52	0
54	MG	1A	3618	1/1	0.88	0.13	42,42,42,42	0
54	MG	2a	1632	1/1	0.88	0.20	59,59,59,59	0
54	MG	1A	4010	1/1	0.88	0.74	31,31,31,31	0
54	MG	2A	3106	1/1	0.88	0.22	46,46,46,46	0
54	MG	2f	3001	1/1	0.88	0.15	44,44,44,44	0
54	MG	2A	3662	1/1	0.88	0.13	56,56,56,56	0
54	MG	1A	3402	1/1	0.88	0.14	50,50,50,50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3055	1/1	0.88	0.12	45,45,45,45	0
54	MG	2a	1667	1/1	0.88	0.27	56,56,56,56	0
54	MG	1A	3355	1/1	0.88	0.14	33,33,33,33	0
54	MG	1P	202	1/1	0.88	0.12	66,66,66,66	0
54	MG	2A	3648	1/1	0.88	0.08	73,73,73,73	0
54	MG	1a	1842	1/1	0.88	0.11	51,51,51,51	0
54	MG	2A	3540	1/1	0.88	0.23	37,37,37,37	0
54	MG	2A	3111	1/1	0.88	0.13	66,66,66,66	0
54	MG	1a	1627	1/1	0.88	0.14	54,54,54,54	0
54	MG	1a	1791	1/1	0.88	0.08	60,60,60,60	0
54	MG	1A	3964	1/1	0.88	0.75	36,36,36,36	0
54	MG	1a	1808	1/1	0.88	0.19	74,74,74,74	0
54	MG	2A	3481	1/1	0.88	0.46	46,46,46,46	0
54	MG	1A	3619	1/1	0.88	0.42	25,25,25,25	0
54	MG	1a	1635	1/1	0.88	0.19	34,34,34,34	0
54	MG	2A	3408	1/1	0.88	0.14	54,54,54,54	0
54	MG	1A	3093	1/1	0.88	0.20	38,38,38,38	0
54	MG	2A	3412	1/1	0.88	0.18	61,61,61,61	0
54	MG	2a	1644	1/1	0.88	0.25	55,55,55,55	0
54	MG	2A	3632	1/1	0.88	0.11	49,49,49,49	0
54	MG	2a	1745	1/1	0.88	0.19	67,67,67,67	0
54	MG	1A	3935	1/1	0.88	0.09	55,55,55,55	0
54	MG	1A	3572	1/1	0.88	0.56	46,46,46,46	0
54	MG	1a	1729	1/1	0.88	0.25	60,60,60,60	0
54	MG	1a	1631	1/1	0.88	0.26	64,64,64,64	0
54	MG	1A	3332	1/1	0.88	0.14	60,60,60,60	0
54	MG	2A	3041	1/1	0.88	0.16	54,54,54,54	0
54	MG	2A	3602	1/1	0.88	0.15	46,46,46,46	0
54	MG	1A	3448	1/1	0.88	0.15	24,24,24,24	0
54	MG	1A	3274	1/1	0.88	0.13	40,40,40,40	0
54	MG	1A	3917	1/1	0.88	0.12	51,51,51,51	0
54	MG	1A	3258	1/1	0.88	0.24	32,32,32,32	0
54	MG	2A	3081	1/1	0.88	0.11	55,55,55,55	0
54	MG	2A	3695	1/1	0.88	0.15	36,36,36,36	0
54	MG	1A	3394	1/1	0.88	0.15	18,18,18,18	0
54	MG	1A	3181	1/1	0.88	0.17	57,57,57,57	0
54	MG	1F	310	1/1	0.88	0.11	42,42,42,42	0
54	MG	1a	1731	1/1	0.88	0.24	56,56,56,56	0
54	MG	1D	307	1/1	0.88	0.18	40,40,40,40	0
54	MG	1a	1742	1/1	0.89	0.25	62,62,62,62	0
54	MG	1A	4007	1/1	0.89	0.33	23,23,23,23	0
54	MG	1A	3404	1/1	0.89	0.19	65,65,65,65	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3705	1/1	0.89	0.17	48,48,48,48	0
54	MG	1A	3399	1/1	0.89	0.16	33,33,33,33	0
54	MG	2A	3375	1/1	0.89	0.15	64,64,64,64	0
54	MG	1a	1743	1/1	0.89	0.11	62,62,62,62	0
54	MG	1A	3124	1/1	0.89	0.20	40,40,40,40	0
54	MG	2A	3301	1/1	0.89	0.10	56,56,56,56	0
54	MG	1G	3001	1/1	0.89	0.15	52,52,52,52	0
54	MG	2a	1601	1/1	0.89	0.17	48,48,48,48	0
54	MG	2A	3538	1/1	0.89	0.11	35,35,35,35	0
59	ZN	2Y	501	1/1	0.89	0.12	79,79,79,79	0
54	MG	1A	3500	1/1	0.89	0.17	44,44,44,44	0
54	MG	1A	3161	1/1	0.89	0.16	34,34,34,34	0
54	MG	2a	1693	1/1	0.89	0.14	55,55,55,55	0
54	MG	2D	307	1/1	0.89	0.50	43,43,43,43	0
54	MG	1A	3708	1/1	0.89	0.10	37,37,37,37	0
54	MG	2A	3450	1/1	0.89	0.11	55,55,55,55	0
54	MG	2B	3010	1/1	0.89	0.14	68,68,68,68	0
54	MG	1U	201	1/1	0.89	0.37	38,38,38,38	0
54	MG	2A	3687	1/1	0.89	0.14	64,64,64,64	0
54	MG	1A	3611	1/1	0.89	0.12	41,41,41,41	0
54	MG	1A	3690	1/1	0.89	0.14	46,46,46,46	0
54	MG	2A	3258	1/1	0.89	0.11	36,36,36,36	0
54	MG	1n	502	1/1	0.89	0.12	51,51,51,51	0
54	MG	2A	3019	1/1	0.89	0.17	56,56,56,56	0
54	MG	2A	3016	1/1	0.89	0.62	37,37,37,37	0
54	MG	1a	1781	1/1	0.89	0.19	58,58,58,58	0
54	MG	1A	3958	1/1	0.89	0.20	53,53,53,53	0
54	MG	2a	1680	1/1	0.89	0.09	58,58,58,58	0
54	MG	1A	3820	1/1	0.89	0.14	50,50,50,50	0
54	MG	2A	3524	1/1	0.89	0.21	26,26,26,26	0
54	MG	2A	3044	1/1	0.89	0.17	46,46,46,46	0
54	MG	1A	3749	1/1	0.89	0.19	36,36,36,36	0
54	MG	2D	301	1/1	0.89	0.10	56,56,56,56	0
54	MG	19	502	1/1	0.89	0.21	50,50,50,50	0
54	MG	2A	3245	1/1	0.89	0.20	60,60,60,60	0
54	MG	2A	3196	1/1	0.89	0.12	50,50,50,50	0
54	MG	2A	3055	1/1	0.89	0.14	38,38,38,38	0
54	MG	1o	3001	1/1	0.89	0.18	44,44,44,44	0
54	MG	1A	3220	1/1	0.89	0.40	31,31,31,31	0
54	MG	2A	3287	1/1	0.89	0.17	42,42,42,42	0
54	MG	1A	3253	1/1	0.89	0.17	59,59,59,59	0
54	MG	2A	3205	1/1	0.89	0.18	60,60,60,60	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3205	1/1	0.89	0.11	42,42,42,42	0
54	MG	1A	3530	1/1	0.89	0.12	44,44,44,44	0
54	MG	1A	3526	1/1	0.89	0.08	40,40,40,40	0
54	MG	1a	1619	1/1	0.89	0.13	54,54,54,54	0
54	MG	1A	3123	1/1	0.89	0.11	32,32,32,32	0
54	MG	2a	1746	1/1	0.89	0.18	60,60,60,60	0
54	MG	2A	3296	1/1	0.89	0.10	36,36,36,36	0
54	MG	1h	3002	1/1	0.89	0.15	64,64,64,64	0
54	MG	1A	3122	1/1	0.89	0.13	32,32,32,32	0
54	MG	2A	3633	1/1	0.89	0.10	43,43,43,43	0
54	MG	2A	3463	1/1	0.89	0.14	62,62,62,62	0
54	MG	1A	3030	1/1	0.89	0.09	54,54,54,54	0
54	MG	1A	3010	1/1	0.89	0.12	38,38,38,38	0
54	MG	2A	3230	1/1	0.89	0.30	55,55,55,55	0
54	MG	1A	3936	1/1	0.89	0.36	33,33,33,33	0
54	MG	1A	3679	1/1	0.89	0.29	52,52,52,52	0
54	MG	1A	3484	1/1	0.89	0.12	35,35,35,35	0
54	MG	1a	1622	1/1	0.89	0.11	51,51,51,51	0
54	MG	1A	3703	1/1	0.89	0.36	47,47,47,47	0
54	MG	2A	3348	1/1	0.89	0.19	42,42,42,42	0
54	MG	1B	229	1/1	0.89	0.11	41,41,41,41	0
54	MG	2A	3280	1/1	0.89	0.11	58,58,58,58	0
54	MG	2a	1649	1/1	0.89	0.16	49,49,49,49	0
54	MG	1a	1844	1/1	0.89	0.19	58,58,58,58	0
54	MG	1S	8001	1/1	0.89	0.12	62,62,62,62	0
54	MG	1A	3718	1/1	0.89	0.13	26,26,26,26	0
54	MG	2A	3468	1/1	0.89	0.16	61,61,61,61	0
54	MG	2A	3384	1/1	0.89	0.39	38,38,38,38	0
54	MG	1A	3654	1/1	0.89	0.48	42,42,42,42	0
54	MG	2A	3594	1/1	0.89	0.25	60,60,60,60	0
54	MG	2A	3156	1/1	0.89	0.12	41,41,41,41	0
54	MG	2A	3200	1/1	0.89	0.12	45,45,45,45	0
54	MG	1A	3241	1/1	0.89	0.15	43,43,43,43	0
54	MG	1A	3184	1/1	0.89	0.13	50,50,50,50	0
54	MG	1A	3810	1/1	0.89	0.09	37,37,37,37	0
54	MG	2e	3001	1/1	0.89	0.32	58,58,58,58	0
54	MG	2A	3593	1/1	0.89	0.07	53,53,53,53	0
54	MG	1A	3666	1/1	0.90	0.10	20,20,20,20	0
54	MG	1A	3573	1/1	0.90	0.70	52,52,52,52	0
54	MG	2a	1661	1/1	0.90	0.41	54,54,54,54	0
54	MG	1A	3301	1/1	0.90	0.20	27,27,27,27	0
54	MG	1A	3070	1/1	0.90	0.17	42,42,42,42	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3058	1/1	0.90	0.21	51,51,51,51	0
54	MG	1A	3610	1/1	0.90	0.14	27,27,27,27	0
54	MG	1a	1778	1/1	0.90	0.15	60,60,60,60	0
54	MG	2A	3483	1/1	0.90	0.13	61,61,61,61	0
54	MG	1A	3071	1/1	0.90	0.49	29,29,29,29	0
54	MG	2A	3671	1/1	0.90	0.13	56,56,56,56	0
54	MG	2Q	3001	1/1	0.90	0.06	61,61,61,61	0
54	MG	2D	303	1/1	0.90	0.52	40,40,40,40	0
54	MG	1A	3928	1/1	0.90	0.12	27,27,27,27	0
54	MG	2A	3613	1/1	0.90	0.18	57,57,57,57	0
54	MG	1a	1673	1/1	0.90	0.35	55,55,55,55	0
54	MG	1A	3784	1/1	0.90	0.11	42,42,42,42	0
54	MG	1A	3534	1/1	0.90	0.15	60,60,60,60	0
54	MG	2A	3504	1/1	0.90	0.10	60,60,60,60	0
54	MG	1A	3781	1/1	0.90	0.07	40,40,40,40	0
54	MG	2A	3317	1/1	0.90	0.11	33,33,33,33	0
54	MG	2a	1720	1/1	0.90	0.18	50,50,50,50	0
54	MG	2a	1621	1/1	0.90	0.14	68,68,68,68	0
54	MG	1A	3696	1/1	0.90	0.16	52,52,52,52	0
54	MG	1A	3077	1/1	0.90	0.41	28,28,28,28	0
54	MG	2G	3002	1/1	0.90	0.16	65,65,65,65	0
54	MG	2B	3004	1/1	0.90	0.12	58,58,58,58	0
54	MG	2A	3457	1/1	0.90	0.13	54,54,54,54	0
54	MG	1A	3415	1/1	0.90	0.08	47,47,47,47	0
54	MG	1A	3751	1/1	0.90	0.31	55,55,55,55	0
54	MG	1A	3704	1/1	0.90	0.12	50,50,50,50	0
54	MG	1a	1806	1/1	0.90	0.20	53,53,53,53	0
54	MG	1A	3004	1/1	0.90	0.23	43,43,43,43	0
54	MG	1A	3256	1/1	0.90	0.15	51,51,51,51	0
54	MG	1A	3347	1/1	0.90	0.12	36,36,36,36	0
54	MG	2a	1672	1/1	0.90	0.13	62,62,62,62	0
54	MG	1a	1819	1/1	0.90	0.20	51,51,51,51	0
54	MG	1A	3079	1/1	0.90	0.63	30,30,30,30	0
54	MG	1a	1837	1/1	0.90	0.16	44,44,44,44	0
54	MG	1B	230	1/1	0.90	0.13	68,68,68,68	0
54	MG	1B	225	1/1	0.90	0.10	40,40,40,40	0
54	MG	2A	3065	1/1	0.90	0.41	49,49,49,49	0
54	MG	1A	3574	1/1	0.90	0.16	26,26,26,26	0
54	MG	15	102	1/1	0.90	0.27	42,42,42,42	0
54	MG	1A	3391	1/1	0.90	0.23	37,37,37,37	0
54	MG	2A	3720	1/1	0.90	0.10	44,44,44,44	0
54	MG	1A	3678	1/1	0.90	0.16	40,40,40,40	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1818	1/1	0.90	0.16	62,62,62,62	0
54	MG	2A	3462	1/1	0.90	0.12	53,53,53,53	0
54	MG	1A	3615	1/1	0.90	0.18	50,50,50,50	0
54	MG	2A	3482	1/1	0.90	0.16	51,51,51,51	0
54	MG	2A	3182	1/1	0.90	0.16	53,53,53,53	0
54	MG	1A	3102	1/1	0.90	0.16	53,53,53,53	0
54	MG	2A	3244	1/1	0.90	1.30	44,44,44,44	0
54	MG	1A	3952	1/1	0.90	0.09	46,46,46,46	0
54	MG	1A	3713	1/1	0.90	0.31	49,49,49,49	0
54	MG	2A	3454	1/1	0.90	0.14	70,70,70,70	0
54	MG	1A	3426	1/1	0.90	0.20	14,14,14,14	0
54	MG	1d	304	1/1	0.90	0.12	56,56,56,56	0
54	MG	2A	3123	1/1	0.90	0.17	49,49,49,49	0
54	MG	2D	308	1/1	0.90	0.14	27,27,27,27	0
54	MG	2A	3406	1/1	0.90	0.14	54,54,54,54	0
54	MG	2A	3236	1/1	0.90	0.12	61,61,61,61	0
54	MG	2A	3063	1/1	0.90	0.47	58,58,58,58	0
54	MG	2A	3250	1/1	0.90	0.14	46,46,46,46	0
54	MG	2A	3143	1/1	0.90	0.08	41,41,41,41	0
54	MG	2F	301	1/1	0.90	0.16	39,39,39,39	0
54	MG	1A	3085	1/1	0.90	0.09	36,36,36,36	0
54	MG	1A	3449	1/1	0.90	0.17	17,17,17,17	0
54	MG	2A	3597	1/1	0.90	0.32	61,61,61,61	0
54	MG	1A	3283	1/1	0.90	0.15	32,32,32,32	0
54	MG	1A	3021	1/1	0.90	0.25	38,38,38,38	0
54	MG	1A	3528	1/1	0.90	0.13	43,43,43,43	0
54	MG	2A	3105	1/1	0.90	0.49	46,46,46,46	0
54	MG	1l	103	1/1	0.90	0.10	42,42,42,42	0
54	MG	1a	1779	1/1	0.90	0.13	58,58,58,58	0
54	MG	2A	3555	1/1	0.90	0.14	61,61,61,61	0
54	MG	1A	3286	1/1	0.90	0.33	56,56,56,56	0
54	MG	1A	3659	1/1	0.90	0.53	52,52,52,52	0
54	MG	2A	3469	1/1	0.90	0.07	61,61,61,61	0
54	MG	2A	3109	1/1	0.90	0.49	39,39,39,39	0
54	MG	1a	1703	1/1	0.90	0.16	60,60,60,60	0
54	MG	1a	1726	1/1	0.90	0.19	62,62,62,62	0
54	MG	1A	3582	1/1	0.90	0.19	41,41,41,41	0
54	MG	1a	1718	1/1	0.90	0.10	56,56,56,56	0
54	MG	1B	221	1/1	0.90	0.18	34,34,34,34	0
54	MG	1A	3050	1/1	0.90	0.34	27,27,27,27	0
54	MG	1A	3558	1/1	0.90	0.10	34,34,34,34	0
54	MG	1y	3003	1/1	0.90	0.17	74,74,74,74	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3519	1/1	0.90	0.15	54,54,54,54	0
54	MG	2A	3607	1/1	0.90	0.16	62,62,62,62	0
54	MG	1a	1697	1/1	0.90	0.13	51,51,51,51	0
54	MG	2A	3290	1/1	0.90	0.15	30,30,30,30	0
54	MG	2A	3644	1/1	0.90	0.15	48,48,48,48	0
54	MG	1A	3363	1/1	0.90	0.15	28,28,28,28	0
54	MG	2a	1608	1/1	0.90	0.14	62,62,62,62	0
54	MG	1B	217	1/1	0.90	0.37	61,61,61,61	0
54	MG	1a	1744	1/1	0.90	0.26	62,62,62,62	0
54	MG	2A	3220	1/1	0.90	0.14	58,58,58,58	0
54	MG	2A	3512	1/1	0.90	0.14	51,51,51,51	0
54	MG	1a	1845	1/1	0.90	0.16	78,78,78,78	0
54	MG	1N	203	1/1	0.90	0.09	53,53,53,53	0
54	MG	1a	1751	1/1	0.90	0.19	69,69,69,69	0
54	MG	2A	3088	1/1	0.90	0.10	56,56,56,56	0
54	MG	2A	3199	1/1	0.90	0.26	47,47,47,47	0
54	MG	1a	1626	1/1	0.90	0.22	59,59,59,59	0
54	MG	1A	3955	1/1	0.90	0.10	39,39,39,39	0
54	MG	2A	3656	1/1	0.90	0.21	48,48,48,48	0
54	MG	1d	305	1/1	0.90	0.19	56,56,56,56	0
54	MG	2A	3478	1/1	0.91	0.11	36,36,36,36	0
54	MG	1A	3296	1/1	0.91	0.14	19,19,19,19	0
54	MG	1A	3667	1/1	0.91	0.13	40,40,40,40	0
54	MG	1A	3411	1/1	0.91	0.12	46,46,46,46	0
54	MG	2A	3224	1/1	0.91	0.63	35,35,35,35	0
54	MG	1A	3532	1/1	0.91	0.17	17,17,17,17	0
54	MG	1A	3213	1/1	0.91	0.20	33,33,33,33	0
54	MG	2a	1617	1/1	0.91	0.19	43,43,43,43	0
54	MG	1F	313	1/1	0.91	0.10	31,31,31,31	0
54	MG	1A	3302	1/1	0.91	0.16	27,27,27,27	0
54	MG	1A	3548	1/1	0.91	0.15	34,34,34,34	0
54	MG	2A	3077	1/1	0.91	0.17	32,32,32,32	0
54	MG	2A	3682	1/1	0.91	0.10	51,51,51,51	0
54	MG	1a	1853	1/1	0.91	0.18	47,47,47,47	0
54	MG	1a	1772	1/1	0.91	0.19	57,57,57,57	0
54	MG	1A	3688	1/1	0.91	0.20	34,34,34,34	0
54	MG	1T	201	1/1	0.91	0.14	54,54,54,54	0
54	MG	2A	3358	1/1	0.91	0.17	38,38,38,38	0
54	MG	11	102	1/1	0.91	0.18	47,47,47,47	0
54	MG	2A	3291	1/1	0.91	0.10	47,47,47,47	0
54	MG	2A	3179	1/1	0.91	0.08	65,65,65,65	0
54	MG	2A	3249	1/1	0.91	0.14	45,45,45,45	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3543	1/1	0.91	0.24	44,44,44,44	0
54	MG	1a	1613	1/1	0.91	0.15	60,60,60,60	0
54	MG	2A	3043	1/1	0.91	0.11	68,68,68,68	0
54	MG	2A	3284	1/1	0.91	0.18	55,55,55,55	0
54	MG	2A	3554	1/1	0.91	0.09	49,49,49,49	0
54	MG	2A	3528	1/1	0.91	0.20	32,32,32,32	0
54	MG	2A	3666	1/1	0.91	0.17	51,51,51,51	0
54	MG	2A	3374	1/1	0.91	0.10	26,26,26,26	0
54	MG	2A	3507	1/1	0.91	0.17	54,54,54,54	0
54	MG	1A	3522	1/1	0.91	0.14	38,38,38,38	0
54	MG	1A	3857	1/1	0.91	0.12	26,26,26,26	0
54	MG	2A	3413	1/1	0.91	0.14	63,63,63,63	0
54	MG	2A	3328	1/1	0.91	0.15	56,56,56,56	0
54	MG	1A	3565	1/1	0.91	0.21	36,36,36,36	0
54	MG	1A	3721	1/1	0.91	0.19	25,25,25,25	0
54	MG	1A	3160	1/1	0.91	0.10	41,41,41,41	0
54	MG	1A	3686	1/1	0.91	0.18	32,32,32,32	0
54	MG	1a	1639	1/1	0.91	0.20	49,49,49,49	0
54	MG	1A	3251	1/1	0.91	0.29	23,23,23,23	0
54	MG	1A	3167	1/1	0.91	0.47	28,28,28,28	0
54	MG	1A	3946	1/1	0.91	0.09	44,44,44,44	0
54	MG	1A	3436	1/1	0.91	0.09	41,41,41,41	0
54	MG	2A	3660	1/1	0.91	0.17	61,61,61,61	0
54	MG	2A	3551	1/1	0.91	0.12	61,61,61,61	0
54	MG	1P	203	1/1	0.91	0.07	29,29,29,29	0
54	MG	1A	3878	1/1	0.91	0.32	57,57,57,57	0
54	MG	1A	3485	1/1	0.91	0.07	47,47,47,47	0
54	MG	1A	3929	1/1	0.91	0.14	38,38,38,38	0
54	MG	2a	1666	1/1	0.91	0.10	57,57,57,57	0
54	MG	2a	1635	1/1	0.91	0.15	71,71,71,71	0
54	MG	2A	3051	1/1	0.91	0.18	38,38,38,38	0
54	MG	1A	3092	1/1	0.91	0.20	32,32,32,32	0
54	MG	2A	3373	1/1	0.91	0.16	55,55,55,55	0
54	MG	2r	8001	1/1	0.91	0.15	65,65,65,65	0
54	MG	2A	3054	1/1	0.91	0.20	63,63,63,63	0
54	MG	1B	203	1/1	0.91	0.13	57,57,57,57	0
54	MG	1A	3460	1/1	0.91	0.18	30,30,30,30	0
54	MG	2B	3008	1/1	0.91	0.08	66,66,66,66	0
54	MG	1A	3051	1/1	0.91	0.60	26,26,26,26	0
54	MG	1A	3140	1/1	0.91	0.46	29,29,29,29	0
54	MG	1a	1669	1/1	0.91	0.16	51,51,51,51	0
54	MG	1d	306	1/1	0.91	0.19	56,56,56,56	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1625	1/1	0.91	0.16	51,51,51,51	0
54	MG	2A	3070	1/1	0.91	0.59	42,42,42,42	0
54	MG	1A	3217	1/1	0.91	0.61	30,30,30,30	0
54	MG	1A	3766	1/1	0.91	0.12	47,47,47,47	0
54	MG	1a	1657	1/1	0.91	0.13	59,59,59,59	0
54	MG	2a	1743	1/1	0.91	0.21	63,63,63,63	0
54	MG	2A	3598	1/1	0.91	0.09	53,53,53,53	0
54	MG	2A	3379	1/1	0.91	0.16	40,40,40,40	0
54	MG	1A	3321	1/1	0.91	0.14	16,16,16,16	0
54	MG	1A	4013	1/1	0.91	0.86	29,29,29,29	0
54	MG	1a	1696	1/1	0.91	0.15	70,70,70,70	0
54	MG	1a	1605	1/1	0.91	0.13	56,56,56,56	0
54	MG	2R	201	1/1	0.91	0.20	35,35,35,35	0
57	MPD	1a	1854	8/8	0.91	0.15	46,63,67,69	0
54	MG	1A	3514	1/1	0.91	0.20	47,47,47,47	0
54	MG	1a	1759	1/1	0.91	0.13	64,64,64,64	0
54	MG	1a	1618	1/1	0.91	0.29	51,51,51,51	0
54	MG	1a	1761	1/1	0.91	0.07	57,57,57,57	0
54	MG	2A	3509	1/1	0.91	0.20	60,60,60,60	0
54	MG	1A	3865	1/1	0.91	0.77	35,35,35,35	0
54	MG	1A	3508	1/1	0.91	0.14	29,29,29,29	0
54	MG	2A	3225	1/1	0.91	0.21	56,56,56,56	0
54	MG	1A	3493	1/1	0.91	0.15	56,56,56,56	0
54	MG	1A	3873	1/1	0.91	0.11	57,57,57,57	0
54	MG	1A	3223	1/1	0.91	0.45	28,28,28,28	0
54	MG	2A	3092	1/1	0.91	0.41	46,46,46,46	0
54	MG	1a	1753	1/1	0.91	0.15	66,66,66,66	0
54	MG	1a	1820	1/1	0.91	0.11	56,56,56,56	0
54	MG	1O	8001	1/1	0.91	0.12	43,43,43,43	0
54	MG	2A	3152	1/1	0.91	0.10	58,58,58,58	0
54	MG	2A	3079	1/1	0.91	0.14	47,47,47,47	0
54	MG	1A	3133	1/1	0.91	0.09	27,27,27,27	0
54	MG	25	502	1/1	0.91	0.24	59,59,59,59	0
54	MG	2A	3369	1/1	0.91	0.27	51,51,51,51	0
54	MG	2A	3005	1/1	0.91	0.27	41,41,41,41	0
54	MG	1A	3831	1/1	0.91	0.13	19,19,19,19	0
54	MG	2A	3573	1/1	0.91	0.16	19,19,19,19	0
54	MG	1A	3419	1/1	0.91	0.21	47,47,47,47	0
54	MG	2P	201	1/1	0.91	0.13	52,52,52,52	0
54	MG	2A	3717	1/1	0.91	0.27	61,61,61,61	0
54	MG	1A	3293	1/1	0.91	0.23	18,18,18,18	0
54	MG	1A	3891	1/1	0.91	0.14	30,30,30,30	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3032	1/1	0.91	0.16	54,54,54,54	0
54	MG	2B	3002	1/1	0.91	0.20	71,71,71,71	0
54	MG	2a	1620	1/1	0.91	0.10	56,56,56,56	0
54	MG	2A	3157	1/1	0.91	0.18	42,42,42,42	0
54	MG	1A	3229	1/1	0.91	0.24	55,55,55,55	0
54	MG	1A	3148	1/1	0.91	0.35	30,30,30,30	0
54	MG	2A	3275	1/1	0.91	0.06	62,62,62,62	0
54	MG	1A	3786	1/1	0.91	0.16	40,40,40,40	0
54	MG	1A	3423	1/1	0.91	0.09	51,51,51,51	0
54	MG	1A	3486	1/1	0.91	0.18	21,21,21,21	0
54	MG	1a	1741	1/1	0.91	0.08	51,51,51,51	0
54	MG	1A	3183	1/1	0.91	0.15	45,45,45,45	0
54	MG	1a	1709	1/1	0.91	0.14	54,54,54,54	0
54	MG	1A	3940	1/1	0.91	0.38	67,67,67,67	0
54	MG	2A	3435	1/1	0.91	0.14	60,60,60,60	0
54	MG	1A	3260	1/1	0.91	0.09	38,38,38,38	0
54	MG	1A	3311	1/1	0.91	0.12	35,35,35,35	0
54	MG	1A	3513	1/1	0.91	0.14	53,53,53,53	0
54	MG	2A	3084	1/1	0.91	0.25	52,52,52,52	0
54	MG	2A	3059	1/1	0.91	0.28	42,42,42,42	0
57	MPD	1T	204	8/8	0.91	0.19	57,64,66,66	0
54	MG	2A	3661	1/1	0.91	0.07	47,47,47,47	0
54	MG	1A	3498	1/1	0.91	0.21	32,32,32,32	0
54	MG	1A	3944	1/1	0.91	0.10	47,47,47,47	0
54	MG	1B	210	1/1	0.91	0.14	50,50,50,50	0
54	MG	1A	3677	1/1	0.91	0.28	43,43,43,43	0
54	MG	2A	3425	1/1	0.91	0.13	68,68,68,68	0
54	MG	1A	3833	1/1	0.91	0.12	30,30,30,30	0
54	MG	2A	3075	1/1	0.91	0.68	42,42,42,42	0
54	MG	2a	1725	1/1	0.91	0.10	64,64,64,64	0
54	MG	1A	3552	1/1	0.91	0.12	45,45,45,45	0
54	MG	1A	3403	1/1	0.92	0.12	50,50,50,50	0
54	MG	2A	3614	1/1	0.92	0.17	58,58,58,58	0
54	MG	1A	3119	1/1	0.92	0.14	38,38,38,38	0
54	MG	1A	3446	1/1	0.92	0.22	20,20,20,20	0
54	MG	2a	1664	1/1	0.92	0.11	61,61,61,61	0
54	MG	2B	3019	1/1	0.92	0.09	65,65,65,65	0
54	MG	1A	3981	1/1	0.92	0.16	51,51,51,51	0
54	MG	1A	3083	1/1	0.92	0.26	40,40,40,40	0
54	MG	2A	3426	1/1	0.92	0.09	58,58,58,58	0
54	MG	1A	3655	1/1	0.92	0.36	30,30,30,30	0
54	MG	1A	3932	1/1	0.92	0.12	58,58,58,58	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3773	1/1	0.92	0.17	64,64,64,64	0
54	MG	2a	1658	1/1	0.92	0.15	60,60,60,60	0
54	MG	2B	3012	1/1	0.92	0.13	50,50,50,50	0
54	MG	1A	3837	1/1	0.92	0.19	56,56,56,56	0
54	MG	1A	3437	1/1	0.92	0.20	41,41,41,41	0
54	MG	2A	3012	1/1	0.92	0.16	43,43,43,43	0
54	MG	1A	3310	1/1	0.92	0.12	38,38,38,38	0
54	MG	1A	3266	1/1	0.92	0.66	40,40,40,40	0
54	MG	2A	3164	1/1	0.92	0.11	69,69,69,69	0
54	MG	2A	3549	1/1	0.92	0.20	38,38,38,38	0
54	MG	1A	3818	1/1	0.92	0.17	31,31,31,31	0
54	MG	2A	3207	1/1	0.92	0.35	55,55,55,55	0
54	MG	2A	3268	1/1	0.92	0.10	29,29,29,29	0
54	MG	1A	3539	1/1	0.92	0.14	22,22,22,22	0
54	MG	1B	208	1/1	0.92	0.24	51,51,51,51	0
54	MG	1A	3538	1/1	0.92	0.11	55,55,55,55	0
54	MG	2A	3506	1/1	0.92	0.10	63,63,63,63	0
54	MG	1a	1839	1/1	0.92	0.08	59,59,59,59	0
54	MG	1A	3210	1/1	0.92	0.32	32,32,32,32	0
54	MG	1A	3061	1/1	0.92	0.10	43,43,43,43	0
54	MG	2F	303	1/1	0.92	0.70	43,43,43,43	0
54	MG	1a	1634	1/1	0.92	0.15	69,69,69,69	0
54	MG	1a	1768	1/1	0.92	0.15	69,69,69,69	0
54	MG	28	8001	1/1	0.92	0.09	46,46,46,46	0
54	MG	1A	3809	1/1	0.92	0.23	39,39,39,39	0
54	MG	1A	3132	1/1	0.92	0.12	40,40,40,40	0
54	MG	1e	3002	1/1	0.92	0.41	53,53,53,53	0
54	MG	1A	3322	1/1	0.92	0.17	21,21,21,21	0
54	MG	2A	3339	1/1	0.92	0.10	71,71,71,71	0
54	MG	1A	3765	1/1	0.92	0.10	39,39,39,39	0
54	MG	1A	3036	1/1	0.92	0.18	38,38,38,38	0
54	MG	2B	3011	1/1	0.92	0.08	65,65,65,65	0
54	MG	1A	3125	1/1	0.92	0.46	30,30,30,30	0
54	MG	1a	1821	1/1	0.92	0.18	44,44,44,44	0
54	MG	1A	3203	1/1	0.92	0.24	55,55,55,55	0
54	MG	1A	3632	1/1	0.92	0.13	63,63,63,63	0
54	MG	1A	3613	1/1	0.92	0.26	50,50,50,50	0
54	MG	2A	3674	1/1	0.92	0.14	63,63,63,63	0
54	MG	1A	3058	1/1	0.92	0.13	34,34,34,34	0
54	MG	2A	3503	1/1	0.92	0.11	54,54,54,54	0
54	MG	10	106	1/1	0.92	0.39	41,41,41,41	0
54	MG	1A	4027	1/1	0.92	0.48	37,37,37,37	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3257	1/1	0.92	0.31	42,42,42,42	0
54	MG	1A	3163	1/1	0.92	0.25	47,47,47,47	0
54	MG	1A	3732	1/1	0.92	0.25	41,41,41,41	0
54	MG	1a	1803	1/1	0.92	0.10	64,64,64,64	0
54	MG	1a	1756	1/1	0.92	0.15	58,58,58,58	0
54	MG	1A	3651	1/1	0.92	0.30	30,30,30,30	0
54	MG	1A	3939	1/1	0.92	0.10	55,55,55,55	0
54	MG	1a	1691	1/1	0.92	0.16	56,56,56,56	0
54	MG	2A	3293	1/1	0.92	0.15	35,35,35,35	0
54	MG	2A	3657	1/1	0.92	0.17	43,43,43,43	0
54	MG	1a	1739	1/1	0.92	0.09	61,61,61,61	0
54	MG	2A	3281	1/1	0.92	0.18	59,59,59,59	0
54	MG	2A	3046	1/1	0.92	0.23	59,59,59,59	0
54	MG	2A	3136	1/1	0.92	0.16	51,51,51,51	0
54	MG	1A	3882	1/1	0.92	0.04	60,60,60,60	0
54	MG	2A	3419	1/1	0.92	0.20	59,59,59,59	0
54	MG	2A	3294	1/1	0.92	0.13	41,41,41,41	0
54	MG	1A	3797	1/1	0.92	0.33	34,34,34,34	0
54	MG	2A	3261	1/1	0.92	0.13	43,43,43,43	0
54	MG	1A	3392	1/1	0.92	0.22	23,23,23,23	0
54	MG	2a	1707	1/1	0.92	0.15	47,47,47,47	0
54	MG	1A	3413	1/1	0.92	0.29	57,57,57,57	0
54	MG	1A	3674	1/1	0.92	0.11	35,35,35,35	0
54	MG	2D	302	1/1	0.92	0.91	38,38,38,38	0
54	MG	2B	3017	1/1	0.92	0.13	80,80,80,80	0
54	MG	2A	3677	1/1	0.92	0.30	50,50,50,50	0
54	MG	1A	3147	1/1	0.92	0.20	39,39,39,39	0
54	MG	1A	3660	1/1	0.92	0.15	51,51,51,51	0
54	MG	1A	3408	1/1	0.92	0.19	50,50,50,50	0
54	MG	1A	3933	1/1	0.92	0.07	41,41,41,41	0
54	MG	1A	3900	1/1	0.92	0.19	40,40,40,40	0
54	MG	1A	3641	1/1	0.92	0.19	29,29,29,29	0
54	MG	2a	1655	1/1	0.92	0.14	63,63,63,63	0
54	MG	2A	3609	1/1	0.92	0.18	45,45,45,45	0
54	MG	1A	3605	1/1	0.92	0.15	44,44,44,44	0
54	MG	1A	3008	1/1	0.92	0.10	33,33,33,33	0
54	MG	1B	222	1/1	0.92	0.14	57,57,57,57	0
54	MG	1a	1812	1/1	0.92	0.10	59,59,59,59	0
54	MG	2T	3001	1/1	0.92	0.24	50,50,50,50	0
54	MG	1A	3780	1/1	0.92	0.21	45,45,45,45	0
54	MG	1h	3001	1/1	0.92	0.12	35,35,35,35	0
54	MG	2A	3211	1/1	0.92	0.48	46,46,46,46	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3186	1/1	0.92	0.19	34,34,34,34	0
54	MG	1A	3118	1/1	0.92	0.17	49,49,49,49	0
54	MG	1a	1730	1/1	0.92	0.12	43,43,43,43	0
54	MG	1A	3549	1/1	0.92	0.14	38,38,38,38	0
54	MG	1A	3521	1/1	0.92	0.17	42,42,42,42	0
54	MG	1A	3739	1/1	0.92	0.20	51,51,51,51	0
54	MG	2a	1606	1/1	0.92	0.12	45,45,45,45	0
54	MG	1A	3212	1/1	0.92	0.57	37,37,37,37	0
54	MG	1a	1856	1/1	0.92	0.19	67,67,67,67	0
54	MG	1A	3197	1/1	0.92	0.14	41,41,41,41	0
54	MG	1A	3924	1/1	0.92	0.16	45,45,45,45	0
54	MG	2A	3047	1/1	0.92	0.14	56,56,56,56	0
54	MG	10	103	1/1	0.92	0.11	43,43,43,43	0
54	MG	1a	1788	1/1	0.92	0.18	54,54,54,54	0
54	MG	2E	302	1/1	0.92	0.39	67,67,67,67	0
54	MG	1a	1664	1/1	0.92	0.21	51,51,51,51	0
54	MG	1A	3038	1/1	0.92	0.13	40,40,40,40	0
54	MG	1A	3767	1/1	0.92	0.11	45,45,45,45	0
54	MG	1b	3001	1/1	0.92	0.18	76,76,76,76	0
54	MG	2A	3323	1/1	0.92	0.17	34,34,34,34	0
54	MG	1a	1689	1/1	0.92	0.18	55,55,55,55	0
54	MG	2a	1626	1/1	0.92	0.21	53,53,53,53	0
54	MG	2A	3108	1/1	0.92	0.19	62,62,62,62	0
54	MG	1A	3337	1/1	0.92	0.10	55,55,55,55	0
54	MG	2A	3153	1/1	0.92	0.47	42,42,42,42	0
54	MG	1A	3142	1/1	0.92	0.21	50,50,50,50	0
54	MG	2A	3453	1/1	0.92	0.31	64,64,64,64	0
54	MG	1A	3428	1/1	0.92	0.31	52,52,52,52	0
54	MG	2A	3456	1/1	0.92	0.14	31,31,31,31	0
54	MG	1A	3172	1/1	0.92	0.86	31,31,31,31	0
54	MG	2A	3139	1/1	0.92	0.10	58,58,58,58	0
54	MG	1A	3823	1/1	0.92	0.30	29,29,29,29	0
54	MG	1A	3292	1/1	0.92	0.17	56,56,56,56	0
54	MG	2A	3371	1/1	0.92	0.17	26,26,26,26	0
54	MG	19	503	1/1	0.92	0.16	50,50,50,50	0
54	MG	1A	3315	1/1	0.92	0.12	25,25,25,25	0
54	MG	2A	3132	1/1	0.92	0.14	43,43,43,43	0
54	MG	1A	3341	1/1	0.92	0.13	36,36,36,36	0
54	MG	1A	3261	1/1	0.92	0.44	36,36,36,36	0
54	MG	2A	3501	1/1	0.92	0.14	43,43,43,43	0
54	MG	1A	3281	1/1	0.92	0.23	36,36,36,36	0
54	MG	1A	3714	1/1	0.92	0.18	37,37,37,37	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3263	1/1	0.92	0.39	25,25,25,25	0
54	MG	2A	3094	1/1	0.92	0.23	49,49,49,49	0
54	MG	2A	3265	1/1	0.92	0.11	57,57,57,57	0
54	MG	2A	3465	1/1	0.92	0.20	56,56,56,56	0
54	MG	1R	201	1/1	0.92	0.36	31,31,31,31	0
54	MG	1A	3966	1/1	0.92	0.43	36,36,36,36	0
54	MG	2A	3566	1/1	0.92	0.12	35,35,35,35	0
54	MG	1A	3116	1/1	0.92	0.23	28,28,28,28	0
54	MG	2A	3460	1/1	0.92	0.16	53,53,53,53	0
54	MG	1A	3075	1/1	0.92	0.39	32,32,32,32	0
54	MG	2A	3154	1/1	0.92	0.19	41,41,41,41	0
54	MG	2A	3283	1/1	0.92	0.07	50,50,50,50	0
54	MG	2A	3402	1/1	0.92	0.09	43,43,43,43	0
54	MG	2A	3702	1/1	0.92	0.09	46,46,46,46	0
54	MG	2a	1650	1/1	0.92	0.11	58,58,58,58	0
54	MG	2A	3151	1/1	0.92	0.21	66,66,66,66	0
54	MG	1A	3353	1/1	0.92	0.13	18,18,18,18	0
54	MG	2A	3680	1/1	0.92	0.12	50,50,50,50	0
54	MG	2A	3031	1/1	0.92	0.19	48,48,48,48	0
54	MG	1A	3608	1/1	0.92	0.18	50,50,50,50	0
54	MG	2A	3114	1/1	0.92	0.20	56,56,56,56	0
54	MG	1a	1836	1/1	0.92	0.09	62,62,62,62	0
54	MG	2A	3558	1/1	0.92	0.09	58,58,58,58	0
54	MG	1A	4005	1/1	0.92	0.31	32,32,32,32	0
54	MG	1A	3512	1/1	0.92	0.19	40,40,40,40	0
54	MG	1A	3848	1/1	0.92	0.14	48,48,48,48	0
54	MG	1B	215	1/1	0.92	0.28	61,61,61,61	0
54	MG	2A	3208	1/1	0.92	0.13	43,43,43,43	0
54	MG	2A	3235	1/1	0.92	0.15	54,54,54,54	0
54	MG	1A	3178	1/1	0.93	0.29	29,29,29,29	0
54	MG	2A	3040	1/1	0.93	0.09	58,58,58,58	0
54	MG	1E	301	1/1	0.93	0.16	35,35,35,35	0
54	MG	1A	3265	1/1	0.93	0.13	46,46,46,46	0
54	MG	2A	3432	1/1	0.93	0.16	57,57,57,57	0
54	MG	1A	3829	1/1	0.93	0.15	54,54,54,54	0
54	MG	2a	1625	1/1	0.93	0.13	67,67,67,67	0
54	MG	2A	3213	1/1	0.93	0.13	67,67,67,67	0
54	MG	1A	3282	1/1	0.93	0.36	24,24,24,24	0
54	MG	1A	4000	1/1	0.93	0.11	30,30,30,30	0
54	MG	2A	3439	1/1	0.93	0.14	64,64,64,64	0
54	MG	2A	3664	1/1	0.93	0.09	57,57,57,57	0
54	MG	2A	3586	1/1	0.93	0.12	84,84,84,84	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3668	1/1	0.93	0.10	48,48,48,48	0
54	MG	2a	1721	1/1	0.93	0.18	76,76,76,76	0
54	MG	2a	1670	1/1	0.93	0.15	59,59,59,59	0
54	MG	1A	3884	1/1	0.93	0.09	48,48,48,48	0
54	MG	1A	3367	1/1	0.93	0.18	18,18,18,18	0
54	MG	1a	1831	1/1	0.93	0.10	54,54,54,54	0
54	MG	2A	3050	1/1	0.93	0.16	58,58,58,58	0
54	MG	2A	3647	1/1	0.93	0.17	57,57,57,57	0
54	MG	1A	3701	1/1	0.93	0.19	29,29,29,29	0
54	MG	1A	3487	1/1	0.93	0.46	51,51,51,51	0
54	MG	1A	3520	1/1	0.93	0.14	38,38,38,38	0
54	MG	1A	3320	1/1	0.93	0.10	24,24,24,24	0
54	MG	1A	4016	1/1	0.93	0.48	41,41,41,41	0
54	MG	1A	3235	1/1	0.93	0.39	39,39,39,39	0
54	MG	2A	3349	1/1	0.93	0.17	56,56,56,56	0
54	MG	1a	1660	1/1	0.93	0.18	46,46,46,46	0
54	MG	1A	3621	1/1	0.93	0.10	52,52,52,52	0
54	MG	2A	3532	1/1	0.93	0.17	52,52,52,52	0
54	MG	1A	3238	1/1	0.93	0.56	40,40,40,40	0
54	MG	2A	3017	1/1	0.93	0.67	41,41,41,41	0
54	MG	1A	3218	1/1	0.93	0.44	30,30,30,30	0
54	MG	1A	3883	1/1	0.93	0.56	47,47,47,47	0
54	MG	1a	1747	1/1	0.93	0.20	56,56,56,56	0
54	MG	1A	3995	1/1	0.93	0.20	26,26,26,26	0
54	MG	2A	3600	1/1	0.93	0.28	54,54,54,54	0
54	MG	2A	3612	1/1	0.93	0.13	40,40,40,40	0
54	MG	2A	3201	1/1	0.93	0.33	50,50,50,50	0
54	MG	2A	3388	1/1	0.93	0.11	51,51,51,51	0
54	MG	1A	3761	1/1	0.93	0.13	32,32,32,32	0
54	MG	2A	3034	1/1	0.93	0.17	42,42,42,42	0
54	MG	1A	3101	1/1	0.93	0.39	30,30,30,30	0
54	MG	1A	3872	1/1	0.93	0.16	50,50,50,50	0
54	MG	1A	3180	1/1	0.93	0.42	37,37,37,37	0
54	MG	2A	3161	1/1	0.93	0.17	46,46,46,46	0
54	MG	1A	3395	1/1	0.93	0.12	13,13,13,13	0
54	MG	1g	3001	1/1	0.93	0.29	52,52,52,52	0
54	MG	1A	3562	1/1	0.93	0.07	32,32,32,32	0
54	MG	2A	3190	1/1	0.93	0.12	47,47,47,47	0
54	MG	1A	3452	1/1	0.93	0.15	21,21,21,21	0
54	MG	2A	3238	1/1	0.93	0.17	44,44,44,44	0
54	MG	1A	4022	1/1	0.93	0.15	30,30,30,30	0
54	MG	1a	1825	1/1	0.93	0.13	54,54,54,54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3500	1/1	0.93	0.12	51,51,51,51	0
54	MG	2A	3212	1/1	0.93	0.38	60,60,60,60	0
54	MG	1A	3864	1/1	0.93	0.08	36,36,36,36	0
54	MG	1a	1648	1/1	0.93	0.07	72,72,72,72	0
54	MG	1a	1655	1/1	0.93	0.26	57,57,57,57	0
54	MG	1A	3457	1/1	0.93	0.09	64,64,64,64	0
54	MG	1F	307	1/1	0.93	0.37	31,31,31,31	0
54	MG	2A	3444	1/1	0.93	0.24	60,60,60,60	0
54	MG	1A	3724	1/1	0.93	0.15	27,27,27,27	0
54	MG	1A	3425	1/1	0.93	0.13	35,35,35,35	0
54	MG	2A	3724	1/1	0.93	0.42	32,32,32,32	0
54	MG	1A	3300	1/1	0.93	0.14	23,23,23,23	0
54	MG	1A	3800	1/1	0.93	0.19	44,44,44,44	0
54	MG	2A	3383	1/1	0.93	0.23	64,64,64,64	0
54	MG	1A	3646	1/1	0.93	0.08	37,37,37,37	0
54	MG	1A	3579	1/1	0.93	0.20	24,24,24,24	0
54	MG	1A	3349	1/1	0.93	0.15	40,40,40,40	0
54	MG	2A	3570	1/1	0.93	0.19	44,44,44,44	0
54	MG	1a	1786	1/1	0.93	0.20	57,57,57,57	0
54	MG	1Z	8001	1/1	0.93	0.19	60,60,60,60	0
54	MG	1A	3463	1/1	0.93	0.13	19,19,19,19	0
54	MG	1A	3106	1/1	0.93	0.42	40,40,40,40	0
59	ZN	24	501	1/1	0.93	0.05	108,108,108,108	0
54	MG	2a	1637	1/1	0.93	0.19	63,63,63,63	0
54	MG	2A	3269	1/1	0.93	0.15	32,32,32,32	0
54	MG	1A	3272	1/1	0.93	0.16	38,38,38,38	0
54	MG	1A	3960	1/1	0.93	0.09	32,32,32,32	0
54	MG	1a	1692	1/1	0.93	0.21	46,46,46,46	0
54	MG	1A	3442	1/1	0.93	0.15	15,15,15,15	0
54	MG	2B	3003	1/1	0.93	0.09	74,74,74,74	0
54	MG	2a	1740	1/1	0.93	0.26	59,59,59,59	0
54	MG	1A	3700	1/1	0.93	0.08	34,34,34,34	0
54	MG	1a	1771	1/1	0.93	0.16	46,46,46,46	0
54	MG	2A	3582	1/1	0.93	0.17	47,47,47,47	0
54	MG	1A	3902	1/1	0.93	0.14	52,52,52,52	0
54	MG	1A	3861	1/1	0.93	0.17	22,22,22,22	0
54	MG	2A	3363	1/1	0.93	0.16	61,61,61,61	0
54	MG	1A	3712	1/1	0.93	0.11	52,52,52,52	0
54	MG	1A	3815	1/1	0.93	0.10	33,33,33,33	0
54	MG	2a	1624	1/1	0.93	0.15	65,65,65,65	0
54	MG	1a	1666	1/1	0.93	0.55	50,50,50,50	0
54	MG	2G	3001	1/1	0.93	0.08	71,71,71,71	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3434	1/1	0.93	0.13	26,26,26,26	0
54	MG	2A	3361	1/1	0.93	0.11	33,33,33,33	0
54	MG	2A	3479	1/1	0.93	0.14	41,41,41,41	0
54	MG	2A	3630	1/1	0.93	0.18	52,52,52,52	0
54	MG	1A	3877	1/1	0.93	0.10	57,57,57,57	0
54	MG	2a	1735	1/1	0.93	0.17	45,45,45,45	0
54	MG	1a	1738	1/1	0.93	0.30	62,62,62,62	0
54	MG	2A	3217	1/1	0.93	0.16	43,43,43,43	0
54	MG	2A	3362	1/1	0.93	0.14	34,34,34,34	0
54	MG	1A	3475	1/1	0.93	0.14	42,42,42,42	0
54	MG	1A	3826	1/1	0.93	0.19	26,26,26,26	0
54	MG	1T	203	1/1	0.93	0.14	52,52,52,52	0
54	MG	2A	3377	1/1	0.93	0.10	43,43,43,43	0
54	MG	2A	3004	1/1	0.93	0.17	44,44,44,44	0
54	MG	1A	3376	1/1	0.93	0.12	29,29,29,29	0
54	MG	1A	3881	1/1	0.93	0.21	43,43,43,43	0
54	MG	1A	3707	1/1	0.93	0.09	40,40,40,40	0
54	MG	2A	3144	1/1	0.93	0.10	54,54,54,54	0
54	MG	2a	1640	1/1	0.93	0.17	53,53,53,53	0
54	MG	1A	3841	1/1	0.93	0.15	29,29,29,29	0
54	MG	1A	3343	1/1	0.93	0.14	56,56,56,56	0
54	MG	1A	3427	1/1	0.93	0.13	37,37,37,37	0
54	MG	2a	1751	1/1	0.93	0.11	53,53,53,53	0
54	MG	1A	3175	1/1	0.93	0.56	35,35,35,35	0
54	MG	2A	3159	1/1	0.93	0.12	50,50,50,50	0
54	MG	1a	1848	1/1	0.93	0.21	53,53,53,53	0
54	MG	2A	3471	1/1	0.93	0.10	61,61,61,61	0
54	MG	2A	3459	1/1	0.93	0.11	38,38,38,38	0
54	MG	1A	3141	1/1	0.93	0.19	38,38,38,38	0
54	MG	2A	3247	1/1	0.93	0.07	50,50,50,50	0
54	MG	1a	1714	1/1	0.93	0.16	56,56,56,56	0
54	MG	2A	3039	1/1	0.93	0.13	56,56,56,56	0
54	MG	1F	302	1/1	0.93	0.13	32,32,32,32	0
54	MG	1A	3717	1/1	0.93	0.41	52,52,52,52	0
54	MG	1E	306	1/1	0.93	0.13	31,31,31,31	0
54	MG	1A	3166	1/1	0.93	0.10	32,32,32,32	0
54	MG	1A	3127	1/1	0.93	0.18	49,49,49,49	0
54	MG	2A	3436	1/1	0.93	0.14	56,56,56,56	0
54	MG	2A	3001	1/1	0.93	0.17	46,46,46,46	0
54	MG	1A	3535	1/1	0.93	0.26	38,38,38,38	0
54	MG	1A	3942	1/1	0.93	0.20	73,73,73,73	0
54	MG	2A	3343	1/1	0.93	0.22	50,50,50,50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1665	1/1	0.93	0.13	59,59,59,59	0
54	MG	1A	3760	1/1	0.93	0.24	61,61,61,61	0
54	MG	1A	3471	1/1	0.93	0.10	31,31,31,31	0
54	MG	2A	3174	1/1	0.93	0.23	45,45,45,45	0
54	MG	1A	3305	1/1	0.93	0.12	39,39,39,39	0
54	MG	2A	3646	1/1	0.93	0.25	60,60,60,60	0
54	MG	1A	3868	1/1	0.93	0.20	23,23,23,23	0
54	MG	1A	3188	1/1	0.93	0.18	53,53,53,53	0
54	MG	2A	3624	1/1	0.93	0.11	37,37,37,37	0
54	MG	1A	3728	1/1	0.93	0.22	38,38,38,38	0
54	MG	2A	3083	1/1	0.93	0.17	49,49,49,49	0
54	MG	1A	3387	1/1	0.93	0.08	54,54,54,54	0
54	MG	1a	1651	1/1	0.93	0.25	59,59,59,59	0
54	MG	2A	3049	1/1	0.93	0.18	53,53,53,53	0
54	MG	1a	1757	1/1	0.93	0.11	77,77,77,77	0
54	MG	1A	3673	1/1	0.93	0.17	28,28,28,28	0
54	MG	2A	3048	1/1	0.93	0.20	61,61,61,61	0
54	MG	1A	3963	1/1	0.93	0.25	38,38,38,38	0
54	MG	1A	3968	1/1	0.93	0.10	11,11,11,11	0
54	MG	1a	1822	1/1	0.93	0.12	60,60,60,60	0
54	MG	1A	3570	1/1	0.93	0.25	47,47,47,47	0
54	MG	1A	3904	1/1	0.93	0.13	60,60,60,60	0
54	MG	1A	3768	1/1	0.93	0.11	54,54,54,54	0
54	MG	2A	3533	1/1	0.93	0.13	51,51,51,51	0
54	MG	1A	3156	1/1	0.93	0.11	49,49,49,49	0
54	MG	2A	3234	1/1	0.93	0.17	52,52,52,52	0
54	MG	2a	1653	1/1	0.93	0.10	53,53,53,53	0
54	MG	2A	3534	1/1	0.93	0.09	65,65,65,65	0
54	MG	2A	3381	1/1	0.93	0.13	53,53,53,53	0
54	MG	1A	3503	1/1	0.93	0.13	58,58,58,58	0
54	MG	2A	3023	1/1	0.93	0.26	55,55,55,55	0
54	MG	2B	3005	1/1	0.93	0.15	61,61,61,61	0
54	MG	2A	3113	1/1	0.93	0.27	59,59,59,59	0
54	MG	1A	3481	1/1	0.93	0.17	48,48,48,48	0
54	MG	1A	3687	1/1	0.93	0.10	44,44,44,44	0
54	MG	2A	3076	1/1	0.93	0.33	44,44,44,44	0
54	MG	1A	3174	1/1	0.93	0.34	34,34,34,34	0
57	MPD	1A	3988	8/8	0.93	0.21	48,52,54,59	0
54	MG	2A	3446	1/1	0.93	0.13	30,30,30,30	0
54	MG	1A	3733	1/1	0.93	0.12	42,42,42,42	0
54	MG	1D	311	1/1	0.93	0.19	66,66,66,66	0
54	MG	2A	3022	1/1	0.93	0.10	39,39,39,39	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3663	1/1	0.93	0.09	61,61,61,61	0
54	MG	1A	3583	1/1	0.93	0.22	20,20,20,20	0
54	MG	1A	3753	1/1	0.93	0.14	35,35,35,35	0
54	MG	1V	203	1/1	0.93	0.20	55,55,55,55	0
54	MG	1A	3417	1/1	0.93	0.16	20,20,20,20	0
54	MG	1a	1705	1/1	0.93	0.13	59,59,59,59	0
54	MG	1A	3335	1/1	0.93	0.15	22,22,22,22	0
54	MG	1A	3196	1/1	0.93	0.57	40,40,40,40	0
54	MG	1A	3954	1/1	0.93	0.09	36,36,36,36	0
57	MPD	2A	3711	8/8	0.93	0.12	48,60,64,64	0
54	MG	2a	1688	1/1	0.93	0.19	54,54,54,54	0
54	MG	2A	3131	1/1	0.93	0.83	44,44,44,44	0
54	MG	1A	3551	1/1	0.93	0.10	43,43,43,43	0
54	MG	2A	3417	1/1	0.93	0.12	37,37,37,37	0
54	MG	1B	218	1/1	0.93	0.10	50,50,50,50	0
54	MG	2A	3028	1/1	0.94	0.12	68,68,68,68	0
54	MG	1A	3599	1/1	0.94	0.24	45,45,45,45	0
54	MG	2A	3336	1/1	0.94	0.15	36,36,36,36	0
54	MG	1B	209	1/1	0.94	0.09	36,36,36,36	0
54	MG	1a	1621	1/1	0.94	0.11	46,46,46,46	0
54	MG	1A	3453	1/1	0.94	0.07	51,51,51,51	0
54	MG	2A	3626	1/1	0.94	0.06	70,70,70,70	0
54	MG	2a	1616	1/1	0.94	0.12	60,60,60,60	0
54	MG	1a	1740	1/1	0.94	0.09	59,59,59,59	0
54	MG	1a	1746	1/1	0.94	0.07	60,60,60,60	0
54	MG	1A	3983	1/1	0.94	0.30	36,36,36,36	0
54	MG	2A	3557	1/1	0.94	0.13	22,22,22,22	0
54	MG	1A	3014	1/1	0.94	0.39	44,44,44,44	0
54	MG	2A	3458	1/1	0.94	0.17	34,34,34,34	0
54	MG	1A	3590	1/1	0.94	0.10	32,32,32,32	0
54	MG	1A	3239	1/1	0.94	0.21	33,33,33,33	0
54	MG	2A	3052	1/1	0.94	0.22	40,40,40,40	0
54	MG	2a	1660	1/1	0.94	0.17	55,55,55,55	0
54	MG	1F	309	1/1	0.94	0.24	43,43,43,43	0
54	MG	1A	3876	1/1	0.94	0.12	27,27,27,27	0
54	MG	1l	3001	1/1	0.94	0.17	47,47,47,47	0
54	MG	1A	3821	1/1	0.94	0.14	26,26,26,26	0
54	MG	1A	4012	1/1	0.94	0.50	25,25,25,25	0
54	MG	1A	3057	1/1	0.94	0.25	27,27,27,27	0
54	MG	1a	1623	1/1	0.94	0.08	47,47,47,47	0
54	MG	1A	3236	1/1	0.94	0.73	38,38,38,38	0
54	MG	1A	3819	1/1	0.94	0.09	39,39,39,39	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3115	1/1	0.94	0.15	63,63,63,63	0
54	MG	1A	3388	1/1	0.94	0.18	22,22,22,22	0
54	MG	1A	3802	1/1	0.94	0.06	47,47,47,47	0
54	MG	1A	3128	1/1	0.94	0.09	32,32,32,32	0
54	MG	2A	3180	1/1	0.94	0.35	63,63,63,63	0
54	MG	2A	3392	1/1	0.94	0.18	56,56,56,56	0
54	MG	1A	3542	1/1	0.94	0.23	31,31,31,31	0
54	MG	1a	1630	1/1	0.94	0.20	46,46,46,46	0
54	MG	1A	3139	1/1	0.94	0.23	29,29,29,29	0
54	MG	2A	3487	1/1	0.94	0.17	46,46,46,46	0
54	MG	2A	3309	1/1	0.94	0.14	25,25,25,25	0
54	MG	1A	3795	1/1	0.94	0.12	32,32,32,32	0
54	MG	1A	3680	1/1	0.94	0.21	25,25,25,25	0
54	MG	2A	3679	1/1	0.94	0.15	57,57,57,57	0
54	MG	2A	3636	1/1	0.94	0.24	47,47,47,47	0
54	MG	2A	3690	1/1	0.94	0.07	67,67,67,67	0
54	MG	1A	3108	1/1	0.94	0.45	42,42,42,42	0
54	MG	1A	3711	1/1	0.94	0.20	30,30,30,30	0
54	MG	1A	3524	1/1	0.94	0.10	46,46,46,46	0
54	MG	2A	3204	1/1	0.94	0.07	47,47,47,47	0
54	MG	1A	3035	1/1	0.94	0.13	38,38,38,38	0
54	MG	2A	3127	1/1	0.94	0.26	36,36,36,36	0
54	MG	1a	1796	1/1	0.94	0.24	50,50,50,50	0
54	MG	1A	3545	1/1	0.94	0.10	39,39,39,39	0
54	MG	2A	3431	1/1	0.94	0.07	53,53,53,53	0
54	MG	1A	3790	1/1	0.94	0.17	39,39,39,39	0
54	MG	1g	3002	1/1	0.94	0.09	60,60,60,60	0
54	MG	1A	4003	1/1	0.94	0.18	27,27,27,27	0
54	MG	1R	202	1/1	0.94	0.14	46,46,46,46	0
54	MG	2A	3297	1/1	0.94	0.17	51,51,51,51	0
54	MG	1A	3009	1/1	0.94	0.23	34,34,34,34	0
54	MG	1A	3626	1/1	0.94	0.14	51,51,51,51	0
54	MG	1a	1800	1/1	0.94	0.23	43,43,43,43	0
54	MG	1A	3974	1/1	0.94	0.14	45,45,45,45	0
54	MG	1A	3697	1/1	0.94	0.21	50,50,50,50	0
54	MG	2A	3583	1/1	0.94	0.14	42,42,42,42	0
54	MG	1A	3706	1/1	0.94	0.10	32,32,32,32	0
54	MG	2A	3706	1/1	0.94	0.21	48,48,48,48	0
54	MG	1A	4009	1/1	0.94	0.69	42,42,42,42	0
54	MG	1A	3370	1/1	0.94	0.14	21,21,21,21	0
54	MG	1A	3591	1/1	0.94	0.14	36,36,36,36	0
54	MG	1A	3469	1/1	0.94	0.09	29,29,29,29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1688	1/1	0.94	0.20	53,53,53,53	0
54	MG	1F	306	1/1	0.94	0.16	31,31,31,31	0
54	MG	1a	1723	1/1	0.94	0.14	50,50,50,50	0
54	MG	2A	3320	1/1	0.94	0.10	59,59,59,59	0
54	MG	1a	1727	1/1	0.94	0.20	43,43,43,43	0
54	MG	2A	3505	1/1	0.94	0.13	55,55,55,55	0
54	MG	1a	1685	1/1	0.94	0.29	40,40,40,40	0
54	MG	1a	1711	1/1	0.94	0.21	58,58,58,58	0
54	MG	1A	3121	1/1	0.94	0.10	57,57,57,57	0
54	MG	1g	3003	1/1	0.94	0.15	45,45,45,45	0
54	MG	1A	3727	1/1	0.94	0.25	22,22,22,22	0
54	MG	1A	3226	1/1	0.94	0.35	32,32,32,32	0
54	MG	1A	3850	1/1	0.94	0.17	48,48,48,48	0
54	MG	1A	3390	1/1	0.94	0.17	40,40,40,40	0
54	MG	1A	3400	1/1	0.94	0.15	35,35,35,35	0
54	MG	1A	3998	1/1	0.94	0.52	32,32,32,32	0
54	MG	1A	3506	1/1	0.94	0.12	33,33,33,33	0
54	MG	1f	3001	1/1	0.94	0.24	64,64,64,64	0
54	MG	2A	3719	1/1	0.94	0.23	48,48,48,48	0
54	MG	2A	3382	1/1	0.94	0.10	43,43,43,43	0
54	MG	2A	3575	1/1	0.94	0.21	41,41,41,41	0
54	MG	2a	1692	1/1	0.94	0.20	48,48,48,48	0
54	MG	1a	1690	1/1	0.94	0.17	45,45,45,45	0
54	MG	2A	3715	1/1	0.94	0.77	37,37,37,37	0
54	MG	1A	3643	1/1	0.94	0.30	56,56,56,56	0
54	MG	1A	3501	1/1	0.94	0.17	59,59,59,59	0
54	MG	2A	3652	1/1	0.94	0.20	44,44,44,44	0
54	MG	1a	1799	1/1	0.94	0.16	58,58,58,58	0
54	MG	1A	3067	1/1	0.94	0.10	38,38,38,38	0
54	MG	1A	3247	1/1	0.94	0.22	40,40,40,40	0
54	MG	1A	3295	1/1	0.94	0.17	19,19,19,19	0
54	MG	1A	3589	1/1	0.94	0.12	54,54,54,54	0
54	MG	1A	3647	1/1	0.94	0.12	38,38,38,38	0
54	MG	1A	3091	1/1	0.94	0.12	41,41,41,41	0
54	MG	1A	3019	1/1	0.94	0.44	33,33,33,33	0
54	MG	1A	3606	1/1	0.94	0.33	42,42,42,42	0
54	MG	1a	1675	1/1	0.94	0.12	42,42,42,42	0
54	MG	1A	3533	1/1	0.94	0.14	35,35,35,35	0
54	MG	2A	3489	1/1	0.94	0.14	69,69,69,69	0
54	MG	2A	3536	1/1	0.94	0.15	57,57,57,57	0
54	MG	1a	1601	1/1	0.94	0.09	56,56,56,56	0
54	MG	1A	3726	1/1	0.94	0.10	32,32,32,32	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	10	101	1/1	0.94	0.07	47,47,47,47	0
54	MG	2A	3140	1/1	0.94	0.15	51,51,51,51	0
54	MG	1A	3560	1/1	0.94	0.10	40,40,40,40	0
54	MG	2a	1612	1/1	0.94	0.17	50,50,50,50	0
54	MG	1A	3250	1/1	0.94	0.38	27,27,27,27	0
54	MG	2A	3712	1/1	0.94	0.39	41,41,41,41	0
54	MG	1A	3681	1/1	0.94	0.17	38,38,38,38	0
54	MG	2a	1719	1/1	0.94	0.16	67,67,67,67	0
54	MG	1A	3859	1/1	0.94	0.14	16,16,16,16	0
54	MG	2A	3568	1/1	0.94	0.15	50,50,50,50	0
54	MG	1A	3313	1/1	0.94	0.10	46,46,46,46	0
54	MG	2A	3422	1/1	0.94	0.07	55,55,55,55	0
54	MG	2A	3525	1/1	0.94	0.18	28,28,28,28	0
54	MG	1A	3289	1/1	0.94	0.16	23,23,23,23	0
54	MG	1A	3461	1/1	0.94	0.10	45,45,45,45	0
54	MG	1A	3026	1/1	0.94	0.41	28,28,28,28	0
54	MG	1W	3001	1/1	0.94	0.22	46,46,46,46	0
54	MG	2A	3178	1/1	0.94	0.15	53,53,53,53	0
54	MG	2A	3122	1/1	0.94	0.20	66,66,66,66	0
54	MG	2a	1677	1/1	0.94	0.22	53,53,53,53	0
54	MG	1A	3980	1/1	0.94	0.25	48,48,48,48	0
54	MG	2a	1697	1/1	0.94	0.20	59,59,59,59	0
54	MG	2A	3176	1/1	0.94	0.21	42,42,42,42	0
54	MG	1A	3504	1/1	0.94	0.11	16,16,16,16	0
54	MG	2A	3315	1/1	0.94	0.17	73,73,73,73	0
54	MG	2A	3329	1/1	0.94	0.20	29,29,29,29	0
54	MG	2A	3665	1/1	0.94	0.20	56,56,56,56	0
54	MG	1A	3764	1/1	0.94	0.20	44,44,44,44	0
54	MG	1B	226	1/1	0.94	0.13	60,60,60,60	0
54	MG	1a	1852	1/1	0.94	0.18	54,54,54,54	0
54	MG	2A	3443	1/1	0.94	0.16	47,47,47,47	0
54	MG	1A	3758	1/1	0.94	0.06	42,42,42,42	0
54	MG	2A	3306	1/1	0.94	0.13	27,27,27,27	0
54	MG	2A	3367	1/1	0.94	0.12	47,47,47,47	0
54	MG	2a	1647	1/1	0.94	0.15	52,52,52,52	0
54	MG	1A	3598	1/1	0.94	0.18	51,51,51,51	0
54	MG	1a	1734	1/1	0.94	0.16	47,47,47,47	0
54	MG	2A	3654	1/1	0.94	0.10	57,57,57,57	0
54	MG	17	101	1/1	0.94	0.49	54,54,54,54	0
54	MG	1A	3483	1/1	0.94	0.17	49,49,49,49	0
54	MG	2N	8001	1/1	0.94	0.14	70,70,70,70	0
54	MG	10	102	1/1	0.94	0.14	36,36,36,36	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3162	1/1	0.94	0.15	41,41,41,41	0
54	MG	1A	3288	1/1	0.94	0.16	16,16,16,16	0
54	MG	2A	3372	1/1	0.94	0.10	51,51,51,51	0
54	MG	2a	1715	1/1	0.94	0.17	60,60,60,60	0
54	MG	1A	3664	1/1	0.94	0.20	30,30,30,30	0
54	MG	1a	1807	1/1	0.94	0.23	67,67,67,67	0
54	MG	2A	3441	1/1	0.94	0.27	47,47,47,47	0
54	MG	2a	1659	1/1	0.94	0.24	48,48,48,48	0
54	MG	1A	3544	1/1	0.94	0.55	34,34,34,34	0
54	MG	2A	3601	1/1	0.94	0.31	57,57,57,57	0
54	MG	2A	3223	1/1	0.94	0.89	43,43,43,43	0
54	MG	1a	1789	1/1	0.94	0.15	69,69,69,69	0
54	MG	1T	202	1/1	0.94	0.09	48,48,48,48	0
54	MG	1A	3198	1/1	0.94	0.49	42,42,42,42	0
54	MG	1A	3581	1/1	0.94	0.17	53,53,53,53	0
54	MG	2A	3093	1/1	0.94	0.18	58,58,58,58	0
54	MG	1a	1687	1/1	0.94	0.22	54,54,54,54	0
54	MG	1A	3604	1/1	0.94	0.07	29,29,29,29	0
54	MG	2A	3494	1/1	0.94	0.21	50,50,50,50	0
54	MG	1a	1678	1/1	0.94	0.15	53,53,53,53	0
54	MG	2A	3639	1/1	0.94	0.12	56,56,56,56	0
54	MG	2A	3700	1/1	0.94	0.15	21,21,21,21	0
54	MG	2a	1723	1/1	0.94	0.19	45,45,45,45	0
54	MG	2A	3595	1/1	0.94	0.21	53,53,53,53	0
54	MG	2A	3239	1/1	0.94	0.14	50,50,50,50	0
54	MG	1a	1785	1/1	0.94	0.10	47,47,47,47	0
54	MG	1A	3816	1/1	0.94	0.13	35,35,35,35	0
59	ZN	2n	501	1/1	0.94	0.08	101,101,101,101	0
54	MG	1D	313	1/1	0.94	0.28	43,43,43,43	0
54	MG	2A	3120	1/1	0.94	0.15	41,41,41,41	0
54	MG	2A	3210	1/1	0.94	0.13	45,45,45,45	0
54	MG	15	104	1/1	0.94	0.15	62,62,62,62	0
54	MG	2A	3138	1/1	0.94	0.13	33,33,33,33	0
54	MG	2A	3642	1/1	0.94	0.16	57,57,57,57	0
54	MG	1A	3793	1/1	0.94	0.19	41,41,41,41	0
54	MG	1A	3496	1/1	0.94	0.14	47,47,47,47	0
54	MG	1A	3948	1/1	0.94	0.09	60,60,60,60	0
54	MG	2A	3233	1/1	0.94	0.13	58,58,58,58	0
54	MG	1a	1719	1/1	0.94	0.13	48,48,48,48	0
54	MG	1A	3634	1/1	0.94	0.13	59,59,59,59	0
54	MG	2a	1696	1/1	0.94	0.15	59,59,59,59	0
54	MG	2A	3693	1/1	0.94	0.10	50,50,50,50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3627	1/1	0.94	0.17	53,53,53,53	0
54	MG	2A	3606	1/1	0.94	0.07	50,50,50,50	0
54	MG	2W	8001	1/1	0.94	0.33	42,42,42,42	0
54	MG	1A	3048	1/1	0.94	0.30	33,33,33,33	0
54	MG	1A	3531	1/1	0.94	0.37	40,40,40,40	0
54	MG	1H	8002	1/1	0.94	0.11	37,37,37,37	0
54	MG	2a	1718	1/1	0.94	0.27	63,63,63,63	0
54	MG	2a	1738	1/1	0.94	0.30	52,52,52,52	0
54	MG	1A	3352	1/1	0.94	0.21	20,20,20,20	0
54	MG	2A	3723	1/1	0.94	0.58	37,37,37,37	0
54	MG	1A	3397	1/1	0.94	0.14	49,49,49,49	0
54	MG	2A	3101	1/1	0.94	0.21	50,50,50,50	0
54	MG	1A	3059	1/1	0.94	0.12	42,42,42,42	0
54	MG	2A	3475	1/1	0.94	0.18	30,30,30,30	0
54	MG	1A	3650	1/1	0.94	0.26	38,38,38,38	0
54	MG	1A	3905	1/1	0.94	0.08	53,53,53,53	0
54	MG	1A	3628	1/1	0.94	0.14	47,47,47,47	0
54	MG	1A	3691	1/1	0.94	0.18	17,17,17,17	0
56	EZP	2A	3709	25/25	0.94	0.46	38,42,50,58	0
54	MG	2A	3527	1/1	0.94	0.17	38,38,38,38	0
54	MG	2t	3001	1/1	0.94	0.11	45,45,45,45	0
54	MG	2A	3414	1/1	0.94	0.14	46,46,46,46	0
54	MG	1A	3871	1/1	0.94	0.24	50,50,50,50	0
54	MG	1A	3137	1/1	0.94	0.14	29,29,29,29	0
54	MG	2A	3429	1/1	0.94	0.12	59,59,59,59	0
54	MG	1A	3693	1/1	0.94	0.10	33,33,33,33	0
54	MG	2A	3591	1/1	0.94	0.26	51,51,51,51	0
54	MG	1N	201	1/1	0.94	0.32	35,35,35,35	0
54	MG	2A	3611	1/1	0.94	0.15	56,56,56,56	0
54	MG	1A	3112	1/1	0.94	0.48	34,34,34,34	0
54	MG	1A	3898	1/1	0.94	0.08	21,21,21,21	0
54	MG	2A	3073	1/1	0.94	0.12	45,45,45,45	0
54	MG	2A	3631	1/1	0.94	0.12	60,60,60,60	0
54	MG	1a	1698	1/1	0.94	0.12	36,36,36,36	0
54	MG	1a	1602	1/1	0.94	0.10	71,71,71,71	0
54	MG	2a	1622	1/1	0.94	0.09	56,56,56,56	0
54	MG	1A	3476	1/1	0.94	0.17	14,14,14,14	0
54	MG	1A	3669	1/1	0.94	0.16	25,25,25,25	0
54	MG	1F	312	1/1	0.94	0.19	51,51,51,51	0
54	MG	1A	3970	1/1	0.94	0.68	40,40,40,40	0
54	MG	1A	3362	1/1	0.94	0.11	36,36,36,36	0
54	MG	2A	3118	1/1	0.94	0.17	54,54,54,54	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3163	1/1	0.94	0.28	53,53,53,53	0
54	MG	1A	3023	1/1	0.94	0.12	19,19,19,19	0
54	MG	1A	3777	1/1	0.94	0.10	19,19,19,19	0
54	MG	1A	3201	1/1	0.94	0.51	39,39,39,39	0
54	MG	1A	3976	1/1	0.94	0.07	38,38,38,38	0
54	MG	2A	3670	1/1	0.94	0.14	49,49,49,49	0
54	MG	1A	3862	1/1	0.94	0.18	33,33,33,33	0
54	MG	2A	3698	1/1	0.94	0.36	40,40,40,40	0
54	MG	2a	1731	1/1	0.94	0.14	61,61,61,61	0
54	MG	2A	3298	1/1	0.94	0.16	27,27,27,27	0
54	MG	2A	3495	1/1	0.94	0.20	45,45,45,45	0
54	MG	1A	3060	1/1	0.94	0.20	28,28,28,28	0
54	MG	10	104	1/1	0.94	0.16	51,51,51,51	0
54	MG	2a	1654	1/1	0.94	0.21	58,58,58,58	0
54	MG	1A	3240	1/1	0.94	0.22	37,37,37,37	0
54	MG	2a	1732	1/1	0.94	0.29	60,60,60,60	0
54	MG	1A	4008	1/1	0.94	0.29	28,28,28,28	0
54	MG	2A	3707	1/1	0.94	0.18	61,61,61,61	0
54	MG	2A	3649	1/1	0.94	0.23	38,38,38,38	0
54	MG	2A	3529	1/1	0.94	0.09	49,49,49,49	0
54	MG	2a	1730	1/1	0.94	0.22	49,49,49,49	0
54	MG	1D	303	1/1	0.94	0.20	44,44,44,44	0
54	MG	1A	3801	1/1	0.94	0.11	34,34,34,34	0
54	MG	1A	3811	1/1	0.94	0.22	31,31,31,31	0
54	MG	2A	3705	1/1	0.94	0.88	45,45,45,45	0
54	MG	1A	3609	1/1	0.94	0.37	41,41,41,41	0
54	MG	1A	3090	1/1	0.95	0.21	12,12,12,12	0
54	MG	1A	3421	1/1	0.95	0.12	30,30,30,30	0
54	MG	2A	3696	1/1	0.95	0.17	52,52,52,52	0
54	MG	2A	3718	1/1	0.95	0.44	44,44,44,44	0
54	MG	2A	3628	1/1	0.95	0.07	60,60,60,60	0
54	MG	1a	1750	1/1	0.95	0.13	59,59,59,59	0
54	MG	2A	3240	1/1	0.95	0.24	49,49,49,49	0
54	MG	1A	3224	1/1	0.95	0.42	36,36,36,36	0
54	MG	2A	3007	1/1	0.95	0.43	36,36,36,36	0
54	MG	1A	3546	1/1	0.95	0.09	52,52,52,52	0
54	MG	2A	3263	1/1	0.95	0.19	32,32,32,32	0
54	MG	1A	3497	1/1	0.95	0.07	46,46,46,46	0
54	MG	2a	1727	1/1	0.95	0.21	61,61,61,61	0
54	MG	1A	3851	1/1	0.95	0.10	41,41,41,41	0
56	EZP	1A	3987	25/25	0.95	0.39	16,28,47,60	0
54	MG	2E	306	1/1	0.95	0.51	44,44,44,44	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3923	1/1	0.95	0.23	50,50,50,50	0
54	MG	1A	3152	1/1	0.95	0.23	31,31,31,31	0
54	MG	2a	1687	1/1	0.95	0.21	67,67,67,67	0
54	MG	1A	3505	1/1	0.95	0.12	27,27,27,27	0
54	MG	1A	3568	1/1	0.95	0.16	48,48,48,48	0
54	MG	2A	3699	1/1	0.95	0.28	61,61,61,61	0
54	MG	2A	3409	1/1	0.95	0.12	51,51,51,51	0
54	MG	1A	3578	1/1	0.95	0.20	23,23,23,23	0
54	MG	2A	3535	1/1	0.95	0.07	42,42,42,42	0
54	MG	1P	201	1/1	0.95	0.35	27,27,27,27	0
54	MG	1A	3230	1/1	0.95	0.19	46,46,46,46	0
54	MG	1A	3013	1/1	0.95	0.12	50,50,50,50	0
54	MG	1A	3916	1/1	0.95	0.09	29,29,29,29	0
54	MG	2a	1722	1/1	0.95	0.25	49,49,49,49	0
54	MG	1a	1712	1/1	0.95	0.18	51,51,51,51	0
54	MG	1A	3973	1/1	0.95	0.12	42,42,42,42	0
54	MG	1A	3762	1/1	0.95	0.15	19,19,19,19	0
54	MG	2A	3264	1/1	0.95	0.14	48,48,48,48	0
54	MG	2A	3550	1/1	0.95	0.16	31,31,31,31	0
54	MG	1A	3466	1/1	0.95	0.13	40,40,40,40	0
54	MG	2A	3074	1/1	0.95	0.41	39,39,39,39	0
54	MG	2A	3185	1/1	0.95	0.09	45,45,45,45	0
54	MG	1a	1694	1/1	0.95	0.21	32,32,32,32	0
54	MG	1a	1721	1/1	0.95	0.12	42,42,42,42	0
54	MG	2A	3484	1/1	0.95	0.36	65,65,65,65	0
54	MG	1A	3443	1/1	0.95	0.14	25,25,25,25	0
54	MG	1B	212	1/1	0.95	0.05	53,53,53,53	0
54	MG	2A	3354	1/1	0.95	0.17	49,49,49,49	0
54	MG	2A	3271	1/1	0.95	0.11	23,23,23,23	0
54	MG	2A	3480	1/1	0.95	0.68	37,37,37,37	0
54	MG	2A	3604	1/1	0.95	0.13	31,31,31,31	0
54	MG	2a	1741	1/1	0.95	0.15	55,55,55,55	0
54	MG	1A	3838	1/1	0.95	0.19	60,60,60,60	0
54	MG	2A	3440	1/1	0.95	0.10	49,49,49,49	0
54	MG	1A	3022	1/1	0.95	0.23	29,29,29,29	0
54	MG	1A	3316	1/1	0.95	0.10	38,38,38,38	0
54	MG	2A	3391	1/1	0.95	0.16	49,49,49,49	0
54	MG	2A	3513	1/1	0.95	0.21	50,50,50,50	0
54	MG	1A	3358	1/1	0.95	0.17	21,21,21,21	0
54	MG	1A	3557	1/1	0.95	0.13	35,35,35,35	0
54	MG	2A	3130	1/1	0.95	0.51	64,64,64,64	0
54	MG	1A	3441	1/1	0.95	0.20	34,34,34,34	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3688	1/1	0.95	0.11	56,56,56,56	0
54	MG	2a	1636	1/1	0.95	0.11	69,69,69,69	0
54	MG	1A	3947	1/1	0.95	0.20	67,67,67,67	0
54	MG	1A	3372	1/1	0.95	0.08	47,47,47,47	0
54	MG	1A	3439	1/1	0.95	0.17	34,34,34,34	0
54	MG	1A	3135	1/1	0.95	0.15	29,29,29,29	0
54	MG	1A	3110	1/1	0.95	0.24	37,37,37,37	0
54	MG	1a	1656	1/1	0.95	0.20	63,63,63,63	0
54	MG	1a	1636	1/1	0.95	0.22	60,60,60,60	0
54	MG	1A	3556	1/1	0.95	0.14	39,39,39,39	0
54	MG	2A	3295	1/1	0.95	0.17	55,55,55,55	0
54	MG	1A	3844	1/1	0.95	0.12	46,46,46,46	0
54	MG	1B	227	1/1	0.95	0.08	52,52,52,52	0
54	MG	2E	305	1/1	0.95	0.24	52,52,52,52	0
54	MG	2A	3322	1/1	0.95	0.13	49,49,49,49	0
54	MG	2A	3045	1/1	0.95	0.10	40,40,40,40	0
54	MG	2A	3253	1/1	0.95	0.19	25,25,25,25	0
54	MG	2B	3009	1/1	0.95	0.08	62,62,62,62	0
54	MG	1A	3371	1/1	0.95	0.19	49,49,49,49	0
54	MG	1A	3040	1/1	0.95	0.15	26,26,26,26	0
54	MG	2A	3541	1/1	0.95	0.07	47,47,47,47	0
54	MG	2A	3531	1/1	0.95	0.11	54,54,54,54	0
54	MG	1A	3262	1/1	0.95	0.15	28,28,28,28	0
54	MG	2a	1717	1/1	0.95	0.18	60,60,60,60	0
54	MG	2a	1619	1/1	0.95	0.19	47,47,47,47	0
54	MG	2A	3655	1/1	0.95	0.16	42,42,42,42	0
54	MG	1A	3255	1/1	0.95	0.60	31,31,31,31	0
54	MG	2A	3556	1/1	0.95	0.25	35,35,35,35	0
54	MG	1A	3502	1/1	0.95	0.13	54,54,54,54	0
54	MG	2a	1657	1/1	0.95	0.11	44,44,44,44	0
54	MG	1a	1811	1/1	0.95	0.16	42,42,42,42	0
54	MG	1a	1616	1/1	0.95	0.12	60,60,60,60	0
54	MG	1A	3709	1/1	0.95	0.08	46,46,46,46	0
54	MG	2A	3543	1/1	0.95	0.27	49,49,49,49	0
54	MG	2a	1690	1/1	0.95	0.15	68,68,68,68	0
54	MG	2A	3360	1/1	0.95	0.13	48,48,48,48	0
54	MG	2A	3577	1/1	0.95	0.12	68,68,68,68	0
54	MG	1E	302	1/1	0.95	0.77	39,39,39,39	0
58	ARG	1B	228	12/12	0.95	0.26	26,40,53,54	0
54	MG	2a	1705	1/1	0.95	0.14	55,55,55,55	0
54	MG	1A	3078	1/1	0.95	0.08	47,47,47,47	0
54	MG	1A	3086	1/1	0.95	0.41	26,26,26,26	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3682	1/1	0.95	0.09	38,38,38,38	0
54	MG	1A	3268	1/1	0.95	0.14	46,46,46,46	0
54	MG	1a	1774	1/1	0.95	0.17	53,53,53,53	0
54	MG	1A	3640	1/1	0.95	0.09	45,45,45,45	0
54	MG	1A	3451	1/1	0.95	0.16	15,15,15,15	0
54	MG	1A	3731	1/1	0.95	0.31	40,40,40,40	0
54	MG	1A	3523	1/1	0.95	0.19	48,48,48,48	0
54	MG	2A	3324	1/1	0.95	0.12	30,30,30,30	0
54	MG	2a	1706	1/1	0.95	0.11	63,63,63,63	0
54	MG	2a	1646	1/1	0.95	0.11	63,63,63,63	0
54	MG	2A	3002	1/1	0.95	0.16	53,53,53,53	0
54	MG	1A	3211	1/1	0.95	0.21	37,37,37,37	0
54	MG	2a	1703	1/1	0.95	0.15	61,61,61,61	0
54	MG	1a	1699	1/1	0.95	0.09	57,57,57,57	0
54	MG	2A	3129	1/1	0.95	0.09	52,52,52,52	0
54	MG	1a	1792	1/1	0.95	0.11	57,57,57,57	0
54	MG	1E	307	1/1	0.95	0.13	53,53,53,53	0
54	MG	2A	3302	1/1	0.95	0.12	25,25,25,25	0
54	MG	1a	1695	1/1	0.95	0.20	37,37,37,37	0
54	MG	1A	3745	1/1	0.95	0.27	60,60,60,60	0
54	MG	1A	3389	1/1	0.95	0.15	27,27,27,27	0
54	MG	2A	3438	1/1	0.95	0.11	50,50,50,50	0
54	MG	1a	1784	1/1	0.95	0.18	59,59,59,59	0
54	MG	2A	3588	1/1	0.95	0.12	48,48,48,48	0
54	MG	2a	1668	1/1	0.95	0.19	45,45,45,45	0
54	MG	1A	3914	1/1	0.95	0.17	38,38,38,38	0
54	MG	1A	3219	1/1	0.95	0.27	25,25,25,25	0
54	MG	1A	3612	1/1	0.95	0.18	22,22,22,22	0
54	MG	1A	3824	1/1	0.95	0.19	17,17,17,17	0
54	MG	2A	3104	1/1	0.95	0.10	42,42,42,42	0
54	MG	1A	3759	1/1	0.95	0.60	43,43,43,43	0
57	MPD	18	102	8/8	0.95	0.36	22,28,35,36	0
54	MG	1A	3094	1/1	0.95	0.46	29,29,29,29	0
54	MG	1A	3143	1/1	0.95	0.06	26,26,26,26	0
54	MG	1A	3368	1/1	0.95	0.19	16,16,16,16	0
54	MG	1A	3366	1/1	0.95	0.24	16,16,16,16	0
54	MG	2A	3546	1/1	0.95	0.26	41,41,41,41	0
54	MG	2A	3394	1/1	0.95	0.08	60,60,60,60	0
54	MG	2A	3292	1/1	0.95	0.23	47,47,47,47	0
54	MG	2a	1734	1/1	0.95	0.21	55,55,55,55	0
54	MG	1A	3863	1/1	0.95	0.12	12,12,12,12	0
54	MG	1A	3098	1/1	0.95	0.38	35,35,35,35	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3310	1/1	0.95	0.15	29,29,29,29	0
54	MG	1B	216	1/1	0.95	0.14	33,33,33,33	0
54	MG	1E	303	1/1	0.95	0.08	32,32,32,32	0
54	MG	1A	3052	1/1	0.95	0.14	36,36,36,36	0
54	MG	2A	3470	1/1	0.95	0.41	43,43,43,43	0
54	MG	1A	3490	1/1	0.95	0.16	50,50,50,50	0
54	MG	1A	3333	1/1	0.95	0.13	25,25,25,25	0
54	MG	1a	1809	1/1	0.95	0.13	66,66,66,66	0
54	MG	2a	1714	1/1	0.95	0.16	48,48,48,48	0
54	MG	1A	3822	1/1	0.95	0.11	40,40,40,40	0
54	MG	1A	3830	1/1	0.95	0.14	41,41,41,41	0
54	MG	1A	3456	1/1	0.95	0.21	27,27,27,27	0
54	MG	1A	3284	1/1	0.95	0.50	32,32,32,32	0
54	MG	2A	3325	1/1	0.95	0.15	40,40,40,40	0
54	MG	1A	3689	1/1	0.95	0.09	22,22,22,22	0
54	MG	2A	3387	1/1	0.95	0.23	45,45,45,45	0
54	MG	1A	3770	1/1	0.95	0.18	27,27,27,27	0
54	MG	2A	3576	1/1	0.95	0.10	62,62,62,62	0
54	MG	1A	3592	1/1	0.95	0.18	44,44,44,44	0
54	MG	1B	223	1/1	0.95	0.07	46,46,46,46	0
54	MG	2a	1711	1/1	0.95	0.22	45,45,45,45	0
54	MG	1W	3002	1/1	0.95	0.14	39,39,39,39	0
54	MG	1a	1654	1/1	0.95	0.08	56,56,56,56	0
54	MG	1A	3002	1/1	0.95	0.11	47,47,47,47	0
54	MG	2A	3082	1/1	0.95	0.07	62,62,62,62	0
54	MG	1B	214	1/1	0.95	0.13	35,35,35,35	0
54	MG	2A	3498	1/1	0.95	0.17	30,30,30,30	0
54	MG	1A	3977	1/1	0.95	0.17	38,38,38,38	0
54	MG	1A	3169	1/1	0.95	0.62	33,33,33,33	0
54	MG	2A	3042	1/1	0.95	0.14	49,49,49,49	0
54	MG	2B	3006	1/1	0.95	0.13	57,57,57,57	0
54	MG	2A	3473	1/1	0.95	0.32	60,60,60,60	0
54	MG	2A	3681	1/1	0.95	0.12	69,69,69,69	0
54	MG	2a	1643	1/1	0.95	0.12	55,55,55,55	0
54	MG	1a	1647	1/1	0.95	0.15	52,52,52,52	0
54	MG	1A	3791	1/1	0.95	0.17	59,59,59,59	0
54	MG	1a	1736	1/1	0.95	0.18	57,57,57,57	0
54	MG	2A	3725	1/1	0.95	0.28	37,37,37,37	0
54	MG	2A	3110	1/1	0.95	0.40	40,40,40,40	0
54	MG	2A	3708	1/1	0.95	0.15	58,58,58,58	0
54	MG	1A	3926	1/1	0.95	0.07	45,45,45,45	0
54	MG	1A	3992	1/1	0.95	0.52	28,28,28,28	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3623	1/1	0.95	0.10	43,43,43,43	0
54	MG	2A	3168	1/1	0.95	0.12	54,54,54,54	0
54	MG	1A	3566	1/1	0.95	0.20	35,35,35,35	0
54	MG	2a	1634	1/1	0.95	0.24	55,55,55,55	0
54	MG	1a	1763	1/1	0.95	0.18	64,64,64,64	0
54	MG	2A	3342	1/1	0.95	0.23	51,51,51,51	0
54	MG	2A	3025	1/1	0.95	0.12	44,44,44,44	0
54	MG	1A	3492	1/1	0.95	0.13	17,17,17,17	0
54	MG	1F	304	1/1	0.95	0.29	24,24,24,24	0
54	MG	2A	3288	1/1	0.95	0.12	49,49,49,49	0
54	MG	2A	3334	1/1	0.95	0.19	35,35,35,35	0
54	MG	2A	3380	1/1	0.95	0.26	56,56,56,56	0
54	MG	2A	3277	1/1	0.95	0.15	38,38,38,38	0
54	MG	1A	3275	1/1	0.95	0.21	29,29,29,29	0
54	MG	2A	3596	1/1	0.95	0.26	50,50,50,50	0
54	MG	1A	3812	1/1	0.95	0.44	35,35,35,35	0
54	MG	1A	3692	1/1	0.95	0.14	34,34,34,34	0
54	MG	1A	3381	1/1	0.95	0.11	40,40,40,40	0
54	MG	1A	3919	1/1	0.95	0.34	45,45,45,45	0
54	MG	1A	3444	1/1	0.95	0.14	24,24,24,24	0
54	MG	1A	3025	1/1	0.95	0.55	29,29,29,29	0
54	MG	1A	3382	1/1	0.95	0.14	19,19,19,19	0
54	MG	2a	1710	1/1	0.95	0.20	56,56,56,56	0
54	MG	1A	3840	1/1	0.95	0.12	33,33,33,33	0
54	MG	1A	3945	1/1	0.95	0.24	36,36,36,36	0
54	MG	1A	3385	1/1	0.95	0.11	51,51,51,51	0
54	MG	1A	3930	1/1	0.95	0.14	60,60,60,60	0
54	MG	2a	1736	1/1	0.95	0.20	61,61,61,61	0
54	MG	1A	4026	1/1	0.95	0.19	35,35,35,35	0
54	MG	1A	3237	1/1	0.95	0.24	28,28,28,28	0
54	MG	1A	3911	1/1	0.95	0.23	46,46,46,46	0
54	MG	1A	3517	1/1	0.95	0.18	48,48,48,48	0
54	MG	1A	3880	1/1	0.95	0.14	37,37,37,37	0
54	MG	2A	3061	1/1	0.95	0.27	51,51,51,51	0
54	MG	1O	8002	1/1	0.95	0.14	46,46,46,46	0
54	MG	2A	3416	1/1	0.95	0.17	54,54,54,54	0
54	MG	2a	1699	1/1	0.95	0.12	71,71,71,71	0
54	MG	2a	1744	1/1	0.95	0.14	50,50,50,50	0
54	MG	1A	3518	1/1	0.95	0.57	51,51,51,51	0
54	MG	2A	3097	1/1	0.95	0.10	67,67,67,67	0
54	MG	2A	3603	1/1	0.95	0.22	32,32,32,32	0
54	MG	1A	3401	1/1	0.95	0.11	45,45,45,45	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3179	1/1	0.95	0.45	36,36,36,36	0
54	MG	1A	3454	1/1	0.95	0.13	22,22,22,22	0
54	MG	2A	3327	1/1	0.95	0.14	48,48,48,48	0
54	MG	1A	3065	1/1	0.95	0.40	26,26,26,26	0
54	MG	2A	3162	1/1	0.95	0.11	53,53,53,53	0
54	MG	2A	3411	1/1	0.95	0.07	55,55,55,55	0
54	MG	1a	1644	1/1	0.95	0.13	60,60,60,60	0
54	MG	1A	3807	1/1	0.95	0.17	40,40,40,40	0
54	MG	1A	3459	1/1	0.95	0.17	23,23,23,23	0
54	MG	2a	1739	1/1	0.95	0.10	51,51,51,51	0
54	MG	1A	3299	1/1	0.95	0.17	19,19,19,19	0
54	MG	1A	3099	1/1	0.95	0.34	30,30,30,30	0
54	MG	2A	3511	1/1	0.95	0.22	43,43,43,43	0
54	MG	2a	1629	1/1	0.96	0.21	60,60,60,60	0
54	MG	1F	301	1/1	0.96	0.75	41,41,41,41	0
54	MG	1A	3338	1/1	0.96	0.12	28,28,28,28	0
54	MG	1A	3623	1/1	0.96	0.13	32,32,32,32	0
54	MG	1A	3105	1/1	0.96	0.16	33,33,33,33	0
54	MG	1A	3462	1/1	0.96	0.11	48,48,48,48	0
54	MG	1A	3827	1/1	0.96	0.16	21,21,21,21	0
54	MG	1a	1610	1/1	0.96	0.15	44,44,44,44	0
54	MG	1F	303	1/1	0.96	0.17	35,35,35,35	0
54	MG	1A	3754	1/1	0.96	0.40	37,37,37,37	0
54	MG	1A	3396	1/1	0.96	0.13	21,21,21,21	0
54	MG	2A	3345	1/1	0.96	0.29	45,45,45,45	0
54	MG	1A	3028	1/1	0.96	0.13	30,30,30,30	0
54	MG	1A	3886	1/1	0.96	0.12	52,52,52,52	0
54	MG	2A	3282	1/1	0.96	0.17	33,33,33,33	0
54	MG	2A	3272	1/1	0.96	0.09	38,38,38,38	0
54	MG	1A	3775	1/1	0.96	0.26	34,34,34,34	0
54	MG	1A	3785	1/1	0.96	0.21	28,28,28,28	0
54	MG	1A	3467	1/1	0.96	0.07	49,49,49,49	0
54	MG	1A	3080	1/1	0.96	0.45	37,37,37,37	0
54	MG	1A	3007	1/1	0.96	0.13	26,26,26,26	0
54	MG	1A	3438	1/1	0.96	0.15	43,43,43,43	0
54	MG	1a	1787	1/1	0.96	0.25	40,40,40,40	0
54	MG	2a	1652	1/1	0.96	0.19	48,48,48,48	0
54	MG	1A	3029	1/1	0.96	0.14	12,12,12,12	0
54	MG	1A	3741	1/1	0.96	0.15	48,48,48,48	0
54	MG	1G	3004	1/1	0.96	0.11	34,34,34,34	0
54	MG	1A	3698	1/1	0.96	0.20	58,58,58,58	0
54	MG	1A	3424	1/1	0.96	0.15	41,41,41,41	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3037	1/1	0.96	0.16	56,56,56,56	0
54	MG	1A	3374	1/1	0.96	0.13	50,50,50,50	0
54	MG	1a	1732	1/1	0.96	0.08	59,59,59,59	0
54	MG	2D	306	1/1	0.96	0.16	56,56,56,56	0
54	MG	2A	3248	1/1	0.96	0.07	55,55,55,55	0
54	MG	1A	3554	1/1	0.96	0.17	40,40,40,40	0
54	MG	2A	3030	1/1	0.96	0.15	53,53,53,53	0
54	MG	1A	3722	1/1	0.96	0.22	39,39,39,39	0
54	MG	1a	1795	1/1	0.96	0.28	49,49,49,49	0
54	MG	1A	3012	1/1	0.96	0.20	17,17,17,17	0
54	MG	2a	1628	1/1	0.96	0.11	31,31,31,31	0
54	MG	1A	3072	1/1	0.96	0.49	26,26,26,26	0
54	MG	2A	3337	1/1	0.96	0.07	38,38,38,38	0
54	MG	1A	3588	1/1	0.96	0.16	23,23,23,23	0
54	MG	1A	3631	1/1	0.96	0.12	48,48,48,48	0
54	MG	15	103	1/1	0.96	0.09	41,41,41,41	0
54	MG	1A	3153	1/1	0.96	0.17	42,42,42,42	0
54	MG	1A	3993	1/1	0.96	0.26	26,26,26,26	0
54	MG	2A	3641	1/1	0.96	0.14	46,46,46,46	0
54	MG	1A	3668	1/1	0.96	0.17	63,63,63,63	0
54	MG	2A	3518	1/1	0.96	0.11	41,41,41,41	0
54	MG	1a	1735	1/1	0.96	0.12	51,51,51,51	0
54	MG	1A	3329	1/1	0.96	0.14	33,33,33,33	0
54	MG	2A	3564	1/1	0.96	0.12	57,57,57,57	0
54	MG	2A	3686	1/1	0.96	0.12	42,42,42,42	0
54	MG	1A	3808	1/1	0.96	0.23	41,41,41,41	0
54	MG	1a	1849	1/1	0.96	0.14	47,47,47,47	0
54	MG	2A	3353	1/1	0.96	0.21	62,62,62,62	0
54	MG	2A	3622	1/1	0.96	0.17	18,18,18,18	0
54	MG	1A	3328	1/1	0.96	0.11	13,13,13,13	0
54	MG	2A	3526	1/1	0.96	0.10	53,53,53,53	0
54	MG	1a	1762	1/1	0.96	0.17	56,56,56,56	0
54	MG	2A	3158	1/1	0.96	0.20	48,48,48,48	0
54	MG	1A	3571	1/1	0.96	0.41	27,27,27,27	0
54	MG	1V	201	1/1	0.96	0.14	50,50,50,50	0
54	MG	1A	3216	1/1	0.96	0.55	29,29,29,29	0
54	MG	2A	3024	1/1	0.96	0.08	35,35,35,35	0
54	MG	2a	1610	1/1	0.96	0.23	45,45,45,45	0
54	MG	1A	3168	1/1	0.96	0.09	46,46,46,46	0
54	MG	1B	201	1/1	0.96	0.53	34,34,34,34	0
54	MG	1A	3617	1/1	0.96	0.15	38,38,38,38	0
54	MG	2A	3099	1/1	0.96	0.08	43,43,43,43	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3750	1/1	0.96	0.16	27,27,27,27	0
54	MG	1A	3200	1/1	0.96	0.34	32,32,32,32	0
54	MG	1A	3088	1/1	0.96	0.25	32,32,32,32	0
54	MG	1A	3814	1/1	0.96	0.15	25,25,25,25	0
54	MG	1A	3215	1/1	0.96	0.31	35,35,35,35	0
54	MG	2A	3312	1/1	0.96	0.20	39,39,39,39	0
54	MG	1A	3429	1/1	0.96	0.15	41,41,41,41	0
54	MG	2A	3565	1/1	0.96	0.12	48,48,48,48	0
54	MG	2A	3254	1/1	0.96	0.14	51,51,51,51	0
54	MG	1A	3561	1/1	0.96	0.12	25,25,25,25	0
54	MG	1A	3972	1/1	0.96	0.36	32,32,32,32	0
54	MG	1A	3068	1/1	0.96	0.15	23,23,23,23	0
54	MG	1A	3465	1/1	0.96	0.19	33,33,33,33	0
54	MG	1B	213	1/1	0.96	0.18	38,38,38,38	0
54	MG	2A	3356	1/1	0.96	0.17	40,40,40,40	0
54	MG	1A	3377	1/1	0.96	0.20	44,44,44,44	0
54	MG	2A	3445	1/1	0.96	0.37	41,41,41,41	0
54	MG	1A	3046	1/1	0.96	0.36	39,39,39,39	0
54	MG	1A	3630	1/1	0.96	0.24	54,54,54,54	0
54	MG	2a	1750	1/1	0.96	0.08	59,59,59,59	0
54	MG	1A	3192	1/1	0.96	0.41	35,35,35,35	0
54	MG	1A	3129	1/1	0.96	0.43	26,26,26,26	0
54	MG	2A	3222	1/1	0.96	0.16	46,46,46,46	0
54	MG	1A	3405	1/1	0.96	0.14	17,17,17,17	0
54	MG	1a	1790	1/1	0.96	0.13	60,60,60,60	0
54	MG	1A	3150	1/1	0.96	0.69	28,28,28,28	0
54	MG	2a	1728	1/1	0.96	0.09	53,53,53,53	0
54	MG	2A	3561	1/1	0.96	0.06	38,38,38,38	0
54	MG	1A	3569	1/1	0.96	0.29	34,34,34,34	0
54	MG	1A	3304	1/1	0.96	0.17	26,26,26,26	0
54	MG	1A	3032	1/1	0.96	0.10	45,45,45,45	0
54	MG	2A	3089	1/1	0.96	0.10	41,41,41,41	0
54	MG	1a	1769	1/1	0.96	0.20	56,56,56,56	0
54	MG	2A	3347	1/1	0.96	0.20	56,56,56,56	0
54	MG	2A	3404	1/1	0.96	0.15	56,56,56,56	0
54	MG	1A	3991	1/1	0.96	0.58	43,43,43,43	0
54	MG	1A	3892	1/1	0.96	0.08	39,39,39,39	0
54	MG	1A	3734	1/1	0.96	0.26	26,26,26,26	0
54	MG	1A	3326	1/1	0.96	0.07	38,38,38,38	0
54	MG	1A	3369	1/1	0.96	0.17	16,16,16,16	0
54	MG	1A	3889	1/1	0.96	0.19	36,36,36,36	0
54	MG	2A	3620	1/1	0.96	0.13	48,48,48,48	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1847	1/1	0.96	0.24	60,60,60,60	0
54	MG	2A	3232	1/1	0.96	0.12	44,44,44,44	0
54	MG	1A	3356	1/1	0.96	0.18	37,37,37,37	0
54	MG	2A	3085	1/1	0.96	0.16	35,35,35,35	0
54	MG	1A	3267	1/1	0.96	0.15	29,29,29,29	0
54	MG	2A	3433	1/1	0.96	0.14	57,57,57,57	0
54	MG	1A	3778	1/1	0.96	0.07	35,35,35,35	0
54	MG	2A	3038	1/1	0.96	0.11	46,46,46,46	0
54	MG	1A	3547	1/1	0.96	0.15	29,29,29,29	0
54	MG	2A	3490	1/1	0.96	0.17	44,44,44,44	0
54	MG	1a	1717	1/1	0.96	0.16	53,53,53,53	0
54	MG	2A	3542	1/1	0.96	0.19	45,45,45,45	0
54	MG	1A	3053	1/1	0.96	0.22	47,47,47,47	0
54	MG	1A	3318	1/1	0.96	0.17	26,26,26,26	0
54	MG	2a	1698	1/1	0.96	0.19	50,50,50,50	0
54	MG	1A	3909	1/1	0.96	0.08	35,35,35,35	0
54	MG	1A	3723	1/1	0.96	0.13	36,36,36,36	0
54	MG	1A	3716	1/1	0.96	0.15	47,47,47,47	0
54	MG	2A	3514	1/1	0.96	0.12	36,36,36,36	0
54	MG	2A	3410	1/1	0.96	0.17	47,47,47,47	0
54	MG	2A	3464	1/1	0.96	0.16	34,34,34,34	0
54	MG	1A	3699	1/1	0.96	0.13	42,42,42,42	0
54	MG	1A	3222	1/1	0.96	0.46	32,32,32,32	0
54	MG	1A	3206	1/1	0.96	0.23	18,18,18,18	0
54	MG	2a	1633	1/1	0.96	0.15	68,68,68,68	0
54	MG	1A	3719	1/1	0.96	0.11	56,56,56,56	0
54	MG	1A	3907	1/1	0.96	0.14	52,52,52,52	0
54	MG	1A	3386	1/1	0.96	0.12	19,19,19,19	0
54	MG	1A	3228	1/1	0.96	0.22	18,18,18,18	0
54	MG	1A	3742	1/1	0.96	0.14	32,32,32,32	0
54	MG	1a	1614	1/1	0.96	0.08	56,56,56,56	0
54	MG	2A	3286	1/1	0.96	0.14	47,47,47,47	0
54	MG	1A	3922	1/1	0.96	0.27	61,61,61,61	0
54	MG	1A	3307	1/1	0.96	0.17	31,31,31,31	0
54	MG	1a	1708	1/1	0.96	0.24	32,32,32,32	0
54	MG	2A	3013	1/1	0.96	0.50	33,33,33,33	0
54	MG	1A	3244	1/1	0.96	0.38	27,27,27,27	0
54	MG	2A	3359	1/1	0.96	0.14	52,52,52,52	0
54	MG	2A	3319	1/1	0.96	0.16	39,39,39,39	0
54	MG	2A	3704	1/1	0.96	0.17	33,33,33,33	0
54	MG	2A	3255	1/1	0.96	0.12	24,24,24,24	0
54	MG	2A	3539	1/1	0.96	0.13	41,41,41,41	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3276	1/1	0.96	0.25	26,26,26,26	0
54	MG	1A	3738	1/1	0.96	0.14	24,24,24,24	0
54	MG	1A	3636	1/1	0.96	0.22	17,17,17,17	0
54	MG	1A	3639	1/1	0.96	0.21	34,34,34,34	0
54	MG	2A	3187	1/1	0.96	0.13	44,44,44,44	0
54	MG	1A	3193	1/1	0.96	0.22	44,44,44,44	0
54	MG	1A	3622	1/1	0.96	0.14	51,51,51,51	0
54	MG	1A	3746	1/1	0.96	0.17	59,59,59,59	0
54	MG	1A	3729	1/1	0.96	0.18	31,31,31,31	0
54	MG	1A	3656	1/1	0.96	0.19	37,37,37,37	0
54	MG	1A	4024	1/1	0.96	0.50	30,30,30,30	0
54	MG	1a	1770	1/1	0.96	0.19	54,54,54,54	0
54	MG	1A	3049	1/1	0.96	0.38	38,38,38,38	0
54	MG	1A	3806	1/1	0.96	0.13	34,34,34,34	0
54	MG	1A	3743	1/1	0.96	0.24	62,62,62,62	0
54	MG	2A	3300	1/1	0.96	0.14	28,28,28,28	0
54	MG	2A	3716	1/1	0.96	0.45	51,51,51,51	0
54	MG	1A	3062	1/1	0.96	0.16	25,25,25,25	0
54	MG	2a	1712	1/1	0.96	0.18	37,37,37,37	0
54	MG	2a	1665	1/1	0.96	0.33	55,55,55,55	0
54	MG	1A	3204	1/1	0.96	0.52	27,27,27,27	0
54	MG	1A	3186	1/1	0.96	0.47	36,36,36,36	0
54	MG	2A	3418	1/1	0.96	0.13	54,54,54,54	0
54	MG	1A	3409	1/1	0.96	0.13	50,50,50,50	0
54	MG	1A	3334	1/1	0.96	0.14	25,25,25,25	0
54	MG	1A	3580	1/1	0.96	0.15	22,22,22,22	0
54	MG	1A	3074	1/1	0.96	0.44	45,45,45,45	0
54	MG	2A	3289	1/1	0.96	0.12	47,47,47,47	0
54	MG	1A	3468	1/1	0.96	0.16	45,45,45,45	0
54	MG	2A	3237	1/1	0.96	0.47	34,34,34,34	0
54	MG	1A	3232	1/1	0.96	0.48	31,31,31,31	0
54	MG	1a	1765	1/1	0.96	0.11	46,46,46,46	0
54	MG	2F	302	1/1	0.96	0.15	49,49,49,49	0
54	MG	1a	1725	1/1	0.96	0.15	46,46,46,46	0
54	MG	1a	1823	1/1	0.96	0.13	48,48,48,48	0
54	MG	1A	3207	1/1	0.96	0.43	39,39,39,39	0
54	MG	1A	4020	1/1	0.96	0.54	27,27,27,27	0
54	MG	13	102	1/1	0.96	0.14	27,27,27,27	0
54	MG	2A	3496	1/1	0.96	0.13	40,40,40,40	0
54	MG	1A	3885	1/1	0.96	0.20	53,53,53,53	0
54	MG	2A	3260	1/1	0.96	0.06	53,53,53,53	0
54	MG	1A	3555	1/1	0.96	0.18	39,39,39,39	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3450	1/1	0.96	0.22	27,27,27,27	0
54	MG	2A	3451	1/1	0.96	0.16	49,49,49,49	0
54	MG	1a	1826	1/1	0.96	0.21	58,58,58,58	0
54	MG	2A	3689	1/1	0.96	0.06	59,59,59,59	0
54	MG	1A	3001	1/1	0.96	0.14	27,27,27,27	0
54	MG	1A	4021	1/1	0.96	0.52	35,35,35,35	0
54	MG	1a	1713	1/1	0.96	0.08	53,53,53,53	0
54	MG	2a	1679	1/1	0.96	0.15	53,53,53,53	0
54	MG	2A	3155	1/1	0.96	0.16	48,48,48,48	0
54	MG	1A	3644	1/1	0.96	0.08	58,58,58,58	0
54	MG	18	101	1/1	0.96	0.06	46,46,46,46	0
54	MG	1a	1611	1/1	0.96	0.18	37,37,37,37	0
54	MG	1D	312	1/1	0.96	0.13	54,54,54,54	0
54	MG	2A	3497	1/1	0.96	0.14	43,43,43,43	0
54	MG	1A	3325	1/1	0.96	0.27	53,53,53,53	0
54	MG	2A	3678	1/1	0.96	0.10	51,51,51,51	0
54	MG	1A	3494	1/1	0.96	0.14	38,38,38,38	0
54	MG	2A	3352	1/1	0.96	0.11	52,52,52,52	0
54	MG	1a	1661	1/1	0.96	0.11	49,49,49,49	0
54	MG	1A	3846	1/1	0.96	0.13	27,27,27,27	0
54	MG	1A	3629	1/1	0.96	0.08	41,41,41,41	0
54	MG	2D	304	1/1	0.96	0.48	42,42,42,42	0
54	MG	1A	3839	1/1	0.96	0.25	32,32,32,32	0
54	MG	1A	3455	1/1	0.96	0.16	10,10,10,10	0
54	MG	2A	3181	1/1	0.96	0.18	47,47,47,47	0
54	MG	1A	3990	1/1	0.96	0.23	20,20,20,20	0
54	MG	1A	3340	1/1	0.96	0.12	28,28,28,28	0
54	MG	2A	3523	1/1	0.96	0.23	49,49,49,49	0
54	MG	1A	3624	1/1	0.96	0.32	45,45,45,45	0
54	MG	1i	3001	1/1	0.96	0.14	53,53,53,53	0
54	MG	2A	3331	1/1	0.96	0.16	49,49,49,49	0
54	MG	2A	3121	1/1	0.96	0.19	53,53,53,53	0
54	MG	1A	3069	1/1	0.96	0.18	23,23,23,23	0
54	MG	2A	3400	1/1	0.96	0.24	36,36,36,36	0
54	MG	2A	3645	1/1	0.96	0.07	40,40,40,40	0
54	MG	1A	3695	1/1	0.96	0.11	49,49,49,49	0
54	MG	2A	3067	1/1	0.96	0.45	45,45,45,45	0
54	MG	1A	3472	1/1	0.97	0.14	20,20,20,20	0
54	MG	1A	4011	1/1	0.97	0.33	29,29,29,29	0
54	MG	2a	1671	1/1	0.97	0.25	47,47,47,47	0
54	MG	1A	3989	1/1	0.97	0.32	50,50,50,50	0
54	MG	2A	3018	1/1	0.97	0.13	40,40,40,40	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3299	1/1	0.97	0.16	28,28,28,28	0
54	MG	2A	3580	1/1	0.97	0.17	36,36,36,36	0
54	MG	1a	1838	1/1	0.97	0.11	55,55,55,55	0
54	MG	1A	3918	1/1	0.97	0.16	38,38,38,38	0
54	MG	2A	3102	1/1	0.97	0.11	42,42,42,42	0
54	MG	2A	3020	1/1	0.97	0.31	57,57,57,57	0
54	MG	1A	4002	1/1	0.97	0.63	29,29,29,29	0
54	MG	2A	3714	1/1	0.97	0.88	45,45,45,45	0
54	MG	1A	3447	1/1	0.97	0.15	34,34,34,34	0
54	MG	1A	3246	1/1	0.97	0.14	58,58,58,58	0
54	MG	1A	3045	1/1	0.97	0.22	35,35,35,35	0
54	MG	1a	1683	1/1	0.97	0.13	59,59,59,59	0
54	MG	1A	3134	1/1	0.97	0.15	22,22,22,22	0
54	MG	2A	3376	1/1	0.97	0.10	47,47,47,47	0
54	MG	1A	3529	1/1	0.97	0.06	47,47,47,47	0
54	MG	1A	3245	1/1	0.97	0.11	27,27,27,27	0
54	MG	2A	3270	1/1	0.97	0.07	37,37,37,37	0
54	MG	1A	3975	1/1	0.97	0.09	39,39,39,39	0
54	MG	1A	3033	1/1	0.97	0.21	34,34,34,34	0
54	MG	2A	3616	1/1	0.97	0.08	45,45,45,45	0
54	MG	2a	1713	1/1	0.97	0.43	55,55,55,55	0
54	MG	2A	3364	1/1	0.97	0.26	58,58,58,58	0
54	MG	2A	3128	1/1	0.97	0.53	45,45,45,45	0
54	MG	2A	3522	1/1	0.97	0.15	47,47,47,47	0
54	MG	1F	305	1/1	0.97	0.49	34,34,34,34	0
54	MG	2A	3578	1/1	0.97	0.16	47,47,47,47	0
54	MG	1a	1710	1/1	0.97	0.12	63,63,63,63	0
54	MG	1A	4019	1/1	0.97	0.21	29,29,29,29	0
54	MG	1A	3308	1/1	0.97	0.20	34,34,34,34	0
54	MG	2E	303	1/1	0.97	0.09	44,44,44,44	0
54	MG	2T	3004	1/1	0.97	0.10	44,44,44,44	0
59	ZN	29	501	1/1	0.97	0.12	62,62,62,62	0
54	MG	2A	3615	1/1	0.97	0.14	35,35,35,35	0
54	MG	1A	3406	1/1	0.97	0.15	52,52,52,52	0
54	MG	1A	3515	1/1	0.97	0.29	30,30,30,30	0
54	MG	2A	3313	1/1	0.97	0.12	33,33,33,33	0
54	MG	2A	3537	1/1	0.97	0.15	42,42,42,42	0
54	MG	1A	3146	1/1	0.97	0.83	34,34,34,34	0
54	MG	2a	1691	1/1	0.97	0.17	56,56,56,56	0
54	MG	2A	3100	1/1	0.97	0.16	48,48,48,48	0
54	MG	1A	3149	1/1	0.97	0.25	21,21,21,21	0
54	MG	1A	3364	1/1	0.97	0.18	13,13,13,13	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1672	1/1	0.97	0.27	51,51,51,51	0
54	MG	2T	3003	1/1	0.97	0.16	61,61,61,61	0
54	MG	1a	1804	1/1	0.97	0.18	59,59,59,59	0
54	MG	1A	3042	1/1	0.97	0.23	8,8,8,8	0
54	MG	1A	3145	1/1	0.97	0.50	43,43,43,43	0
54	MG	1a	1722	1/1	0.97	0.15	56,56,56,56	0
54	MG	1A	3653	1/1	0.97	0.45	41,41,41,41	0
54	MG	1A	3507	1/1	0.97	0.10	29,29,29,29	0
54	MG	2A	3638	1/1	0.97	0.09	32,32,32,32	0
54	MG	1A	3772	1/1	0.97	0.44	24,24,24,24	0
54	MG	1A	3294	1/1	0.97	0.10	46,46,46,46	0
54	MG	1A	3109	1/1	0.97	0.57	31,31,31,31	0
54	MG	2A	3701	1/1	0.97	0.17	47,47,47,47	0
54	MG	14	502	1/1	0.97	0.06	72,72,72,72	0
54	MG	1A	3087	1/1	0.97	0.53	26,26,26,26	0
54	MG	1A	3931	1/1	0.97	0.21	34,34,34,34	0
54	MG	2A	3141	1/1	0.97	0.37	39,39,39,39	0
54	MG	1F	308	1/1	0.97	0.39	29,29,29,29	0
54	MG	1a	1682	1/1	0.97	0.10	59,59,59,59	0
54	MG	1A	3107	1/1	0.97	0.26	27,27,27,27	0
54	MG	1A	3111	1/1	0.97	0.45	31,31,31,31	0
54	MG	2A	3474	1/1	0.97	0.13	50,50,50,50	0
54	MG	1a	1645	1/1	0.97	0.19	41,41,41,41	0
54	MG	2A	3390	1/1	0.97	0.13	31,31,31,31	0
54	MG	1X	102	1/1	0.97	0.16	31,31,31,31	0
54	MG	1a	1615	1/1	0.97	0.17	59,59,59,59	0
54	MG	1A	3348	1/1	0.97	0.13	41,41,41,41	0
54	MG	2A	3150	1/1	0.97	0.15	62,62,62,62	0
54	MG	1a	1603	1/1	0.97	0.15	45,45,45,45	0
54	MG	1A	3541	1/1	0.97	0.17	19,19,19,19	0
54	MG	2O	201	1/1	0.97	0.12	48,48,48,48	0
54	MG	2A	3015	1/1	0.97	0.42	43,43,43,43	0
54	MG	1A	3910	1/1	0.97	0.12	59,59,59,59	0
54	MG	1A	3254	1/1	0.97	0.36	30,30,30,30	0
54	MG	1A	3410	1/1	0.97	0.17	18,18,18,18	0
54	MG	1A	3715	1/1	0.97	0.11	19,19,19,19	0
54	MG	2A	3086	1/1	0.97	0.13	48,48,48,48	0
54	MG	1A	3912	1/1	0.97	0.21	43,43,43,43	0
54	MG	1A	3509	1/1	0.97	0.14	41,41,41,41	0
54	MG	1A	3586	1/1	0.97	0.10	23,23,23,23	0
54	MG	2A	3209	1/1	0.97	0.65	43,43,43,43	0
54	MG	1A	3491	1/1	0.97	0.07	36,36,36,36	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1l	101	1/1	0.97	0.23	44,44,44,44	0
54	MG	1A	3607	1/1	0.97	0.14	50,50,50,50	0
54	MG	1e	3001	1/1	0.97	0.36	56,56,56,56	0
54	MG	1a	1632	1/1	0.97	0.13	35,35,35,35	0
54	MG	2A	3455	1/1	0.97	0.08	48,48,48,48	0
54	MG	1A	3600	1/1	0.97	0.21	27,27,27,27	0
54	MG	2A	3437	1/1	0.97	0.08	58,58,58,58	0
54	MG	1A	3893	1/1	0.97	0.11	50,50,50,50	0
54	MG	1A	3126	1/1	0.97	0.48	33,33,33,33	0
54	MG	2E	301	1/1	0.97	0.12	43,43,43,43	0
54	MG	1A	3027	1/1	0.97	0.26	34,34,34,34	0
54	MG	1A	3015	1/1	0.97	0.55	29,29,29,29	0
54	MG	1A	3984	1/1	0.97	0.12	37,37,37,37	0
54	MG	1a	1827	1/1	0.97	0.11	33,33,33,33	0
54	MG	2A	3634	1/1	0.97	0.15	42,42,42,42	0
54	MG	1A	3897	1/1	0.97	0.17	23,23,23,23	0
54	MG	1A	3478	1/1	0.97	0.17	16,16,16,16	0
54	MG	2A	3592	1/1	0.97	0.14	47,47,47,47	0
54	MG	1a	1643	1/1	0.97	0.10	52,52,52,52	0
54	MG	1A	3312	1/1	0.97	0.18	17,17,17,17	0
54	MG	1a	1733	1/1	0.97	0.12	55,55,55,55	0
54	MG	2A	3722	1/1	0.97	0.30	48,48,48,48	0
54	MG	1A	3357	1/1	0.97	0.13	20,20,20,20	0
54	MG	2A	3228	1/1	0.97	0.13	58,58,58,58	0
54	MG	2a	1701	1/1	0.97	0.26	42,42,42,42	0
54	MG	2A	3256	1/1	0.97	0.17	51,51,51,51	0
54	MG	1A	3855	1/1	0.97	0.18	25,25,25,25	0
54	MG	1A	3852	1/1	0.97	0.32	30,30,30,30	0
54	MG	1A	3176	1/1	0.97	0.17	49,49,49,49	0
54	MG	1A	3710	1/1	0.97	0.16	38,38,38,38	0
54	MG	2A	3571	1/1	0.97	0.20	42,42,42,42	0
54	MG	1a	1642	1/1	0.97	0.20	39,39,39,39	0
54	MG	1A	3248	1/1	0.97	0.14	31,31,31,31	0
54	MG	2A	3499	1/1	0.97	0.21	30,30,30,30	0
54	MG	1a	1829	1/1	0.97	0.18	42,42,42,42	0
54	MG	2A	3057	1/1	0.97	0.12	39,39,39,39	0
54	MG	2A	3033	1/1	0.97	0.17	46,46,46,46	0
54	MG	1a	1798	1/1	0.97	0.12	61,61,61,61	0
54	MG	1A	3073	1/1	0.97	0.40	30,30,30,30	0
54	MG	1A	3979	1/1	0.97	0.28	47,47,47,47	0
54	MG	2A	3279	1/1	0.97	0.12	63,63,63,63	0
54	MG	1A	3375	1/1	0.97	0.15	16,16,16,16	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2a	1724	1/1	0.97	0.20	41,41,41,41	0
54	MG	1A	3113	1/1	0.97	0.15	18,18,18,18	0
54	MG	1a	1646	1/1	0.97	0.23	48,48,48,48	0
54	MG	1A	3925	1/1	0.97	0.14	49,49,49,49	0
54	MG	1A	3792	1/1	0.97	0.14	12,12,12,12	0
54	MG	2A	3221	1/1	0.97	0.40	57,57,57,57	0
54	MG	1A	3888	1/1	0.97	0.12	18,18,18,18	0
54	MG	1A	3227	1/1	0.97	0.35	25,25,25,25	0
54	MG	2a	1674	1/1	0.97	0.16	43,43,43,43	0
54	MG	1A	3414	1/1	0.97	0.14	49,49,49,49	0
54	MG	1A	3856	1/1	0.97	0.19	42,42,42,42	0
54	MG	1A	3978	1/1	0.97	0.34	26,26,26,26	0
54	MG	1A	3771	1/1	0.97	0.22	27,27,27,27	0
54	MG	2A	3008	1/1	0.97	0.10	57,57,57,57	0
54	MG	1A	3231	1/1	0.97	0.52	34,34,34,34	0
54	MG	1A	3685	1/1	0.97	0.10	42,42,42,42	0
54	MG	2A	3517	1/1	0.97	0.20	46,46,46,46	0
54	MG	1A	3041	1/1	0.97	0.12	12,12,12,12	0
54	MG	1A	3130	1/1	0.97	0.61	25,25,25,25	0
54	MG	1A	3066	1/1	0.97	0.50	30,30,30,30	0
54	MG	1E	304	1/1	0.97	0.17	16,16,16,16	0
54	MG	1A	3849	1/1	0.97	0.11	58,58,58,58	0
54	MG	2a	1702	1/1	0.97	0.13	73,73,73,73	0
54	MG	2A	3366	1/1	0.97	0.14	31,31,31,31	0
54	MG	1Q	201	1/1	0.97	0.12	38,38,38,38	0
54	MG	2A	3259	1/1	0.97	0.10	32,32,32,32	0
54	MG	1A	3997	1/1	0.97	0.25	23,23,23,23	0
54	MG	1A	3638	1/1	0.97	0.09	38,38,38,38	0
54	MG	1a	1745	1/1	0.97	0.09	47,47,47,47	0
54	MG	2B	3016	1/1	0.97	0.14	52,52,52,52	0
54	MG	1D	308	1/1	0.97	0.27	31,31,31,31	0
54	MG	2A	3307	1/1	0.97	0.19	51,51,51,51	0
54	MG	1a	1609	1/1	0.97	0.34	51,51,51,51	0
54	MG	2A	3125	1/1	0.97	0.20	38,38,38,38	0
54	MG	2A	3035	1/1	0.97	0.13	29,29,29,29	0
54	MG	2A	3011	1/1	0.97	0.13	21,21,21,21	0
54	MG	1A	3154	1/1	0.97	0.13	41,41,41,41	0
54	MG	1A	3097	1/1	0.97	0.58	23,23,23,23	0
54	MG	1A	3959	1/1	0.97	0.48	47,47,47,47	0
54	MG	1A	3658	1/1	0.97	0.10	24,24,24,24	0
54	MG	2A	3069	1/1	0.97	0.11	40,40,40,40	0
54	MG	1A	3249	1/1	0.97	0.41	34,34,34,34	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1Q	204	1/1	0.97	0.17	31,31,31,31	0
54	MG	1B	205	1/1	0.97	0.11	40,40,40,40	0
54	MG	2A	3427	1/1	0.97	0.10	57,57,57,57	0
54	MG	1A	3796	1/1	0.97	0.19	45,45,45,45	0
54	MG	2a	1708	1/1	0.97	0.27	52,52,52,52	0
54	MG	1A	3314	1/1	0.97	0.14	46,46,46,46	0
54	MG	1A	3813	1/1	0.97	0.13	56,56,56,56	0
54	MG	1A	3020	1/1	0.97	0.25	33,33,33,33	0
54	MG	1A	3063	1/1	0.97	0.24	32,32,32,32	0
54	MG	1A	3458	1/1	0.97	0.19	21,21,21,21	0
54	MG	1A	3018	1/1	0.97	0.41	24,24,24,24	0
54	MG	2a	1733	1/1	0.97	0.32	52,52,52,52	0
54	MG	2A	3516	1/1	0.97	0.20	19,19,19,19	0
54	MG	1A	3234	1/1	0.97	0.49	24,24,24,24	0
54	MG	1A	3587	1/1	0.97	0.15	26,26,26,26	0
54	MG	1A	3564	1/1	0.97	0.11	39,39,39,39	0
54	MG	2A	3227	1/1	0.97	0.66	38,38,38,38	0
54	MG	1A	3676	1/1	0.97	0.17	28,28,28,28	0
54	MG	2A	3395	1/1	0.97	0.12	56,56,56,56	0
54	MG	1a	1663	1/1	0.97	0.15	59,59,59,59	0
54	MG	2A	3267	1/1	0.97	0.14	52,52,52,52	0
54	MG	1A	3157	1/1	0.97	0.13	28,28,28,28	0
54	MG	2A	3351	1/1	0.97	0.17	25,25,25,25	0
54	MG	1A	3596	1/1	0.97	0.40	38,38,38,38	0
54	MG	2A	3062	1/1	0.97	0.43	35,35,35,35	0
54	MG	1a	1728	1/1	0.97	0.10	51,51,51,51	0
54	MG	2A	3574	1/1	0.97	0.15	52,52,52,52	0
54	MG	1A	3482	1/1	0.97	0.18	17,17,17,17	0
54	MG	1A	3350	1/1	0.97	0.17	29,29,29,29	0
54	MG	1A	3360	1/1	0.97	0.16	18,18,18,18	0
54	MG	2a	1686	1/1	0.97	0.09	52,52,52,52	0
54	MG	1A	4001	1/1	0.97	0.20	37,37,37,37	0
54	MG	2A	3584	1/1	0.97	0.13	46,46,46,46	0
54	MG	1A	3044	1/1	0.97	0.15	23,23,23,23	0
54	MG	1Q	202	1/1	0.97	0.14	29,29,29,29	0
54	MG	1A	3171	1/1	0.98	0.23	23,23,23,23	0
54	MG	1A	3114	1/1	0.98	0.15	22,22,22,22	0
54	MG	1A	3774	1/1	0.98	0.10	12,12,12,12	0
54	MG	1A	3269	1/1	0.98	0.15	12,12,12,12	0
54	MG	2A	3276	1/1	0.98	0.12	44,44,44,44	0
54	MG	1A	3115	1/1	0.98	0.17	22,22,22,22	0
54	MG	2A	3378	1/1	0.98	0.10	28,28,28,28	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3572	1/1	0.98	0.10	21,21,21,21	0
54	MG	1A	3874	1/1	0.98	0.15	43,43,43,43	0
54	MG	1A	3195	1/1	0.98	0.33	33,33,33,33	0
54	MG	1A	3890	1/1	0.98	0.17	46,46,46,46	0
54	MG	1A	3273	1/1	0.98	0.11	30,30,30,30	0
54	MG	1A	3393	1/1	0.98	0.17	18,18,18,18	0
54	MG	1A	3351	1/1	0.98	0.14	18,18,18,18	0
54	MG	1A	3416	1/1	0.98	0.10	48,48,48,48	0
54	MG	1D	301	1/1	0.98	0.30	25,25,25,25	0
60	SF4	1d	302	8/8	0.98	0.17	48,59,66,72	0
54	MG	1A	3185	1/1	0.98	0.31	42,42,42,42	0
54	MG	1a	1607	1/1	0.98	0.11	51,51,51,51	0
54	MG	1A	4006	1/1	0.98	0.23	31,31,31,31	0
54	MG	1A	3474	1/1	0.98	0.15	44,44,44,44	0
54	MG	2A	3407	1/1	0.98	0.11	50,50,50,50	0
54	MG	1A	3412	1/1	0.98	0.16	45,45,45,45	0
54	MG	1a	1670	1/1	0.98	0.22	50,50,50,50	0
54	MG	1A	3344	1/1	0.98	0.12	21,21,21,21	0
54	MG	1A	3985	1/1	0.98	0.35	36,36,36,36	0
54	MG	1A	3860	1/1	0.98	0.31	43,43,43,43	0
54	MG	1a	1706	1/1	0.98	0.17	28,28,28,28	0
54	MG	1A	3489	1/1	0.98	0.14	21,21,21,21	0
54	MG	1A	3202	1/1	0.98	0.66	32,32,32,32	0
54	MG	1A	3585	1/1	0.98	0.11	36,36,36,36	0
54	MG	1A	3470	1/1	0.98	0.12	36,36,36,36	0
54	MG	1A	3553	1/1	0.98	0.14	18,18,18,18	0
54	MG	2A	3135	1/1	0.98	0.13	67,67,67,67	0
54	MG	1A	3306	1/1	0.98	0.13	23,23,23,23	0
54	MG	2A	3424	1/1	0.98	0.12	52,52,52,52	0
54	MG	2A	3559	1/1	0.98	0.19	32,32,32,32	0
54	MG	1A	3076	1/1	0.98	0.36	27,27,27,27	0
54	MG	1A	3776	1/1	0.98	0.13	26,26,26,26	0
54	MG	1A	3290	1/1	0.98	0.16	32,32,32,32	0
54	MG	2A	3064	1/1	0.98	0.23	21,21,21,21	0
54	MG	1A	3763	1/1	0.98	0.24	46,46,46,46	0
54	MG	1A	3433	1/1	0.98	0.12	32,32,32,32	0
60	SF4	2d	501	8/8	0.98	0.14	61,71,81,92	0
54	MG	1A	3999	1/1	0.98	0.53	32,32,32,32	0
54	MG	1A	3155	1/1	0.98	0.19	26,26,26,26	0
54	MG	1A	3495	1/1	0.98	0.14	18,18,18,18	0
54	MG	2A	3169	1/1	0.98	0.35	38,38,38,38	0
54	MG	1A	4025	1/1	0.98	0.37	30,30,30,30	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3464	1/1	0.98	0.14	56,56,56,56	0
54	MG	2V	201	1/1	0.98	0.16	60,60,60,60	0
54	MG	1A	3317	1/1	0.98	0.10	56,56,56,56	0
54	MG	1A	3996	1/1	0.98	0.40	27,27,27,27	0
54	MG	2A	3119	1/1	0.98	0.09	64,64,64,64	0
54	MG	1A	3684	1/1	0.98	0.12	46,46,46,46	0
54	MG	1A	3652	1/1	0.98	0.29	44,44,44,44	0
54	MG	2A	3344	1/1	0.98	0.17	37,37,37,37	0
54	MG	1A	3510	1/1	0.98	0.15	34,34,34,34	0
54	MG	1Q	203	1/1	0.98	0.24	36,36,36,36	0
54	MG	1A	3345	1/1	0.98	0.22	50,50,50,50	0
54	MG	1a	1815	1/1	0.98	0.10	44,44,44,44	0
54	MG	1A	3853	1/1	0.98	0.14	15,15,15,15	0
54	MG	2A	3266	1/1	0.98	0.14	40,40,40,40	0
54	MG	1A	3037	1/1	0.98	0.16	39,39,39,39	0
54	MG	2T	3002	1/1	0.98	0.11	61,61,61,61	0
54	MG	1A	3407	1/1	0.98	0.12	38,38,38,38	0
54	MG	1A	3089	1/1	0.98	0.29	26,26,26,26	0
54	MG	2a	1609	1/1	0.98	0.17	46,46,46,46	0
54	MG	1A	3243	1/1	0.98	0.13	35,35,35,35	0
54	MG	1A	3614	1/1	0.98	0.16	17,17,17,17	0
54	MG	1A	3516	1/1	0.98	0.14	31,31,31,31	0
54	MG	1A	3920	1/1	0.98	0.15	21,21,21,21	0
54	MG	2A	3605	1/1	0.98	0.10	62,62,62,62	0
54	MG	1A	3136	1/1	0.98	0.20	24,24,24,24	0
54	MG	1a	1758	1/1	0.98	0.20	52,52,52,52	0
54	MG	2A	3340	1/1	0.98	0.19	55,55,55,55	0
54	MG	2A	3311	1/1	0.98	0.13	43,43,43,43	0
54	MG	1A	3842	1/1	0.98	0.10	42,42,42,42	0
54	MG	2A	3491	1/1	0.98	0.11	46,46,46,46	0
54	MG	2A	3066	1/1	0.98	0.16	51,51,51,51	0
54	MG	2A	3333	1/1	0.98	0.09	28,28,28,28	0
54	MG	2A	3485	1/1	0.98	0.10	45,45,45,45	0
54	MG	1A	3270	1/1	0.98	0.12	11,11,11,11	0
54	MG	1A	3747	1/1	0.98	0.19	44,44,44,44	0
54	MG	1A	3633	1/1	0.98	0.19	51,51,51,51	0
54	MG	1A	3104	1/1	0.98	0.38	23,23,23,23	0
54	MG	1A	3199	1/1	0.98	0.66	38,38,38,38	0
54	MG	1A	3648	1/1	0.98	0.21	32,32,32,32	0
54	MG	1A	3525	1/1	0.98	0.17	37,37,37,37	0
54	MG	1A	3965	1/1	0.98	0.20	10,10,10,10	0
54	MG	1A	3803	1/1	0.98	0.48	34,34,34,34	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3277	1/1	0.98	0.35	28,28,28,28	0
54	MG	2A	3452	1/1	0.98	0.17	38,38,38,38	0
54	MG	1A	3418	1/1	0.98	0.14	22,22,22,22	0
54	MG	1A	3834	1/1	0.98	0.14	31,31,31,31	0
54	MG	2A	3625	1/1	0.98	0.12	16,16,16,16	0
54	MG	1A	3331	1/1	0.98	0.10	12,12,12,12	0
54	MG	1A	3671	1/1	0.98	0.10	15,15,15,15	0
54	MG	1A	3480	1/1	0.98	0.14	36,36,36,36	0
54	MG	1A	3540	1/1	0.98	0.14	25,25,25,25	0
54	MG	1A	3164	1/1	0.98	0.44	22,22,22,22	0
54	MG	2A	3145	1/1	0.98	0.63	44,44,44,44	0
54	MG	1A	3024	1/1	0.98	0.33	29,29,29,29	0
54	MG	1A	3725	1/1	0.98	0.08	36,36,36,36	0
54	MG	2A	3107	1/1	0.98	0.13	43,43,43,43	0
54	MG	1A	3378	1/1	0.98	0.09	20,20,20,20	0
54	MG	2A	3415	1/1	0.98	0.14	41,41,41,41	0
54	MG	1A	3005	1/1	0.98	0.17	15,15,15,15	0
54	MG	1A	3694	1/1	0.98	0.09	40,40,40,40	0
54	MG	2A	3026	1/1	0.98	0.42	41,41,41,41	0
54	MG	13	101	1/1	0.98	0.15	53,53,53,53	0
59	ZN	15	101	1/1	0.98	0.20	39,39,39,39	0
54	MG	2A	3090	1/1	0.98	0.14	19,19,19,19	0
59	ZN	14	501	1/1	0.98	0.14	80,80,80,80	0
54	MG	1A	3616	1/1	0.98	0.23	16,16,16,16	0
54	MG	2A	3006	1/1	0.98	0.54	43,43,43,43	0
54	MG	1A	3064	1/1	0.98	0.40	29,29,29,29	0
54	MG	1a	1760	1/1	0.98	0.19	52,52,52,52	0
54	MG	1A	3593	1/1	0.98	0.16	40,40,40,40	0
54	MG	2A	3530	1/1	0.98	0.13	25,25,25,25	0
54	MG	1A	3319	1/1	0.98	0.14	15,15,15,15	0
54	MG	1A	3225	1/1	0.98	0.30	32,32,32,32	0
54	MG	1A	3971	1/1	0.98	0.13	16,16,16,16	0
54	MG	2A	3278	1/1	0.98	0.10	25,25,25,25	0
54	MG	1A	3736	1/1	0.98	0.16	41,41,41,41	0
54	MG	2A	3241	1/1	0.98	0.20	47,47,47,47	0
54	MG	1A	3788	1/1	0.98	0.16	23,23,23,23	0
54	MG	2A	3357	1/1	0.98	0.15	41,41,41,41	0
54	MG	1A	3384	1/1	0.98	0.15	14,14,14,14	0
54	MG	1A	3006	1/1	0.98	0.17	17,17,17,17	0
54	MG	2A	3492	1/1	0.98	0.25	66,66,66,66	0
54	MG	2A	3643	1/1	0.98	0.17	34,34,34,34	0
54	MG	2A	3515	1/1	0.98	0.17	54,54,54,54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3713	1/1	0.98	0.82	40,40,40,40	0
54	MG	1a	1850	1/1	0.98	0.07	45,45,45,45	0
54	MG	1a	1764	1/1	0.98	0.10	61,61,61,61	0
54	MG	2A	3316	1/1	0.98	0.18	41,41,41,41	0
54	MG	1A	3595	1/1	0.98	0.20	16,16,16,16	0
54	MG	1A	3435	1/1	0.98	0.22	37,37,37,37	0
54	MG	1A	3165	1/1	0.98	0.35	28,28,28,28	0
54	MG	2A	3133	1/1	0.98	0.14	47,47,47,47	0
54	MG	1A	3359	1/1	0.98	0.14	15,15,15,15	0
54	MG	1A	3627	1/1	0.98	0.26	30,30,30,30	0
54	MG	1A	3285	1/1	0.98	0.29	36,36,36,36	0
54	MG	1A	3967	1/1	0.98	0.15	19,19,19,19	0
54	MG	1A	3845	1/1	0.98	0.17	37,37,37,37	0
54	MG	1A	4018	1/1	0.98	0.23	36,36,36,36	0
54	MG	1a	1724	1/1	0.98	0.18	41,41,41,41	0
54	MG	2A	3617	1/1	0.98	0.14	46,46,46,46	0
54	MG	1A	3365	1/1	0.98	0.15	13,13,13,13	0
54	MG	1a	1693	1/1	0.98	0.08	42,42,42,42	0
54	MG	1A	3537	1/1	0.98	0.18	46,46,46,46	0
54	MG	1A	3956	1/1	0.98	0.09	24,24,24,24	0
54	MG	2A	3396	1/1	0.98	0.21	29,29,29,29	0
54	MG	1a	1801	1/1	0.98	0.15	43,43,43,43	0
54	MG	1A	4015	1/1	0.98	0.38	39,39,39,39	0
54	MG	1D	305	1/1	0.98	0.26	39,39,39,39	0
54	MG	1A	3264	1/1	0.98	0.64	42,42,42,42	0
54	MG	1A	3477	1/1	0.98	0.16	16,16,16,16	0
54	MG	2A	3637	1/1	0.98	0.15	30,30,30,30	0
54	MG	1A	3096	1/1	0.98	0.33	25,25,25,25	0
54	MG	1A	3431	1/1	0.98	0.13	34,34,34,34	0
54	MG	1A	3103	1/1	0.98	0.47	25,25,25,25	0
54	MG	2A	3653	1/1	0.98	0.28	48,48,48,48	0
54	MG	1A	3536	1/1	0.98	0.19	26,26,26,26	0
54	MG	1A	3336	1/1	0.98	0.12	33,33,33,33	0
54	MG	1A	3896	1/1	0.98	0.12	22,22,22,22	0
54	MG	1A	3432	1/1	0.98	0.23	35,35,35,35	0
54	MG	1A	3915	1/1	0.99	0.11	25,25,25,25	0
59	ZN	26	501	1/1	0.99	0.18	59,59,59,59	0
54	MG	1a	1716	1/1	0.99	0.12	39,39,39,39	0
54	MG	2A	3003	1/1	0.99	0.16	37,37,37,37	0
55	K	2A	3246	1/1	0.99	0.11	30,30,30,30	0
54	MG	1A	3117	1/1	0.99	0.17	39,39,39,39	0
54	MG	1A	3740	1/1	0.99	0.18	29,29,29,29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3017	1/1	0.99	0.36	25,25,25,25	0
54	MG	2A	3650	1/1	0.99	0.16	36,36,36,36	0
54	MG	1A	3003	1/1	0.99	0.10	31,31,31,31	0
54	MG	1A	3601	1/1	0.99	0.14	31,31,31,31	0
54	MG	1A	3843	1/1	0.99	0.23	30,30,30,30	0
54	MG	1A	3420	1/1	0.99	0.13	50,50,50,50	0
54	MG	1A	3657	1/1	0.99	0.29	31,31,31,31	0
54	MG	1A	3309	1/1	0.99	0.10	34,34,34,34	0
54	MG	2A	3117	1/1	0.99	0.26	36,36,36,36	0
54	MG	1A	3221	1/1	0.99	0.51	24,24,24,24	0
54	MG	1A	3170	1/1	0.99	0.26	28,28,28,28	0
54	MG	1A	3683	1/1	0.99	0.14	25,25,25,25	0
54	MG	1A	3016	1/1	0.99	0.49	17,17,17,17	0
54	MG	1A	3769	1/1	0.99	0.17	19,19,19,19	0
54	MG	1A	3879	1/1	0.99	0.12	33,33,33,33	0
54	MG	1A	4014	1/1	0.99	0.40	28,28,28,28	0
54	MG	1A	3828	1/1	0.99	0.15	13,13,13,13	0
54	MG	1A	3511	1/1	0.99	0.07	32,32,32,32	0
54	MG	1A	4004	1/1	0.99	0.25	25,25,25,25	0
54	MG	1D	306	1/1	0.99	0.15	11,11,11,11	0
54	MG	1A	3620	1/1	0.99	0.06	44,44,44,44	0
54	MG	2A	3091	1/1	0.99	0.15	61,61,61,61	0
54	MG	2A	3243	1/1	0.99	0.15	18,18,18,18	0
54	MG	1A	3645	1/1	0.99	0.12	35,35,35,35	0
54	MG	2A	3257	1/1	0.99	0.18	43,43,43,43	0
54	MG	1A	3298	1/1	0.99	0.18	14,14,14,14	0
54	MG	2A	3346	1/1	0.99	0.21	52,52,52,52	0
54	MG	1A	3034	1/1	0.99	0.10	33,33,33,33	0
54	MG	2A	3461	1/1	0.99	0.10	55,55,55,55	0
54	MG	1A	3994	1/1	0.99	0.31	26,26,26,26	0
54	MG	1D	304	1/1	0.99	0.18	33,33,33,33	0
55	K	1A	3287	1/1	0.99	0.06	27,27,27,27	0
54	MG	2A	3009	1/1	0.99	0.20	30,30,30,30	0
54	MG	1A	3787	1/1	0.99	0.23	40,40,40,40	0
59	ZN	16	501	1/1	0.99	0.27	46,46,46,46	0
54	MG	2A	3365	1/1	0.99	0.23	32,32,32,32	0
54	MG	2A	3442	1/1	0.99	0.16	27,27,27,27	0
54	MG	1V	202	1/1	0.99	0.15	47,47,47,47	0
54	MG	1a	1638	1/1	0.99	0.16	44,44,44,44	0
54	MG	2A	3560	1/1	0.99	0.15	43,43,43,43	0
54	MG	2A	3027	1/1	0.99	0.13	30,30,30,30	0
54	MG	1A	3081	1/1	0.99	0.43	34,34,34,34	0

*Continued on next page...*

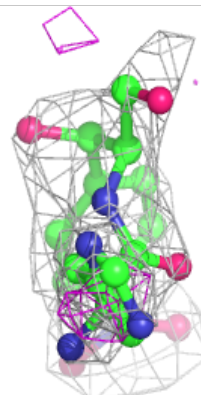
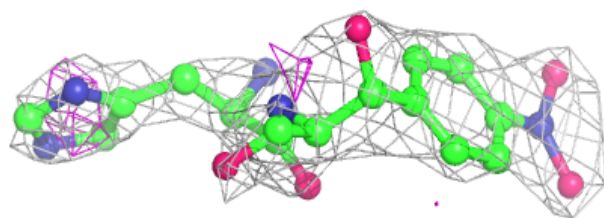
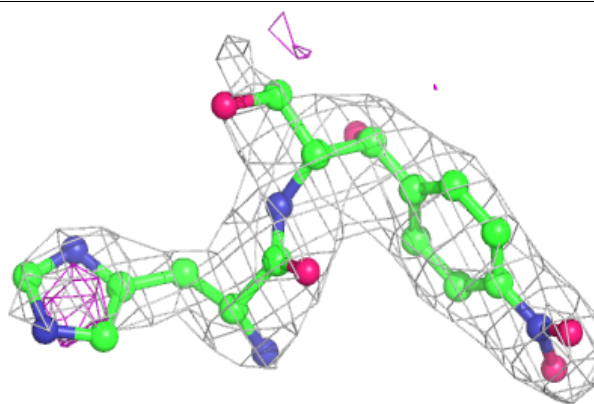
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3323	1/1	0.99	0.14	18,18,18,18	0
54	MG	1A	3661	1/1	0.99	0.11	32,32,32,32	0
54	MG	2A	3420	1/1	0.99	0.17	28,28,28,28	0
54	MG	1A	3054	1/1	0.99	0.12	21,21,21,21	0
54	MG	1A	3895	1/1	0.99	0.11	16,16,16,16	0
54	MG	2E	304	1/1	0.99	0.13	29,29,29,29	0
54	MG	2A	3403	1/1	0.99	0.29	57,57,57,57	0
59	ZN	1n	501	1/1	0.99	0.15	60,60,60,60	0
54	MG	1B	220	1/1	0.99	0.15	20,20,20,20	0
59	ZN	19	501	1/1	0.99	0.23	39,39,39,39	0
54	MG	1A	3084	1/1	0.99	0.21	33,33,33,33	0
54	MG	1A	3869	1/1	0.99	0.14	56,56,56,56	0
54	MG	2A	3585	1/1	0.99	0.14	57,57,57,57	0
54	MG	1A	3625	1/1	0.99	0.10	35,35,35,35	0
59	ZN	1Y	501	1/1	0.99	0.20	46,46,46,46	0
59	ZN	25	501	1/1	0.99	0.22	44,44,44,44	0

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

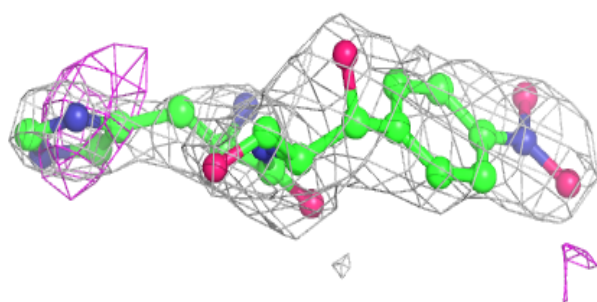
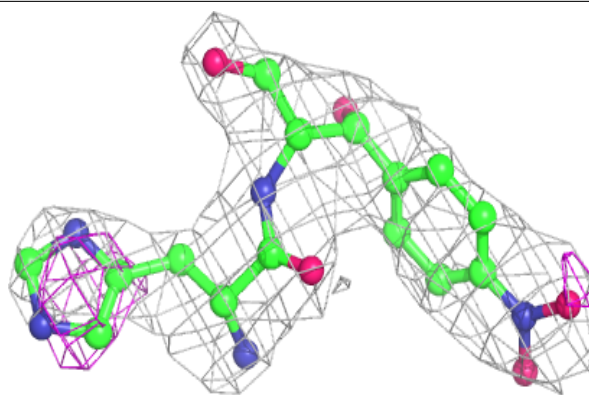
**Electron density around EZP 2A 3709:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around EZP 1A 3987:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.