



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 11:05 PM EDT

PDB ID : 8T8C / pdb_00008t8c
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with protein Y, A-site aminoacyl-tRNA analog ACC-PMN, and P-site formyl-MFI-tripeptidyl-tRNA analog ACCA-IFMf at 2.60Å resolution
Authors : Thaler, J.; Syroegin, E.A.; Breuker, K.; Polikanov, Y.S.; Micura, R.
Deposited on : 2023-06-22
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

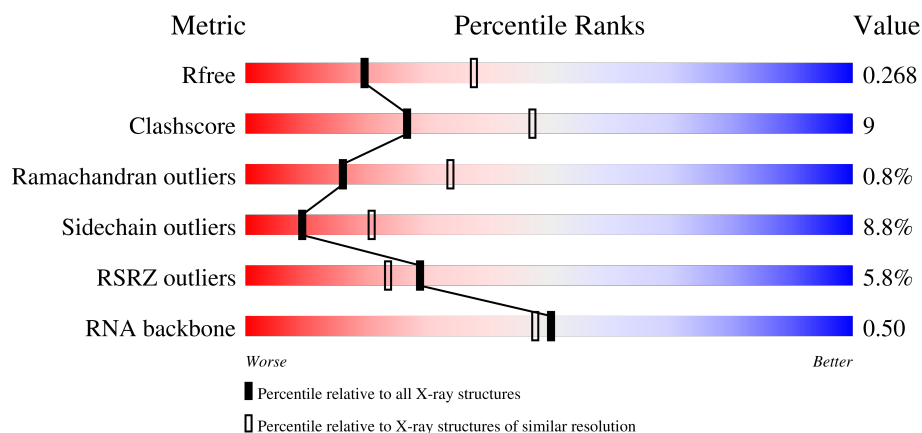
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



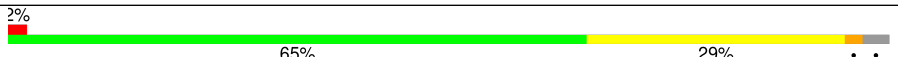
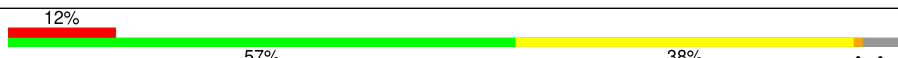
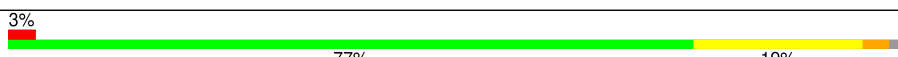
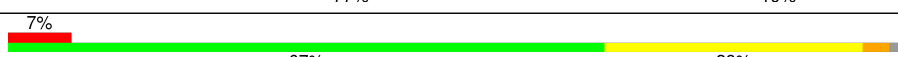
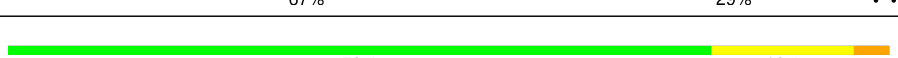
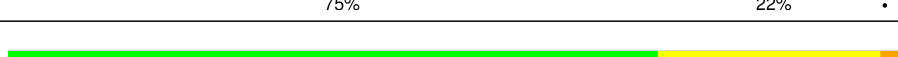
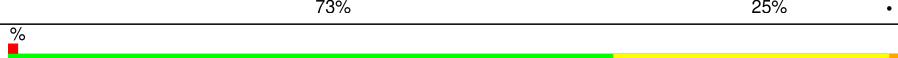
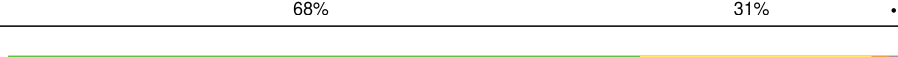
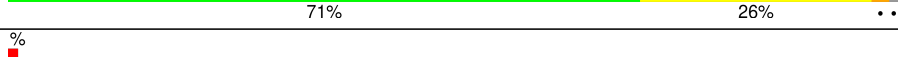
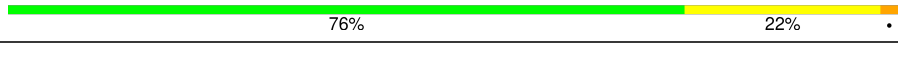
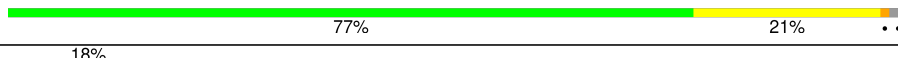
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	4% 64% 29% 6%
1	2A	2915	5% 57% 34% 7%
2	1B	121	% 64% 31% ••
2	2B	121	16% 53% 41% 5%

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	

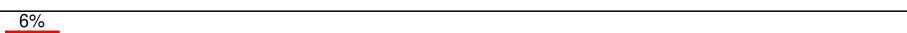
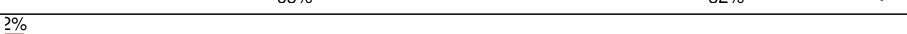
Continued on next page...

Continued from previous page...

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

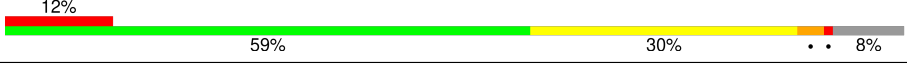
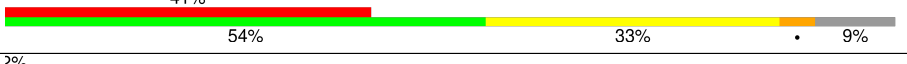
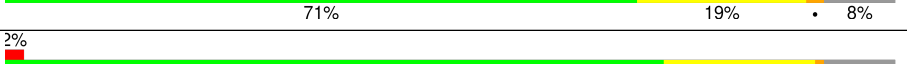
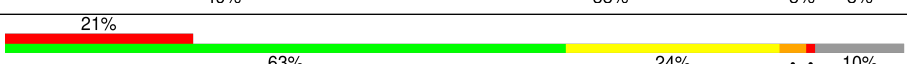
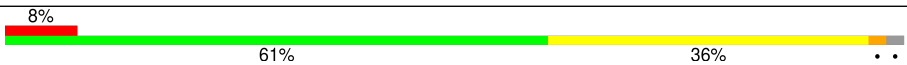
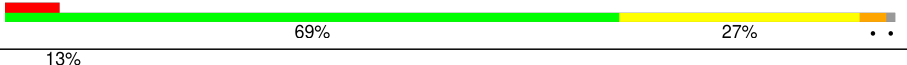
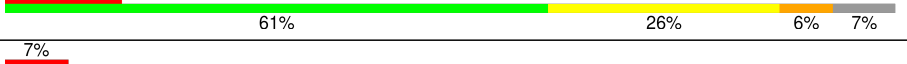
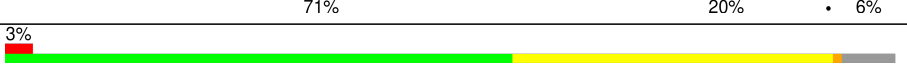
Continued on next page...

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	
54	1w	4	
54	2w	4	
55	1x	4	
55	2x	4	
56	1v	3	
56	2v	3	

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
57	MG	1a	1871	-	-	-	X
57	MG	2A	3090	-	-	-	X
57	MG	2A	3291	-	-	-	X
61	SF4	2d	501	-	-	X	-

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 296459 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	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			650	401	139	109	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			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 a RNA chain called A-site Aminoacyl-tRNA Analog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	4	Total	C	N	O	P	0	0	1
			78	40	13	22	3			
54	2w	4	Total	C	N	O	P	0	0	1
			78	40	13	22	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1x	4	Total	C	N	O	P	0	0	1
			63	28	12	20	3			
55	2x	4	Total	C	N	O	P	0	0	1
			63	28	12	20	3			

- Molecule 56 is a protein called P-site Peptidyl-tRNA Analog Peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1v	3	Total	C	N	O	S	0	0	0
			29	21	3	4	1			
56	2v	3	Total	C	N	O	S	0	0	0
			29	21	3	4	1			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1029	Total	Mg	0	0
			1029	1029		
57	1B	29	Total	Mg	0	0
			29	29		
57	1D	16	Total	Mg	0	0
			16	16		
57	1E	9	Total	Mg	0	0
			9	9		
57	1F	15	Total	Mg	0	0
			15	15		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1G	4	Total 4	Mg 4	0	0
57	1H	2	Total 2	Mg 2	0	0
57	1N	4	Total 4	Mg 4	0	0
57	1O	2	Total 2	Mg 2	0	0
57	1P	3	Total 3	Mg 3	0	0
57	1Q	5	Total 5	Mg 5	0	0
57	1R	5	Total 5	Mg 5	0	0
57	1T	5	Total 5	Mg 5	0	0
57	1U	7	Total 7	Mg 7	0	0
57	1V	6	Total 6	Mg 6	0	0
57	1W	4	Total 4	Mg 4	0	0
57	1Y	1	Total 1	Mg 1	0	0
57	1Z	1	Total 1	Mg 1	0	0
57	10	10	Total 10	Mg 10	0	0
57	11	3	Total 3	Mg 3	0	0
57	13	4	Total 4	Mg 4	0	0
57	15	9	Total 9	Mg 9	0	0
57	17	5	Total 5	Mg 5	0	0
57	18	2	Total 2	Mg 2	0	0
57	19	3	Total 3	Mg 3	0	0
57	1a	272	Total 272	Mg 272	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1b	1	Total 1	Mg 1	0	0
57	1d	5	Total 5	Mg 5	0	0
57	1e	3	Total 3	Mg 3	0	0
57	1f	2	Total 2	Mg 2	0	0
57	1g	2	Total 2	Mg 2	0	0
57	1h	2	Total 2	Mg 2	0	0
57	1i	1	Total 1	Mg 1	0	0
57	1l	2	Total 2	Mg 2	0	0
57	1m	1	Total 1	Mg 1	0	0
57	1n	3	Total 3	Mg 3	0	0
57	1o	1	Total 1	Mg 1	0	0
57	1t	1	Total 1	Mg 1	0	0
57	1u	1	Total 1	Mg 1	0	0
57	1y	3	Total 3	Mg 3	0	0
57	1w	1	Total 1	Mg 1	0	0
57	1x	2	Total 2	Mg 2	0	0
57	2A	734	Total 734	Mg 734	0	0
57	2B	17	Total 17	Mg 17	0	0
57	2D	11	Total 11	Mg 11	0	0
57	2E	8	Total 8	Mg 8	0	0
57	2F	4	Total 4	Mg 4	0	0

Continued on next page...

Continued from previous page...

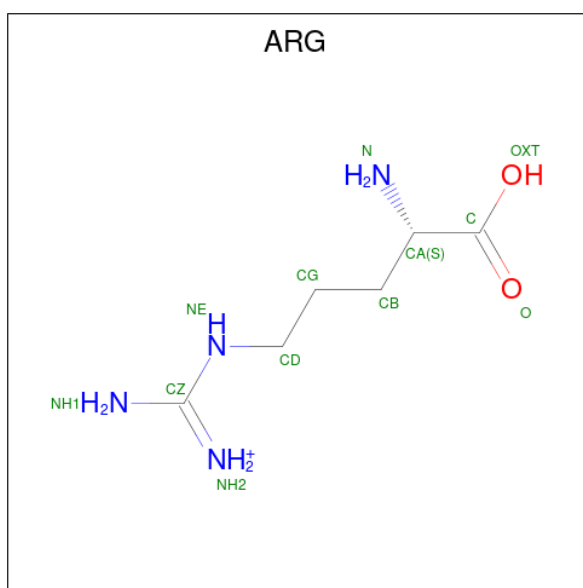
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2G	2	Total 2	Mg 2	0	0
57	2I	1	Total 1	Mg 1	0	0
57	2N	1	Total 1	Mg 1	0	0
57	2P	2	Total 2	Mg 2	0	0
57	2Q	2	Total 2	Mg 2	0	0
57	2R	2	Total 2	Mg 2	0	0
57	2T	4	Total 4	Mg 4	0	0
57	2V	2	Total 2	Mg 2	0	0
57	2W	3	Total 3	Mg 3	0	0
57	2X	1	Total 1	Mg 1	0	0
57	2Y	1	Total 1	Mg 1	0	0
57	20	1	Total 1	Mg 1	0	0
57	21	4	Total 4	Mg 4	0	0
57	23	1	Total 1	Mg 1	0	0
57	25	4	Total 4	Mg 4	0	0
57	27	1	Total 1	Mg 1	0	0
57	28	1	Total 1	Mg 1	0	0
57	29	1	Total 1	Mg 1	0	0
57	2a	188	Total 188	Mg 188	0	0
57	2e	2	Total 2	Mg 2	0	0
57	2f	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

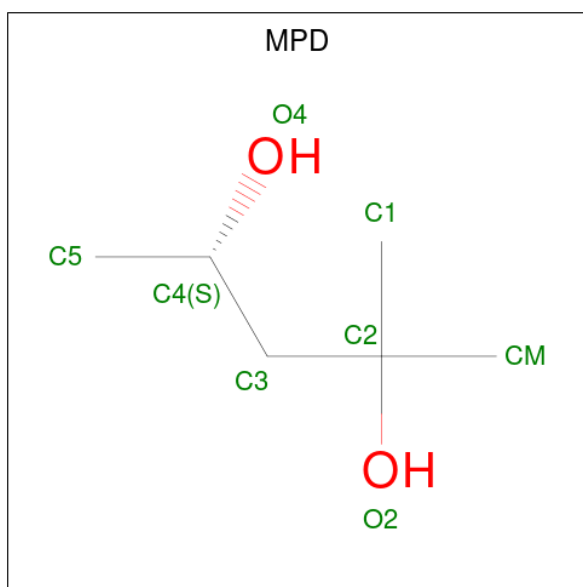
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2j	1	Total	Mg	0	0
			1	1		
57	2n	1	Total	Mg	0	0
			1	1		
57	2p	1	Total	Mg	0	0
			1	1		
57	2t	1	Total	Mg	0	0
			1	1		
57	2x	1	Total	Mg	0	0
			1	1		

- Molecule 58 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



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

- Molecule 59 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1	Total C O 8 6 2	0	0
59	18	1	Total C O 8 6 2	0	0
59	1a	1	Total C O 8 6 2	0	0
59	1a	1	Total C O 8 6 2	0	0
59	2A	1	Total C O 8 6 2	0	0
59	2A	1	Total C O 8 6 2	0	0
59	2A	1	Total C O 8 6 2	0	0

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

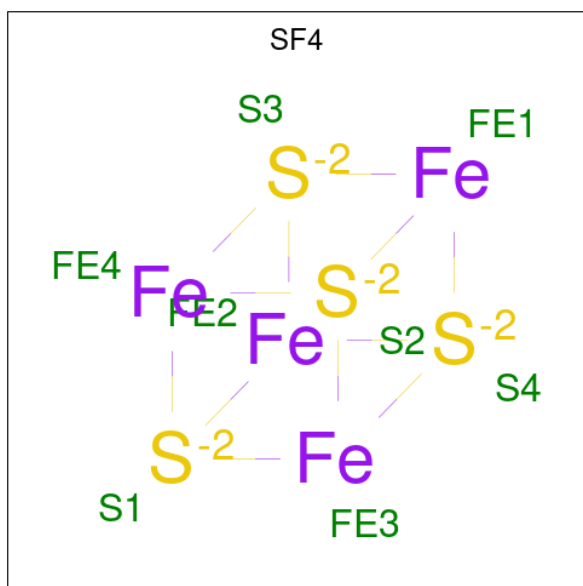
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1Y	1	Total Zn 1 1	0	0
60	14	1	Total Zn 1 1	0	0
60	15	1	Total Zn 1 1	0	0
60	16	1	Total Zn 1 1	0	0
60	19	1	Total Zn 1 1	0	0

Continued on next page...

Continued from previous page...

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

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



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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	3560	Total 3560	O 3560	0	0
62	1B	89	Total 89	O 89	0	0
62	1D	98	Total 98	O 98	0	0
62	1E	69	Total 69	O 69	0	0
62	1F	51	Total 51	O 51	0	0
62	1G	15	Total 15	O 15	0	0
62	1H	6	Total 6	O 6	0	0
62	1I	4	Total 4	O 4	0	0
62	1N	43	Total 43	O 43	0	0
62	1O	22	Total 22	O 22	0	0
62	1P	63	Total 63	O 63	0	0
62	1Q	33	Total 33	O 33	0	0
62	1R	30	Total 30	O 30	0	0
62	1S	8	Total 8	O 8	0	0
62	1T	24	Total 24	O 24	0	0
62	1U	45	Total 45	O 45	0	0
62	1V	30	Total 30	O 30	0	0
62	1W	26	Total 26	O 26	0	0
62	1X	23	Total 23	O 23	0	0
62	1Y	12	Total 12	O 12	0	0
62	1Z	9	Total 9	O 9	0	0
62	10	22	Total 22	O 22	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	11	24	Total 24	O 24	0	0
62	12	10	Total 10	O 10	0	0
62	13	19	Total 19	O 19	0	0
62	14	2	Total 2	O 2	0	0
62	15	24	Total 24	O 24	0	0
62	16	15	Total 15	O 15	0	0
62	17	14	Total 14	O 14	0	0
62	18	21	Total 21	O 21	0	0
62	19	7	Total 7	O 7	0	0
62	1a	382	Total 382	O 382	0	0
62	1d	5	Total 5	O 5	0	0
62	1e	3	Total 3	O 3	0	0
62	1f	2	Total 2	O 2	0	0
62	1h	1	Total 1	O 1	0	0
62	1i	1	Total 1	O 1	0	0
62	1j	1	Total 1	O 1	0	0
62	1l	3	Total 3	O 3	0	0
62	1o	3	Total 3	O 3	0	0
62	1p	2	Total 2	O 2	0	0
62	1u	1	Total 1	O 1	0	0
62	1y	3	Total 3	O 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1w	4	Total 4	O 4	0	0
62	1x	4	Total 4	O 4	0	0
62	2A	1737	Total 1737	O 1737	0	0
62	2B	33	Total 33	O 33	0	0
62	2D	32	Total 32	O 32	0	0
62	2E	22	Total 22	O 22	0	0
62	2F	20	Total 20	O 20	0	0
62	2G	2	Total 2	O 2	0	0
62	2I	2	Total 2	O 2	0	0
62	2N	3	Total 3	O 3	0	0
62	2O	11	Total 11	O 11	0	0
62	2P	18	Total 18	O 18	0	0
62	2Q	7	Total 7	O 7	0	0
62	2R	14	Total 14	O 14	0	0
62	2S	2	Total 2	O 2	0	0
62	2T	6	Total 6	O 6	0	0
62	2U	7	Total 7	O 7	0	0
62	2V	5	Total 5	O 5	0	0
62	2W	7	Total 7	O 7	0	0
62	2X	4	Total 4	O 4	0	0
62	2Y	2	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2Z	9	Total 9	O 9	0	0
62	20	7	Total 7	O 7	0	0
62	21	17	Total 17	O 17	0	0
62	25	7	Total 7	O 7	0	0
62	26	1	Total 1	O 1	0	0
62	27	4	Total 4	O 4	0	0
62	28	12	Total 12	O 12	0	0
62	2a	224	Total 224	O 224	0	0
62	2d	3	Total 3	O 3	0	0
62	2e	2	Total 2	O 2	0	0
62	2f	1	Total 1	O 1	0	0
62	2j	1	Total 1	O 1	0	0
62	2l	3	Total 3	O 3	0	0
62	2o	3	Total 3	O 3	0	0
62	2p	1	Total 1	O 1	0	0
62	2q	1	Total 1	O 1	0	0
62	2r	2	Total 2	O 2	0	0
62	2t	1	Total 1	O 1	0	0
62	2y	1	Total 1	O 1	0	0
62	2w	3	Total 3	O 3	0	0
62	2x	2	Total 2	O 2	0	0

Continued on next page...

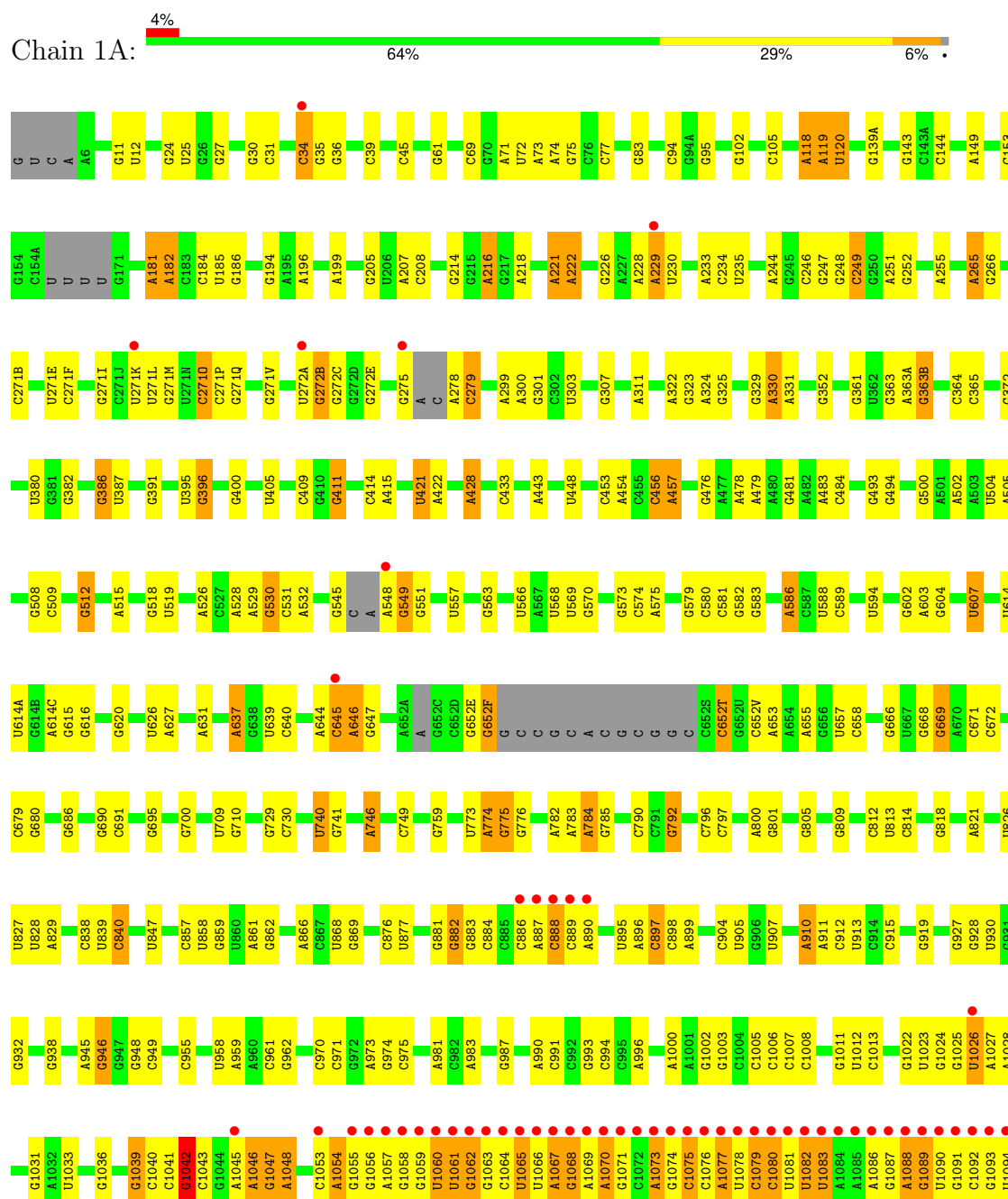
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2v	1	Total	O	0	0
			1	1		

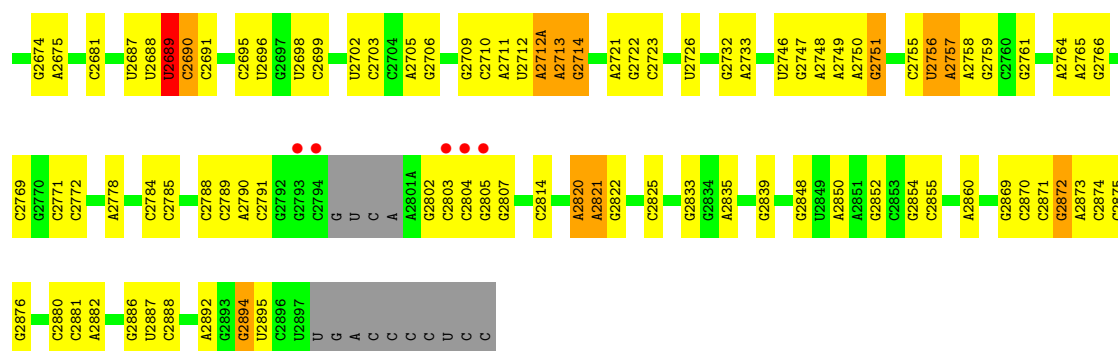
3 Residue-property plots

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

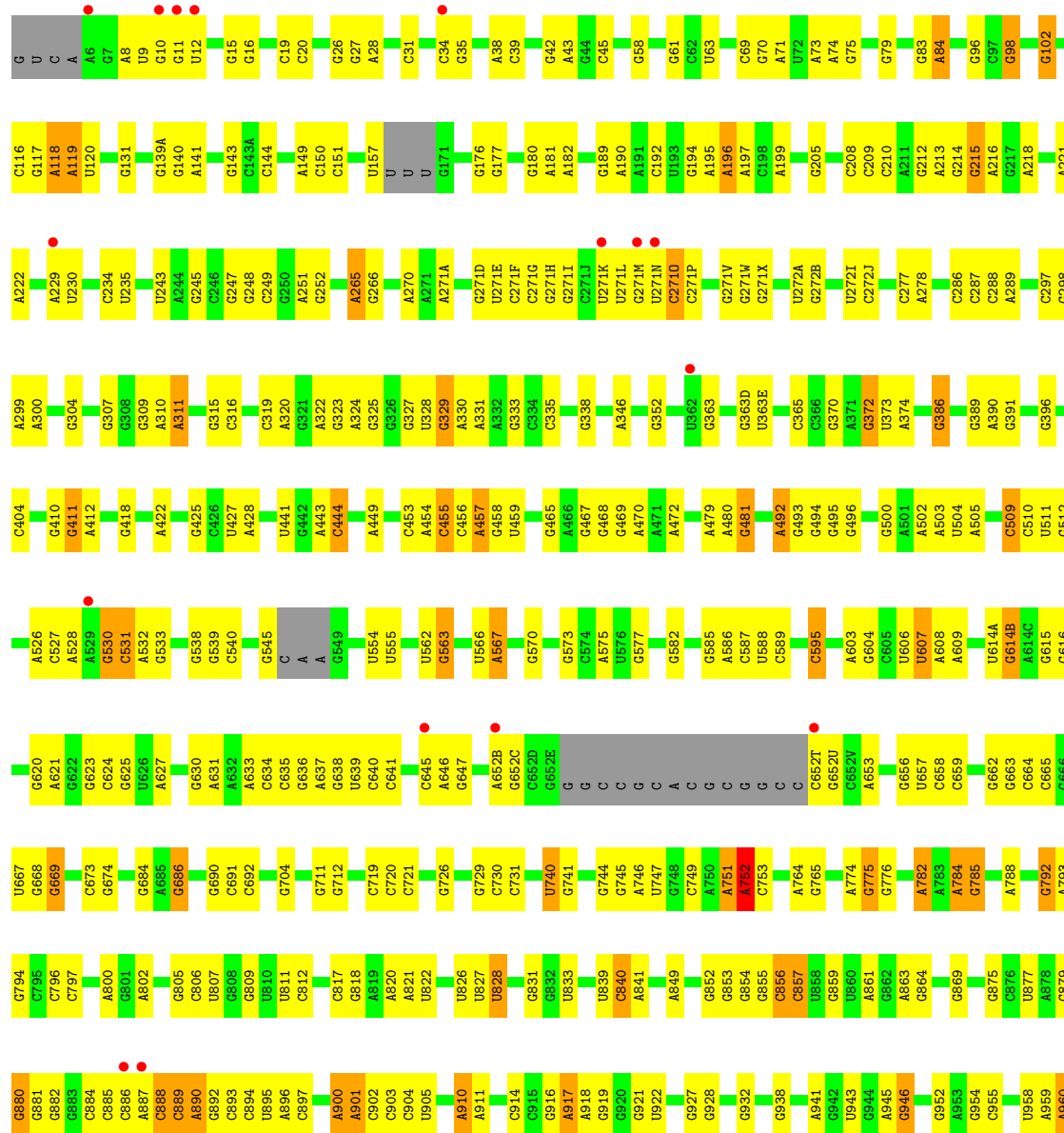
• Molecule 1: 23S Ribosomal RNA



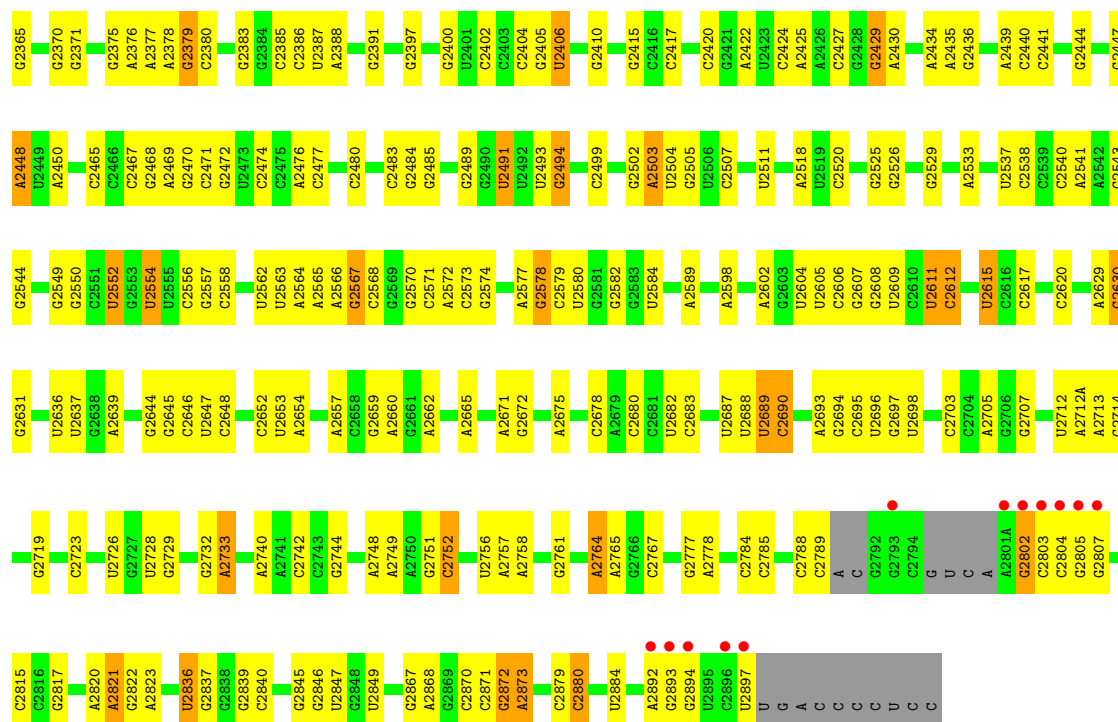
U2555	G2429	C2324	A2208	C2137	A2060	G1930	A1802	U1688	G1459	A1095
A2561	U2431	G2325	G2223	C2138	G2061	U1931	A1803	A1558	A1460	U1096
U2562	A2432	G2326	G2224	C2139	C2065	A1932	U1805	U1352	A1210	U1097
U2563						G1933		A1566	U1211	A1098
A2564	A2435	G2329	C2226	C2142	G2069	A1936	A1810	G1696	A1220	G1099
A2565	U2439	G2330	A2227	C2143		A1937	A1811	G1697		C1100
A2566	C2440	G2331	G2228	U2144	G2072	A1938	A1812	A1698	A1226	U1101
G2567	C2441	G2334	G2238	C2145	U2074	U1939	A1815	A1701	A1470	C1102
C2568		A2335	G2239	G2146	U2075	U1940	G1816	A1702	G1475	A1103
		A2336	C2240	C2147		C1941		G1703	A1476	C1104
C2573	G2445			G2148	G2080	G1942	A1823	A1709	A1477	U1105
G2574	G2446			U2149	G2086	U1943		C1582	G1478	G1106
	U2447	G2341	U2243	U2150	G2087	U1944		A1583		
U2584	A2448	C2342	U2244	G2151	U2086	U1955	A1824	C1584	G1239	C1109
U2585				G2152	G2087		A1825	A1586	U1240	G1110
C2586	G2454	G2345	C2248	G2153				G1494	A1241	A1111
		A2346		G2154	G2090	A1960	A1829	A1587	G1245	U1113
A2590	A2476	C2347	G2251	G2155		C1961		C1588		U1114
C2591		U2348	G2251	G2156	G2093	U1962	A1840	A1486	G1252	G1115
G2592	C2483	C2349	C2258	G2157		G1963		G1487	A1253	C1116
U2593		C2350		A2158	U2096	G1964	A1847	A1490		
C2594	A2488		A2267	G2159	C2097	C1967	G1721	A1608	G1256	C1124
A2602	U2491	C2355	A2268	C2160	U2098	U1968	A1853	A1609	C1257	G1125
G2603	U2492	C2359	A2269	C2161	G2099	A1969	A1854	A1610		
U2604	U2493	A2360	A2273	C2162	G2100	A1970	G1857	A1616	G1260	G1131
U2605			A2274	C2163	G2101	A1971	G1858			
C2606	C2498	C2364		G2164	U2102	A1972		U1629	G1266	C1135
G2607	C2499	C2365	G2277	U2165	C2103		G1865	G1750	U1336	U1137
			A2278	G2166		A1981			A1401	G1138
G2608			G2279	C2167					A1507	C1270
C2610	G2502	G2375	G2279	A2168	C2106	U1993	A1877	G1753	C1506	A1268
U2611	U2503	A2376	G2280	C2169	C2107		G1878	C1754	A1508	A1269
C2612	U2504	A2377		A2170	U2108	C1996	G1883	A1755	C1509	G1271
	G2505	A2378	C2283	A2171	C2109	G1987		G1756	A1509A	A1272
	U2506			U2172	G2110		A1889		A1509B	U1273
	C2507	G2379		A2173	C2111			A1762	G1510	C1407
C2617	G2508	C2380	A2286	C2174	G2112	G2000	A1890	G1763	C1511	C1416
G2618	U2508	C2381	A2287	U2180	U2113	A2001	G1896	G1764	U1512	A1275
C2619			A2288	C2181	A2114	G2002			C1513	A1276
	A2518	G2382	A2288	G2182	G2115		G1899	G1772	U1514	G1277
G2623	U2519	C2383	G2289	G2183	C2116	G2012	A1900	A1773		A1278
	C2520	G2384	G2290	G2184	A2117	A2013			U1518	G1281
C2628	U2521	C2385	U2291	C2185	A2119		G1906	A1780	G1423	G1169
A2629	U2522		C2292	G2186		A2020		C1781	G1424	G1170
G2630		G2399	A2305	C2187	U2122	G2023	U1911	G1782	G1529	C1295
	G2525	C2404	G2308	G2188	G2123		A1912	A1783	C1530	G1296
C2635	U2528	G2405	A2309	U2189	G2124	A2031	G1913		G1531	A1174
G2641	G2529	U2406	A2310	C2190	G2125	G2032	C1914	A1786	C1532	U1175
	A2530	G2407	U2311	G2191	A2126	A2033	U1915	C1790	G	A1177
C2646			U2312	G2192	G2127		A1916	A1791	U	G1176
U2647	G2534	C2417		G2193	C2128	G2038	U1917		A	U1300
	U2535		C2316		C2129		A1918	U1794	C	A1178
A2654	C2536	A2422	C2317	U2197	U2130	C2043	A1919	C1795	G1537	C1179
	U2537	U2423	G2318	A2198				U1671		G1186
C2658	C2538	A2424	G2319		U2132	C2055	C1920	G1796	A1445	G1187
		A2425	G2320	U2203	G2133			C1797	A1449	U1188
A2662	U2552	A2426	G2321	U2205	C2134	A2057	U1924	G1798	G1455	U1199
	C2627	G2553	C2322	G2006	A2135	A2058	C1924	G1799		C1200
U2667	U2554	C2659	C2323	C2027	C2136	U2059	C1929	C1801	C1546	U1340
									C1547	U1341



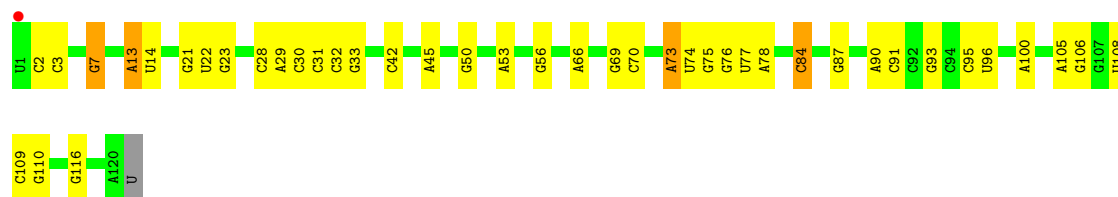
• Molecule 1: 23S Ribosomal RNA



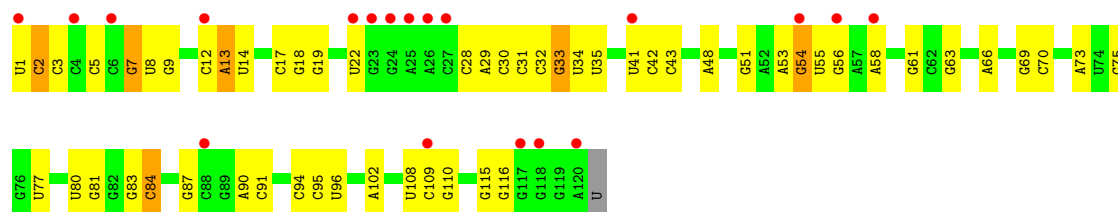
G2290	C2188	G2127	C1942	G1801	G1649	U	U1420	G1302	G1106	A1046	C961
U2291	U2189	C2128	A1952	A1802	G1650	A	G1421	G1203	G1107	G1047	
C2292	G2190	U2129		A1803	G1651	C1536	G1422	A1204	U1108	A1048	C965
G2293	G2191	U2130	U1955		A1852	G1539		C1314	C1109	C1049	
C2294	G2192	G2131	U1960	G1816	G1653	G1542	C1428	C1208	A1050	G1051	C971
G2295	A2198	U2132	A1961	G1817	A1654	A1542	G1429	G1315	G1110	G1052	C972
U2296	C2199	C2133	C1962	U1818	A1655	C1543	C1430	U1316	G1111	C1053	A973
C2297	A2199	A2134	U1963	C1827	G1656	C1544	C1430	A1317	G1112	C1052	A973
A2298	G2200	A2135	U1963	G1828	C1657	C1546	C1442	G1319	G1113	C1053	G974
G2299	C2202	C2136	U1963	G1829	C1658	C1547	G1442	G1216	A1054	A1054	C975
G2300	G2203	C2137	U1963	G1830	A1664	C1548	A1445	A1220	G1055	G1056	G979
C2301	C2205	C2138	G1967			C1550	A1449	G1225	G1115	A1057	
A2305	G2206	C2140	A1969	U1833	A1668	C1550	A1449	G1225	G1116	A1057	A983
G2308	G2207	G2141	A1970	U1833	A1669	A1568	G1450	G1229	G1117	G1058	A984
A2309	U2218	C2142	A1971	U1835	C1670	A1569	C1450A	G1237	G1118	G1059	A984
A2310	G2219	A1972	A1972	G1839	U1671	A1570	G1455	G1237	U	U1060	C986
A2311	A2225	C1983		G1842	U1673	A1578	G1459	A1237	G1122		
U2312	G2226	U1991	U1991		G1674	A1587		U1240	G1123	G1062	G993
G2313	A2227	G1992	G1992	G1845	U1688	G1588	C1464	A1241	G1124	G1063	C994
G2314	G2227	U1993	U1993	G1846	G1465	A1570	G1465	G1252	G1125	C1064	C994
G2315	G2227	C1994	C1994	A1847	C1467	A1587	C1467	A1254	G1126	U1066	C995
G2316	A2232	U1995	U1995	A1848	A1700	A1579		U1255	A1128	U1066	A996
C2317	U2233	C1996	C1996	G1861	G1702	A1580		G1256	G1129	A1067	G997
G2318	G2234	G1997	G1997		G1703	A1581	A1471	G1257	U1130	G1068	
G2319	G2238	U1998	U1998	A1876	U1720	G1583		C1258	G1131		G1002
A2320	G2242	C2000	C2000	A1877	G1721	C1584	U1489	G1264	G1132	A1069	G1003
G2321	U2243	A2001	A2001	G1878	A1722	A1586	A1490	A1265	G1133	G1070	G1004
A2322	U2244	G2002	G2002		U1739	A1587	G1491	G1266	G1071	G1072	C1005
G2323				A1889	A1889	C1588	G1492	G1266	C1073	G1073	C1006
G2324	G2250	A2005	A2005	A1890	C1754	G1593	A1493	A1269	U1076	G1076	A1010
G2325	G2251	G2012	G2012	G1899	G1755	G1594	A1494	C1270	U1078	A1077	G1011
A2326	G2251	A2013	A2013	A1900	G1756	G1595	A1495	A1366	G1080	C1079	G1012
G2327	G2255	A2014	A2014	A1901	A1762	A1596	U1497	G1367	U1081	U1014	U1014
G2328	C2261	A2019	A2019	G1906	G1763	A1597	C1498	G1368	G1154	U1082	G1015
A2329	U2262	A2020	A2020	U1911	G1764	C1598		U1372	A1155	U1083	G1016
G2330	C2263	G2021	G2021	G1914	C1771	C1599	U1503	C1376	C1161	A1084	G1017
G2331	A2267	U2022	U2022	U1915	G1772	C1602	C1504	A1278	G1162	A1085	A1020
A2332	A2268	G2023	G2023	U1916	A1773	C1607	A1508	G1281	U1165	G1086	G1022
G2333	A2269	U2028	U2028	U1917	A1780	A1608	C1509	A1287	G1166	G1087	U1023
G2334	G2270	G2029	G2029	G1917	C1781	A1609	A1509A	U1288	U1167	U1088	G1024
A2335	G2271	A2030	A2030	G1920	C1782	C1622	U1512	C1289	G1171	G1089	G1025
G2336	U2272	A2031	A2031	G1921	A1786	U1629	C1513	G1291	G	G1091	U1026
G2337	A2273	G2032	G2032	G1921	A1786	U1629	C1514	C1292	A	C1092	A1027
A2338	G2274	A2033	A2033	A1927	A1786	U1629	U1514	U1293	U	G1093	A1028
G2339	C2275	G2036	G2036	A1928	A1791	G1633	G1525	U1294	A	U1094	G1029
G2340	G2276	G2037	G2037	A1929	U1794	G1633	G1526	C1295	G1178	A1095	G1030
A2341	U2277	G2038	G2038	G1930	U1796	C1640	G1529	G1296	C1179	G1099	G1031
G2342	A2278	C2039	C2039	A1937	U1797	G1642	C1530	U1300	G1184	U1101	U1035
C2343	G2283	G2040	G2040	U1938	C1797	G1642	C1531	A1301	U1102	C1102	G1036
G2344	A2286	U2041	U2041	U1939	U1798	G1647	C1532	A1302	U1103	C1103	C1041
A2345	A2287	G2042	G2042	U1939	G1799	C1647	G1532	A1302	C1104	U1105	A1045
G2346	G2289	C2043	C2043	C1800	C1800	C1648	G1533	G1303			



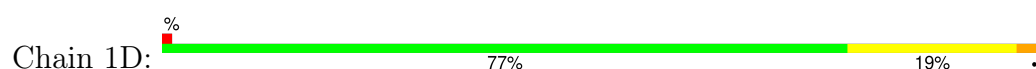
• Molecule 2: 5S Ribosomal RNA

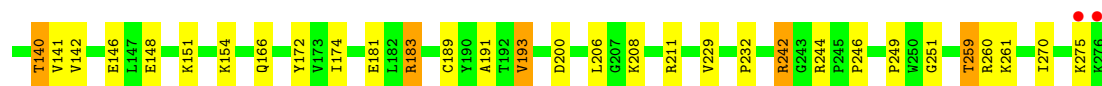


• Molecule 2: 5S Ribosomal RNA

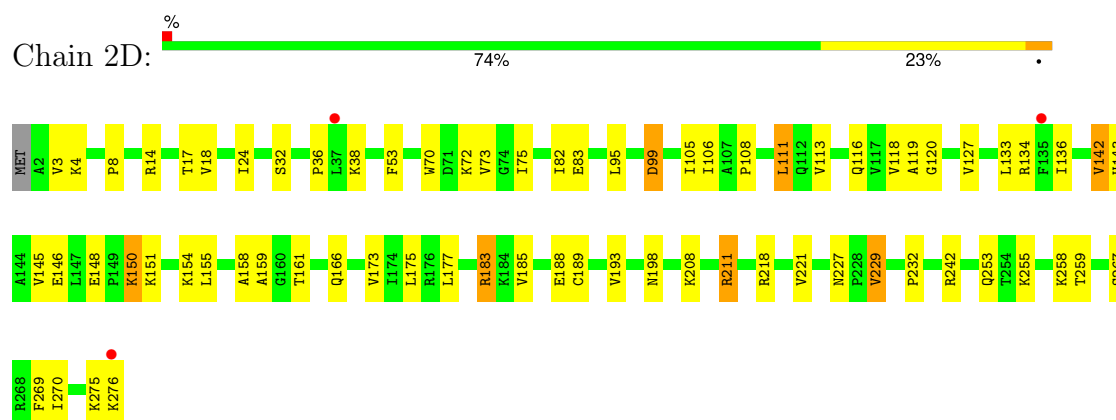


• Molecule 3: 50S ribosomal protein L2

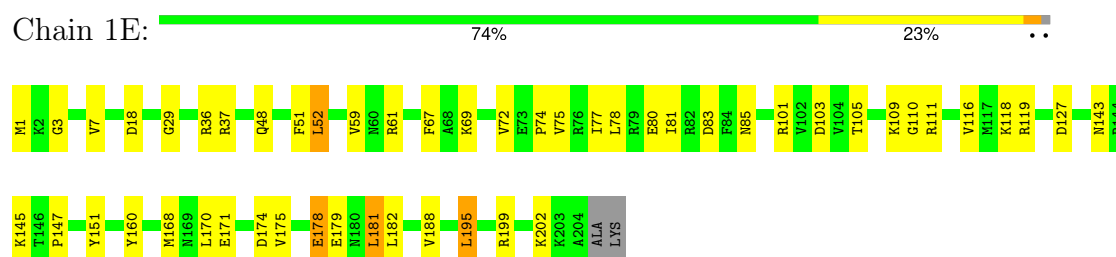




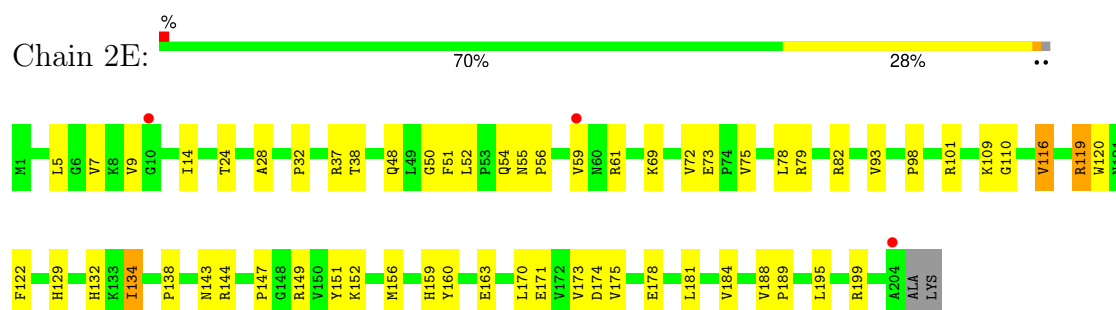
- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3



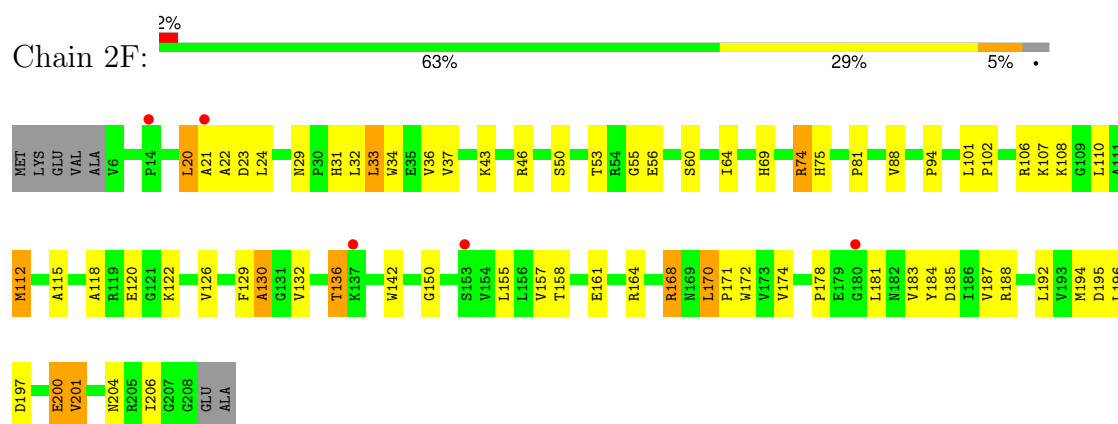
- Molecule 4: 50S ribosomal protein L3



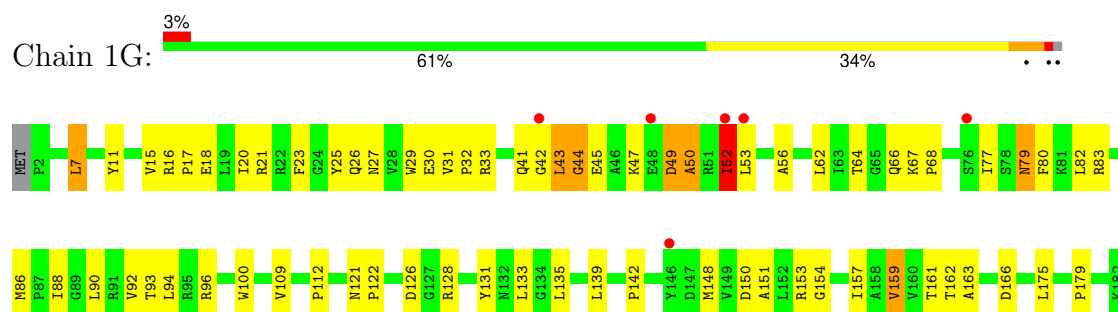
- Molecule 5: 50S ribosomal protein L4



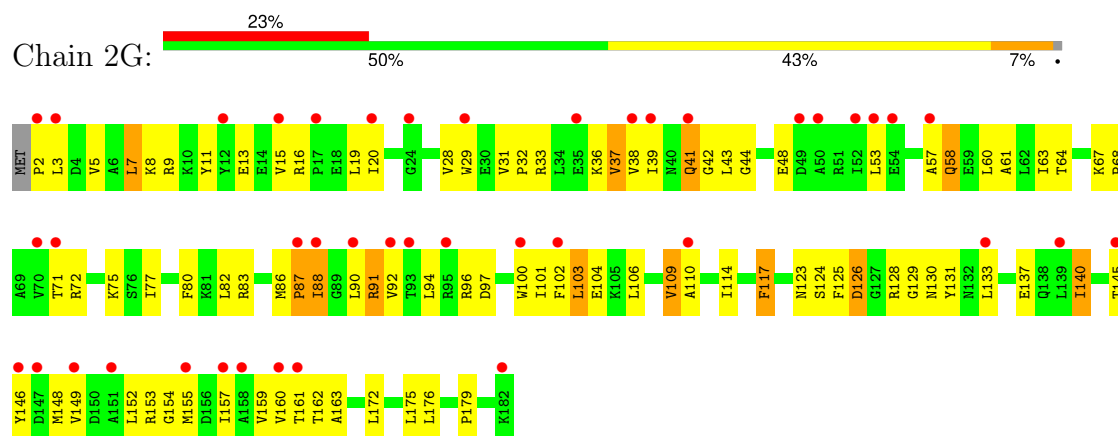
- Molecule 5: 50S ribosomal protein L4



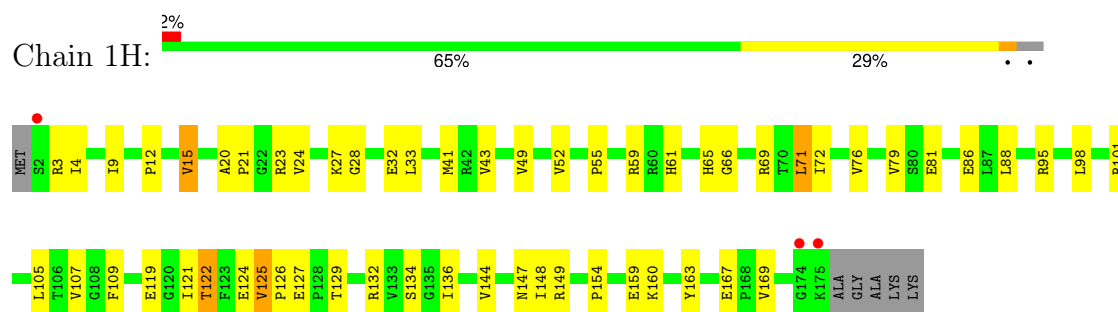
• Molecule 6: 50S ribosomal protein L5



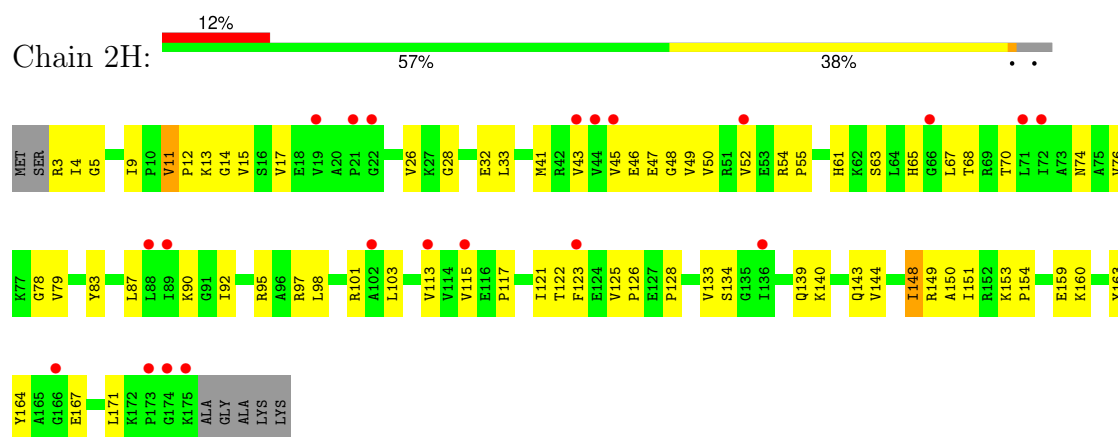
• Molecule 6: 50S ribosomal protein L5



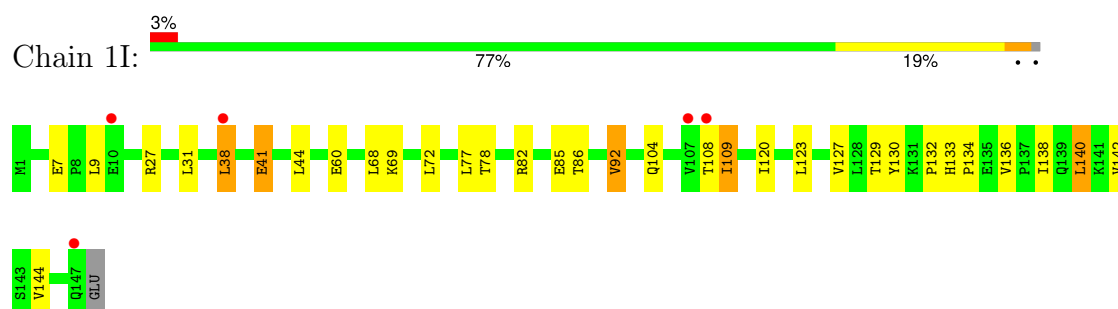
• Molecule 7: 50S ribosomal protein L6



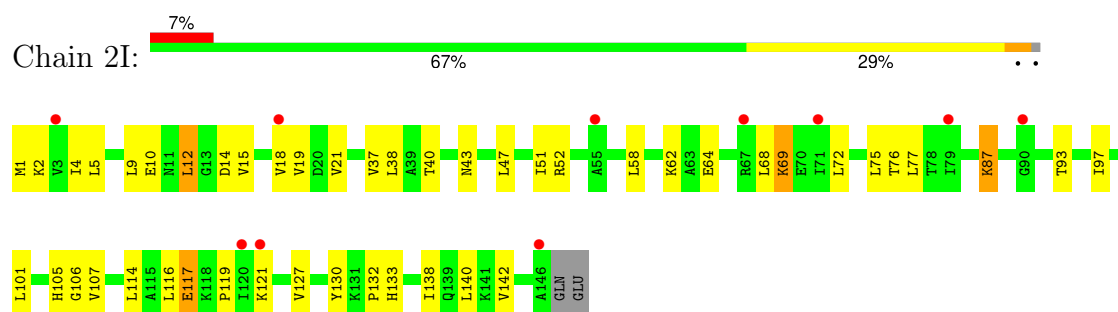
• Molecule 7: 50S ribosomal protein L6



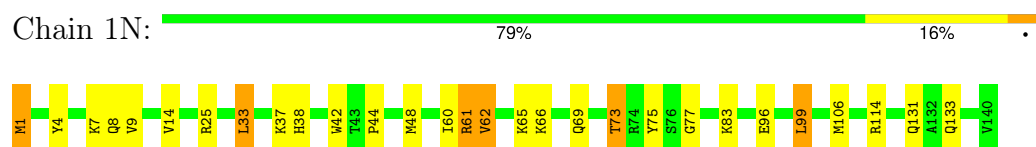
- Molecule 8: 50S ribosomal protein L9



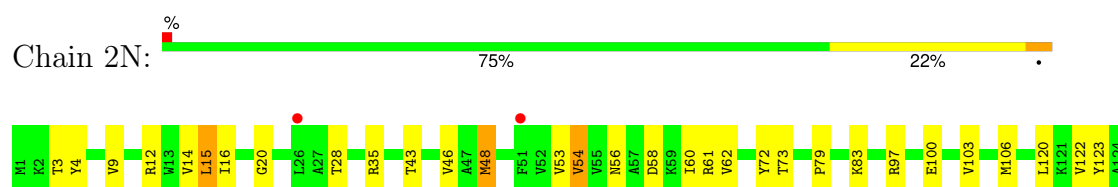
- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13



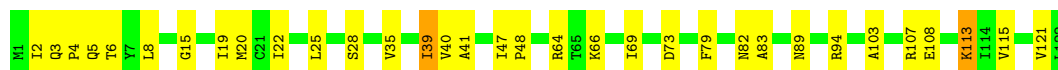
- Molecule 9: 50S ribosomal protein L13





- Molecule 10: 50S ribosomal protein L14

Chain 1O: 73% 25%



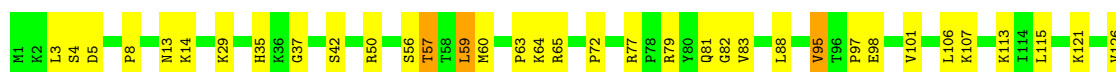
- Molecule 10: 50S ribosomal protein L14

Chain 2O: 68% 31%



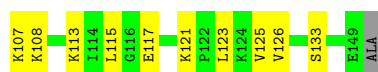
- Molecule 11: 50S ribosomal protein L15

Chain 1P: 71% 26%



- Molecule 11: 50S ribosomal protein L15

Chain 2P: 68% 29%

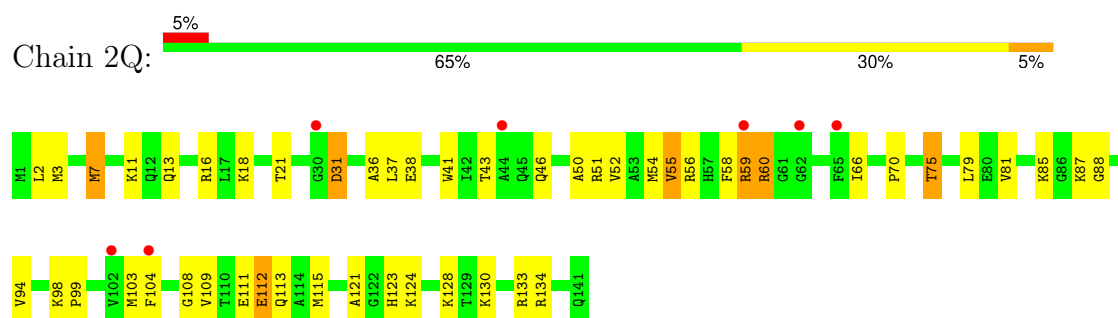


- Molecule 12: 50S ribosomal protein L16

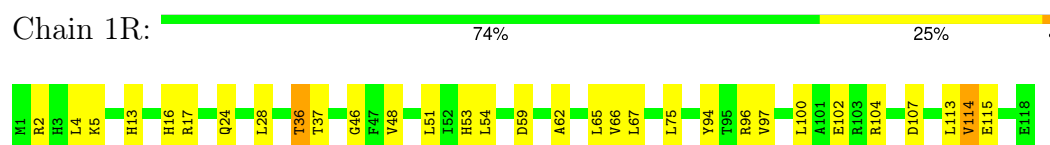
Chain 1Q: 83% 16%



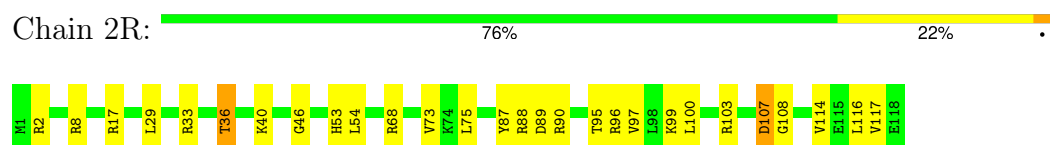
- Molecule 12: 50S ribosomal protein L16



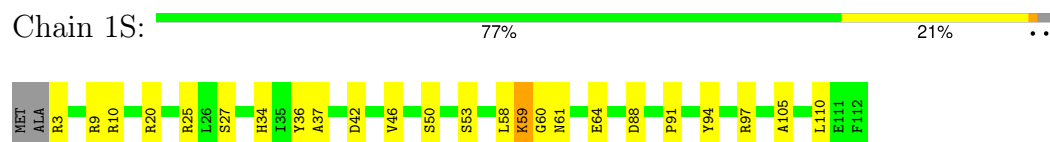
- Molecule 13: 50S ribosomal protein L17



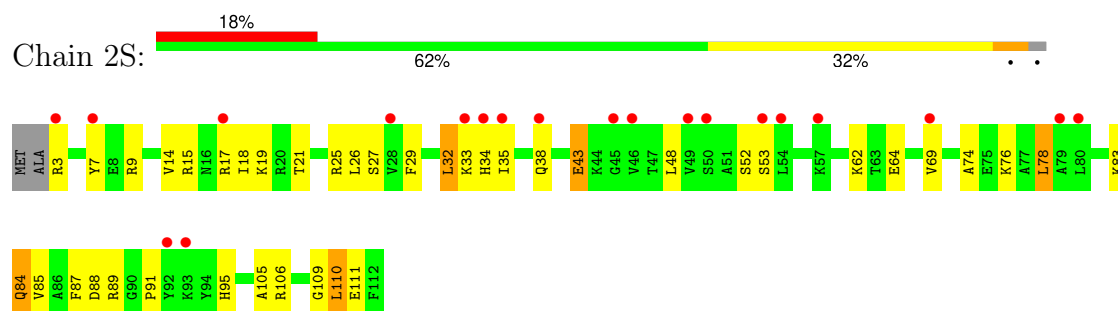
- Molecule 13: 50S ribosomal protein L17



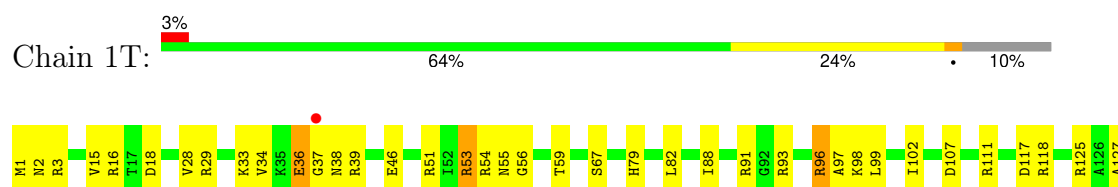
- Molecule 14: 50S ribosomal protein L18

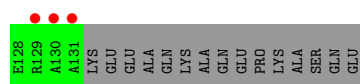


- Molecule 14: 50S ribosomal protein L18



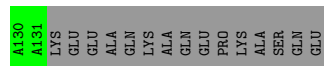
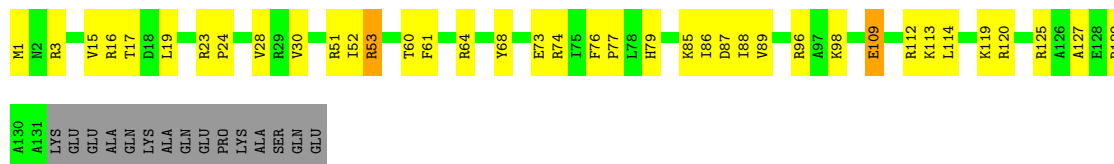
- Molecule 15: 50S ribosomal protein L19





- Molecule 15: 50S ribosomal protein L19

Chain 2T: 64% 25% 10%



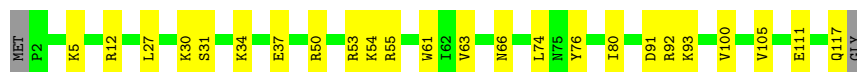
- Molecule 16: 50S ribosomal protein L20

Chain 1U: 80% 18% ..



- Molecule 16: 50S ribosomal protein L20

Chain 2U: 78% 20% ..



- Molecule 17: 50S ribosomal protein L21

Chain 1V: 86% 11% ..



- Molecule 17: 50S ribosomal protein L21

Chain 2V: 2% 73% 24% ..

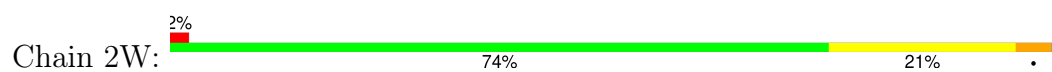


- Molecule 18: 50S ribosomal protein L22

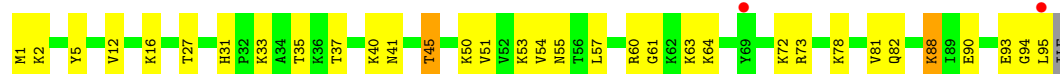
Chain 1W: 80% 18% ..



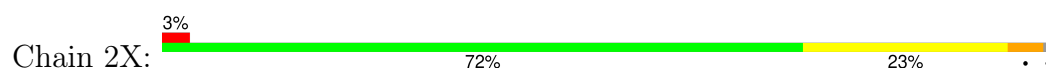
- Molecule 18: 50S ribosomal protein L22



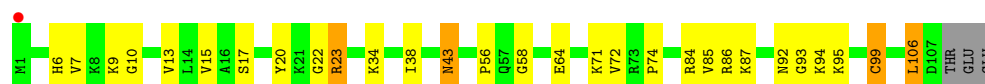
- Molecule 19: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L23



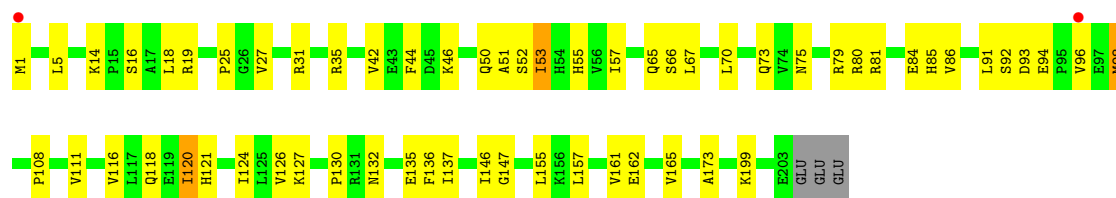
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

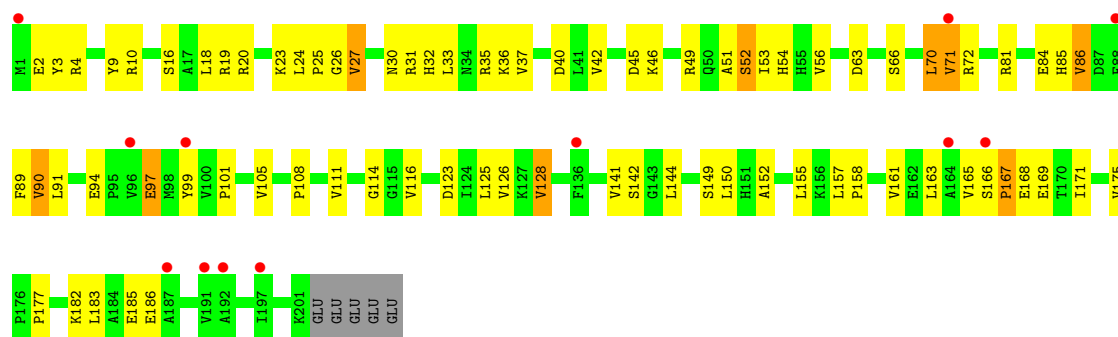


- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25





- Molecule 22: 50S ribosomal protein L27

Chain 10: 76% 19% ..



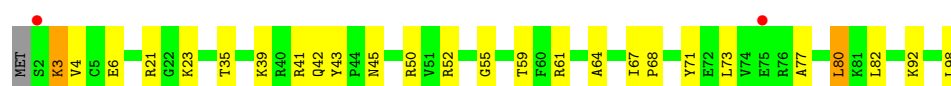
- Molecule 22: 50S ribosomal protein L27

Chain 20: 4% 73% 22% ..



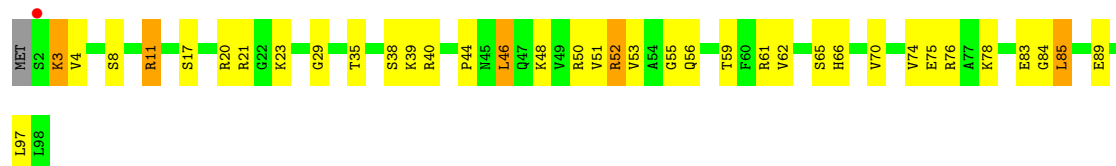
- Molecule 23: 50S ribosomal protein L28

Chain 11: 2% 72% 24% ..



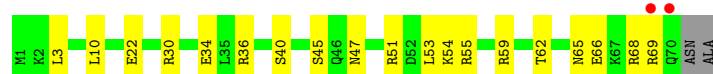
- Molecule 23: 50S ribosomal protein L28

Chain 21: 1% 61% 33% 5% .

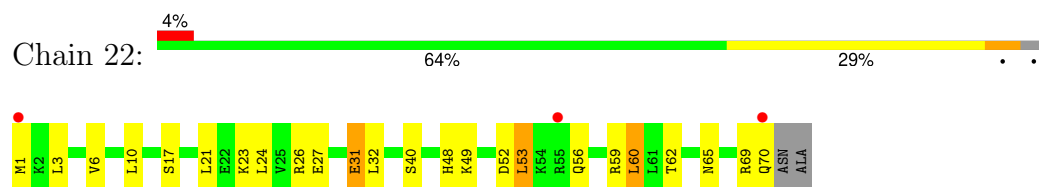


- Molecule 24: 50S ribosomal protein L29

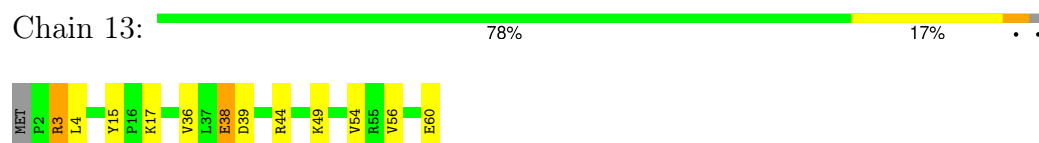
Chain 12: 3% 71% 26% .



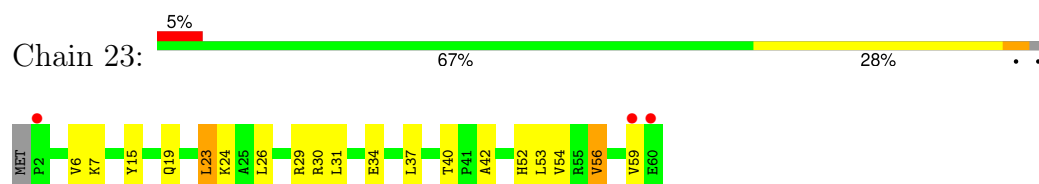
- Molecule 24: 50S ribosomal protein L29



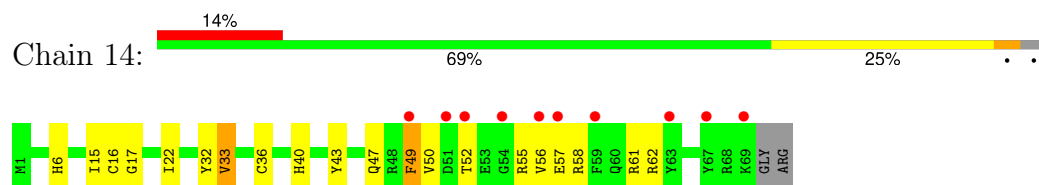
- Molecule 25: 50S ribosomal protein L30



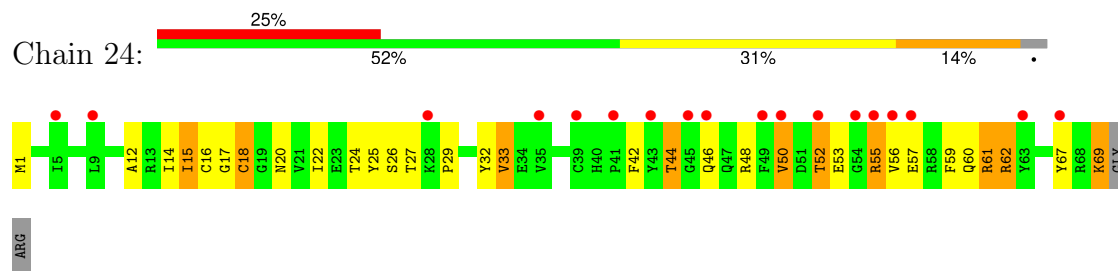
- Molecule 25: 50S ribosomal protein L30



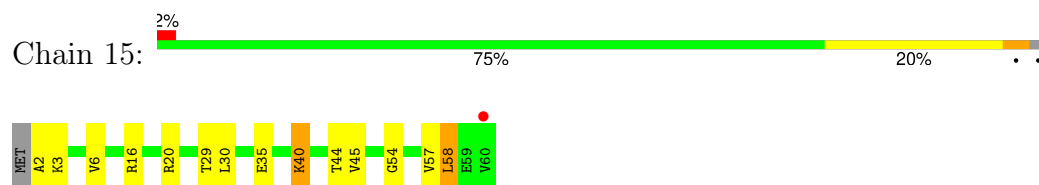
- Molecule 26: 50S ribosomal protein L31



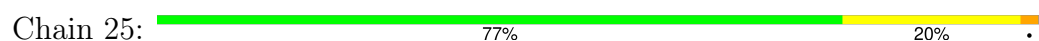
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32





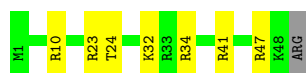
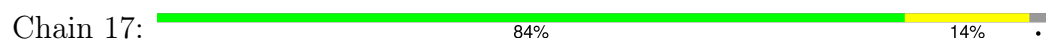
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



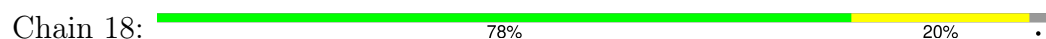
- Molecule 29: 50S ribosomal protein L34



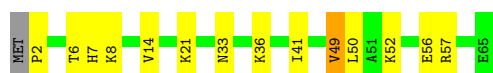
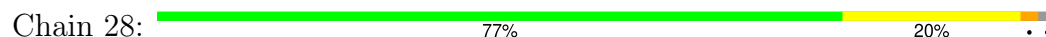
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35

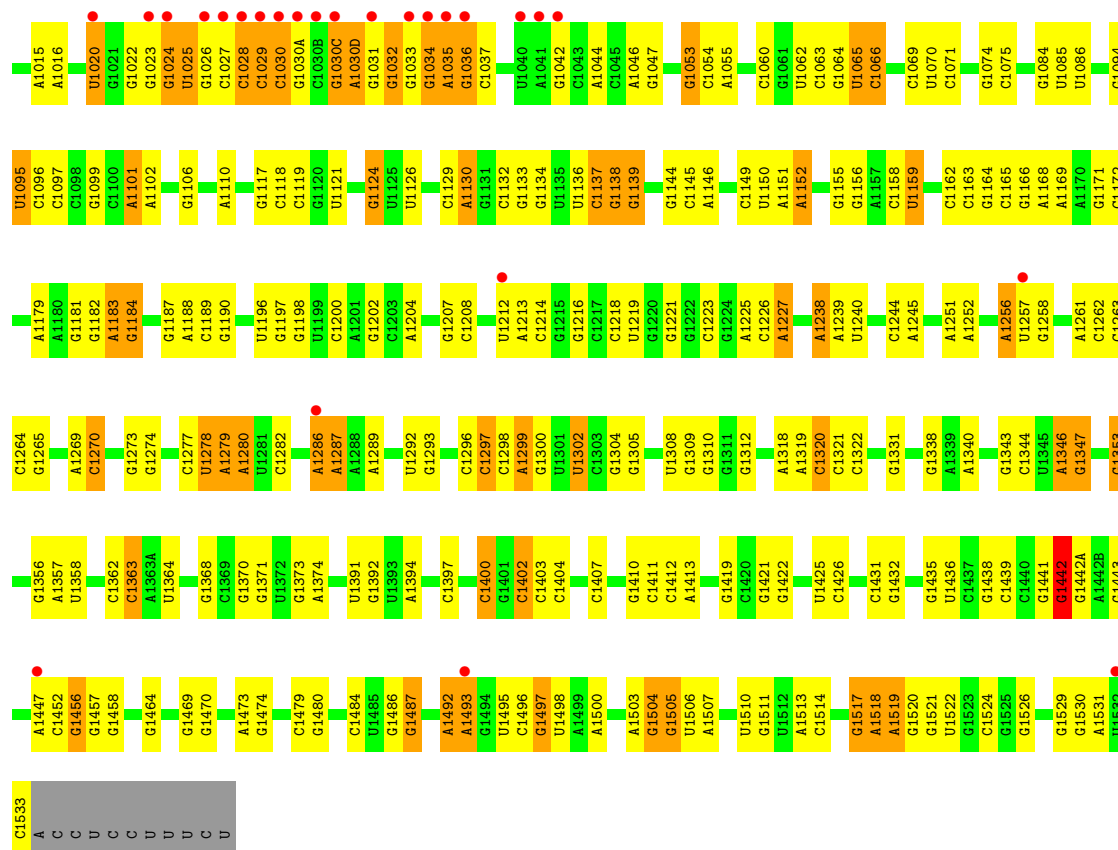


- Molecule 30: 50S ribosomal protein L35

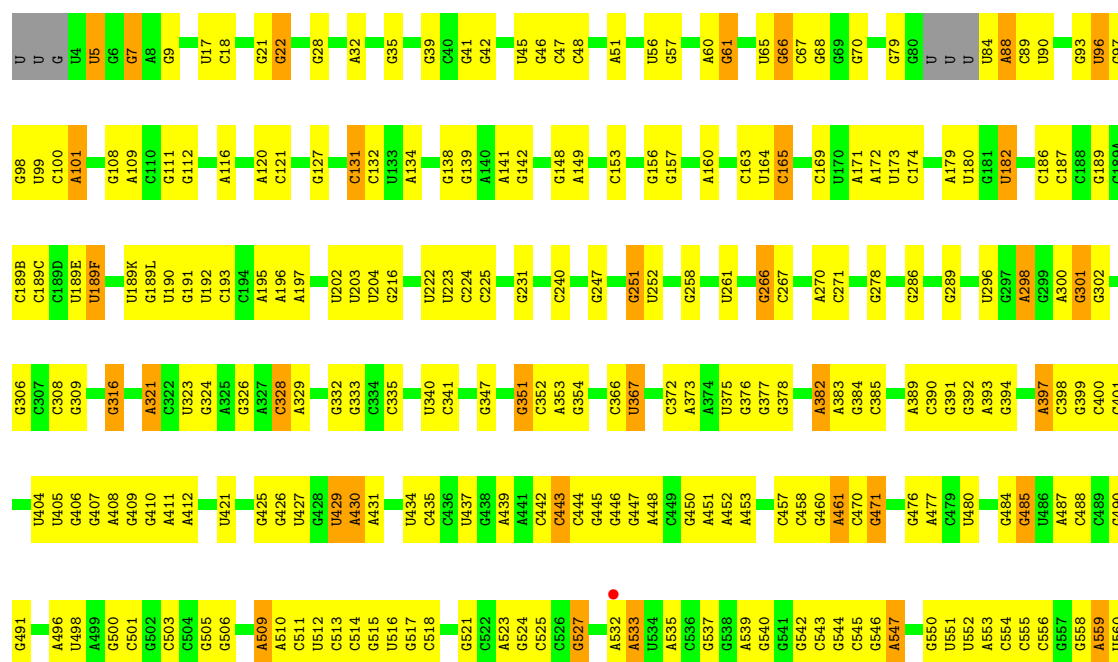


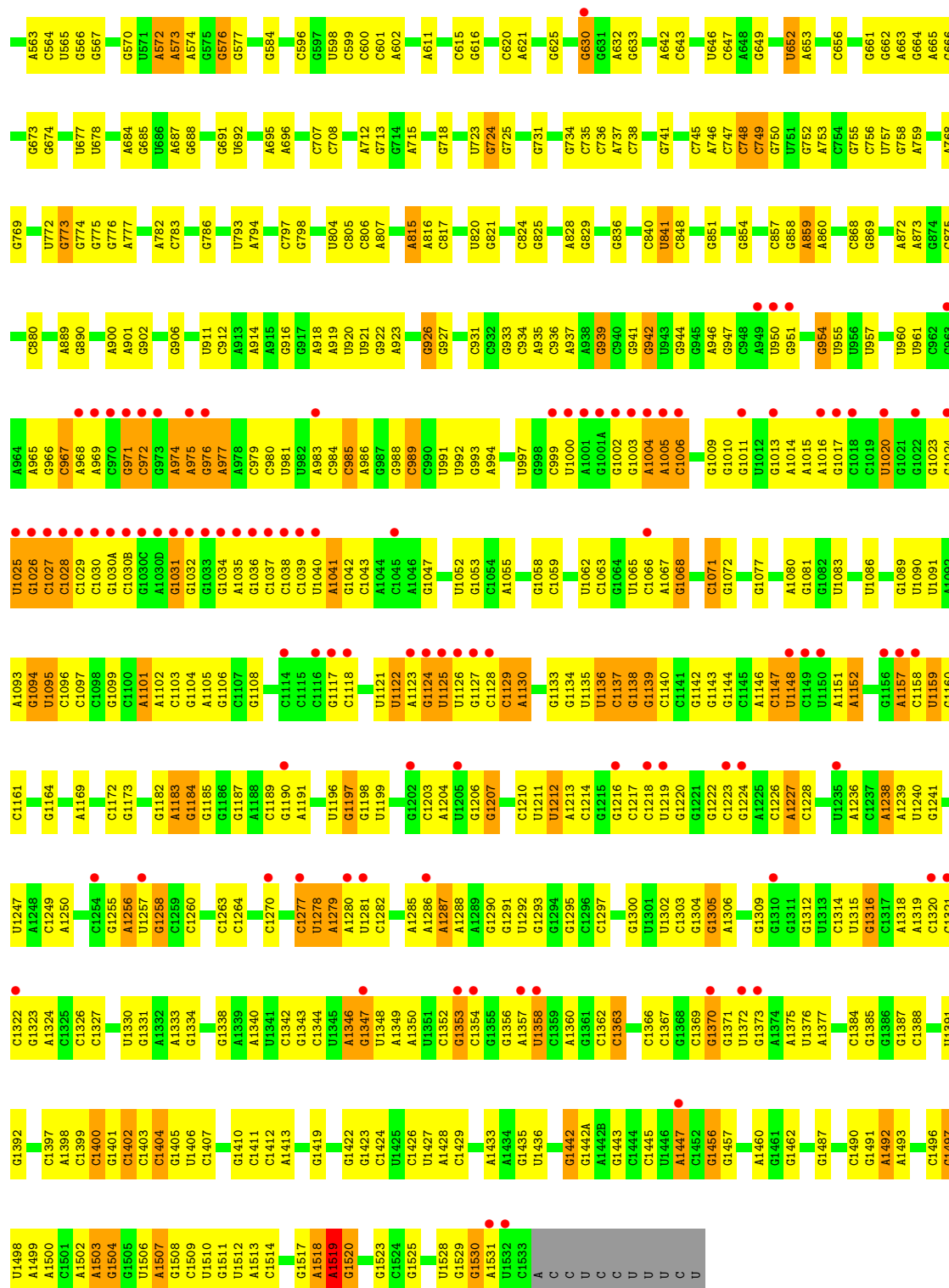
- Molecule 31: 50S ribosomal protein L36

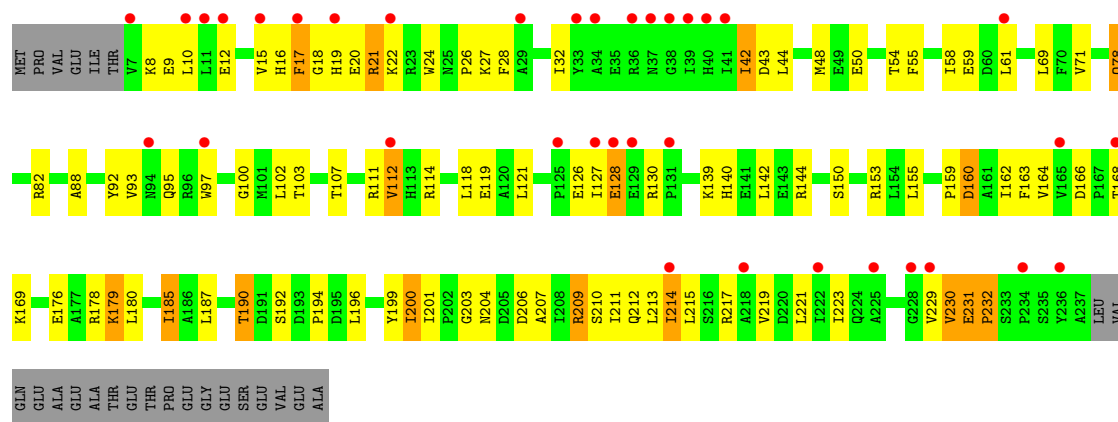




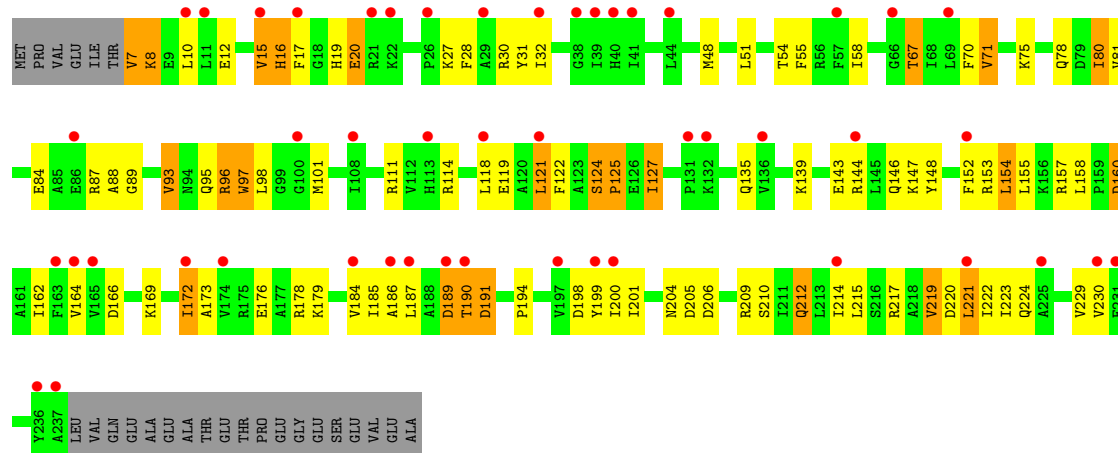
• Molecule 32: 16S Ribosomal RNA



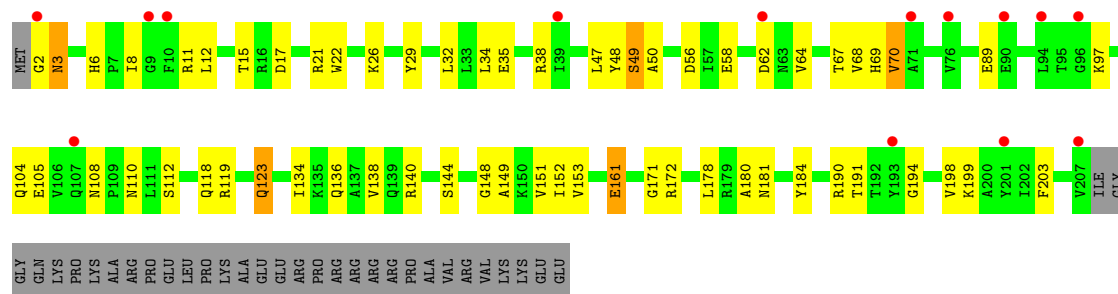




• Molecule 33: 30S ribosomal protein S2

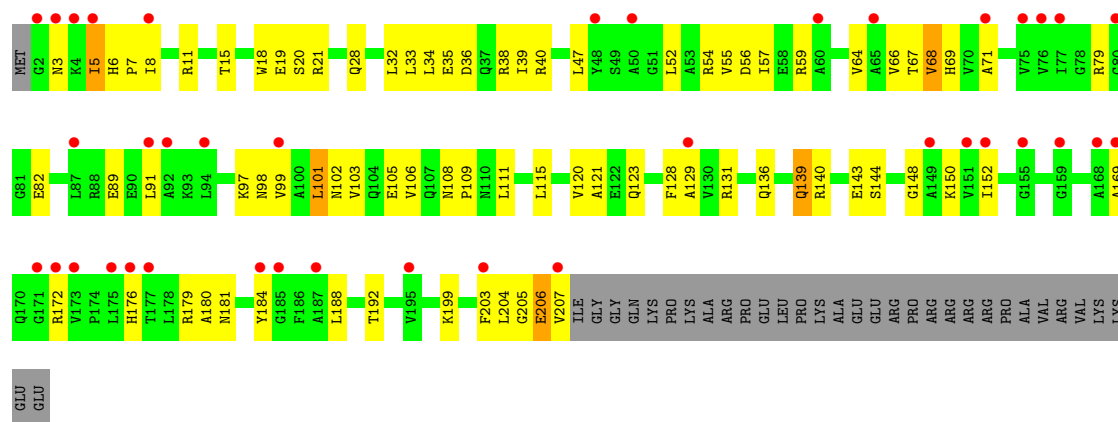


• Molecule 34: 30S ribosomal protein S3

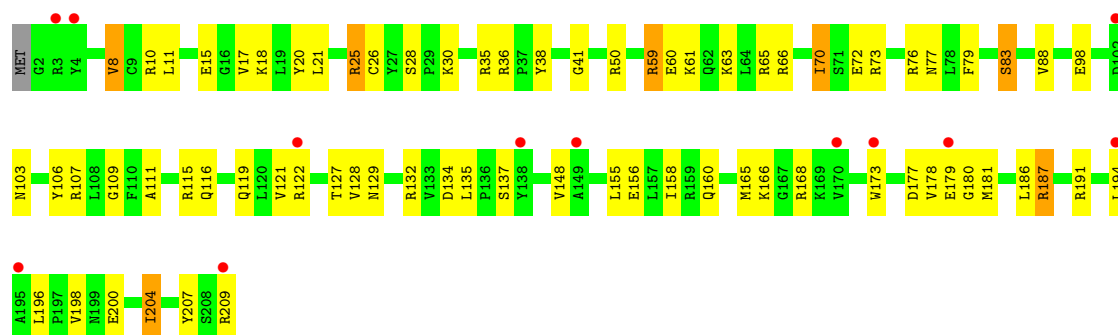


• Molecule 34: 30S ribosomal protein S3

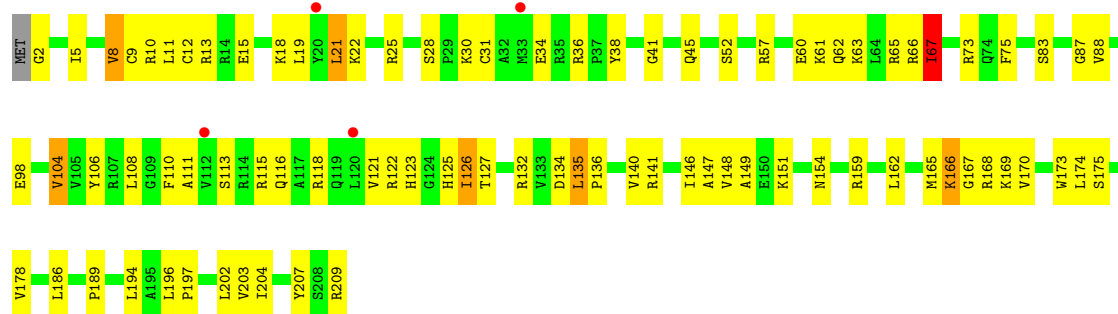




• Molecule 35: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S4

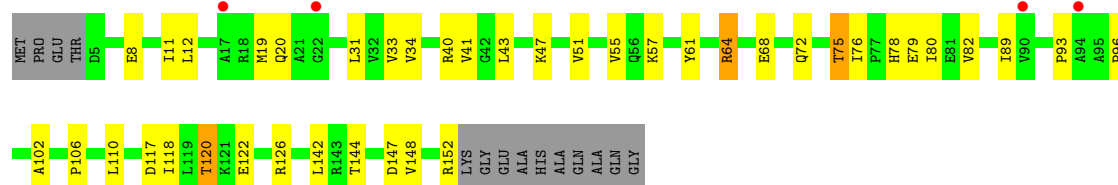


• Molecule 36: 30S ribosomal protein S5

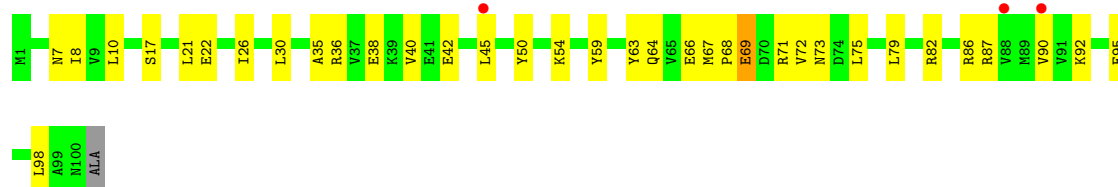




- Molecule 36: 30S ribosomal protein S5



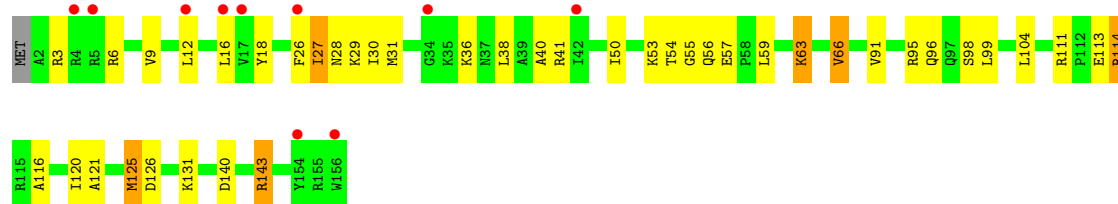
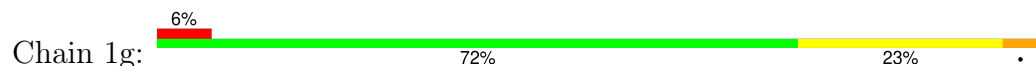
- Molecule 37: 30S ribosomal protein S6



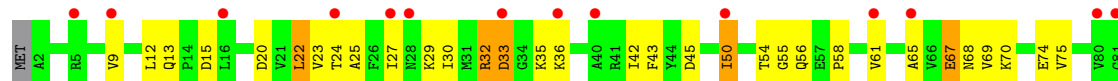
- Molecule 37: 30S ribosomal protein S6

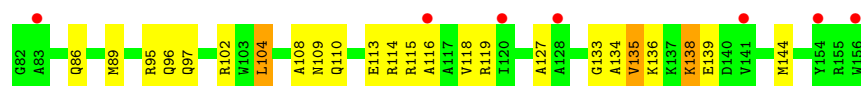


- Molecule 38: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S7

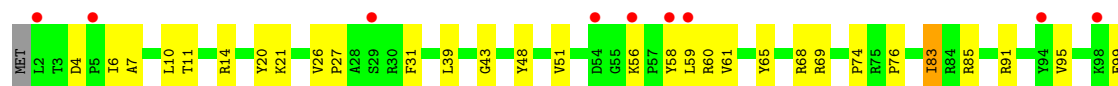




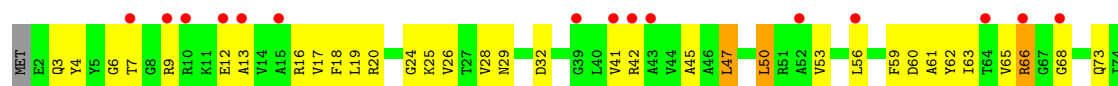
- Molecule 39: 30S ribosomal protein S8



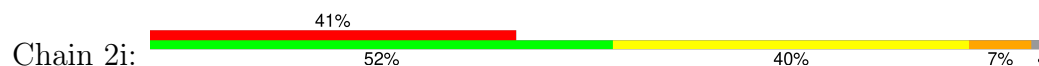
- Molecule 39: 30S ribosomal protein S8



- Molecule 40: 30S ribosomal protein S9

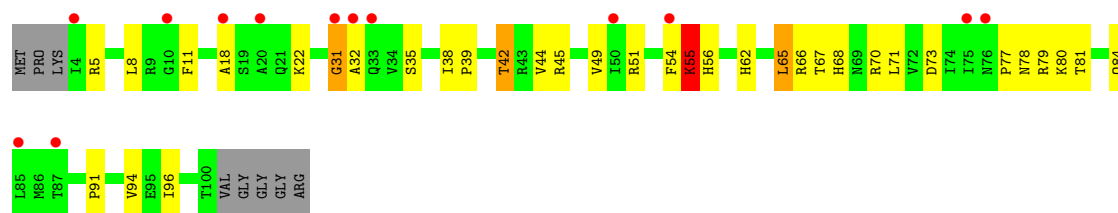


- Molecule 40: 30S ribosomal protein S9

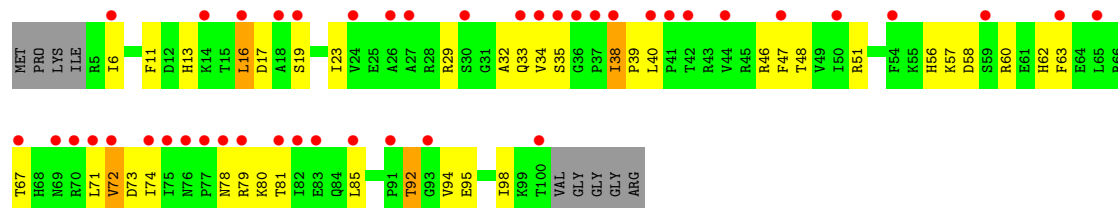
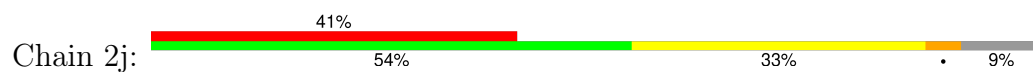


- Molecule 41: 30S ribosomal protein S10

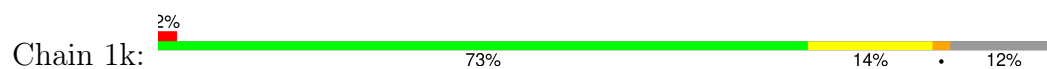




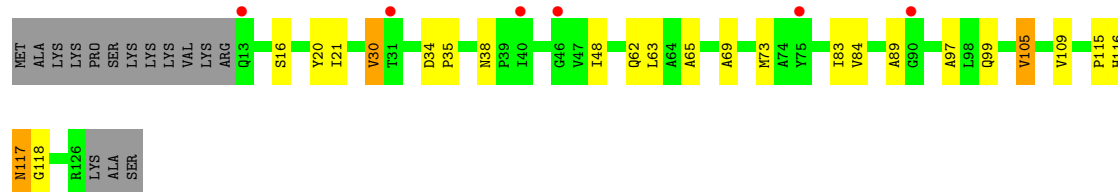
• Molecule 41: 30S ribosomal protein S10



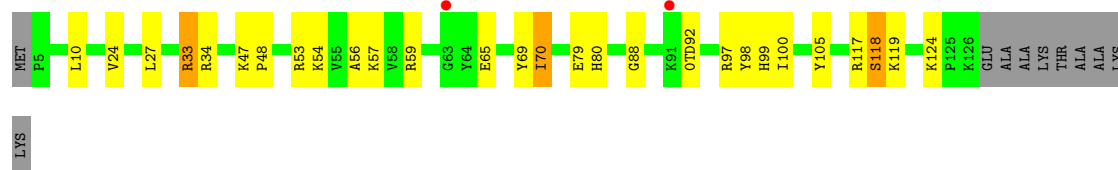
• Molecule 42: 30S ribosomal protein S11



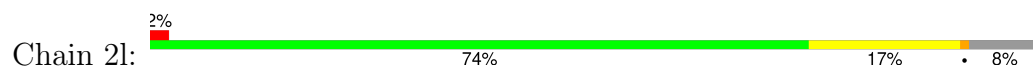
• Molecule 42: 30S ribosomal protein S11

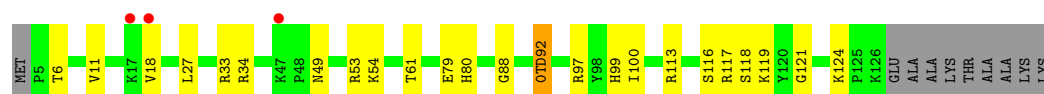


• Molecule 43: 30S ribosomal protein S12

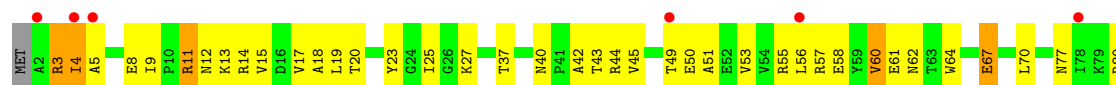


• Molecule 43: 30S ribosomal protein S12

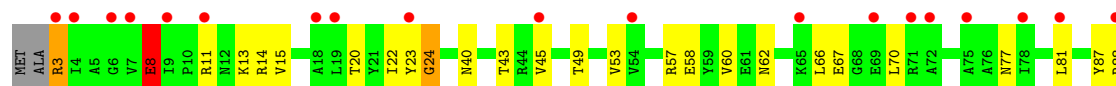




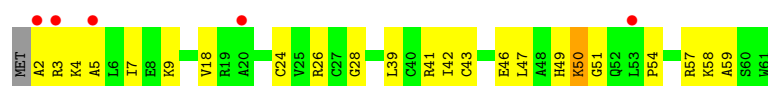
- Molecule 44: 30S ribosomal protein S13



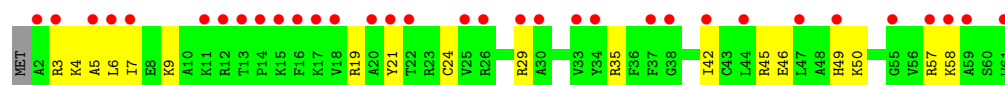
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



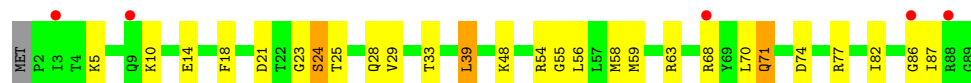
- Molecule 45: 30S ribosomal protein S14 type Z



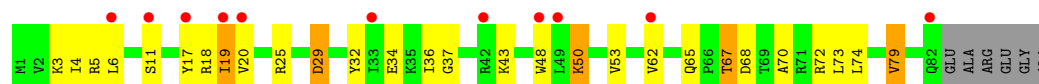
- Molecule 46: 30S ribosomal protein S15



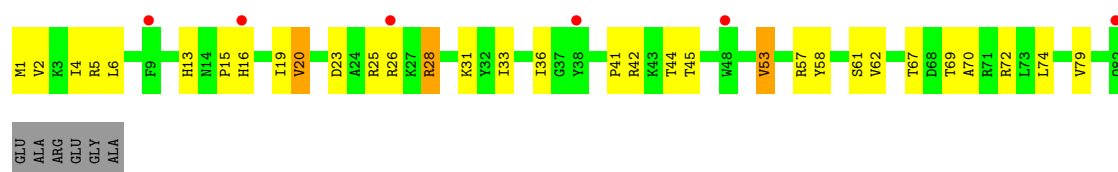
- Molecule 46: 30S ribosomal protein S15



• Molecule 47: 30S ribosomal protein S16



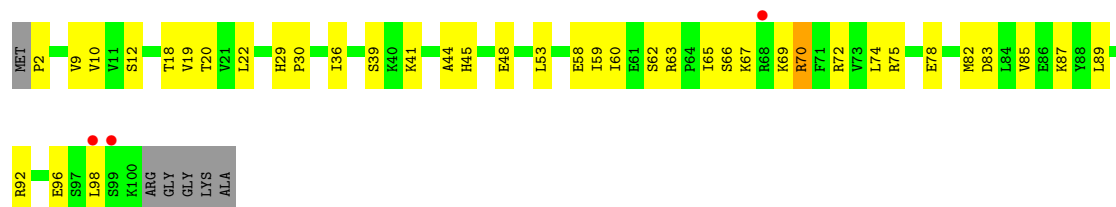
• Molecule 47: 30S ribosomal protein S16



• Molecule 48: 30S ribosomal protein S17



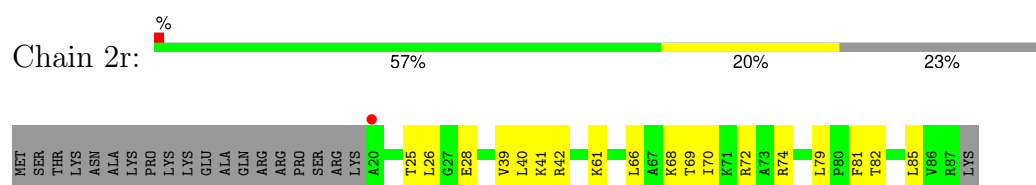
• Molecule 48: 30S ribosomal protein S17



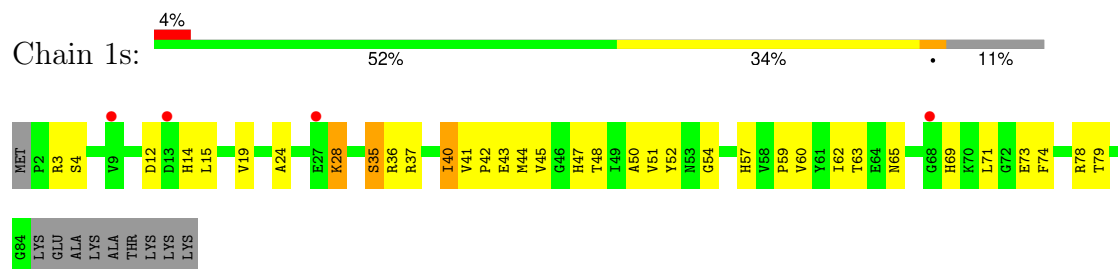
• Molecule 49: 30S ribosomal protein S18



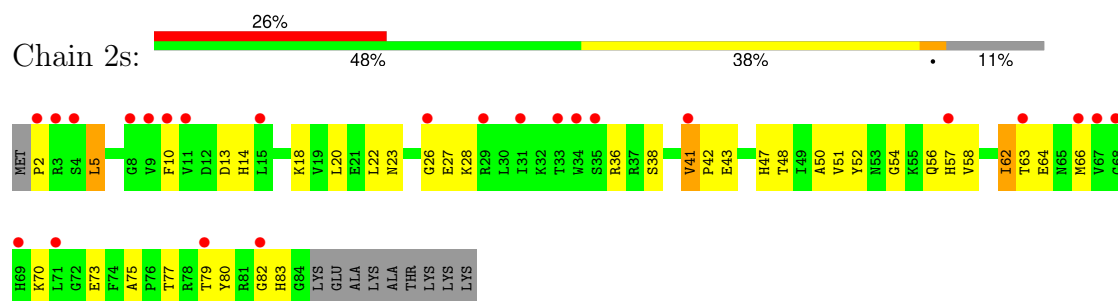
• Molecule 49: 30S ribosomal protein S18



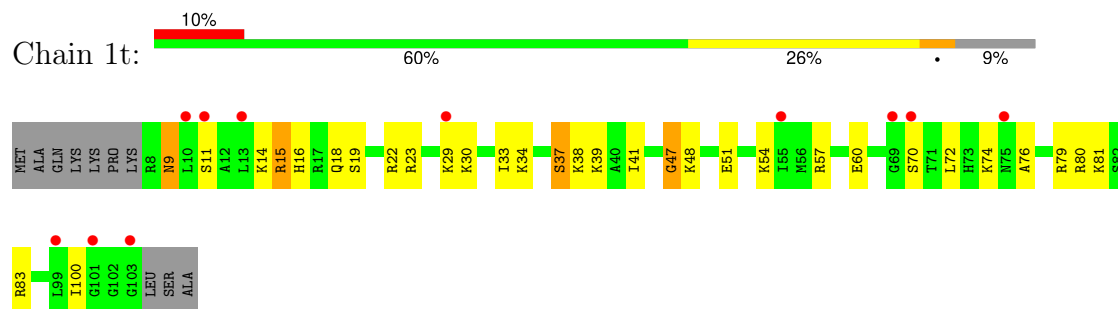
- Molecule 50: 30S ribosomal protein S19



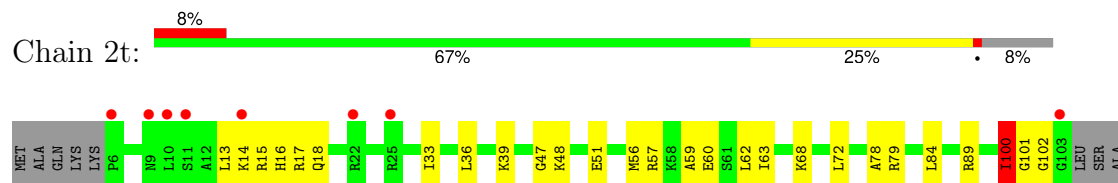
- Molecule 50: 30S ribosomal protein S19



- Molecule 51: 30S ribosomal protein S20

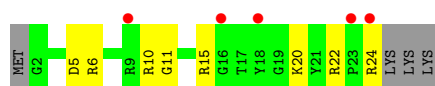


- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx

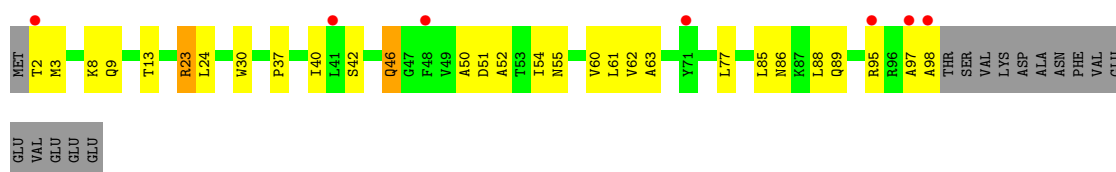




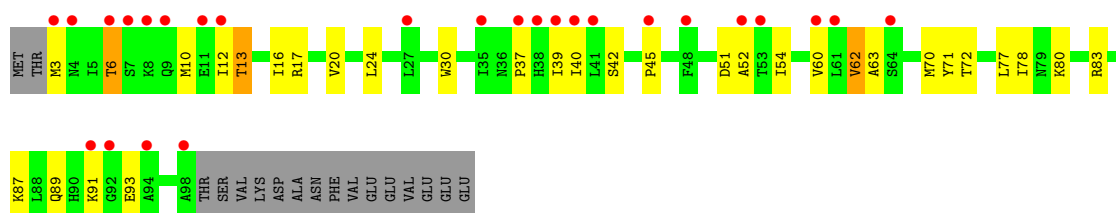
- Molecule 52: 30S ribosomal protein Thx



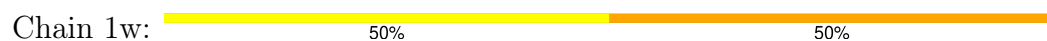
- Molecule 53: Ribosome-associated inhibitor A



- Molecule 53: Ribosome-associated inhibitor A



- Molecule 54: A-site Aminoacyl-tRNA Analog



- Molecule 54: A-site Aminoacyl-tRNA Analog

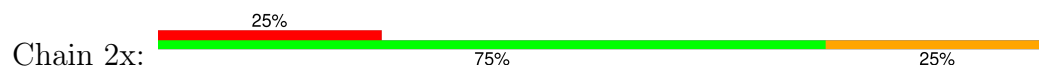


- Molecule 55: P-site Peptidyl-tRNA Analog RNA





- Molecule 55: P-site Peptidyl-tRNA Analog RNA



- Molecule 56: P-site Peptidyl-tRNA Analog Peptide



- Molecule 56: P-site Peptidyl-tRNA Analog Peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.83Å 450.39Å 621.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.10 – 2.60 122.10 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (122.10-2.60) 99.5 (122.10-2.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.220 , 0.269 0.221 , 0.268	Depositor DCC
R_{free} test set	88928 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	296459	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, M2G, 2MU, OMG, MA6, 4OC, 0TD, PPU, MPD, FME, 5MC, UR3, 8AN, SF4, OMC, 2MA, ZN, MG, G7M, 5MU, 2MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.28	0/69030	0.47	3/107750 (0.0%)
1	2A	0.22	0/68902	0.41	2/107548 (0.0%)
2	1B	0.24	0/2876	0.42	0/4486
2	2B	0.20	0/2878	0.37	0/4490
3	1D	0.28	0/2181	0.51	0/2940
3	2D	0.22	0/2186	0.47	0/2944
4	1E	0.26	0/1592	0.51	0/2149
4	2E	0.21	0/1592	0.43	0/2149
5	1F	0.26	0/1619	0.48	0/2193
5	2F	0.21	0/1615	0.46	0/2188
6	1G	0.22	0/1451	0.48	1/1961 (0.1%)
6	2G	0.22	0/1449	0.47	0/1957
7	1H	0.22	0/1356	0.41	0/1834
7	2H	0.20	0/1350	0.40	0/1826
8	1I	0.20	0/1109	0.44	0/1512
8	2I	0.19	0/1091	0.41	0/1490
9	1N	0.25	0/1148	0.48	0/1547
9	2N	0.20	0/1144	0.39	0/1543
10	1O	0.26	0/943	0.46	0/1269
10	2O	0.21	0/943	0.43	0/1269
11	1P	0.27	0/1152	0.50	0/1533
11	2P	0.20	0/1152	0.46	0/1533
12	1Q	0.26	0/1143	0.48	0/1527
12	2Q	0.19	0/1143	0.42	0/1527
13	1R	0.28	0/982	0.50	0/1312
13	2R	0.21	0/982	0.46	0/1312
14	1S	0.22	0/887	0.49	0/1180
14	2S	0.20	0/880	0.44	0/1172
15	1T	0.24	0/1105	0.47	0/1477
15	2T	0.21	0/1097	0.44	0/1468
16	1U	0.28	0/977	0.47	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.38	0/1301
17	1V	0.27	0/786	0.48	0/1053
17	2V	0.20	0/782	0.41	0/1049
18	1W	0.27	0/897	0.50	0/1205
18	2W	0.20	0/897	0.42	0/1205
19	1X	0.27	0/764	0.49	0/1025
19	2X	0.20	0/764	0.42	0/1025
20	1Y	0.23	0/823	0.47	0/1099
20	2Y	0.20	0/823	0.43	0/1100
21	1Z	0.24	0/1620	0.48	1/2200 (0.0%)
21	2Z	0.21	0/1590	0.43	0/2162
22	10	0.27	0/662	0.50	0/881
22	20	0.22	0/659	0.49	0/877
23	11	0.25	0/761	0.46	0/1013
23	21	0.22	0/766	0.42	0/1018
24	12	0.22	0/590	0.43	0/781
24	22	0.20	0/594	0.38	0/785
25	13	0.28	0/474	0.53	0/635
25	23	0.19	0/469	0.39	0/630
26	14	0.25	0/559	0.58	0/754
26	24	0.27	0/549	0.59	0/741
27	15	0.28	0/473	0.52	0/639
27	25	0.24	0/469	0.49	0/635
28	16	0.25	0/460	0.46	0/613
28	26	0.20	0/456	0.42	0/608
29	17	0.31	0/426	0.54	0/561
29	27	0.24	0/426	0.50	0/561
30	18	0.27	0/525	0.50	0/691
30	28	0.20	0/525	0.39	0/691
31	19	0.29	0/310	0.46	0/407
31	29	0.20	0/310	0.40	0/407
32	1a	0.20	0/35795	0.39	1/55864 (0.0%)
32	2a	0.20	0/35890	0.38	0/56012
33	1b	0.21	0/1876	0.49	0/2533
33	2b	0.23	0/1860	0.48	0/2518
34	1c	0.19	0/1582	0.42	0/2137
34	2c	0.21	0/1566	0.43	0/2119
35	1d	0.20	0/1695	0.43	0/2274
35	2d	0.19	0/1698	0.48	1/2277 (0.0%)
36	1e	0.20	0/1149	0.45	0/1548
36	2e	0.20	0/1149	0.44	0/1548
37	1f	0.21	0/827	0.40	0/1120
37	2f	0.19	0/829	0.41	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.18	0/1254	0.37	0/1683
38	2g	0.20	0/1248	0.41	0/1676
39	1h	0.19	0/1118	0.41	0/1506
39	2h	0.19	0/1108	0.41	0/1494
40	1i	0.20	0/1005	0.42	0/1351
40	2i	0.21	0/985	0.46	0/1329
41	1j	0.20	0/732	0.43	0/993
41	2j	0.22	0/723	0.45	0/984
42	1k	0.19	0/849	0.40	0/1150
42	2k	0.18	0/848	0.44	1/1149 (0.1%)
43	1l	0.20	0/937	0.42	0/1260
43	2l	0.22	0/937	0.42	0/1260
44	1m	0.19	0/924	0.45	0/1242
44	2m	0.23	0/905	0.46	0/1217
45	1n	0.20	0/501	0.45	0/664
45	2n	0.22	0/501	0.43	0/664
46	1o	0.19	0/739	0.38	0/985
46	2o	0.19	0/739	0.39	0/985
47	1p	0.21	0/697	0.47	0/939
47	2p	0.19	0/693	0.45	1/935 (0.1%)
48	1q	0.20	0/836	0.43	0/1117
48	2q	0.19	0/836	0.42	0/1117
49	1r	0.20	0/560	0.42	0/746
49	2r	0.20	0/560	0.38	0/746
50	1s	0.17	0/663	0.44	0/895
50	2s	0.23	0/660	0.42	0/893
51	1t	0.21	0/734	0.45	0/969
51	2t	0.19	0/736	0.45	0/976
52	1u	0.20	0/203	0.45	0/266
52	2u	0.23	0/203	0.44	0/266
53	1y	0.20	0/776	0.40	0/1048
53	2y	0.21	0/761	0.40	0/1030
54	1w	1.86	2/44 (4.5%)	1.54	1/67 (1.5%)
54	2w	1.56	1/44 (2.3%)	1.06	0/67
55	1x	0.44	0/44	0.52	0/67
55	2x	0.29	0/44	0.44	0/67
56	1v	0.29	0/19	0.37	0/24
56	2v	0.24	0/19	0.41	0/24
All	All	0.23	3/310242 (0.0%)	0.43	12/463663 (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
11	1P	0	1
11	2P	0	1
14	1S	0	1
26	24	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	74	C	O3'-P	-5.64	1.52	1.61
54	2w	74	C	O3'-P	-5.44	1.52	1.61
54	1w	75	C	P-OP1	-5.43	1.38	1.49

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	75	C	C3'-C2'-O2'	-9.42	96.56	110.70
1	1A	1042	G	OP1-P-O3'	-9.31	80.08	108.00
35	2d	67	ILE	N-CA-C	-7.06	105.90	112.96
1	1A	1042	G	OP2-P-O3'	-6.86	87.42	108.00
6	1G	96	ARG	CB-CA-C	-5.96	109.69	116.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
14	1S	58	LEU	Peptide
26	24	18	CYS	Peptide
11	2P	35	HIS	Peptide

5.2 Too-close contacts

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	31204	647	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2A	61758	0	31152	789	0
2	1B	2572	0	1305	29	0
2	2B	2573	0	1306	34	0
3	1D	2131	0	2207	45	0
3	2D	2136	0	2218	48	0
4	1E	1559	0	1618	33	0
4	2E	1559	0	1617	38	0
5	1F	1584	0	1625	37	0
5	2F	1580	0	1619	46	0
6	1G	1426	0	1445	52	0
6	2G	1424	0	1441	67	0
7	1H	1330	0	1407	33	0
7	2H	1324	0	1402	37	0
8	1I	1094	0	1127	16	0
8	2I	1076	0	1094	19	0
9	1N	1121	0	1195	25	0
9	2N	1117	0	1184	21	0
10	1O	933	0	996	25	0
10	2O	933	0	996	29	0
11	1P	1135	0	1212	30	0
11	2P	1135	0	1212	37	0
12	1Q	1122	0	1179	20	0
12	2Q	1122	0	1179	35	0
13	1R	968	0	1033	22	0
13	2R	968	0	1033	19	0
14	1S	877	0	938	17	0
14	2S	870	0	923	30	0
15	1T	1091	0	1151	31	0
15	2T	1083	0	1136	28	0
16	1U	959	0	1019	14	0
16	2U	959	0	1019	20	0
17	1V	775	0	841	8	0
17	2V	771	0	830	14	0
18	1W	886	0	940	11	0
18	2W	886	0	940	16	0
19	1X	750	0	814	26	0
19	2X	750	0	814	15	0
20	1Y	810	0	892	18	0
20	2Y	810	0	887	25	0
21	1Z	1587	0	1598	31	0
21	2Z	1557	0	1564	55	0
22	10	653	0	674	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	650	0	665	20	0
23	11	754	0	823	20	0
23	21	759	0	837	28	0
24	12	588	0	643	13	0
24	22	592	0	654	11	0
25	13	469	0	518	6	0
25	23	464	0	514	9	0
26	14	546	0	522	14	0
26	24	536	0	514	22	0
27	15	459	0	476	12	0
27	25	455	0	465	10	0
28	16	453	0	473	7	0
28	26	449	0	469	10	0
29	17	418	0	467	5	0
29	27	418	0	467	12	0
30	18	517	0	582	10	0
30	28	517	0	582	8	0
31	19	307	0	335	2	0
31	29	307	0	335	7	0
32	1a	32246	0	16295	430	0
32	2a	32331	0	16338	508	0
33	1b	1842	0	1862	63	0
33	2b	1825	0	1828	69	0
34	1c	1558	0	1557	36	0
34	2c	1542	0	1517	53	0
35	1d	1665	0	1687	56	0
35	2d	1668	0	1703	64	0
36	1e	1133	0	1191	35	0
36	2e	1133	0	1191	29	0
37	1f	814	0	808	20	0
37	2f	816	0	808	18	0
38	1g	1235	0	1249	24	0
38	2g	1229	0	1238	36	0
39	1h	1098	0	1143	29	0
39	2h	1088	0	1126	36	0
40	1i	986	0	990	38	0
40	2i	966	0	953	50	0
41	1j	719	0	672	26	0
41	2j	710	0	661	25	0
42	1k	834	0	838	11	0
42	2k	833	0	836	14	0
43	1l	932	0	981	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	2l	932	0	981	17	0
44	1m	914	0	954	37	0
44	2m	895	0	920	28	0
45	1n	492	0	529	19	0
45	2n	492	0	529	16	0
46	1o	728	0	760	17	0
46	2o	728	0	760	19	0
47	1p	681	0	697	22	0
47	2p	677	0	686	19	0
48	1q	823	0	891	15	0
48	2q	823	0	891	23	0
49	1r	555	0	618	9	0
49	2r	555	0	618	9	0
50	1s	648	0	658	22	0
50	2s	645	0	635	34	0
51	1t	732	0	809	22	0
51	2t	733	0	795	19	0
52	1u	199	0	208	8	0
52	2u	199	0	208	10	0
53	1y	764	0	786	20	0
53	2y	749	0	757	22	0
54	1w	78	0	50	3	0
54	2w	78	0	49	4	0
55	1x	63	0	33	0	0
55	2x	63	0	33	2	0
56	1v	29	0	30	1	0
56	2v	29	0	30	3	0
57	10	10	0	0	0	0
57	11	3	0	0	0	0
57	13	4	0	0	0	0
57	15	9	0	0	0	0
57	17	5	0	0	0	0
57	18	2	0	0	0	0
57	19	3	0	0	0	0
57	1A	1029	0	0	0	0
57	1B	29	0	0	0	0
57	1D	16	0	0	0	0
57	1E	9	0	0	0	0
57	1F	15	0	0	0	0
57	1G	4	0	0	0	0
57	1H	2	0	0	0	0
57	1N	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1O	2	0	0	0	0
57	1P	3	0	0	0	0
57	1Q	5	0	0	0	0
57	1R	5	0	0	0	0
57	1T	5	0	0	0	0
57	1U	7	0	0	0	0
57	1V	6	0	0	0	0
57	1W	4	0	0	0	0
57	1Y	1	0	0	0	0
57	1Z	1	0	0	0	0
57	1a	272	0	0	0	0
57	1b	1	0	0	0	0
57	1d	5	0	0	0	0
57	1e	3	0	0	0	0
57	1f	2	0	0	0	0
57	1g	2	0	0	0	0
57	1h	2	0	0	0	0
57	1i	1	0	0	0	0
57	1l	2	0	0	0	0
57	1m	1	0	0	0	0
57	1n	3	0	0	0	0
57	1o	1	0	0	0	0
57	1t	1	0	0	0	0
57	1u	1	0	0	0	0
57	1w	1	0	0	0	0
57	1x	2	0	0	0	0
57	1y	3	0	0	0	0
57	20	1	0	0	0	0
57	21	4	0	0	0	0
57	23	1	0	0	0	0
57	25	4	0	0	0	0
57	27	1	0	0	0	0
57	28	1	0	0	0	0
57	29	1	0	0	0	0
57	2A	734	0	0	0	0
57	2B	17	0	0	0	0
57	2D	11	0	0	0	0
57	2E	8	0	0	0	0
57	2F	4	0	0	0	0
57	2G	2	0	0	0	0
57	2I	1	0	0	0	0
57	2N	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2P	2	0	0	0	0
57	2Q	2	0	0	0	0
57	2R	2	0	0	0	0
57	2T	4	0	0	0	0
57	2V	2	0	0	0	0
57	2W	3	0	0	0	0
57	2X	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2a	188	0	0	0	0
57	2e	2	0	0	0	0
57	2f	1	0	0	0	0
57	2j	1	0	0	0	0
57	2n	1	0	0	0	0
57	2p	1	0	0	0	0
57	2t	1	0	0	0	0
57	2x	1	0	0	0	0
58	1A	12	0	12	4	0
58	1B	12	0	12	0	0
59	18	8	0	14	0	0
59	1A	8	0	14	1	0
59	1a	16	0	28	4	0
59	2A	24	0	42	1	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	0	0
61	2d	8	0	0	2	0
62	10	22	0	0	1	0
62	11	24	0	0	2	0
62	12	10	0	0	3	0
62	13	19	0	0	1	0
62	14	2	0	0	0	0
62	15	24	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	16	15	0	0	1	0
62	17	14	0	0	1	0
62	18	21	0	0	2	0
62	19	7	0	0	0	0
62	1A	3560	0	0	122	0
62	1B	89	0	0	3	0
62	1D	98	0	0	4	0
62	1E	69	0	0	2	0
62	1F	51	0	0	1	0
62	1G	15	0	0	1	0
62	1H	6	0	0	1	0
62	1I	4	0	0	0	0
62	1N	43	0	0	3	0
62	1O	22	0	0	3	0
62	1P	63	0	0	4	0
62	1Q	33	0	0	3	0
62	1R	30	0	0	2	0
62	1S	8	0	0	1	0
62	1T	24	0	0	4	0
62	1U	45	0	0	3	0
62	1V	30	0	0	1	0
62	1W	26	0	0	1	0
62	1X	23	0	0	1	0
62	1Y	12	0	0	1	0
62	1Z	9	0	0	2	0
62	1a	382	0	0	27	0
62	1d	5	0	0	1	0
62	1e	3	0	0	0	0
62	1f	2	0	0	0	0
62	1h	1	0	0	0	0
62	1i	1	0	0	0	0
62	1j	1	0	0	0	0
62	1l	3	0	0	1	0
62	1o	3	0	0	0	0
62	1p	2	0	0	0	0
62	1u	1	0	0	0	0
62	1w	4	0	0	1	0
62	1x	4	0	0	0	0
62	1y	3	0	0	0	0
62	20	7	0	0	0	0
62	21	17	0	0	4	0
62	25	7	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	26	1	0	0	0	0
62	27	4	0	0	0	0
62	28	12	0	0	0	0
62	2A	1737	0	0	121	0
62	2B	33	0	0	4	0
62	2D	32	0	0	1	0
62	2E	22	0	0	1	0
62	2F	20	0	0	1	0
62	2G	2	0	0	0	0
62	2I	2	0	0	0	0
62	2N	3	0	0	1	0
62	2O	11	0	0	1	0
62	2P	18	0	0	2	0
62	2Q	7	0	0	0	0
62	2R	14	0	0	2	0
62	2S	2	0	0	0	0
62	2T	6	0	0	0	0
62	2U	7	0	0	1	0
62	2V	5	0	0	0	0
62	2W	7	0	0	0	0
62	2X	4	0	0	0	0
62	2Y	2	0	0	0	0
62	2Z	9	0	0	2	0
62	2a	224	0	0	19	0
62	2d	3	0	0	0	0
62	2e	2	0	0	0	0
62	2f	1	0	0	0	0
62	2j	1	0	0	0	0
62	2l	3	0	0	1	0
62	2o	3	0	0	0	0
62	2p	1	0	0	0	0
62	2q	1	0	0	0	0
62	2r	2	0	0	0	0
62	2t	1	0	0	0	0
62	2v	1	0	0	0	0
62	2w	3	0	0	0	0
62	2x	2	0	0	0	0
62	2y	1	0	0	0	0
All	All	296459	0	194836	4310	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 9.

The worst 5 of 4310 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)
54:1w:73:A:O3'	62:1w:201:HOH:O	1.60	1.20
1:1A:1082:U:H3	1:1A:1086:A:N6	1.41	1.17
1:2A:2139:C:N4	1:2A:2152:G:H1	1.44	1.14
1:1A:2137:C:N4	1:1A:2154:G:H1	1.56	1.04
1:1A:1082:U:O4	1:1A:1086:A:N1	1.92	1.01

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	257 (94%)	16 (6%)	0	100	100
4	1E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	24	46
4	2E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	24	46
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	24	46
5	2F	201/210 (96%)	185 (92%)	15 (8%)	1 (0%)	24	46
6	1G	179/182 (98%)	159 (89%)	15 (8%)	5 (3%)	4	6
6	2G	179/182 (98%)	146 (82%)	28 (16%)	5 (3%)	4	6
7	1H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	21	42
7	2H	171/180 (95%)	146 (85%)	22 (13%)	3 (2%)	6	14
8	1I	145/148 (98%)	122 (84%)	22 (15%)	1 (1%)	18	38
8	2I	144/148 (97%)	124 (86%)	18 (12%)	2 (1%)	9	19
9	1N	138/140 (99%)	128 (93%)	10 (7%)	0	100	100
9	2N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	34
11	1P	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	18	38
11	2P	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	18	38
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
12	2Q	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	18	38
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	108 (93%)	7 (6%)	1 (1%)	14	30
14	1S	108/112 (96%)	103 (95%)	4 (4%)	1 (1%)	14	30
14	2S	108/112 (96%)	100 (93%)	8 (7%)	0	100	100
15	1T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	16	34
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12	28
17	2V	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	6	12
18	1W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	11	25
19	2X	93/96 (97%)	86 (92%)	6 (6%)	1 (1%)	11	25
20	1Y	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
20	2Y	105/110 (96%)	93 (89%)	12 (11%)	0	100	100
21	1Z	201/206 (98%)	184 (92%)	17 (8%)	0	100	100
21	2Z	199/206 (97%)	172 (86%)	24 (12%)	3 (2%)	8	18
22	10	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
22	20	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	10	23
23	11	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11	25
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	25
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	50 (75%)	16 (24%)	1 (2%)	8	18
26	24	67/71 (94%)	48 (72%)	16 (24%)	3 (4%)	2	2
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
27	25	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	199 (87%)	24 (10%)	6 (3%)	4	7
33	2b	229/256 (90%)	191 (83%)	32 (14%)	6 (3%)	4	7
34	1c	204/239 (85%)	182 (89%)	21 (10%)	1 (0%)	24	46
34	2c	204/239 (85%)	163 (80%)	38 (19%)	3 (2%)	8	18
35	1d	206/209 (99%)	188 (91%)	17 (8%)	1 (0%)	24	46
35	2d	206/209 (99%)	187 (91%)	18 (9%)	1 (0%)	24	46
36	1e	146/162 (90%)	135 (92%)	9 (6%)	2 (1%)	9	19
36	2e	146/162 (90%)	133 (91%)	13 (9%)	0	100	100
37	1f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
37	2f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
38	1g	153/156 (98%)	142 (93%)	10 (6%)	1 (1%)	18	38
38	2g	153/156 (98%)	139 (91%)	12 (8%)	2 (1%)	9	21
39	1h	135/138 (98%)	125 (93%)	10 (7%)	0	100	100
39	2h	135/138 (98%)	124 (92%)	10 (7%)	1 (1%)	18	38
40	1i	125/128 (98%)	107 (86%)	18 (14%)	0	100	100
40	2i	124/128 (97%)	111 (90%)	13 (10%)	0	100	100
41	1j	95/105 (90%)	81 (85%)	9 (10%)	5 (5%)	1	1
41	2j	94/105 (90%)	79 (84%)	13 (14%)	2 (2%)	5	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	1k	112/129 (87%)	97 (87%)	14 (12%)	1 (1%)	14	30
42	2k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	14	30
43	1l	119/132 (90%)	110 (92%)	9 (8%)	0	100	100
43	2l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
44	1m	114/126 (90%)	99 (87%)	12 (10%)	3 (3%)	4	7
44	2m	112/126 (89%)	91 (81%)	19 (17%)	2 (2%)	6	14
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
46	1o	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	5	9
46	2o	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
47	1p	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
47	2p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
48	1q	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	12	28
48	2q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
49	1r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/93 (87%)	73 (90%)	7 (9%)	1 (1%)	10	23
50	2s	81/93 (87%)	66 (82%)	14 (17%)	1 (1%)	10	23
51	1t	94/106 (89%)	85 (90%)	8 (8%)	1 (1%)	11	25
51	2t	96/106 (91%)	88 (92%)	6 (6%)	2 (2%)	5	11
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	16 (76%)	5 (24%)	0	100	100
53	1y	95/113 (84%)	93 (98%)	2 (2%)	0	100	100
53	2y	94/113 (83%)	86 (92%)	7 (7%)	1 (1%)	11	25
56	1v	1/3 (33%)	1 (100%)	0	0	100	100
56	2v	1/3 (33%)	1 (100%)	0	0	100	100
All	All	11643/12360 (94%)	10671 (92%)	882 (8%)	90 (1%)	16	34

5 of 90 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	44	GLY
7	1H	126	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	1X	94	GLY
33	1b	17	PHE
33	1b	127	ILE

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	20
3	2D	215/218 (99%)	198 (92%)	17 (8%)	11	26
4	1E	164/166 (99%)	154 (94%)	10 (6%)	17	37
4	2E	164/166 (99%)	152 (93%)	12 (7%)	13	29
5	1F	160/166 (96%)	143 (89%)	17 (11%)	6	14
5	2F	159/166 (96%)	139 (87%)	20 (13%)	4	9
6	1G	144/156 (92%)	136 (94%)	8 (6%)	19	40
6	2G	142/156 (91%)	128 (90%)	14 (10%)	7	16
7	1H	144/148 (97%)	129 (90%)	15 (10%)	7	14
7	2H	143/148 (97%)	126 (88%)	17 (12%)	5	10
8	1I	111/124 (90%)	96 (86%)	15 (14%)	4	7
8	2I	108/124 (87%)	88 (82%)	20 (18%)	1	3
9	1N	119/119 (100%)	110 (92%)	9 (8%)	12	27
9	2N	118/119 (99%)	109 (92%)	9 (8%)	12	27
10	1O	100/100 (100%)	95 (95%)	5 (5%)	22	46
10	2O	100/100 (100%)	95 (95%)	5 (5%)	22	46
11	1P	115/116 (99%)	108 (94%)	7 (6%)	17	37
11	2P	115/116 (99%)	109 (95%)	6 (5%)	21	44
12	1Q	111/111 (100%)	107 (96%)	4 (4%)	31	58
12	2Q	111/111 (100%)	100 (90%)	11 (10%)	7	16
13	1R	101/101 (100%)	93 (92%)	8 (8%)	11	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	2R	101/101 (100%)	95 (94%)	6 (6%)	18	38
14	1S	87/88 (99%)	84 (97%)	3 (3%)	32	60
14	2S	85/88 (97%)	72 (85%)	13 (15%)	3	5
15	1T	115/127 (91%)	108 (94%)	7 (6%)	17	37
15	2T	113/127 (89%)	108 (96%)	5 (4%)	25	50
16	1U	93/94 (99%)	87 (94%)	6 (6%)	15	35
16	2U	93/94 (99%)	88 (95%)	5 (5%)	20	42
17	1V	81/82 (99%)	75 (93%)	6 (7%)	13	29
17	2V	80/82 (98%)	70 (88%)	10 (12%)	4	9
18	1W	90/92 (98%)	83 (92%)	7 (8%)	11	26
18	2W	90/92 (98%)	83 (92%)	7 (8%)	11	26
19	1X	77/78 (99%)	75 (97%)	2 (3%)	40	68
19	2X	77/78 (99%)	70 (91%)	7 (9%)	9	19
20	1Y	86/91 (94%)	76 (88%)	10 (12%)	5	11
20	2Y	86/91 (94%)	77 (90%)	9 (10%)	6	14
21	1Z	169/179 (94%)	152 (90%)	17 (10%)	7	15
21	2Z	165/179 (92%)	150 (91%)	15 (9%)	9	19
22	10	65/67 (97%)	59 (91%)	6 (9%)	8	19
22	20	64/67 (96%)	62 (97%)	2 (3%)	35	63
23	11	79/83 (95%)	78 (99%)	1 (1%)	61	82
23	21	81/83 (98%)	75 (93%)	6 (7%)	13	29
24	12	65/67 (97%)	63 (97%)	2 (3%)	35	63
24	22	66/67 (98%)	56 (85%)	10 (15%)	3	5
25	13	51/52 (98%)	46 (90%)	5 (10%)	7	17
25	23	50/52 (96%)	42 (84%)	8 (16%)	2	4
26	14	58/63 (92%)	53 (91%)	5 (9%)	10	22
26	24	54/63 (86%)	45 (83%)	9 (17%)	2	4
27	15	51/52 (98%)	48 (94%)	3 (6%)	18	38
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	25
28	16	51/52 (98%)	48 (94%)	3 (6%)	18	38
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	17	41/42 (98%)	40 (98%)	1 (2%)	43	70
29	27	41/42 (98%)	39 (95%)	2 (5%)	22	47
30	18	54/55 (98%)	53 (98%)	1 (2%)	50	75
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	29
31	19	34/34 (100%)	32 (94%)	2 (6%)	18	38
31	29	34/34 (100%)	31 (91%)	3 (9%)	9	21
33	1b	191/220 (87%)	168 (88%)	23 (12%)	5	10
33	2b	187/220 (85%)	160 (86%)	27 (14%)	3	6
34	1c	144/188 (77%)	132 (92%)	12 (8%)	10	23
34	2c	140/188 (74%)	124 (89%)	16 (11%)	5	11
35	1d	171/181 (94%)	154 (90%)	17 (10%)	7	16
35	2d	172/181 (95%)	150 (87%)	22 (13%)	4	8
36	1e	114/123 (93%)	100 (88%)	14 (12%)	4	9
36	2e	114/123 (93%)	104 (91%)	10 (9%)	9	21
37	1f	85/90 (94%)	76 (89%)	9 (11%)	6	14
37	2f	85/90 (94%)	78 (92%)	7 (8%)	10	24
38	1g	120/127 (94%)	107 (89%)	13 (11%)	6	13
38	2g	119/127 (94%)	106 (89%)	13 (11%)	6	13
39	1h	116/119 (98%)	105 (90%)	11 (10%)	8	18
39	2h	114/119 (96%)	106 (93%)	8 (7%)	14	31
40	1i	91/99 (92%)	80 (88%)	11 (12%)	5	10
40	2i	88/99 (89%)	75 (85%)	13 (15%)	3	6
41	1j	68/92 (74%)	62 (91%)	6 (9%)	9	21
41	2j	68/92 (74%)	57 (84%)	11 (16%)	2	4
42	1k	83/99 (84%)	78 (94%)	5 (6%)	17	37
42	2k	83/99 (84%)	79 (95%)	4 (5%)	23	47
43	1l	96/108 (89%)	93 (97%)	3 (3%)	35	63
43	2l	96/108 (89%)	92 (96%)	4 (4%)	26	52
44	1m	90/101 (89%)	82 (91%)	8 (9%)	9	20
44	2m	87/101 (86%)	81 (93%)	6 (7%)	14	32
45	1n	49/50 (98%)	45 (92%)	4 (8%)	10	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	2n	49/50 (98%)	47 (96%)	2 (4%)	27	54
46	1o	78/80 (98%)	73 (94%)	5 (6%)	16	35
46	2o	78/80 (98%)	69 (88%)	9 (12%)	5	11
47	1p	69/74 (93%)	61 (88%)	8 (12%)	5	11
47	2p	68/74 (92%)	59 (87%)	9 (13%)	4	8
48	1q	94/97 (97%)	85 (90%)	9 (10%)	8	17
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13	29
49	1r	59/77 (77%)	53 (90%)	6 (10%)	7	15
49	2r	59/77 (77%)	54 (92%)	5 (8%)	10	22
50	1s	68/80 (85%)	62 (91%)	6 (9%)	9	21
50	2s	67/80 (84%)	60 (90%)	7 (10%)	7	14
51	1t	71/82 (87%)	62 (87%)	9 (13%)	4	9
51	2t	70/82 (85%)	67 (96%)	3 (4%)	26	51
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	40
52	2u	18/22 (82%)	18 (100%)	0	100	100
53	1y	82/98 (84%)	74 (90%)	8 (10%)	7	17
53	2y	79/98 (81%)	71 (90%)	8 (10%)	7	15
56	1v	2/2 (100%)	2 (100%)	0	100	100
56	2v	2/2 (100%)	2 (100%)	0	100	100
All	All	9535/10264 (93%)	8691 (91%)	844 (9%)	9	20

5 of 844 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	2H	68	THR
19	2X	66	LEU
46	2o	24	SER
8	2I	40	THR
7	2H	67	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 164 such sidechains are listed below:

Mol	Chain	Res	Type
33	2b	135	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	2j	69	ASN
34	2c	108	ASN
37	2f	32	ASN
46	2o	13	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	419 (14%)	28 (0%)
1	2A	2858/2915 (98%)	476 (16%)	30 (1%)
2	1B	119/121 (98%)	11 (9%)	0
2	2B	119/121 (98%)	19 (15%)	0
32	1a	1497/1521 (98%)	255 (17%)	0
32	2a	1501/1521 (98%)	272 (18%)	0
54	1w	1/4 (25%)	0	0
54	2w	1/4 (25%)	0	0
55	1x	1/4 (25%)	0	0
55	2x	1/4 (25%)	0	0
All	All	8963/9130 (98%)	1452 (16%)	58 (0%)

5 of 1452 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	34	C
1	1A	36	G
1	1A	45	C
1	1A	61	G
1	1A	71	A

5 of 58 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	196	A
1	2A	2439	A
1	2A	856	C
1	2A	2406	U
1	2A	1992	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	2MA	1A	2503	1,57	22,25,26	1.46	5 (22%)	32,37,40	2.26	8 (25%)
1	PSU	1A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	2.04	4 (19%)
32	4OC	2a	1402	32	20,23,24	0.76	0	25,32,35	0.97	1 (4%)
56	FME	2v	1	56	8,9,10	0.94	0	8,9,11	0.77	0
1	OMG	1A	2251	1,57,55	23,26,27	1.31	3 (13%)	32,38,41	1.99	5 (15%)
54	PPU	1w	76	54,1	37,40,41	2.88	22 (59%)	47,57,60	2.15	14 (29%)
32	5MC	1a	967	32	19,22,23	1.66	3 (15%)	26,32,35	1.18	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.76	0	25,32,35	0.90	1 (4%)
1	PSU	1A	2605	1	18,21,22	1.35	2 (11%)	21,30,33	2.15	4 (19%)
32	UR3	1a	1498	32	19,22,23	0.94	1 (5%)	26,32,35	1.70	2 (7%)
32	5MC	2a	1400	32	19,22,23	1.64	3 (15%)	26,32,35	1.16	3 (11%)
32	5MC	2a	1407	32	19,22,23	1.70	2 (10%)	26,32,35	1.13	3 (11%)
1	2MA	2A	2503	1,57	22,25,26	1.43	4 (18%)	32,37,40	2.41	9 (28%)
32	PSU	1a	516	57,32	18,21,22	1.39	3 (16%)	21,30,33	2.11	4 (19%)
32	5MC	1a	1400	32	19,22,23	1.69	3 (15%)	26,32,35	1.19	2 (7%)
32	G7M	2a	527	32	23,26,27	1.52	3 (13%)	34,39,42	1.69	4 (11%)
32	5MC	1a	1404	32	19,22,23	1.51	3 (15%)	26,32,35	1.13	3 (11%)
32	M2G	1a	966	32	24,27,28	1.32	3 (12%)	33,40,43	1.89	5 (15%)
1	PSU	2A	1911	1	18,21,22	1.40	3 (16%)	21,30,33	2.04	3 (14%)
32	MA6	2a	1518	32	23,26,27	0.38	0	33,38,41	2.01	9 (27%)
55	8AN	1x	76	57,55,56	21,24,25	1.32	3 (14%)	26,35,38	2.38	10 (38%)
1	5MC	2A	1942	1	19,22,23	1.74	3 (15%)	26,32,35	1.27	2 (7%)
32	M2G	2a	966	32	24,27,28	1.36	3 (12%)	33,40,43	1.85	5 (15%)
1	OMG	2A	2251	1,57,55	23,26,27	1.28	3 (13%)	32,38,41	1.96	6 (18%)
54	PPU	2w	76	54,1	37,40,41	2.43	17 (45%)	47,57,60	2.21	14 (29%)
56	FME	1v	1	56	8,9,10	1.02	0	8,9,11	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	2a	967	32	19,22,23	1.83	3 (15%)	26,32,35	1.11	2 (7%)
32	MA6	1a	1519	32	23,26,27	0.43	0	33,38,41	1.99	8 (24%)
32	5MC	1a	1407	32	19,22,23	1.57	2 (10%)	26,32,35	1.17	3 (11%)
1	5MC	2A	1962	1	19,22,23	1.61	3 (15%)	26,32,35	1.10	2 (7%)
1	OMC	2A	1920	1	19,22,23	0.81	0	25,31,34	1.03	1 (4%)
1	5MU	1A	1915	1,57	19,22,23	1.45	4 (21%)	27,32,35	2.38	10 (37%)
43	0TD	1l	92	43	8,9,10	4.77	1 (12%)	6,11,13	5.36	3 (50%)
32	5MC	2a	1404	32	19,22,23	1.84	2 (10%)	26,32,35	1.19	3 (11%)
32	UR3	2a	1498	32	19,22,23	0.96	1 (5%)	26,32,35	1.66	3 (11%)
1	2MU	2A	2552	1,57	19,22,24	1.28	3 (15%)	25,31,36	1.83	5 (20%)
1	5MC	1A	1942	1	19,22,23	1.56	3 (15%)	26,32,35	1.22	3 (11%)
32	MA6	1a	1518	32	23,26,27	0.41	0	33,38,41	1.96	10 (30%)
1	5MU	2A	1939	1,57	19,22,23	1.46	5 (26%)	27,32,35	2.15	8 (29%)
32	MA6	2a	1519	32	23,26,27	0.41	0	33,38,41	2.11	9 (27%)
1	PSU	1A	1917	1	18,21,22	1.36	2 (11%)	21,30,33	2.03	3 (14%)
1	5MC	1A	1962	1,57	19,22,23	1.71	3 (15%)	26,32,35	1.13	3 (11%)
43	0TD	2l	92	43	8,9,10	4.49	1 (12%)	6,11,13	1.75	2 (33%)
1	5MU	2A	1915	1	19,22,23	1.47	4 (21%)	27,32,35	2.11	8 (29%)
32	2MG	2a	1207	32	23,26,27	1.24	4 (17%)	33,38,41	2.11	8 (24%)
1	PSU	2A	1917	1	18,21,22	1.39	2 (11%)	21,30,33	2.02	3 (14%)
32	PSU	2a	516	57,32	18,21,22	1.38	3 (16%)	21,30,33	2.04	5 (23%)
32	G7M	1a	527	57,32	23,26,27	1.58	3 (13%)	34,39,42	1.69	4 (11%)
1	2MU	1A	2552	1,57	19,22,24	1.30	4 (21%)	25,31,36	2.11	6 (24%)
32	2MG	1a	1207	57,32	23,26,27	1.23	4 (17%)	33,38,41	2.33	10 (30%)
1	PSU	2A	2605	1	18,21,22	1.35	3 (16%)	21,30,33	1.97	4 (19%)
1	5MU	1A	1939	1,57	19,22,23	1.39	4 (21%)	27,32,35	2.10	6 (22%)
55	8AN	2x	76	57,55,56	21,24,25	1.38	3 (14%)	26,35,38	2.34	11 (42%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	1.14	3 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MA	1A	2503	1,57	-	1/7/25/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
56	FME	2v	1	56	-	1/7/9/11	-
1	OMG	1A	2251	1,57,55	-	0/9/27/28	0/3/3/3
54	PPU	1w	76	54,1	-	2/25/43/44	0/4/4/4
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	4/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,57	-	1/7/25/26	0/3/3/3
32	PSU	1a	516	57,32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32	-	3/7/25/26	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	1/11/29/30	0/3/3/3
55	8AN	1x	76	57,55,56	-	1/7/25/26	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	OMG	2A	2251	1,57,55	-	0/9/27/28	0/3/3/3
54	PPU	2w	76	54,1	-	2/25/43/44	0/4/4/4
56	FME	1v	1	56	-	5/7/9/11	-
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1	-	2/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
1	5MU	1A	1915	1,57	-	2/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1,57	-	0/9/27/28	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	5MU	2A	1939	1,57	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1A	1962	1,57	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	57,32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	57,32	-	0/7/25/26	0/3/3/3
1	2MU	1A	2552	1,57	-	0/9/27/28	0/2/2/2
32	2MG	1a	1207	57,32	-	0/9/27/28	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,57	-	0/7/25/26	0/2/2/2
55	8AN	2x	76	57,55,56	-	3/7/25/26	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2

The worst 5 of 161 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-13.04	1.69	1.82
43	2l	92	0TD	CB-SB	-12.36	1.69	1.82
32	2a	1404	5MC	C5-C4	6.93	1.49	1.44
32	2a	967	5MC	C5-C4	6.77	1.49	1.44
1	2A	1942	5MC	C5-C4	6.28	1.48	1.44

The worst 5 of 269 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-12.44	80.00	102.36
1	2A	2503	2MA	C5-C4-N3	-8.60	118.12	127.18
1	1A	2503	2MA	C5-C4-N3	-7.85	118.91	127.18
32	1a	1207	2MG	C2-N3-C4	7.25	121.06	112.00
32	1a	1498	UR3	C4-N3-C2	-6.89	119.04	124.58

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
32	2a	1519	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

29 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1402	4OC	1	0
56	2v	1	FME	2	0
1	1A	2251	OMG	1	0
54	1w	76	PPU	1	0
32	1a	967	5MC	1	0
32	1a	1402	4OC	1	0
32	2a	1400	5MC	2	0
1	2A	2503	2MA	1	0
32	1a	1400	5MC	2	0
32	2a	1518	MA6	2	0
1	2A	2251	OMG	1	0
54	2w	76	PPU	4	0
56	1v	1	FME	1	0
32	2a	967	5MC	1	0
32	1a	1519	MA6	2	0
1	2A	1962	5MC	1	0
1	2A	1920	OMC	1	0
32	2a	1404	5MC	1	0
1	2A	2552	2MU	2	0
1	1A	1942	5MC	1	0
32	1a	1518	MA6	4	0
1	2A	1939	5MU	1	0
32	2a	1519	MA6	3	0
43	2l	92	0TD	4	0
32	2a	1207	2MG	1	0
1	2A	1917	PSU	1	0
1	1A	1939	5MU	1	0
55	2x	76	8AN	2	0
1	1A	1920	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2513 ligands modelled in this entry, 2502 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	MPD	2A	3737	-	7,7,7	0.34	0	9,10,10	0.24	0
58	ARG	1A	4030	-	10,11,11	0.70	0	9,13,13	0.98	1 (11%)
59	MPD	2A	3736	-	7,7,7	0.34	0	9,10,10	0.27	0
59	MPD	1a	1874	-	7,7,7	0.41	0	9,10,10	0.38	0
59	MPD	1a	1873	-	7,7,7	0.30	0	9,10,10	0.36	0
61	SF4	2d	501	35	0,12,12	-	-	-	-	-
59	MPD	18	103	-	7,7,7	0.36	0	9,10,10	0.76	0
58	ARG	1B	230	57	10,11,11	0.81	1 (10%)	9,13,13	1.20	1 (11%)
61	SF4	1d	306	35	0,12,12	-	-	-	-	-
59	MPD	2A	3735	-	7,7,7	0.33	0	9,10,10	0.33	0
59	MPD	1A	4031	-	7,7,7	0.36	0	9,10,10	0.18	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
59	MPD	2A	3737	-	-	2/5/5/5	-
58	ARG	1A	4030	-	-	1/11/11/11	-
59	MPD	2A	3736	-	-	0/5/5/5	-
59	MPD	1a	1874	-	-	1/5/5/5	-
59	MPD	1a	1873	-	-	1/5/5/5	-
61	SF4	2d	501	35	-	-	0/6/5/5
59	MPD	18	103	-	-	3/5/5/5	-
58	ARG	1B	230	57	-	3/11/11/11	-
61	SF4	1d	306	35	-	-	0/6/5/5
59	MPD	2A	3735	-	-	1/5/5/5	-
59	MPD	1A	4031	-	-	2/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1B	230	ARG	OXT-C	-2.38	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1B	230	ARG	OXT-C-O	-3.48	116.18	124.08
58	1A	4030	ARG	OXT-C-O	-2.80	117.72	124.08

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	18	103	MPD	C2-C3-C4-C5
58	1B	230	ARG	NE-CD-CG-CB
58	1A	4030	ARG	C-CA-CB-CG
59	18	103	MPD	CM-C2-C3-C4
59	2A	3737	MPD	C1-C2-C3-C4

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	1A	4030	ARG	4	0
59	1a	1874	MPD	2	0
59	1a	1873	MPD	2	0
61	2d	501	SF4	2	0
59	2A	3735	MPD	1	0
59	1A	4031	MPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2861/2915 (98%)	-0.49	125 (4%) 39 33	17, 35, 88, 103	0
1	2A	2856/2915 (97%)	0.05	152 (5%) 32 26	31, 56, 91, 102	0
2	1B	120/121 (99%)	-0.29	1 (0%) 82 80	28, 49, 63, 77	0
2	2B	120/121 (99%)	1.18	19 (15%) 5 4	58, 78, 87, 92	0
3	1D	275/276 (99%)	-0.24	2 (0%) 84 82	21, 35, 49, 69	0
3	2D	275/276 (99%)	0.20	3 (1%) 78 74	32, 49, 61, 78	0
4	1E	204/206 (99%)	-0.16	0 100 100	20, 41, 58, 75	0
4	2E	204/206 (99%)	0.24	3 (1%) 72 68	32, 56, 68, 77	0
5	1F	203/210 (96%)	-0.16	1 (0%) 87 85	19, 41, 66, 77	0
5	2F	203/210 (96%)	0.53	5 (2%) 58 52	35, 63, 75, 82	0
6	1G	181/182 (99%)	0.57	6 (3%) 49 43	45, 61, 73, 85	0
6	2G	181/182 (99%)	1.54	42 (23%) 2 1	68, 78, 83, 89	0
7	1H	174/180 (96%)	0.10	3 (1%) 69 64	38, 52, 63, 71	0
7	2H	173/180 (96%)	1.12	21 (12%) 8 6	65, 76, 81, 86	0
8	1I	147/148 (99%)	0.66	5 (3%) 48 42	41, 68, 78, 84	0
8	2I	146/148 (98%)	1.06	10 (6%) 23 19	51, 71, 79, 84	0
9	1N	140/140 (100%)	-0.30	0 100 100	25, 38, 57, 70	0
9	2N	140/140 (100%)	0.47	2 (1%) 73 69	44, 62, 73, 76	0
10	1O	122/122 (100%)	-0.14	0 100 100	29, 41, 60, 65	0
10	2O	122/122 (100%)	0.17	1 (0%) 82 80	40, 53, 65, 77	0
11	1P	149/150 (99%)	0.03	0 100 100	20, 45, 66, 77	0
11	2P	149/150 (99%)	0.52	1 (0%) 84 82	38, 62, 77, 86	0
12	1Q	141/141 (100%)	-0.22	0 100 100	25, 38, 51, 60	0
12	2Q	141/141 (100%)	0.84	7 (4%) 34 28	42, 62, 70, 76	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.28	0 100 100	26, 35, 48, 56	0
13	2R	118/118 (100%)	0.13	0 100 100	39, 51, 60, 68	0
14	1S	110/112 (98%)	0.26	0 100 100	38, 49, 61, 64	0
14	2S	110/112 (98%)	1.34	20 (18%) 3 3	63, 72, 77, 78	0
15	1T	131/146 (89%)	-0.01	4 (3%) 51 45	33, 44, 64, 78	0
15	2T	131/146 (89%)	0.32	0 100 100	48, 56, 74, 77	0
16	1U	116/118 (98%)	-0.41	0 100 100	21, 30, 46, 58	0
16	2U	116/118 (98%)	0.36	0 100 100	38, 58, 70, 79	0
17	1V	101/101 (100%)	-0.21	0 100 100	21, 40, 54, 65	0
17	2V	101/101 (100%)	0.63	2 (1%) 65 60	44, 67, 74, 78	0
18	1W	112/113 (99%)	-0.30	0 100 100	23, 31, 50, 78	0
18	2W	112/113 (99%)	0.14	2 (1%) 67 63	38, 49, 65, 81	0
19	1X	95/96 (98%)	-0.14	2 (2%) 63 58	27, 36, 60, 74	0
19	2X	95/96 (98%)	0.74	3 (3%) 50 44	51, 60, 72, 79	0
20	1Y	107/110 (97%)	0.16	1 (0%) 81 78	32, 48, 67, 75	0
20	2Y	107/110 (97%)	0.94	2 (1%) 66 61	56, 68, 76, 81	0
21	1Z	203/206 (98%)	0.29	2 (0%) 79 76	39, 55, 69, 77	0
21	2Z	201/206 (97%)	1.13	12 (5%) 27 22	64, 73, 80, 84	0
22	10	83/85 (97%)	-0.17	0 100 100	23, 37, 50, 56	0
22	20	83/85 (97%)	0.74	3 (3%) 46 40	48, 62, 70, 75	0
23	11	97/98 (98%)	0.08	2 (2%) 63 58	28, 41, 65, 70	0
23	21	97/98 (98%)	0.22	1 (1%) 79 76	36, 54, 70, 76	0
24	12	70/72 (97%)	0.14	2 (2%) 53 48	35, 50, 60, 70	0
24	22	70/72 (97%)	0.81	3 (4%) 40 34	57, 68, 74, 79	0
25	13	59/60 (98%)	-0.23	0 100 100	27, 36, 60, 66	0
25	23	59/60 (98%)	0.59	3 (5%) 33 28	51, 60, 73, 81	0
26	14	69/71 (97%)	0.96	10 (14%) 6 4	51, 75, 84, 87	0
26	24	69/71 (97%)	1.59	18 (26%) 1 1	75, 83, 90, 92	0
27	15	59/60 (98%)	-0.34	1 (1%) 69 64	20, 31, 47, 61	0
27	25	59/60 (98%)	0.05	0 100 100	37, 49, 63, 70	0
28	16	53/54 (98%)	-0.30	0 100 100	34, 42, 54, 60	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.23	0 100 100	52, 59, 65, 71	0
29	17	48/49 (97%)	-0.33	0 100 100	20, 28, 54, 64	0
29	27	48/49 (97%)	0.06	3 (6%) 26 20	33, 43, 58, 70	0
30	18	64/65 (98%)	-0.34	0 100 100	25, 34, 41, 55	0
30	28	64/65 (98%)	0.45	0 100 100	42, 54, 59, 67	0
31	19	37/37 (100%)	-0.07	0 100 100	28, 39, 54, 57	0
31	29	37/37 (100%)	0.93	1 (2%) 56 50	54, 63, 73, 75	0
32	1a	1488/1521 (97%)	0.38	36 (2%) 59 54	35, 67, 88, 100	0
32	2a	1492/1521 (98%)	0.62	101 (6%) 23 19	42, 72, 90, 102	0
33	1b	231/256 (90%)	1.16	36 (15%) 5 4	65, 74, 83, 88	0
33	2b	231/256 (90%)	1.40	48 (20%) 2 2	68, 78, 85, 92	0
34	1c	206/239 (86%)	1.00	14 (6%) 23 19	60, 72, 80, 83	0
34	2c	206/239 (86%)	1.38	39 (18%) 3 2	69, 79, 84, 87	0
35	1d	208/209 (99%)	0.76	12 (5%) 29 23	56, 69, 78, 82	0
35	2d	208/209 (99%)	0.78	4 (1%) 66 61	57, 67, 75, 83	0
36	1e	148/162 (91%)	0.58	3 (2%) 65 60	46, 63, 73, 85	0
36	2e	148/162 (91%)	0.79	4 (2%) 56 50	59, 68, 76, 85	0
37	1f	100/101 (99%)	0.57	3 (3%) 52 47	49, 63, 72, 76	0
37	2f	100/101 (99%)	0.45	1 (1%) 79 76	55, 65, 75, 79	0
38	1g	155/156 (99%)	0.71	10 (6%) 25 19	59, 68, 76, 82	0
38	2g	155/156 (99%)	1.12	21 (13%) 7 5	67, 76, 82, 87	0
39	1h	137/138 (99%)	0.74	5 (3%) 46 40	55, 65, 72, 77	0
39	2h	137/138 (99%)	1.00	10 (7%) 21 17	60, 69, 75, 77	0
40	1i	127/128 (99%)	1.29	24 (18%) 3 2	57, 75, 81, 83	0
40	2i	126/128 (98%)	1.99	53 (42%) 0 0	69, 81, 86, 91	0
41	1j	97/105 (92%)	1.32	13 (13%) 7 5	61, 75, 83, 87	0
41	2j	96/105 (91%)	2.05	43 (44%) 0 0	73, 81, 86, 89	0
42	1k	114/129 (88%)	0.56	3 (2%) 57 51	40, 61, 72, 75	0
42	2k	114/129 (88%)	0.72	6 (5%) 32 26	57, 69, 77, 79	0
43	1l	121/132 (91%)	0.40	2 (1%) 69 64	48, 59, 67, 73	0
43	2l	121/132 (91%)	0.59	3 (2%) 58 52	54, 63, 69, 74	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	0.96	8 (6%) 23 18	60, 70, 76, 79	0
44	2m	114/126 (90%)	1.55	27 (23%) 2 1	73, 79, 83, 86	0
45	1n	60/61 (98%)	1.07	5 (8%) 17 13	61, 69, 75, 76	0
45	2n	60/61 (98%)	2.12	33 (55%) 0 0	70, 79, 83, 85	0
46	1o	88/89 (98%)	0.77	6 (6%) 23 19	45, 63, 75, 82	0
46	2o	88/89 (98%)	0.84	5 (5%) 29 24	54, 67, 75, 81	0
47	1p	82/88 (93%)	1.24	11 (13%) 7 5	60, 70, 78, 83	0
47	2p	82/88 (93%)	0.93	6 (7%) 21 17	59, 66, 76, 81	0
48	1q	99/105 (94%)	0.94	5 (5%) 33 28	53, 65, 73, 77	0
48	2q	99/105 (94%)	0.67	3 (3%) 52 47	55, 66, 74, 75	0
49	1r	68/88 (77%)	0.59	1 (1%) 72 68	52, 61, 73, 81	0
49	2r	68/88 (77%)	0.71	1 (1%) 72 68	58, 68, 75, 80	0
50	1s	83/93 (89%)	0.95	4 (4%) 35 30	60, 72, 80, 84	0
50	2s	83/93 (89%)	1.65	24 (28%) 1 1	71, 81, 85, 88	0
51	1t	96/106 (90%)	1.05	11 (11%) 9 7	62, 70, 78, 81	0
51	2t	98/106 (92%)	0.78	8 (8%) 17 14	54, 66, 75, 79	0
52	1u	23/27 (85%)	1.18	5 (21%) 2 2	66, 70, 74, 77	0
52	2u	23/27 (85%)	2.00	10 (43%) 0 0	73, 78, 82, 86	0
53	1y	97/113 (85%)	0.69	7 (7%) 21 17	49, 60, 71, 75	0
53	2y	96/113 (84%)	1.61	26 (27%) 1 1	66, 75, 80, 86	0
54	1w	3/4 (75%)	-0.40	0 100 100	30, 30, 35, 47	0
54	2w	3/4 (75%)	-0.75	0 100 100	44, 44, 45, 52	0
55	1x	3/4 (75%)	-0.50	0 100 100	23, 23, 25, 35	0
55	2x	3/4 (75%)	0.22	1 (33%) 1 1	35, 35, 43, 47	0
56	1v	2/3 (66%)	-0.03	0 100 100	27, 27, 27, 30	0
56	2v	2/3 (66%)	0.02	0 100 100	44, 44, 44, 47	0
All	All	20794/21490 (96%)	0.36	1207 (5%) 29 23	17, 61, 84, 103	0

The worst 5 of 1207 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1087	G	8.4
53	1y	98	ALA	6.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1076	C	6.4
45	2n	2	ALA	6.4
1	1A	1071	G	5.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	5MU	2A	1915	21/22	0.83	0.11	77,82,87,96	0
32	M2G	2a	966	25/26	0.86	0.16	61,70,84,98	0
1	PSU	2A	1917	20/21	0.88	0.09	73,79,99,100	0
1	5MU	1A	1915	21/22	0.88	0.12	67,73,81,92	0
32	5MC	2a	967	21/22	0.88	0.15	55,73,79,83	0
32	2MG	2a	1207	24/25	0.89	0.11	77,84,88,94	0
1	PSU	2A	1911	20/21	0.90	0.10	64,73,77,77	0
1	PSU	1A	1917	20/21	0.90	0.10	56,68,75,79	0
32	2MG	1a	1207	24/25	0.90	0.12	67,75,79,80	0
32	PSU	2a	516	20/21	0.91	0.11	68,75,81,84	0
43	0TD	1l	92	10/11	0.91	0.13	62,64,67,72	0
32	G7M	2a	527	24/25	0.92	0.11	57,68,73,78	0
32	4OC	2a	1402	22/23	0.93	0.12	61,65,72,75	0
32	5MC	2a	1404	21/22	0.93	0.11	55,61,63,67	0
1	OMC	2A	1920	21/22	0.93	0.11	59,67,72,73	0
43	0TD	1l	92	10/11	0.94	0.10	44,56,60,71	0
1	5MC	2A	1942	21/22	0.94	0.12	43,56,62,69	0
32	PSU	1a	516	20/21	0.94	0.10	61,66,71,75	0
32	5MC	1a	967	21/22	0.94	0.11	60,63,71,76	0
1	PSU	1A	1911	20/21	0.94	0.09	53,66,68,68	0
56	FME	1v	1	10/11	0.94	0.15	22,37,47,68	0
32	5MC	2a	1400	21/22	0.95	0.11	62,69,72,75	0
32	MA6	1a	1519	24/25	0.95	0.10	38,47,52,53	0
32	M2G	1a	966	25/26	0.95	0.10	52,59,70,78	0
32	UR3	2a	1498	21/22	0.95	0.10	58,62,69,71	0
32	MA6	2a	1518	24/25	0.95	0.12	57,63,70,70	0
32	5MC	1a	1407	21/22	0.95	0.09	47,53,57,62	0
32	UR3	1a	1498	21/22	0.95	0.11	47,51,57,63	0
56	FME	2v	1	10/11	0.95	0.13	47,57,60,77	0
32	5MC	2a	1407	21/22	0.96	0.09	50,62,68,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	G7M	1a	527	24/25	0.96	0.09	45,55,58,65	0
1	2MA	2A	2503	23/24	0.96	0.08	31,36,39,39	0
32	MA6	2a	1519	24/25	0.96	0.12	59,63,70,74	0
1	OMC	1A	1920	21/22	0.96	0.09	47,55,59,60	0
55	8AN	2x	76	22/23	0.96	0.08	34,39,42,45	0
32	5MC	1a	1400	21/22	0.96	0.10	53,58,64,65	0
32	5MC	1a	1404	21/22	0.96	0.08	44,49,52,56	0
32	4OC	1a	1402	22/23	0.97	0.08	48,53,55,60	0
1	OMG	2A	2251	24/25	0.97	0.09	30,37,44,45	0
1	5MC	1A	1942	21/22	0.97	0.07	28,34,41,42	0
1	2MU	2A	2552	21/23	0.97	0.07	32,38,42,47	0
54	PPU	1w	76	37/38	0.97	0.07	18,23,27,31	0
54	PPU	2w	76	37/38	0.97	0.09	29,38,42,49	0
1	PSU	2A	2605	20/21	0.97	0.09	30,39,44,50	0
32	MA6	1a	1518	24/25	0.97	0.09	41,46,48,53	0
1	5MU	2A	1939	21/22	0.97	0.09	36,41,47,48	0
1	OMG	1A	2251	24/25	0.98	0.06	19,21,24,25	0
1	2MA	1A	2503	23/24	0.98	0.07	18,22,26,28	0
1	2MU	1A	2552	21/23	0.98	0.07	21,31,34,35	0
1	PSU	1A	2605	20/21	0.98	0.08	21,29,32,35	0
1	5MU	1A	1939	21/22	0.98	0.06	22,27,29,30	0
1	5MC	2A	1962	21/22	0.98	0.08	37,44,49,56	0
1	5MC	1A	1962	21/22	0.98	0.07	30,34,39,44	0
55	8AN	1x	76	22/23	0.99	0.05	18,21,26,27	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3703	1/1	0.37	0.22	67,67,67,67	0
57	MG	2A	3483	1/1	0.57	0.30	76,76,76,76	0
57	MG	1A	3468	1/1	0.59	0.29	70,70,70,70	0
57	MG	2a	3048	1/1	0.60	0.28	89,89,89,89	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	4004	1/1	0.61	0.27	66,66,66,66	0
57	MG	2n	101	1/1	0.62	0.34	76,76,76,76	0
57	MG	2A	3533	1/1	0.65	0.21	65,65,65,65	0
57	MG	1A	3729	1/1	0.66	0.14	64,64,64,64	0
57	MG	1a	1753	1/1	0.66	0.34	71,71,71,71	0
57	MG	1A	3995	1/1	0.66	0.17	76,76,76,76	0
57	MG	1a	1863	1/1	0.67	0.31	71,71,71,71	0
57	MG	2A	3719	1/1	0.67	0.19	71,71,71,71	0
57	MG	2A	3449	1/1	0.69	0.20	89,89,89,89	0
57	MG	1A	3650	1/1	0.69	0.24	57,57,57,57	0
57	MG	1a	1794	1/1	0.70	0.32	77,77,77,77	0
57	MG	2A	3536	1/1	0.70	0.19	71,71,71,71	0
57	MG	1A	3765	1/1	0.70	0.26	55,55,55,55	0
57	MG	2A	3724	1/1	0.70	0.19	77,77,77,77	0
57	MG	2a	3022	1/1	0.70	0.35	71,71,71,71	0
57	MG	2A	3504	1/1	0.70	0.15	72,72,72,72	0
57	MG	2a	3114	1/1	0.70	0.26	64,64,64,64	0
57	MG	2A	3516	1/1	0.70	0.22	74,74,74,74	0
57	MG	1A	3710	1/1	0.71	0.17	75,75,75,75	0
57	MG	1a	1696	1/1	0.71	0.20	79,79,79,79	0
57	MG	2A	3297	1/1	0.71	0.14	78,78,78,78	0
57	MG	1A	3736	1/1	0.71	0.18	42,42,42,42	0
57	MG	1a	1785	1/1	0.71	0.14	84,84,84,84	0
57	MG	1a	1866	1/1	0.72	0.15	69,69,69,69	0
57	MG	1A	4024	1/1	0.72	0.25	69,69,69,69	0
57	MG	2A	3532	1/1	0.72	0.16	61,61,61,61	0
57	MG	1A	3806	1/1	0.72	0.12	78,78,78,78	0
57	MG	1A	3853	1/1	0.72	0.16	72,72,72,72	0
57	MG	2A	3661	1/1	0.72	0.27	73,73,73,73	0
57	MG	1a	1827	1/1	0.73	0.15	75,75,75,75	0
57	MG	2B	207	1/1	0.73	0.27	83,83,83,83	0
57	MG	1a	1871	1/1	0.73	0.43	88,88,88,88	0
57	MG	2A	3491	1/1	0.73	0.21	72,72,72,72	0
57	MG	1A	3816	1/1	0.73	0.19	72,72,72,72	0
57	MG	2a	3121	1/1	0.73	0.26	72,72,72,72	0
57	MG	2A	3389	1/1	0.73	0.16	74,74,74,74	0
57	MG	1a	1666	1/1	0.74	0.18	75,75,75,75	0
57	MG	1a	1782	1/1	0.74	0.22	74,74,74,74	0
57	MG	2A	3085	1/1	0.74	0.24	77,77,77,77	0
57	MG	2A	3291	1/1	0.74	0.55	74,74,74,74	0
57	MG	2A	3484	1/1	0.74	0.26	71,71,71,71	0
57	MG	2p	101	1/1	0.74	0.36	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3470	1/1	0.75	0.20	64,64,64,64	0
57	MG	2a	3057	1/1	0.75	0.29	74,74,74,74	0
57	MG	1A	3339	1/1	0.75	0.16	69,69,69,69	0
57	MG	2A	3279	1/1	0.75	0.33	73,73,73,73	0
57	MG	2A	3538	1/1	0.75	0.17	82,82,82,82	0
57	MG	2A	3575	1/1	0.75	0.28	70,70,70,70	0
57	MG	1a	1868	1/1	0.76	0.30	80,80,80,80	0
57	MG	1A	4008	1/1	0.76	0.13	45,45,45,45	0
57	MG	1d	301	1/1	0.76	0.18	79,79,79,79	0
57	MG	2A	3355	1/1	0.76	0.16	76,76,76,76	0
57	MG	2a	3066	1/1	0.76	0.25	72,72,72,72	0
57	MG	1a	1836	1/1	0.76	0.17	78,78,78,78	0
57	MG	2A	3238	1/1	0.76	0.21	68,68,68,68	0
57	MG	2A	3468	1/1	0.76	0.20	72,72,72,72	0
57	MG	2A	3728	1/1	0.76	0.19	78,78,78,78	0
57	MG	1a	1754	1/1	0.77	0.11	56,56,56,56	0
57	MG	1a	1736	1/1	0.77	0.15	81,81,81,81	0
57	MG	2a	3076	1/1	0.77	0.15	74,74,74,74	0
57	MG	1A	3460	1/1	0.77	0.28	65,65,65,65	0
57	MG	2A	3157	1/1	0.77	0.19	66,66,66,66	0
57	MG	2A	3621	1/1	0.77	0.12	80,80,80,80	0
57	MG	2A	3229	1/1	0.77	0.27	61,61,61,61	0
57	MG	2A	3269	1/1	0.78	0.19	63,63,63,63	0
57	MG	2A	3275	1/1	0.78	0.17	59,59,59,59	0
57	MG	1a	1813	1/1	0.78	0.32	76,76,76,76	0
57	MG	2B	214	1/1	0.78	0.15	79,79,79,79	0
57	MG	1A	3606	1/1	0.78	0.13	36,36,36,36	0
57	MG	1d	302	1/1	0.78	0.18	76,76,76,76	0
57	MG	2A	3325	1/1	0.78	0.26	60,60,60,60	0
57	MG	1A	3929	1/1	0.78	0.15	53,53,53,53	0
57	MG	2A	3106	1/1	0.78	0.17	65,65,65,65	0
57	MG	2A	3118	1/1	0.78	0.36	66,66,66,66	0
57	MG	1B	206	1/1	0.78	0.33	63,63,63,63	0
57	MG	1a	1787	1/1	0.78	0.20	83,83,83,83	0
57	MG	1V	205	1/1	0.78	0.14	63,63,63,63	0
57	MG	1a	1810	1/1	0.79	0.17	79,79,79,79	0
57	MG	2A	3509	1/1	0.79	0.17	64,64,64,64	0
57	MG	1A	3992	1/1	0.79	0.18	59,59,59,59	0
57	MG	2P	201	1/1	0.79	0.25	61,61,61,61	0
57	MG	2a	3002	1/1	0.79	0.31	65,65,65,65	0
57	MG	1A	3342	1/1	0.79	0.12	58,58,58,58	0
57	MG	1a	1763	1/1	0.79	0.20	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3391	1/1	0.79	0.19	60,60,60,60	0
57	MG	1a	1772	1/1	0.79	0.14	65,65,65,65	0
57	MG	1A	3322	1/1	0.79	0.21	64,64,64,64	0
57	MG	2a	3086	1/1	0.79	0.29	72,72,72,72	0
57	MG	2a	3094	1/1	0.79	0.39	64,64,64,64	0
57	MG	1a	1698	1/1	0.79	0.27	74,74,74,74	0
57	MG	1a	1702	1/1	0.79	0.14	68,68,68,68	0
57	MG	2a	3144	1/1	0.79	0.16	66,66,66,66	0
57	MG	1B	211	1/1	0.79	0.23	63,63,63,63	0
57	MG	1a	1809	1/1	0.79	0.23	69,69,69,69	0
57	MG	1a	1662	1/1	0.80	0.15	74,74,74,74	0
57	MG	2A	3090	1/1	0.80	0.42	79,79,79,79	0
57	MG	1A	3528	1/1	0.80	0.21	75,75,75,75	0
57	MG	2A	3288	1/1	0.80	0.33	67,67,67,67	0
57	MG	1A	3399	1/1	0.80	0.19	66,66,66,66	0
57	MG	2A	3146	1/1	0.80	0.34	60,60,60,60	0
57	MG	1B	220	1/1	0.80	0.12	30,30,30,30	0
57	MG	2A	3328	1/1	0.80	0.28	71,71,71,71	0
57	MG	2A	3731	1/1	0.80	0.19	65,65,65,65	0
57	MG	2A	3214	1/1	0.80	0.24	60,60,60,60	0
57	MG	1A	3803	1/1	0.80	0.21	63,63,63,63	0
57	MG	2a	3166	1/1	0.80	0.23	72,72,72,72	0
57	MG	2I	201	1/1	0.80	0.15	76,76,76,76	0
57	MG	2A	3070	1/1	0.80	0.34	76,76,76,76	0
57	MG	1a	1803	1/1	0.81	0.29	74,74,74,74	0
57	MG	2A	3040	1/1	0.81	0.24	68,68,68,68	0
57	MG	2B	212	1/1	0.81	0.14	81,81,81,81	0
57	MG	1a	1673	1/1	0.81	0.22	68,68,68,68	0
57	MG	2A	3512	1/1	0.81	0.18	70,70,70,70	0
57	MG	1A	3720	1/1	0.81	0.21	52,52,52,52	0
57	MG	2T	203	1/1	0.81	0.17	71,71,71,71	0
57	MG	2A	3526	1/1	0.81	0.18	48,48,48,48	0
57	MG	1A	3689	1/1	0.81	0.17	61,61,61,61	0
57	MG	1a	1824	1/1	0.81	0.26	72,72,72,72	0
57	MG	1A	3435	1/1	0.81	0.19	60,60,60,60	0
57	MG	2a	3059	1/1	0.81	0.34	81,81,81,81	0
57	MG	2a	3062	1/1	0.81	0.24	65,65,65,65	0
57	MG	1a	1828	1/1	0.81	0.26	74,74,74,74	0
57	MG	1a	1703	1/1	0.81	0.28	70,70,70,70	0
57	MG	1a	1784	1/1	0.81	0.17	69,69,69,69	0
57	MG	2A	3659	1/1	0.81	0.11	54,54,54,54	0
57	MG	1a	1718	1/1	0.81	0.14	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3689	1/1	0.81	0.15	71,71,71,71	0
57	MG	2A	3712	1/1	0.81	0.28	75,75,75,75	0
57	MG	1A	3200	1/1	0.81	0.12	64,64,64,64	0
57	MG	1a	1793	1/1	0.81	0.15	83,83,83,83	0
57	MG	1a	1748	1/1	0.81	0.15	79,79,79,79	0
57	MG	2A	3366	1/1	0.82	0.12	48,48,48,48	0
57	MG	2A	3694	1/1	0.82	0.17	61,61,61,61	0
57	MG	2A	3709	1/1	0.82	0.23	63,63,63,63	0
57	MG	1A	3698	1/1	0.82	0.16	59,59,59,59	0
57	MG	2A	3716	1/1	0.82	0.17	74,74,74,74	0
57	MG	1a	1636	1/1	0.82	0.24	68,68,68,68	0
57	MG	1a	1849	1/1	0.82	0.13	66,66,66,66	0
57	MG	2A	3464	1/1	0.82	0.22	63,63,63,63	0
57	MG	1a	1722	1/1	0.82	0.20	68,68,68,68	0
57	MG	1A	3389	1/1	0.82	0.13	50,50,50,50	0
57	MG	1A	3757	1/1	0.82	0.13	63,63,63,63	0
57	MG	2A	3223	1/1	0.82	0.27	60,60,60,60	0
57	MG	1A	3863	1/1	0.82	0.13	27,27,27,27	0
57	MG	2A	3230	1/1	0.82	0.23	65,65,65,65	0
57	MG	1a	1676	1/1	0.82	0.26	66,66,66,66	0
57	MG	1A	3892	1/1	0.82	0.28	62,62,62,62	0
57	MG	1n	103	1/1	0.82	0.25	70,70,70,70	0
57	MG	2A	3021	1/1	0.82	0.17	71,71,71,71	0
57	MG	1A	3192	1/1	0.82	0.24	56,56,56,56	0
57	MG	2A	3041	1/1	0.82	0.17	55,55,55,55	0
57	MG	2A	3055	1/1	0.82	0.25	58,58,58,58	0
57	MG	1a	1777	1/1	0.82	0.17	76,76,76,76	0
57	MG	2a	3071	1/1	0.82	0.37	78,78,78,78	0
57	MG	2A	3557	1/1	0.82	0.19	65,65,65,65	0
57	MG	2A	3559	1/1	0.82	0.11	74,74,74,74	0
57	MG	2A	3075	1/1	0.82	0.22	67,67,67,67	0
57	MG	2A	3613	1/1	0.82	0.19	60,60,60,60	0
57	MG	2A	3617	1/1	0.82	0.20	71,71,71,71	0
57	MG	2A	3329	1/1	0.82	0.23	75,75,75,75	0
57	MG	2A	3351	1/1	0.82	0.18	67,67,67,67	0
57	MG	2a	3180	1/1	0.82	0.25	70,70,70,70	0
57	MG	1A	3574	1/1	0.82	0.23	55,55,55,55	0
57	MG	2A	3688	1/1	0.82	0.12	66,66,66,66	0
57	MG	2A	3564	1/1	0.83	0.12	70,70,70,70	0
57	MG	1A	3454	1/1	0.83	0.13	25,25,25,25	0
57	MG	2A	3583	1/1	0.83	0.13	54,54,54,54	0
57	MG	2A	3607	1/1	0.83	0.11	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1B	227	1/1	0.83	0.13	58,58,58,58	0
57	MG	1A	3224	1/1	0.83	0.14	66,66,66,66	0
57	MG	2a	3006	1/1	0.83	0.15	55,55,55,55	0
57	MG	1a	1631	1/1	0.83	0.22	66,66,66,66	0
57	MG	2a	3024	1/1	0.83	0.35	65,65,65,65	0
57	MG	1A	3696	1/1	0.83	0.14	65,65,65,65	0
57	MG	2a	3049	1/1	0.83	0.19	68,68,68,68	0
57	MG	2a	3056	1/1	0.83	0.19	71,71,71,71	0
57	MG	1a	1650	1/1	0.83	0.20	66,66,66,66	0
57	MG	2A	3684	1/1	0.83	0.11	65,65,65,65	0
57	MG	2A	3125	1/1	0.83	0.22	62,62,62,62	0
57	MG	1A	3193	1/1	0.83	0.32	71,71,71,71	0
57	MG	1A	3515	1/1	0.83	0.12	35,35,35,35	0
57	MG	1A	3395	1/1	0.83	0.13	55,55,55,55	0
57	MG	2A	3710	1/1	0.83	0.11	75,75,75,75	0
57	MG	1a	1823	1/1	0.83	0.13	63,63,63,63	0
57	MG	2A	3226	1/1	0.83	0.16	49,49,49,49	0
57	MG	2A	3376	1/1	0.83	0.14	54,54,54,54	0
57	MG	1A	3338	1/1	0.83	0.13	60,60,60,60	0
57	MG	2a	3154	1/1	0.83	0.12	73,73,73,73	0
57	MG	1A	3188	1/1	0.83	0.26	52,52,52,52	0
57	MG	2A	3404	1/1	0.83	0.14	53,53,53,53	0
57	MG	2A	3732	1/1	0.83	0.22	69,69,69,69	0
57	MG	1A	3889	1/1	0.83	0.15	45,45,45,45	0
59	MPD	2A	3736	8/8	0.83	0.28	67,72,77,77	0
57	MG	1A	3537	1/1	0.84	0.12	47,47,47,47	0
57	MG	1a	1786	1/1	0.84	0.18	71,71,71,71	0
57	MG	2A	3730	1/1	0.84	0.19	76,76,76,76	0
57	MG	15	3108	1/1	0.84	0.12	57,57,57,57	0
57	MG	1a	1605	1/1	0.84	0.23	67,67,67,67	0
57	MG	2A	3733	1/1	0.84	0.26	68,68,68,68	0
57	MG	1a	1607	1/1	0.84	0.17	61,61,61,61	0
57	MG	1a	1801	1/1	0.84	0.15	69,69,69,69	0
57	MG	1A	3521	1/1	0.84	0.13	52,52,52,52	0
57	MG	1a	1726	1/1	0.84	0.15	54,54,54,54	0
57	MG	1a	1634	1/1	0.84	0.25	71,71,71,71	0
57	MG	2A	3321	1/1	0.84	0.24	67,67,67,67	0
57	MG	28	101	1/1	0.84	0.18	62,62,62,62	0
57	MG	1A	4022	1/1	0.84	0.21	66,66,66,66	0
57	MG	2A	3083	1/1	0.84	0.21	77,77,77,77	0
57	MG	2a	3014	1/1	0.84	0.23	71,71,71,71	0
57	MG	1a	1822	1/1	0.84	0.18	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3338	1/1	0.84	0.24	71,71,71,71	0
57	MG	1A	3576	1/1	0.84	0.14	46,46,46,46	0
57	MG	2A	3610	1/1	0.84	0.18	51,51,51,51	0
57	MG	1A	3946	1/1	0.84	0.08	79,79,79,79	0
57	MG	2A	3615	1/1	0.84	0.12	67,67,67,67	0
57	MG	1a	1758	1/1	0.84	0.16	66,66,66,66	0
57	MG	1A	3300	1/1	0.84	0.15	56,56,56,56	0
57	MG	2a	3064	1/1	0.84	0.16	75,75,75,75	0
57	MG	2A	3636	1/1	0.84	0.10	59,59,59,59	0
57	MG	2A	3135	1/1	0.84	0.20	54,54,54,54	0
57	MG	2A	3136	1/1	0.84	0.17	66,66,66,66	0
57	MG	2A	3670	1/1	0.84	0.25	61,61,61,61	0
57	MG	1A	3534	1/1	0.84	0.17	32,32,32,32	0
57	MG	2A	3426	1/1	0.84	0.27	75,75,75,75	0
57	MG	2A	3150	1/1	0.84	0.17	52,52,52,52	0
57	MG	2a	3128	1/1	0.84	0.12	62,62,62,62	0
57	MG	2A	3691	1/1	0.84	0.26	76,76,76,76	0
57	MG	1a	1775	1/1	0.84	0.20	61,61,61,61	0
57	MG	2A	3159	1/1	0.84	0.24	84,84,84,84	0
57	MG	2a	3175	1/1	0.84	0.16	55,55,55,55	0
57	MG	2A	3191	1/1	0.84	0.23	72,72,72,72	0
57	MG	1A	3997	1/1	0.84	0.18	67,67,67,67	0
57	MG	1a	1692	1/1	0.84	0.22	63,63,63,63	0
57	MG	1F	314	1/1	0.84	0.12	48,48,48,48	0
57	MG	1A	3776	1/1	0.85	0.13	48,48,48,48	0
57	MG	1a	1682	1/1	0.85	0.24	68,68,68,68	0
57	MG	2E	305	1/1	0.85	0.13	32,32,32,32	0
57	MG	1A	3778	1/1	0.85	0.15	65,65,65,65	0
57	MG	1A	3292	1/1	0.85	0.10	75,75,75,75	0
57	MG	1A	3294	1/1	0.85	0.11	72,72,72,72	0
57	MG	2I	102	1/1	0.85	0.11	49,49,49,49	0
57	MG	1A	3593	1/1	0.85	0.14	63,63,63,63	0
57	MG	2A	3086	1/1	0.85	0.13	76,76,76,76	0
57	MG	2a	3004	1/1	0.85	0.16	60,60,60,60	0
57	MG	1A	3844	1/1	0.85	0.10	47,47,47,47	0
57	MG	1a	1705	1/1	0.85	0.18	73,73,73,73	0
57	MG	1A	3596	1/1	0.85	0.18	54,54,54,54	0
57	MG	2A	3357	1/1	0.85	0.23	67,67,67,67	0
57	MG	1A	3010	1/1	0.85	0.15	51,51,51,51	0
57	MG	2A	3622	1/1	0.85	0.26	54,54,54,54	0
57	MG	1A	3872	1/1	0.85	0.10	37,37,37,37	0
57	MG	1a	1734	1/1	0.85	0.14	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3876	1/1	0.85	0.12	61,61,61,61	0
57	MG	2A	3148	1/1	0.85	0.12	66,66,66,66	0
57	MG	15	3106	1/1	0.85	0.27	36,36,36,36	0
57	MG	1A	3721	1/1	0.85	0.11	60,60,60,60	0
57	MG	1A	3724	1/1	0.85	0.16	53,53,53,53	0
57	MG	2A	3465	1/1	0.85	0.13	72,72,72,72	0
57	MG	2A	3167	1/1	0.85	0.30	66,66,66,66	0
57	MG	1a	1862	1/1	0.85	0.24	71,71,71,71	0
57	MG	2a	3097	1/1	0.85	0.30	72,72,72,72	0
57	MG	1A	3900	1/1	0.85	0.15	58,58,58,58	0
57	MG	1a	1760	1/1	0.85	0.17	75,75,75,75	0
57	MG	1A	3308	1/1	0.85	0.12	40,40,40,40	0
57	MG	1A	3938	1/1	0.85	0.11	63,63,63,63	0
57	MG	1A	3559	1/1	0.85	0.18	47,47,47,47	0
57	MG	2a	3165	1/1	0.85	0.22	67,67,67,67	0
57	MG	1A	3975	1/1	0.85	0.13	64,64,64,64	0
57	MG	2a	3168	1/1	0.85	0.21	69,69,69,69	0
57	MG	2A	3243	1/1	0.85	0.11	53,53,53,53	0
57	MG	2A	3268	1/1	0.85	0.22	71,71,71,71	0
57	MG	1A	3692	1/1	0.85	0.10	51,51,51,51	0
57	MG	1A	3694	1/1	0.85	0.12	58,58,58,58	0
59	MPD	2A	3735	8/8	0.85	0.27	38,48,56,61	0
57	MG	1A	3775	1/1	0.85	0.12	54,54,54,54	0
59	MPD	2A	3737	8/8	0.85	0.20	56,68,70,73	0
57	MG	2A	3723	1/1	0.86	0.25	69,69,69,69	0
57	MG	2A	3395	1/1	0.86	0.20	75,75,75,75	0
57	MG	1A	3786	1/1	0.86	0.13	24,24,24,24	0
57	MG	1A	3983	1/1	0.86	0.10	68,68,68,68	0
57	MG	2A	3119	1/1	0.86	0.22	66,66,66,66	0
57	MG	1A	3988	1/1	0.86	0.22	42,42,42,42	0
57	MG	1A	3990	1/1	0.86	0.18	38,38,38,38	0
57	MG	1A	3789	1/1	0.86	0.09	29,29,29,29	0
57	MG	1A	3600	1/1	0.86	0.38	48,48,48,48	0
57	MG	1A	3601	1/1	0.86	0.23	53,53,53,53	0
57	MG	1A	3539	1/1	0.86	0.14	47,47,47,47	0
57	MG	1A	3622	1/1	0.86	0.12	31,31,31,31	0
57	MG	2A	3495	1/1	0.86	0.21	66,66,66,66	0
57	MG	1A	4021	1/1	0.86	0.20	51,51,51,51	0
57	MG	1A	3002	1/1	0.86	0.17	58,58,58,58	0
57	MG	2A	3173	1/1	0.86	0.10	68,68,68,68	0
57	MG	2A	3187	1/1	0.86	0.26	65,65,65,65	0
57	MG	1A	3678	1/1	0.86	0.17	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	4027	1/1	0.86	0.16	62,62,62,62	0
57	MG	1A	3569	1/1	0.86	0.13	67,67,67,67	0
57	MG	2a	3017	1/1	0.86	0.12	67,67,67,67	0
57	MG	2A	3224	1/1	0.86	0.12	59,59,59,59	0
57	MG	1a	1706	1/1	0.86	0.17	60,60,60,60	0
57	MG	2a	3031	1/1	0.86	0.28	65,65,65,65	0
57	MG	1a	1707	1/1	0.86	0.25	69,69,69,69	0
57	MG	1a	1711	1/1	0.86	0.26	72,72,72,72	0
57	MG	1a	1716	1/1	0.86	0.15	64,64,64,64	0
57	MG	1B	209	1/1	0.86	0.12	55,55,55,55	0
57	MG	2A	3582	1/1	0.86	0.10	51,51,51,51	0
57	MG	1a	1864	1/1	0.86	0.10	68,68,68,68	0
57	MG	1A	3350	1/1	0.86	0.13	50,50,50,50	0
57	MG	2A	3270	1/1	0.86	0.11	77,77,77,77	0
57	MG	2A	3612	1/1	0.86	0.12	47,47,47,47	0
57	MG	1A	3761	1/1	0.86	0.09	28,28,28,28	0
57	MG	1B	226	1/1	0.86	0.17	69,69,69,69	0
57	MG	1A	3764	1/1	0.86	0.19	52,52,52,52	0
57	MG	1E	305	1/1	0.86	0.11	49,49,49,49	0
57	MG	2a	3105	1/1	0.86	0.20	48,48,48,48	0
57	MG	1d	305	1/1	0.86	0.08	85,85,85,85	0
57	MG	2A	3313	1/1	0.86	0.26	76,76,76,76	0
57	MG	1A	3383	1/1	0.86	0.10	43,43,43,43	0
57	MG	1G	202	1/1	0.86	0.10	50,50,50,50	0
57	MG	1A	3261	1/1	0.86	0.25	60,60,60,60	0
57	MG	1A	3937	1/1	0.86	0.13	46,46,46,46	0
57	MG	2A	3044	1/1	0.86	0.22	68,68,68,68	0
57	MG	2A	3343	1/1	0.86	0.21	62,62,62,62	0
57	MG	1A	3176	1/1	0.86	0.22	45,45,45,45	0
57	MG	15	3109	1/1	0.86	0.18	72,72,72,72	0
57	MG	2j	201	1/1	0.86	0.13	68,68,68,68	0
57	MG	1A	3943	1/1	0.86	0.18	73,73,73,73	0
57	MG	1a	1776	1/1	0.86	0.11	83,83,83,83	0
58	ARG	1A	4030	12/12	0.86	0.17	45,63,76,76	0
57	MG	1A	3699	1/1	0.86	0.13	68,68,68,68	0
57	MG	1a	1609	1/1	0.86	0.16	48,48,48,48	0
57	MG	1A	3954	1/1	0.86	0.12	52,52,52,52	0
57	MG	10	104	1/1	0.87	0.09	45,45,45,45	0
57	MG	2G	202	1/1	0.87	0.19	76,76,76,76	0
57	MG	2A	3153	1/1	0.87	0.17	60,60,60,60	0
57	MG	2N	201	1/1	0.87	0.11	72,72,72,72	0
57	MG	1A	3926	1/1	0.87	0.13	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3568	1/1	0.87	0.14	37,37,37,37	0
57	MG	2A	3569	1/1	0.87	0.11	43,43,43,43	0
57	MG	1A	3640	1/1	0.87	0.15	44,44,44,44	0
57	MG	2A	3579	1/1	0.87	0.12	51,51,51,51	0
57	MG	2A	3350	1/1	0.87	0.09	59,59,59,59	0
57	MG	1A	3428	1/1	0.87	0.23	54,54,54,54	0
57	MG	1A	3817	1/1	0.87	0.17	26,26,26,26	0
57	MG	2a	3016	1/1	0.87	0.22	64,64,64,64	0
57	MG	1a	1791	1/1	0.87	0.22	75,75,75,75	0
57	MG	2A	3190	1/1	0.87	0.25	67,67,67,67	0
57	MG	1A	4025	1/1	0.87	0.14	63,63,63,63	0
57	MG	2A	3209	1/1	0.87	0.23	65,65,65,65	0
57	MG	1A	3827	1/1	0.87	0.14	34,34,34,34	0
57	MG	1B	203	1/1	0.87	0.14	62,62,62,62	0
57	MG	2a	3052	1/1	0.87	0.22	61,61,61,61	0
57	MG	1A	3676	1/1	0.87	0.14	54,54,54,54	0
57	MG	2A	3409	1/1	0.87	0.15	62,62,62,62	0
57	MG	2A	3644	1/1	0.87	0.14	66,66,66,66	0
57	MG	2a	3060	1/1	0.87	0.15	74,74,74,74	0
57	MG	2A	3414	1/1	0.87	0.13	39,39,39,39	0
57	MG	2A	3417	1/1	0.87	0.13	58,58,58,58	0
57	MG	2A	3418	1/1	0.87	0.11	50,50,50,50	0
57	MG	2A	3678	1/1	0.87	0.13	57,57,57,57	0
57	MG	1a	1733	1/1	0.87	0.16	60,60,60,60	0
57	MG	2a	3080	1/1	0.87	0.18	76,76,76,76	0
57	MG	2a	3085	1/1	0.87	0.14	59,59,59,59	0
57	MG	1A	3386	1/1	0.87	0.15	34,34,34,34	0
57	MG	2A	3460	1/1	0.87	0.14	43,43,43,43	0
57	MG	1A	3481	1/1	0.87	0.16	32,32,32,32	0
57	MG	2A	3078	1/1	0.87	0.22	57,57,57,57	0
57	MG	1B	215	1/1	0.87	0.12	53,53,53,53	0
57	MG	2a	3116	1/1	0.87	0.14	72,72,72,72	0
57	MG	1a	1663	1/1	0.87	0.16	66,66,66,66	0
57	MG	1A	3489	1/1	0.87	0.12	55,55,55,55	0
57	MG	2a	3131	1/1	0.87	0.09	72,72,72,72	0
57	MG	2a	3134	1/1	0.87	0.12	82,82,82,82	0
57	MG	1A	3610	1/1	0.87	0.19	51,51,51,51	0
57	MG	2a	3149	1/1	0.87	0.18	68,68,68,68	0
57	MG	1A	3881	1/1	0.87	0.08	50,50,50,50	0
57	MG	2A	3278	1/1	0.87	0.24	65,65,65,65	0
57	MG	1a	1835	1/1	0.87	0.18	78,78,78,78	0
57	MG	2A	3285	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
57	MG	1A	3360	1/1	0.87	0.12	57,57,57,57	0
57	MG	1a	1767	1/1	0.87	0.24	60,60,60,60	0
57	MG	2A	3294	1/1	0.87	0.17	54,54,54,54	0
57	MG	1E	309	1/1	0.87	0.15	63,63,63,63	0
57	MG	2B	203	1/1	0.87	0.19	74,74,74,74	0
57	MG	1A	3891	1/1	0.87	0.18	54,54,54,54	0
57	MG	2B	211	1/1	0.87	0.15	54,54,54,54	0
57	MG	1A	3798	1/1	0.87	0.23	63,63,63,63	0
57	MG	1A	3637	1/1	0.87	0.13	24,24,24,24	0
57	MG	2F	303	1/1	0.88	0.17	50,50,50,50	0
57	MG	2A	3544	1/1	0.88	0.13	53,53,53,53	0
57	MG	2A	3554	1/1	0.88	0.16	71,71,71,71	0
57	MG	2A	3092	1/1	0.88	0.16	60,60,60,60	0
57	MG	1a	1816	1/1	0.88	0.16	68,68,68,68	0
57	MG	1a	1821	1/1	0.88	0.12	66,66,66,66	0
57	MG	1A	3715	1/1	0.88	0.20	68,68,68,68	0
57	MG	23	101	1/1	0.88	0.16	63,63,63,63	0
57	MG	1a	1610	1/1	0.88	0.14	58,58,58,58	0
57	MG	2A	3129	1/1	0.88	0.24	63,63,63,63	0
57	MG	2A	3131	1/1	0.88	0.23	62,62,62,62	0
57	MG	2A	3581	1/1	0.88	0.12	67,67,67,67	0
57	MG	2a	3012	1/1	0.88	0.17	71,71,71,71	0
57	MG	1A	3580	1/1	0.88	0.16	63,63,63,63	0
57	MG	1A	3662	1/1	0.88	0.17	67,67,67,67	0
57	MG	1a	1739	1/1	0.88	0.21	79,79,79,79	0
57	MG	1A	3674	1/1	0.88	0.09	37,37,37,37	0
57	MG	1a	1644	1/1	0.88	0.16	63,63,63,63	0
57	MG	1A	3535	1/1	0.88	0.10	36,36,36,36	0
57	MG	1a	1851	1/1	0.88	0.10	52,52,52,52	0
57	MG	2A	3381	1/1	0.88	0.22	59,59,59,59	0
57	MG	2A	3618	1/1	0.88	0.10	56,56,56,56	0
57	MG	2a	3054	1/1	0.88	0.26	62,62,62,62	0
57	MG	1a	1859	1/1	0.88	0.15	84,84,84,84	0
57	MG	1A	3041	1/1	0.88	0.13	52,52,52,52	0
57	MG	1A	3832	1/1	0.88	0.09	15,15,15,15	0
57	MG	2A	3184	1/1	0.88	0.29	54,54,54,54	0
57	MG	1A	3972	1/1	0.88	0.14	48,48,48,48	0
57	MG	1A	3756	1/1	0.88	0.16	59,59,59,59	0
57	MG	1A	3688	1/1	0.88	0.12	55,55,55,55	0
57	MG	2A	3672	1/1	0.88	0.14	55,55,55,55	0
57	MG	1B	228	1/1	0.88	0.14	65,65,65,65	0
57	MG	1a	1684	1/1	0.88	0.14	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3860	1/1	0.88	0.10	64,64,64,64	0
57	MG	1A	3213	1/1	0.88	0.06	47,47,47,47	0
57	MG	2a	3091	1/1	0.88	0.29	63,63,63,63	0
57	MG	1A	3552	1/1	0.88	0.19	58,58,58,58	0
57	MG	1A	3993	1/1	0.88	0.36	54,54,54,54	0
57	MG	2a	3098	1/1	0.88	0.32	63,63,63,63	0
57	MG	2A	3703	1/1	0.88	0.11	63,63,63,63	0
57	MG	2A	3029	1/1	0.88	0.17	60,60,60,60	0
57	MG	1A	3874	1/1	0.88	0.11	38,38,38,38	0
57	MG	1A	3553	1/1	0.88	0.09	28,28,28,28	0
57	MG	13	103	1/1	0.88	0.18	64,64,64,64	0
57	MG	1A	3088	1/1	0.88	0.16	61,61,61,61	0
57	MG	1a	1709	1/1	0.88	0.16	61,61,61,61	0
57	MG	2A	3271	1/1	0.88	0.11	61,61,61,61	0
57	MG	2a	3146	1/1	0.88	0.19	70,70,70,70	0
57	MG	2A	3273	1/1	0.88	0.20	49,49,49,49	0
57	MG	1a	1800	1/1	0.88	0.19	70,70,70,70	0
57	MG	1A	3462	1/1	0.88	0.20	62,62,62,62	0
57	MG	2A	3082	1/1	0.88	0.16	44,44,44,44	0
57	MG	2A	3530	1/1	0.88	0.35	48,48,48,48	0
57	MG	1A	3464	1/1	0.88	0.10	35,35,35,35	0
57	MG	2B	205	1/1	0.88	0.20	58,58,58,58	0
57	MG	2a	3184	1/1	0.88	0.21	63,63,63,63	0
57	MG	1A	3032	1/1	0.88	0.25	55,55,55,55	0
57	MG	1a	1720	1/1	0.88	0.12	63,63,63,63	0
57	MG	2A	3537	1/1	0.88	0.14	55,55,55,55	0
57	MG	1A	3645	1/1	0.88	0.15	54,54,54,54	0
57	MG	2B	216	1/1	0.88	0.12	70,70,70,70	0
57	MG	2A	3543	1/1	0.88	0.15	64,64,64,64	0
57	MG	2F	302	1/1	0.88	0.10	47,47,47,47	0
57	MG	1A	3869	1/1	0.89	0.11	43,43,43,43	0
57	MG	1A	3289	1/1	0.89	0.30	46,46,46,46	0
57	MG	1A	3744	1/1	0.89	0.09	43,43,43,43	0
57	MG	2A	3361	1/1	0.89	0.23	59,59,59,59	0
57	MG	1A	3752	1/1	0.89	0.14	54,54,54,54	0
57	MG	2A	3370	1/1	0.89	0.09	38,38,38,38	0
57	MG	1A	3560	1/1	0.89	0.09	25,25,25,25	0
57	MG	2A	3091	1/1	0.89	0.14	66,66,66,66	0
57	MG	1a	1788	1/1	0.89	0.22	62,62,62,62	0
57	MG	2A	3093	1/1	0.89	0.16	60,60,60,60	0
57	MG	1a	1789	1/1	0.89	0.16	64,64,64,64	0
57	MG	1B	202	1/1	0.89	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
57	MG	1a	1677	1/1	0.89	0.13	70,70,70,70	0
57	MG	1a	1678	1/1	0.89	0.14	65,65,65,65	0
57	MG	2A	3126	1/1	0.89	0.14	60,60,60,60	0
57	MG	1a	1796	1/1	0.89	0.17	67,67,67,67	0
57	MG	1a	1797	1/1	0.89	0.13	71,71,71,71	0
57	MG	2A	3440	1/1	0.89	0.12	44,44,44,44	0
57	MG	2A	3133	1/1	0.89	0.18	63,63,63,63	0
57	MG	2E	304	1/1	0.89	0.17	54,54,54,54	0
57	MG	2A	3450	1/1	0.89	0.13	61,61,61,61	0
57	MG	1a	1799	1/1	0.89	0.12	66,66,66,66	0
57	MG	1A	3110	1/1	0.89	0.12	67,67,67,67	0
57	MG	1A	3405	1/1	0.89	0.11	52,52,52,52	0
57	MG	1a	1691	1/1	0.89	0.11	60,60,60,60	0
57	MG	1B	207	1/1	0.89	0.29	63,63,63,63	0
57	MG	2A	3472	1/1	0.89	0.15	68,68,68,68	0
57	MG	1A	3425	1/1	0.89	0.09	21,21,21,21	0
57	MG	1A	3682	1/1	0.89	0.12	27,27,27,27	0
57	MG	1a	1701	1/1	0.89	0.16	63,63,63,63	0
57	MG	1A	3922	1/1	0.89	0.13	28,28,28,28	0
57	MG	2A	3496	1/1	0.89	0.18	66,66,66,66	0
57	MG	1A	3683	1/1	0.89	0.09	48,48,48,48	0
57	MG	1A	3501	1/1	0.89	0.11	34,34,34,34	0
57	MG	1A	3931	1/1	0.89	0.10	53,53,53,53	0
57	MG	1A	3325	1/1	0.89	0.13	69,69,69,69	0
57	MG	2A	3521	1/1	0.89	0.20	70,70,70,70	0
57	MG	2A	3522	1/1	0.89	0.11	63,63,63,63	0
57	MG	1a	1708	1/1	0.89	0.17	62,62,62,62	0
57	MG	2A	3193	1/1	0.89	0.17	57,57,57,57	0
57	MG	2a	3030	1/1	0.89	0.20	64,64,64,64	0
57	MG	2A	3201	1/1	0.89	0.30	69,69,69,69	0
57	MG	2a	3039	1/1	0.89	0.21	63,63,63,63	0
57	MG	2a	3044	1/1	0.89	0.17	72,72,72,72	0
57	MG	2a	3046	1/1	0.89	0.10	61,61,61,61	0
57	MG	2A	3206	1/1	0.89	0.14	58,58,58,58	0
57	MG	1A	3378	1/1	0.89	0.08	17,17,17,17	0
57	MG	1A	3523	1/1	0.89	0.12	48,48,48,48	0
57	MG	2a	3053	1/1	0.89	0.13	56,56,56,56	0
57	MG	1a	1843	1/1	0.89	0.11	48,48,48,48	0
57	MG	2A	3539	1/1	0.89	0.12	59,59,59,59	0
57	MG	1a	1715	1/1	0.89	0.15	61,61,61,61	0
57	MG	1A	3441	1/1	0.89	0.14	71,71,71,71	0
57	MG	2A	3552	1/1	0.89	0.11	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3447	1/1	0.89	0.12	33,33,33,33	0
57	MG	1A	3958	1/1	0.89	0.10	70,70,70,70	0
57	MG	1A	3971	1/1	0.89	0.16	48,48,48,48	0
57	MG	2a	3069	1/1	0.89	0.09	71,71,71,71	0
57	MG	2A	3242	1/1	0.89	0.10	51,51,51,51	0
57	MG	1A	3449	1/1	0.89	0.08	28,28,28,28	0
57	MG	2A	3245	1/1	0.89	0.14	59,59,59,59	0
57	MG	1a	1727	1/1	0.89	0.13	65,65,65,65	0
57	MG	1A	3814	1/1	0.89	0.10	52,52,52,52	0
57	MG	1A	3980	1/1	0.89	0.10	54,54,54,54	0
57	MG	1A	3335	1/1	0.89	0.16	58,58,58,58	0
57	MG	1A	3625	1/1	0.89	0.11	46,46,46,46	0
57	MG	2A	3585	1/1	0.89	0.19	53,53,53,53	0
57	MG	2A	3588	1/1	0.89	0.11	45,45,45,45	0
57	MG	2a	3111	1/1	0.89	0.23	59,59,59,59	0
57	MG	1d	303	1/1	0.89	0.14	74,74,74,74	0
57	MG	1d	304	1/1	0.89	0.14	55,55,55,55	0
57	MG	1a	1606	1/1	0.89	0.11	64,64,64,64	0
57	MG	2a	3123	1/1	0.89	0.10	67,67,67,67	0
57	MG	1g	201	1/1	0.89	0.30	68,68,68,68	0
57	MG	2A	3286	1/1	0.89	0.19	56,56,56,56	0
57	MG	2A	3287	1/1	0.89	0.16	52,52,52,52	0
57	MG	1A	3632	1/1	0.89	0.10	43,43,43,43	0
57	MG	1A	3718	1/1	0.89	0.15	33,33,33,33	0
57	MG	2A	3292	1/1	0.89	0.22	62,62,62,62	0
57	MG	1A	3457	1/1	0.89	0.15	58,58,58,58	0
57	MG	1a	1617	1/1	0.89	0.11	69,69,69,69	0
57	MG	2A	3655	1/1	0.89	0.12	71,71,71,71	0
57	MG	2a	3167	1/1	0.89	0.07	89,89,89,89	0
57	MG	2A	3300	1/1	0.89	0.10	63,63,63,63	0
57	MG	2a	3169	1/1	0.89	0.13	84,84,84,84	0
57	MG	2a	3171	1/1	0.89	0.13	59,59,59,59	0
57	MG	1a	1629	1/1	0.89	0.10	52,52,52,52	0
57	MG	2A	3320	1/1	0.89	0.23	60,60,60,60	0
57	MG	1A	3080	1/1	0.89	0.14	43,43,43,43	0
57	MG	2A	3050	1/1	0.89	0.17	66,66,66,66	0
57	MG	1A	3858	1/1	0.89	0.10	37,37,37,37	0
57	MG	2A	3062	1/1	0.89	0.13	60,60,60,60	0
57	MG	2A	3330	1/1	0.89	0.17	30,30,30,30	0
59	MPD	1a	1873	8/8	0.89	0.15	53,68,74,75	0
57	MG	1a	1635	1/1	0.89	0.09	50,50,50,50	0
57	MG	1A	3643	1/1	0.89	0.12	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3203	1/1	0.89	0.19	40,40,40,40	0
57	MG	2A	3385	1/1	0.90	0.12	38,38,38,38	0
57	MG	2A	3722	1/1	0.90	0.12	52,52,52,52	0
57	MG	1A	3911	1/1	0.90	0.07	22,22,22,22	0
57	MG	1A	3484	1/1	0.90	0.17	62,62,62,62	0
57	MG	2A	3726	1/1	0.90	0.07	76,76,76,76	0
57	MG	1A	3779	1/1	0.90	0.11	55,55,55,55	0
57	MG	1a	1680	1/1	0.90	0.26	76,76,76,76	0
57	MG	2A	3405	1/1	0.90	0.13	68,68,68,68	0
57	MG	1A	3337	1/1	0.90	0.16	54,54,54,54	0
57	MG	1B	217	1/1	0.90	0.10	60,60,60,60	0
57	MG	2A	3734	1/1	0.90	0.14	58,58,58,58	0
57	MG	2A	3415	1/1	0.90	0.16	49,49,49,49	0
57	MG	2A	3416	1/1	0.90	0.11	63,63,63,63	0
57	MG	1a	1687	1/1	0.90	0.16	60,60,60,60	0
57	MG	1a	1688	1/1	0.90	0.13	67,67,67,67	0
57	MG	2A	3422	1/1	0.90	0.13	58,58,58,58	0
57	MG	1A	3557	1/1	0.90	0.19	49,49,49,49	0
57	MG	2A	3434	1/1	0.90	0.19	63,63,63,63	0
57	MG	2A	3435	1/1	0.90	0.09	38,38,38,38	0
57	MG	1a	1811	1/1	0.90	0.08	55,55,55,55	0
57	MG	2E	306	1/1	0.90	0.09	60,60,60,60	0
57	MG	1B	224	1/1	0.90	0.13	45,45,45,45	0
57	MG	1A	3936	1/1	0.90	0.09	50,50,50,50	0
57	MG	2A	3160	1/1	0.90	0.11	52,52,52,52	0
57	MG	1A	3791	1/1	0.90	0.20	56,56,56,56	0
57	MG	1A	3795	1/1	0.90	0.14	59,59,59,59	0
57	MG	2A	3176	1/1	0.90	0.14	68,68,68,68	0
57	MG	2A	3180	1/1	0.90	0.11	56,56,56,56	0
57	MG	1B	229	1/1	0.90	0.11	50,50,50,50	0
57	MG	2A	3480	1/1	0.90	0.11	54,54,54,54	0
57	MG	1D	314	1/1	0.90	0.12	59,59,59,59	0
57	MG	1a	1704	1/1	0.90	0.15	67,67,67,67	0
57	MG	1A	3272	1/1	0.90	0.09	48,48,48,48	0
57	MG	1A	3277	1/1	0.90	0.12	48,48,48,48	0
57	MG	2a	3007	1/1	0.90	0.29	67,67,67,67	0
57	MG	1A	3950	1/1	0.90	0.11	31,31,31,31	0
57	MG	2A	3205	1/1	0.90	0.14	67,67,67,67	0
57	MG	1A	3711	1/1	0.90	0.12	57,57,57,57	0
57	MG	2A	3208	1/1	0.90	0.12	64,64,64,64	0
57	MG	1N	203	1/1	0.90	0.08	62,62,62,62	0
57	MG	1R	203	1/1	0.90	0.26	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	3027	1/1	0.90	0.20	64,64,64,64	0
57	MG	2A	3217	1/1	0.90	0.12	63,63,63,63	0
57	MG	1a	1713	1/1	0.90	0.22	57,57,57,57	0
57	MG	2a	3038	1/1	0.90	0.09	76,76,76,76	0
57	MG	1T	203	1/1	0.90	0.17	63,63,63,63	0
57	MG	2a	3040	1/1	0.90	0.25	64,64,64,64	0
57	MG	2a	3043	1/1	0.90	0.14	72,72,72,72	0
57	MG	1A	3564	1/1	0.90	0.07	33,33,33,33	0
57	MG	1W	204	1/1	0.90	0.13	48,48,48,48	0
57	MG	1a	1719	1/1	0.90	0.14	58,58,58,58	0
57	MG	2A	3234	1/1	0.90	0.24	44,44,44,44	0
57	MG	2a	3050	1/1	0.90	0.25	63,63,63,63	0
57	MG	2A	3235	1/1	0.90	0.20	66,66,66,66	0
57	MG	1a	1867	1/1	0.90	0.12	65,65,65,65	0
57	MG	1A	3311	1/1	0.90	0.12	41,41,41,41	0
57	MG	10	110	1/1	0.90	0.17	37,37,37,37	0
57	MG	2A	3244	1/1	0.90	0.28	63,63,63,63	0
57	MG	13	102	1/1	0.90	0.09	36,36,36,36	0
57	MG	1A	3572	1/1	0.90	0.08	30,30,30,30	0
57	MG	2a	3061	1/1	0.90	0.30	63,63,63,63	0
57	MG	1A	3658	1/1	0.90	0.13	58,58,58,58	0
57	MG	1A	3345	1/1	0.90	0.09	37,37,37,37	0
57	MG	1A	3837	1/1	0.90	0.15	48,48,48,48	0
57	MG	1A	3838	1/1	0.90	0.11	47,47,47,47	0
57	MG	2A	3572	1/1	0.90	0.09	47,47,47,47	0
57	MG	2a	3075	1/1	0.90	0.21	63,63,63,63	0
57	MG	1n	102	1/1	0.90	0.14	66,66,66,66	0
57	MG	2A	3576	1/1	0.90	0.15	54,54,54,54	0
57	MG	1a	1745	1/1	0.90	0.10	59,59,59,59	0
57	MG	1w	101	1/1	0.90	0.13	63,63,63,63	0
57	MG	1A	3668	1/1	0.90	0.10	47,47,47,47	0
57	MG	1a	1750	1/1	0.90	0.32	61,61,61,61	0
57	MG	1A	3526	1/1	0.90	0.09	43,43,43,43	0
57	MG	1A	3401	1/1	0.90	0.19	53,53,53,53	0
57	MG	2a	3100	1/1	0.90	0.16	68,68,68,68	0
57	MG	2A	3597	1/1	0.90	0.13	70,70,70,70	0
57	MG	2a	3110	1/1	0.90	0.18	65,65,65,65	0
57	MG	1A	3747	1/1	0.90	0.14	52,52,52,52	0
57	MG	2a	3112	1/1	0.90	0.26	65,65,65,65	0
57	MG	1A	3677	1/1	0.90	0.10	31,31,31,31	0
57	MG	2A	3051	1/1	0.90	0.27	70,70,70,70	0
57	MG	1A	3753	1/1	0.90	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
57	MG	2A	3059	1/1	0.90	0.20	61,61,61,61	0
57	MG	2a	3126	1/1	0.90	0.14	75,75,75,75	0
57	MG	2a	3127	1/1	0.90	0.12	65,65,65,65	0
57	MG	2A	3310	1/1	0.90	0.22	53,53,53,53	0
57	MG	2a	3129	1/1	0.90	0.12	72,72,72,72	0
57	MG	1a	1765	1/1	0.90	0.14	67,67,67,67	0
57	MG	2A	3315	1/1	0.90	0.15	47,47,47,47	0
57	MG	2a	3136	1/1	0.90	0.12	73,73,73,73	0
57	MG	2A	3064	1/1	0.90	0.27	55,55,55,55	0
57	MG	2A	3624	1/1	0.90	0.28	67,67,67,67	0
57	MG	1a	1630	1/1	0.90	0.23	66,66,66,66	0
57	MG	2a	3150	1/1	0.90	0.10	69,69,69,69	0
57	MG	2a	3151	1/1	0.90	0.23	64,64,64,64	0
57	MG	1A	4006	1/1	0.90	0.12	44,44,44,44	0
57	MG	2a	3155	1/1	0.90	0.15	68,68,68,68	0
57	MG	1A	3531	1/1	0.90	0.07	24,24,24,24	0
57	MG	1A	3594	1/1	0.90	0.10	62,62,62,62	0
57	MG	1A	3079	1/1	0.90	0.20	49,49,49,49	0
57	MG	1a	1780	1/1	0.90	0.15	65,65,65,65	0
57	MG	2A	3339	1/1	0.90	0.12	64,64,64,64	0
57	MG	1A	3090	1/1	0.90	0.08	53,53,53,53	0
57	MG	2A	3679	1/1	0.90	0.11	67,67,67,67	0
57	MG	1A	3374	1/1	0.90	0.19	48,48,48,48	0
57	MG	2a	3181	1/1	0.90	0.23	60,60,60,60	0
57	MG	1a	1658	1/1	0.90	0.12	65,65,65,65	0
57	MG	2a	3187	1/1	0.90	0.15	74,74,74,74	0
57	MG	1a	1661	1/1	0.90	0.18	65,65,65,65	0
57	MG	1A	3768	1/1	0.90	0.14	53,53,53,53	0
57	MG	2A	3099	1/1	0.90	0.23	64,64,64,64	0
57	MG	2x	101	1/1	0.90	0.19	47,47,47,47	0
57	MG	2A	3363	1/1	0.90	0.13	57,57,57,57	0
57	MG	1A	3072	1/1	0.90	0.11	45,45,45,45	0
59	MPD	1a	1874	8/8	0.90	0.16	57,66,70,71	0
57	MG	1A	3893	1/1	0.90	0.11	54,54,54,54	0
57	MG	1a	1667	1/1	0.90	0.14	65,65,65,65	0
57	MG	1A	3548	1/1	0.90	0.14	61,61,61,61	0
57	MG	1a	1814	1/1	0.91	0.26	64,64,64,64	0
57	MG	2A	3729	1/1	0.91	0.18	59,59,59,59	0
57	MG	2A	3151	1/1	0.91	0.09	55,55,55,55	0
57	MG	1A	3398	1/1	0.91	0.09	63,63,63,63	0
57	MG	1A	3098	1/1	0.91	0.14	54,54,54,54	0
57	MG	1T	201	1/1	0.91	0.06	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
57	MG	1A	3282	1/1	0.91	0.14	55,55,55,55	0
57	MG	2A	3423	1/1	0.91	0.12	47,47,47,47	0
57	MG	1A	3669	1/1	0.91	0.29	48,48,48,48	0
57	MG	2A	3430	1/1	0.91	0.09	40,40,40,40	0
57	MG	2B	210	1/1	0.91	0.25	69,69,69,69	0
57	MG	1A	3985	1/1	0.91	0.17	54,54,54,54	0
57	MG	2A	3174	1/1	0.91	0.17	58,58,58,58	0
57	MG	1Y	201	1/1	0.91	0.15	61,61,61,61	0
57	MG	1a	1830	1/1	0.91	0.09	62,62,62,62	0
57	MG	2D	309	1/1	0.91	0.09	33,33,33,33	0
57	MG	2E	301	1/1	0.91	0.17	68,68,68,68	0
57	MG	1A	3847	1/1	0.91	0.12	43,43,43,43	0
57	MG	1A	3181	1/1	0.91	0.16	52,52,52,52	0
57	MG	2A	3461	1/1	0.91	0.14	59,59,59,59	0
57	MG	1a	1840	1/1	0.91	0.19	68,68,68,68	0
57	MG	1l	102	1/1	0.91	0.11	62,62,62,62	0
57	MG	2G	201	1/1	0.91	0.10	70,70,70,70	0
57	MG	1a	1712	1/1	0.91	0.12	57,57,57,57	0
57	MG	1a	1850	1/1	0.91	0.16	50,50,50,50	0
57	MG	1A	3504	1/1	0.91	0.11	31,31,31,31	0
57	MG	2A	3473	1/1	0.91	0.13	64,64,64,64	0
57	MG	2A	3475	1/1	0.91	0.10	59,59,59,59	0
57	MG	2V	202	1/1	0.91	0.26	57,57,57,57	0
57	MG	2W	202	1/1	0.91	0.22	57,57,57,57	0
57	MG	1a	1857	1/1	0.91	0.10	60,60,60,60	0
57	MG	1A	3340	1/1	0.91	0.29	53,53,53,53	0
57	MG	1A	3204	1/1	0.91	0.11	50,50,50,50	0
57	MG	29	101	1/1	0.91	0.23	67,67,67,67	0
57	MG	2A	3487	1/1	0.91	0.09	55,55,55,55	0
57	MG	15	3107	1/1	0.91	0.12	44,44,44,44	0
57	MG	1A	3038	1/1	0.91	0.19	48,48,48,48	0
57	MG	2A	3219	1/1	0.91	0.23	72,72,72,72	0
57	MG	2a	3008	1/1	0.91	0.09	61,61,61,61	0
57	MG	2a	3009	1/1	0.91	0.11	50,50,50,50	0
57	MG	1A	4000	1/1	0.91	0.16	50,50,50,50	0
57	MG	2A	3505	1/1	0.91	0.12	49,49,49,49	0
57	MG	1a	1604	1/1	0.91	0.13	61,61,61,61	0
57	MG	1A	3762	1/1	0.91	0.18	56,56,56,56	0
57	MG	2a	3020	1/1	0.91	0.10	80,80,80,80	0
57	MG	1A	3216	1/1	0.91	0.18	35,35,35,35	0
57	MG	1A	3443	1/1	0.91	0.14	62,62,62,62	0
57	MG	1A	4019	1/1	0.91	0.08	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3128	1/1	0.91	0.17	57,57,57,57	0
57	MG	1A	3886	1/1	0.91	0.12	27,27,27,27	0
57	MG	2a	3033	1/1	0.91	0.25	65,65,65,65	0
57	MG	2a	3034	1/1	0.91	0.15	61,61,61,61	0
57	MG	2a	3037	1/1	0.91	0.09	69,69,69,69	0
57	MG	1a	1741	1/1	0.91	0.08	61,61,61,61	0
57	MG	1e	203	1/1	0.91	0.36	68,68,68,68	0
57	MG	2A	3535	1/1	0.91	0.12	52,52,52,52	0
57	MG	2a	3041	1/1	0.91	0.27	64,64,64,64	0
57	MG	1A	3772	1/1	0.91	0.14	50,50,50,50	0
57	MG	1A	3774	1/1	0.91	0.07	34,34,34,34	0
57	MG	2a	3045	1/1	0.91	0.22	58,58,58,58	0
57	MG	2A	3266	1/1	0.91	0.23	57,57,57,57	0
57	MG	1A	3533	1/1	0.91	0.10	23,23,23,23	0
57	MG	2A	3541	1/1	0.91	0.10	60,60,60,60	0
57	MG	1u	101	1/1	0.91	0.22	74,74,74,74	0
57	MG	1y	202	1/1	0.91	0.09	60,60,60,60	0
57	MG	1a	1751	1/1	0.91	0.11	63,63,63,63	0
57	MG	1a	1633	1/1	0.91	0.09	45,45,45,45	0
57	MG	2A	3024	1/1	0.91	0.13	52,52,52,52	0
57	MG	1A	3448	1/1	0.91	0.10	27,27,27,27	0
57	MG	2A	3561	1/1	0.91	0.11	61,61,61,61	0
57	MG	2A	3031	1/1	0.91	0.17	60,60,60,60	0
57	MG	2A	3566	1/1	0.91	0.10	60,60,60,60	0
57	MG	2A	3281	1/1	0.91	0.09	53,53,53,53	0
57	MG	1A	3225	1/1	0.91	0.11	52,52,52,52	0
57	MG	2A	3571	1/1	0.91	0.11	39,39,39,39	0
57	MG	1B	205	1/1	0.91	0.08	52,52,52,52	0
57	MG	2a	3070	1/1	0.91	0.10	61,61,61,61	0
57	MG	2A	3042	1/1	0.91	0.20	61,61,61,61	0
57	MG	1A	3619	1/1	0.91	0.12	34,34,34,34	0
57	MG	1A	3781	1/1	0.91	0.10	39,39,39,39	0
57	MG	1a	1656	1/1	0.91	0.30	66,66,66,66	0
57	MG	1a	1769	1/1	0.91	0.12	53,53,53,53	0
57	MG	1a	1771	1/1	0.91	0.11	63,63,63,63	0
57	MG	1A	3784	1/1	0.91	0.10	41,41,41,41	0
57	MG	2A	3306	1/1	0.91	0.15	44,44,44,44	0
57	MG	2A	3309	1/1	0.91	0.32	59,59,59,59	0
57	MG	2A	3605	1/1	0.91	0.16	52,52,52,52	0
57	MG	1a	1659	1/1	0.91	0.16	57,57,57,57	0
57	MG	1A	3321	1/1	0.91	0.14	59,59,59,59	0
57	MG	2a	3109	1/1	0.91	0.32	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1B	212	1/1	0.91	0.09	56,56,56,56	0
57	MG	2A	3076	1/1	0.91	0.18	67,67,67,67	0
57	MG	1A	3246	1/1	0.91	0.09	58,58,58,58	0
57	MG	2A	3616	1/1	0.91	0.14	39,39,39,39	0
57	MG	2A	3323	1/1	0.91	0.23	69,69,69,69	0
57	MG	1A	3541	1/1	0.91	0.21	57,57,57,57	0
57	MG	1A	3133	1/1	0.91	0.24	32,32,32,32	0
57	MG	1a	1669	1/1	0.91	0.25	62,62,62,62	0
57	MG	1A	3712	1/1	0.91	0.17	39,39,39,39	0
57	MG	2A	3333	1/1	0.91	0.12	55,55,55,55	0
57	MG	2A	3639	1/1	0.91	0.10	54,54,54,54	0
57	MG	1A	3713	1/1	0.91	0.18	36,36,36,36	0
57	MG	2A	3650	1/1	0.91	0.10	75,75,75,75	0
57	MG	2A	3652	1/1	0.91	0.08	50,50,50,50	0
57	MG	1A	3326	1/1	0.91	0.26	56,56,56,56	0
57	MG	1A	3393	1/1	0.91	0.11	51,51,51,51	0
57	MG	1A	3953	1/1	0.91	0.12	50,50,50,50	0
57	MG	2A	3098	1/1	0.91	0.25	60,60,60,60	0
57	MG	1D	311	1/1	0.91	0.10	47,47,47,47	0
57	MG	2A	3675	1/1	0.91	0.18	55,55,55,55	0
57	MG	2A	3676	1/1	0.91	0.11	60,60,60,60	0
57	MG	1A	3198	1/1	0.91	0.09	47,47,47,47	0
57	MG	1a	1686	1/1	0.91	0.14	47,47,47,47	0
57	MG	1A	3955	1/1	0.91	0.09	54,54,54,54	0
57	MG	2A	3686	1/1	0.91	0.28	47,47,47,47	0
57	MG	2A	3122	1/1	0.91	0.22	73,73,73,73	0
57	MG	2a	3170	1/1	0.91	0.09	57,57,57,57	0
57	MG	1A	3648	1/1	0.91	0.09	23,23,23,23	0
57	MG	2a	3172	1/1	0.91	0.12	78,78,78,78	0
57	MG	2a	3174	1/1	0.91	0.10	78,78,78,78	0
57	MG	1A	3968	1/1	0.91	0.10	37,37,37,37	0
57	MG	2a	3179	1/1	0.91	0.07	76,76,76,76	0
57	MG	2A	3380	1/1	0.91	0.16	61,61,61,61	0
57	MG	2A	3697	1/1	0.91	0.09	66,66,66,66	0
57	MG	2a	3183	1/1	0.91	0.25	56,56,56,56	0
57	MG	1F	315	1/1	0.91	0.11	55,55,55,55	0
57	MG	2a	3186	1/1	0.91	0.15	77,77,77,77	0
57	MG	1a	1694	1/1	0.91	0.10	53,53,53,53	0
57	MG	2f	201	1/1	0.91	0.10	53,53,53,53	0
57	MG	1a	1805	1/1	0.91	0.17	55,55,55,55	0
57	MG	2A	3711	1/1	0.91	0.23	46,46,46,46	0
57	MG	2A	3134	1/1	0.91	0.09	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3392	1/1	0.91	0.09	38,38,38,38	0
57	MG	2A	3718	1/1	0.91	0.23	64,64,64,64	0
57	MG	1a	1695	1/1	0.91	0.27	61,61,61,61	0
57	MG	1A	3478	1/1	0.91	0.11	60,60,60,60	0
57	MG	1G	203	1/1	0.91	0.08	49,49,49,49	0
57	MG	2A	3408	1/1	0.91	0.11	59,59,59,59	0
57	MG	1a	1700	1/1	0.91	0.13	68,68,68,68	0
57	MG	1a	1613	1/1	0.92	0.10	71,71,71,71	0
57	MG	1A	3586	1/1	0.92	0.15	45,45,45,45	0
57	MG	2A	3365	1/1	0.92	0.09	29,29,29,29	0
57	MG	1a	1625	1/1	0.92	0.08	51,51,51,51	0
57	MG	1a	1768	1/1	0.92	0.15	53,53,53,53	0
57	MG	1a	1628	1/1	0.92	0.18	53,53,53,53	0
57	MG	2A	3087	1/1	0.92	0.17	47,47,47,47	0
57	MG	2A	3725	1/1	0.92	0.23	66,66,66,66	0
57	MG	2A	3089	1/1	0.92	0.27	70,70,70,70	0
57	MG	2A	3727	1/1	0.92	0.11	76,76,76,76	0
57	MG	1A	3998	1/1	0.92	0.10	68,68,68,68	0
57	MG	2A	3388	1/1	0.92	0.08	40,40,40,40	0
57	MG	1A	3397	1/1	0.92	0.13	42,42,42,42	0
57	MG	1A	3841	1/1	0.92	0.09	44,44,44,44	0
57	MG	1A	3843	1/1	0.92	0.08	33,33,33,33	0
57	MG	2A	3394	1/1	0.92	0.14	46,46,46,46	0
57	MG	1A	3169	1/1	0.92	0.15	43,43,43,43	0
57	MG	2A	3396	1/1	0.92	0.15	52,52,52,52	0
57	MG	2B	204	1/1	0.92	0.26	61,61,61,61	0
57	MG	1A	3498	1/1	0.92	0.07	18,18,18,18	0
57	MG	1A	4020	1/1	0.92	0.17	69,69,69,69	0
57	MG	2A	3407	1/1	0.92	0.06	36,36,36,36	0
57	MG	2A	3107	1/1	0.92	0.17	60,60,60,60	0
57	MG	2A	3109	1/1	0.92	0.27	57,57,57,57	0
57	MG	2A	3110	1/1	0.92	0.12	51,51,51,51	0
57	MG	1A	3599	1/1	0.92	0.17	43,43,43,43	0
57	MG	1a	1645	1/1	0.92	0.20	55,55,55,55	0
57	MG	1A	3855	1/1	0.92	0.09	41,41,41,41	0
57	MG	2A	3123	1/1	0.92	0.25	58,58,58,58	0
57	MG	2A	3124	1/1	0.92	0.24	65,65,65,65	0
57	MG	1a	1654	1/1	0.92	0.16	71,71,71,71	0
57	MG	1A	4023	1/1	0.92	0.12	61,61,61,61	0
57	MG	1a	1657	1/1	0.92	0.11	62,62,62,62	0
57	MG	1A	3103	1/1	0.92	0.11	53,53,53,53	0
57	MG	1a	1792	1/1	0.92	0.16	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3075	1/1	0.92	0.12	41,41,41,41	0
57	MG	2A	3445	1/1	0.92	0.17	59,59,59,59	0
57	MG	1a	1660	1/1	0.92	0.17	69,69,69,69	0
57	MG	2R	202	1/1	0.92	0.15	60,60,60,60	0
57	MG	1A	3507	1/1	0.92	0.07	22,22,22,22	0
57	MG	2A	3453	1/1	0.92	0.08	40,40,40,40	0
57	MG	2A	3456	1/1	0.92	0.18	56,56,56,56	0
57	MG	1B	201	1/1	0.92	0.17	46,46,46,46	0
57	MG	1A	3866	1/1	0.92	0.08	46,46,46,46	0
57	MG	25	102	1/1	0.92	0.24	43,43,43,43	0
57	MG	25	103	1/1	0.92	0.08	56,56,56,56	0
57	MG	1A	3513	1/1	0.92	0.08	28,28,28,28	0
57	MG	1A	3618	1/1	0.92	0.07	31,31,31,31	0
57	MG	1A	3242	1/1	0.92	0.14	34,34,34,34	0
57	MG	2A	3154	1/1	0.92	0.16	48,48,48,48	0
57	MG	1a	1671	1/1	0.92	0.11	69,69,69,69	0
57	MG	1a	1807	1/1	0.92	0.20	60,60,60,60	0
57	MG	1A	3621	1/1	0.92	0.13	52,52,52,52	0
57	MG	2A	3476	1/1	0.92	0.22	39,39,39,39	0
57	MG	2A	3477	1/1	0.92	0.07	57,57,57,57	0
57	MG	1a	1674	1/1	0.92	0.14	48,48,48,48	0
57	MG	2A	3170	1/1	0.92	0.22	35,35,35,35	0
57	MG	1A	3743	1/1	0.92	0.08	46,46,46,46	0
57	MG	2a	3018	1/1	0.92	0.11	47,47,47,47	0
57	MG	1B	210	1/1	0.92	0.16	60,60,60,60	0
57	MG	1A	3406	1/1	0.92	0.11	35,35,35,35	0
57	MG	2A	3493	1/1	0.92	0.11	58,58,58,58	0
57	MG	2a	3026	1/1	0.92	0.24	59,59,59,59	0
57	MG	1A	3887	1/1	0.92	0.13	57,57,57,57	0
57	MG	2A	3183	1/1	0.92	0.20	71,71,71,71	0
57	MG	1a	1818	1/1	0.92	0.19	55,55,55,55	0
57	MG	2A	3186	1/1	0.92	0.23	55,55,55,55	0
57	MG	1A	3423	1/1	0.92	0.10	19,19,19,19	0
57	MG	1A	3151	1/1	0.92	0.11	45,45,45,45	0
57	MG	1A	3307	1/1	0.92	0.18	71,71,71,71	0
57	MG	2A	3520	1/1	0.92	0.08	75,75,75,75	0
57	MG	1A	3258	1/1	0.92	0.18	43,43,43,43	0
57	MG	2A	3198	1/1	0.92	0.21	43,43,43,43	0
57	MG	2A	3524	1/1	0.92	0.17	63,63,63,63	0
57	MG	1A	3439	1/1	0.92	0.11	22,22,22,22	0
57	MG	1A	3907	1/1	0.92	0.07	43,43,43,43	0
57	MG	2A	3531	1/1	0.92	0.13	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3644	1/1	0.92	0.10	50,50,50,50	0
57	MG	1a	1833	1/1	0.92	0.12	53,53,53,53	0
57	MG	1A	3920	1/1	0.92	0.09	48,48,48,48	0
57	MG	2a	3051	1/1	0.92	0.22	66,66,66,66	0
57	MG	2A	3213	1/1	0.92	0.07	50,50,50,50	0
57	MG	1D	307	1/1	0.92	0.09	47,47,47,47	0
57	MG	1A	3351	1/1	0.92	0.12	15,15,15,15	0
57	MG	1a	1697	1/1	0.92	0.19	53,53,53,53	0
57	MG	1A	3357	1/1	0.92	0.09	15,15,15,15	0
57	MG	1A	3445	1/1	0.92	0.09	35,35,35,35	0
57	MG	1A	3654	1/1	0.92	0.21	29,29,29,29	0
57	MG	1A	3538	1/1	0.92	0.07	59,59,59,59	0
57	MG	1A	3359	1/1	0.92	0.11	37,37,37,37	0
57	MG	2A	3555	1/1	0.92	0.25	59,59,59,59	0
57	MG	1a	1861	1/1	0.92	0.11	79,79,79,79	0
57	MG	1A	3667	1/1	0.92	0.23	44,44,44,44	0
57	MG	1A	3191	1/1	0.92	0.09	44,44,44,44	0
57	MG	2A	3240	1/1	0.92	0.10	65,65,65,65	0
57	MG	2A	3565	1/1	0.92	0.13	59,59,59,59	0
57	MG	2A	3241	1/1	0.92	0.10	53,53,53,53	0
57	MG	1A	3367	1/1	0.92	0.19	61,61,61,61	0
57	MG	1N	204	1/1	0.92	0.16	57,57,57,57	0
57	MG	1Q	202	1/1	0.92	0.14	53,53,53,53	0
57	MG	1A	3948	1/1	0.92	0.08	27,27,27,27	0
57	MG	2A	3259	1/1	0.92	0.20	67,67,67,67	0
57	MG	2a	3095	1/1	0.92	0.28	54,54,54,54	0
57	MG	2A	3263	1/1	0.92	0.11	39,39,39,39	0
57	MG	1A	3551	1/1	0.92	0.08	47,47,47,47	0
57	MG	1A	3675	1/1	0.92	0.10	25,25,25,25	0
57	MG	2a	3102	1/1	0.92	0.33	53,53,53,53	0
57	MG	1A	3783	1/1	0.92	0.09	32,32,32,32	0
57	MG	2a	3108	1/1	0.92	0.18	46,46,46,46	0
57	MG	1W	201	1/1	0.92	0.26	51,51,51,51	0
57	MG	1A	3319	1/1	0.92	0.06	30,30,30,30	0
57	MG	1A	3957	1/1	0.92	0.10	44,44,44,44	0
57	MG	1A	3456	1/1	0.92	0.10	37,37,37,37	0
57	MG	10	107	1/1	0.92	0.09	48,48,48,48	0
57	MG	2a	3115	1/1	0.92	0.14	54,54,54,54	0
57	MG	2A	3606	1/1	0.92	0.13	68,68,68,68	0
57	MG	1i	201	1/1	0.92	0.17	67,67,67,67	0
57	MG	1l	201	1/1	0.92	0.22	57,57,57,57	0
57	MG	2a	3124	1/1	0.92	0.15	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1l	202	1/1	0.92	0.07	64,64,64,64	0
57	MG	10	108	1/1	0.92	0.12	57,57,57,57	0
57	MG	1a	1724	1/1	0.92	0.16	65,65,65,65	0
57	MG	1A	3320	1/1	0.92	0.30	47,47,47,47	0
57	MG	1A	3271	1/1	0.92	0.15	29,29,29,29	0
57	MG	1a	1728	1/1	0.92	0.10	52,52,52,52	0
57	MG	2A	3619	1/1	0.92	0.09	73,73,73,73	0
57	MG	2a	3137	1/1	0.92	0.09	57,57,57,57	0
57	MG	2a	3142	1/1	0.92	0.15	48,48,48,48	0
57	MG	2A	3620	1/1	0.92	0.07	63,63,63,63	0
57	MG	2A	3001	1/1	0.92	0.32	65,65,65,65	0
57	MG	2A	3002	1/1	0.92	0.11	52,52,52,52	0
57	MG	2A	3298	1/1	0.92	0.27	61,61,61,61	0
57	MG	2A	3626	1/1	0.92	0.13	75,75,75,75	0
57	MG	2a	3152	1/1	0.92	0.15	66,66,66,66	0
57	MG	2A	3014	1/1	0.92	0.21	65,65,65,65	0
57	MG	2A	3019	1/1	0.92	0.07	45,45,45,45	0
57	MG	2a	3161	1/1	0.92	0.12	62,62,62,62	0
57	MG	2A	3307	1/1	0.92	0.17	62,62,62,62	0
57	MG	2A	3646	1/1	0.92	0.11	41,41,41,41	0
57	MG	2A	3308	1/1	0.92	0.30	61,61,61,61	0
57	MG	1a	1731	1/1	0.92	0.09	66,66,66,66	0
57	MG	1A	3461	1/1	0.92	0.06	15,15,15,15	0
57	MG	1A	3209	1/1	0.92	0.15	39,39,39,39	0
57	MG	2A	3660	1/1	0.92	0.10	45,45,45,45	0
57	MG	1A	3976	1/1	0.92	0.13	53,53,53,53	0
57	MG	2a	3173	1/1	0.92	0.11	60,60,60,60	0
57	MG	2A	3319	1/1	0.92	0.28	52,52,52,52	0
57	MG	1A	3273	1/1	0.92	0.17	53,53,53,53	0
57	MG	1A	3390	1/1	0.92	0.07	32,32,32,32	0
57	MG	1a	1742	1/1	0.92	0.13	71,71,71,71	0
57	MG	1A	3477	1/1	0.92	0.10	49,49,49,49	0
57	MG	1a	1746	1/1	0.92	0.15	69,69,69,69	0
57	MG	18	102	1/1	0.92	0.26	40,40,40,40	0
57	MG	2A	3685	1/1	0.92	0.14	59,59,59,59	0
57	MG	2A	3054	1/1	0.92	0.16	58,58,58,58	0
57	MG	2e	202	1/1	0.92	0.08	70,70,70,70	0
57	MG	2A	3687	1/1	0.92	0.07	65,65,65,65	0
57	MG	1A	3695	1/1	0.92	0.08	52,52,52,52	0
57	MG	1A	3157	1/1	0.92	0.16	55,55,55,55	0
57	MG	1a	1752	1/1	0.92	0.17	68,68,68,68	0
57	MG	1A	3819	1/1	0.92	0.10	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3067	1/1	0.92	0.10	49,49,49,49	0
57	MG	2A	3701	1/1	0.92	0.16	69,69,69,69	0
57	MG	1A	3578	1/1	0.92	0.10	50,50,50,50	0
57	MG	2A	3353	1/1	0.92	0.09	50,50,50,50	0
57	MG	1A	3994	1/1	0.92	0.18	31,31,31,31	0
57	MG	1A	3278	1/1	0.92	0.19	52,52,52,52	0
57	MG	1A	3767	1/1	0.93	0.07	34,34,34,34	0
57	MG	2A	3382	1/1	0.93	0.07	29,29,29,29	0
57	MG	1a	1672	1/1	0.93	0.23	68,68,68,68	0
57	MG	1B	223	1/1	0.93	0.12	58,58,58,58	0
57	MG	1A	3913	1/1	0.93	0.08	18,18,18,18	0
57	MG	1a	1675	1/1	0.93	0.19	49,49,49,49	0
57	MG	1A	3440	1/1	0.93	0.12	24,24,24,24	0
57	MG	1A	3502	1/1	0.93	0.12	25,25,25,25	0
57	MG	1A	3670	1/1	0.93	0.09	59,59,59,59	0
57	MG	1A	3060	1/1	0.93	0.13	55,55,55,55	0
57	MG	1A	3341	1/1	0.93	0.11	52,52,52,52	0
57	MG	1A	3159	1/1	0.93	0.33	40,40,40,40	0
57	MG	1a	1685	1/1	0.93	0.25	71,71,71,71	0
57	MG	1D	313	1/1	0.93	0.15	57,57,57,57	0
57	MG	1A	3579	1/1	0.93	0.07	41,41,41,41	0
57	MG	2A	3410	1/1	0.93	0.21	61,61,61,61	0
57	MG	1A	3780	1/1	0.93	0.09	22,22,22,22	0
57	MG	1E	307	1/1	0.93	0.07	49,49,49,49	0
57	MG	1A	3940	1/1	0.93	0.17	60,60,60,60	0
57	MG	1a	1826	1/1	0.93	0.28	67,67,67,67	0
57	MG	2B	201	1/1	0.93	0.09	67,67,67,67	0
57	MG	1A	3190	1/1	0.93	0.25	31,31,31,31	0
57	MG	1A	3584	1/1	0.93	0.11	42,42,42,42	0
57	MG	1A	3519	1/1	0.93	0.09	64,64,64,64	0
57	MG	1A	3949	1/1	0.93	0.11	22,22,22,22	0
57	MG	1a	1834	1/1	0.93	0.12	45,45,45,45	0
57	MG	1A	3785	1/1	0.93	0.08	34,34,34,34	0
57	MG	1A	3349	1/1	0.93	0.12	25,25,25,25	0
57	MG	2B	213	1/1	0.93	0.13	71,71,71,71	0
57	MG	2A	3439	1/1	0.93	0.15	67,67,67,67	0
57	MG	1A	3522	1/1	0.93	0.08	52,52,52,52	0
57	MG	2D	306	1/1	0.93	0.18	51,51,51,51	0
57	MG	2A	3443	1/1	0.93	0.08	50,50,50,50	0
57	MG	2D	310	1/1	0.93	0.08	54,54,54,54	0
57	MG	2D	311	1/1	0.93	0.30	59,59,59,59	0
57	MG	1a	1841	1/1	0.93	0.18	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3790	1/1	0.93	0.14	47,47,47,47	0
57	MG	1a	1846	1/1	0.93	0.11	61,61,61,61	0
57	MG	2A	3179	1/1	0.93	0.21	67,67,67,67	0
57	MG	1A	3027	1/1	0.93	0.06	58,58,58,58	0
57	MG	2A	3181	1/1	0.93	0.13	58,58,58,58	0
57	MG	1T	202	1/1	0.93	0.09	67,67,67,67	0
57	MG	1A	3693	1/1	0.93	0.10	47,47,47,47	0
57	MG	2A	3185	1/1	0.93	0.17	63,63,63,63	0
57	MG	2A	3467	1/1	0.93	0.08	45,45,45,45	0
57	MG	1V	203	1/1	0.93	0.10	43,43,43,43	0
57	MG	2Q	201	1/1	0.93	0.29	65,65,65,65	0
57	MG	2A	3469	1/1	0.93	0.09	56,56,56,56	0
57	MG	1A	3960	1/1	0.93	0.08	49,49,49,49	0
57	MG	2V	201	1/1	0.93	0.07	63,63,63,63	0
57	MG	2A	3471	1/1	0.93	0.10	49,49,49,49	0
57	MG	1a	1860	1/1	0.93	0.13	54,54,54,54	0
57	MG	20	101	1/1	0.93	0.18	53,53,53,53	0
57	MG	21	101	1/1	0.93	0.07	53,53,53,53	0
57	MG	1A	3961	1/1	0.93	0.10	53,53,53,53	0
57	MG	2A	3192	1/1	0.93	0.11	51,51,51,51	0
57	MG	25	101	1/1	0.93	0.41	46,46,46,46	0
57	MG	1A	3524	1/1	0.93	0.09	44,44,44,44	0
57	MG	2A	3196	1/1	0.93	0.15	62,62,62,62	0
57	MG	1A	3175	1/1	0.93	0.08	43,43,43,43	0
57	MG	1A	3323	1/1	0.93	0.12	30,30,30,30	0
57	MG	1a	1865	1/1	0.93	0.10	60,60,60,60	0
57	MG	1A	3529	1/1	0.93	0.11	53,53,53,53	0
57	MG	1A	3530	1/1	0.93	0.08	38,38,38,38	0
57	MG	1A	3979	1/1	0.93	0.10	56,56,56,56	0
57	MG	2A	3210	1/1	0.93	0.09	59,59,59,59	0
57	MG	1a	1870	1/1	0.93	0.19	76,76,76,76	0
57	MG	2A	3500	1/1	0.93	0.09	36,36,36,36	0
57	MG	1a	1717	1/1	0.93	0.13	71,71,71,71	0
57	MG	2A	3215	1/1	0.93	0.10	61,61,61,61	0
57	MG	2A	3506	1/1	0.93	0.17	47,47,47,47	0
57	MG	2A	3508	1/1	0.93	0.13	63,63,63,63	0
57	MG	2a	3019	1/1	0.93	0.16	49,49,49,49	0
57	MG	11	101	1/1	0.93	0.10	59,59,59,59	0
57	MG	1A	3701	1/1	0.93	0.09	38,38,38,38	0
57	MG	2A	3514	1/1	0.93	0.11	57,57,57,57	0
57	MG	2a	3025	1/1	0.93	0.18	65,65,65,65	0
57	MG	2A	3515	1/1	0.93	0.15	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3220	1/1	0.93	0.18	40,40,40,40	0
57	MG	1A	3612	1/1	0.93	0.10	44,44,44,44	0
57	MG	1A	3614	1/1	0.93	0.07	31,31,31,31	0
57	MG	2a	3032	1/1	0.93	0.17	67,67,67,67	0
57	MG	2A	3225	1/1	0.93	0.26	54,54,54,54	0
57	MG	1A	3617	1/1	0.93	0.07	47,47,47,47	0
57	MG	2a	3036	1/1	0.93	0.15	63,63,63,63	0
57	MG	1e	201	1/1	0.93	0.19	52,52,52,52	0
57	MG	1e	202	1/1	0.93	0.12	50,50,50,50	0
57	MG	1A	3291	1/1	0.93	0.09	42,42,42,42	0
57	MG	1A	3991	1/1	0.93	0.14	53,53,53,53	0
57	MG	2A	3236	1/1	0.93	0.15	54,54,54,54	0
57	MG	1h	202	1/1	0.93	0.11	67,67,67,67	0
57	MG	1A	3402	1/1	0.93	0.09	42,42,42,42	0
57	MG	1A	3259	1/1	0.93	0.09	44,44,44,44	0
57	MG	19	102	1/1	0.93	0.12	57,57,57,57	0
57	MG	1a	1601	1/1	0.93	0.15	58,58,58,58	0
57	MG	2A	3540	1/1	0.93	0.15	54,54,54,54	0
57	MG	1a	1603	1/1	0.93	0.22	57,57,57,57	0
57	MG	2A	3542	1/1	0.93	0.12	52,52,52,52	0
57	MG	1o	3101	1/1	0.93	0.19	51,51,51,51	0
57	MG	2A	3251	1/1	0.93	0.22	44,44,44,44	0
57	MG	2A	3547	1/1	0.93	0.14	38,38,38,38	0
57	MG	2A	3550	1/1	0.93	0.11	50,50,50,50	0
57	MG	2A	3254	1/1	0.93	0.25	43,43,43,43	0
57	MG	2A	3256	1/1	0.93	0.10	62,62,62,62	0
57	MG	1A	3125	1/1	0.93	0.17	47,47,47,47	0
57	MG	1A	3623	1/1	0.93	0.22	28,28,28,28	0
57	MG	1A	3419	1/1	0.93	0.05	40,40,40,40	0
57	MG	2A	3267	1/1	0.93	0.20	54,54,54,54	0
57	MG	1x	101	1/1	0.93	0.07	39,39,39,39	0
57	MG	1x	102	1/1	0.93	0.11	34,34,34,34	0
57	MG	1A	3467	1/1	0.93	0.12	52,52,52,52	0
57	MG	1A	3728	1/1	0.93	0.34	34,34,34,34	0
57	MG	2A	3006	1/1	0.93	0.10	40,40,40,40	0
57	MG	2A	3570	1/1	0.93	0.09	77,77,77,77	0
57	MG	1A	4001	1/1	0.93	0.13	72,72,72,72	0
57	MG	2A	3277	1/1	0.93	0.27	61,61,61,61	0
57	MG	2A	3015	1/1	0.93	0.15	60,60,60,60	0
57	MG	2a	3090	1/1	0.93	0.12	56,56,56,56	0
57	MG	2A	3018	1/1	0.93	0.14	39,39,39,39	0
57	MG	1A	4003	1/1	0.93	0.14	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3284	1/1	0.93	0.15	44,44,44,44	0
57	MG	2a	3096	1/1	0.93	0.28	58,58,58,58	0
57	MG	1A	3422	1/1	0.93	0.07	20,20,20,20	0
57	MG	2A	3022	1/1	0.93	0.12	60,60,60,60	0
57	MG	2a	3099	1/1	0.93	0.33	59,59,59,59	0
57	MG	1a	1618	1/1	0.93	0.09	52,52,52,52	0
57	MG	2a	3101	1/1	0.93	0.23	60,60,60,60	0
57	MG	2A	3586	1/1	0.93	0.09	47,47,47,47	0
57	MG	2A	3026	1/1	0.93	0.13	58,58,58,58	0
57	MG	2A	3589	1/1	0.93	0.16	44,44,44,44	0
57	MG	2A	3591	1/1	0.93	0.12	59,59,59,59	0
57	MG	2A	3596	1/1	0.93	0.09	37,37,37,37	0
57	MG	1a	1619	1/1	0.93	0.14	66,66,66,66	0
57	MG	2A	3601	1/1	0.93	0.10	58,58,58,58	0
57	MG	1A	3732	1/1	0.93	0.09	30,30,30,30	0
57	MG	1A	3734	1/1	0.93	0.08	34,34,34,34	0
57	MG	1A	3469	1/1	0.93	0.15	62,62,62,62	0
57	MG	2a	3119	1/1	0.93	0.10	64,64,64,64	0
57	MG	2A	3608	1/1	0.93	0.14	62,62,62,62	0
57	MG	1A	3868	1/1	0.93	0.07	41,41,41,41	0
57	MG	1A	3738	1/1	0.93	0.07	49,49,49,49	0
57	MG	2A	3303	1/1	0.93	0.17	61,61,61,61	0
57	MG	2A	3045	1/1	0.93	0.10	54,54,54,54	0
57	MG	2A	3046	1/1	0.93	0.25	63,63,63,63	0
57	MG	2A	3049	1/1	0.93	0.11	50,50,50,50	0
57	MG	2a	3130	1/1	0.93	0.24	72,72,72,72	0
57	MG	1A	3370	1/1	0.93	0.10	50,50,50,50	0
57	MG	1A	3373	1/1	0.93	0.10	40,40,40,40	0
57	MG	1A	3875	1/1	0.93	0.07	39,39,39,39	0
57	MG	1A	3267	1/1	0.93	0.13	49,49,49,49	0
57	MG	2a	3138	1/1	0.93	0.20	56,56,56,56	0
57	MG	2A	3316	1/1	0.93	0.37	45,45,45,45	0
57	MG	1A	3482	1/1	0.93	0.07	14,14,14,14	0
57	MG	1a	1773	1/1	0.93	0.19	70,70,70,70	0
57	MG	2A	3627	1/1	0.93	0.10	52,52,52,52	0
57	MG	2A	3634	1/1	0.93	0.08	65,65,65,65	0
57	MG	1a	1774	1/1	0.93	0.16	58,58,58,58	0
57	MG	1A	3554	1/1	0.93	0.09	40,40,40,40	0
57	MG	1a	1649	1/1	0.93	0.18	63,63,63,63	0
57	MG	2A	3327	1/1	0.93	0.08	53,53,53,53	0
57	MG	2a	3159	1/1	0.93	0.16	61,61,61,61	0
57	MG	2A	3648	1/1	0.93	0.07	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	3162	1/1	0.93	0.13	63,63,63,63	0
57	MG	2a	3163	1/1	0.93	0.10	58,58,58,58	0
57	MG	1A	3755	1/1	0.93	0.09	55,55,55,55	0
57	MG	2A	3651	1/1	0.93	0.09	76,76,76,76	0
57	MG	1A	3651	1/1	0.93	0.13	44,44,44,44	0
57	MG	2A	3077	1/1	0.93	0.10	52,52,52,52	0
57	MG	1B	204	1/1	0.93	0.09	52,52,52,52	0
57	MG	1A	3890	1/1	0.93	0.07	47,47,47,47	0
57	MG	1A	3432	1/1	0.93	0.08	37,37,37,37	0
57	MG	2A	3667	1/1	0.93	0.13	37,37,37,37	0
57	MG	1A	3486	1/1	0.93	0.08	44,44,44,44	0
57	MG	2A	3346	1/1	0.93	0.08	40,40,40,40	0
57	MG	2A	3674	1/1	0.93	0.10	45,45,45,45	0
57	MG	2a	3176	1/1	0.93	0.07	63,63,63,63	0
57	MG	1A	3661	1/1	0.93	0.17	30,30,30,30	0
57	MG	1A	3894	1/1	0.93	0.17	30,30,30,30	0
57	MG	2A	3352	1/1	0.93	0.22	60,60,60,60	0
57	MG	1A	3197	1/1	0.93	0.10	55,55,55,55	0
57	MG	1a	1790	1/1	0.93	0.13	74,74,74,74	0
57	MG	2A	3356	1/1	0.93	0.14	61,61,61,61	0
57	MG	1A	3905	1/1	0.93	0.07	58,58,58,58	0
57	MG	2e	201	1/1	0.93	0.11	65,65,65,65	0
57	MG	1A	3219	1/1	0.93	0.18	55,55,55,55	0
57	MG	1A	3909	1/1	0.93	0.10	21,21,21,21	0
57	MG	1a	1668	1/1	0.93	0.27	64,64,64,64	0
57	MG	2A	3690	1/1	0.93	0.08	59,59,59,59	0
57	MG	1B	218	1/1	0.93	0.07	48,48,48,48	0
57	MG	2A	3105	1/1	0.93	0.11	53,53,53,53	0
57	MG	1a	1670	1/1	0.93	0.15	59,59,59,59	0
59	MPD	1A	4031	8/8	0.93	0.18	50,54,58,60	0
57	MG	2A	3377	1/1	0.93	0.12	45,45,45,45	0
57	MG	2A	3702	1/1	0.93	0.14	60,60,60,60	0
57	MG	1a	1798	1/1	0.93	0.09	49,49,49,49	0
57	MG	2A	3707	1/1	0.93	0.12	66,66,66,66	0
57	MG	2A	3708	1/1	0.93	0.12	63,63,63,63	0
57	MG	1A	3251	1/1	0.94	0.12	55,55,55,55	0
57	MG	2A	3047	1/1	0.94	0.14	48,48,48,48	0
57	MG	2A	3048	1/1	0.94	0.17	43,43,43,43	0
57	MG	2A	3336	1/1	0.94	0.14	40,40,40,40	0
57	MG	1A	3011	1/1	0.94	0.09	44,44,44,44	0
57	MG	1A	3076	1/1	0.94	0.14	34,34,34,34	0
57	MG	2A	3342	1/1	0.94	0.15	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	10	109	1/1	0.94	0.08	50,50,50,50	0
57	MG	1A	3540	1/1	0.94	0.06	24,24,24,24	0
57	MG	2A	3347	1/1	0.94	0.07	42,42,42,42	0
57	MG	2A	3348	1/1	0.94	0.07	40,40,40,40	0
57	MG	1a	1749	1/1	0.94	0.16	41,41,41,41	0
57	MG	2A	3057	1/1	0.94	0.21	69,69,69,69	0
57	MG	1A	3777	1/1	0.94	0.06	20,20,20,20	0
57	MG	2A	3060	1/1	0.94	0.06	47,47,47,47	0
57	MG	2A	3061	1/1	0.94	0.06	45,45,45,45	0
57	MG	1A	3166	1/1	0.94	0.25	58,58,58,58	0
57	MG	1A	3262	1/1	0.94	0.13	48,48,48,48	0
57	MG	1A	3659	1/1	0.94	0.17	50,50,50,50	0
57	MG	2A	3715	1/1	0.94	0.10	58,58,58,58	0
57	MG	15	3102	1/1	0.94	0.07	34,34,34,34	0
57	MG	1a	1756	1/1	0.94	0.17	58,58,58,58	0
57	MG	15	3104	1/1	0.94	0.12	38,38,38,38	0
57	MG	2A	3720	1/1	0.94	0.20	61,61,61,61	0
57	MG	2A	3721	1/1	0.94	0.11	56,56,56,56	0
57	MG	1A	3959	1/1	0.94	0.09	59,59,59,59	0
57	MG	1a	1761	1/1	0.94	0.12	54,54,54,54	0
57	MG	2A	3081	1/1	0.94	0.17	45,45,45,45	0
57	MG	1A	3388	1/1	0.94	0.14	61,61,61,61	0
57	MG	1A	3782	1/1	0.94	0.06	38,38,38,38	0
57	MG	1a	1766	1/1	0.94	0.09	61,61,61,61	0
57	MG	1A	3966	1/1	0.94	0.13	42,42,42,42	0
57	MG	2A	3386	1/1	0.94	0.12	63,63,63,63	0
57	MG	18	101	1/1	0.94	0.08	39,39,39,39	0
57	MG	1A	3324	1/1	0.94	0.15	53,53,53,53	0
57	MG	1a	1770	1/1	0.94	0.11	55,55,55,55	0
57	MG	1A	3664	1/1	0.94	0.08	41,41,41,41	0
57	MG	1A	3665	1/1	0.94	0.08	56,56,56,56	0
57	MG	1A	3264	1/1	0.94	0.07	39,39,39,39	0
57	MG	2A	3094	1/1	0.94	0.09	63,63,63,63	0
57	MG	2A	3402	1/1	0.94	0.09	41,41,41,41	0
57	MG	1A	3167	1/1	0.94	0.08	47,47,47,47	0
57	MG	2B	206	1/1	0.94	0.14	61,61,61,61	0
57	MG	1A	3470	1/1	0.94	0.13	52,52,52,52	0
57	MG	1A	3558	1/1	0.94	0.14	22,22,22,22	0
57	MG	1A	3792	1/1	0.94	0.10	49,49,49,49	0
57	MG	1A	3476	1/1	0.94	0.08	62,62,62,62	0
57	MG	2A	3108	1/1	0.94	0.10	56,56,56,56	0
57	MG	1A	3329	1/1	0.94	0.24	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3989	1/1	0.94	0.10	37,37,37,37	0
57	MG	2A	3111	1/1	0.94	0.15	63,63,63,63	0
57	MG	1a	1614	1/1	0.94	0.11	63,63,63,63	0
57	MG	1a	1616	1/1	0.94	0.10	63,63,63,63	0
57	MG	2A	3419	1/1	0.94	0.09	50,50,50,50	0
57	MG	2A	3421	1/1	0.94	0.10	34,34,34,34	0
57	MG	2E	303	1/1	0.94	0.10	47,47,47,47	0
57	MG	1A	3065	1/1	0.94	0.08	50,50,50,50	0
57	MG	1A	3804	1/1	0.94	0.14	49,49,49,49	0
57	MG	1A	3567	1/1	0.94	0.10	39,39,39,39	0
57	MG	2F	301	1/1	0.94	0.11	49,49,49,49	0
57	MG	1a	1624	1/1	0.94	0.10	68,68,68,68	0
57	MG	2A	3432	1/1	0.94	0.09	35,35,35,35	0
57	MG	1A	3807	1/1	0.94	0.08	29,29,29,29	0
57	MG	2A	3127	1/1	0.94	0.29	60,60,60,60	0
57	MG	2A	3436	1/1	0.94	0.14	74,74,74,74	0
57	MG	2A	3437	1/1	0.94	0.10	39,39,39,39	0
57	MG	1a	1626	1/1	0.94	0.23	65,65,65,65	0
57	MG	1A	3810	1/1	0.94	0.10	38,38,38,38	0
57	MG	2A	3442	1/1	0.94	0.17	59,59,59,59	0
57	MG	2T	202	1/1	0.94	0.12	52,52,52,52	0
57	MG	1A	3171	1/1	0.94	0.11	32,32,32,32	0
57	MG	1A	3815	1/1	0.94	0.29	52,52,52,52	0
57	MG	1A	3679	1/1	0.94	0.09	18,18,18,18	0
57	MG	1A	3999	1/1	0.94	0.12	47,47,47,47	0
57	MG	2Y	201	1/1	0.94	0.14	52,52,52,52	0
57	MG	2A	3451	1/1	0.94	0.07	56,56,56,56	0
57	MG	2A	3138	1/1	0.94	0.16	50,50,50,50	0
57	MG	2A	3454	1/1	0.94	0.26	61,61,61,61	0
57	MG	2I	103	1/1	0.94	0.11	55,55,55,55	0
57	MG	2A	3140	1/1	0.94	0.17	58,58,58,58	0
57	MG	1A	3570	1/1	0.94	0.22	61,61,61,61	0
57	MG	1A	3571	1/1	0.94	0.13	25,25,25,25	0
57	MG	1A	4002	1/1	0.94	0.13	33,33,33,33	0
57	MG	27	101	1/1	0.94	0.13	46,46,46,46	0
57	MG	1a	1637	1/1	0.94	0.27	63,63,63,63	0
57	MG	1a	1638	1/1	0.94	0.10	69,69,69,69	0
57	MG	1a	1640	1/1	0.94	0.15	63,63,63,63	0
57	MG	2a	3003	1/1	0.94	0.27	53,53,53,53	0
57	MG	2A	3156	1/1	0.94	0.20	46,46,46,46	0
57	MG	1a	1808	1/1	0.94	0.13	66,66,66,66	0
57	MG	1a	1641	1/1	0.94	0.16	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1643	1/1	0.94	0.20	49,49,49,49	0
57	MG	2A	3162	1/1	0.94	0.10	61,61,61,61	0
57	MG	2A	3166	1/1	0.94	0.12	55,55,55,55	0
57	MG	1A	3687	1/1	0.94	0.10	44,44,44,44	0
57	MG	2a	3015	1/1	0.94	0.13	54,54,54,54	0
57	MG	2A	3168	1/1	0.94	0.06	63,63,63,63	0
57	MG	1A	3069	1/1	0.94	0.17	43,43,43,43	0
57	MG	2A	3482	1/1	0.94	0.20	59,59,59,59	0
57	MG	1a	1648	1/1	0.94	0.12	50,50,50,50	0
57	MG	1A	3120	1/1	0.94	0.13	29,29,29,29	0
57	MG	2A	3175	1/1	0.94	0.11	59,59,59,59	0
57	MG	2A	3489	1/1	0.94	0.08	61,61,61,61	0
57	MG	1A	3178	1/1	0.94	0.16	36,36,36,36	0
57	MG	2A	3492	1/1	0.94	0.08	65,65,65,65	0
57	MG	1a	1653	1/1	0.94	0.16	50,50,50,50	0
57	MG	2a	3028	1/1	0.94	0.14	67,67,67,67	0
57	MG	2a	3029	1/1	0.94	0.08	56,56,56,56	0
57	MG	1A	3839	1/1	0.94	0.10	46,46,46,46	0
57	MG	1A	3403	1/1	0.94	0.13	47,47,47,47	0
57	MG	2A	3182	1/1	0.94	0.12	53,53,53,53	0
57	MG	2A	3503	1/1	0.94	0.07	57,57,57,57	0
57	MG	1A	3842	1/1	0.94	0.08	36,36,36,36	0
57	MG	1A	3492	1/1	0.94	0.05	25,25,25,25	0
57	MG	1A	3493	1/1	0.94	0.12	48,48,48,48	0
57	MG	1A	3582	1/1	0.94	0.12	54,54,54,54	0
57	MG	1A	3496	1/1	0.94	0.12	22,22,22,22	0
57	MG	2A	3188	1/1	0.94	0.23	54,54,54,54	0
57	MG	1a	1831	1/1	0.94	0.11	54,54,54,54	0
57	MG	1A	3083	1/1	0.94	0.19	51,51,51,51	0
57	MG	1A	3590	1/1	0.94	0.11	41,41,41,41	0
57	MG	1A	3859	1/1	0.94	0.10	45,45,45,45	0
57	MG	1A	3499	1/1	0.94	0.07	29,29,29,29	0
57	MG	2A	3197	1/1	0.94	0.09	48,48,48,48	0
57	MG	1a	1837	1/1	0.94	0.18	70,70,70,70	0
57	MG	2A	3199	1/1	0.94	0.07	56,56,56,56	0
57	MG	2A	3529	1/1	0.94	0.16	54,54,54,54	0
57	MG	1A	3706	1/1	0.94	0.10	41,41,41,41	0
57	MG	1A	3865	1/1	0.94	0.09	48,48,48,48	0
57	MG	1A	3707	1/1	0.94	0.07	47,47,47,47	0
57	MG	2a	3055	1/1	0.94	0.17	64,64,64,64	0
57	MG	1A	3085	1/1	0.94	0.09	46,46,46,46	0
57	MG	2A	3534	1/1	0.94	0.17	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	3058	1/1	0.94	0.20	64,64,64,64	0
57	MG	1a	1848	1/1	0.94	0.14	52,52,52,52	0
57	MG	1A	3595	1/1	0.94	0.11	25,25,25,25	0
57	MG	2A	3211	1/1	0.94	0.11	56,56,56,56	0
57	MG	1A	3418	1/1	0.94	0.07	37,37,37,37	0
57	MG	1A	3343	1/1	0.94	0.14	45,45,45,45	0
57	MG	2a	3065	1/1	0.94	0.10	64,64,64,64	0
57	MG	1a	1852	1/1	0.94	0.15	60,60,60,60	0
57	MG	2a	3068	1/1	0.94	0.14	61,61,61,61	0
57	MG	2A	3216	1/1	0.94	0.09	52,52,52,52	0
57	MG	1A	3022	1/1	0.94	0.11	43,43,43,43	0
57	MG	2A	3218	1/1	0.94	0.23	55,55,55,55	0
57	MG	2a	3073	1/1	0.94	0.15	62,62,62,62	0
57	MG	1A	3716	1/1	0.94	0.16	34,34,34,34	0
57	MG	2A	3545	1/1	0.94	0.10	37,37,37,37	0
57	MG	1A	3346	1/1	0.94	0.13	37,37,37,37	0
57	MG	2a	3082	1/1	0.94	0.28	64,64,64,64	0
57	MG	2A	3222	1/1	0.94	0.26	49,49,49,49	0
57	MG	1A	3347	1/1	0.94	0.09	46,46,46,46	0
57	MG	2A	3553	1/1	0.94	0.07	52,52,52,52	0
57	MG	1A	3609	1/1	0.94	0.15	58,58,58,58	0
57	MG	1A	3517	1/1	0.94	0.11	52,52,52,52	0
57	MG	1A	3230	1/1	0.94	0.12	38,38,38,38	0
57	MG	2A	3558	1/1	0.94	0.07	36,36,36,36	0
57	MG	2A	3227	1/1	0.94	0.10	49,49,49,49	0
57	MG	1A	3293	1/1	0.94	0.09	43,43,43,43	0
57	MG	1A	3731	1/1	0.94	0.15	33,33,33,33	0
57	MG	2A	3232	1/1	0.94	0.18	60,60,60,60	0
57	MG	1A	3615	1/1	0.94	0.08	48,48,48,48	0
57	MG	1A	3616	1/1	0.94	0.07	36,36,36,36	0
57	MG	1A	3895	1/1	0.94	0.11	28,28,28,28	0
57	MG	1D	309	1/1	0.94	0.22	38,38,38,38	0
57	MG	1A	3896	1/1	0.94	0.10	56,56,56,56	0
57	MG	1A	3433	1/1	0.94	0.17	53,53,53,53	0
57	MG	1A	3904	1/1	0.94	0.10	59,59,59,59	0
57	MG	1D	315	1/1	0.94	0.10	55,55,55,55	0
57	MG	2a	3113	1/1	0.94	0.07	47,47,47,47	0
57	MG	2A	3577	1/1	0.94	0.08	60,60,60,60	0
57	MG	1A	3737	1/1	0.94	0.09	42,42,42,42	0
57	MG	1a	1699	1/1	0.94	0.22	68,68,68,68	0
57	MG	2a	3118	1/1	0.94	0.17	53,53,53,53	0
57	MG	1A	3232	1/1	0.94	0.44	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3352	1/1	0.94	0.09	20,20,20,20	0
57	MG	2a	3122	1/1	0.94	0.13	53,53,53,53	0
57	MG	2A	3255	1/1	0.94	0.18	51,51,51,51	0
57	MG	1f	201	1/1	0.94	0.14	63,63,63,63	0
57	MG	2A	3587	1/1	0.94	0.15	53,53,53,53	0
57	MG	1f	202	1/1	0.94	0.09	46,46,46,46	0
57	MG	2A	3261	1/1	0.94	0.08	50,50,50,50	0
57	MG	1A	3620	1/1	0.94	0.10	51,51,51,51	0
57	MG	1h	201	1/1	0.94	0.17	56,56,56,56	0
57	MG	1A	3353	1/1	0.94	0.21	49,49,49,49	0
57	MG	2a	3133	1/1	0.94	0.07	33,33,33,33	0
57	MG	2A	3599	1/1	0.94	0.11	45,45,45,45	0
57	MG	2a	3135	1/1	0.94	0.19	53,53,53,53	0
57	MG	1G	201	1/1	0.94	0.06	67,67,67,67	0
57	MG	2A	3602	1/1	0.94	0.08	55,55,55,55	0
57	MG	2A	3604	1/1	0.94	0.07	38,38,38,38	0
57	MG	2a	3141	1/1	0.94	0.15	68,68,68,68	0
57	MG	1A	3915	1/1	0.94	0.15	26,26,26,26	0
57	MG	1A	3919	1/1	0.94	0.17	39,39,39,39	0
57	MG	1G	204	1/1	0.94	0.11	46,46,46,46	0
57	MG	1A	3527	1/1	0.94	0.07	24,24,24,24	0
57	MG	1A	3237	1/1	0.94	0.14	29,29,29,29	0
57	MG	2A	3611	1/1	0.94	0.07	63,63,63,63	0
57	MG	1a	1710	1/1	0.94	0.20	51,51,51,51	0
57	MG	2a	3153	1/1	0.94	0.07	57,57,57,57	0
57	MG	1y	201	1/1	0.94	0.08	58,58,58,58	0
57	MG	2A	3614	1/1	0.94	0.11	74,74,74,74	0
57	MG	1O	202	1/1	0.94	0.08	56,56,56,56	0
57	MG	1A	3143	1/1	0.94	0.17	42,42,42,42	0
57	MG	1Q	204	1/1	0.94	0.08	31,31,31,31	0
57	MG	1A	3927	1/1	0.94	0.09	47,47,47,47	0
57	MG	1R	205	1/1	0.94	0.14	50,50,50,50	0
57	MG	1A	3629	1/1	0.94	0.15	35,35,35,35	0
57	MG	2A	3004	1/1	0.94	0.12	57,57,57,57	0
57	MG	1A	3089	1/1	0.94	0.14	44,44,44,44	0
57	MG	2A	3007	1/1	0.94	0.15	40,40,40,40	0
57	MG	2A	3293	1/1	0.94	0.19	52,52,52,52	0
57	MG	2A	3009	1/1	0.94	0.13	66,66,66,66	0
57	MG	2A	3631	1/1	0.94	0.13	51,51,51,51	0
57	MG	2A	3011	1/1	0.94	0.12	55,55,55,55	0
57	MG	1A	3633	1/1	0.94	0.10	46,46,46,46	0
57	MG	1T	204	1/1	0.94	0.08	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1721	1/1	0.94	0.16	63,63,63,63	0
57	MG	2A	3304	1/1	0.94	0.22	66,66,66,66	0
57	MG	2A	3305	1/1	0.94	0.08	49,49,49,49	0
57	MG	1U	206	1/1	0.94	0.10	37,37,37,37	0
57	MG	1A	3635	1/1	0.94	0.13	57,57,57,57	0
57	MG	1a	1725	1/1	0.94	0.15	51,51,51,51	0
57	MG	2A	3654	1/1	0.94	0.10	55,55,55,55	0
57	MG	1A	3362	1/1	0.94	0.05	40,40,40,40	0
57	MG	1A	3366	1/1	0.94	0.07	37,37,37,37	0
57	MG	1W	202	1/1	0.94	0.14	45,45,45,45	0
57	MG	1A	3248	1/1	0.94	0.11	50,50,50,50	0
57	MG	2A	3663	1/1	0.94	0.14	58,58,58,58	0
57	MG	2A	3664	1/1	0.94	0.10	41,41,41,41	0
57	MG	2A	3032	1/1	0.94	0.12	54,54,54,54	0
57	MG	2A	3033	1/1	0.94	0.10	49,49,49,49	0
57	MG	2A	3038	1/1	0.94	0.14	47,47,47,47	0
57	MG	1A	3314	1/1	0.94	0.10	35,35,35,35	0
57	MG	1Z	301	1/1	0.94	0.14	44,44,44,44	0
57	MG	10	101	1/1	0.94	0.28	40,40,40,40	0
57	MG	1a	1737	1/1	0.94	0.11	68,68,68,68	0
57	MG	10	103	1/1	0.94	0.09	50,50,50,50	0
57	MG	2A	3682	1/1	0.94	0.11	60,60,60,60	0
57	MG	2A	3359	1/1	0.95	0.09	59,59,59,59	0
57	MG	2A	3100	1/1	0.95	0.19	60,60,60,60	0
57	MG	2A	3362	1/1	0.95	0.09	51,51,51,51	0
57	MG	1a	1621	1/1	0.95	0.07	66,66,66,66	0
57	MG	1A	3544	1/1	0.95	0.06	49,49,49,49	0
57	MG	1A	3331	1/1	0.95	0.12	40,40,40,40	0
57	MG	2A	3368	1/1	0.95	0.09	47,47,47,47	0
57	MG	2A	3692	1/1	0.95	0.17	53,53,53,53	0
57	MG	2A	3693	1/1	0.95	0.08	34,34,34,34	0
57	MG	1A	3549	1/1	0.95	0.11	56,56,56,56	0
57	MG	2A	3695	1/1	0.95	0.08	41,41,41,41	0
57	MG	2A	3372	1/1	0.95	0.11	38,38,38,38	0
57	MG	2A	3698	1/1	0.95	0.23	61,61,61,61	0
57	MG	1a	1627	1/1	0.95	0.15	57,57,57,57	0
57	MG	1a	1795	1/1	0.95	0.10	48,48,48,48	0
57	MG	2A	3378	1/1	0.95	0.08	30,30,30,30	0
57	MG	2A	3706	1/1	0.95	0.09	50,50,50,50	0
57	MG	1A	3671	1/1	0.95	0.11	48,48,48,48	0
57	MG	2A	3114	1/1	0.95	0.18	44,44,44,44	0
57	MG	2A	3116	1/1	0.95	0.22	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3813	1/1	0.95	0.07	46,46,46,46	0
57	MG	1A	3236	1/1	0.95	0.20	57,57,57,57	0
57	MG	2A	3387	1/1	0.95	0.07	48,48,48,48	0
57	MG	1A	3008	1/1	0.95	0.12	39,39,39,39	0
57	MG	1A	3239	1/1	0.95	0.14	35,35,35,35	0
57	MG	2A	3390	1/1	0.95	0.06	33,33,33,33	0
57	MG	1A	3241	1/1	0.95	0.18	38,38,38,38	0
57	MG	1A	3818	1/1	0.95	0.09	43,43,43,43	0
57	MG	1a	1804	1/1	0.95	0.29	59,59,59,59	0
57	MG	1A	3555	1/1	0.95	0.08	48,48,48,48	0
57	MG	1A	3820	1/1	0.95	0.10	52,52,52,52	0
57	MG	2A	3401	1/1	0.95	0.09	59,59,59,59	0
57	MG	1A	3821	1/1	0.95	0.06	42,42,42,42	0
57	MG	1A	3823	1/1	0.95	0.07	40,40,40,40	0
57	MG	1A	3825	1/1	0.95	0.07	58,58,58,58	0
57	MG	1A	4016	1/1	0.95	0.06	40,40,40,40	0
57	MG	1A	3095	1/1	0.95	0.10	39,39,39,39	0
57	MG	2A	3137	1/1	0.95	0.15	38,38,38,38	0
57	MG	1A	3831	1/1	0.95	0.09	48,48,48,48	0
57	MG	2A	3411	1/1	0.95	0.06	59,59,59,59	0
57	MG	2A	3412	1/1	0.95	0.07	63,63,63,63	0
57	MG	2A	3413	1/1	0.95	0.07	33,33,33,33	0
57	MG	2A	3139	1/1	0.95	0.21	61,61,61,61	0
57	MG	1A	3096	1/1	0.95	0.08	15,15,15,15	0
57	MG	2A	3142	1/1	0.95	0.13	55,55,55,55	0
57	MG	2A	3145	1/1	0.95	0.13	63,63,63,63	0
57	MG	1A	3833	1/1	0.95	0.22	38,38,38,38	0
57	MG	2A	3147	1/1	0.95	0.10	45,45,45,45	0
57	MG	2B	209	1/1	0.95	0.16	55,55,55,55	0
57	MG	1a	1820	1/1	0.95	0.06	69,69,69,69	0
57	MG	1A	3835	1/1	0.95	0.06	23,23,23,23	0
57	MG	1a	1651	1/1	0.95	0.08	49,49,49,49	0
57	MG	2A	3424	1/1	0.95	0.09	44,44,44,44	0
57	MG	2A	3425	1/1	0.95	0.14	61,61,61,61	0
57	MG	1A	3836	1/1	0.95	0.06	41,41,41,41	0
57	MG	2D	303	1/1	0.95	0.14	53,53,53,53	0
57	MG	2D	304	1/1	0.95	0.37	43,43,43,43	0
57	MG	2A	3429	1/1	0.95	0.11	50,50,50,50	0
57	MG	2D	308	1/1	0.95	0.07	48,48,48,48	0
57	MG	1A	3247	1/1	0.95	0.20	51,51,51,51	0
57	MG	2A	3155	1/1	0.95	0.09	50,50,50,50	0
57	MG	1A	3097	1/1	0.95	0.07	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3562	1/1	0.95	0.10	42,42,42,42	0
57	MG	2A	3158	1/1	0.95	0.24	63,63,63,63	0
57	MG	1A	3451	1/1	0.95	0.07	17,17,17,17	0
57	MG	1A	3691	1/1	0.95	0.08	66,66,66,66	0
57	MG	1A	3565	1/1	0.95	0.23	50,50,50,50	0
57	MG	2E	308	1/1	0.95	0.15	59,59,59,59	0
57	MG	2A	3441	1/1	0.95	0.10	63,63,63,63	0
57	MG	2A	3165	1/1	0.95	0.10	43,43,43,43	0
57	MG	1A	3173	1/1	0.95	0.10	35,35,35,35	0
57	MG	2A	3444	1/1	0.95	0.22	59,59,59,59	0
57	MG	1A	3253	1/1	0.95	0.09	35,35,35,35	0
57	MG	2A	3448	1/1	0.95	0.27	57,57,57,57	0
57	MG	1A	3174	1/1	0.95	0.06	44,44,44,44	0
57	MG	2A	3169	1/1	0.95	0.09	46,46,46,46	0
57	MG	1A	3348	1/1	0.95	0.09	46,46,46,46	0
57	MG	1A	3004	1/1	0.95	0.07	40,40,40,40	0
57	MG	1a	1839	1/1	0.95	0.14	70,70,70,70	0
57	MG	1A	3260	1/1	0.95	0.06	46,46,46,46	0
57	MG	2T	204	1/1	0.95	0.11	50,50,50,50	0
57	MG	2A	3457	1/1	0.95	0.06	38,38,38,38	0
57	MG	2A	3459	1/1	0.95	0.11	55,55,55,55	0
57	MG	1A	3575	1/1	0.95	0.07	41,41,41,41	0
57	MG	1A	3702	1/1	0.95	0.15	40,40,40,40	0
57	MG	2A	3463	1/1	0.95	0.10	65,65,65,65	0
57	MG	1A	3100	1/1	0.95	0.09	43,43,43,43	0
57	MG	1a	1847	1/1	0.95	0.15	67,67,67,67	0
57	MG	2A	3466	1/1	0.95	0.06	70,70,70,70	0
57	MG	1A	3042	1/1	0.95	0.06	30,30,30,30	0
57	MG	1A	3107	1/1	0.95	0.14	28,28,28,28	0
57	MG	1A	3355	1/1	0.95	0.06	21,21,21,21	0
57	MG	1A	3266	1/1	0.95	0.07	67,67,67,67	0
57	MG	1A	3471	1/1	0.95	0.07	45,45,45,45	0
57	MG	1A	3475	1/1	0.95	0.12	57,57,57,57	0
57	MG	1A	3589	1/1	0.95	0.05	55,55,55,55	0
57	MG	2A	3474	1/1	0.95	0.10	56,56,56,56	0
57	MG	1a	1679	1/1	0.95	0.21	60,60,60,60	0
57	MG	1A	3877	1/1	0.95	0.08	29,29,29,29	0
57	MG	2a	3005	1/1	0.95	0.07	52,52,52,52	0
57	MG	1a	1681	1/1	0.95	0.11	66,66,66,66	0
57	MG	1D	305	1/1	0.95	0.12	34,34,34,34	0
57	MG	2A	3194	1/1	0.95	0.08	41,41,41,41	0
57	MG	1a	1683	1/1	0.95	0.08	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3186	1/1	0.95	0.09	32,32,32,32	0
57	MG	2A	3485	1/1	0.95	0.07	48,48,48,48	0
57	MG	1A	3591	1/1	0.95	0.07	40,40,40,40	0
57	MG	1A	3108	1/1	0.95	0.07	34,34,34,34	0
57	MG	2A	3490	1/1	0.95	0.09	32,32,32,32	0
57	MG	1D	312	1/1	0.95	0.14	36,36,36,36	0
57	MG	2A	3202	1/1	0.95	0.13	60,60,60,60	0
57	MG	2A	3203	1/1	0.95	0.08	50,50,50,50	0
57	MG	2A	3204	1/1	0.95	0.06	46,46,46,46	0
57	MG	1a	1869	1/1	0.95	0.17	55,55,55,55	0
57	MG	2A	3497	1/1	0.95	0.07	42,42,42,42	0
57	MG	1A	3047	1/1	0.95	0.19	48,48,48,48	0
57	MG	2A	3501	1/1	0.95	0.14	56,56,56,56	0
57	MG	2A	3207	1/1	0.95	0.25	61,61,61,61	0
57	MG	1a	1690	1/1	0.95	0.18	67,67,67,67	0
57	MG	1a	1872	1/1	0.95	0.07	45,45,45,45	0
57	MG	1A	3723	1/1	0.95	0.06	55,55,55,55	0
57	MG	2A	3507	1/1	0.95	0.06	44,44,44,44	0
57	MG	1A	3479	1/1	0.95	0.07	58,58,58,58	0
57	MG	1E	304	1/1	0.95	0.07	21,21,21,21	0
57	MG	2a	3035	1/1	0.95	0.06	46,46,46,46	0
57	MG	2A	3510	1/1	0.95	0.11	49,49,49,49	0
57	MG	2A	3511	1/1	0.95	0.10	55,55,55,55	0
57	MG	1A	3725	1/1	0.95	0.14	41,41,41,41	0
57	MG	2A	3513	1/1	0.95	0.09	60,60,60,60	0
57	MG	1A	3052	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3056	1/1	0.95	0.10	42,42,42,42	0
57	MG	1F	307	1/1	0.95	0.28	27,27,27,27	0
57	MG	2A	3517	1/1	0.95	0.07	44,44,44,44	0
57	MG	2A	3519	1/1	0.95	0.13	58,58,58,58	0
57	MG	1F	313	1/1	0.95	0.10	42,42,42,42	0
57	MG	2a	3047	1/1	0.95	0.26	63,63,63,63	0
57	MG	1A	3730	1/1	0.95	0.26	39,39,39,39	0
57	MG	1A	3483	1/1	0.95	0.07	25,25,25,25	0
57	MG	2A	3523	1/1	0.95	0.09	61,61,61,61	0
57	MG	1A	3126	1/1	0.95	0.18	52,52,52,52	0
57	MG	1A	3903	1/1	0.95	0.06	33,33,33,33	0
57	MG	1A	3485	1/1	0.95	0.08	46,46,46,46	0
57	MG	1A	3608	1/1	0.95	0.10	57,57,57,57	0
57	MG	1A	3281	1/1	0.95	0.14	58,58,58,58	0
57	MG	1A	3908	1/1	0.95	0.06	15,15,15,15	0
57	MG	2A	3228	1/1	0.95	0.21	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1m	201	1/1	0.95	0.06	72,72,72,72	0
57	MG	1O	201	1/1	0.95	0.06	48,48,48,48	0
57	MG	2A	3231	1/1	0.95	0.15	48,48,48,48	0
57	MG	1A	3082	1/1	0.95	0.08	33,33,33,33	0
57	MG	1P	202	1/1	0.95	0.14	25,25,25,25	0
57	MG	1t	201	1/1	0.95	0.12	60,60,60,60	0
57	MG	1A	3739	1/1	0.95	0.06	31,31,31,31	0
57	MG	2A	3237	1/1	0.95	0.22	47,47,47,47	0
57	MG	1A	3129	1/1	0.95	0.18	68,68,68,68	0
57	MG	1R	202	1/1	0.95	0.17	33,33,33,33	0
57	MG	1A	3379	1/1	0.95	0.11	34,34,34,34	0
57	MG	1A	3290	1/1	0.95	0.12	56,56,56,56	0
57	MG	2A	3546	1/1	0.95	0.14	55,55,55,55	0
57	MG	2a	3074	1/1	0.95	0.09	59,59,59,59	0
57	MG	1A	3199	1/1	0.95	0.16	56,56,56,56	0
57	MG	2A	3548	1/1	0.95	0.12	26,26,26,26	0
57	MG	1A	3131	1/1	0.95	0.06	35,35,35,35	0
57	MG	2a	3081	1/1	0.95	0.06	69,69,69,69	0
57	MG	1A	3923	1/1	0.95	0.05	23,23,23,23	0
57	MG	2a	3083	1/1	0.95	0.22	66,66,66,66	0
57	MG	2a	3084	1/1	0.95	0.07	65,65,65,65	0
57	MG	1A	3201	1/1	0.95	0.21	50,50,50,50	0
57	MG	2A	3253	1/1	0.95	0.10	32,32,32,32	0
57	MG	2a	3087	1/1	0.95	0.10	61,61,61,61	0
57	MG	1T	205	1/1	0.95	0.06	49,49,49,49	0
57	MG	2A	3556	1/1	0.95	0.08	63,63,63,63	0
57	MG	2a	3092	1/1	0.95	0.33	58,58,58,58	0
57	MG	1U	201	1/1	0.95	0.18	29,29,29,29	0
57	MG	2A	3008	1/1	0.95	0.08	43,43,43,43	0
57	MG	2A	3258	1/1	0.95	0.45	61,61,61,61	0
57	MG	1a	1723	1/1	0.95	0.16	56,56,56,56	0
57	MG	1A	3202	1/1	0.95	0.07	31,31,31,31	0
57	MG	1U	207	1/1	0.95	0.16	49,49,49,49	0
57	MG	2A	3265	1/1	0.95	0.12	30,30,30,30	0
57	MG	1A	3928	1/1	0.95	0.11	48,48,48,48	0
57	MG	1A	3035	1/1	0.95	0.12	44,44,44,44	0
57	MG	2a	3103	1/1	0.95	0.15	50,50,50,50	0
57	MG	1A	3394	1/1	0.95	0.07	47,47,47,47	0
57	MG	2A	3020	1/1	0.95	0.21	45,45,45,45	0
57	MG	1A	3933	1/1	0.95	0.11	38,38,38,38	0
57	MG	1A	3512	1/1	0.95	0.09	60,60,60,60	0
57	MG	2A	3023	1/1	0.95	0.13	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
57	MG	2A	3274	1/1	0.95	0.12	61,61,61,61	0
57	MG	1A	3302	1/1	0.95	0.12	34,34,34,34	0
57	MG	2A	3025	1/1	0.95	0.06	34,34,34,34	0
57	MG	1A	3396	1/1	0.95	0.10	34,34,34,34	0
57	MG	1A	3134	1/1	0.95	0.21	35,35,35,35	0
57	MG	2A	3030	1/1	0.95	0.17	52,52,52,52	0
57	MG	2A	3283	1/1	0.95	0.07	53,53,53,53	0
57	MG	2a	3120	1/1	0.95	0.10	57,57,57,57	0
57	MG	1A	3941	1/1	0.95	0.05	27,27,27,27	0
57	MG	1A	3141	1/1	0.95	0.07	41,41,41,41	0
57	MG	1A	3944	1/1	0.95	0.07	35,35,35,35	0
57	MG	2A	3036	1/1	0.95	0.20	56,56,56,56	0
57	MG	2a	3125	1/1	0.95	0.10	61,61,61,61	0
57	MG	2A	3593	1/1	0.95	0.13	58,58,58,58	0
57	MG	1A	3945	1/1	0.95	0.06	47,47,47,47	0
57	MG	1A	3771	1/1	0.95	0.07	44,44,44,44	0
57	MG	2A	3598	1/1	0.95	0.06	33,33,33,33	0
57	MG	1a	1747	1/1	0.95	0.09	65,65,65,65	0
57	MG	1A	3309	1/1	0.95	0.09	48,48,48,48	0
57	MG	1A	3773	1/1	0.95	0.12	47,47,47,47	0
57	MG	2A	3603	1/1	0.95	0.10	44,44,44,44	0
57	MG	2A	3295	1/1	0.95	0.21	54,54,54,54	0
57	MG	1A	3212	1/1	0.95	0.15	46,46,46,46	0
57	MG	1A	3312	1/1	0.95	0.05	16,16,16,16	0
57	MG	1A	3638	1/1	0.95	0.06	22,22,22,22	0
57	MG	2a	3140	1/1	0.95	0.12	58,58,58,58	0
57	MG	2A	3302	1/1	0.95	0.20	53,53,53,53	0
57	MG	1A	3063	1/1	0.95	0.14	52,52,52,52	0
57	MG	1A	3956	1/1	0.95	0.07	54,54,54,54	0
57	MG	15	3105	1/1	0.95	0.06	38,38,38,38	0
57	MG	2a	3148	1/1	0.95	0.09	68,68,68,68	0
57	MG	1A	3641	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	3148	1/1	0.95	0.21	59,59,59,59	0
57	MG	1A	3217	1/1	0.95	0.09	31,31,31,31	0
57	MG	1a	1762	1/1	0.95	0.11	55,55,55,55	0
57	MG	1A	3410	1/1	0.95	0.05	32,32,32,32	0
57	MG	2A	3311	1/1	0.95	0.14	52,52,52,52	0
57	MG	17	101	1/1	0.95	0.06	33,33,33,33	0
57	MG	2a	3156	1/1	0.95	0.11	69,69,69,69	0
57	MG	2A	3314	1/1	0.95	0.24	50,50,50,50	0
57	MG	1A	3413	1/1	0.95	0.08	27,27,27,27	0
57	MG	1A	3963	1/1	0.95	0.07	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	19	101	1/1	0.95	0.14	51,51,51,51	0
57	MG	2A	3065	1/1	0.95	0.07	51,51,51,51	0
57	MG	1A	3965	1/1	0.95	0.07	41,41,41,41	0
57	MG	2A	3322	1/1	0.95	0.18	57,57,57,57	0
57	MG	1A	3414	1/1	0.95	0.09	21,21,21,21	0
57	MG	2A	3072	1/1	0.95	0.12	63,63,63,63	0
57	MG	2A	3638	1/1	0.95	0.12	58,58,58,58	0
57	MG	1a	1602	1/1	0.95	0.10	63,63,63,63	0
57	MG	1A	3086	1/1	0.95	0.16	39,39,39,39	0
57	MG	2A	3645	1/1	0.95	0.13	39,39,39,39	0
57	MG	1A	3222	1/1	0.95	0.07	26,26,26,26	0
57	MG	1A	3153	1/1	0.95	0.06	59,59,59,59	0
57	MG	1A	3037	1/1	0.95	0.09	42,42,42,42	0
57	MG	2a	3177	1/1	0.95	0.10	64,64,64,64	0
57	MG	2a	3178	1/1	0.95	0.10	74,74,74,74	0
57	MG	2A	3334	1/1	0.95	0.08	23,23,23,23	0
57	MG	1A	3228	1/1	0.95	0.13	34,34,34,34	0
57	MG	1A	3427	1/1	0.95	0.18	61,61,61,61	0
57	MG	2A	3084	1/1	0.95	0.07	40,40,40,40	0
57	MG	1a	1778	1/1	0.95	0.13	46,46,46,46	0
57	MG	1A	3066	1/1	0.95	0.09	39,39,39,39	0
57	MG	2A	3344	1/1	0.95	0.10	58,58,58,58	0
57	MG	2a	3188	1/1	0.95	0.18	47,47,47,47	0
57	MG	1a	1781	1/1	0.95	0.23	67,67,67,67	0
57	MG	1a	1611	1/1	0.95	0.10	58,58,58,58	0
57	MG	1a	1783	1/1	0.95	0.07	62,62,62,62	0
57	MG	2A	3669	1/1	0.95	0.07	56,56,56,56	0
57	MG	1A	3982	1/1	0.95	0.21	46,46,46,46	0
57	MG	2A	3671	1/1	0.95	0.11	47,47,47,47	0
57	MG	2t	201	1/1	0.95	0.10	43,43,43,43	0
57	MG	1A	3793	1/1	0.95	0.15	33,33,33,33	0
57	MG	1A	3327	1/1	0.95	0.10	55,55,55,55	0
58	ARG	1B	230	12/12	0.95	0.09	28,43,53,54	0
57	MG	1A	3666	1/1	0.95	0.07	54,54,54,54	0
59	MPD	18	103	8/8	0.95	0.13	28,35,38,40	0
57	MG	2A	3354	1/1	0.95	0.06	31,31,31,31	0
57	MG	2A	3095	1/1	0.95	0.12	56,56,56,56	0
57	MG	1A	3800	1/1	0.95	0.09	47,47,47,47	0
57	MG	1A	3164	1/1	0.95	0.19	36,36,36,36	0
57	MG	2A	3358	1/1	0.95	0.09	34,34,34,34	0
60	ZN	24	501	1/1	0.95	0.14	136,136,136,136	0
57	MG	1A	3935	1/1	0.96	0.09	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3714	1/1	0.96	0.07	53,53,53,53	0
57	MG	1A	3751	1/1	0.96	0.10	39,39,39,39	0
57	MG	1A	3487	1/1	0.96	0.06	58,58,58,58	0
57	MG	2A	3717	1/1	0.96	0.11	52,52,52,52	0
57	MG	1A	3611	1/1	0.96	0.06	24,24,24,24	0
57	MG	1A	3939	1/1	0.96	0.07	49,49,49,49	0
57	MG	1A	3754	1/1	0.96	0.09	45,45,45,45	0
57	MG	1A	3091	1/1	0.96	0.11	37,37,37,37	0
57	MG	17	102	1/1	0.96	0.14	35,35,35,35	0
57	MG	2A	3141	1/1	0.96	0.10	46,46,46,46	0
57	MG	17	104	1/1	0.96	0.13	51,51,51,51	0
57	MG	2A	3143	1/1	0.96	0.20	48,48,48,48	0
57	MG	1A	3942	1/1	0.96	0.11	48,48,48,48	0
57	MG	1A	3303	1/1	0.96	0.06	48,48,48,48	0
57	MG	1A	3391	1/1	0.96	0.08	22,22,22,22	0
57	MG	1A	3758	1/1	0.96	0.13	54,54,54,54	0
57	MG	2A	3420	1/1	0.96	0.10	48,48,48,48	0
57	MG	2A	3149	1/1	0.96	0.16	66,66,66,66	0
57	MG	19	103	1/1	0.96	0.06	68,68,68,68	0
57	MG	1A	3759	1/1	0.96	0.06	24,24,24,24	0
57	MG	1A	3494	1/1	0.96	0.08	37,37,37,37	0
57	MG	1A	3392	1/1	0.96	0.08	48,48,48,48	0
57	MG	2B	202	1/1	0.96	0.25	69,69,69,69	0
57	MG	1a	1806	1/1	0.96	0.14	64,64,64,64	0
57	MG	1A	3763	1/1	0.96	0.15	54,54,54,54	0
57	MG	1A	3951	1/1	0.96	0.07	50,50,50,50	0
57	MG	2A	3431	1/1	0.96	0.16	51,51,51,51	0
57	MG	1A	3304	1/1	0.96	0.10	32,32,32,32	0
57	MG	2B	208	1/1	0.96	0.11	52,52,52,52	0
57	MG	1A	3306	1/1	0.96	0.18	43,43,43,43	0
57	MG	1a	1608	1/1	0.96	0.08	56,56,56,56	0
57	MG	2A	3161	1/1	0.96	0.19	62,62,62,62	0
57	MG	1A	3766	1/1	0.96	0.05	32,32,32,32	0
57	MG	2A	3164	1/1	0.96	0.11	43,43,43,43	0
57	MG	1A	3221	1/1	0.96	0.15	54,54,54,54	0
57	MG	2B	215	1/1	0.96	0.14	64,64,64,64	0
57	MG	1A	3092	1/1	0.96	0.10	47,47,47,47	0
57	MG	2B	217	1/1	0.96	0.06	69,69,69,69	0
57	MG	1a	1817	1/1	0.96	0.19	66,66,66,66	0
57	MG	1A	3769	1/1	0.96	0.08	40,40,40,40	0
57	MG	2D	305	1/1	0.96	0.13	37,37,37,37	0
57	MG	1A	3503	1/1	0.96	0.06	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2D	307	1/1	0.96	0.18	41,41,41,41	0
57	MG	1A	3007	1/1	0.96	0.10	37,37,37,37	0
57	MG	2A	3446	1/1	0.96	0.14	45,45,45,45	0
57	MG	2A	3171	1/1	0.96	0.12	53,53,53,53	0
57	MG	1A	3506	1/1	0.96	0.09	27,27,27,27	0
57	MG	1A	3626	1/1	0.96	0.15	28,28,28,28	0
57	MG	1A	3964	1/1	0.96	0.14	34,34,34,34	0
57	MG	1a	1825	1/1	0.96	0.08	51,51,51,51	0
57	MG	2A	3178	1/1	0.96	0.12	51,51,51,51	0
57	MG	1A	3310	1/1	0.96	0.11	35,35,35,35	0
57	MG	1A	3509	1/1	0.96	0.14	18,18,18,18	0
57	MG	1A	3062	1/1	0.96	0.07	36,36,36,36	0
57	MG	1A	3634	1/1	0.96	0.08	35,35,35,35	0
57	MG	1A	3400	1/1	0.96	0.07	26,26,26,26	0
57	MG	1A	3227	1/1	0.96	0.05	40,40,40,40	0
57	MG	1A	3313	1/1	0.96	0.15	36,36,36,36	0
57	MG	1A	3977	1/1	0.96	0.08	55,55,55,55	0
57	MG	1A	3978	1/1	0.96	0.06	44,44,44,44	0
57	MG	1A	3132	1/1	0.96	0.12	46,46,46,46	0
57	MG	1A	3520	1/1	0.96	0.08	48,48,48,48	0
57	MG	1A	3981	1/1	0.96	0.07	24,24,24,24	0
57	MG	1A	3642	1/1	0.96	0.13	45,45,45,45	0
57	MG	1a	1842	1/1	0.96	0.06	58,58,58,58	0
57	MG	1A	3229	1/1	0.96	0.08	39,39,39,39	0
57	MG	1a	1845	1/1	0.96	0.06	64,64,64,64	0
57	MG	1A	3045	1/1	0.96	0.09	23,23,23,23	0
57	MG	2W	201	1/1	0.96	0.23	45,45,45,45	0
57	MG	1A	3986	1/1	0.96	0.06	45,45,45,45	0
57	MG	1A	3407	1/1	0.96	0.06	40,40,40,40	0
57	MG	2A	3200	1/1	0.96	0.11	51,51,51,51	0
57	MG	2A	3479	1/1	0.96	0.07	57,57,57,57	0
57	MG	1a	1642	1/1	0.96	0.17	58,58,58,58	0
57	MG	1A	3647	1/1	0.96	0.06	31,31,31,31	0
57	MG	1A	3409	1/1	0.96	0.05	25,25,25,25	0
57	MG	1A	3525	1/1	0.96	0.07	39,39,39,39	0
57	MG	1a	1853	1/1	0.96	0.16	50,50,50,50	0
57	MG	1a	1855	1/1	0.96	0.10	60,60,60,60	0
57	MG	1a	1647	1/1	0.96	0.13	50,50,50,50	0
57	MG	1A	3034	1/1	0.96	0.05	40,40,40,40	0
57	MG	1A	3794	1/1	0.96	0.12	24,24,24,24	0
57	MG	1A	3652	1/1	0.96	0.08	37,37,37,37	0
57	MG	1A	3796	1/1	0.96	0.06	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3212	1/1	0.96	0.05	43,43,43,43	0
57	MG	1A	3653	1/1	0.96	0.14	41,41,41,41	0
57	MG	1A	3799	1/1	0.96	0.12	54,54,54,54	0
57	MG	1a	1655	1/1	0.96	0.12	50,50,50,50	0
57	MG	1A	3411	1/1	0.96	0.06	29,29,29,29	0
57	MG	1A	3801	1/1	0.96	0.09	31,31,31,31	0
57	MG	2a	3010	1/1	0.96	0.09	52,52,52,52	0
57	MG	2a	3011	1/1	0.96	0.08	62,62,62,62	0
57	MG	1A	3802	1/1	0.96	0.07	43,43,43,43	0
57	MG	1A	3655	1/1	0.96	0.06	23,23,23,23	0
57	MG	1A	3234	1/1	0.96	0.14	34,34,34,34	0
57	MG	2A	3221	1/1	0.96	0.12	50,50,50,50	0
57	MG	1A	3136	1/1	0.96	0.10	43,43,43,43	0
57	MG	1A	4005	1/1	0.96	0.06	30,30,30,30	0
57	MG	1A	3417	1/1	0.96	0.09	25,25,25,25	0
57	MG	1a	1665	1/1	0.96	0.07	69,69,69,69	0
57	MG	2a	3021	1/1	0.96	0.09	50,50,50,50	0
57	MG	1A	3180	1/1	0.96	0.17	21,21,21,21	0
57	MG	1A	4010	1/1	0.96	0.09	57,57,57,57	0
57	MG	1A	4014	1/1	0.96	0.06	40,40,40,40	0
57	MG	1A	3811	1/1	0.96	0.09	34,34,34,34	0
57	MG	1A	4017	1/1	0.96	0.20	29,29,29,29	0
57	MG	1A	3663	1/1	0.96	0.10	29,29,29,29	0
57	MG	2A	3518	1/1	0.96	0.06	65,65,65,65	0
57	MG	1A	3137	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3420	1/1	0.96	0.09	14,14,14,14	0
57	MG	1A	3182	1/1	0.96	0.10	28,28,28,28	0
57	MG	1A	3183	1/1	0.96	0.10	55,55,55,55	0
57	MG	1A	3328	1/1	0.96	0.13	48,48,48,48	0
57	MG	1A	3426	1/1	0.96	0.09	28,28,28,28	0
57	MG	2A	3239	1/1	0.96	0.12	54,54,54,54	0
57	MG	2A	3528	1/1	0.96	0.06	39,39,39,39	0
57	MG	1A	3184	1/1	0.96	0.31	40,40,40,40	0
57	MG	1A	4029	1/1	0.96	0.06	52,52,52,52	0
57	MG	1A	3140	1/1	0.96	0.07	44,44,44,44	0
57	MG	1n	101	1/1	0.96	0.13	55,55,55,55	0
57	MG	2a	3042	1/1	0.96	0.20	48,48,48,48	0
57	MG	1A	3822	1/1	0.96	0.07	38,38,38,38	0
57	MG	1A	3672	1/1	0.96	0.12	51,51,51,51	0
57	MG	2A	3247	1/1	0.96	0.08	47,47,47,47	0
57	MG	2A	3248	1/1	0.96	0.07	43,43,43,43	0
57	MG	1A	3430	1/1	0.96	0.06	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3545	1/1	0.96	0.07	37,37,37,37	0
57	MG	1A	3334	1/1	0.96	0.19	40,40,40,40	0
57	MG	1A	3049	1/1	0.96	0.09	38,38,38,38	0
57	MG	1A	3189	1/1	0.96	0.15	35,35,35,35	0
57	MG	1y	203	1/1	0.96	0.08	68,68,68,68	0
57	MG	1A	3142	1/1	0.96	0.08	51,51,51,51	0
57	MG	2A	3260	1/1	0.96	0.25	55,55,55,55	0
57	MG	1a	1689	1/1	0.96	0.15	45,45,45,45	0
57	MG	1A	3680	1/1	0.96	0.06	38,38,38,38	0
57	MG	1A	3254	1/1	0.96	0.29	34,34,34,34	0
57	MG	1A	3256	1/1	0.96	0.22	45,45,45,45	0
57	MG	1a	1693	1/1	0.96	0.17	58,58,58,58	0
57	MG	1B	216	1/1	0.96	0.11	44,44,44,44	0
57	MG	1A	3684	1/1	0.96	0.06	51,51,51,51	0
57	MG	1A	3840	1/1	0.96	0.09	36,36,36,36	0
57	MG	2a	3063	1/1	0.96	0.29	62,62,62,62	0
57	MG	1A	3257	1/1	0.96	0.22	44,44,44,44	0
57	MG	1A	3556	1/1	0.96	0.09	54,54,54,54	0
57	MG	1A	3444	1/1	0.96	0.10	24,24,24,24	0
57	MG	2a	3067	1/1	0.96	0.18	54,54,54,54	0
57	MG	1B	225	1/1	0.96	0.06	57,57,57,57	0
57	MG	2A	3016	1/1	0.96	0.29	42,42,42,42	0
57	MG	1A	3690	1/1	0.96	0.11	30,30,30,30	0
57	MG	2A	3563	1/1	0.96	0.07	74,74,74,74	0
57	MG	2a	3072	1/1	0.96	0.25	40,40,40,40	0
57	MG	1A	3084	1/1	0.96	0.28	40,40,40,40	0
57	MG	2A	3280	1/1	0.96	0.18	48,48,48,48	0
57	MG	1A	3852	1/1	0.96	0.11	49,49,49,49	0
57	MG	2A	3282	1/1	0.96	0.07	42,42,42,42	0
57	MG	2a	3077	1/1	0.96	0.14	49,49,49,49	0
57	MG	2a	3078	1/1	0.96	0.13	62,62,62,62	0
57	MG	2a	3079	1/1	0.96	0.39	59,59,59,59	0
57	MG	1A	3446	1/1	0.96	0.16	36,36,36,36	0
57	MG	1D	304	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	3145	1/1	0.96	0.06	38,38,38,38	0
57	MG	1A	3856	1/1	0.96	0.06	29,29,29,29	0
57	MG	1A	3067	1/1	0.96	0.09	42,42,42,42	0
57	MG	1A	3195	1/1	0.96	0.13	30,30,30,30	0
57	MG	2A	3289	1/1	0.96	0.14	38,38,38,38	0
57	MG	2A	3290	1/1	0.96	0.21	43,43,43,43	0
57	MG	2a	3089	1/1	0.96	0.19	53,53,53,53	0
57	MG	1A	3196	1/1	0.96	0.22	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3453	1/1	0.96	0.10	44,44,44,44	0
57	MG	1A	3568	1/1	0.96	0.13	38,38,38,38	0
57	MG	1A	3039	1/1	0.96	0.11	39,39,39,39	0
57	MG	1a	1714	1/1	0.96	0.14	56,56,56,56	0
57	MG	2A	3296	1/1	0.96	0.25	58,58,58,58	0
57	MG	1A	3455	1/1	0.96	0.07	28,28,28,28	0
57	MG	1A	3152	1/1	0.96	0.10	39,39,39,39	0
57	MG	1A	3871	1/1	0.96	0.06	36,36,36,36	0
57	MG	2A	3592	1/1	0.96	0.08	60,60,60,60	0
57	MG	2A	3301	1/1	0.96	0.06	56,56,56,56	0
57	MG	2A	3594	1/1	0.96	0.07	61,61,61,61	0
57	MG	1A	3704	1/1	0.96	0.07	52,52,52,52	0
57	MG	2a	3104	1/1	0.96	0.14	56,56,56,56	0
57	MG	1F	305	1/1	0.96	0.12	37,37,37,37	0
57	MG	2a	3106	1/1	0.96	0.36	60,60,60,60	0
57	MG	1A	3873	1/1	0.96	0.06	43,43,43,43	0
57	MG	1F	309	1/1	0.96	0.19	47,47,47,47	0
57	MG	1A	3705	1/1	0.96	0.10	57,57,57,57	0
57	MG	1A	3020	1/1	0.96	0.29	35,35,35,35	0
57	MG	1A	3573	1/1	0.96	0.07	43,43,43,43	0
57	MG	1A	3708	1/1	0.96	0.05	34,34,34,34	0
57	MG	1A	3878	1/1	0.96	0.06	46,46,46,46	0
57	MG	1A	3880	1/1	0.96	0.05	27,27,27,27	0
57	MG	2A	3052	1/1	0.96	0.24	60,60,60,60	0
57	MG	2a	3117	1/1	0.96	0.06	77,77,77,77	0
57	MG	1A	3268	1/1	0.96	0.07	40,40,40,40	0
57	MG	1H	201	1/1	0.96	0.06	51,51,51,51	0
57	MG	2A	3056	1/1	0.96	0.08	38,38,38,38	0
57	MG	2A	3317	1/1	0.96	0.21	59,59,59,59	0
57	MG	2A	3318	1/1	0.96	0.09	51,51,51,51	0
57	MG	1H	202	1/1	0.96	0.10	61,61,61,61	0
57	MG	1N	201	1/1	0.96	0.10	44,44,44,44	0
57	MG	1a	1735	1/1	0.96	0.07	55,55,55,55	0
57	MG	1A	3882	1/1	0.96	0.11	34,34,34,34	0
57	MG	1A	3883	1/1	0.96	0.06	24,24,24,24	0
57	MG	2A	3324	1/1	0.96	0.23	73,73,73,73	0
57	MG	1a	1738	1/1	0.96	0.09	33,33,33,33	0
57	MG	1A	3154	1/1	0.96	0.10	45,45,45,45	0
57	MG	1A	3156	1/1	0.96	0.07	35,35,35,35	0
57	MG	2A	3623	1/1	0.96	0.07	50,50,50,50	0
57	MG	2A	3069	1/1	0.96	0.08	51,51,51,51	0
57	MG	1A	3114	1/1	0.96	0.12	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3331	1/1	0.96	0.17	60,60,60,60	0
57	MG	2A	3071	1/1	0.96	0.06	45,45,45,45	0
57	MG	1a	1744	1/1	0.96	0.17	60,60,60,60	0
57	MG	2a	3139	1/1	0.96	0.15	67,67,67,67	0
57	MG	2A	3073	1/1	0.96	0.09	48,48,48,48	0
57	MG	2A	3074	1/1	0.96	0.07	52,52,52,52	0
57	MG	1P	203	1/1	0.96	0.12	37,37,37,37	0
57	MG	2a	3143	1/1	0.96	0.07	68,68,68,68	0
57	MG	2A	3642	1/1	0.96	0.05	50,50,50,50	0
57	MG	1Q	201	1/1	0.96	0.05	28,28,28,28	0
57	MG	2a	3147	1/1	0.96	0.15	51,51,51,51	0
57	MG	1A	3714	1/1	0.96	0.10	45,45,45,45	0
57	MG	1A	3158	1/1	0.96	0.21	40,40,40,40	0
57	MG	2A	3079	1/1	0.96	0.13	48,48,48,48	0
57	MG	1A	3073	1/1	0.96	0.06	27,27,27,27	0
57	MG	1A	3581	1/1	0.96	0.06	57,57,57,57	0
57	MG	2A	3349	1/1	0.96	0.05	41,41,41,41	0
57	MG	1A	3206	1/1	0.96	0.08	46,46,46,46	0
57	MG	1A	3160	1/1	0.96	0.09	33,33,33,33	0
57	MG	2A	3656	1/1	0.96	0.09	58,58,58,58	0
57	MG	2a	3157	1/1	0.96	0.07	66,66,66,66	0
57	MG	1A	3283	1/1	0.96	0.05	40,40,40,40	0
57	MG	1A	3898	1/1	0.96	0.12	40,40,40,40	0
57	MG	1a	1755	1/1	0.96	0.11	54,54,54,54	0
57	MG	2A	3088	1/1	0.96	0.07	49,49,49,49	0
57	MG	2a	3164	1/1	0.96	0.12	61,61,61,61	0
57	MG	1A	3472	1/1	0.96	0.07	44,44,44,44	0
57	MG	2A	3666	1/1	0.96	0.07	62,62,62,62	0
57	MG	1A	3901	1/1	0.96	0.06	37,37,37,37	0
57	MG	2A	3668	1/1	0.96	0.08	42,42,42,42	0
57	MG	1A	3902	1/1	0.96	0.06	21,21,21,21	0
57	MG	1U	203	1/1	0.96	0.23	35,35,35,35	0
57	MG	2A	3360	1/1	0.96	0.08	51,51,51,51	0
57	MG	1U	205	1/1	0.96	0.19	37,37,37,37	0
57	MG	2A	3673	1/1	0.96	0.06	43,43,43,43	0
57	MG	1A	3286	1/1	0.96	0.08	45,45,45,45	0
57	MG	1A	3726	1/1	0.96	0.05	30,30,30,30	0
57	MG	2A	3097	1/1	0.96	0.12	56,56,56,56	0
57	MG	1A	3727	1/1	0.96	0.09	31,31,31,31	0
57	MG	2A	3367	1/1	0.96	0.14	55,55,55,55	0
57	MG	1A	3210	1/1	0.96	0.24	55,55,55,55	0
57	MG	2A	3683	1/1	0.96	0.06	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3369	1/1	0.96	0.09	58,58,58,58	0
57	MG	1A	3371	1/1	0.96	0.11	67,67,67,67	0
57	MG	1A	3161	1/1	0.96	0.13	34,34,34,34	0
57	MG	1A	3163	1/1	0.96	0.23	28,28,28,28	0
57	MG	1A	3480	1/1	0.96	0.06	61,61,61,61	0
57	MG	1A	3597	1/1	0.96	0.09	23,23,23,23	0
57	MG	1A	3918	1/1	0.96	0.06	44,44,44,44	0
57	MG	1A	3214	1/1	0.96	0.21	49,49,49,49	0
57	MG	1A	3123	1/1	0.96	0.10	35,35,35,35	0
57	MG	10	105	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	3057	1/1	0.96	0.16	47,47,47,47	0
57	MG	2A	3117	1/1	0.96	0.08	40,40,40,40	0
57	MG	1A	3605	1/1	0.96	0.07	44,44,44,44	0
57	MG	1a	1779	1/1	0.96	0.16	63,63,63,63	0
57	MG	2A	3700	1/1	0.96	0.06	49,49,49,49	0
57	MG	1A	3924	1/1	0.96	0.09	56,56,56,56	0
57	MG	1A	3741	1/1	0.96	0.07	35,35,35,35	0
57	MG	1A	3742	1/1	0.96	0.10	36,36,36,36	0
57	MG	1A	3385	1/1	0.96	0.07	45,45,45,45	0
57	MG	13	101	1/1	0.96	0.10	27,27,27,27	0
57	MG	1A	3218	1/1	0.96	0.35	38,38,38,38	0
57	MG	2A	3398	1/1	0.96	0.14	46,46,46,46	0
57	MG	1A	3301	1/1	0.96	0.07	29,29,29,29	0
57	MG	1A	3749	1/1	0.96	0.10	48,48,48,48	0
57	MG	2A	3276	1/1	0.97	0.07	39,39,39,39	0
57	MG	1A	3879	1/1	0.97	0.15	26,26,26,26	0
57	MG	1A	3518	1/1	0.97	0.10	20,20,20,20	0
57	MG	2E	302	1/1	0.97	0.08	41,41,41,41	0
57	MG	1a	1639	1/1	0.97	0.10	53,53,53,53	0
57	MG	1A	3421	1/1	0.97	0.05	18,18,18,18	0
57	MG	2A	3080	1/1	0.97	0.07	35,35,35,35	0
57	MG	1B	208	1/1	0.97	0.07	46,46,46,46	0
57	MG	1A	3624	1/1	0.97	0.08	55,55,55,55	0
57	MG	1A	3269	1/1	0.97	0.14	30,30,30,30	0
57	MG	1a	1802	1/1	0.97	0.12	49,49,49,49	0
57	MG	1A	3033	1/1	0.97	0.05	39,39,39,39	0
57	MG	1A	3748	1/1	0.97	0.06	28,28,28,28	0
57	MG	1a	1646	1/1	0.97	0.09	51,51,51,51	0
57	MG	1A	3888	1/1	0.97	0.07	33,33,33,33	0
57	MG	1A	3628	1/1	0.97	0.21	30,30,30,30	0
57	MG	1A	3059	1/1	0.97	0.10	50,50,50,50	0
57	MG	2P	202	1/1	0.97	0.06	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3631	1/1	0.97	0.14	30,30,30,30	0
57	MG	2Q	202	1/1	0.97	0.31	57,57,57,57	0
57	MG	1B	219	1/1	0.97	0.05	27,27,27,27	0
57	MG	2A	3525	1/1	0.97	0.07	64,64,64,64	0
57	MG	1A	3130	1/1	0.97	0.03	26,26,26,26	0
57	MG	2A	3527	1/1	0.97	0.06	60,60,60,60	0
57	MG	1a	1812	1/1	0.97	0.10	62,62,62,62	0
57	MG	1B	221	1/1	0.97	0.05	48,48,48,48	0
57	MG	2A	3096	1/1	0.97	0.12	42,42,42,42	0
57	MG	1B	222	1/1	0.97	0.05	38,38,38,38	0
57	MG	2W	203	1/1	0.97	0.10	60,60,60,60	0
57	MG	1A	3274	1/1	0.97	0.10	36,36,36,36	0
57	MG	1A	3276	1/1	0.97	0.12	26,26,26,26	0
57	MG	1A	3087	1/1	0.97	0.40	40,40,40,40	0
57	MG	2A	3101	1/1	0.97	0.05	37,37,37,37	0
57	MG	2A	3103	1/1	0.97	0.07	53,53,53,53	0
57	MG	2I	104	1/1	0.97	0.13	51,51,51,51	0
57	MG	1A	3431	1/1	0.97	0.07	21,21,21,21	0
57	MG	1A	3017	1/1	0.97	0.23	29,29,29,29	0
57	MG	1A	3279	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3434	1/1	0.97	0.04	25,25,25,25	0
57	MG	1A	3061	1/1	0.97	0.10	36,36,36,36	0
57	MG	1A	3436	1/1	0.97	0.04	35,35,35,35	0
57	MG	1A	3437	1/1	0.97	0.06	35,35,35,35	0
57	MG	2a	3001	1/1	0.97	0.09	42,42,42,42	0
57	MG	2A	3312	1/1	0.97	0.07	38,38,38,38	0
57	MG	2A	3112	1/1	0.97	0.07	47,47,47,47	0
57	MG	2A	3113	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3177	1/1	0.97	0.09	29,29,29,29	0
57	MG	1D	310	1/1	0.97	0.12	23,23,23,23	0
57	MG	1A	3906	1/1	0.97	0.07	49,49,49,49	0
57	MG	2A	3551	1/1	0.97	0.06	67,67,67,67	0
57	MG	1A	3018	1/1	0.97	0.14	26,26,26,26	0
57	MG	1a	1832	1/1	0.97	0.14	54,54,54,54	0
57	MG	2A	3120	1/1	0.97	0.09	54,54,54,54	0
57	MG	2A	3121	1/1	0.97	0.11	39,39,39,39	0
57	MG	2a	3013	1/1	0.97	0.05	48,48,48,48	0
57	MG	1A	3285	1/1	0.97	0.05	37,37,37,37	0
57	MG	1A	3649	1/1	0.97	0.07	56,56,56,56	0
57	MG	1A	3442	1/1	0.97	0.04	28,28,28,28	0
57	MG	1E	301	1/1	0.97	0.12	35,35,35,35	0
57	MG	2A	3326	1/1	0.97	0.10	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3562	1/1	0.97	0.06	52,52,52,52	0
57	MG	1A	3135	1/1	0.97	0.19	33,33,33,33	0
57	MG	1A	3288	1/1	0.97	0.07	22,22,22,22	0
57	MG	1A	3916	1/1	0.97	0.06	40,40,40,40	0
57	MG	2a	3023	1/1	0.97	0.06	39,39,39,39	0
57	MG	2A	3130	1/1	0.97	0.18	46,46,46,46	0
57	MG	1A	3542	1/1	0.97	0.09	57,57,57,57	0
57	MG	2A	3332	1/1	0.97	0.05	28,28,28,28	0
57	MG	1A	3226	1/1	0.97	0.15	32,32,32,32	0
57	MG	1A	3019	1/1	0.97	0.18	25,25,25,25	0
57	MG	1A	3921	1/1	0.97	0.09	53,53,53,53	0
57	MG	2A	3573	1/1	0.97	0.06	56,56,56,56	0
57	MG	1F	311	1/1	0.97	0.09	49,49,49,49	0
57	MG	1A	3657	1/1	0.97	0.12	33,33,33,33	0
57	MG	2A	3340	1/1	0.97	0.18	39,39,39,39	0
57	MG	2A	3578	1/1	0.97	0.08	60,60,60,60	0
57	MG	2A	3341	1/1	0.97	0.10	49,49,49,49	0
57	MG	1A	3547	1/1	0.97	0.25	21,21,21,21	0
57	MG	1A	3064	1/1	0.97	0.07	28,28,28,28	0
57	MG	1A	3925	1/1	0.97	0.07	58,58,58,58	0
57	MG	1A	3361	1/1	0.97	0.08	28,28,28,28	0
57	MG	1A	3138	1/1	0.97	0.13	26,26,26,26	0
57	MG	1A	3363	1/1	0.97	0.09	35,35,35,35	0
57	MG	2A	3144	1/1	0.97	0.06	41,41,41,41	0
57	MG	1a	1854	1/1	0.97	0.06	56,56,56,56	0
57	MG	1A	3139	1/1	0.97	0.22	28,28,28,28	0
57	MG	1A	3231	1/1	0.97	0.07	35,35,35,35	0
57	MG	1A	3295	1/1	0.97	0.07	53,53,53,53	0
57	MG	1A	3298	1/1	0.97	0.11	45,45,45,45	0
57	MG	2A	3595	1/1	0.97	0.09	48,48,48,48	0
57	MG	1A	3372	1/1	0.97	0.10	26,26,26,26	0
57	MG	1A	3458	1/1	0.97	0.07	40,40,40,40	0
57	MG	1A	3459	1/1	0.97	0.05	58,58,58,58	0
57	MG	1A	3299	1/1	0.97	0.07	28,28,28,28	0
57	MG	2A	3600	1/1	0.97	0.05	38,38,38,38	0
57	MG	1A	3093	1/1	0.97	0.18	32,32,32,32	0
57	MG	1A	3375	1/1	0.97	0.08	28,28,28,28	0
57	MG	1A	3463	1/1	0.97	0.06	40,40,40,40	0
57	MG	1A	3566	1/1	0.97	0.05	30,30,30,30	0
57	MG	1Q	205	1/1	0.97	0.08	51,51,51,51	0
57	MG	1A	3377	1/1	0.97	0.04	27,27,27,27	0
57	MG	1A	3797	1/1	0.97	0.05	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
57	MG	1A	3465	1/1	0.97	0.07	50,50,50,50	0
57	MG	2A	3609	1/1	0.97	0.05	29,29,29,29	0
57	MG	2A	3163	1/1	0.97	0.15	50,50,50,50	0
57	MG	1b	301	1/1	0.97	0.12	60,60,60,60	0
57	MG	1A	3947	1/1	0.97	0.06	24,24,24,24	0
57	MG	1A	3187	1/1	0.97	0.21	37,37,37,37	0
57	MG	2A	3373	1/1	0.97	0.07	28,28,28,28	0
57	MG	2A	3375	1/1	0.97	0.08	44,44,44,44	0
57	MG	1A	3235	1/1	0.97	0.15	28,28,28,28	0
57	MG	1A	3681	1/1	0.97	0.11	56,56,56,56	0
57	MG	1A	3380	1/1	0.97	0.06	25,25,25,25	0
57	MG	1A	3381	1/1	0.97	0.06	45,45,45,45	0
57	MG	1A	3382	1/1	0.97	0.07	51,51,51,51	0
57	MG	1A	3805	1/1	0.97	0.11	55,55,55,55	0
57	MG	1A	3685	1/1	0.97	0.06	44,44,44,44	0
57	MG	1A	3006	1/1	0.97	0.05	31,31,31,31	0
57	MG	1A	3013	1/1	0.97	0.04	20,20,20,20	0
57	MG	2A	3625	1/1	0.97	0.05	58,58,58,58	0
57	MG	2A	3177	1/1	0.97	0.07	61,61,61,61	0
57	MG	1g	202	1/1	0.97	0.06	55,55,55,55	0
57	MG	2A	3629	1/1	0.97	0.12	54,54,54,54	0
57	MG	1A	3238	1/1	0.97	0.15	32,32,32,32	0
57	MG	2A	3632	1/1	0.97	0.07	38,38,38,38	0
57	MG	1A	3812	1/1	0.97	0.10	51,51,51,51	0
57	MG	1A	3577	1/1	0.97	0.12	41,41,41,41	0
57	MG	2A	3393	1/1	0.97	0.13	39,39,39,39	0
57	MG	1A	3040	1/1	0.97	0.10	38,38,38,38	0
57	MG	2A	3640	1/1	0.97	0.08	56,56,56,56	0
57	MG	1A	3240	1/1	0.97	0.14	22,22,22,22	0
57	MG	1A	3023	1/1	0.97	0.07	28,28,28,28	0
57	MG	1A	3024	1/1	0.97	0.10	27,27,27,27	0
57	MG	10	102	1/1	0.97	0.09	29,29,29,29	0
57	MG	1A	3243	1/1	0.97	0.19	35,35,35,35	0
57	MG	2A	3649	1/1	0.97	0.05	49,49,49,49	0
57	MG	2A	3403	1/1	0.97	0.18	54,54,54,54	0
57	MG	1A	3970	1/1	0.97	0.08	37,37,37,37	0
57	MG	2A	3189	1/1	0.97	0.13	53,53,53,53	0
57	MG	1A	3583	1/1	0.97	0.14	49,49,49,49	0
57	MG	1A	3697	1/1	0.97	0.14	52,52,52,52	0
57	MG	1a	1729	1/1	0.97	0.08	42,42,42,42	0
57	MG	2A	3658	1/1	0.97	0.05	41,41,41,41	0
57	MG	1a	1730	1/1	0.97	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
57	MG	1A	3244	1/1	0.97	0.13	33,33,33,33	0
57	MG	2A	3195	1/1	0.97	0.08	54,54,54,54	0
57	MG	2a	3107	1/1	0.97	0.29	64,64,64,64	0
57	MG	1A	3585	1/1	0.97	0.07	47,47,47,47	0
57	MG	1A	3150	1/1	0.97	0.10	24,24,24,24	0
57	MG	1A	3587	1/1	0.97	0.07	13,13,13,13	0
57	MG	1A	3826	1/1	0.97	0.10	21,21,21,21	0
57	MG	1A	3588	1/1	0.97	0.05	29,29,29,29	0
57	MG	1A	3828	1/1	0.97	0.07	36,36,36,36	0
57	MG	2A	3005	1/1	0.97	0.15	38,38,38,38	0
57	MG	1A	3194	1/1	0.97	0.12	27,27,27,27	0
57	MG	1a	1740	1/1	0.97	0.11	37,37,37,37	0
57	MG	1A	3315	1/1	0.97	0.18	34,34,34,34	0
57	MG	15	3103	1/1	0.97	0.15	30,30,30,30	0
57	MG	2A	3010	1/1	0.97	0.12	48,48,48,48	0
57	MG	1A	3984	1/1	0.97	0.07	38,38,38,38	0
57	MG	2A	3677	1/1	0.97	0.06	54,54,54,54	0
57	MG	2A	3013	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3317	1/1	0.97	0.19	35,35,35,35	0
57	MG	2A	3680	1/1	0.97	0.11	47,47,47,47	0
57	MG	1A	3592	1/1	0.97	0.06	35,35,35,35	0
57	MG	1A	3044	1/1	0.97	0.07	31,31,31,31	0
57	MG	2A	3017	1/1	0.97	0.13	54,54,54,54	0
57	MG	2A	3433	1/1	0.97	0.08	63,63,63,63	0
57	MG	1A	3709	1/1	0.97	0.14	48,48,48,48	0
57	MG	1A	3106	1/1	0.97	0.05	30,30,30,30	0
57	MG	1A	3025	1/1	0.97	0.16	38,38,38,38	0
57	MG	1A	3014	1/1	0.97	0.08	43,43,43,43	0
57	MG	2A	3438	1/1	0.97	0.07	34,34,34,34	0
57	MG	17	103	1/1	0.97	0.09	37,37,37,37	0
57	MG	1A	3255	1/1	0.97	0.12	28,28,28,28	0
57	MG	17	105	1/1	0.97	0.06	40,40,40,40	0
57	MG	1A	3109	1/1	0.97	0.13	32,32,32,32	0
57	MG	1A	3028	1/1	0.97	0.18	25,25,25,25	0
57	MG	2A	3696	1/1	0.97	0.08	46,46,46,46	0
57	MG	2A	3028	1/1	0.97	0.08	31,31,31,31	0
57	MG	1a	1757	1/1	0.97	0.07	61,61,61,61	0
57	MG	2A	3699	1/1	0.97	0.04	37,37,37,37	0
57	MG	1A	3030	1/1	0.97	0.07	25,25,25,25	0
57	MG	2A	3447	1/1	0.97	0.06	51,51,51,51	0
57	MG	1a	1759	1/1	0.97	0.11	58,58,58,58	0
57	MG	1A	3717	1/1	0.97	0.07	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3848	1/1	0.97	0.06	29,29,29,29	0
57	MG	2A	3034	1/1	0.97	0.13	64,64,64,64	0
57	MG	2A	3452	1/1	0.97	0.07	47,47,47,47	0
57	MG	2A	3035	1/1	0.97	0.10	45,45,45,45	0
57	MG	1A	3849	1/1	0.97	0.18	43,43,43,43	0
57	MG	2A	3455	1/1	0.97	0.07	53,53,53,53	0
57	MG	2A	3037	1/1	0.97	0.18	52,52,52,52	0
57	MG	1A	3850	1/1	0.97	0.06	53,53,53,53	0
57	MG	2A	3458	1/1	0.97	0.09	56,56,56,56	0
57	MG	2A	3039	1/1	0.97	0.06	27,27,27,27	0
57	MG	1A	3602	1/1	0.97	0.08	48,48,48,48	0
57	MG	1A	3603	1/1	0.97	0.07	36,36,36,36	0
57	MG	2A	3462	1/1	0.97	0.05	46,46,46,46	0
57	MG	1A	3854	1/1	0.97	0.04	42,42,42,42	0
57	MG	1A	3604	1/1	0.97	0.14	42,42,42,42	0
57	MG	1A	3722	1/1	0.97	0.08	24,24,24,24	0
57	MG	1A	4007	1/1	0.97	0.31	43,43,43,43	0
57	MG	1A	3857	1/1	0.97	0.14	38,38,38,38	0
57	MG	1A	4009	1/1	0.97	0.05	50,50,50,50	0
57	MG	1A	3500	1/1	0.97	0.05	21,21,21,21	0
57	MG	1a	1612	1/1	0.97	0.07	27,27,27,27	0
57	MG	2A	3246	1/1	0.97	0.18	38,38,38,38	0
57	MG	1A	4011	1/1	0.97	0.07	38,38,38,38	0
57	MG	1A	3081	1/1	0.97	0.05	34,34,34,34	0
57	MG	2A	3249	1/1	0.97	0.15	52,52,52,52	0
57	MG	2A	3250	1/1	0.97	0.09	29,29,29,29	0
57	MG	1A	3408	1/1	0.97	0.08	28,28,28,28	0
57	MG	2A	3252	1/1	0.97	0.07	46,46,46,46	0
57	MG	2A	3478	1/1	0.97	0.09	33,33,33,33	0
57	MG	1A	3121	1/1	0.97	0.10	18,18,18,18	0
57	MG	1A	3053	1/1	0.97	0.10	29,29,29,29	0
57	MG	2a	3182	1/1	0.97	0.07	57,57,57,57	0
57	MG	1A	3124	1/1	0.97	0.05	35,35,35,35	0
57	MG	2A	3058	1/1	0.97	0.10	38,38,38,38	0
57	MG	2a	3185	1/1	0.97	0.08	57,57,57,57	0
57	MG	1a	1620	1/1	0.97	0.04	47,47,47,47	0
57	MG	1A	3867	1/1	0.97	0.09	41,41,41,41	0
57	MG	2A	3486	1/1	0.97	0.07	47,47,47,47	0
57	MG	1A	3332	1/1	0.97	0.07	52,52,52,52	0
57	MG	2A	3488	1/1	0.97	0.05	45,45,45,45	0
57	MG	1A	3508	1/1	0.97	0.06	46,46,46,46	0
57	MG	2A	3262	1/1	0.97	0.16	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3063	1/1	0.97	0.08	46,46,46,46	0
57	MG	2A	3264	1/1	0.97	0.30	36,36,36,36	0
57	MG	1A	3054	1/1	0.97	0.19	24,24,24,24	0
57	MG	1A	3510	1/1	0.97	0.08	25,25,25,25	0
57	MG	1A	4026	1/1	0.97	0.10	49,49,49,49	0
57	MG	2D	301	1/1	0.97	0.14	42,42,42,42	0
57	MG	2D	302	1/1	0.97	0.26	33,33,33,33	0
57	MG	1A	3016	1/1	0.97	0.12	35,35,35,35	0
57	MG	1A	4028	1/1	0.97	0.08	44,44,44,44	0
57	MG	1A	3336	1/1	0.97	0.06	23,23,23,23	0
57	MG	1A	3514	1/1	0.97	0.05	24,24,24,24	0
57	MG	1A	3127	1/1	0.97	0.09	37,37,37,37	0
57	MG	1A	3168	1/1	0.97	0.10	28,28,28,28	0
57	MG	1A	3740	1/1	0.97	0.05	50,50,50,50	0
57	MG	1F	312	1/1	0.98	0.08	34,34,34,34	0
57	MG	1A	3368	1/1	0.98	0.08	57,57,57,57	0
57	MG	1a	1664	1/1	0.98	0.08	52,52,52,52	0
57	MG	1A	3750	1/1	0.98	0.04	16,16,16,16	0
57	MG	1a	1815	1/1	0.98	0.16	65,65,65,65	0
57	MG	1A	3036	1/1	0.98	0.03	28,28,28,28	0
57	MG	1A	3851	1/1	0.98	0.03	20,20,20,20	0
57	MG	1A	3223	1/1	0.98	0.04	29,29,29,29	0
57	MG	1A	3099	1/1	0.98	0.09	28,28,28,28	0
57	MG	2A	3427	1/1	0.98	0.04	32,32,32,32	0
57	MG	2A	3428	1/1	0.98	0.08	42,42,42,42	0
57	MG	1A	3967	1/1	0.98	0.05	27,27,27,27	0
57	MG	1A	3155	1/1	0.98	0.19	33,33,33,33	0
57	MG	1A	3969	1/1	0.98	0.06	51,51,51,51	0
57	MG	1A	3316	1/1	0.98	0.06	16,16,16,16	0
57	MG	1N	202	1/1	0.98	0.12	37,37,37,37	0
57	MG	1A	3438	1/1	0.98	0.05	25,25,25,25	0
57	MG	1A	3012	1/1	0.98	0.26	41,41,41,41	0
57	MG	1A	3973	1/1	0.98	0.09	18,18,18,18	0
57	MG	1a	1829	1/1	0.98	0.08	55,55,55,55	0
57	MG	1A	3376	1/1	0.98	0.04	20,20,20,20	0
57	MG	2A	3257	1/1	0.98	0.07	22,22,22,22	0
57	MG	1A	3318	1/1	0.98	0.11	15,15,15,15	0
57	MG	1A	3516	1/1	0.98	0.06	42,42,42,42	0
57	MG	2A	3628	1/1	0.98	0.05	62,62,62,62	0
57	MG	1A	3861	1/1	0.98	0.04	43,43,43,43	0
57	MG	2A	3630	1/1	0.98	0.05	40,40,40,40	0
57	MG	1A	3270	1/1	0.98	0.16	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1Q	203	1/1	0.98	0.06	39,39,39,39	0
57	MG	1A	3864	1/1	0.98	0.06	31,31,31,31	0
57	MG	2A	3635	1/1	0.98	0.06	54,54,54,54	0
57	MG	1A	3673	1/1	0.98	0.07	32,32,32,32	0
57	MG	2A	3637	1/1	0.98	0.11	56,56,56,56	0
57	MG	1a	1838	1/1	0.98	0.10	57,57,57,57	0
57	MG	1A	3101	1/1	0.98	0.16	35,35,35,35	0
57	MG	1A	3102	1/1	0.98	0.25	27,27,27,27	0
57	MG	1R	204	1/1	0.98	0.06	40,40,40,40	0
57	MG	2A	3643	1/1	0.98	0.06	40,40,40,40	0
57	MG	1A	3046	1/1	0.98	0.09	10,10,10,10	0
57	MG	1A	3105	1/1	0.98	0.21	25,25,25,25	0
57	MG	2A	3104	1/1	0.98	0.06	52,52,52,52	0
57	MG	2A	3647	1/1	0.98	0.05	37,37,37,37	0
57	MG	1a	1844	1/1	0.98	0.04	53,53,53,53	0
57	MG	1A	3870	1/1	0.98	0.05	54,54,54,54	0
57	MG	1A	3987	1/1	0.98	0.04	21,21,21,21	0
57	MG	1A	3275	1/1	0.98	0.17	30,30,30,30	0
57	MG	1A	3384	1/1	0.98	0.04	15,15,15,15	0
57	MG	1A	3005	1/1	0.98	0.09	17,17,17,17	0
57	MG	1U	202	1/1	0.98	0.11	41,41,41,41	0
57	MG	1A	3598	1/1	0.98	0.11	33,33,33,33	0
57	MG	2A	3657	1/1	0.98	0.05	43,43,43,43	0
57	MG	1U	204	1/1	0.98	0.18	27,27,27,27	0
57	MG	1A	3450	1/1	0.98	0.10	21,21,21,21	0
57	MG	2A	3115	1/1	0.98	0.10	45,45,45,45	0
57	MG	1A	3003	1/1	0.98	0.04	26,26,26,26	0
57	MG	2A	3662	1/1	0.98	0.03	38,38,38,38	0
57	MG	1A	3387	1/1	0.98	0.10	16,16,16,16	0
57	MG	1V	201	1/1	0.98	0.08	21,21,21,21	0
57	MG	2A	3665	1/1	0.98	0.05	58,58,58,58	0
57	MG	1a	1858	1/1	0.98	0.06	60,60,60,60	0
57	MG	1A	3233	1/1	0.98	0.13	37,37,37,37	0
57	MG	1V	204	1/1	0.98	0.06	32,32,32,32	0
57	MG	1A	3996	1/1	0.98	0.04	44,44,44,44	0
57	MG	1V	206	1/1	0.98	0.05	56,56,56,56	0
57	MG	1A	3686	1/1	0.98	0.07	40,40,40,40	0
57	MG	1A	3078	1/1	0.98	0.09	33,33,33,33	0
57	MG	1A	3280	1/1	0.98	0.15	43,43,43,43	0
57	MG	1A	3330	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3532	1/1	0.98	0.04	24,24,24,24	0
57	MG	1A	3885	1/1	0.98	0.04	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
57	MG	1A	3607	1/1	0.98	0.05	29,29,29,29	0
57	MG	2A	3299	1/1	0.98	0.03	49,49,49,49	0
57	MG	2A	3481	1/1	0.98	0.08	45,45,45,45	0
57	MG	1A	3050	1/1	0.98	0.10	34,34,34,34	0
57	MG	2A	3681	1/1	0.98	0.04	53,53,53,53	0
57	MG	1A	3051	1/1	0.98	0.33	46,46,46,46	0
57	MG	1A	3112	1/1	0.98	0.23	28,28,28,28	0
57	MG	10	106	1/1	0.98	0.03	47,47,47,47	0
57	MG	1A	3536	1/1	0.98	0.07	15,15,15,15	0
57	MG	1A	3787	1/1	0.98	0.06	41,41,41,41	0
57	MG	1A	3788	1/1	0.98	0.07	39,39,39,39	0
57	MG	1A	3284	1/1	0.98	0.14	32,32,32,32	0
57	MG	1A	3613	1/1	0.98	0.13	39,39,39,39	0
57	MG	1A	4012	1/1	0.98	0.03	32,32,32,32	0
57	MG	11	103	1/1	0.98	0.10	33,33,33,33	0
57	MG	1A	4013	1/1	0.98	0.04	55,55,55,55	0
57	MG	2A	3494	1/1	0.98	0.10	49,49,49,49	0
57	MG	2a	3088	1/1	0.98	0.17	45,45,45,45	0
57	MG	1A	3113	1/1	0.98	0.11	40,40,40,40	0
57	MG	1A	4015	1/1	0.98	0.07	37,37,37,37	0
57	MG	13	104	1/1	0.98	0.06	37,37,37,37	0
57	MG	2A	3499	1/1	0.98	0.06	56,56,56,56	0
57	MG	2a	3093	1/1	0.98	0.15	45,45,45,45	0
57	MG	1A	3001	1/1	0.98	0.04	31,31,31,31	0
57	MG	1A	3287	1/1	0.98	0.07	27,27,27,27	0
57	MG	2A	3502	1/1	0.98	0.06	49,49,49,49	0
57	MG	1A	4018	1/1	0.98	0.13	47,47,47,47	0
57	MG	1a	1732	1/1	0.98	0.07	40,40,40,40	0
57	MG	2A	3152	1/1	0.98	0.05	38,38,38,38	0
57	MG	2A	3704	1/1	0.98	0.04	22,22,22,22	0
57	MG	2A	3705	1/1	0.98	0.08	42,42,42,42	0
57	MG	1A	3172	1/1	0.98	0.23	31,31,31,31	0
57	MG	1A	3116	1/1	0.98	0.07	39,39,39,39	0
57	MG	1A	3205	1/1	0.98	0.06	46,46,46,46	0
57	MG	1A	3117	1/1	0.98	0.09	31,31,31,31	0
57	MG	1A	3546	1/1	0.98	0.04	23,23,23,23	0
57	MG	1A	3207	1/1	0.98	0.18	45,45,45,45	0
57	MG	1A	3344	1/1	0.98	0.10	25,25,25,25	0
57	MG	2A	3713	1/1	0.98	0.17	46,46,46,46	0
57	MG	1A	3208	1/1	0.98	0.17	42,42,42,42	0
57	MG	1A	3550	1/1	0.98	0.04	23,23,23,23	0
57	MG	1A	3118	1/1	0.98	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
57	MG	1a	1743	1/1	0.98	0.06	58,58,58,58	0
57	MG	1A	3910	1/1	0.98	0.05	29,29,29,29	0
57	MG	1A	3627	1/1	0.98	0.16	30,30,30,30	0
57	MG	1A	3912	1/1	0.98	0.04	26,26,26,26	0
57	MG	1A	3119	1/1	0.98	0.17	31,31,31,31	0
57	MG	2A	3335	1/1	0.98	0.07	60,60,60,60	0
57	MG	1A	3297	1/1	0.98	0.11	17,17,17,17	0
57	MG	1A	3630	1/1	0.98	0.06	28,28,28,28	0
57	MG	1A	3917	1/1	0.98	0.04	15,15,15,15	0
57	MG	1A	3809	1/1	0.98	0.08	42,42,42,42	0
57	MG	2A	3172	1/1	0.98	0.07	60,60,60,60	0
57	MG	1A	3249	1/1	0.98	0.23	27,27,27,27	0
57	MG	1A	3211	1/1	0.98	0.13	40,40,40,40	0
57	MG	1A	3412	1/1	0.98	0.09	35,35,35,35	0
57	MG	2A	3345	1/1	0.98	0.07	39,39,39,39	0
57	MG	1A	3719	1/1	0.98	0.05	40,40,40,40	0
57	MG	1A	3144	1/1	0.98	0.18	22,22,22,22	0
57	MG	1B	213	1/1	0.98	0.08	49,49,49,49	0
57	MG	2A	3012	1/1	0.98	0.05	27,27,27,27	0
57	MG	2a	3132	1/1	0.98	0.04	57,57,57,57	0
57	MG	1B	214	1/1	0.98	0.04	33,33,33,33	0
57	MG	1A	3094	1/1	0.98	0.13	26,26,26,26	0
57	MG	1A	3636	1/1	0.98	0.04	42,42,42,42	0
57	MG	1A	3415	1/1	0.98	0.06	20,20,20,20	0
57	MG	1A	3416	1/1	0.98	0.06	23,23,23,23	0
57	MG	1a	1615	1/1	0.98	0.09	56,56,56,56	0
57	MG	1a	1764	1/1	0.98	0.06	60,60,60,60	0
57	MG	1A	3561	1/1	0.98	0.06	33,33,33,33	0
57	MG	1A	3146	1/1	0.98	0.07	32,32,32,32	0
57	MG	1A	3563	1/1	0.98	0.05	24,24,24,24	0
57	MG	1A	3932	1/1	0.98	0.05	53,53,53,53	0
57	MG	1A	3354	1/1	0.98	0.04	22,22,22,22	0
57	MG	2a	3145	1/1	0.98	0.08	68,68,68,68	0
57	MG	1A	3215	1/1	0.98	0.06	34,34,34,34	0
57	MG	1a	1622	1/1	0.98	0.14	49,49,49,49	0
57	MG	2A	3549	1/1	0.98	0.05	54,54,54,54	0
57	MG	2A	3364	1/1	0.98	0.10	55,55,55,55	0
57	MG	2A	3027	1/1	0.98	0.05	41,41,41,41	0
57	MG	1a	1623	1/1	0.98	0.14	54,54,54,54	0
57	MG	1A	3824	1/1	0.98	0.06	49,49,49,49	0
57	MG	1A	3356	1/1	0.98	0.03	30,30,30,30	0
57	MG	1A	3026	1/1	0.98	0.13	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
57	MG	1A	3305	1/1	0.98	0.05	31,31,31,31	0
57	MG	1A	3733	1/1	0.98	0.05	25,25,25,25	0
57	MG	1D	301	1/1	0.98	0.12	41,41,41,41	0
57	MG	2a	3158	1/1	0.98	0.08	40,40,40,40	0
57	MG	1D	302	1/1	0.98	0.08	39,39,39,39	0
57	MG	2a	3160	1/1	0.98	0.09	51,51,51,51	0
57	MG	1D	303	1/1	0.98	0.04	33,33,33,33	0
57	MG	1a	1632	1/1	0.98	0.08	35,35,35,35	0
57	MG	1A	3829	1/1	0.98	0.18	30,30,30,30	0
57	MG	1A	3830	1/1	0.98	0.19	34,34,34,34	0
57	MG	1A	3149	1/1	0.98	0.05	26,26,26,26	0
57	MG	1A	3495	1/1	0.98	0.07	50,50,50,50	0
57	MG	2A	3567	1/1	0.98	0.08	58,58,58,58	0
57	MG	2A	3383	1/1	0.98	0.05	37,37,37,37	0
57	MG	2A	3384	1/1	0.98	0.05	36,36,36,36	0
57	MG	1A	3424	1/1	0.98	0.06	19,19,19,19	0
57	MG	2A	3043	1/1	0.98	0.24	56,56,56,56	0
57	MG	1A	3834	1/1	0.98	0.06	31,31,31,31	0
57	MG	1A	3497	1/1	0.98	0.07	37,37,37,37	0
57	MG	2A	3574	1/1	0.98	0.08	30,30,30,30	0
57	MG	1A	3122	1/1	0.98	0.06	26,26,26,26	0
57	MG	1A	3021	1/1	0.98	0.08	35,35,35,35	0
57	MG	1A	3220	1/1	0.98	0.16	26,26,26,26	0
57	MG	1A	3656	1/1	0.98	0.08	33,33,33,33	0
57	MG	1E	302	1/1	0.98	0.26	38,38,38,38	0
57	MG	2A	3580	1/1	0.98	0.05	53,53,53,53	0
57	MG	2R	201	1/1	0.98	0.06	53,53,53,53	0
57	MG	1E	303	1/1	0.98	0.04	26,26,26,26	0
57	MG	2T	201	1/1	0.98	0.14	59,59,59,59	0
57	MG	1A	3952	1/1	0.98	0.07	38,38,38,38	0
57	MG	2A	3053	1/1	0.98	0.10	44,44,44,44	0
57	MG	2A	3584	1/1	0.98	0.06	52,52,52,52	0
57	MG	1A	3364	1/1	0.98	0.07	27,27,27,27	0
57	MG	1E	306	1/1	0.98	0.07	29,29,29,29	0
57	MG	1A	3055	1/1	0.98	0.10	33,33,33,33	0
57	MG	1E	308	1/1	0.98	0.04	35,35,35,35	0
57	MG	1A	3745	1/1	0.98	0.09	27,27,27,27	0
57	MG	2X	101	1/1	0.98	0.11	54,54,54,54	0
57	MG	1a	1652	1/1	0.98	0.10	58,58,58,58	0
57	MG	2A	3406	1/1	0.98	0.07	44,44,44,44	0
57	MG	1F	301	1/1	0.98	0.09	23,23,23,23	0
57	MG	1F	302	1/1	0.98	0.16	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1F	304	1/1	0.98	0.18	30,30,30,30	0
57	MG	1A	3746	1/1	0.98	0.06	44,44,44,44	0
57	MG	1F	306	1/1	0.98	0.04	31,31,31,31	0
57	MG	1A	3263	1/1	0.98	0.12	27,27,27,27	0
57	MG	2A	3233	1/1	0.98	0.27	44,44,44,44	0
57	MG	2A	3066	1/1	0.98	0.17	38,38,38,38	0
57	MG	25	104	1/1	0.98	0.09	57,57,57,57	0
57	MG	1A	3845	1/1	0.98	0.09	52,52,52,52	0
57	MG	1F	310	1/1	0.98	0.06	31,31,31,31	0
60	ZN	14	501	1/1	0.98	0.10	112,112,112,112	0
60	ZN	2Y	202	1/1	0.98	0.05	82,82,82,82	0
57	MG	1A	3660	1/1	0.98	0.12	49,49,49,49	0
60	ZN	29	102	1/1	0.98	0.04	63,63,63,63	0
60	ZN	2n	102	1/1	0.98	0.04	88,88,88,88	0
61	SF4	1d	306	8/8	0.98	0.04	55,64,73,75	0
61	SF4	2d	501	8/8	0.98	0.05	58,70,76,78	0
57	MG	1A	3250	1/1	0.99	0.15	32,32,32,32	0
57	MG	1A	3165	1/1	0.99	0.04	33,33,33,33	0
57	MG	1F	308	1/1	0.99	0.06	26,26,26,26	0
57	MG	1A	3252	1/1	0.99	0.18	28,28,28,28	0
57	MG	1A	3646	1/1	0.99	0.08	22,22,22,22	0
57	MG	2A	3068	1/1	0.99	0.09	22,22,22,22	0
57	MG	2E	307	1/1	0.99	0.07	33,33,33,33	0
57	MG	1A	3029	1/1	0.99	0.04	27,27,27,27	0
57	MG	1A	3358	1/1	0.99	0.07	34,34,34,34	0
57	MG	1A	3488	1/1	0.99	0.04	40,40,40,40	0
57	MG	2A	3003	1/1	0.99	0.03	40,40,40,40	0
57	MG	2F	304	1/1	0.99	0.08	47,47,47,47	0
57	MG	1A	3735	1/1	0.99	0.05	43,43,43,43	0
57	MG	1A	3452	1/1	0.99	0.05	29,29,29,29	0
57	MG	1A	3490	1/1	0.99	0.04	36,36,36,36	0
57	MG	1A	3491	1/1	0.99	0.07	22,22,22,22	0
57	MG	15	3101	1/1	0.99	0.07	26,26,26,26	0
57	MG	1A	3930	1/1	0.99	0.03	25,25,25,25	0
57	MG	1A	3015	1/1	0.99	0.05	35,35,35,35	0
57	MG	2A	3371	1/1	0.99	0.05	41,41,41,41	0
57	MG	1A	3104	1/1	0.99	0.06	20,20,20,20	0
57	MG	1A	3333	1/1	0.99	0.07	33,33,33,33	0
57	MG	2A	3374	1/1	0.99	0.08	31,31,31,31	0
57	MG	1A	3934	1/1	0.99	0.07	32,32,32,32	0
57	MG	1A	3068	1/1	0.99	0.07	32,32,32,32	0
57	MG	1A	3170	1/1	0.99	0.05	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
57	MG	1A	3048	1/1	0.99	0.08	22,22,22,22	0
57	MG	2A	3379	1/1	0.99	0.08	37,37,37,37	0
57	MG	1A	3884	1/1	0.99	0.03	48,48,48,48	0
57	MG	1A	3365	1/1	0.99	0.06	39,39,39,39	0
57	MG	1P	201	1/1	0.99	0.09	26,26,26,26	0
57	MG	1A	3070	1/1	0.99	0.19	26,26,26,26	0
57	MG	1a	1856	1/1	0.99	0.10	35,35,35,35	0
57	MG	1A	3071	1/1	0.99	0.16	31,31,31,31	0
57	MG	1A	3429	1/1	0.99	0.03	25,25,25,25	0
57	MG	1A	3043	1/1	0.99	0.07	19,19,19,19	0
57	MG	1A	3369	1/1	0.99	0.08	23,23,23,23	0
57	MG	1A	3543	1/1	0.99	0.06	18,18,18,18	0
57	MG	1A	3031	1/1	0.99	0.09	15,15,15,15	0
57	MG	1R	201	1/1	0.99	0.09	32,32,32,32	0
57	MG	2A	3633	1/1	0.99	0.09	43,43,43,43	0
57	MG	1A	3505	1/1	0.99	0.11	35,35,35,35	0
57	MG	1A	3111	1/1	0.99	0.16	24,24,24,24	0
57	MG	1A	3846	1/1	0.99	0.04	30,30,30,30	0
57	MG	1A	3074	1/1	0.99	0.05	29,29,29,29	0
57	MG	2A	3102	1/1	0.99	0.05	54,54,54,54	0
57	MG	2A	3397	1/1	0.99	0.04	38,38,38,38	0
57	MG	1A	3897	1/1	0.99	0.04	30,30,30,30	0
57	MG	2A	3641	1/1	0.99	0.08	48,48,48,48	0
57	MG	2A	3400	1/1	0.99	0.03	42,42,42,42	0
57	MG	2A	3560	1/1	0.99	0.04	22,22,22,22	0
57	MG	1A	3265	1/1	0.99	0.12	30,30,30,30	0
57	MG	1D	306	1/1	0.99	0.05	16,16,16,16	0
57	MG	1A	3899	1/1	0.99	0.06	39,39,39,39	0
57	MG	1D	308	1/1	0.99	0.10	30,30,30,30	0
57	MG	1A	3404	1/1	0.99	0.04	40,40,40,40	0
57	MG	1A	3009	1/1	0.99	0.08	24,24,24,24	0
57	MG	1A	3511	1/1	0.99	0.06	35,35,35,35	0
57	MG	1A	3760	1/1	0.99	0.08	31,31,31,31	0
57	MG	1A	3179	1/1	0.99	0.08	29,29,29,29	0
57	MG	2A	3653	1/1	0.99	0.02	34,34,34,34	0
57	MG	1A	3473	1/1	0.99	0.04	20,20,20,20	0
57	MG	1A	3808	1/1	0.99	0.09	26,26,26,26	0
57	MG	1D	316	1/1	0.99	0.05	38,38,38,38	0
57	MG	1V	202	1/1	0.99	0.18	29,29,29,29	0
57	MG	1A	3058	1/1	0.99	0.04	22,22,22,22	0
57	MG	1A	3962	1/1	0.99	0.04	41,41,41,41	0
57	MG	1A	3115	1/1	0.99	0.14	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3337	1/1	0.99	0.08	44,44,44,44	0
57	MG	1A	3245	1/1	0.99	0.13	23,23,23,23	0
57	MG	1a	1819	1/1	0.99	0.07	48,48,48,48	0
57	MG	1A	3296	1/1	0.99	0.13	21,21,21,21	0
57	MG	1A	3162	1/1	0.99	0.10	30,30,30,30	0
57	MG	1W	203	1/1	0.99	0.15	25,25,25,25	0
57	MG	1A	3639	1/1	0.99	0.09	28,28,28,28	0
57	MG	1A	3862	1/1	0.99	0.04	33,33,33,33	0
57	MG	1A	3914	1/1	0.99	0.06	33,33,33,33	0
57	MG	2A	3272	1/1	0.99	0.05	38,38,38,38	0
57	MG	2A	3128	1/1	0.99	0.07	29,29,29,29	0
60	ZN	1Y	202	1/1	0.99	0.03	59,59,59,59	0
57	MG	1A	3077	1/1	0.99	0.15	31,31,31,31	0
60	ZN	19	104	1/1	0.99	0.06	42,42,42,42	0
57	MG	1A	3770	1/1	0.99	0.17	32,32,32,32	0
57	MG	2A	3590	1/1	0.99	0.04	35,35,35,35	0
60	ZN	26	501	1/1	0.99	0.02	56,56,56,56	0
57	MG	1F	303	1/1	0.99	0.15	30,30,30,30	0
57	MG	2A	3132	1/1	0.99	0.10	50,50,50,50	0
57	MG	1A	3147	1/1	0.99	0.03	31,31,31,31	0
57	MG	1A	3185	1/1	0.99	0.05	26,26,26,26	0
57	MG	2A	3399	1/1	1.00	0.03	30,30,30,30	0
60	ZN	1n	104	1/1	1.00	0.02	66,66,66,66	0
57	MG	1A	3700	1/1	1.00	0.05	32,32,32,32	0
57	MG	1A	3974	1/1	1.00	0.02	25,25,25,25	0
60	ZN	25	105	1/1	1.00	0.04	53,53,53,53	0
57	MG	1A	3474	1/1	1.00	0.06	17,17,17,17	0
57	MG	2A	3498	1/1	1.00	0.04	35,35,35,35	0
57	MG	1A	3466	1/1	1.00	0.02	19,19,19,19	0
60	ZN	15	3110	1/1	1.00	0.04	40,40,40,40	0
60	ZN	16	501	1/1	1.00	0.05	41,41,41,41	0

6.5 Other polymers

There are no such residues in this entry.