



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 03:51 AM EDT

PDB ID : 9D7S / pdb_00009d7s
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with Api antimicrobial peptide, mRNA, A-site release factor 1, and deacylated P-site and E-site tRNA^{phe} at 2.85Å resolution
Authors : Aleksandrova, E.V.; Huang, W.; Baliga, C.; Atkinson, G.C.; Vazquez-Laslop, N.; Mankin, A.S.; Polikanov, Y.S.
Deposited on : 2024-08-17
Resolution : 2.85 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

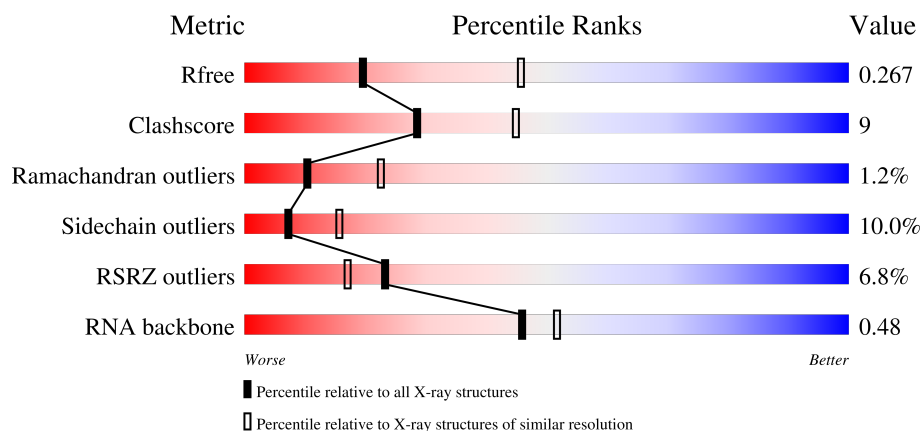
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)
RNA backbone	3983	1009 (3.06-2.66)

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	 4% 58% 31% 7% .
2	1B	121	 76% 19% .

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	25	60	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	1i	128	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	354	
54	2w	354	
55	1x	76	
55	1y	76	
55	2x	76	
55	2y	76	
56	1z	18	
56	2z	18	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1A	3600	-	-	-	X
57	MG	1a	1662	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 299015 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1085	693	189	202	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1061	680	186	194	1			

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			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
			771	495	140	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	1X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	2X	95	Total	C	N	O	S	0	0	0
			746	485	134	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	183	Total	C	N	O	S	0	0	0
			1437	919	256	260	2			
21	2Z	186	Total	C	N	O	S	0	0	0
			1451	928	256	265	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	76	Total	C	N	O	S	0	0	0
			604	373	128	102	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			548	347	99	97	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	68	Total	C	N	O	S	0	0	0
			517	330	92	90	5			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	18	64	Total	C	N	O	S	0	0	0
			511	328	99	82	2			
30	28	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1554	977	302	274	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
			1659	1040	326	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1130	714	214	199	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			810	513	143	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
			1231	766	243	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			983	623	193	167			
40	2i	123	Total	C	N	O	0	0	0
			940	593	185	162			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	98	Total	C	N	O	0	0	0
			721	449	140	132			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	131			

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	118	Total	C	N	O	S	0	0	0
			923	569	191	161	2			
44	2m	115	Total	C	N	O	S	0	0	0
			889	546	183	158	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
			486	309	101	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
			551	353	108	90				

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

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

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

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

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

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

- Molecule 53 is a RNA chain called PHE-Stop mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			274	124	48	89	13			
53	2v	13	Total	C	N	O	P	0	0	0
			274	124	48	89	13			

- Molecule 54 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	249	Total	C	N	O	S	0	0	0
			1939	1199	360	371	9			
54	2w	253	Total	C	N	O	S	0	0	0
			1957	1210	361	377	9			

- Molecule 55 is a RNA chain called P-site and E-site Deacylated tRNA^{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	75	Total	C	N	O	P	S	0	0	0
			1612	722	288	525	75	2			
55	1y	74	Total	C	N	O	P	S	0	0	0
			1590	712	285	517	74	2			
55	2x	75	Total	C	N	O	P	S	0	0	0
			1612	722	288	525	75	2			
55	2y	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			

- Molecule 56 is a protein called Api Antimicrobial Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	1z	14	Total	C	N	O	0	0	0
			119	79	23	17			
56	2z	14	Total	C	N	O	0	0	0
			119	79	23	17			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	793	Total	Mg	0	0
			793	793		
57	1B	20	Total	Mg	0	0
			20	20		
57	1D	9	Total	Mg	0	0
			9	9		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1E	7	Total 7	Mg 7	0	0
57	1F	14	Total 14	Mg 14	0	0
57	1G	3	Total 3	Mg 3	0	0
57	1N	3	Total 3	Mg 3	0	0
57	1O	1	Total 1	Mg 1	0	0
57	1P	4	Total 4	Mg 4	0	0
57	1Q	5	Total 5	Mg 5	0	0
57	1R	2	Total 2	Mg 2	0	0
57	1T	1	Total 1	Mg 1	0	0
57	1U	8	Total 8	Mg 8	0	0
57	1V	5	Total 5	Mg 5	0	0
57	1W	3	Total 3	Mg 3	0	0
57	1X	3	Total 3	Mg 3	0	0
57	1Z	2	Total 2	Mg 2	0	0
57	10	4	Total 4	Mg 4	0	0
57	11	3	Total 3	Mg 3	0	0
57	12	1	Total 1	Mg 1	0	0
57	13	1	Total 1	Mg 1	0	0
57	15	7	Total 7	Mg 7	0	0
57	16	1	Total 1	Mg 1	0	0
57	17	7	Total 7	Mg 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	18	2	Total 2	Mg 2	0	0
57	19	1	Total 1	Mg 1	0	0
57	1a	167	Total 167	Mg 167	0	0
57	1f	1	Total 1	Mg 1	0	0
57	1i	1	Total 1	Mg 1	0	0
57	1k	1	Total 1	Mg 1	0	0
57	1m	1	Total 1	Mg 1	0	0
57	1n	1	Total 1	Mg 1	0	0
57	1v	3	Total 3	Mg 3	0	0
57	1w	3	Total 3	Mg 3	0	0
57	1x	10	Total 10	Mg 10	0	0
57	1y	3	Total 3	Mg 3	0	0
57	2A	657	Total 657	Mg 657	0	0
57	2B	10	Total 10	Mg 10	0	0
57	2D	7	Total 7	Mg 7	0	0
57	2E	7	Total 7	Mg 7	0	0
57	2F	5	Total 5	Mg 5	0	0
57	2O	1	Total 1	Mg 1	0	0
57	2P	1	Total 1	Mg 1	0	0
57	2Q	3	Total 3	Mg 3	0	0
57	2R	1	Total 1	Mg 1	0	0

Continued on next page...

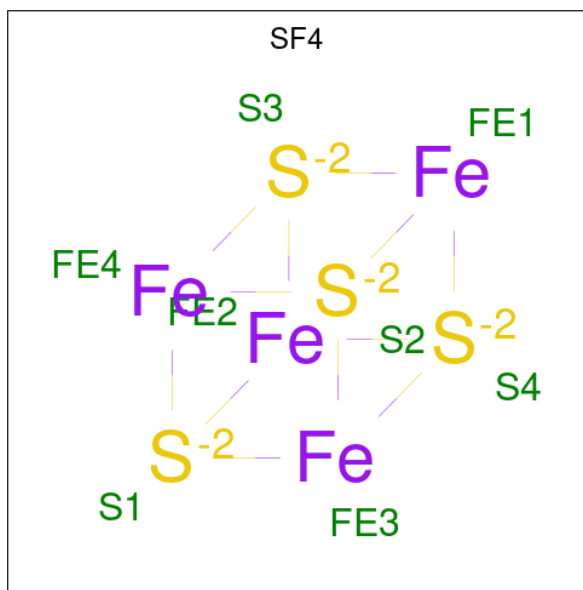
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2U	2	Total 2	Mg 2	0	0
57	2V	2	Total 2	Mg 2	0	0
57	2W	1	Total 1	Mg 1	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	1	Total 1	Mg 1	0	0
57	23	2	Total 2	Mg 2	0	0
57	25	2	Total 2	Mg 2	0	0
57	26	1	Total 1	Mg 1	0	0
57	28	1	Total 1	Mg 1	0	0
57	2a	165	Total 165	Mg 165	0	0
57	2e	3	Total 3	Mg 3	0	0
57	2f	1	Total 1	Mg 1	0	0
57	2j	1	Total 1	Mg 1	0	0
57	2k	2	Total 2	Mg 2	0	0
57	2t	1	Total 1	Mg 1	0	0
57	2v	2	Total 2	Mg 2	0	0
57	2x	9	Total 9	Mg 9	0	0

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total 1	Zn 1	0	0
58	14	1	Total 1	Zn 1	0	0
58	15	1	Total 1	Zn 1	0	0
58	16	1	Total 1	Zn 1	0	0
58	19	1	Total 1	Zn 1	0	0
58	1n	1	Total 1	Zn 1	0	0
58	2Y	1	Total 1	Zn 1	0	0
58	24	1	Total 1	Zn 1	0	0
58	25	1	Total 1	Zn 1	0	0
58	26	1	Total 1	Zn 1	0	0
58	29	1	Total 1	Zn 1	0	0
58	2n	1	Total 1	Zn 1	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	1d	1	Total	Fe	S	0	0
			8	4	4		
59	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	1368	Total	O	0	0
			1368	1368		
60	1B	27	Total	O	0	0
			27	27		
60	1D	14	Total	O	0	0
			14	14		
60	1E	14	Total	O	0	0
			14	14		
60	1F	10	Total	O	0	0
			10	10		
60	1G	1	Total	O	0	0
			1	1		
60	1N	3	Total	O	0	0
			3	3		
60	1O	3	Total	O	0	0
			3	3		
60	1P	18	Total	O	0	0
			18	18		
60	1Q	7	Total	O	0	0
			7	7		
60	1R	1	Total	O	0	0
			1	1		
60	1T	1	Total	O	0	0
			1	1		
60	1U	6	Total	O	0	0
			6	6		
60	1V	2	Total	O	0	0
			2	2		
60	1W	2	Total	O	0	0
			2	2		
60	1X	3	Total	O	0	0
			3	3		
60	10	3	Total	O	0	0
			3	3		
60	11	2	Total	O	0	0
			2	2		

Continued on next page...

Continued from previous page...

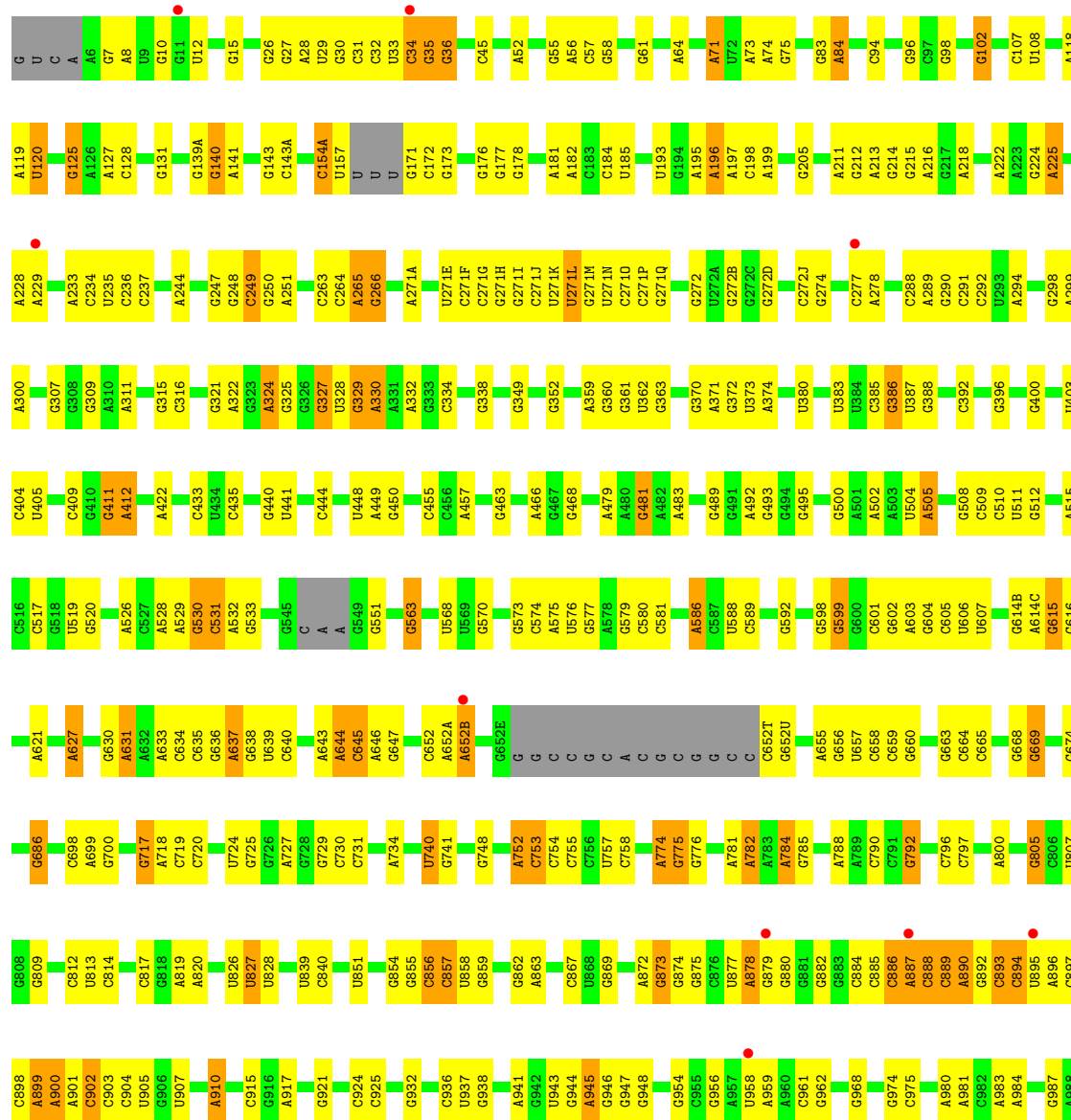
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	13	2	Total 2	O 2	0	0
60	15	6	Total 6	O 6	0	0
60	16	1	Total 1	O 1	0	0
60	17	3	Total 3	O 3	0	0
60	18	6	Total 6	O 6	0	0
60	19	1	Total 1	O 1	0	0
60	1a	164	Total 164	O 164	0	0
60	1d	2	Total 2	O 2	0	0
60	1e	1	Total 1	O 1	0	0
60	1l	2	Total 2	O 2	0	0
60	1p	1	Total 1	O 1	0	0
60	1v	3	Total 3	O 3	0	0
60	1w	5	Total 5	O 5	0	0
60	1x	20	Total 20	O 20	0	0
60	1y	1	Total 1	O 1	0	0
60	1z	3	Total 3	O 3	0	0
60	2A	949	Total 949	O 949	0	0
60	2B	5	Total 5	O 5	0	0
60	2D	13	Total 13	O 13	0	0
60	2E	8	Total 8	O 8	0	0
60	2F	6	Total 6	O 6	0	0

Continued on next page...

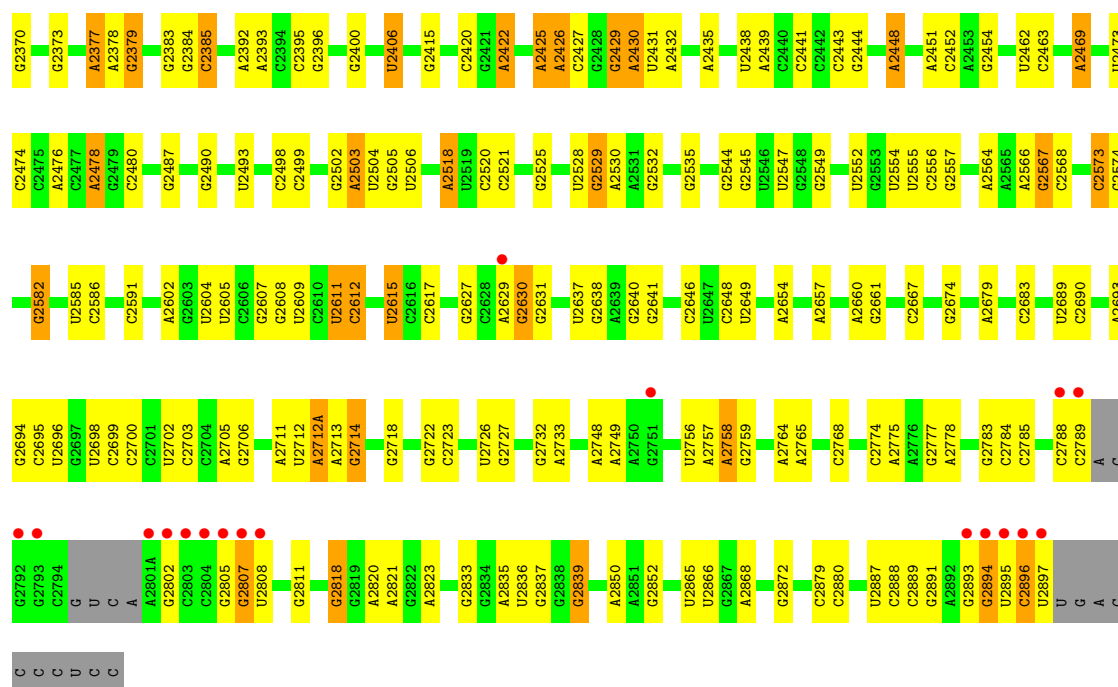
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2N	2	Total 2	O 2	0	0
60	2P	7	Total 7	O 7	0	0
60	2R	2	Total 2	O 2	0	0
60	2T	1	Total 1	O 1	0	0
60	2U	1	Total 1	O 1	0	0
60	2V	1	Total 1	O 1	0	0
60	2W	1	Total 1	O 1	0	0
60	2X	2	Total 2	O 2	0	0
60	2Y	1	Total 1	O 1	0	0
60	20	6	Total 6	O 6	0	0
60	21	2	Total 2	O 2	0	0
60	23	2	Total 2	O 2	0	0
60	27	2	Total 2	O 2	0	0
60	28	2	Total 2	O 2	0	0
60	2a	154	Total 154	O 154	0	0
60	2d	1	Total 1	O 1	0	0
60	2q	1	Total 1	O 1	0	0
60	2v	3	Total 3	O 3	0	0
60	2w	2	Total 2	O 2	0	0
60	2x	11	Total 11	O 11	0	0
60	2z	1	Total 1	O 1	0	0

G2532	A2435	G2224	C2138	G2055	U1931	G1813	A1669	C1432	C1314	G1088
A2533	A2439	G2226	C2139	C2056	A1932	A1814	U1673	U1433	C1315	G1089
A2534	A2440	G2224	C2140	G2057	G1933	A1815	G1674	A1543	U1187	U1090
G2535	G2441	G2234	G2141	A2060	C1934	A1816	C1686	C1437	G1188	G1091
U2537	C2442	G2234	C2142	G2061	G1935	G1817	C1687	U1438	G1192	G1092
G2538	C2443	G2239	C2143	A2062	A1936	U1818	U1688	A1588	G1199	G1093
U2547	C2444	G2239	C2145	G2069	A1937	A1819	G1687	A1439	U1094	A1095
U2552	G2445	G2239	C2146	G2070	U1938	G1826	G1688	G1442	C1200	U1096
U2554	G2446	G2239	C2147	G2071	U1939	A1828	G1696	A1445	C1201	U1097
A2564	G2447	U2244	G2148	U2074	C1942	G1839	A1700	G1448	G1212	A1098
A2565	A2448	U2244	G2149	U2075	U1945	U1839	A1701	A1449	C1218	G1099
G2567	C2452	G2251	G2150	G2076	U1955	G1845	G1702	G1450	U1101	C1102
C2568	A2460	G2251	G2151	C2081	C1962	A1846	G1703	A1555	G1358	A1103
A2572	U2462	U2557	G2152	A2082	G1963	U1847	G1704	G1455	A1359	
G2573	C2374	U2577	G2153	C2086	U1964	A1847	G1705	A1580	A1360	
G2574	A2469	A2274	C2162	U2086	C1965	U1851	G1705	A1460	A1226	
G2575	G2470	G2277	G2163	G2095	A1966	A1852	U1709	G1461	G1236	
G2576	C2471	G2278	C2164	C2096	C1967	G1857	G1711	A1586	G1239	
A2577	G2472	G2279	G2165	U2096	U1968	A1858	C1712	G1464	U1240	
U2583	A2476	G2283	C2166	C2097	C1969	A1859	U1713	G1466	A1241	
U2584	C2477	G2284	U2167	U2098	A1972	U1864	A1722	C1467	G1371	
U2585	A2478	C2284	G2168	G2100	G1975	A1866	U1739	A1471	U1372	
A2589	C2483	C2285	A2169	G2101	U1981	A1876	G1756	G1478	G1244	
A2590	U2491	A2287	A2170	C2107	U1983	A1877	C1762	A1482	A1253	
G2591	U2491	A2287	A2171	U2109	C1986	A1879	G1763	C1493	G1256	
G2592	U2491	A2287	A2172	G2110	G1987	C1883	G1764	A1495	A1127	
C2601	G2494	C2292	A2173	C2111	C2001	A1884	C1771	A1496	A1262	
A2602	G2495	C2292	C2174	G2112	A2001	U1889	G1772	A1507	U1263	
G2603	C2496	U2297	C2175	A2114	G2002	A1889	A1773	C1508	G1264	
U2604	C2499	C2297	A2176	G2115	C2012	C1895	U1779	A1509A	A1265	
U2605	C2499	C2299	C2178	A2117	G2012	C1895	A1780	A1509B	U1267	
U2609	G2502	G2304	U2179	U2118	A2020	G1899	G1781	G1400	G1401	
C2610	U2503	A2305	U2180	A2119	C2021	A1900	C1782	G1401	G1271	
U2611	G2505	C2306	G2182	G2120	U2022	G1903	A1783	U1512	A1272	
G2612	G2506	G2307	C2183	U2122	G2023	G1903	A1784	C1513	A1273	
U2615	C2507	G2308	G2184	G2123	G2029	G1906	A1786	U1514	U1406	
C2616	G2508	G2407	C2188	G2124	A2030	U1911	G1791	C1516	A1278	
G2617	U2513	U2312	U2189	A2125	C2031	U1911	G1792	G1517	C1289	
G2618	U2514	G2319	G2190	G2126	G2032	C1914	G1792	U1518	U1165	
G2619	C2515	G2319	G2191	C2128	A2033	U1915	U1796	A1652	C1290	
G2627	A2518	A2321	G2192	C2129	C2036	C1917	C1797	A1528	C1291	
C2628	U2519	A2322	G2193	U2130	C2036	U1917	U1798	C1532	C1292	
A2629	G2520	G2323	U2203	C2131	C2040	A1918	G1799	G	G1296	
G2630	U2520	G2324	U2203	U2132	U2041	A1919	C1800	U	U1300	
G2631	G2529	C2325	G2206	C2133	C2043	A1919	G1801	A	A1301	
G2634	U2530	G2326	G2207	A2135	C2043	G1921	A1810	C	A1302	
	U2531	A2327	G2207	G2136	C2051	G1928	G1811		A1303	
		A2420	A2328	C2137	C2052	G1929	A1812		G1303	

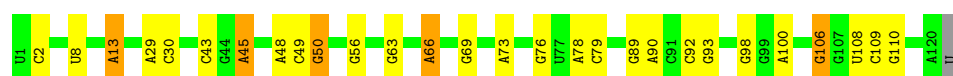


G2990	G2182	U2122	A2030	A1918	G1801	G1681	U1578	G1479	G1364	A1241	A1129	G	G989
U2291	C2183	G2123	A2031	A1919	U1808	G1682	A1579	G1480	A1365	A1242	U1130	C	C994
C2292	C2184	G2124	G2032	C1920	A1809	C1683	A1580	U1481	C1370	G1243	G1131	U	C995
C2293	G2185	G2125	A2033	G1921	A1810	C1684	C1581	G1482	U1371	G1250	G1135	A	A996
C2294	G2186	A2126	C2036	G1922	G1811	U1688	C1582	A1490	U1372	A1253	G1136	G	G997
C2295	G2187	G2127	G2037	C1923	A1812	A1689	C1583	U1493	A1379	G1265	G1139	A	A1000
U2296	C2188	C2128	G2038	C1924	U1816	G1696	C1584	C1493	G1380	G1256	C1140	G	A1005
C2297	U2189	C2129	C2039	A1927	G1816	G1697	C1588	C1494	G1381	C1257	U1141	C	C1006
A2298	G2190	G2131	C2040	A1928	A1819	G1698	C1589	A1495	A1384	A1267	U1142	A	A1009
C2299	G2191	U2132	C2041	G1929	U1820	G1699	C1592	U1496	A1385	G1264	A1142A	C	A1010
G2300	G2192	G2133	C2043	C1930	U1821	A1700	G1593	U1497	G1385	A1265	A1143	C	G1011
C2301	A2198	U1931	C2050	U1932	A1822	A1701	A1596	U1503	U1394	G1266	A1143	C	A1012
A2305	U2203	A1932	G2051	G1933	G1822	U1709	A1597	C1504	U1395	G1267	G1149	A	U1013
C2306	C2205	C2137	A2052	C1934	C1827	C1710	C1598	C1505	U1396	A1268	C1150	U	U1014
G2307	G2206	G2138	G2053	G1935	A1829	U1720	C1599	A1507	C1402	A1269	G1153	C	U1019
G2308	G2207	C2139	C2055	A1936	G1830	U1721	C1607	U1508	G1411	G1271	A1156	U	G1022
A2311	A2208	G2140	G2056	A1937	U1835	G1722	A1608	C1509	A1412	A1272	U1165	A	U1023
U2312	U2218	C2141	A2057	U1938	C1836	G1723	A1609	A1509A	G1413	U1273	C1166	A	G1024
C2313	G2224	C2142	A2058	U1939	C1837	U1739	A1610	A1509B	G1414	A1274	U1167	A	G1025
C2314	G2225	C2143	A2059	U1940	C1837	U1740	A1611	G1510	U1415	A1278	G1168	G	U1026
G2315	C2226	U2144	A2060	C1942	G1840	A1741	A1614	U1514	G1416	C1289	G1169	A	A1027
C2316	C2226	C2145	G2061	U1943	U1843	G1746	C1615	G1515	C1417	C1290	G1170	U	U1028
C2317	C2246	C2146	C2065	U1955	A1847	G1747	A1616	U1518	G1418	G1297	G1171	G	G1030
G2318	U2232	G2147	C2066	U1956	U1848	G1753	A1617	G1519	A1419	U1300	G	U	G1031
C2319	U2233	G2148	G2067	C1957	G1849	C1754	U1629	G1526	G1423	A1301	A	U	A1032
A2320	G2234	C2149	G2068	C1958	U1850	G1755	G1630	G1527	G1424	C1314	C1178	A	U1033
G2321	G2235	U2150	G2069	C1958	G1851	G1756	C1631	A1528	C1428	C1315	C1179	A	G1037
A2322	G2238	G2151	G2070	C1962	U1852	U1757	A1631A	G1529	U1431	U1316	C1180	A	C1038
G2325	G2239	G2152	U2074	U1963	C1852	G1758	A1632	G1530	A1434	A1317	G1186	C	G1039
C2326	C2240	C2153	U2075	G1964	C1853	G1759	C1633	C1531	C1437	C1318	G1187	C	G1040
A2327	A2241	G2154	G2086	C1965	A1859	G1763	A1637	C1532	U	G1319	U1188	U	C1041
A2328	G2246	G2155	U2086	A1966	U1859	G1764	C1638	C1533	A1445	A1321	A1189	A	G1042
G2329	A2247	G2156	G2087	C1967	A1876	U1769	C1640	A1537	G1449	G1332	G1192	C	C1043
A2333	G2251	G2157	G2088	U1970	A1877	G1770	A1641	G1538	A1450	C1333	G1203	G	A
C2334	C2264	C2162	G2100	A1971	G1878	G1771	G1642	A1539	G1451	U1341	A1204	G	A
A2335	A2268	G2163	G2101	U1972	U1883	A1773	C1648	G1541	G1455	U1342	U1205	C	A
G2343	A2269	C2164	C2103	U1993	A1889	A1780	G1651	A1542	A1471	A1349	C1207	A	A
U2344	G2270	G2165	G2104	C1996	A1890	C1781	A1652	C1543	A1460	A1349	C1208	C	A
G2345	G2271	G2166	C2105	G1997	G1899	C1782	A1653	C1544	G1466	U1352	G1209	C	C
A2346	U2272	G2167	G2106	C2006	A1900	A1783	A1654	C1545	C1467	G1355	A1210	A	A
C2347	A2273	G2168	C2107	C2006	G1906	U1786	C1658	C1546	A1477	G1356	U1211	G	G
U2348	A2274	A2169	U2109	G2111	G1907	C1790	A1664	C1547	A1471	U1357	A1220	A	A
G2349	C2275	A2170	G2110	A2013	C1908	A1791	A1665	A1588	A1474	G1358	G1224	G	G
C2350	A2278	U2172	G2111	A2014	U1911	U1794	G1666	A1566	C1474	A1359	A1237	U	U
G2354	A2279	C2174	A2113	C2021	U1912	U1795	A1667	A1567	G1475	A1360	G1125	G	G
A2360	C2283	G2175	A2114	U2022	A1913	U1796	A1668	A1568	C1477	C1363	A1126	U	U
A2361	G2284	G2176	G2115	G2023	C1914	C1797	A1669	G1568	A1477	G1478	G1112	G	G
C2364	A2286	C2177	A2117	G2024	U1915	C1797	A1674	A1569	A1477	G1478	G1113	A	A
G2365	A2287	C2178	U2118	C2025	A1916	C1797	A1674	A1569	A1477	G1478	G1114	G	G
A2369	G2289	U2180	G2120	G2026	A1916	C1797	A1674	A1569	A1477	G1478	G1115	G	G
		G2181	G2121	G2027	A1916	C1797	A1674	A1569	A1477	G1478	G1116	G	G
					A1916	C1797	A1674	A1569	A1477	G1478	G1117	A	A
					A1916	C1797	A1674	A1569	A1477	G1478	G1118	A	A



- Molecule 2: 5S Ribosomal RNA

Chain 1B: 76% 19%



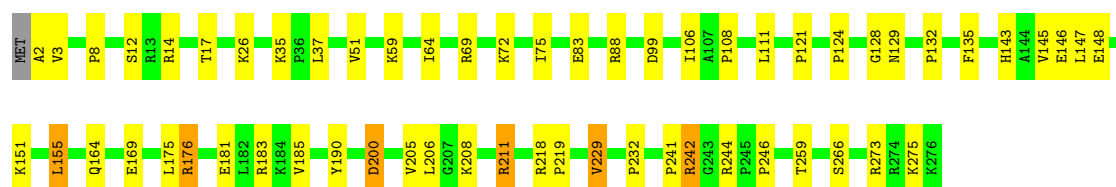
- Molecule 2: 5S Ribosomal RNA

Chain 2B: 55% 39% 6%

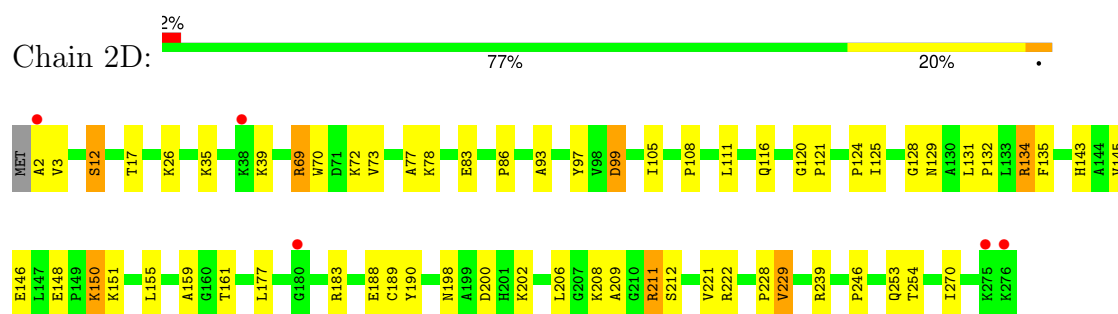


- Molecule 3: 50S ribosomal protein L2

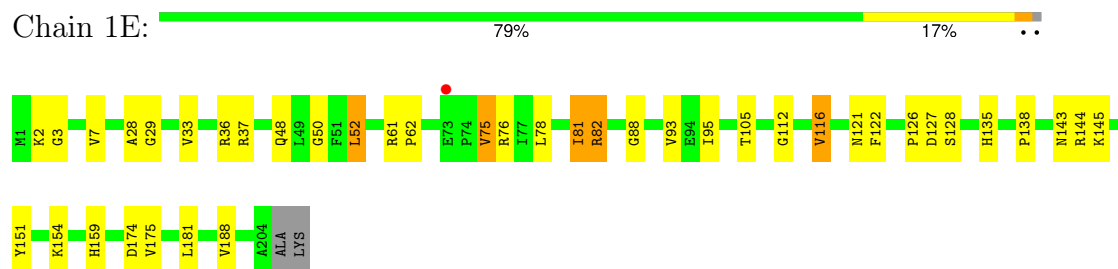
Chain 1D: 78% 19%



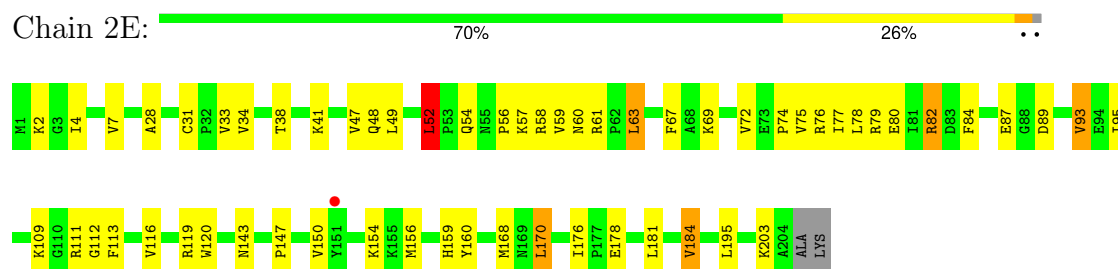
- Molecule 3: 50S ribosomal protein L2



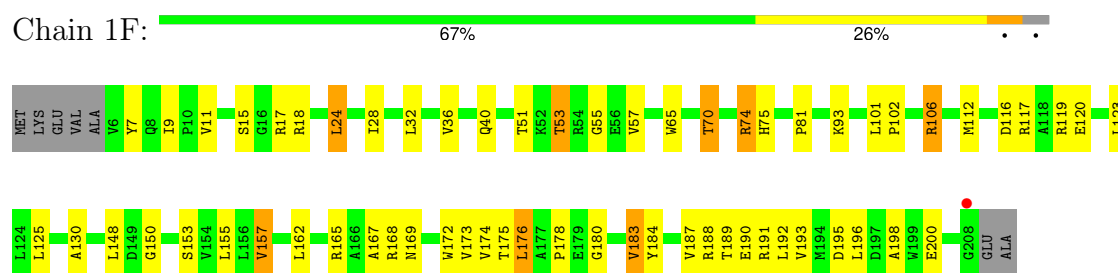
• Molecule 4: 50S ribosomal protein L3



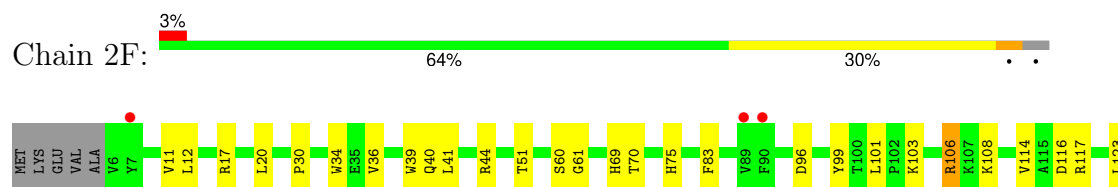
• Molecule 4: 50S ribosomal protein L3

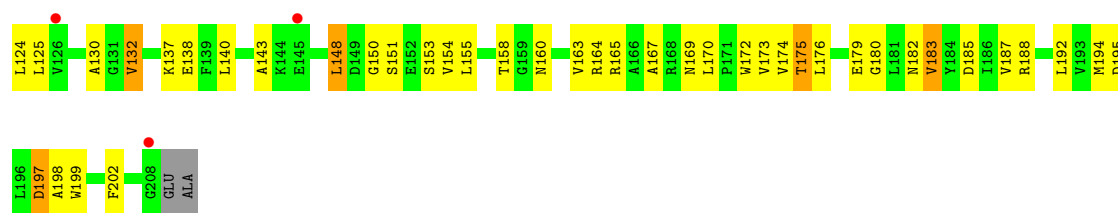


• Molecule 5: 50S ribosomal protein L4

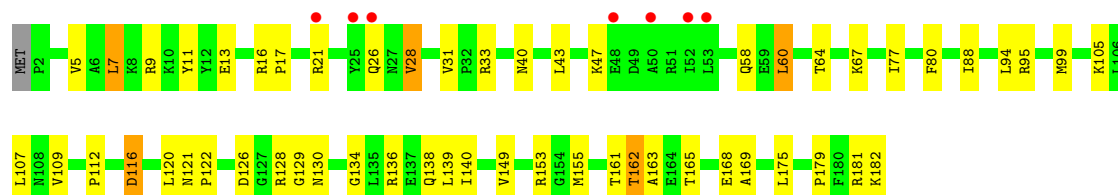


• Molecule 5: 50S ribosomal protein L4

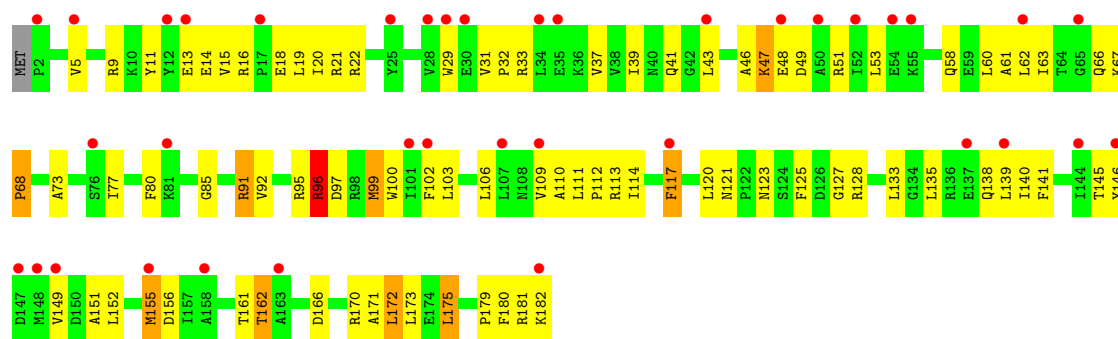




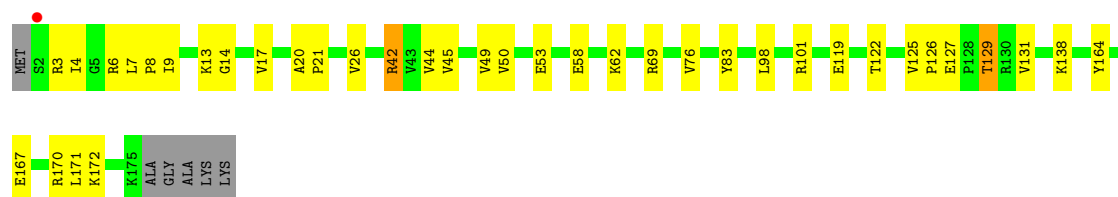
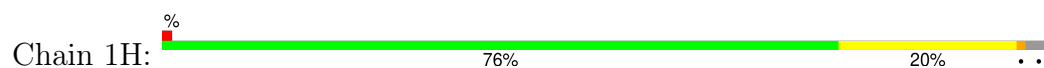
• Molecule 6: 50S ribosomal protein L5



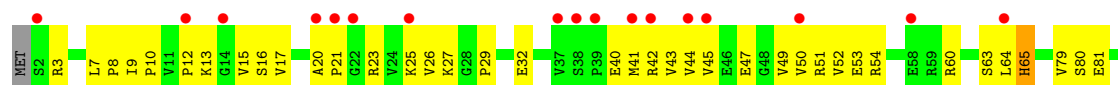
• Molecule 6: 50S ribosomal protein L5

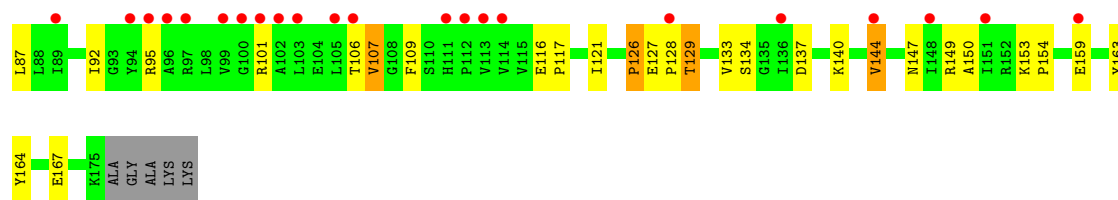


• Molecule 7: 50S ribosomal protein L6

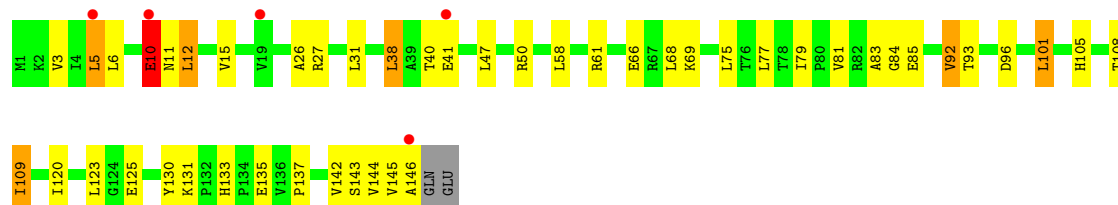


• Molecule 7: 50S ribosomal protein L6

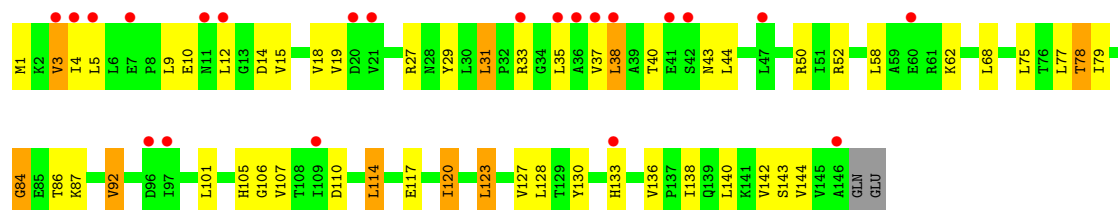




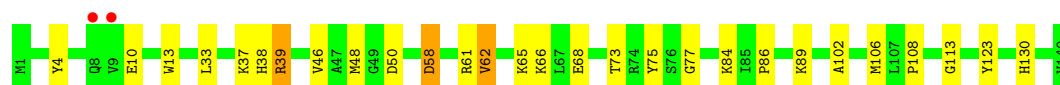
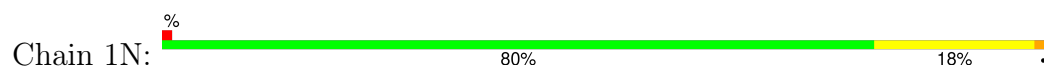
• Molecule 8: 50S ribosomal protein L9



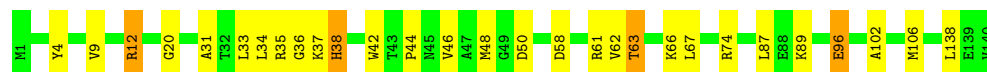
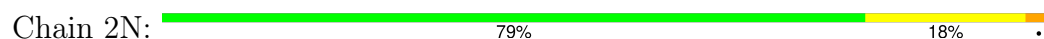
• Molecule 8: 50S ribosomal protein L9



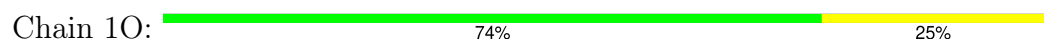
• Molecule 9: 50S ribosomal protein L13



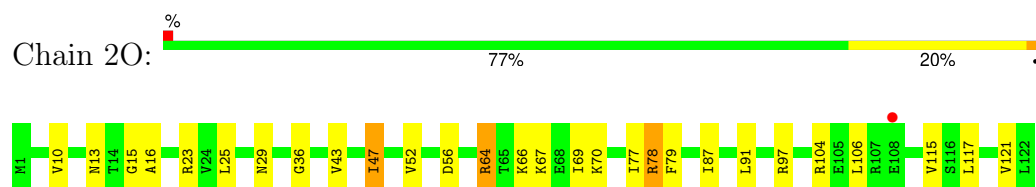
• Molecule 9: 50S ribosomal protein L13



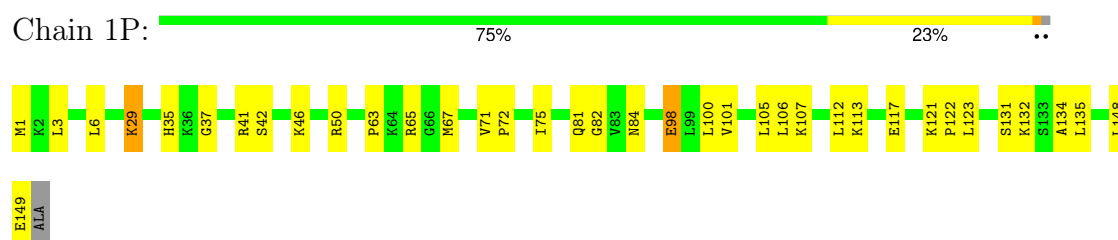
• Molecule 10: 50S ribosomal protein L14



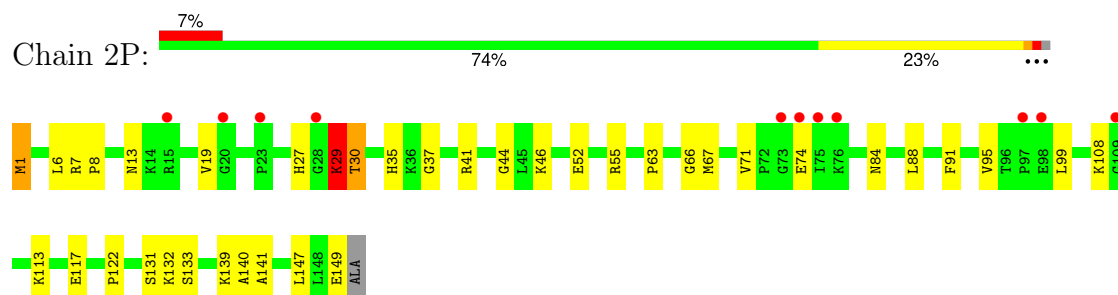
- Molecule 10: 50S ribosomal protein L14



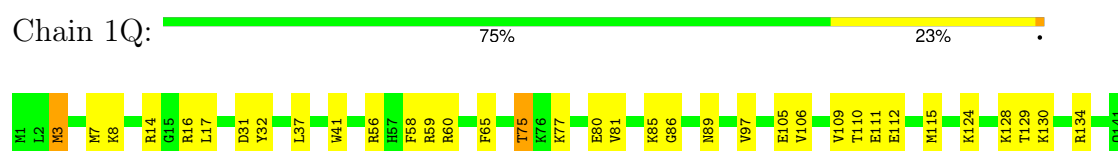
- Molecule 11: 50S ribosomal protein L15



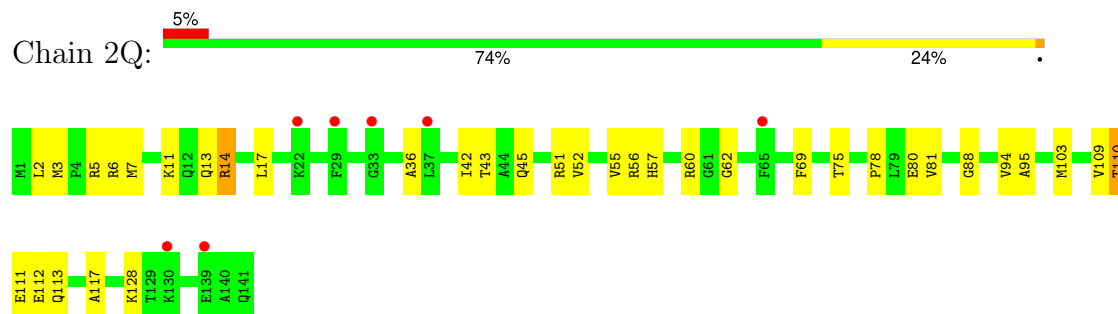
- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L16

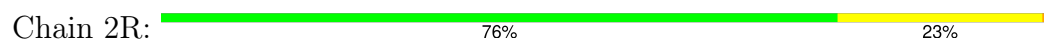


- Molecule 13: 50S ribosomal protein L17

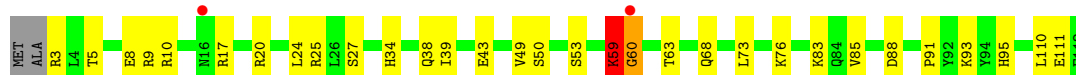




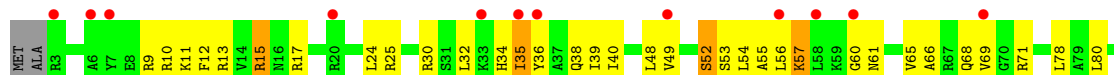
- Molecule 13: 50S ribosomal protein L17



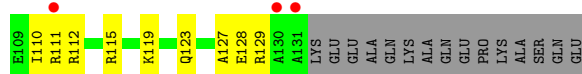
- Molecule 14: 50S ribosomal protein L18



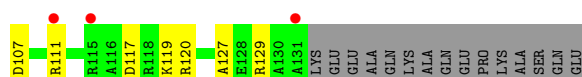
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19

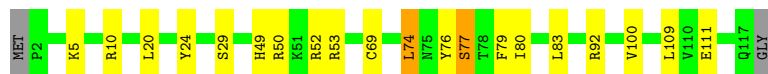


- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20

Chain 1U:  81% 15% ..



- Molecule 16: 50S ribosomal protein L20

Chain 2U:  81% 16% ..



- Molecule 17: 50S ribosomal protein L21

Chain 1V:  80% 17% ..



- Molecule 17: 50S ribosomal protein L21

Chain 2V:  83% 15% ..



- Molecule 18: 50S ribosomal protein L22

Chain 1W:  75% 23% ..



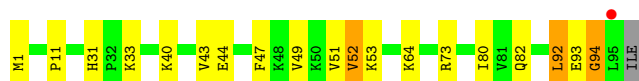
- Molecule 18: 50S ribosomal protein L22

Chain 2W:  77% 22% ..

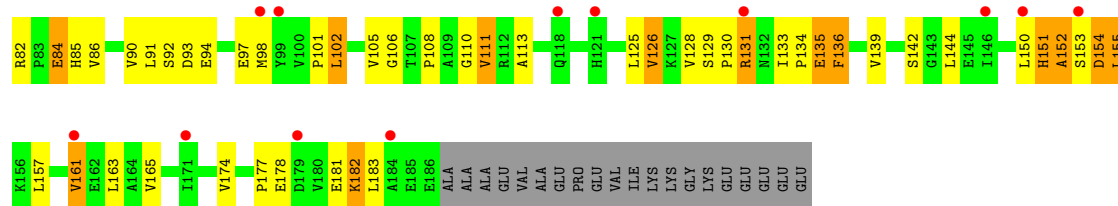


- Molecule 19: 50S ribosomal protein L23

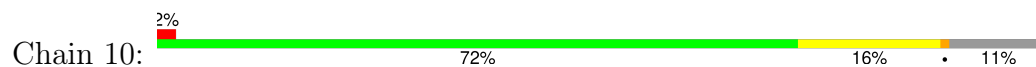
Chain 1X:  79% 17% ..



- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|----|----|----|----|--|----|-----|-----|--|-----|--|-----|-----|--|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|--|-----|--|-----|-----|-----|-----|--|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|-----|-----|-----|-----|-----|-----|--|-----|--|-----|-----|
| M1 | E2 | Y3 | R4 | L5 | | Y9 | R10 | E11 | | P15 | | L18 | R19 | | P25 | | M28 | Y29 | N30 | R31 | H32 | L33 | N34 | R35 | | Y38 | | V39 | D40 | L41 | V42 | | D45 | | F48 | R49 | Q50 | A51 | S52 | I53 | H54 | H55 | V56 | I57 | V58 | L59 | E60 | L61 | | P68 | T69 | L70 | R71 | R72 | Q73 | | D77 | | R80 | Y81 |
|----|----|----|----|----|--|----|-----|-----|--|-----|--|-----|-----|--|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|--|-----|--|-----|-----|-----|-----|--|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|-----|-----|-----|-----|-----|-----|--|-----|--|-----|-----|



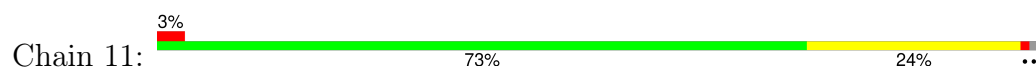
- Molecule 22: 50S ribosomal protein L27



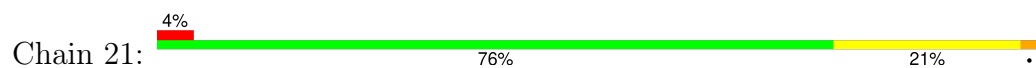
- Molecule 22: 50S ribosomal protein L27



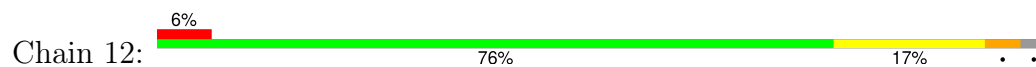
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29

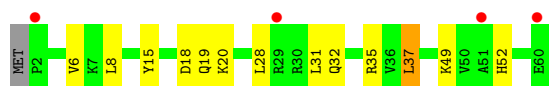
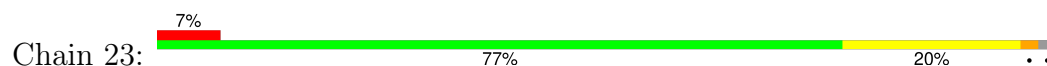




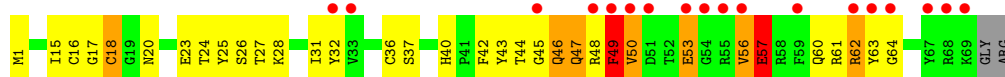
- Molecule 25: 50S ribosomal protein L30



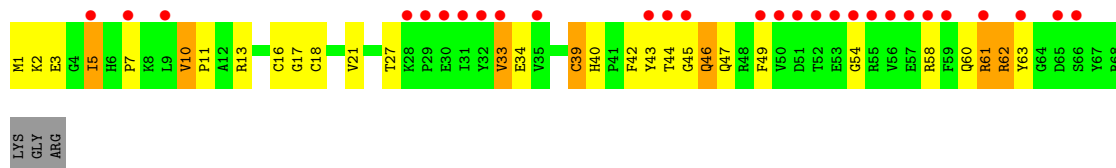
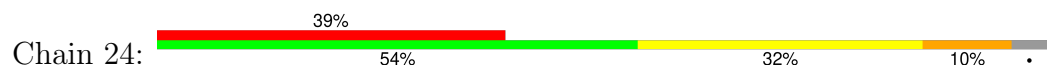
- Molecule 25: 50S ribosomal protein L30



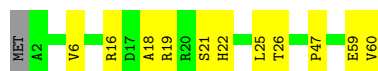
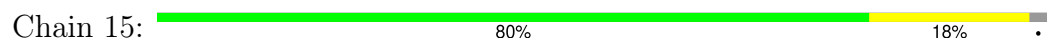
- Molecule 26: 50S ribosomal protein L31



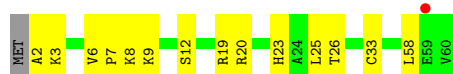
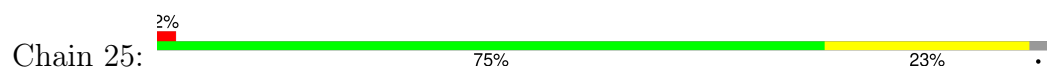
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32

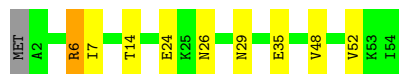


- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33

Chain 16:  81% 15% ..



- Molecule 28: 50S ribosomal protein L33

Chain 26:  4% 78% 19% ..



- Molecule 29: 50S ribosomal protein L34

Chain 17:  4% 71% 24% ..



- Molecule 29: 50S ribosomal protein L34

Chain 27:  8% 84% 12% ..



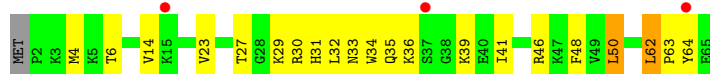
- Molecule 30: 50S ribosomal protein L35

Chain 18:  65% 32% ..



- Molecule 30: 50S ribosomal protein L35

Chain 28:  5% 66% 29% ..



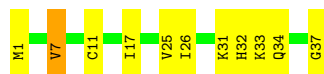
- Molecule 31: 50S ribosomal protein L36

Chain 19:  68% 30% ..



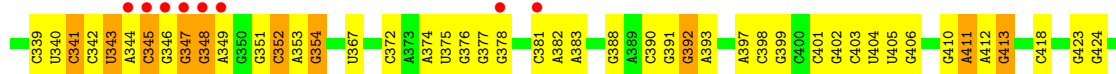
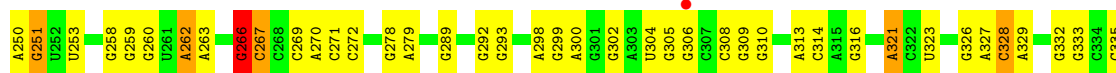
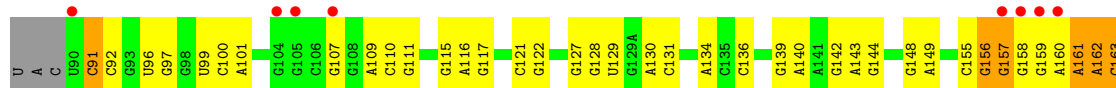
• Molecule 31: 50S ribosomal protein L36

Chain 29:  70% 27% .

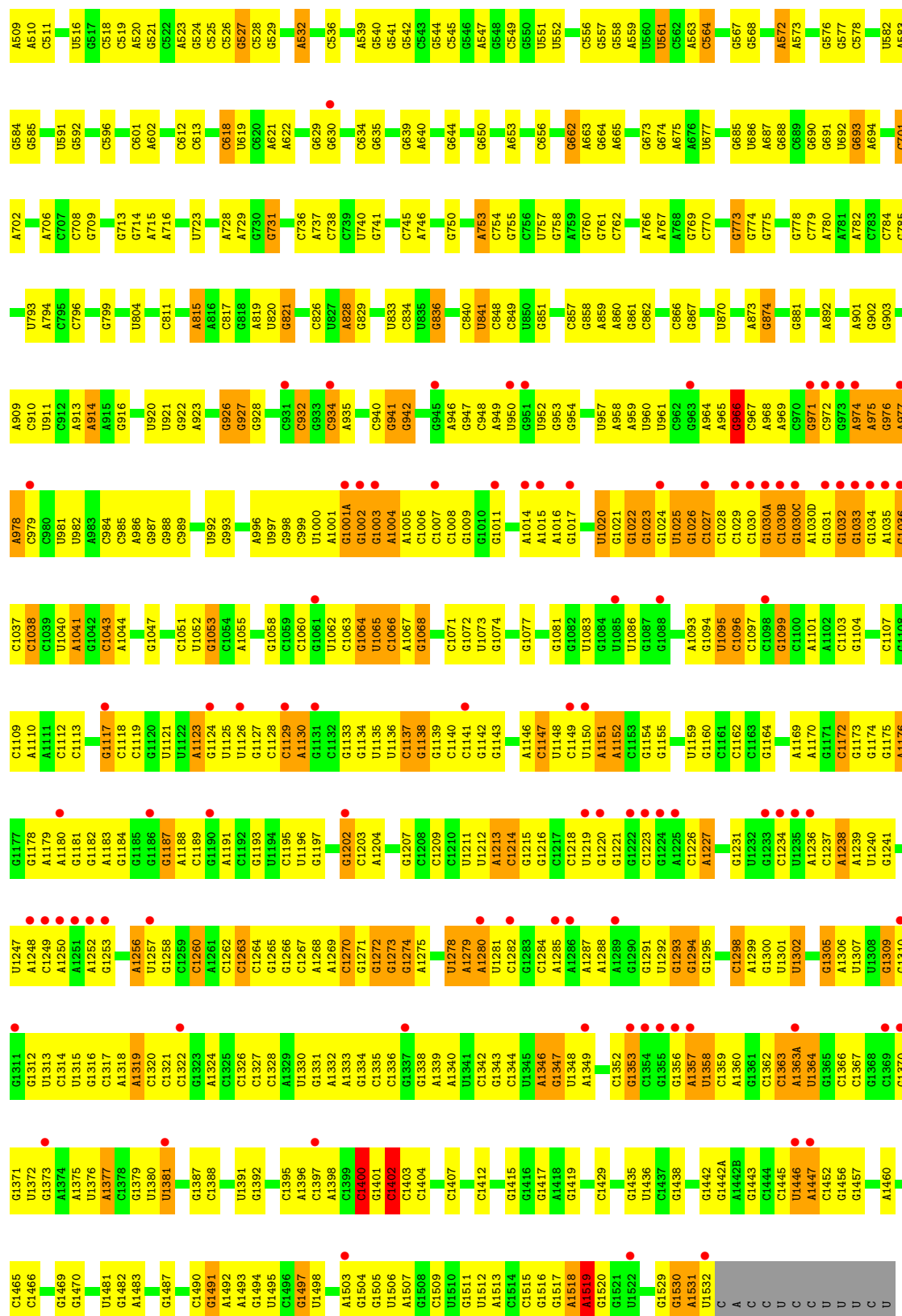


• Molecule 32: 16S Ribosomal RNA

Chain 1a:  5% 49% 42% 7% .

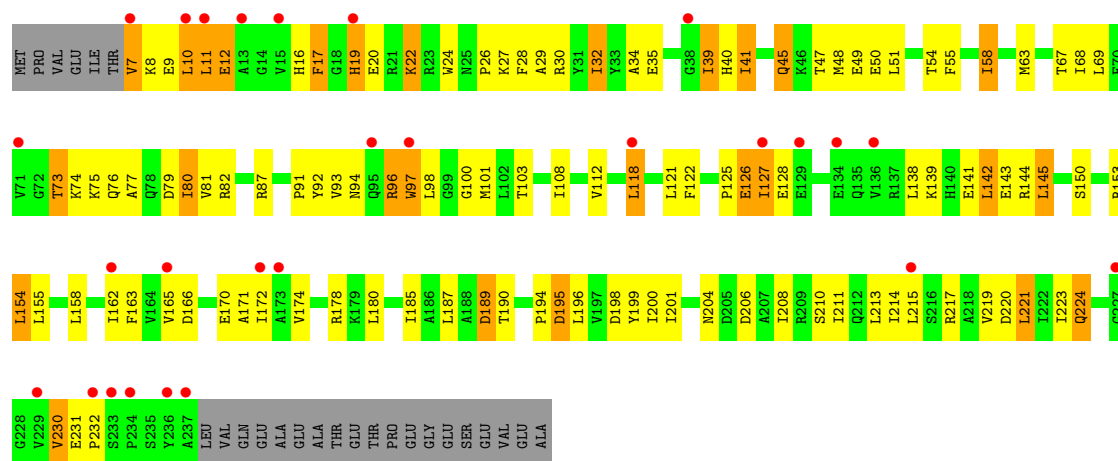




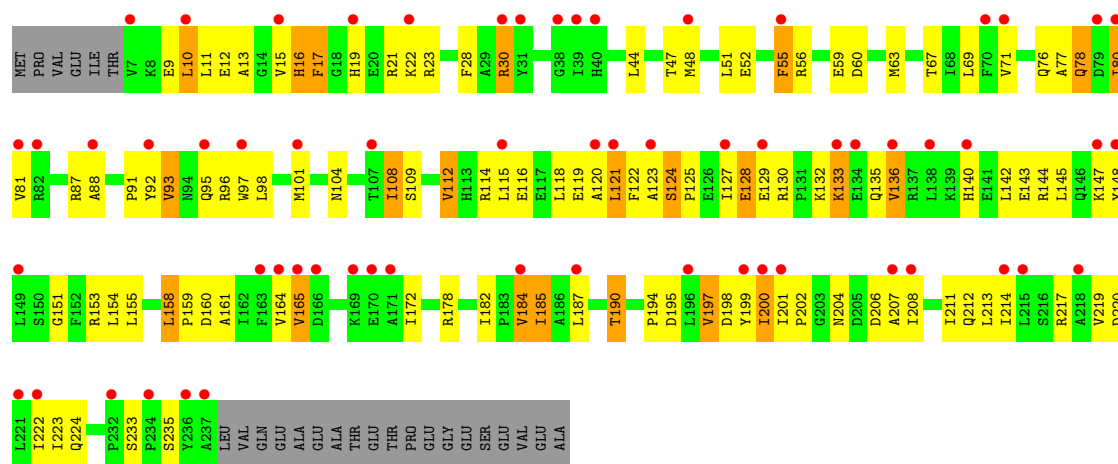


• Molecule 33: 30S ribosomal protein S2

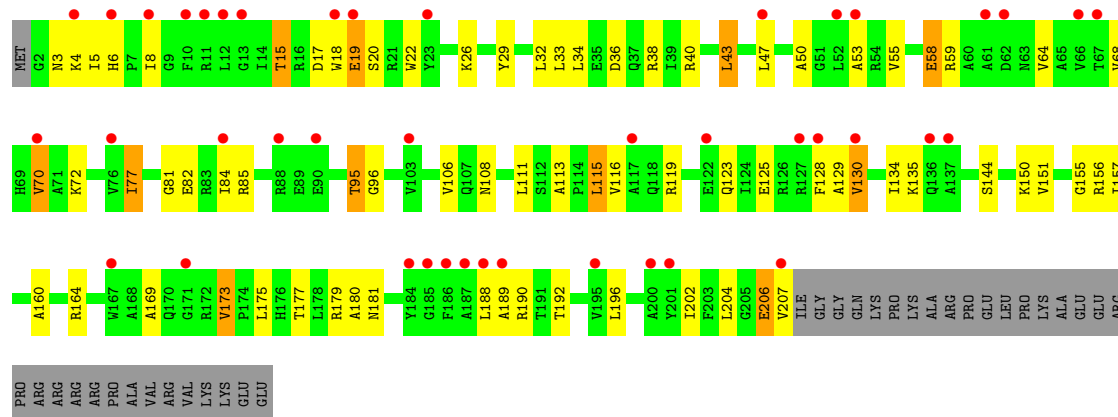




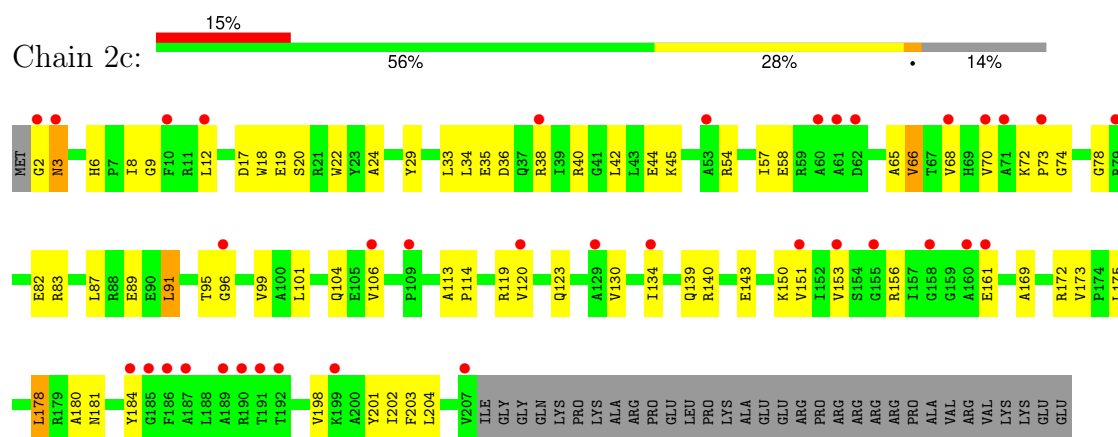
• Molecule 33: 30S ribosomal protein S2



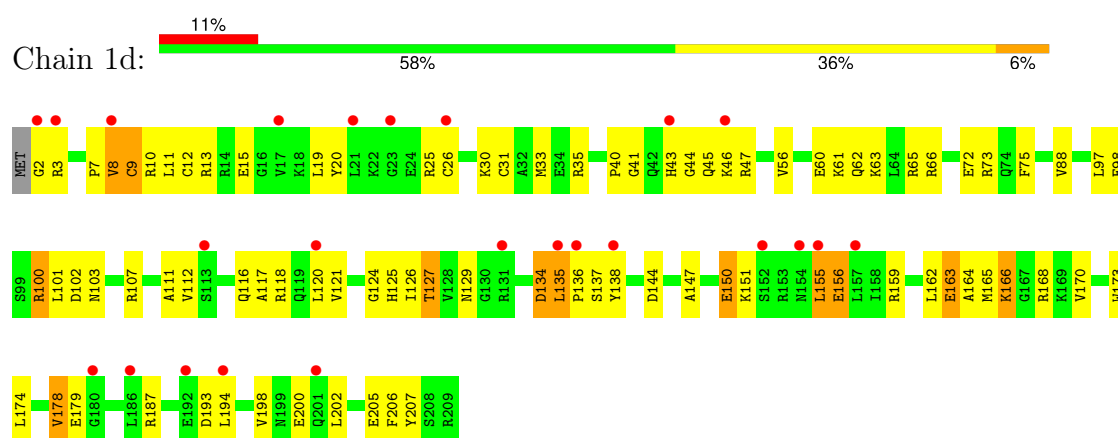
• Molecule 34: 30S ribosomal protein S3



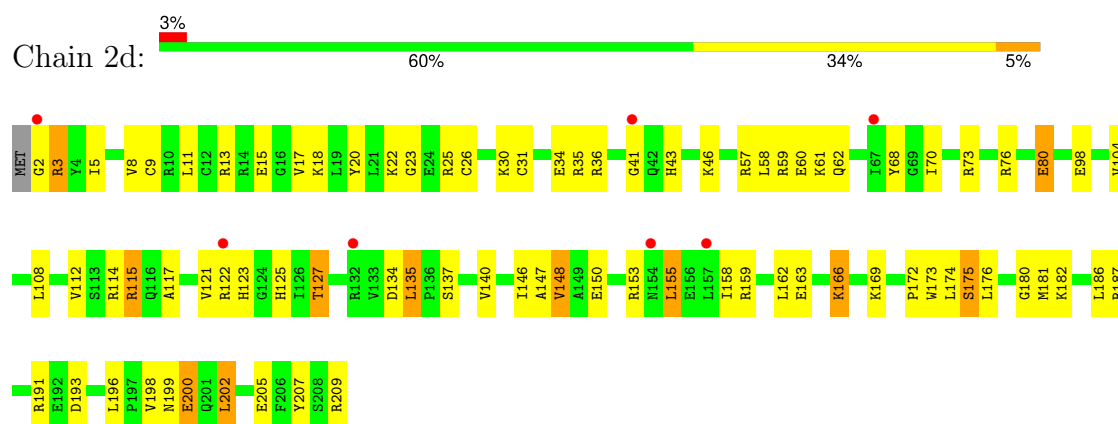
• Molecule 34: 30S ribosomal protein S3



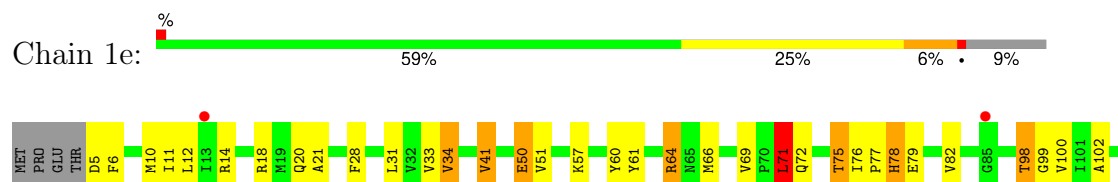
• Molecule 35: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S4



• Molecule 36: 30S ribosomal protein S5

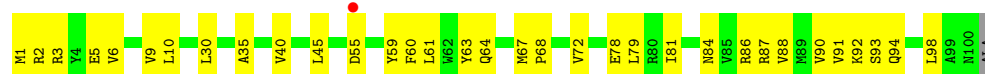




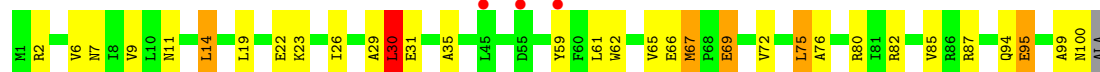
- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6



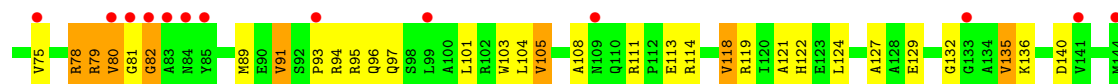
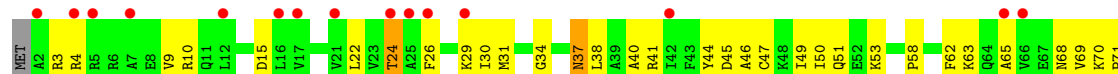
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7

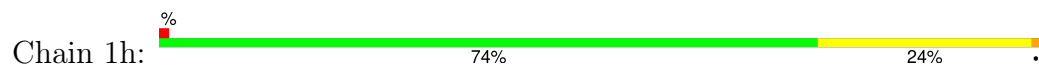


- Molecule 38: 30S ribosomal protein S7

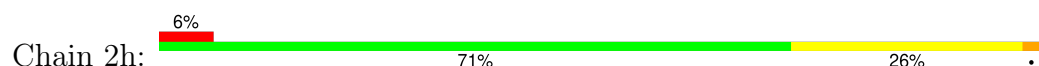




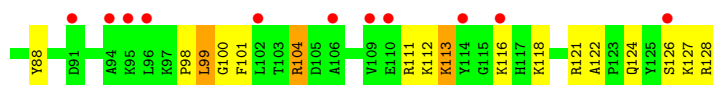
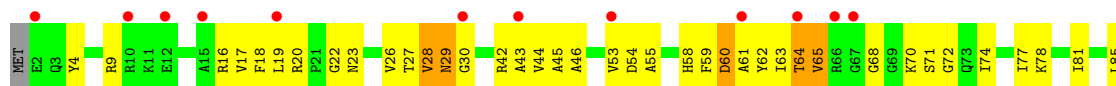
- Molecule 39: 30S ribosomal protein S8



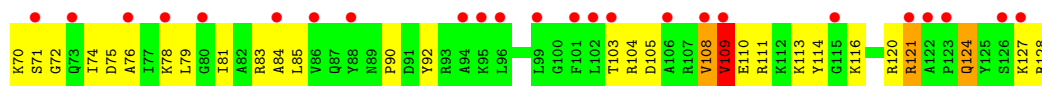
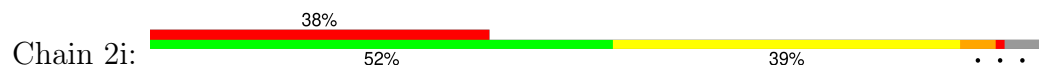
- Molecule 39: 30S ribosomal protein S8



- Molecule 40: 30S ribosomal protein S9

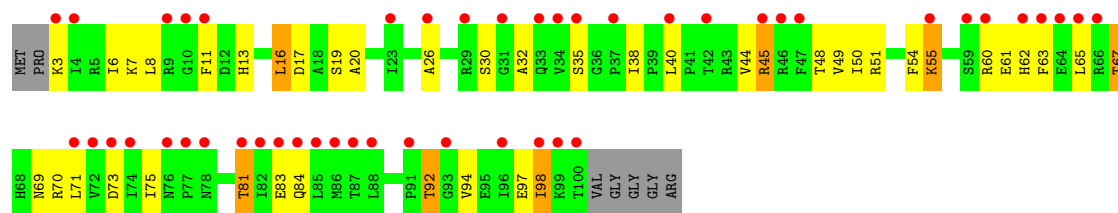


- Molecule 40: 30S ribosomal protein S9

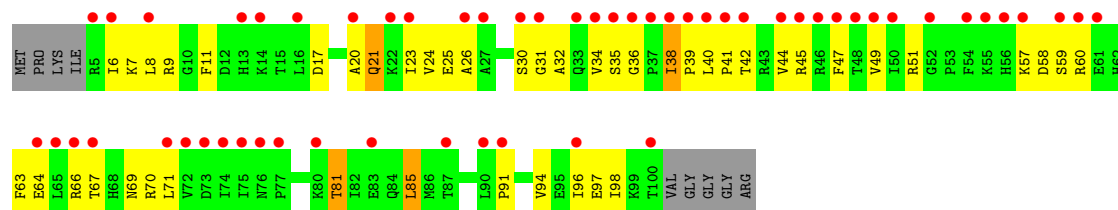


- Molecule 41: 30S ribosomal protein S10

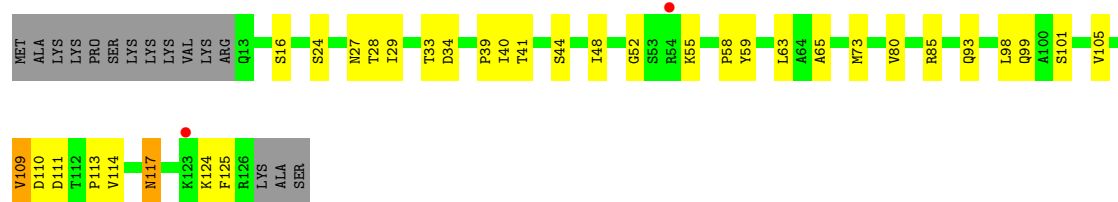




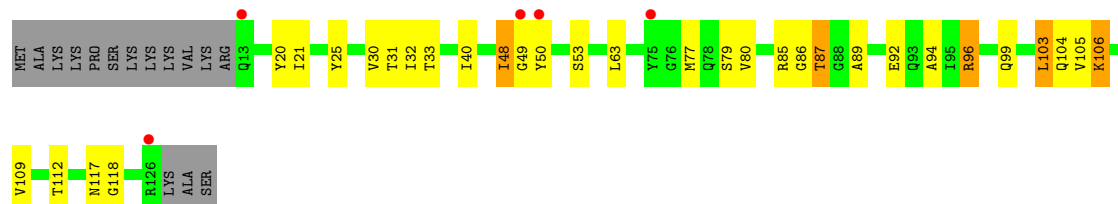
• Molecule 41: 30S ribosomal protein S10



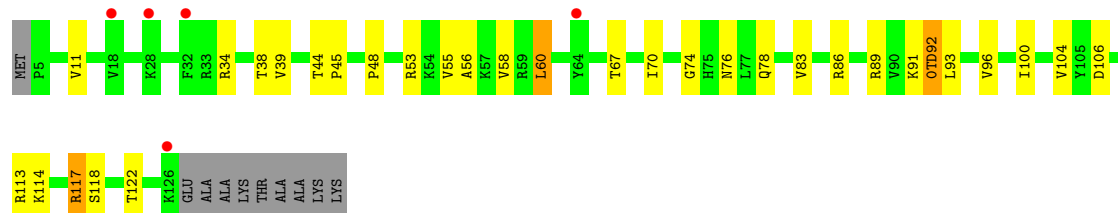
• Molecule 42: 30S ribosomal protein S11



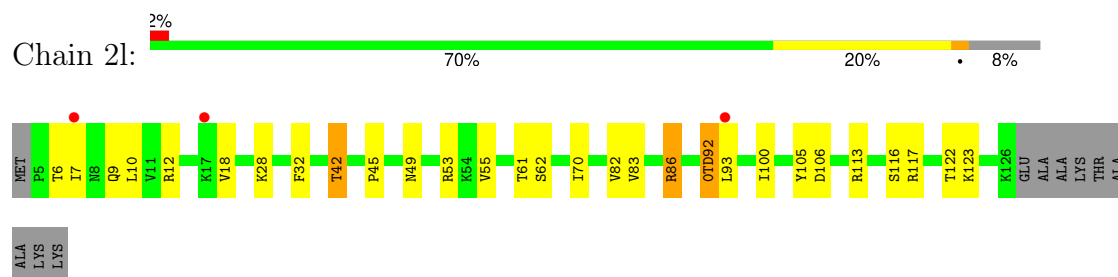
• Molecule 42: 30S ribosomal protein S11



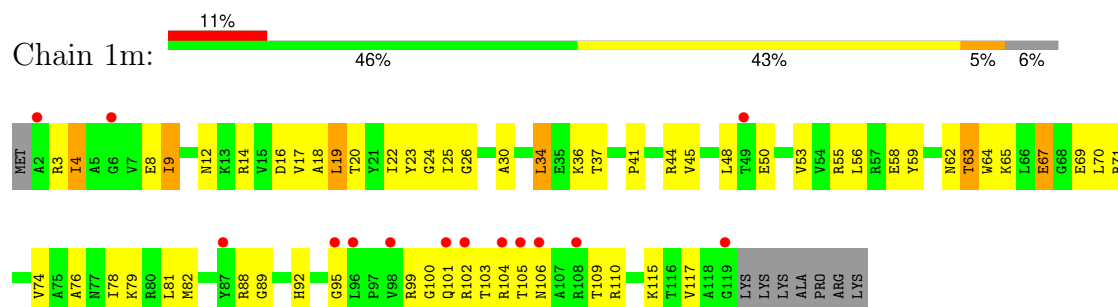
• Molecule 43: 30S ribosomal protein S12



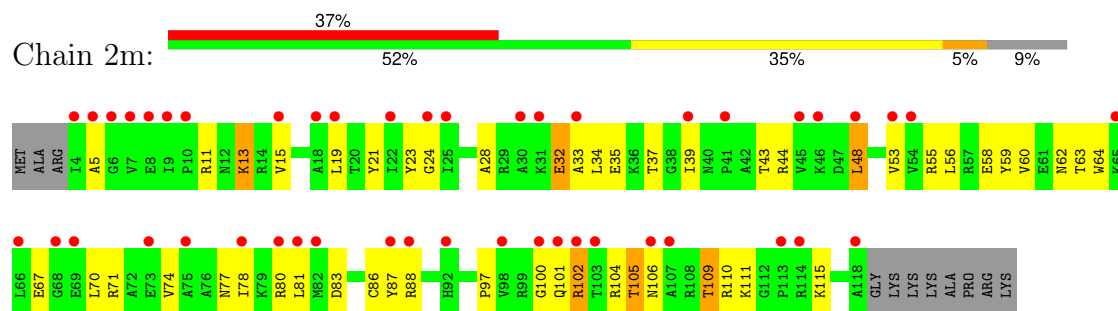
- Molecule 43: 30S ribosomal protein S12



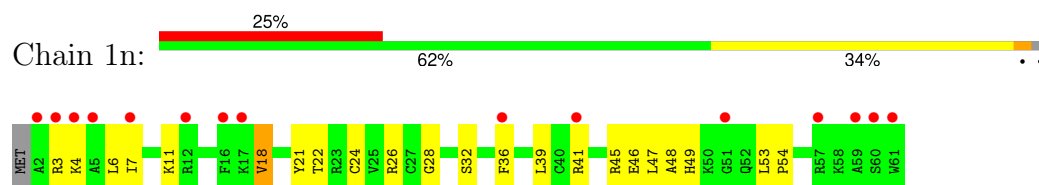
- Molecule 44: 30S ribosomal protein S13



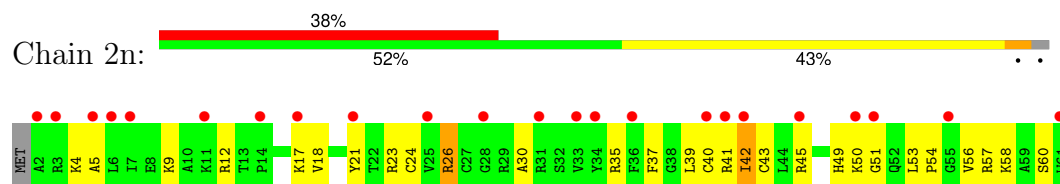
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15

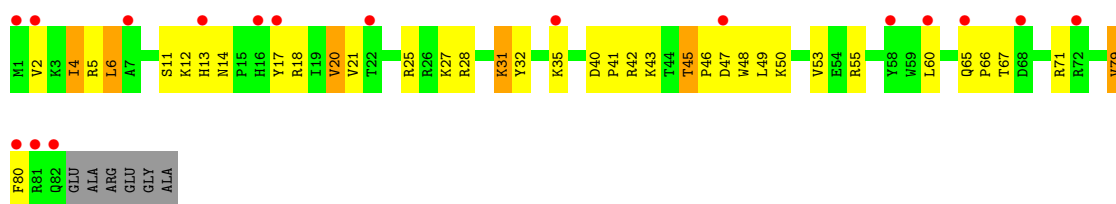




- Molecule 46: 30S ribosomal protein S15



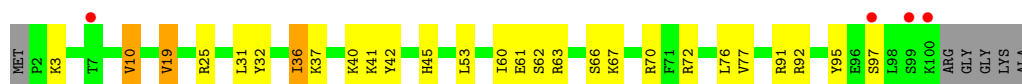
- Molecule 47: 30S ribosomal protein S16



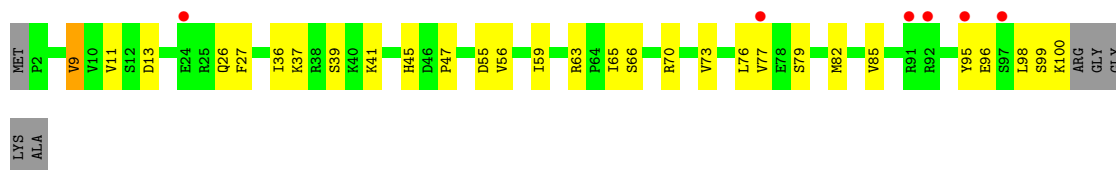
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17

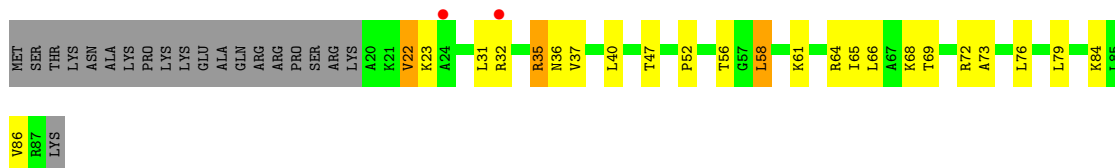


- Molecule 49: 30S ribosomal protein S18

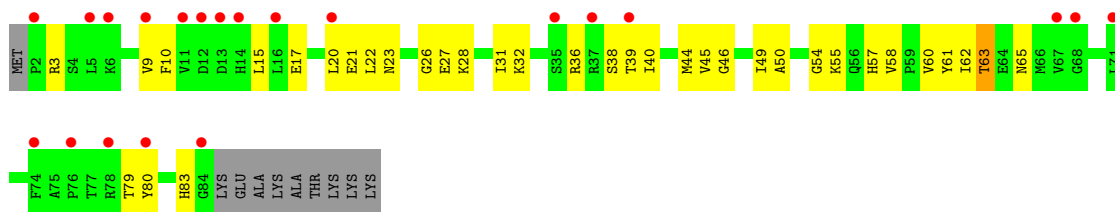




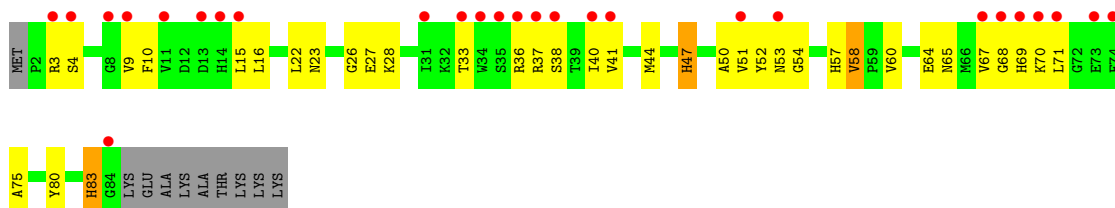
- Molecule 49: 30S ribosomal protein S18



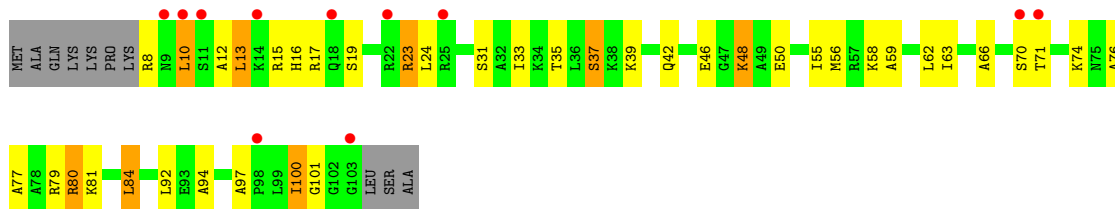
- Molecule 50: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S19

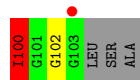


- Molecule 51: 30S ribosomal protein S20

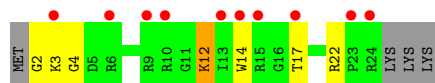
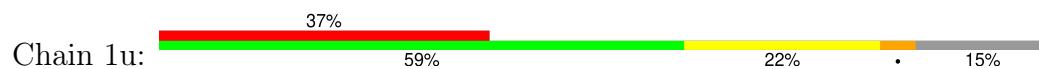


- Molecule 51: 30S ribosomal protein S20

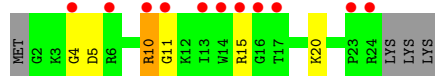
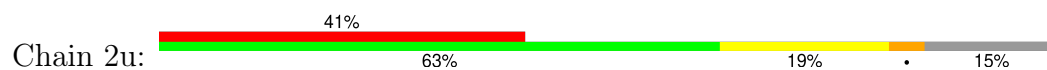




• Molecule 52: 30S ribosomal protein Thx



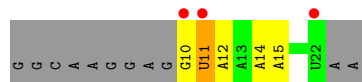
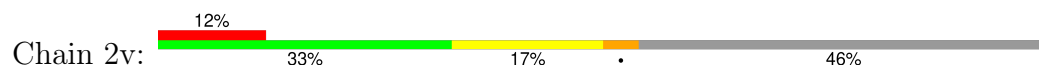
• Molecule 52: 30S ribosomal protein Thx



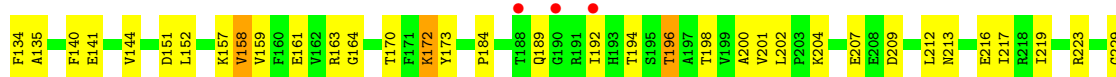
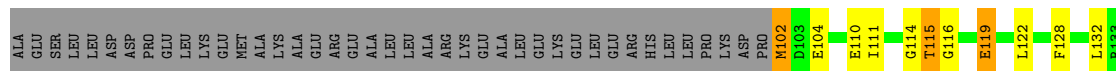
• Molecule 53: PHE-Stop mRNA

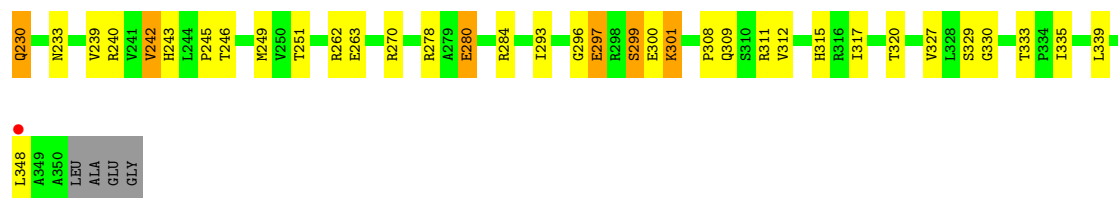


• Molecule 53: PHE-Stop mRNA

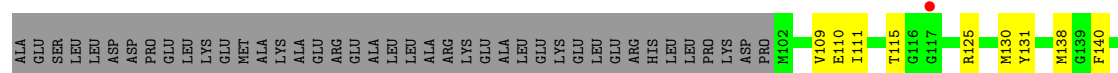


• Molecule 54: Peptide chain release factor 1





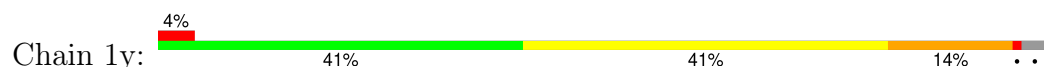
• Molecule 54: Peptide chain release factor 1



• Molecule 55: P-site and E-site Deacylated tRNAphe

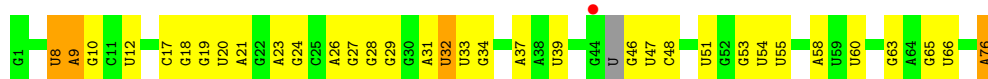


• Molecule 55: P-site and E-site Deacylated tRNAphe

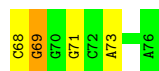


• Molecule 55: P-site and E-site Deacylated tRNAphe

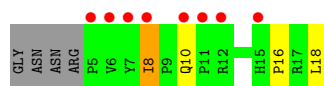
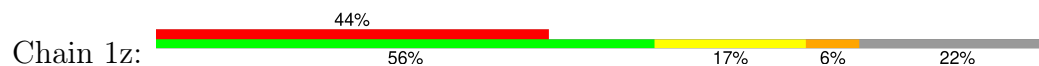




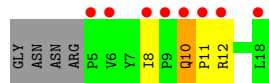
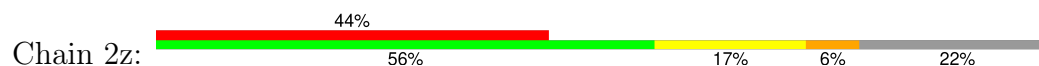
- Molecule 55: P-site and E-site Deacylated tRNA^{phe}



- Molecule 56: Api Antimicrobial Peptide



- Molecule 56: Api Antimicrobial Peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.35Å 451.32Å 625.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.43 – 2.85 102.43 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.1 (102.43-2.85) 99.1 (102.43-2.85)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.218 , 0.268 0.220 , 0.267	Depositor DCC
R_{free} test set	68034 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	299015	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% 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: SF4, 4OC, 2MG, MA6, OMG, 5MU, MG, G7M, MIA, 5MC, 4SU, OMU, ZN, OMC, PSU, 0TD, 2MA, UR3, M2G, MEQ

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	0/69011	0.45	1/107720 (0.0%)
1	2A	0.21	0/67295	0.39	1/105042 (0.0%)
2	1B	0.21	0/2881	0.38	0/4494
2	2B	0.18	0/2881	0.33	0/4494
3	1D	0.26	0/2186	0.50	0/2944
3	2D	0.22	0/2186	0.44	0/2944
4	1E	0.28	0/1592	0.49	0/2149
4	2E	0.21	0/1592	0.44	0/2149
5	1F	0.27	0/1619	0.51	0/2193
5	2F	0.21	0/1615	0.46	0/2188
6	1G	0.20	0/1450	0.44	0/1959
6	2G	0.21	0/1449	0.45	0/1958
7	1H	0.22	0/1356	0.43	0/1834
7	2H	0.18	0/1356	0.37	0/1834
8	1I	0.21	0/1100	0.49	1/1501 (0.1%)
8	2I	0.19	0/1076	0.44	0/1471
9	1N	0.27	0/1144	0.46	0/1543
9	2N	0.18	0/1144	0.39	0/1543
10	1O	0.28	0/943	0.50	0/1269
10	2O	0.21	0/943	0.42	0/1269
11	1P	0.26	0/1152	0.55	0/1533
11	2P	0.20	0/1152	0.44	0/1533
12	1Q	0.25	0/1143	0.48	0/1527
12	2Q	0.19	0/1143	0.41	0/1527
13	1R	0.27	0/982	0.52	0/1312
13	2R	0.20	0/982	0.45	0/1312
14	1S	0.22	0/887	0.55	1/1180 (0.1%)
14	2S	0.21	0/880	0.46	0/1172
15	1T	0.26	0/1105	0.48	0/1477
15	2T	0.20	0/1097	0.47	0/1468
16	1U	0.30	0/977	0.46	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	0.25	0/782	0.45	0/1049
17	2V	0.20	0/782	0.43	0/1049
18	1W	0.29	0/897	0.48	0/1205
18	2W	0.22	0/897	0.47	0/1205
19	1X	0.24	0/764	0.44	0/1025
19	2X	0.21	0/760	0.38	0/1021
20	1Y	0.24	0/819	0.50	0/1095
20	2Y	0.21	0/823	0.47	0/1100
21	1Z	0.21	0/1469	0.47	0/1998
21	2Z	0.19	0/1483	0.42	0/2018
22	10	0.25	0/612	0.53	0/816
22	20	0.21	0/616	0.48	0/821
23	11	0.23	0/762	0.41	0/1014
23	21	0.23	0/762	0.45	0/1014
24	12	0.25	0/590	0.38	0/781
24	22	0.18	0/590	0.36	0/781
25	13	0.27	0/474	0.48	0/635
25	23	0.21	0/469	0.40	0/630
26	14	0.25	0/561	0.61	0/756
26	24	0.28	0/530	0.66	1/719 (0.1%)
27	15	0.29	0/469	0.53	0/635
27	25	0.22	0/469	0.41	0/635
28	16	0.23	0/460	0.46	0/613
28	26	0.20	0/456	0.41	0/608
29	17	0.31	0/426	0.53	0/561
29	27	0.25	0/426	0.50	0/561
30	18	0.28	0/519	0.47	0/684
30	28	0.18	0/525	0.39	0/691
31	19	0.27	0/310	0.45	0/407
31	29	0.21	0/310	0.43	0/407
32	1a	0.20	0/35795	0.38	2/55864 (0.0%)
32	2a	0.20	0/35886	0.38	0/56005
33	1b	0.21	0/1881	0.48	0/2542
33	2b	0.24	0/1860	0.54	1/2518 (0.0%)
34	1c	0.19	0/1578	0.43	1/2133 (0.0%)
34	2c	0.20	0/1566	0.46	1/2119 (0.0%)
35	1d	0.19	0/1689	0.42	0/2267
35	2d	0.21	0/1704	0.43	0/2284
36	1e	0.20	0/1145	0.46	0/1543
36	2e	0.21	0/1146	0.45	0/1545
37	1f	0.20	0/823	0.45	0/1116
37	2f	0.19	0/829	0.39	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.21	0/1250	0.41	0/1679
38	2g	0.20	0/1254	0.45	0/1683
39	1h	0.19	0/1108	0.41	0/1494
39	2h	0.20	0/1108	0.42	0/1494
40	1i	0.21	0/1002	0.51	0/1346
40	2i	0.25	0/957	0.51	0/1288
41	1j	0.21	0/734	0.43	0/997
41	2j	0.22	0/727	0.44	0/988
42	1k	0.19	0/844	0.38	0/1145
42	2k	0.19	0/848	0.39	0/1149
43	1l	0.21	0/937	0.43	0/1260
43	2l	0.21	0/937	0.45	0/1260
44	1m	0.21	0/933	0.51	0/1254
44	2m	0.21	0/899	0.49	0/1212
45	1n	0.20	0/501	0.47	0/664
45	2n	0.21	0/495	0.44	0/657
46	1o	0.20	0/739	0.40	0/985
46	2o	0.18	0/739	0.37	0/985
47	1p	0.20	0/697	0.45	0/939
47	2p	0.21	0/693	0.45	0/935
48	1q	0.19	0/836	0.41	0/1117
48	2q	0.19	0/836	0.40	0/1117
49	1r	0.19	0/560	0.44	0/746
49	2r	0.21	0/556	0.47	0/741
50	1s	0.21	0/667	0.43	0/900
50	2s	0.19	0/661	0.40	0/893
51	1t	0.20	0/730	0.46	0/965
51	2t	0.19	0/729	0.41	0/965
52	1u	0.20	0/203	0.48	0/266
52	2u	0.19	0/203	0.44	0/266
53	1v	0.24	0/306	0.41	0/473
53	2v	0.22	0/306	0.38	0/473
54	1w	0.20	0/1956	0.41	0/2634
54	2w	0.19	0/1974	0.38	0/2657
55	1x	0.28	1/1629 (0.1%)	0.40	0/2535
55	1y	0.26	1/1602 (0.1%)	0.35	0/2488
55	2x	0.26	2/1629 (0.1%)	0.35	0/2535
55	2y	0.28	1/1606 (0.1%)	0.35	0/2497
56	1z	0.25	0/126	0.43	0/173
56	2z	0.23	0/126	0.41	0/173
All	All	0.23	5/317653 (0.0%)	0.42	10/474762 (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
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2y	46	G7M	O3'-P	5.59	1.61	1.56
55	2x	46	G7M	O3'-P	5.35	1.61	1.56
55	1y	46	G7M	O3'-P	5.22	1.61	1.56
55	1x	8	4SU	O3'-P	5.11	1.61	1.56
55	2x	8	4SU	O3'-P	5.08	1.61	1.56

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	24	54	GLY	N-CA-C	-7.39	105.53	115.36
8	1I	68	LEU	N-CA-C	-7.16	106.46	114.62
14	1S	59	LYS	N-CA-C	6.48	118.42	108.12
34	2c	66	VAL	N-CA-C	6.28	112.93	106.21
34	1c	19	GLU	N-CA-C	-6.17	106.12	113.21

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	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	61852	0	31195	582	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2A	60322	0	30426	659	0
2	1B	2576	0	1305	20	0
2	2B	2576	0	1305	39	0
3	1D	2136	0	2218	41	0
3	2D	2136	0	2218	45	0
4	1E	1559	0	1618	26	0
4	2E	1559	0	1618	38	0
5	1F	1584	0	1624	39	0
5	2F	1580	0	1619	46	0
6	1G	1425	0	1443	32	0
6	2G	1424	0	1434	54	0
7	1H	1330	0	1407	19	0
7	2H	1330	0	1407	35	0
8	1I	1085	0	1114	30	0
8	2I	1061	0	1080	33	0
9	1N	1117	0	1184	17	0
9	2N	1117	0	1184	18	0
10	1O	933	0	996	24	0
10	2O	933	0	996	21	0
11	1P	1135	0	1212	27	0
11	2P	1135	0	1212	28	0
12	1Q	1122	0	1178	19	0
12	2Q	1122	0	1179	21	0
13	1R	968	0	1033	18	0
13	2R	968	0	1033	17	0
14	1S	877	0	938	21	0
14	2S	870	0	923	32	0
15	1T	1091	0	1151	28	0
15	2T	1083	0	1136	30	0
16	1U	959	0	1019	15	0
16	2U	959	0	1019	17	0
17	1V	771	0	830	14	0
17	2V	771	0	830	12	0
18	1W	886	0	940	15	0
18	2W	886	0	940	14	0
19	1X	750	0	814	13	0
19	2X	746	0	803	10	0
20	1Y	806	0	881	23	0
20	2Y	810	0	887	20	0
21	1Z	1437	0	1446	38	0
21	2Z	1451	0	1450	54	0
22	10	604	0	619	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	608	0	622	15	0
23	11	755	0	826	16	0
23	21	755	0	826	14	0
24	12	588	0	643	10	0
24	22	588	0	643	16	0
25	13	469	0	518	11	0
25	23	464	0	514	8	0
26	14	548	0	529	22	0
26	24	517	0	479	23	0
27	15	455	0	465	6	0
27	25	455	0	465	8	0
28	16	453	0	472	4	0
28	26	449	0	469	8	0
29	17	418	0	467	8	0
29	27	418	0	467	6	0
30	18	511	0	571	20	0
30	28	517	0	582	14	0
31	19	307	0	335	8	0
31	29	307	0	335	8	0
32	1a	32246	0	16294	477	0
32	2a	32327	0	16338	509	0
33	1b	1846	0	1867	76	0
33	2b	1825	0	1828	83	0
34	1c	1554	0	1551	42	0
34	2c	1542	0	1517	44	0
35	1d	1659	0	1676	61	0
35	2d	1674	0	1714	61	0
36	1e	1129	0	1185	37	0
36	2e	1130	0	1184	32	0
37	1f	810	0	797	19	0
37	2f	816	0	808	23	0
38	1g	1231	0	1238	23	0
38	2g	1235	0	1249	46	0
39	1h	1088	0	1126	24	0
39	2h	1088	0	1126	26	0
40	1i	983	0	986	43	0
40	2i	940	0	938	40	0
41	1j	721	0	672	33	0
41	2j	714	0	672	37	0
42	1k	829	0	825	18	0
42	2k	833	0	836	20	0
43	1l	932	0	980	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	2l	932	0	980	18	0
44	1m	923	0	962	45	0
44	2m	889	0	901	35	0
45	1n	492	0	529	22	0
45	2n	486	0	518	30	0
46	1o	728	0	760	14	0
46	2o	728	0	760	20	0
47	1p	681	0	697	30	0
47	2p	677	0	686	21	0
48	1q	823	0	891	21	0
48	2q	823	0	891	17	0
49	1r	555	0	618	8	0
49	2r	551	0	614	21	0
50	1s	652	0	662	23	0
50	2s	646	0	644	28	0
51	1t	728	0	798	26	0
51	2t	727	0	796	19	0
52	1u	199	0	208	6	0
52	2u	199	0	208	4	0
53	1v	274	0	139	8	0
53	2v	274	0	139	4	0
54	1w	1939	0	1925	51	0
54	2w	1957	0	1937	37	0
55	1x	1612	0	829	12	0
55	1y	1590	0	815	19	0
55	2x	1612	0	829	14	0
55	2y	1592	0	818	19	0
56	1z	119	0	123	3	0
56	2z	119	0	123	2	0
57	10	4	0	0	0	0
57	11	3	0	0	0	0
57	12	1	0	0	0	0
57	13	1	0	0	0	0
57	15	7	0	0	0	0
57	16	1	0	0	0	0
57	17	7	0	0	0	0
57	18	2	0	0	0	0
57	19	1	0	0	0	0
57	1A	793	0	0	0	0
57	1B	20	0	0	0	0
57	1D	9	0	0	0	0
57	1E	7	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1F	14	0	0	0	0
57	1G	3	0	0	0	0
57	1N	3	0	0	0	0
57	1O	1	0	0	0	0
57	1P	4	0	0	0	0
57	1Q	5	0	0	0	0
57	1R	2	0	0	0	0
57	1T	1	0	0	0	0
57	1U	8	0	0	0	0
57	1V	5	0	0	0	0
57	1W	3	0	0	0	0
57	1X	3	0	0	0	0
57	1Z	2	0	0	0	0
57	1a	167	0	0	0	0
57	1f	1	0	0	0	0
57	1i	1	0	0	0	0
57	1k	1	0	0	0	0
57	1m	1	0	0	0	0
57	1n	1	0	0	0	0
57	1v	3	0	0	0	0
57	1w	3	0	0	0	0
57	1x	10	0	0	0	0
57	1y	3	0	0	0	0
57	20	1	0	0	0	0
57	21	1	0	0	0	0
57	23	2	0	0	0	0
57	25	2	0	0	0	0
57	26	1	0	0	0	0
57	28	1	0	0	0	0
57	2A	657	0	0	0	0
57	2B	10	0	0	0	0
57	2D	7	0	0	0	0
57	2E	7	0	0	0	0
57	2F	5	0	0	0	0
57	2O	1	0	0	0	0
57	2P	1	0	0	0	0
57	2Q	3	0	0	0	0
57	2R	1	0	0	0	0
57	2U	2	0	0	0	0
57	2V	2	0	0	0	0
57	2W	1	0	0	0	0
57	2X	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	2Y	1	0	0	0	0
57	2a	165	0	0	0	0
57	2e	3	0	0	0	0
57	2f	1	0	0	0	0
57	2j	1	0	0	0	0
57	2k	2	0	0	0	0
57	2t	1	0	0	0	0
57	2v	2	0	0	0	0
57	2x	9	0	0	0	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	0	0
59	2d	8	0	0	1	0
60	10	3	0	0	0	0
60	11	2	0	0	0	0
60	13	2	0	0	1	0
60	15	6	0	0	0	0
60	16	1	0	0	0	0
60	17	3	0	0	0	0
60	18	6	0	0	0	0
60	19	1	0	0	1	0
60	1A	1368	0	0	78	0
60	1B	27	0	0	0	0
60	1D	14	0	0	0	0
60	1E	14	0	0	2	0
60	1F	10	0	0	0	0
60	1G	1	0	0	0	0
60	1N	3	0	0	0	0
60	1O	3	0	0	0	0
60	1P	18	0	0	1	0
60	1Q	7	0	0	0	0
60	1R	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1T	1	0	0	0	0
60	1U	6	0	0	0	0
60	1V	2	0	0	0	0
60	1W	2	0	0	0	0
60	1X	3	0	0	0	0
60	1a	164	0	0	14	0
60	1d	2	0	0	0	0
60	1e	1	0	0	0	0
60	1l	2	0	0	0	0
60	1p	1	0	0	0	0
60	1v	3	0	0	0	0
60	1w	5	0	0	0	0
60	1x	20	0	0	2	0
60	1y	1	0	0	0	0
60	1z	3	0	0	0	0
60	20	6	0	0	0	0
60	21	2	0	0	0	0
60	23	2	0	0	0	0
60	27	2	0	0	0	0
60	28	2	0	0	0	0
60	2A	949	0	0	89	0
60	2B	5	0	0	0	0
60	2D	13	0	0	2	0
60	2E	8	0	0	0	0
60	2F	6	0	0	0	0
60	2N	2	0	0	0	0
60	2P	7	0	0	1	0
60	2R	2	0	0	0	0
60	2T	1	0	0	0	0
60	2U	1	0	0	0	0
60	2V	1	0	0	0	0
60	2W	1	0	0	0	0
60	2X	2	0	0	0	0
60	2Y	1	0	0	0	0
60	2a	154	0	0	14	0
60	2d	1	0	0	0	0
60	2q	1	0	0	0	0
60	2v	3	0	0	0	0
60	2w	2	0	0	1	0
60	2x	11	0	0	1	0
60	2z	1	0	0	0	0
All	All	299015	0	199299	4238	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 4238 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2129:C:N4	1:2A:2159:G:H1	1.47	1.12
32:2a:1256:A:H61	32:2a:1278:U:H1'	1.26	1.00
1:1A:1057:A:N6	1:1A:1081:U:H3	1.60	0.99
1:1A:2124:G:H1	1:1A:2174:C:H42	1.07	0.97
32:1a:875:C:H1'	39:1h:15:ASN:HD21	1.33	0.93

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%)	259 (95%)	14 (5%)	0	100	100
3	2D	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	30	48
4	1E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	24	42
4	2E	202/206 (98%)	187 (93%)	13 (6%)	2 (1%)	12	25
5	1F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	24	42
5	2F	201/210 (96%)	191 (95%)	8 (4%)	2 (1%)	12	25
6	1G	179/182 (98%)	160 (89%)	18 (10%)	1 (1%)	21	38
6	2G	179/182 (98%)	156 (87%)	20 (11%)	3 (2%)	7	16
7	1H	172/180 (96%)	159 (92%)	12 (7%)	1 (1%)	21	38
7	2H	172/180 (96%)	152 (88%)	16 (9%)	4 (2%)	5	11
8	1I	144/148 (97%)	126 (88%)	15 (10%)	3 (2%)	5	13
8	2I	144/148 (97%)	121 (84%)	19 (13%)	4 (3%)	4	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
10	1O	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
11	1P	147/150 (98%)	137 (93%)	8 (5%)	2 (1%)	9	19
11	2P	147/150 (98%)	137 (93%)	7 (5%)	3 (2%)	6	13
12	1Q	139/141 (99%)	132 (95%)	6 (4%)	1 (1%)	18	35
12	2Q	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	18	35
13	1R	116/118 (98%)	113 (97%)	2 (2%)	1 (1%)	14	28
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	14	28
14	2S	108/112 (96%)	93 (86%)	13 (12%)	2 (2%)	6	14
15	1T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	6	13
17	2V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	12	25
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	106 (96%)	3 (3%)	1 (1%)	14	28
19	1X	93/96 (97%)	91 (98%)	0	2 (2%)	5	12
19	2X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	1Y	105/110 (96%)	95 (90%)	9 (9%)	1 (1%)	12	25
20	2Y	105/110 (96%)	95 (90%)	9 (9%)	1 (1%)	12	25
21	1Z	181/206 (88%)	159 (88%)	20 (11%)	2 (1%)	11	24
21	2Z	184/206 (89%)	153 (83%)	26 (14%)	5 (3%)	4	9
22	10	74/85 (87%)	67 (90%)	6 (8%)	1 (1%)	9	19
22	20	75/85 (88%)	67 (89%)	7 (9%)	1 (1%)	9	21
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	24
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	24
24	12	68/72 (94%)	64 (94%)	4 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	42 (63%)	18 (27%)	7 (10%)	0	0
26	24	66/71 (93%)	44 (67%)	20 (30%)	2 (3%)	3	8
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
29	27	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
31	19	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	187 (82%)	37 (16%)	5 (2%)	5	12
33	2b	229/256 (90%)	193 (84%)	27 (12%)	9 (4%)	2	4
34	1c	204/239 (85%)	178 (87%)	24 (12%)	2 (1%)	12	25
34	2c	204/239 (85%)	180 (88%)	21 (10%)	3 (2%)	8	18
35	1d	206/209 (99%)	185 (90%)	16 (8%)	5 (2%)	4	10
35	2d	206/209 (99%)	189 (92%)	15 (7%)	2 (1%)	12	25
36	1e	146/162 (90%)	133 (91%)	11 (8%)	2 (1%)	9	19
36	2e	146/162 (90%)	133 (91%)	10 (7%)	3 (2%)	5	13
37	1f	98/101 (97%)	89 (91%)	9 (9%)	0	100	100
37	2f	98/101 (97%)	89 (91%)	8 (8%)	1 (1%)	12	25
38	1g	153/156 (98%)	138 (90%)	12 (8%)	3 (2%)	6	13
38	2g	153/156 (98%)	134 (88%)	16 (10%)	3 (2%)	6	13
39	1h	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
39	2h	135/138 (98%)	124 (92%)	11 (8%)	0	100	100
40	1i	125/128 (98%)	103 (82%)	16 (13%)	6 (5%)	2	3
40	2i	121/128 (94%)	96 (79%)	23 (19%)	2 (2%)	7	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	1j	96/105 (91%)	84 (88%)	11 (12%)	1 (1%)	12	25
41	2j	94/105 (90%)	80 (85%)	12 (13%)	2 (2%)	5	13
42	1k	112/129 (87%)	98 (88%)	14 (12%)	0	100	100
42	2k	112/129 (87%)	98 (88%)	10 (9%)	4 (4%)	2	5
43	1l	119/132 (90%)	111 (93%)	7 (6%)	1 (1%)	16	31
43	2l	119/132 (90%)	107 (90%)	11 (9%)	1 (1%)	16	31
44	1m	116/126 (92%)	102 (88%)	11 (10%)	3 (3%)	4	9
44	2m	113/126 (90%)	94 (83%)	17 (15%)	2 (2%)	6	15
45	1n	58/61 (95%)	50 (86%)	8 (14%)	0	100	100
45	2n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
46	1o	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
46	2o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	10	22
47	1p	80/88 (91%)	64 (80%)	15 (19%)	1 (1%)	9	21
47	2p	80/88 (91%)	67 (84%)	13 (16%)	0	100	100
48	1q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
48	2q	97/105 (92%)	84 (87%)	12 (12%)	1 (1%)	12	25
49	1r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
49	2r	66/88 (75%)	59 (89%)	7 (11%)	0	100	100
50	1s	81/93 (87%)	68 (84%)	12 (15%)	1 (1%)	10	22
50	2s	81/93 (87%)	68 (84%)	13 (16%)	0	100	100
51	1t	94/106 (89%)	82 (87%)	10 (11%)	2 (2%)	5	13
51	2t	94/106 (89%)	83 (88%)	5 (5%)	6 (6%)	1	1
52	1u	21/27 (78%)	21 (100%)	0	0	100	100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
54	1w	246/354 (70%)	228 (93%)	14 (6%)	4 (2%)	7	17
54	2w	250/354 (71%)	229 (92%)	20 (8%)	1 (0%)	30	48
56	1z	12/18 (67%)	10 (83%)	2 (17%)	0	100	100
56	2z	12/18 (67%)	10 (83%)	2 (17%)	0	100	100
All	All	11922/12872 (93%)	10834 (91%)	949 (8%)	139 (1%)	10	22

5 of 139 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
8	1I	10	GLU
14	1S	60	GLY
17	1V	79	VAL
23	11	3	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	206 (96%)	9 (4%)	26	51
3	2D	215/218 (99%)	204 (95%)	11 (5%)	21	43
4	1E	164/166 (99%)	153 (93%)	11 (7%)	15	31
4	2E	164/166 (99%)	146 (89%)	18 (11%)	6	12
5	1F	160/166 (96%)	142 (89%)	18 (11%)	5	11
5	2F	159/166 (96%)	143 (90%)	16 (10%)	7	15
6	1G	143/156 (92%)	126 (88%)	17 (12%)	5	10
6	2G	142/156 (91%)	120 (84%)	22 (16%)	2	5
7	1H	144/148 (97%)	135 (94%)	9 (6%)	16	34
7	2H	144/148 (97%)	127 (88%)	17 (12%)	5	10
8	1I	110/124 (89%)	96 (87%)	14 (13%)	4	8
8	2I	104/124 (84%)	86 (83%)	18 (17%)	2	3
9	1N	118/119 (99%)	110 (93%)	8 (7%)	14	30
9	2N	118/119 (99%)	110 (93%)	8 (7%)	14	30
10	1O	100/100 (100%)	98 (98%)	2 (2%)	48	71
10	2O	100/100 (100%)	94 (94%)	6 (6%)	17	36
11	1P	115/116 (99%)	109 (95%)	6 (5%)	21	43
11	2P	115/116 (99%)	103 (90%)	12 (10%)	7	14
12	1Q	111/111 (100%)	98 (88%)	13 (12%)	5	10
12	2Q	111/111 (100%)	101 (91%)	10 (9%)	9	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	1R	101/101 (100%)	89 (88%)	12 (12%)	5	10
13	2R	101/101 (100%)	97 (96%)	4 (4%)	28	53
14	1S	87/88 (99%)	77 (88%)	10 (12%)	5	10
14	2S	85/88 (97%)	75 (88%)	10 (12%)	5	10
15	1T	115/127 (91%)	108 (94%)	7 (6%)	17	35
15	2T	113/127 (89%)	107 (95%)	6 (5%)	20	42
16	1U	93/94 (99%)	88 (95%)	5 (5%)	20	42
16	2U	93/94 (99%)	92 (99%)	1 (1%)	65	81
17	1V	80/82 (98%)	77 (96%)	3 (4%)	29	54
17	2V	80/82 (98%)	76 (95%)	4 (5%)	22	44
18	1W	90/92 (98%)	85 (94%)	5 (6%)	19	40
18	2W	90/92 (98%)	85 (94%)	5 (6%)	19	40
19	1X	77/78 (99%)	74 (96%)	3 (4%)	28	54
19	2X	76/78 (97%)	70 (92%)	6 (8%)	11	24
20	1Y	85/91 (93%)	76 (89%)	9 (11%)	6	13
20	2Y	86/91 (94%)	77 (90%)	9 (10%)	6	13
21	1Z	155/179 (87%)	141 (91%)	14 (9%)	9	19
21	2Z	155/179 (87%)	127 (82%)	28 (18%)	2	2
22	10	61/67 (91%)	58 (95%)	3 (5%)	22	45
22	20	61/67 (91%)	55 (90%)	6 (10%)	7	16
23	11	80/83 (96%)	75 (94%)	5 (6%)	16	34
23	21	80/83 (96%)	74 (92%)	6 (8%)	12	26
24	12	65/67 (97%)	61 (94%)	4 (6%)	16	34
24	22	65/67 (97%)	62 (95%)	3 (5%)	24	48
25	13	51/52 (98%)	46 (90%)	5 (10%)	7	16
25	23	50/52 (96%)	46 (92%)	4 (8%)	11	24
26	14	58/63 (92%)	50 (86%)	8 (14%)	3	7
26	24	51/63 (81%)	42 (82%)	9 (18%)	2	3
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	36
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	24
28	16	51/52 (98%)	47 (92%)	4 (8%)	11	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	16
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	27
29	27	41/42 (98%)	39 (95%)	2 (5%)	22	45
30	18	53/55 (96%)	49 (92%)	4 (8%)	12	26
30	28	54/55 (98%)	48 (89%)	6 (11%)	6	12
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	61
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	61
33	1b	192/220 (87%)	150 (78%)	42 (22%)	1	1
33	2b	187/220 (85%)	162 (87%)	25 (13%)	4	7
34	1c	144/188 (77%)	122 (85%)	22 (15%)	3	5
34	2c	140/188 (74%)	123 (88%)	17 (12%)	5	9
35	1d	170/181 (94%)	148 (87%)	22 (13%)	4	7
35	2d	173/181 (96%)	153 (88%)	20 (12%)	5	10
36	1e	113/123 (92%)	97 (86%)	16 (14%)	3	6
36	2e	113/123 (92%)	94 (83%)	19 (17%)	2	3
37	1f	84/90 (93%)	78 (93%)	6 (7%)	13	28
37	2f	85/90 (94%)	76 (89%)	9 (11%)	6	13
38	1g	119/127 (94%)	107 (90%)	12 (10%)	7	15
38	2g	120/127 (94%)	106 (88%)	14 (12%)	5	10
39	1h	114/119 (96%)	107 (94%)	7 (6%)	17	35
39	2h	114/119 (96%)	108 (95%)	6 (5%)	20	42
40	1i	90/99 (91%)	80 (89%)	10 (11%)	6	12
40	2i	86/99 (87%)	73 (85%)	13 (15%)	3	5
41	1j	68/92 (74%)	56 (82%)	12 (18%)	2	3
41	2j	69/92 (75%)	61 (88%)	8 (12%)	5	10
42	1k	82/99 (83%)	73 (89%)	9 (11%)	6	12
42	2k	83/99 (84%)	75 (90%)	8 (10%)	8	17
43	1l	96/108 (89%)	86 (90%)	10 (10%)	7	14
43	2l	96/108 (89%)	89 (93%)	7 (7%)	13	27
44	1m	90/101 (89%)	81 (90%)	9 (10%)	7	16
44	2m	85/101 (84%)	74 (87%)	11 (13%)	4	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	1n	49/50 (98%)	46 (94%)	3 (6%)	17	35
45	2n	48/50 (96%)	44 (92%)	4 (8%)	10	22
46	1o	78/80 (98%)	75 (96%)	3 (4%)	29	54
46	2o	78/80 (98%)	72 (92%)	6 (8%)	12	25
47	1p	69/74 (93%)	60 (87%)	9 (13%)	4	7
47	2p	68/74 (92%)	62 (91%)	6 (9%)	9	20
48	1q	94/97 (97%)	88 (94%)	6 (6%)	16	33
48	2q	94/97 (97%)	88 (94%)	6 (6%)	16	33
49	1r	59/77 (77%)	51 (86%)	8 (14%)	3	7
49	2r	58/77 (75%)	51 (88%)	7 (12%)	5	9
50	1s	69/80 (86%)	60 (87%)	9 (13%)	4	7
50	2s	67/80 (84%)	58 (87%)	9 (13%)	4	7
51	1t	70/82 (85%)	59 (84%)	11 (16%)	2	4
51	2t	70/82 (85%)	63 (90%)	7 (10%)	7	16
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	40
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	12
54	1w	203/298 (68%)	176 (87%)	27 (13%)	4	7
54	2w	203/298 (68%)	167 (82%)	36 (18%)	2	3
56	1z	14/17 (82%)	12 (86%)	2 (14%)	3	6
56	2z	14/17 (82%)	11 (79%)	3 (21%)	1	1
All	All	9748/10694 (91%)	8777 (90%)	971 (10%)	7	16

5 of 971 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
54	1w	315	HIS
45	2n	26	ARG
9	2N	9	VAL
44	2m	34	LEU
54	2w	222	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 156 such sidechains are listed below:

Mol	Chain	Res	Type
26	24	46	GLN
41	2j	21	GLN
33	2b	19	HIS
36	2e	73	ASN
49	2r	63	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	446 (15%)	27 (0%)
1	2A	2791/2915 (95%)	484 (17%)	22 (0%)
2	1B	119/121 (98%)	11 (9%)	0
2	2B	119/121 (98%)	19 (15%)	0
32	1a	1497/1521 (98%)	294 (19%)	0
32	2a	1501/1521 (98%)	315 (20%)	0
53	1v	10/24 (41%)	2 (20%)	0
53	2v	10/24 (41%)	2 (20%)	0
55	1x	73/76 (96%)	12 (16%)	0
55	1y	71/76 (93%)	23 (32%)	0
55	2x	73/76 (96%)	12 (16%)	0
55	2y	72/76 (94%)	28 (38%)	0
All	All	9200/9466 (97%)	1648 (17%)	49 (0%)

5 of 1648 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	15	G
1	1A	27	G
1	1A	34	C

5 of 49 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	228	A
1	2A	856	C
1	2A	266	G
1	2A	528	A
1	2A	1210	A

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

78 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
43	0TD	1l	92	43	8,9,10	4.24	1 (12%)	6,11,13	13.49	1 (16%)
1	OMG	2A	2251	55,1	23,26,27	1.22	3 (13%)	32,38,41	1.97	6 (18%)
55	4SU	1y	8	55	18,21,22	1.78	4 (22%)	25,30,33	2.20	5 (20%)
55	MIA	2x	37	55	28,31,32	2.37	6 (21%)	38,44,47	2.73	14 (36%)
1	5MC	2A	1962	57,1	19,22,23	1.62	3 (15%)	26,32,35	1.07	2 (7%)
1	OMC	2A	1920	1	19,22,23	0.79	0	25,31,34	0.90	0
32	PSU	2a	516	57,32	18,21,22	1.35	2 (11%)	21,30,33	1.90	4 (19%)
32	MA6	1a	1519	32	23,26,27	0.44	0	33,38,41	2.01	10 (30%)
55	G7M	2y	46	55	23,26,27	1.54	4 (17%)	34,39,42	1.79	5 (14%)
32	2MG	2a	1207	32	23,26,27	1.22	2 (8%)	33,38,41	2.21	8 (24%)
1	5MU	2A	1939	57,1	19,22,23	1.42	4 (21%)	27,32,35	2.30	6 (22%)
1	OMU	2A	2552	57,1	19,22,23	1.28	3 (15%)	25,31,34	1.78	5 (20%)
32	5MC	1a	1400	32	19,22,23	1.69	3 (15%)	26,32,35	1.13	2 (7%)
1	OMU	1A	2552	57,1	19,22,23	1.21	3 (15%)	25,31,34	1.92	5 (20%)
55	PSU	1x	32	55	18,21,22	1.35	2 (11%)	21,30,33	2.03	3 (14%)
55	4SU	2x	8	55	18,21,22	1.83	5 (27%)	25,30,33	1.73	5 (20%)
55	PSU	1y	39	55	18,21,22	1.42	2 (11%)	21,30,33	1.99	3 (14%)
32	G7M	1a	527	32	23,26,27	1.54	3 (13%)	34,39,42	1.79	5 (14%)
32	4OC	2a	1402	57,32	20,23,24	0.80	0	25,32,35	0.99	2 (8%)
55	G7M	1y	46	55	23,26,27	1.58	4 (17%)	34,39,42	1.84	5 (14%)
32	MA6	2a	1519	32	23,26,27	0.43	0	33,38,41	2.09	9 (27%)
54	MEQ	2w	230	54	8,9,10	0.69	0	5,10,12	0.67	0
1	5MU	1A	1939	57,1	19,22,23	1.38	5 (26%)	27,32,35	2.26	6 (22%)
55	PSU	2x	32	55	18,21,22	1.38	2 (11%)	21,30,33	2.02	4 (19%)
55	PSU	2y	32	55	18,21,22	1.34	2 (11%)	21,30,33	1.95	3 (14%)
1	PSU	2A	2605	1	18,21,22	1.32	3 (16%)	21,30,33	2.18	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	2MG	1a	1207	32	23,26,27	1.25	4 (17%)	33,38,41	2.10	7 (21%)
55	PSU	2x	39	55	18,21,22	1.42	2 (11%)	21,30,33	1.70	4 (19%)
32	UR3	2a	1498	32	19,22,23	0.98	0	26,32,35	1.69	2 (7%)
1	5MU	1A	1915	54,57,1	19,22,23	1.46	6 (31%)	27,32,35	2.31	6 (22%)
1	PSU	1A	1917	1	18,21,22	1.44	2 (11%)	21,30,33	2.05	3 (14%)
32	5MC	2a	1407	32	19,22,23	1.52	2 (10%)	26,32,35	1.05	3 (11%)
55	PSU	1y	32	55	18,21,22	1.38	2 (11%)	21,30,33	1.95	4 (19%)
55	G7M	1x	46	55	23,26,27	1.53	3 (13%)	34,39,42	1.71	5 (14%)
1	2MA	1A	2503	57,1	22,25,26	1.42	5 (22%)	32,37,40	2.39	9 (28%)
32	5MC	2a	1404	32	19,22,23	1.76	3 (15%)	26,32,35	1.24	3 (11%)
1	OMG	1A	2251	55,57,1	23,26,27	1.21	3 (13%)	32,38,41	2.04	6 (18%)
32	MA6	2a	1518	32	23,26,27	0.41	0	33,38,41	2.03	8 (24%)
55	4SU	1x	8	55	18,21,22	1.71	4 (22%)	25,30,33	1.69	4 (16%)
55	5MU	2x	54	55	19,22,23	1.38	5 (26%)	27,32,35	2.08	8 (29%)
55	PSU	2x	55	55	18,21,22	1.38	2 (11%)	21,30,33	2.05	4 (19%)
32	G7M	2a	527	32	23,26,27	1.51	3 (13%)	34,39,42	1.67	5 (14%)
32	5MC	2a	967	32	19,22,23	1.73	3 (15%)	26,32,35	1.18	2 (7%)
55	G7M	2x	46	55	23,26,27	1.55	3 (13%)	34,39,42	1.81	5 (14%)
55	MIA	1x	37	55	28,31,32	2.49	7 (25%)	38,44,47	2.53	13 (34%)
55	PSU	1x	55	55	18,21,22	1.29	2 (11%)	21,30,33	1.93	4 (19%)
55	5MU	2y	54	55	19,22,23	1.49	4 (21%)	27,32,35	1.97	7 (25%)
55	PSU	2y	55	55	18,21,22	1.38	2 (11%)	21,30,33	1.97	4 (19%)
1	PSU	2A	1917	1	18,21,22	1.36	2 (11%)	21,30,33	2.03	3 (14%)
55	MIA	2y	37	55	28,31,32	2.33	6 (21%)	38,44,47	2.91	15 (39%)
1	PSU	2A	1911	1	18,21,22	1.40	2 (11%)	21,30,33	2.04	4 (19%)
32	M2G	1a	966	32	24,27,28	1.28	4 (16%)	33,40,43	1.91	6 (18%)
32	5MC	1a	1407	32	19,22,23	1.50	2 (10%)	26,32,35	1.05	2 (7%)
54	MEQ	1w	230	54	8,9,10	0.78	0	5,10,12	1.34	1 (20%)
1	PSU	1A	1911	1	18,21,22	1.40	2 (11%)	21,30,33	2.13	4 (19%)
32	5MC	1a	967	32	19,22,23	1.72	3 (15%)	26,32,35	1.14	3 (11%)
1	5MC	1A	1942	1	19,22,23	1.44	3 (15%)	26,32,35	1.19	2 (7%)
32	M2G	2a	966	32	24,27,28	1.27	4 (16%)	33,40,43	1.92	6 (18%)
32	5MC	1a	1404	32	19,22,23	1.61	3 (15%)	26,32,35	1.07	2 (7%)
32	UR3	1a	1498	57,32	19,22,23	1.05	2 (10%)	26,32,35	1.65	3 (11%)
1	5MU	2A	1915	57,1	19,22,23	1.50	6 (31%)	27,32,35	2.14	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1A	2605	57,1	18,21,22	1.39	2 (11%)	21,30,33	2.19	3 (14%)
55	PSU	2y	39	55	18,21,22	1.35	2 (11%)	21,30,33	1.94	3 (14%)
43	0TD	2l	92	43	8,9,10	4.66	2 (25%)	6,11,13	1.61	1 (16%)
1	5MC	2A	1942	1	19,22,23	1.53	3 (15%)	26,32,35	1.12	2 (7%)
1	2MA	2A	2503	57,1	22,25,26	1.47	4 (18%)	32,37,40	2.35	7 (21%)
32	4OC	1a	1402	57,32	20,23,24	0.76	0	25,32,35	1.04	2 (8%)
55	4SU	2y	8	55	18,21,22	1.70	3 (16%)	25,30,33	2.34	5 (20%)
55	5MU	1y	54	55	19,22,23	1.46	5 (26%)	27,32,35	2.02	7 (25%)
55	PSU	1y	55	55	18,21,22	1.36	2 (11%)	21,30,33	2.05	3 (14%)
32	PSU	1a	516	57,32	18,21,22	1.42	2 (11%)	21,30,33	2.04	5 (23%)
32	MA6	1a	1518	32	23,26,27	0.37	0	33,38,41	2.07	9 (27%)
55	5MU	1x	54	55	19,22,23	1.42	4 (21%)	27,32,35	1.88	6 (22%)
32	5MC	2a	1400	32	19,22,23	1.59	3 (15%)	26,32,35	1.16	2 (7%)
1	OMC	1A	1920	1	19,22,23	0.80	0	25,31,34	0.93	1 (4%)
1	5MC	1A	1962	57,1	19,22,23	1.44	3 (15%)	26,32,35	1.16	4 (15%)
55	PSU	1x	39	55	18,21,22	1.42	3 (16%)	21,30,33	1.78	3 (14%)
55	MIA	1y	37	55	28,31,32	2.24	6 (21%)	38,44,47	2.69	13 (34%)

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
43	0TD	1l	92	43	-	5/7/12/14	-
1	OMG	2A	2251	55,1	-	0/9/27/28	0/3/3/3
55	4SU	1y	8	55	-	1/7/25/26	0/2/2/2
55	MIA	2x	37	55	-	6/15/33/34	0/3/3/3
1	5MC	2A	1962	57,1	-	1/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
32	PSU	2a	516	57,32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
55	G7M	2y	46	55	-	2/7/25/26	0/3/3/3
32	2MG	2a	1207	32	-	2/9/27/28	0/3/3/3
1	5MU	2A	1939	57,1	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	57,1	-	0/9/27/28	0/2/2/2
32	5MC	1a	1400	32	-	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	OMU	1A	2552	57,1	-	0/9/27/28	0/2/2/2
55	PSU	1x	32	55	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
55	PSU	1y	39	55	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32	-	3/7/25/26	0/3/3/3
32	4OC	2a	1402	57,32	-	2/9/29/30	0/2/2/2
55	G7M	1y	46	55	-	3/7/25/26	0/3/3/3
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
54	MEQ	2w	230	54	-	2/8/9/11	-
1	5MU	1A	1939	57,1	-	0/7/25/26	0/2/2/2
55	PSU	2x	32	55	-	0/7/25/26	0/2/2/2
55	PSU	2y	32	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
55	PSU	2x	39	55	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	54,57,1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
55	PSU	1y	32	55	-	0/7/25/26	0/2/2/2
55	G7M	1x	46	55	-	3/7/25/26	0/3/3/3
1	2MA	1A	2503	57,1	-	0/7/25/26	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	55,57,1	-	0/9/27/28	0/3/3/3
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32	-	1/7/25/26	0/3/3/3
32	5MC	2a	967	32	-	1/7/25/26	0/2/2/2
55	G7M	2x	46	55	-	3/7/25/26	0/3/3/3
55	MIA	1x	37	55	-	5/15/33/34	0/3/3/3
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
55	5MU	2y	54	55	-	2/7/25/26	0/2/2/2
55	PSU	2y	55	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
55	MIA	2y	37	55	-	2/15/33/34	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	MEQ	1w	230	54	-	4/8/9/11	-
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	57,32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	57,1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	57,1	-	0/7/25/26	0/2/2/2
55	PSU	2y	39	55	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	4/7/12/14	-
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	57,1	-	2/7/25/26	0/3/3/3
32	4OC	1a	1402	57,32	-	2/9/29/30	0/2/2/2
55	4SU	2y	8	55	-	0/7/25/26	0/2/2/2
55	5MU	1y	54	55	-	0/7/25/26	0/2/2/2
55	PSU	1y	55	55	-	2/7/25/26	0/2/2/2
32	PSU	1a	516	57,32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
1	5MC	1A	1962	57,1	-	0/7/25/26	0/2/2/2
55	PSU	1x	39	55	-	0/7/25/26	0/2/2/2
55	MIA	1y	37	55	-	6/15/33/34	0/3/3/3

The worst 5 of 216 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.60	1.69	1.82
43	1l	92	0TD	CB-SB	-11.52	1.70	1.82
55	1x	37	MIA	C2-S10	-8.24	1.68	1.75
55	1x	37	MIA	C13-C14	7.08	1.53	1.32
55	2x	37	MIA	C13-C14	6.96	1.53	1.32

The worst 5 of 372 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	32.94	161.58	102.36
55	2y	37	MIA	C12-C13-C14	-10.01	109.05	127.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2503	2MA	C5-C4-N3	-8.59	118.14	127.18
1	1A	2503	2MA	C5-C4-N3	-8.25	118.49	127.18
55	2x	37	MIA	C5-C4-N3	-8.18	118.56	127.18

There are no chirality outliers.

5 of 73 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	CA-CB-SB-CSB
54	1w	230	MEQ	CG-CD-NE2-CE
55	1x	37	MIA	C5-C6-N6-C12
55	1x	37	MIA	C12-C13-C14-C15

There are no ring outliers.

30 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	1l	92	0TD	2	0
55	1y	8	4SU	1	0
1	2A	1920	OMC	1	0
32	1a	1519	MA6	2	0
1	2A	1939	5MU	2	0
1	1A	2552	OMU	1	0
55	2x	8	4SU	1	0
55	1y	39	PSU	1	0
32	2a	1402	4OC	3	0
55	1y	46	G7M	3	0
32	2a	1519	MA6	1	0
54	2w	230	MEQ	1	0
1	1A	1939	5MU	1	0
55	2x	32	PSU	1	0
55	1x	46	G7M	1	0
32	2a	1518	MA6	2	0
55	1x	8	4SU	1	0
32	2a	527	G7M	1	0
55	1x	37	MIA	2	0
55	2y	55	PSU	1	0
54	1w	230	MEQ	1	0
32	2a	966	M2G	1	0
55	2y	39	PSU	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	2l	92	0TD	2	0
1	2A	2503	2MA	2	0
32	1a	1402	4OC	3	0
55	2y	8	4SU	1	0
32	1a	1518	MA6	1	0
32	2a	1400	5MC	1	0
1	1A	1920	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2006 ligands modelled in this entry, 2004 are monoatomic - leaving 2 for Mogul analysis.

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

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	2d	501	SF4	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	2860/2915 (98%)	-0.39	105 (3%)	45	35	12, 28, 89, 107	0
1	2A	2789/2915 (95%)	0.09	108 (3%)	43	34	25, 51, 91, 106	0
2	1B	120/121 (99%)	-0.32	0	100	100	23, 48, 63, 77	0
2	2B	120/121 (99%)	0.89	7 (5%)	29	21	57, 79, 92, 96	0
3	1D	275/276 (99%)	-0.28	0	100	100	13, 29, 46, 68	0
3	2D	275/276 (99%)	0.18	5 (1%)	67	61	26, 45, 59, 77	0
4	1E	204/206 (99%)	-0.34	1 (0%)	87	85	12, 28, 52, 67	0
4	2E	204/206 (99%)	0.15	1 (0%)	87	85	27, 48, 63, 72	0
5	1F	203/210 (96%)	-0.13	1 (0%)	87	85	13, 33, 60, 80	0
5	2F	203/210 (96%)	0.59	6 (2%)	52	44	28, 59, 73, 86	0
6	1G	181/182 (99%)	0.63	7 (3%)	43	34	45, 56, 69, 84	0
6	2G	181/182 (99%)	1.41	37 (20%)	3	2	63, 78, 84, 89	0
7	1H	174/180 (96%)	0.07	1 (0%)	85	82	32, 44, 58, 70	0
7	2H	174/180 (96%)	1.39	39 (22%)	2	2	62, 76, 85, 93	0
8	1I	146/148 (98%)	0.65	5 (3%)	48	38	37, 62, 74, 82	0
8	2I	146/148 (98%)	1.09	22 (15%)	5	4	48, 68, 76, 82	0
9	1N	140/140 (100%)	-0.19	2 (1%)	73	67	17, 28, 52, 67	0
9	2N	140/140 (100%)	0.43	0	100	100	41, 57, 71, 78	0
10	1O	122/122 (100%)	-0.14	0	100	100	18, 32, 49, 56	0
10	2O	122/122 (100%)	0.03	1 (0%)	82	78	33, 44, 60, 65	0
11	1P	149/150 (99%)	0.02	0	100	100	13, 35, 56, 64	0
11	2P	149/150 (99%)	0.70	11 (7%)	20	14	34, 60, 76, 83	0
12	1Q	141/141 (100%)	-0.01	0	100	100	20, 32, 46, 59	0
12	2Q	141/141 (100%)	0.67	7 (4%)	34	27	42, 60, 69, 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%)	-0.45	0 100 100	16, 26, 43, 54	0
13	2R	118/118 (100%)	0.39	0 100 100	33, 47, 57, 65	0
14	1S	110/112 (98%)	0.03	2 (1%) 67 61	35, 46, 59, 64	0
14	2S	110/112 (98%)	1.35	16 (14%) 6 4	63, 73, 80, 84	0
15	1T	131/146 (89%)	0.04	4 (3%) 51 43	24, 35, 63, 79	0
15	2T	131/146 (89%)	0.34	3 (2%) 61 52	36, 49, 69, 81	0
16	1U	116/118 (98%)	-0.44	0 100 100	13, 22, 33, 54	0
16	2U	116/118 (98%)	0.41	1 (0%) 81 76	36, 53, 68, 75	0
17	1V	101/101 (100%)	-0.33	0 100 100	15, 30, 46, 55	0
17	2V	101/101 (100%)	0.69	4 (3%) 42 33	40, 62, 72, 80	0
18	1W	112/113 (99%)	-0.44	1 (0%) 81 76	14, 22, 37, 76	0
18	2W	112/113 (99%)	0.20	0 100 100	33, 43, 59, 84	0
19	1X	95/96 (98%)	-0.10	1 (1%) 78 73	20, 31, 55, 71	0
19	2X	95/96 (98%)	0.68	6 (6%) 26 19	41, 59, 69, 74	0
20	1Y	107/110 (97%)	0.28	2 (1%) 66 59	28, 41, 63, 75	0
20	2Y	107/110 (97%)	1.12	16 (14%) 5 4	48, 65, 77, 83	0
21	1Z	183/206 (88%)	0.53	10 (5%) 30 23	35, 52, 66, 73	0
21	2Z	186/206 (90%)	1.09	15 (8%) 18 13	61, 72, 80, 87	0
22	10	76/85 (89%)	-0.15	2 (2%) 57 48	23, 31, 49, 64	0
22	20	77/85 (90%)	0.75	5 (6%) 25 18	42, 60, 68, 74	0
23	11	97/98 (98%)	0.03	3 (3%) 51 43	18, 37, 63, 72	0
23	21	97/98 (98%)	0.76	4 (4%) 41 32	38, 53, 72, 77	0
24	12	70/72 (97%)	0.33	4 (5%) 29 22	27, 44, 55, 76	0
24	22	70/72 (97%)	0.66	3 (4%) 40 31	55, 65, 73, 76	0
25	13	59/60 (98%)	-0.29	0 100 100	20, 28, 51, 68	0
25	23	59/60 (98%)	0.47	4 (6%) 23 17	45, 56, 70, 76	0
26	14	69/71 (97%)	1.20	18 (26%) 1 1	52, 73, 88, 93	0
26	24	68/71 (95%)	1.88	28 (41%) 0 0	72, 84, 91, 94	0
27	15	59/60 (98%)	-0.36	0 100 100	11, 23, 44, 54	0
27	25	59/60 (98%)	0.23	1 (1%) 69 63	30, 45, 63, 76	0
28	16	53/54 (98%)	-0.13	0 100 100	30, 37, 50, 56	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.56	2 (3%)	44	35	49, 60, 67, 73	0
29	17	48/49 (97%)	-0.04	2 (4%)	40	32	15, 22, 45, 65	0
29	27	48/49 (97%)	0.27	4 (8%)	17	13	27, 38, 63, 68	0
30	18	64/65 (98%)	-0.19	0	100	100	17, 27, 34, 41	0
30	28	64/65 (98%)	0.64	3 (4%)	36	28	41, 49, 57, 64	0
31	19	37/37 (100%)	-0.17	0	100	100	23, 30, 46, 50	0
31	29	37/37 (100%)	0.77	0	100	100	52, 61, 69, 75	0
32	1a	1488/1521 (97%)	0.56	83 (5%)	30	22	26, 68, 92, 106	0
32	2a	1491/1521 (98%)	0.69	94 (6%)	26	19	35, 69, 93, 105	0
33	1b	231/256 (90%)	1.08	27 (11%)	9	7	59, 73, 84, 90	0
33	2b	231/256 (90%)	1.51	62 (26%)	1	1	67, 78, 86, 90	0
34	1c	206/239 (86%)	1.45	42 (20%)	3	2	63, 75, 82, 85	0
34	2c	206/239 (86%)	1.36	36 (17%)	4	3	65, 77, 85, 89	0
35	1d	208/209 (99%)	1.10	24 (11%)	9	7	46, 67, 78, 83	0
35	2d	208/209 (99%)	0.76	7 (3%)	48	38	50, 61, 71, 75	0
36	1e	148/162 (91%)	0.51	2 (1%)	73	67	47, 58, 70, 80	0
36	2e	148/162 (91%)	0.84	8 (5%)	31	23	42, 65, 74, 88	0
37	1f	100/101 (99%)	0.47	1 (1%)	79	74	52, 63, 74, 77	0
37	2f	100/101 (99%)	0.74	3 (3%)	52	44	53, 69, 77, 81	0
38	1g	155/156 (99%)	0.93	12 (7%)	19	14	58, 70, 80, 84	0
38	2g	155/156 (99%)	1.37	30 (19%)	3	3	64, 77, 84, 88	0
39	1h	137/138 (99%)	0.51	2 (1%)	72	65	51, 60, 67, 72	0
39	2h	137/138 (99%)	0.86	8 (5%)	29	21	52, 66, 73, 78	0
40	1i	127/128 (99%)	1.43	23 (18%)	3	3	58, 76, 82, 87	0
40	2i	123/128 (96%)	1.87	49 (39%)	1	0	70, 81, 87, 91	0
41	1j	98/105 (93%)	1.99	47 (47%)	0	0	63, 79, 86, 92	0
41	2j	96/105 (91%)	2.27	56 (58%)	0	0	71, 81, 88, 93	0
42	1k	114/129 (88%)	0.49	2 (1%)	67	61	40, 60, 71, 76	0
42	2k	114/129 (88%)	0.77	5 (4%)	39	30	48, 68, 76, 83	0
43	1l	121/132 (91%)	0.71	5 (4%)	41	32	37, 55, 65, 70	0
43	2l	121/132 (91%)	0.63	3 (2%)	58	49	45, 54, 62, 68	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	118/126 (93%)	1.26	14 (11%) 9 7	63, 74, 80, 87	0
44	2m	115/126 (91%)	1.81	46 (40%) 1 0	70, 80, 86, 91	0
45	1n	60/61 (98%)	1.57	15 (25%) 2 1	61, 73, 82, 85	0
45	2n	60/61 (98%)	1.92	23 (38%) 1 0	70, 78, 83, 86	0
46	1o	88/89 (98%)	0.54	2 (2%) 61 52	42, 58, 72, 74	0
46	2o	88/89 (98%)	0.83	5 (5%) 29 22	49, 64, 76, 82	0
47	1p	82/88 (93%)	1.42	17 (20%) 2 2	54, 67, 78, 86	0
47	2p	82/88 (93%)	0.85	3 (3%) 45 35	49, 61, 68, 77	0
48	1q	99/105 (94%)	0.68	4 (4%) 42 33	47, 59, 70, 73	0
48	2q	99/105 (94%)	0.83	6 (6%) 27 20	50, 63, 72, 76	0
49	1r	68/88 (77%)	0.67	1 (1%) 72 65	48, 58, 76, 81	0
49	2r	68/88 (77%)	0.75	2 (2%) 53 45	56, 65, 73, 80	0
50	1s	83/93 (89%)	1.44	21 (25%) 1 1	69, 77, 85, 89	0
50	2s	83/93 (89%)	1.63	27 (32%) 1 1	72, 81, 88, 92	0
51	1t	96/106 (90%)	1.00	11 (11%) 9 7	55, 63, 73, 77	0
51	2t	96/106 (90%)	1.00	8 (8%) 17 13	51, 65, 77, 81	0
52	1u	23/27 (85%)	1.80	10 (43%) 0 0	65, 71, 76, 79	0
52	2u	23/27 (85%)	1.80	11 (47%) 0 0	72, 79, 83, 84	0
53	1v	13/24 (54%)	0.81	3 (23%) 2 2	45, 53, 91, 91	0
53	2v	13/24 (54%)	1.30	3 (23%) 2 2	59, 69, 99, 101	0
54	1w	248/354 (70%)	0.35	4 (1%) 70 64	26, 62, 77, 84	0
54	2w	252/354 (71%)	0.78	18 (7%) 22 16	44, 69, 83, 91	0
55	1x	68/76 (89%)	0.05	1 (1%) 72 65	23, 54, 69, 88	0
55	1y	67/76 (88%)	0.67	3 (4%) 38 29	32, 86, 95, 101	0
55	2x	68/76 (89%)	0.39	1 (1%) 72 65	42, 71, 82, 91	0
55	2y	67/76 (88%)	1.20	6 (8%) 15 12	55, 94, 100, 102	0
56	1z	14/18 (77%)	1.97	8 (57%) 0 0	29, 52, 72, 75	0
56	2z	14/18 (77%)	2.17	8 (57%) 0 0	52, 67, 76, 79	0
All	All	21290/22338 (95%)	0.43	1442 (6%) 23 17	11, 58, 85, 107	0

The worst 5 of 1442 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	2F	89	VAL	7.1
1	1A	1068	G	6.8
44	1m	2	ALA	6.7
38	2g	16	LEU	6.4
1	2A	2115	G	6.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
55	G7M	1y	46	24/25	0.58	0.16	85,90,107,120	0
55	4SU	2y	8	20/21	0.61	0.14	89,97,111,122	0
55	5MU	2y	54	21/22	0.63	0.16	88,98,108,120	0
55	G7M	2y	46	24/25	0.64	0.13	85,96,105,129	0
55	PSU	2y	55	20/21	0.67	0.17	88,98,106,116	0
55	PSU	2y	32	20/21	0.69	0.14	83,87,93,96	0
55	PSU	1y	55	20/21	0.72	0.12	82,92,101,109	0
55	PSU	2y	39	20/21	0.75	0.14	75,87,90,93	0
55	5MU	1y	54	21/22	0.77	0.11	81,86,98,113	0
55	PSU	1y	32	20/21	0.78	0.15	67,82,88,89	0
55	4SU	1y	8	20/21	0.79	0.12	86,91,99,99	0
55	MIA	2y	37	29/30	0.79	0.16	76,82,95,106	0
55	PSU	1y	39	20/21	0.80	0.14	64,74,79,82	0
55	G7M	2x	46	24/25	0.81	0.14	68,74,79,100	0
32	2MG	1a	1207	24/25	0.83	0.13	75,79,83,90	0
32	2MG	2a	1207	24/25	0.85	0.12	62,78,83,85	0
55	MIA	1y	37	29/30	0.87	0.14	62,73,78,78	0
43	0TD	1l	92	10/11	0.88	0.14	45,55,58,59	0
55	PSU	2x	55	20/21	0.88	0.10	63,72,79,81	0
55	G7M	1x	46	24/25	0.88	0.10	44,54,82,100	0
55	PSU	2x	32	20/21	0.89	0.11	52,69,82,83	0
32	5MC	2a	967	21/22	0.89	0.12	59,66,76,82	0
1	5MU	2A	1915	21/22	0.91	0.11	52,62,73,78	0
55	5MU	2x	54	21/22	0.91	0.10	60,69,77,80	0
32	PSU	2a	516	20/21	0.91	0.10	61,67,70,70	0
32	G7M	2a	527	24/25	0.91	0.12	56,63,68,79	0
1	5MU	1A	1915	21/22	0.91	0.11	37,51,62,63	0
55	5MU	1x	54	21/22	0.91	0.11	50,58,62,69	0
32	5MC	2a	1400	21/22	0.91	0.12	52,65,70,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
43	0TD	2l	92	10/11	0.91	0.14	50,55,63,64	0
55	4SU	2x	8	20/21	0.91	0.11	63,68,71,72	0
32	PSU	1a	516	20/21	0.91	0.12	45,67,73,73	0
32	M2G	2a	966	25/26	0.92	0.11	56,62,73,78	0
55	PSU	2x	39	20/21	0.92	0.10	41,65,71,71	0
1	PSU	2A	1911	20/21	0.92	0.10	52,56,59,67	0
32	M2G	1a	966	25/26	0.92	0.13	47,53,65,72	0
32	5MC	2a	1404	21/22	0.93	0.12	43,50,55,56	0
32	5MC	1a	967	21/22	0.93	0.12	49,55,64,66	0
55	PSU	1x	32	20/21	0.93	0.11	53,59,66,73	0
55	PSU	1x	55	20/21	0.93	0.09	53,59,62,64	0
32	4OC	2a	1402	22/23	0.93	0.12	44,52,58,62	0
32	MA6	2a	1518	24/25	0.94	0.12	42,57,62,66	0
32	G7M	1a	527	24/25	0.94	0.11	48,58,65,66	0
1	PSU	1A	1917	20/21	0.94	0.08	38,47,60,61	0
1	PSU	2A	1917	20/21	0.95	0.08	45,53,56,59	0
32	MA6	2a	1519	24/25	0.95	0.13	43,52,59,60	0
1	OMC	2A	1920	21/22	0.95	0.10	51,53,59,62	0
54	MEQ	2w	230	10/11	0.95	0.12	47,51,53,54	0
32	5MC	1a	1400	21/22	0.95	0.11	45,56,61,62	0
55	MIA	1x	37	29/30	0.95	0.11	36,51,59,67	0
55	MIA	2x	37	29/30	0.95	0.12	60,66,71,71	0
55	PSU	1x	39	20/21	0.95	0.10	44,54,60,61	0
32	5MC	2a	1407	21/22	0.95	0.09	39,47,54,60	0
32	5MC	1a	1404	21/22	0.96	0.09	34,39,42,46	0
32	5MC	1a	1407	21/22	0.96	0.09	27,38,42,43	0
1	5MC	2A	1962	21/22	0.96	0.10	25,32,38,41	0
1	PSU	1A	1911	20/21	0.96	0.09	37,46,55,55	0
1	OMC	1A	1920	21/22	0.96	0.09	32,40,45,48	0
32	UR3	2a	1498	21/22	0.96	0.10	42,49,54,56	0
1	5MC	1A	1942	21/22	0.96	0.07	20,26,30,36	0
32	4OC	1a	1402	22/23	0.96	0.09	30,38,46,53	0
55	4SU	1x	8	20/21	0.97	0.08	36,44,49,49	0
32	MA6	1a	1518	24/25	0.97	0.09	31,35,38,38	0
32	MA6	1a	1519	24/25	0.97	0.09	28,33,37,38	0
1	5MU	2A	1939	21/22	0.97	0.09	28,32,36,37	0
1	5MC	2A	1942	21/22	0.97	0.09	37,46,48,50	0
1	5MC	1A	1962	21/22	0.97	0.07	22,27,30,37	0
1	OMG	2A	2251	24/25	0.97	0.09	30,36,39,44	0
1	2MA	2A	2503	23/24	0.97	0.07	25,29,31,33	0
54	MEQ	1w	230	10/11	0.97	0.09	20,29,32,32	0
1	5MU	1A	1939	21/22	0.98	0.06	15,19,23,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	OMG	1A	2251	24/25	0.98	0.06	14,18,21,23	0
1	OMU	2A	2552	21/22	0.98	0.07	23,30,34,38	0
1	PSU	2A	2605	20/21	0.98	0.07	23,30,35,36	0
1	2MA	1A	2503	23/24	0.98	0.06	11,14,17,19	0
1	OMU	1A	2552	21/22	0.98	0.07	14,19,25,26	0
32	UR3	1a	1498	21/22	0.98	0.07	29,35,41,44	0
1	PSU	1A	2605	20/21	0.98	0.07	14,18,23,23	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	3636	1/1	0.46	0.26	56,56,56,56	0
57	MG	2a	1764	1/1	0.46	0.18	77,77,77,77	0
57	MG	1a	1662	1/1	0.48	0.40	73,73,73,73	0
57	MG	2A	3631	1/1	0.59	0.30	79,79,79,79	0
57	MG	1A	3649	1/1	0.60	0.17	49,49,49,49	0
57	MG	2a	1732	1/1	0.61	0.19	58,58,58,58	0
57	MG	2A	3491	1/1	0.61	0.19	65,65,65,65	0
57	MG	2A	3569	1/1	0.62	0.21	54,54,54,54	0
57	MG	2A	3340	1/1	0.62	0.29	77,77,77,77	0
57	MG	2A	3100	1/1	0.63	0.15	79,79,79,79	0
57	MG	2A	3632	1/1	0.63	0.29	70,70,70,70	0
57	MG	2A	3510	1/1	0.66	0.20	51,51,51,51	0
57	MG	1A	3749	1/1	0.66	0.37	34,34,34,34	0
57	MG	2A	3236	1/1	0.66	0.17	73,73,73,73	0
57	MG	1A	3480	1/1	0.66	0.16	62,62,62,62	0
57	MG	2A	3345	1/1	0.66	0.13	79,79,79,79	0
57	MG	1a	1763	1/1	0.66	0.22	64,64,64,64	0
57	MG	1a	1751	1/1	0.67	0.17	71,71,71,71	0
57	MG	2A	3591	1/1	0.67	0.20	69,69,69,69	0
57	MG	2A	3271	1/1	0.68	0.21	59,59,59,59	0
57	MG	2A	3070	1/1	0.69	0.15	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	3112	1/1	0.69	0.21	61,61,61,61	0
57	MG	2A	3460	1/1	0.70	0.17	59,59,59,59	0
57	MG	1A	3793	1/1	0.70	0.13	67,67,67,67	0
57	MG	2a	1762	1/1	0.70	0.26	76,76,76,76	0
57	MG	2A	3451	1/1	0.70	0.15	56,56,56,56	0
57	MG	2A	3026	1/1	0.71	0.14	62,62,62,62	0
57	MG	2A	3111	1/1	0.71	0.37	69,69,69,69	0
57	MG	1A	3740	1/1	0.71	0.18	40,40,40,40	0
57	MG	1A	3363	1/1	0.72	0.15	58,58,58,58	0
57	MG	1Q	204	1/1	0.72	0.17	58,58,58,58	0
57	MG	2A	3471	1/1	0.72	0.23	68,68,68,68	0
57	MG	2A	3091	1/1	0.73	0.20	62,62,62,62	0
57	MG	1A	3154	1/1	0.73	0.08	70,70,70,70	0
57	MG	1A	3707	1/1	0.74	0.16	43,43,43,43	0
57	MG	2A	3594	1/1	0.74	0.22	82,82,82,82	0
57	MG	2A	3605	1/1	0.74	0.21	56,56,56,56	0
57	MG	1a	1704	1/1	0.74	0.26	68,68,68,68	0
57	MG	2v	102	1/1	0.74	0.22	67,67,67,67	0
57	MG	2x	108	1/1	0.74	0.27	67,67,67,67	0
57	MG	2a	1605	1/1	0.75	0.18	57,57,57,57	0
57	MG	2a	1676	1/1	0.75	0.35	66,66,66,66	0
57	MG	2A	3463	1/1	0.75	0.13	65,65,65,65	0
57	MG	2a	1750	1/1	0.75	0.16	48,48,48,48	0
57	MG	1a	1697	1/1	0.75	0.32	59,59,59,59	0
57	MG	1A	3592	1/1	0.75	0.33	51,51,51,51	0
57	MG	1A	3437	1/1	0.75	0.25	63,63,63,63	0
57	MG	1A	3540	1/1	0.75	0.16	16,16,16,16	0
57	MG	2a	1705	1/1	0.76	0.22	77,77,77,77	0
57	MG	2A	3110	1/1	0.76	0.34	68,68,68,68	0
57	MG	2a	1737	1/1	0.76	0.21	62,62,62,62	0
57	MG	2A	3566	1/1	0.76	0.18	56,56,56,56	0
57	MG	1a	1735	1/1	0.76	0.15	60,60,60,60	0
57	MG	2F	304	1/1	0.76	0.18	40,40,40,40	0
57	MG	1a	1609	1/1	0.76	0.25	64,64,64,64	0
57	MG	2A	3034	1/1	0.76	0.31	52,52,52,52	0
57	MG	2A	3472	1/1	0.77	0.15	41,41,41,41	0
57	MG	1A	3725	1/1	0.77	0.13	15,15,15,15	0
57	MG	2A	3425	1/1	0.77	0.15	61,61,61,61	0
57	MG	1a	1674	1/1	0.77	0.39	70,70,70,70	0
57	MG	2A	3306	1/1	0.77	0.24	60,60,60,60	0
57	MG	2A	3327	1/1	0.77	0.17	66,66,66,66	0
57	MG	1A	3340	1/1	0.77	0.17	57,57,57,57	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	1v	103	1/1	0.78	0.21	68,68,68,68	0
57	MG	2A	3488	1/1	0.78	0.16	58,58,58,58	0
57	MG	1x	104	1/1	0.78	0.28	63,63,63,63	0
57	MG	2a	1609	1/1	0.78	0.23	70,70,70,70	0
57	MG	2A	3346	1/1	0.78	0.18	67,67,67,67	0
57	MG	2a	1681	1/1	0.78	0.15	66,66,66,66	0
57	MG	2A	3540	1/1	0.78	0.19	66,66,66,66	0
57	MG	2a	1723	1/1	0.78	0.20	64,64,64,64	0
57	MG	1A	3431	1/1	0.78	0.10	53,53,53,53	0
57	MG	2A	3434	1/1	0.78	0.16	67,67,67,67	0
57	MG	2A	3576	1/1	0.78	0.15	69,69,69,69	0
57	MG	1a	1721	1/1	0.78	0.23	52,52,52,52	0
57	MG	1A	3510	1/1	0.78	0.13	45,45,45,45	0
57	MG	1A	3462	1/1	0.78	0.17	55,55,55,55	0
57	MG	1A	3465	1/1	0.78	0.13	31,31,31,31	0
57	MG	1A	3350	1/1	0.79	0.19	49,49,49,49	0
57	MG	2A	3646	1/1	0.79	0.28	56,56,56,56	0
57	MG	2F	301	1/1	0.79	0.19	47,47,47,47	0
57	MG	1A	3506	1/1	0.79	0.15	30,30,30,30	0
57	MG	1a	1666	1/1	0.79	0.36	65,65,65,65	0
57	MG	1a	1767	1/1	0.79	0.18	58,58,58,58	0
57	MG	2A	3492	1/1	0.79	0.17	59,59,59,59	0
57	MG	1A	3746	1/1	0.79	0.33	32,32,32,32	0
57	MG	2A	3371	1/1	0.79	0.17	70,70,70,70	0
57	MG	2A	3555	1/1	0.79	0.30	66,66,66,66	0
57	MG	2A	3403	1/1	0.79	0.16	45,45,45,45	0
57	MG	1A	3424	1/1	0.79	0.19	61,61,61,61	0
57	MG	2A	3144	1/1	0.79	0.11	61,61,61,61	0
57	MG	2A	3445	1/1	0.79	0.14	55,55,55,55	0
57	MG	2A	3148	1/1	0.79	0.28	69,69,69,69	0
57	MG	1A	3670	1/1	0.79	0.20	55,55,55,55	0
57	MG	1A	3476	1/1	0.79	0.24	75,75,75,75	0
57	MG	1a	1646	1/1	0.80	0.24	63,63,63,63	0
57	MG	1A	3326	1/1	0.80	0.15	32,32,32,32	0
57	MG	2a	1654	1/1	0.80	0.27	70,70,70,70	0
57	MG	1B	211	1/1	0.80	0.15	52,52,52,52	0
57	MG	1A	3600	1/1	0.80	0.52	37,37,37,37	0
57	MG	1a	1682	1/1	0.80	0.23	64,64,64,64	0
57	MG	1A	3784	1/1	0.80	0.13	68,68,68,68	0
57	MG	2A	3486	1/1	0.80	0.11	65,65,65,65	0
57	MG	1a	1634	1/1	0.80	0.22	64,64,64,64	0
57	MG	2A	3391	1/1	0.80	0.21	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1752	1/1	0.80	0.17	58,58,58,58	0
57	MG	1a	1635	1/1	0.80	0.28	65,65,65,65	0
57	MG	2A	3055	1/1	0.80	0.23	63,63,63,63	0
57	MG	2A	3261	1/1	0.80	0.25	53,53,53,53	0
57	MG	2I	101	1/1	0.80	0.23	58,58,58,58	0
57	MG	2A	3559	1/1	0.81	0.12	61,61,61,61	0
57	MG	2A	3190	1/1	0.81	0.16	59,59,59,59	0
57	MG	2a	1653	1/1	0.81	0.36	52,52,52,52	0
57	MG	2A	3228	1/1	0.81	0.14	46,46,46,46	0
57	MG	2A	3348	1/1	0.81	0.15	67,67,67,67	0
57	MG	2A	3589	1/1	0.81	0.12	58,58,58,58	0
57	MG	2A	3360	1/1	0.81	0.14	53,53,53,53	0
57	MG	2A	3039	1/1	0.81	0.15	54,54,54,54	0
57	MG	2A	3598	1/1	0.81	0.11	60,60,60,60	0
57	MG	1A	3582	1/1	0.81	0.12	30,30,30,30	0
57	MG	2A	3398	1/1	0.81	0.16	53,53,53,53	0
57	MG	2A	3068	1/1	0.81	0.23	47,47,47,47	0
57	MG	1a	1618	1/1	0.81	0.25	60,60,60,60	0
57	MG	2A	3084	1/1	0.81	0.14	49,49,49,49	0
57	MG	2A	3444	1/1	0.81	0.18	49,49,49,49	0
57	MG	1a	1619	1/1	0.81	0.14	51,51,51,51	0
57	MG	10	104	1/1	0.82	0.09	42,42,42,42	0
57	MG	2Q	201	1/1	0.82	0.22	58,58,58,58	0
57	MG	2A	3195	1/1	0.82	0.17	56,56,56,56	0
57	MG	1a	1621	1/1	0.82	0.16	59,59,59,59	0
57	MG	2A	3453	1/1	0.82	0.40	52,52,52,52	0
57	MG	2a	1646	1/1	0.82	0.19	54,54,54,54	0
57	MG	1A	3696	1/1	0.82	0.15	40,40,40,40	0
57	MG	2A	3578	1/1	0.82	0.24	55,55,55,55	0
57	MG	2A	3583	1/1	0.82	0.16	71,71,71,71	0
57	MG	2A	3118	1/1	0.82	0.14	51,51,51,51	0
57	MG	1a	1717	1/1	0.82	0.26	48,48,48,48	0
57	MG	2a	1713	1/1	0.82	0.19	68,68,68,68	0
57	MG	2A	3275	1/1	0.82	0.16	39,39,39,39	0
57	MG	2A	3279	1/1	0.82	0.14	57,57,57,57	0
57	MG	2A	3602	1/1	0.82	0.30	42,42,42,42	0
57	MG	2A	3402	1/1	0.82	0.18	50,50,50,50	0
57	MG	2a	1751	1/1	0.82	0.18	72,72,72,72	0
57	MG	2A	3612	1/1	0.82	0.11	61,61,61,61	0
57	MG	2a	1757	1/1	0.82	0.17	78,78,78,78	0
57	MG	2A	3293	1/1	0.82	0.11	40,40,40,40	0
57	MG	2A	3409	1/1	0.82	0.18	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	2k	201	1/1	0.82	0.16	58,58,58,58	0
57	MG	1A	3667	1/1	0.82	0.20	59,59,59,59	0
57	MG	2A	3184	1/1	0.82	0.22	53,53,53,53	0
57	MG	2A	3062	1/1	0.83	0.19	59,59,59,59	0
57	MG	2A	3367	1/1	0.83	0.15	44,44,44,44	0
57	MG	1A	3353	1/1	0.83	0.12	31,31,31,31	0
57	MG	23	102	1/1	0.83	0.26	63,63,63,63	0
57	MG	1a	1615	1/1	0.83	0.12	51,51,51,51	0
57	MG	1A	3574	1/1	0.83	0.13	59,59,59,59	0
57	MG	2a	1645	1/1	0.83	0.20	51,51,51,51	0
57	MG	2A	3401	1/1	0.83	0.16	55,55,55,55	0
57	MG	2a	1649	1/1	0.83	0.22	62,62,62,62	0
57	MG	2A	3090	1/1	0.83	0.15	50,50,50,50	0
57	MG	1A	3626	1/1	0.83	0.08	38,38,38,38	0
57	MG	2A	3269	1/1	0.83	0.14	47,47,47,47	0
57	MG	1A	3504	1/1	0.83	0.19	54,54,54,54	0
57	MG	2A	3107	1/1	0.83	0.21	69,69,69,69	0
57	MG	1x	106	1/1	0.83	0.20	59,59,59,59	0
57	MG	2A	3290	1/1	0.83	0.17	56,56,56,56	0
57	MG	2A	3450	1/1	0.83	0.17	46,46,46,46	0
57	MG	2A	3024	1/1	0.83	0.20	66,66,66,66	0
57	MG	2A	3297	1/1	0.83	0.11	41,41,41,41	0
57	MG	1a	1622	1/1	0.83	0.31	66,66,66,66	0
57	MG	1A	3718	1/1	0.83	0.14	51,51,51,51	0
57	MG	2A	3619	1/1	0.83	0.10	66,66,66,66	0
57	MG	2A	3629	1/1	0.83	0.21	60,60,60,60	0
57	MG	2A	3134	1/1	0.83	0.23	59,59,59,59	0
57	MG	2A	3143	1/1	0.83	0.12	50,50,50,50	0
57	MG	1A	3591	1/1	0.83	0.12	29,29,29,29	0
57	MG	1A	3663	1/1	0.83	0.11	39,39,39,39	0
57	MG	2A	3509	1/1	0.84	0.12	48,48,48,48	0
57	MG	2A	3399	1/1	0.84	0.14	43,43,43,43	0
57	MG	2A	3526	1/1	0.84	0.17	60,60,60,60	0
57	MG	2A	3076	1/1	0.84	0.17	53,53,53,53	0
57	MG	1a	1747	1/1	0.84	0.11	48,48,48,48	0
57	MG	1A	3396	1/1	0.84	0.12	20,20,20,20	0
57	MG	1a	1756	1/1	0.84	0.19	57,57,57,57	0
57	MG	1A	3206	1/1	0.84	0.08	15,15,15,15	0
57	MG	1a	1651	1/1	0.84	0.28	67,67,67,67	0
57	MG	1A	3553	1/1	0.84	0.13	38,38,38,38	0
57	MG	11	102	1/1	0.84	0.23	64,64,64,64	0
57	MG	1A	3638	1/1	0.84	0.21	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	2a	1668	1/1	0.84	0.20	60,60,60,60	0
57	MG	1y	103	1/1	0.84	0.29	81,81,81,81	0
57	MG	2a	1677	1/1	0.84	0.18	59,59,59,59	0
57	MG	1A	3644	1/1	0.84	0.11	54,54,54,54	0
57	MG	1A	3120	1/1	0.84	0.17	68,68,68,68	0
57	MG	1A	3436	1/1	0.84	0.05	9,9,9,9	0
57	MG	1A	3780	1/1	0.84	0.17	43,43,43,43	0
57	MG	2A	3047	1/1	0.84	0.12	48,48,48,48	0
57	MG	1A	3044	1/1	0.84	0.11	57,57,57,57	0
57	MG	2a	1739	1/1	0.84	0.20	58,58,58,58	0
57	MG	1a	1726	1/1	0.84	0.21	70,70,70,70	0
57	MG	1a	1734	1/1	0.84	0.23	54,54,54,54	0
57	MG	1A	3456	1/1	0.84	0.13	36,36,36,36	0
57	MG	2A	3643	1/1	0.84	0.12	45,45,45,45	0
57	MG	2A	3500	1/1	0.84	0.12	47,47,47,47	0
57	MG	2A	3656	1/1	0.84	0.27	49,49,49,49	0
57	MG	2B	206	1/1	0.84	0.35	54,54,54,54	0
57	MG	2D	306	1/1	0.84	0.19	62,62,62,62	0
57	MG	2D	307	1/1	0.84	0.16	56,56,56,56	0
57	MG	1a	1714	1/1	0.85	0.28	61,61,61,61	0
57	MG	1A	3007	1/1	0.85	0.08	30,30,30,30	0
57	MG	2A	3249	1/1	0.85	0.26	52,52,52,52	0
57	MG	2A	3254	1/1	0.85	0.17	63,63,63,63	0
57	MG	1A	3123	1/1	0.85	0.18	21,21,21,21	0
57	MG	1A	3634	1/1	0.85	0.18	56,56,56,56	0
57	MG	1A	3447	1/1	0.85	0.14	37,37,37,37	0
57	MG	1A	3221	1/1	0.85	0.18	49,49,49,49	0
57	MG	1a	1744	1/1	0.85	0.22	70,70,70,70	0
57	MG	1A	3266	1/1	0.85	0.12	59,59,59,59	0
57	MG	2A	3476	1/1	0.85	0.20	49,49,49,49	0
57	MG	2F	303	1/1	0.85	0.16	57,57,57,57	0
57	MG	1A	3307	1/1	0.85	0.20	54,54,54,54	0
57	MG	1a	1755	1/1	0.85	0.25	63,63,63,63	0
57	MG	1a	1640	1/1	0.85	0.17	61,61,61,61	0
57	MG	1A	3318	1/1	0.85	0.28	51,51,51,51	0
57	MG	2A	3496	1/1	0.85	0.30	57,57,57,57	0
57	MG	1A	3585	1/1	0.85	0.15	24,24,24,24	0
57	MG	2a	1633	1/1	0.85	0.18	60,60,60,60	0
57	MG	2A	3508	1/1	0.85	0.20	55,55,55,55	0
57	MG	1A	3149	1/1	0.85	0.23	47,47,47,47	0
57	MG	2a	1648	1/1	0.85	0.19	53,53,53,53	0
57	MG	1A	3673	1/1	0.85	0.17	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	3516	1/1	0.85	0.17	51,51,51,51	0
57	MG	1A	3684	1/1	0.85	0.12	42,42,42,42	0
57	MG	2a	1658	1/1	0.85	0.20	54,54,54,54	0
57	MG	2a	1661	1/1	0.85	0.29	66,66,66,66	0
57	MG	2a	1666	1/1	0.85	0.30	70,70,70,70	0
57	MG	1a	1675	1/1	0.85	0.22	57,57,57,57	0
57	MG	2A	3546	1/1	0.85	0.24	59,59,59,59	0
57	MG	2A	3365	1/1	0.85	0.17	64,64,64,64	0
57	MG	2a	1678	1/1	0.85	0.14	65,65,65,65	0
57	MG	2A	3556	1/1	0.85	0.14	50,50,50,50	0
57	MG	2a	1698	1/1	0.85	0.14	71,71,71,71	0
57	MG	2A	3014	1/1	0.85	0.17	48,48,48,48	0
57	MG	2A	3370	1/1	0.85	0.15	53,53,53,53	0
57	MG	2a	1716	1/1	0.85	0.17	80,80,80,80	0
57	MG	1A	3502	1/1	0.85	0.14	30,30,30,30	0
57	MG	2a	1731	1/1	0.85	0.18	56,56,56,56	0
57	MG	2A	3573	1/1	0.85	0.12	82,82,82,82	0
57	MG	2A	3154	1/1	0.85	0.20	59,59,59,59	0
57	MG	2A	3176	1/1	0.85	0.26	53,53,53,53	0
57	MG	2a	1742	1/1	0.85	0.14	66,66,66,66	0
57	MG	1a	1684	1/1	0.85	0.14	57,57,57,57	0
57	MG	2A	3586	1/1	0.85	0.15	81,81,81,81	0
57	MG	1a	1603	1/1	0.85	0.19	54,54,54,54	0
57	MG	1A	3698	1/1	0.85	0.15	53,53,53,53	0
57	MG	2A	3197	1/1	0.85	0.14	62,62,62,62	0
57	MG	2A	3203	1/1	0.85	0.16	57,57,57,57	0
57	MG	2e	201	1/1	0.85	0.18	66,66,66,66	0
57	MG	2A	3411	1/1	0.85	0.13	26,26,26,26	0
57	MG	2A	3207	1/1	0.85	0.13	58,58,58,58	0
57	MG	2x	104	1/1	0.85	0.19	69,69,69,69	0
57	MG	2A	3429	1/1	0.85	0.14	33,33,33,33	0
57	MG	2A	3350	1/1	0.86	0.17	48,48,48,48	0
57	MG	2A	3167	1/1	0.86	0.23	43,43,43,43	0
57	MG	2A	3174	1/1	0.86	0.20	58,58,58,58	0
57	MG	2a	1604	1/1	0.86	0.17	59,59,59,59	0
57	MG	1A	3575	1/1	0.86	0.11	17,17,17,17	0
57	MG	2A	3533	1/1	0.86	0.07	65,65,65,65	0
57	MG	1A	3113	1/1	0.86	0.16	32,32,32,32	0
57	MG	1A	3351	1/1	0.86	0.14	46,46,46,46	0
57	MG	2A	3389	1/1	0.86	0.15	50,50,50,50	0
57	MG	1a	1742	1/1	0.86	0.26	86,86,86,86	0
57	MG	1A	3650	1/1	0.86	0.11	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	2a	1652	1/1	0.86	0.30	44,44,44,44	0
57	MG	2A	3199	1/1	0.86	0.15	55,55,55,55	0
57	MG	2A	3400	1/1	0.86	0.11	54,54,54,54	0
57	MG	2a	1655	1/1	0.86	0.24	56,56,56,56	0
57	MG	1a	1746	1/1	0.86	0.17	62,62,62,62	0
57	MG	1A	3066	1/1	0.86	0.32	51,51,51,51	0
57	MG	2A	3216	1/1	0.86	0.14	40,40,40,40	0
57	MG	2A	3581	1/1	0.86	0.10	52,52,52,52	0
57	MG	2A	3226	1/1	0.86	0.17	51,51,51,51	0
57	MG	1A	3073	1/1	0.86	0.51	62,62,62,62	0
57	MG	2A	3077	1/1	0.86	0.27	63,63,63,63	0
57	MG	2A	3248	1/1	0.86	0.18	39,39,39,39	0
57	MG	2a	1687	1/1	0.86	0.13	56,56,56,56	0
57	MG	1a	1677	1/1	0.86	0.23	58,58,58,58	0
57	MG	2A	3595	1/1	0.86	0.13	63,63,63,63	0
57	MG	2a	1709	1/1	0.86	0.13	47,47,47,47	0
57	MG	2A	3251	1/1	0.86	0.18	62,62,62,62	0
57	MG	1a	1678	1/1	0.86	0.20	57,57,57,57	0
57	MG	1a	1757	1/1	0.86	0.22	57,57,57,57	0
57	MG	1a	1681	1/1	0.86	0.39	74,74,74,74	0
57	MG	2A	3102	1/1	0.86	0.34	67,67,67,67	0
57	MG	1A	3334	1/1	0.86	0.12	39,39,39,39	0
57	MG	1i	201	1/1	0.86	0.23	70,70,70,70	0
57	MG	1a	1683	1/1	0.86	0.19	60,60,60,60	0
57	MG	1A	3768	1/1	0.86	0.10	15,15,15,15	0
57	MG	1A	3775	1/1	0.86	0.19	62,62,62,62	0
57	MG	2A	3650	1/1	0.86	0.17	61,61,61,61	0
57	MG	1A	3411	1/1	0.86	0.13	39,39,39,39	0
57	MG	2B	204	1/1	0.86	0.14	49,49,49,49	0
57	MG	2A	3314	1/1	0.86	0.18	47,47,47,47	0
57	MG	2A	3140	1/1	0.86	0.10	51,51,51,51	0
57	MG	1A	3681	1/1	0.86	0.27	20,20,20,20	0
57	MG	2v	101	1/1	0.86	0.23	67,67,67,67	0
57	MG	2A	3015	1/1	0.86	0.20	42,42,42,42	0
57	MG	1A	3421	1/1	0.86	0.09	49,49,49,49	0
57	MG	1A	3106	1/1	0.86	0.14	45,45,45,45	0
57	MG	1B	209	1/1	0.87	0.15	59,59,59,59	0
57	MG	1a	1637	1/1	0.87	0.27	62,62,62,62	0
57	MG	2R	201	1/1	0.87	0.14	51,51,51,51	0
57	MG	2A	3069	1/1	0.87	0.24	61,61,61,61	0
57	MG	2A	3522	1/1	0.87	0.26	64,64,64,64	0
57	MG	1A	3714	1/1	0.87	0.26	25,25,25,25	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	3532	1/1	0.87	0.19	54,54,54,54	0
57	MG	2A	3205	1/1	0.87	0.12	39,39,39,39	0
57	MG	2a	1625	1/1	0.87	0.29	61,61,61,61	0
57	MG	2A	3373	1/1	0.87	0.09	33,33,33,33	0
57	MG	1B	220	1/1	0.87	0.14	44,44,44,44	0
57	MG	1a	1647	1/1	0.87	0.14	53,53,53,53	0
57	MG	2A	3392	1/1	0.87	0.18	59,59,59,59	0
57	MG	2A	3397	1/1	0.87	0.17	45,45,45,45	0
57	MG	2A	3221	1/1	0.87	0.32	56,56,56,56	0
57	MG	2A	3568	1/1	0.87	0.10	39,39,39,39	0
57	MG	1E	307	1/1	0.87	0.18	42,42,42,42	0
57	MG	1a	1658	1/1	0.87	0.19	54,54,54,54	0
57	MG	2A	3230	1/1	0.87	0.12	50,50,50,50	0
57	MG	1P	204	1/1	0.87	0.11	43,43,43,43	0
57	MG	1A	3402	1/1	0.87	0.11	24,24,24,24	0
57	MG	2a	1667	1/1	0.87	0.15	55,55,55,55	0
57	MG	1a	1667	1/1	0.87	0.27	59,59,59,59	0
57	MG	1V	204	1/1	0.87	0.14	30,30,30,30	0
57	MG	1A	3580	1/1	0.87	0.14	16,16,16,16	0
57	MG	1A	3646	1/1	0.87	0.10	36,36,36,36	0
57	MG	2A	3593	1/1	0.87	0.17	57,57,57,57	0
57	MG	18	101	1/1	0.87	0.21	44,44,44,44	0
57	MG	1A	3359	1/1	0.87	0.12	12,12,12,12	0
57	MG	2A	3124	1/1	0.87	0.27	49,49,49,49	0
57	MG	1A	3685	1/1	0.87	0.10	59,59,59,59	0
57	MG	1a	1613	1/1	0.87	0.15	41,41,41,41	0
57	MG	2A	3607	1/1	0.87	0.18	31,31,31,31	0
57	MG	2a	1719	1/1	0.87	0.14	61,61,61,61	0
57	MG	1A	3694	1/1	0.87	0.16	45,45,45,45	0
57	MG	1a	1687	1/1	0.87	0.12	38,38,38,38	0
57	MG	2A	3299	1/1	0.87	0.12	45,45,45,45	0
57	MG	1A	3631	1/1	0.87	0.13	33,33,33,33	0
57	MG	1A	3096	1/1	0.87	0.14	33,33,33,33	0
57	MG	2a	1741	1/1	0.87	0.18	62,62,62,62	0
57	MG	1a	1708	1/1	0.87	0.15	64,64,64,64	0
57	MG	2A	3645	1/1	0.87	0.14	65,65,65,65	0
57	MG	2A	3479	1/1	0.87	0.20	42,42,42,42	0
57	MG	2A	3481	1/1	0.87	0.13	40,40,40,40	0
57	MG	1A	3705	1/1	0.87	0.17	27,27,27,27	0
57	MG	2A	3657	1/1	0.87	0.27	68,68,68,68	0
57	MG	2B	202	1/1	0.87	0.17	64,64,64,64	0
57	MG	1A	3006	1/1	0.87	0.14	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2f	201	1/1	0.87	0.18	53,53,53,53	0
57	MG	1B	208	1/1	0.87	0.18	52,52,52,52	0
57	MG	1a	1723	1/1	0.87	0.11	53,53,53,53	0
57	MG	2A	3191	1/1	0.87	0.26	55,55,55,55	0
57	MG	2A	3351	1/1	0.87	0.12	45,45,45,45	0
57	MG	2A	3359	1/1	0.87	0.09	63,63,63,63	0
57	MG	2A	3394	1/1	0.88	0.13	39,39,39,39	0
57	MG	1A	3011	1/1	0.88	0.11	47,47,47,47	0
57	MG	2A	3123	1/1	0.88	0.12	52,52,52,52	0
57	MG	1a	1730	1/1	0.88	0.15	46,46,46,46	0
57	MG	1a	1670	1/1	0.88	0.22	53,53,53,53	0
57	MG	2a	1614	1/1	0.88	0.15	49,49,49,49	0
57	MG	1G	203	1/1	0.88	0.09	39,39,39,39	0
57	MG	2a	1626	1/1	0.88	0.17	47,47,47,47	0
57	MG	2A	3562	1/1	0.88	0.16	68,68,68,68	0
57	MG	2a	1644	1/1	0.88	0.24	58,58,58,58	0
57	MG	1A	3770	1/1	0.88	0.11	45,45,45,45	0
57	MG	1A	3060	1/1	0.88	0.12	41,41,41,41	0
57	MG	1a	1626	1/1	0.88	0.14	45,45,45,45	0
57	MG	2A	3277	1/1	0.88	0.11	67,67,67,67	0
57	MG	2A	3413	1/1	0.88	0.23	45,45,45,45	0
57	MG	2A	3417	1/1	0.88	0.19	74,74,74,74	0
57	MG	2A	3150	1/1	0.88	0.22	52,52,52,52	0
57	MG	1a	1628	1/1	0.88	0.26	55,55,55,55	0
57	MG	1a	1750	1/1	0.88	0.24	66,66,66,66	0
57	MG	2A	3171	1/1	0.88	0.12	37,37,37,37	0
57	MG	2A	3064	1/1	0.88	0.13	47,47,47,47	0
57	MG	1A	3322	1/1	0.88	0.28	13,13,13,13	0
57	MG	1Z	301	1/1	0.88	0.11	48,48,48,48	0
57	MG	1A	3482	1/1	0.88	0.17	51,51,51,51	0
57	MG	1a	1638	1/1	0.88	0.08	56,56,56,56	0
57	MG	2A	3462	1/1	0.88	0.20	38,38,38,38	0
57	MG	2A	3193	1/1	0.88	0.15	40,40,40,40	0
57	MG	2a	1686	1/1	0.88	0.18	43,43,43,43	0
57	MG	1A	3134	1/1	0.88	0.09	36,36,36,36	0
57	MG	2A	3080	1/1	0.88	0.29	61,61,61,61	0
57	MG	2A	3617	1/1	0.88	0.10	53,53,53,53	0
57	MG	1A	3373	1/1	0.88	0.16	42,42,42,42	0
57	MG	2A	3478	1/1	0.88	0.17	65,65,65,65	0
57	MG	1a	1601	1/1	0.88	0.12	53,53,53,53	0
57	MG	2A	3357	1/1	0.88	0.09	53,53,53,53	0
57	MG	2A	3641	1/1	0.88	0.24	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	2A	3482	1/1	0.88	0.12	45,45,45,45	0
57	MG	2A	3485	1/1	0.88	0.19	64,64,64,64	0
57	MG	1A	3226	1/1	0.88	0.09	37,37,37,37	0
57	MG	1x	103	1/1	0.88	0.17	51,51,51,51	0
57	MG	2A	3361	1/1	0.88	0.16	47,47,47,47	0
57	MG	1A	3090	1/1	0.88	0.34	38,38,38,38	0
57	MG	2a	1749	1/1	0.88	0.21	57,57,57,57	0
57	MG	2A	3105	1/1	0.88	0.11	43,43,43,43	0
57	MG	2A	3223	1/1	0.88	0.11	68,68,68,68	0
57	MG	1A	3276	1/1	0.88	0.26	44,44,44,44	0
57	MG	2B	207	1/1	0.88	0.23	60,60,60,60	0
57	MG	2a	1758	1/1	0.88	0.13	65,65,65,65	0
57	MG	2D	301	1/1	0.88	0.18	34,34,34,34	0
57	MG	1E	303	1/1	0.88	0.20	49,49,49,49	0
57	MG	2A	3376	1/1	0.88	0.18	52,52,52,52	0
57	MG	2A	3383	1/1	0.88	0.19	55,55,55,55	0
57	MG	2A	3001	1/1	0.88	0.23	50,50,50,50	0
57	MG	2A	3525	1/1	0.88	0.20	61,61,61,61	0
57	MG	2A	3010	1/1	0.88	0.10	55,55,55,55	0
57	MG	2A	3242	1/1	0.88	0.12	44,44,44,44	0
57	MG	2V	201	1/1	0.88	0.24	46,46,46,46	0
57	MG	2x	109	1/1	0.88	0.18	60,60,60,60	0
57	MG	1A	3622	1/1	0.89	0.17	60,60,60,60	0
57	MG	1y	102	1/1	0.89	0.24	63,63,63,63	0
57	MG	1A	3246	1/1	0.89	0.22	66,66,66,66	0
57	MG	1A	3629	1/1	0.89	0.15	29,29,29,29	0
57	MG	1A	3264	1/1	0.89	0.12	34,34,34,34	0
57	MG	1A	3027	1/1	0.89	0.09	40,40,40,40	0
57	MG	25	102	1/1	0.89	0.12	54,54,54,54	0
57	MG	1A	3270	1/1	0.89	0.34	56,56,56,56	0
57	MG	1A	3152	1/1	0.89	0.09	66,66,66,66	0
57	MG	2a	1606	1/1	0.89	0.22	50,50,50,50	0
57	MG	2a	1608	1/1	0.89	0.32	49,49,49,49	0
57	MG	1A	3277	1/1	0.89	0.40	36,36,36,36	0
57	MG	2A	3536	1/1	0.89	0.14	49,49,49,49	0
57	MG	2a	1615	1/1	0.89	0.25	58,58,58,58	0
57	MG	2a	1624	1/1	0.89	0.14	54,54,54,54	0
57	MG	1a	1696	1/1	0.89	0.11	45,45,45,45	0
57	MG	2A	3544	1/1	0.89	0.16	56,56,56,56	0
57	MG	2a	1628	1/1	0.89	0.09	45,45,45,45	0
57	MG	1A	3443	1/1	0.89	0.10	22,22,22,22	0
57	MG	2a	1641	1/1	0.89	0.11	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	2A	3553	1/1	0.89	0.10	26,26,26,26	0
57	MG	1A	3761	1/1	0.89	0.08	39,39,39,39	0
57	MG	2A	3048	1/1	0.89	0.19	64,64,64,64	0
57	MG	2A	3053	1/1	0.89	0.16	51,51,51,51	0
57	MG	2A	3054	1/1	0.89	0.20	33,33,33,33	0
57	MG	1A	3559	1/1	0.89	0.10	26,26,26,26	0
57	MG	1a	1713	1/1	0.89	0.14	46,46,46,46	0
57	MG	1A	3567	1/1	0.89	0.11	45,45,45,45	0
57	MG	1A	3652	1/1	0.89	0.15	43,43,43,43	0
57	MG	2A	3574	1/1	0.89	0.11	50,50,50,50	0
57	MG	1A	3658	1/1	0.89	0.13	39,39,39,39	0
57	MG	1a	1624	1/1	0.89	0.18	49,49,49,49	0
57	MG	1A	3445	1/1	0.89	0.14	33,33,33,33	0
57	MG	1a	1627	1/1	0.89	0.13	51,51,51,51	0
57	MG	2a	1670	1/1	0.89	0.28	58,58,58,58	0
57	MG	1A	3122	1/1	0.89	0.27	37,37,37,37	0
57	MG	2A	3081	1/1	0.89	0.21	49,49,49,49	0
57	MG	2A	3412	1/1	0.89	0.22	66,66,66,66	0
57	MG	1a	1629	1/1	0.89	0.11	37,37,37,37	0
57	MG	1A	3029	1/1	0.89	0.14	65,65,65,65	0
57	MG	1A	3378	1/1	0.89	0.14	45,45,45,45	0
57	MG	2A	3597	1/1	0.89	0.15	35,35,35,35	0
57	MG	2A	3098	1/1	0.89	0.16	46,46,46,46	0
57	MG	2A	3099	1/1	0.89	0.08	46,46,46,46	0
57	MG	2a	1710	1/1	0.89	0.17	56,56,56,56	0
57	MG	1A	3674	1/1	0.89	0.09	49,49,49,49	0
57	MG	1A	3380	1/1	0.89	0.19	46,46,46,46	0
57	MG	1E	302	1/1	0.89	0.10	16,16,16,16	0
57	MG	2a	1721	1/1	0.89	0.16	47,47,47,47	0
57	MG	1A	3683	1/1	0.89	0.11	55,55,55,55	0
57	MG	2A	3278	1/1	0.89	0.15	58,58,58,58	0
57	MG	2A	3622	1/1	0.89	0.27	58,58,58,58	0
57	MG	1A	3466	1/1	0.89	0.24	56,56,56,56	0
57	MG	2A	3289	1/1	0.89	0.13	41,41,41,41	0
57	MG	1F	301	1/1	0.89	0.15	39,39,39,39	0
57	MG	2A	3468	1/1	0.89	0.16	58,58,58,58	0
57	MG	2a	1747	1/1	0.89	0.24	53,53,53,53	0
57	MG	2A	3292	1/1	0.89	0.09	30,30,30,30	0
57	MG	1F	305	1/1	0.89	0.33	31,31,31,31	0
57	MG	2A	3117	1/1	0.89	0.29	59,59,59,59	0
57	MG	1a	1761	1/1	0.89	0.10	45,45,45,45	0
57	MG	2A	3654	1/1	0.89	0.15	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	3064	1/1	0.89	0.19	45,45,45,45	0
57	MG	2A	3310	1/1	0.89	0.19	29,29,29,29	0
57	MG	1a	1664	1/1	0.89	0.25	53,53,53,53	0
57	MG	2A	3125	1/1	0.89	0.27	45,45,45,45	0
57	MG	2A	3333	1/1	0.89	0.21	61,61,61,61	0
57	MG	2A	3132	1/1	0.89	0.06	51,51,51,51	0
57	MG	2A	3490	1/1	0.89	0.16	55,55,55,55	0
57	MG	1N	203	1/1	0.89	0.12	41,41,41,41	0
57	MG	2x	103	1/1	0.89	0.18	47,47,47,47	0
57	MG	1A	3136	1/1	0.89	0.36	46,46,46,46	0
57	MG	1A	3621	1/1	0.89	0.16	60,60,60,60	0
57	MG	1V	202	1/1	0.89	0.39	30,30,30,30	0
57	MG	2A	3257	1/1	0.90	0.13	53,53,53,53	0
57	MG	2B	203	1/1	0.90	0.17	57,57,57,57	0
57	MG	1A	3699	1/1	0.90	0.23	51,51,51,51	0
57	MG	1A	3602	1/1	0.90	0.10	48,48,48,48	0
57	MG	1a	1719	1/1	0.90	0.15	48,48,48,48	0
57	MG	2B	210	1/1	0.90	0.08	60,60,60,60	0
57	MG	1A	3611	1/1	0.90	0.16	43,43,43,43	0
57	MG	1A	3618	1/1	0.90	0.15	38,38,38,38	0
57	MG	1A	3620	1/1	0.90	0.12	53,53,53,53	0
57	MG	2A	3093	1/1	0.90	0.19	48,48,48,48	0
57	MG	2A	3483	1/1	0.90	0.10	46,46,46,46	0
57	MG	2A	3484	1/1	0.90	0.40	39,39,39,39	0
57	MG	2A	3094	1/1	0.90	0.17	51,51,51,51	0
57	MG	1A	3720	1/1	0.90	0.14	51,51,51,51	0
57	MG	2A	3487	1/1	0.90	0.14	46,46,46,46	0
57	MG	1a	1732	1/1	0.90	0.10	50,50,50,50	0
57	MG	1A	3019	1/1	0.90	0.12	44,44,44,44	0
57	MG	1a	1617	1/1	0.90	0.28	48,48,48,48	0
57	MG	1a	1741	1/1	0.90	0.17	63,63,63,63	0
57	MG	2A	3106	1/1	0.90	0.18	58,58,58,58	0
57	MG	2A	3308	1/1	0.90	0.07	39,39,39,39	0
57	MG	2a	1607	1/1	0.90	0.19	47,47,47,47	0
57	MG	2A	3505	1/1	0.90	0.16	39,39,39,39	0
57	MG	1A	3107	1/1	0.90	0.09	31,31,31,31	0
57	MG	2a	1612	1/1	0.90	0.23	60,60,60,60	0
57	MG	1A	3267	1/1	0.90	0.23	24,24,24,24	0
57	MG	1A	3747	1/1	0.90	0.19	16,16,16,16	0
57	MG	2A	3331	1/1	0.90	0.14	35,35,35,35	0
57	MG	1A	3627	1/1	0.90	0.09	14,14,14,14	0
57	MG	2A	3524	1/1	0.90	0.11	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3757	1/1	0.90	0.13	39,39,39,39	0
57	MG	1A	3170	1/1	0.90	0.09	53,53,53,53	0
57	MG	2a	1635	1/1	0.90	0.12	65,65,65,65	0
57	MG	2a	1640	1/1	0.90	0.20	39,39,39,39	0
57	MG	1A	3467	1/1	0.90	0.12	28,28,28,28	0
57	MG	2a	1642	1/1	0.90	0.20	44,44,44,44	0
57	MG	1A	3471	1/1	0.90	0.15	32,32,32,32	0
57	MG	1A	3177	1/1	0.90	0.20	44,44,44,44	0
57	MG	1A	3384	1/1	0.90	0.14	40,40,40,40	0
57	MG	2A	3354	1/1	0.90	0.14	35,35,35,35	0
57	MG	1a	1762	1/1	0.90	0.14	50,50,50,50	0
57	MG	1A	3389	1/1	0.90	0.11	18,18,18,18	0
57	MG	2A	3554	1/1	0.90	0.20	50,50,50,50	0
57	MG	2A	3142	1/1	0.90	0.17	42,42,42,42	0
57	MG	1a	1766	1/1	0.90	0.13	54,54,54,54	0
57	MG	1A	3785	1/1	0.90	0.11	61,61,61,61	0
57	MG	1A	3786	1/1	0.90	0.08	19,19,19,19	0
57	MG	2a	1662	1/1	0.90	0.10	54,54,54,54	0
57	MG	2A	3563	1/1	0.90	0.23	57,57,57,57	0
57	MG	1v	101	1/1	0.90	0.14	48,48,48,48	0
57	MG	1A	3790	1/1	0.90	0.22	45,45,45,45	0
57	MG	2A	3156	1/1	0.90	0.18	51,51,51,51	0
57	MG	2a	1674	1/1	0.90	0.16	60,60,60,60	0
57	MG	2a	1675	1/1	0.90	0.13	59,59,59,59	0
57	MG	2A	3572	1/1	0.90	0.16	56,56,56,56	0
57	MG	1a	1645	1/1	0.90	0.13	66,66,66,66	0
57	MG	2A	3382	1/1	0.90	0.17	47,47,47,47	0
57	MG	2a	1679	1/1	0.90	0.13	59,59,59,59	0
57	MG	2A	3575	1/1	0.90	0.25	53,53,53,53	0
57	MG	1A	3792	1/1	0.90	0.11	41,41,41,41	0
57	MG	1A	3393	1/1	0.90	0.10	20,20,20,20	0
57	MG	2a	1695	1/1	0.90	0.10	61,61,61,61	0
57	MG	2A	3580	1/1	0.90	0.13	61,61,61,61	0
57	MG	2a	1702	1/1	0.90	0.24	57,57,57,57	0
57	MG	1B	201	1/1	0.90	0.12	58,58,58,58	0
57	MG	2a	1707	1/1	0.90	0.16	49,49,49,49	0
57	MG	1B	202	1/1	0.90	0.22	43,43,43,43	0
57	MG	2A	3393	1/1	0.90	0.12	19,19,19,19	0
57	MG	1A	3179	1/1	0.90	0.11	38,38,38,38	0
57	MG	2A	3590	1/1	0.90	0.18	45,45,45,45	0
57	MG	2A	3396	1/1	0.90	0.13	56,56,56,56	0
57	MG	1A	3287	1/1	0.90	0.08	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	1A	3190	1/1	0.90	0.12	29,29,29,29	0
57	MG	2a	1725	1/1	0.90	0.28	57,57,57,57	0
57	MG	2a	1726	1/1	0.90	0.22	58,58,58,58	0
57	MG	2a	1730	1/1	0.90	0.12	44,44,44,44	0
57	MG	1A	3520	1/1	0.90	0.14	23,23,23,23	0
57	MG	1D	302	1/1	0.90	0.37	36,36,36,36	0
57	MG	1A	3204	1/1	0.90	0.22	42,42,42,42	0
57	MG	2A	3200	1/1	0.90	0.15	55,55,55,55	0
57	MG	1A	3049	1/1	0.90	0.12	43,43,43,43	0
57	MG	1E	305	1/1	0.90	0.11	46,46,46,46	0
57	MG	2a	1745	1/1	0.90	0.13	59,59,59,59	0
57	MG	2A	3043	1/1	0.90	0.16	59,59,59,59	0
57	MG	1A	3213	1/1	0.90	0.14	41,41,41,41	0
57	MG	1A	3097	1/1	0.90	0.10	32,32,32,32	0
57	MG	1A	3144	1/1	0.90	0.19	28,28,28,28	0
57	MG	2A	3626	1/1	0.90	0.08	47,47,47,47	0
57	MG	2A	3627	1/1	0.90	0.12	54,54,54,54	0
57	MG	1A	3439	1/1	0.90	0.08	49,49,49,49	0
57	MG	2A	3227	1/1	0.90	0.19	46,46,46,46	0
57	MG	1A	3238	1/1	0.90	0.10	38,38,38,38	0
57	MG	2A	3640	1/1	0.90	0.17	37,37,37,37	0
57	MG	1A	3444	1/1	0.90	0.10	24,24,24,24	0
57	MG	1A	3121	1/1	0.90	0.09	34,34,34,34	0
57	MG	1A	3692	1/1	0.90	0.09	31,31,31,31	0
57	MG	1A	3446	1/1	0.90	0.09	23,23,23,23	0
57	MG	1A	3253	1/1	0.90	0.15	48,48,48,48	0
57	MG	2A	3072	1/1	0.90	0.16	53,53,53,53	0
57	MG	2x	106	1/1	0.90	0.24	68,68,68,68	0
57	MG	2A	3252	1/1	0.90	0.14	49,49,49,49	0
57	MG	1A	3454	1/1	0.90	0.10	19,19,19,19	0
57	MG	2A	3637	1/1	0.91	0.14	34,34,34,34	0
57	MG	2A	3188	1/1	0.91	0.10	51,51,51,51	0
57	MG	2A	3005	1/1	0.91	0.15	52,52,52,52	0
57	MG	1A	3268	1/1	0.91	0.14	30,30,30,30	0
57	MG	2A	3192	1/1	0.91	0.16	47,47,47,47	0
57	MG	1A	3100	1/1	0.91	0.25	35,35,35,35	0
57	MG	2A	3416	1/1	0.91	0.07	34,34,34,34	0
57	MG	2A	3653	1/1	0.91	0.12	49,49,49,49	0
57	MG	1a	1676	1/1	0.91	0.10	41,41,41,41	0
57	MG	2A	3020	1/1	0.91	0.10	51,51,51,51	0
57	MG	2A	3428	1/1	0.91	0.22	50,50,50,50	0
57	MG	1P	203	1/1	0.91	0.15	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	3232	1/1	0.91	0.12	31,31,31,31	0
57	MG	2A	3201	1/1	0.91	0.14	45,45,45,45	0
57	MG	2B	205	1/1	0.91	0.14	53,53,53,53	0
57	MG	2A	3027	1/1	0.91	0.41	47,47,47,47	0
57	MG	2A	3448	1/1	0.91	0.22	55,55,55,55	0
57	MG	1a	1680	1/1	0.91	0.17	39,39,39,39	0
57	MG	2A	3036	1/1	0.91	0.10	49,49,49,49	0
57	MG	1A	3358	1/1	0.91	0.09	33,33,33,33	0
57	MG	2A	3220	1/1	0.91	0.17	50,50,50,50	0
57	MG	2E	302	1/1	0.91	0.28	40,40,40,40	0
57	MG	1U	207	1/1	0.91	0.11	31,31,31,31	0
57	MG	2A	3044	1/1	0.91	0.12	55,55,55,55	0
57	MG	2A	3464	1/1	0.91	0.10	52,52,52,52	0
57	MG	1A	3512	1/1	0.91	0.08	36,36,36,36	0
57	MG	2A	3469	1/1	0.91	0.14	63,63,63,63	0
57	MG	1A	3159	1/1	0.91	0.12	28,28,28,28	0
57	MG	1a	1686	1/1	0.91	0.23	44,44,44,44	0
57	MG	2A	3229	1/1	0.91	0.08	38,38,38,38	0
57	MG	25	101	1/1	0.91	0.30	42,42,42,42	0
57	MG	1A	3730	1/1	0.91	0.11	36,36,36,36	0
57	MG	1Z	302	1/1	0.91	0.17	44,44,44,44	0
57	MG	2A	3238	1/1	0.91	0.22	49,49,49,49	0
57	MG	2A	3241	1/1	0.91	0.16	60,60,60,60	0
57	MG	1A	3168	1/1	0.91	0.16	42,42,42,42	0
57	MG	2A	3063	1/1	0.91	0.09	55,55,55,55	0
57	MG	1A	3742	1/1	0.91	0.09	54,54,54,54	0
57	MG	2a	1610	1/1	0.91	0.11	51,51,51,51	0
57	MG	2a	1611	1/1	0.91	0.12	58,58,58,58	0
57	MG	2A	3067	1/1	0.91	0.07	44,44,44,44	0
57	MG	15	103	1/1	0.91	0.21	28,28,28,28	0
57	MG	1A	3745	1/1	0.91	0.12	34,34,34,34	0
57	MG	2a	1620	1/1	0.91	0.13	59,59,59,59	0
57	MG	2A	3489	1/1	0.91	0.10	56,56,56,56	0
57	MG	1A	3368	1/1	0.91	0.10	34,34,34,34	0
57	MG	1A	3036	1/1	0.91	0.39	39,39,39,39	0
57	MG	2A	3263	1/1	0.91	0.09	34,34,34,34	0
57	MG	2A	3073	1/1	0.91	0.17	48,48,48,48	0
57	MG	1A	3312	1/1	0.91	0.10	36,36,36,36	0
57	MG	2A	3272	1/1	0.91	0.12	46,46,46,46	0
57	MG	1A	3647	1/1	0.91	0.08	50,50,50,50	0
57	MG	1A	3568	1/1	0.91	0.07	33,33,33,33	0
57	MG	1A	3573	1/1	0.91	0.14	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	3452	1/1	0.91	0.11	42,42,42,42	0
57	MG	1a	1731	1/1	0.91	0.14	64,64,64,64	0
57	MG	1A	3771	1/1	0.91	0.09	33,33,33,33	0
57	MG	1A	3657	1/1	0.91	0.09	26,26,26,26	0
57	MG	1A	3314	1/1	0.91	0.10	14,14,14,14	0
57	MG	2A	3527	1/1	0.91	0.12	60,60,60,60	0
57	MG	1A	3577	1/1	0.91	0.11	11,11,11,11	0
57	MG	1a	1625	1/1	0.91	0.17	48,48,48,48	0
57	MG	2a	1656	1/1	0.91	0.11	50,50,50,50	0
57	MG	2A	3534	1/1	0.91	0.16	60,60,60,60	0
57	MG	2A	3301	1/1	0.91	0.10	30,30,30,30	0
57	MG	2A	3539	1/1	0.91	0.15	37,37,37,37	0
57	MG	1A	3666	1/1	0.91	0.13	38,38,38,38	0
57	MG	2A	3542	1/1	0.91	0.17	58,58,58,58	0
57	MG	1A	3256	1/1	0.91	0.27	35,35,35,35	0
57	MG	1A	3457	1/1	0.91	0.13	38,38,38,38	0
57	MG	2a	1671	1/1	0.91	0.29	57,57,57,57	0
57	MG	2a	1673	1/1	0.91	0.16	80,80,80,80	0
57	MG	1a	1749	1/1	0.91	0.08	55,55,55,55	0
57	MG	1A	3261	1/1	0.91	0.20	32,32,32,32	0
57	MG	1A	3172	1/1	0.91	0.11	32,32,32,32	0
57	MG	1a	1752	1/1	0.91	0.17	67,67,67,67	0
57	MG	1a	1753	1/1	0.91	0.17	64,64,64,64	0
57	MG	2A	3560	1/1	0.91	0.11	44,44,44,44	0
57	MG	1A	3677	1/1	0.91	0.13	38,38,38,38	0
57	MG	1A	3332	1/1	0.91	0.09	45,45,45,45	0
57	MG	2A	3565	1/1	0.91	0.09	59,59,59,59	0
57	MG	2a	1690	1/1	0.91	0.09	41,41,41,41	0
57	MG	2A	3347	1/1	0.91	0.10	22,22,22,22	0
57	MG	1A	3117	1/1	0.91	0.25	53,53,53,53	0
57	MG	2a	1700	1/1	0.91	0.17	36,36,36,36	0
57	MG	1a	1759	1/1	0.91	0.12	49,49,49,49	0
57	MG	1A	3406	1/1	0.91	0.09	19,19,19,19	0
57	MG	2A	3126	1/1	0.91	0.12	49,49,49,49	0
57	MG	2a	1708	1/1	0.91	0.16	65,65,65,65	0
57	MG	2A	3356	1/1	0.91	0.17	67,67,67,67	0
57	MG	2A	3130	1/1	0.91	0.09	34,34,34,34	0
57	MG	1a	1644	1/1	0.91	0.27	55,55,55,55	0
57	MG	2A	3133	1/1	0.91	0.16	57,57,57,57	0
57	MG	2a	1718	1/1	0.91	0.21	52,52,52,52	0
57	MG	1A	3474	1/1	0.91	0.09	53,53,53,53	0
57	MG	2A	3139	1/1	0.91	0.17	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	3582	1/1	0.91	0.10	50,50,50,50	0
57	MG	1A	3689	1/1	0.91	0.10	39,39,39,39	0
57	MG	2A	3584	1/1	0.91	0.09	61,61,61,61	0
57	MG	2a	1729	1/1	0.91	0.13	57,57,57,57	0
57	MG	1A	3613	1/1	0.91	0.17	26,26,26,26	0
57	MG	1a	1648	1/1	0.91	0.16	53,53,53,53	0
57	MG	1A	3615	1/1	0.91	0.10	31,31,31,31	0
57	MG	2a	1734	1/1	0.91	0.26	56,56,56,56	0
57	MG	2A	3147	1/1	0.91	0.09	40,40,40,40	0
57	MG	2A	3377	1/1	0.91	0.09	36,36,36,36	0
57	MG	2A	3379	1/1	0.91	0.16	62,62,62,62	0
57	MG	2A	3381	1/1	0.91	0.14	54,54,54,54	0
57	MG	1A	3338	1/1	0.91	0.07	21,21,21,21	0
57	MG	1w	401	1/1	0.91	0.30	44,44,44,44	0
57	MG	2A	3599	1/1	0.91	0.16	44,44,44,44	0
57	MG	1w	403	1/1	0.91	0.10	43,43,43,43	0
57	MG	2A	3604	1/1	0.91	0.53	57,57,57,57	0
57	MG	1A	3225	1/1	0.91	0.14	33,33,33,33	0
57	MG	2a	1756	1/1	0.91	0.10	59,59,59,59	0
57	MG	2A	3158	1/1	0.91	0.20	47,47,47,47	0
57	MG	2A	3163	1/1	0.91	0.12	59,59,59,59	0
57	MG	2A	3613	1/1	0.91	0.12	62,62,62,62	0
57	MG	2A	3614	1/1	0.91	0.19	54,54,54,54	0
57	MG	1A	3343	1/1	0.91	0.13	29,29,29,29	0
57	MG	2A	3170	1/1	0.91	0.13	45,45,45,45	0
57	MG	2A	3620	1/1	0.91	0.12	48,48,48,48	0
57	MG	2t	201	1/1	0.91	0.12	50,50,50,50	0
57	MG	1A	3700	1/1	0.91	0.10	40,40,40,40	0
57	MG	2A	3172	1/1	0.91	0.17	50,50,50,50	0
57	MG	1A	3703	1/1	0.91	0.10	46,46,46,46	0
57	MG	1F	311	1/1	0.91	0.41	38,38,38,38	0
57	MG	2A	3180	1/1	0.91	0.33	59,59,59,59	0
57	MG	1a	1671	1/1	0.91	0.23	65,65,65,65	0
57	MG	2A	3636	1/1	0.91	0.17	46,46,46,46	0
57	MG	1A	3563	1/1	0.92	0.11	44,44,44,44	0
57	MG	2A	3013	1/1	0.92	0.11	40,40,40,40	0
57	MG	1a	1650	1/1	0.92	0.24	36,36,36,36	0
57	MG	1A	3150	1/1	0.92	0.11	41,41,41,41	0
57	MG	2A	3414	1/1	0.92	0.22	42,42,42,42	0
57	MG	2A	3194	1/1	0.92	0.14	44,44,44,44	0
57	MG	1a	1654	1/1	0.92	0.23	53,53,53,53	0
57	MG	2A	3649	1/1	0.92	0.23	38,38,38,38	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	1655	1/1	0.92	0.13	38,38,38,38	0
57	MG	2A	3652	1/1	0.92	0.11	45,45,45,45	0
57	MG	1A	3050	1/1	0.92	0.22	40,40,40,40	0
57	MG	1a	1659	1/1	0.92	0.22	51,51,51,51	0
57	MG	2A	3433	1/1	0.92	0.08	29,29,29,29	0
57	MG	2A	3029	1/1	0.92	0.29	34,34,34,34	0
57	MG	2B	201	1/1	0.92	0.12	68,68,68,68	0
57	MG	2A	3438	1/1	0.92	0.07	33,33,33,33	0
57	MG	2A	3202	1/1	0.92	0.21	44,44,44,44	0
57	MG	1A	3212	1/1	0.92	0.14	26,26,26,26	0
57	MG	1B	205	1/1	0.92	0.07	55,55,55,55	0
57	MG	2A	3449	1/1	0.92	0.07	50,50,50,50	0
57	MG	2A	3206	1/1	0.92	0.17	43,43,43,43	0
57	MG	2B	208	1/1	0.92	0.48	59,59,59,59	0
57	MG	2A	3038	1/1	0.92	0.13	51,51,51,51	0
57	MG	2A	3208	1/1	0.92	0.19	45,45,45,45	0
57	MG	2D	303	1/1	0.92	0.15	38,38,38,38	0
57	MG	2A	3458	1/1	0.92	0.09	62,62,62,62	0
57	MG	2A	3209	1/1	0.92	0.32	67,67,67,67	0
57	MG	1A	3352	1/1	0.92	0.08	36,36,36,36	0
57	MG	2A	3219	1/1	0.92	0.21	38,38,38,38	0
57	MG	1A	3273	1/1	0.92	0.26	53,53,53,53	0
57	MG	2A	3466	1/1	0.92	0.18	40,40,40,40	0
57	MG	2O	201	1/1	0.92	0.16	51,51,51,51	0
57	MG	1A	3356	1/1	0.92	0.14	35,35,35,35	0
57	MG	1A	3058	1/1	0.92	0.10	25,25,25,25	0
57	MG	2U	201	1/1	0.92	0.14	50,50,50,50	0
57	MG	2A	3470	1/1	0.92	0.15	42,42,42,42	0
57	MG	2W	201	1/1	0.92	0.16	39,39,39,39	0
57	MG	1A	3581	1/1	0.92	0.09	19,19,19,19	0
57	MG	1A	3059	1/1	0.92	0.07	30,30,30,30	0
57	MG	2A	3475	1/1	0.92	0.17	68,68,68,68	0
57	MG	1A	3686	1/1	0.92	0.12	24,24,24,24	0
57	MG	1A	3165	1/1	0.92	0.12	56,56,56,56	0
57	MG	2A	3057	1/1	0.92	0.24	62,62,62,62	0
57	MG	1A	3366	1/1	0.92	0.10	26,26,26,26	0
57	MG	1A	3693	1/1	0.92	0.12	43,43,43,43	0
57	MG	1A	3367	1/1	0.92	0.09	16,16,16,16	0
57	MG	2A	3066	1/1	0.92	0.13	46,46,46,46	0
57	MG	2A	3243	1/1	0.92	0.08	23,23,23,23	0
57	MG	1F	307	1/1	0.92	0.10	34,34,34,34	0
57	MG	1A	3458	1/1	0.92	0.12	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3697	1/1	0.92	0.14	51,51,51,51	0
57	MG	1N	202	1/1	0.92	0.13	33,33,33,33	0
57	MG	1A	3304	1/1	0.92	0.09	24,24,24,24	0
57	MG	1A	3610	1/1	0.92	0.09	39,39,39,39	0
57	MG	1A	3010	1/1	0.92	0.09	25,25,25,25	0
57	MG	2A	3493	1/1	0.92	0.12	60,60,60,60	0
57	MG	2a	1627	1/1	0.92	0.27	51,51,51,51	0
57	MG	1A	3308	1/1	0.92	0.11	17,17,17,17	0
57	MG	1U	204	1/1	0.92	0.23	27,27,27,27	0
57	MG	2A	3501	1/1	0.92	0.11	54,54,54,54	0
57	MG	2a	1636	1/1	0.92	0.19	45,45,45,45	0
57	MG	2a	1637	1/1	0.92	0.19	39,39,39,39	0
57	MG	2a	1638	1/1	0.92	0.21	52,52,52,52	0
57	MG	2A	3504	1/1	0.92	0.19	51,51,51,51	0
57	MG	1a	1711	1/1	0.92	0.14	29,29,29,29	0
57	MG	2A	3082	1/1	0.92	0.10	41,41,41,41	0
57	MG	2a	1643	1/1	0.92	0.25	47,47,47,47	0
57	MG	1A	3309	1/1	0.92	0.09	40,40,40,40	0
57	MG	1A	3381	1/1	0.92	0.21	57,57,57,57	0
57	MG	1A	3708	1/1	0.92	0.35	29,29,29,29	0
57	MG	1W	202	1/1	0.92	0.07	25,25,25,25	0
57	MG	2A	3287	1/1	0.92	0.17	57,57,57,57	0
57	MG	1A	3230	1/1	0.92	0.37	28,28,28,28	0
57	MG	1A	3716	1/1	0.92	0.26	23,23,23,23	0
57	MG	1A	3313	1/1	0.92	0.10	45,45,45,45	0
57	MG	2A	3530	1/1	0.92	0.09	51,51,51,51	0
57	MG	1A	3478	1/1	0.92	0.18	46,46,46,46	0
57	MG	2A	3101	1/1	0.92	0.21	46,46,46,46	0
57	MG	2A	3298	1/1	0.92	0.11	58,58,58,58	0
57	MG	12	101	1/1	0.92	0.10	43,43,43,43	0
57	MG	2a	1664	1/1	0.92	0.23	54,54,54,54	0
57	MG	1A	3124	1/1	0.92	0.18	29,29,29,29	0
57	MG	15	107	1/1	0.92	0.07	42,42,42,42	0
57	MG	17	106	1/1	0.92	0.13	51,51,51,51	0
57	MG	1a	1736	1/1	0.92	0.17	55,55,55,55	0
57	MG	2A	3312	1/1	0.92	0.10	35,35,35,35	0
57	MG	2A	3547	1/1	0.92	0.08	36,36,36,36	0
57	MG	2A	3552	1/1	0.92	0.22	28,28,28,28	0
57	MG	1A	3729	1/1	0.92	0.17	41,41,41,41	0
57	MG	2A	3315	1/1	0.92	0.08	32,32,32,32	0
57	MG	1A	3039	1/1	0.92	0.09	33,33,33,33	0
57	MG	2A	3113	1/1	0.92	0.18	25,25,25,25	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	3558	1/1	0.92	0.08	63,63,63,63	0
57	MG	1A	3732	1/1	0.92	0.10	36,36,36,36	0
57	MG	1A	3735	1/1	0.92	0.12	19,19,19,19	0
57	MG	2A	3343	1/1	0.92	0.08	35,35,35,35	0
57	MG	2A	3344	1/1	0.92	0.12	40,40,40,40	0
57	MG	2A	3121	1/1	0.92	0.26	59,59,59,59	0
57	MG	1a	1610	1/1	0.92	0.12	33,33,33,33	0
57	MG	1a	1612	1/1	0.92	0.12	33,33,33,33	0
57	MG	1A	3738	1/1	0.92	0.11	22,22,22,22	0
57	MG	2A	3349	1/1	0.92	0.17	47,47,47,47	0
57	MG	1A	3486	1/1	0.92	0.09	40,40,40,40	0
57	MG	1A	3500	1/1	0.92	0.10	10,10,10,10	0
57	MG	1A	3501	1/1	0.92	0.12	22,22,22,22	0
57	MG	1A	3635	1/1	0.92	0.09	35,35,35,35	0
57	MG	2a	1711	1/1	0.92	0.15	52,52,52,52	0
57	MG	1a	1620	1/1	0.92	0.15	43,43,43,43	0
57	MG	2a	1715	1/1	0.92	0.12	66,66,66,66	0
57	MG	2A	3135	1/1	0.92	0.17	30,30,30,30	0
57	MG	2A	3136	1/1	0.92	0.26	53,53,53,53	0
57	MG	1A	3400	1/1	0.92	0.10	37,37,37,37	0
57	MG	1A	3021	1/1	0.92	0.23	30,30,30,30	0
57	MG	2a	1722	1/1	0.92	0.10	56,56,56,56	0
57	MG	1a	1623	1/1	0.92	0.21	50,50,50,50	0
57	MG	2a	1724	1/1	0.92	0.24	57,57,57,57	0
57	MG	1A	3751	1/1	0.92	0.11	46,46,46,46	0
57	MG	1A	3753	1/1	0.92	0.09	43,43,43,43	0
57	MG	1A	3324	1/1	0.92	0.09	29,29,29,29	0
57	MG	1A	3758	1/1	0.92	0.11	35,35,35,35	0
57	MG	2A	3592	1/1	0.92	0.17	64,64,64,64	0
57	MG	1A	3067	1/1	0.92	0.10	43,43,43,43	0
57	MG	2A	3151	1/1	0.92	0.30	55,55,55,55	0
57	MG	2a	1735	1/1	0.92	0.17	55,55,55,55	0
57	MG	2a	1736	1/1	0.92	0.20	60,60,60,60	0
57	MG	1A	3762	1/1	0.92	0.19	52,52,52,52	0
57	MG	1a	1632	1/1	0.92	0.15	48,48,48,48	0
57	MG	1A	3180	1/1	0.92	0.24	23,23,23,23	0
57	MG	2A	3384	1/1	0.92	0.07	45,45,45,45	0
57	MG	2A	3387	1/1	0.92	0.20	61,61,61,61	0
57	MG	1A	3648	1/1	0.92	0.10	27,27,27,27	0
57	MG	2A	3390	1/1	0.92	0.09	20,20,20,20	0
57	MG	1x	102	1/1	0.92	0.12	37,37,37,37	0
57	MG	2A	3168	1/1	0.92	0.15	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3188	1/1	0.92	0.08	33,33,33,33	0
57	MG	2a	1754	1/1	0.92	0.18	63,63,63,63	0
57	MG	1A	3531	1/1	0.92	0.09	10,10,10,10	0
57	MG	2A	3616	1/1	0.92	0.09	48,48,48,48	0
57	MG	1A	3427	1/1	0.92	0.11	31,31,31,31	0
57	MG	2A	3618	1/1	0.92	0.22	38,38,38,38	0
57	MG	1A	3653	1/1	0.92	0.06	31,31,31,31	0
57	MG	2a	1765	1/1	0.92	0.15	75,75,75,75	0
57	MG	1A	3548	1/1	0.92	0.09	33,33,33,33	0
57	MG	2e	202	1/1	0.92	0.07	64,64,64,64	0
57	MG	2A	3621	1/1	0.92	0.08	47,47,47,47	0
57	MG	2A	3177	1/1	0.92	0.12	60,60,60,60	0
57	MG	2A	3624	1/1	0.92	0.12	48,48,48,48	0
57	MG	2A	3625	1/1	0.92	0.12	45,45,45,45	0
57	MG	1A	3031	1/1	0.92	0.07	34,34,34,34	0
57	MG	2x	101	1/1	0.92	0.24	71,71,71,71	0
57	MG	2x	102	1/1	0.92	0.42	64,64,64,64	0
57	MG	2A	3182	1/1	0.92	0.24	51,51,51,51	0
57	MG	1A	3193	1/1	0.92	0.17	51,51,51,51	0
57	MG	2A	3007	1/1	0.92	0.14	47,47,47,47	0
57	MG	2A	3404	1/1	0.92	0.09	50,50,50,50	0
57	MG	2A	3635	1/1	0.92	0.14	55,55,55,55	0
57	MG	2X	101	1/1	0.93	0.17	44,44,44,44	0
57	MG	20	101	1/1	0.93	0.15	62,62,62,62	0
57	MG	1X	101	1/1	0.93	0.18	37,37,37,37	0
57	MG	2A	3035	1/1	0.93	0.13	62,62,62,62	0
57	MG	1A	3479	1/1	0.93	0.09	41,41,41,41	0
57	MG	2A	3037	1/1	0.93	0.12	38,38,38,38	0
57	MG	26	101	1/1	0.93	0.11	62,62,62,62	0
57	MG	1A	3662	1/1	0.93	0.09	44,44,44,44	0
57	MG	1A	3228	1/1	0.93	0.10	25,25,25,25	0
57	MG	1A	3750	1/1	0.93	0.10	39,39,39,39	0
57	MG	1A	3433	1/1	0.93	0.06	14,14,14,14	0
57	MG	2A	3183	1/1	0.93	0.12	36,36,36,36	0
57	MG	2A	3045	1/1	0.93	0.26	46,46,46,46	0
57	MG	2A	3186	1/1	0.93	0.18	50,50,50,50	0
57	MG	1A	3108	1/1	0.93	0.17	58,58,58,58	0
57	MG	2A	3372	1/1	0.93	0.11	59,59,59,59	0
57	MG	1a	1705	1/1	0.93	0.10	56,56,56,56	0
57	MG	2A	3549	1/1	0.93	0.08	48,48,48,48	0
57	MG	2a	1617	1/1	0.93	0.17	53,53,53,53	0
57	MG	2A	3551	1/1	0.93	0.18	23,23,23,23	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	1623	1/1	0.93	0.30	40,40,40,40	0
57	MG	2A	3375	1/1	0.93	0.18	39,39,39,39	0
57	MG	2A	3051	1/1	0.93	0.08	49,49,49,49	0
57	MG	15	104	1/1	0.93	0.23	28,28,28,28	0
57	MG	1A	3492	1/1	0.93	0.10	45,45,45,45	0
57	MG	17	103	1/1	0.93	0.17	33,33,33,33	0
57	MG	2A	3056	1/1	0.93	0.11	37,37,37,37	0
57	MG	2A	3196	1/1	0.93	0.10	58,58,58,58	0
57	MG	1A	3094	1/1	0.93	0.21	32,32,32,32	0
57	MG	2A	3385	1/1	0.93	0.13	62,62,62,62	0
57	MG	2A	3061	1/1	0.93	0.11	52,52,52,52	0
57	MG	2a	1639	1/1	0.93	0.20	56,56,56,56	0
57	MG	2A	3564	1/1	0.93	0.13	47,47,47,47	0
57	MG	2A	3388	1/1	0.93	0.17	45,45,45,45	0
57	MG	1A	3595	1/1	0.93	0.12	55,55,55,55	0
57	MG	1A	3676	1/1	0.93	0.13	14,14,14,14	0
57	MG	1A	3767	1/1	0.93	0.09	37,37,37,37	0
57	MG	1A	3327	1/1	0.93	0.15	32,32,32,32	0
57	MG	2A	3204	1/1	0.93	0.20	29,29,29,29	0
57	MG	1A	3769	1/1	0.93	0.09	14,14,14,14	0
57	MG	2A	3395	1/1	0.93	0.11	31,31,31,31	0
57	MG	2a	1650	1/1	0.93	0.12	48,48,48,48	0
57	MG	1A	3678	1/1	0.93	0.13	27,27,27,27	0
57	MG	1A	3200	1/1	0.93	0.13	40,40,40,40	0
57	MG	2A	3579	1/1	0.93	0.23	47,47,47,47	0
57	MG	1A	3773	1/1	0.93	0.14	53,53,53,53	0
57	MG	1A	3682	1/1	0.93	0.13	33,33,33,33	0
57	MG	1A	3777	1/1	0.93	0.14	38,38,38,38	0
57	MG	2A	3074	1/1	0.93	0.11	61,61,61,61	0
57	MG	1A	3503	1/1	0.93	0.07	11,11,11,11	0
57	MG	2a	1663	1/1	0.93	0.12	51,51,51,51	0
57	MG	1a	1737	1/1	0.93	0.20	46,46,46,46	0
57	MG	2A	3222	1/1	0.93	0.17	49,49,49,49	0
57	MG	1A	3782	1/1	0.93	0.07	29,29,29,29	0
57	MG	2A	3224	1/1	0.93	0.18	62,62,62,62	0
57	MG	1A	3239	1/1	0.93	0.07	16,16,16,16	0
57	MG	1A	3283	1/1	0.93	0.33	44,44,44,44	0
57	MG	1A	3038	1/1	0.93	0.25	35,35,35,35	0
57	MG	2A	3415	1/1	0.93	0.15	32,32,32,32	0
57	MG	1A	3687	1/1	0.93	0.07	42,42,42,42	0
57	MG	1A	3791	1/1	0.93	0.12	43,43,43,43	0
57	MG	2A	3418	1/1	0.93	0.10	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3422	1/1	0.93	0.10	39,39,39,39	0
57	MG	2A	3603	1/1	0.93	0.09	43,43,43,43	0
57	MG	1A	3616	1/1	0.93	0.08	43,43,43,43	0
57	MG	2a	1682	1/1	0.93	0.24	52,52,52,52	0
57	MG	1A	3617	1/1	0.93	0.13	47,47,47,47	0
57	MG	1A	3511	1/1	0.93	0.12	46,46,46,46	0
57	MG	2A	3608	1/1	0.93	0.09	37,37,37,37	0
57	MG	2A	3430	1/1	0.93	0.07	45,45,45,45	0
57	MG	2a	1697	1/1	0.93	0.11	48,48,48,48	0
57	MG	1A	3619	1/1	0.93	0.09	50,50,50,50	0
57	MG	1B	203	1/1	0.93	0.10	45,45,45,45	0
57	MG	2A	3245	1/1	0.93	0.16	25,25,25,25	0
57	MG	2a	1703	1/1	0.93	0.20	64,64,64,64	0
57	MG	2a	1704	1/1	0.93	0.18	53,53,53,53	0
57	MG	2A	3439	1/1	0.93	0.17	33,33,33,33	0
57	MG	2A	3443	1/1	0.93	0.16	45,45,45,45	0
57	MG	1A	3294	1/1	0.93	0.15	39,39,39,39	0
57	MG	1A	3391	1/1	0.93	0.08	25,25,25,25	0
57	MG	1A	3524	1/1	0.93	0.15	36,36,36,36	0
57	MG	1A	3623	1/1	0.93	0.48	25,25,25,25	0
57	MG	2A	3253	1/1	0.93	0.14	48,48,48,48	0
57	MG	2a	1714	1/1	0.93	0.16	43,43,43,43	0
57	MG	1B	212	1/1	0.93	0.06	46,46,46,46	0
57	MG	1A	3527	1/1	0.93	0.10	29,29,29,29	0
57	MG	1a	1764	1/1	0.93	0.20	70,70,70,70	0
57	MG	1A	3250	1/1	0.93	0.12	35,35,35,35	0
57	MG	2A	3461	1/1	0.93	0.15	48,48,48,48	0
57	MG	1D	308	1/1	0.93	0.10	41,41,41,41	0
57	MG	2A	3270	1/1	0.93	0.12	65,65,65,65	0
57	MG	1A	3533	1/1	0.93	0.11	16,16,16,16	0
57	MG	1A	3045	1/1	0.93	0.09	30,30,30,30	0
57	MG	1A	3543	1/1	0.93	0.10	43,43,43,43	0
57	MG	2a	1727	1/1	0.93	0.10	44,44,44,44	0
57	MG	2A	3122	1/1	0.93	0.30	61,61,61,61	0
57	MG	1A	3711	1/1	0.93	0.18	23,23,23,23	0
57	MG	1A	3254	1/1	0.93	0.11	48,48,48,48	0
57	MG	2A	3284	1/1	0.93	0.13	55,55,55,55	0
57	MG	2a	1733	1/1	0.93	0.20	49,49,49,49	0
57	MG	1A	3551	1/1	0.93	0.07	25,25,25,25	0
57	MG	2A	3288	1/1	0.93	0.13	51,51,51,51	0
57	MG	1A	3173	1/1	0.93	0.41	36,36,36,36	0
57	MG	1A	3639	1/1	0.93	0.19	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	1x	105	1/1	0.93	0.19	26,26,26,26	0
57	MG	1A	3723	1/1	0.93	0.09	32,32,32,32	0
57	MG	1A	3405	1/1	0.93	0.09	11,11,11,11	0
57	MG	1a	1665	1/1	0.93	0.23	49,49,49,49	0
57	MG	2a	1746	1/1	0.93	0.20	40,40,40,40	0
57	MG	1A	3074	1/1	0.93	0.25	46,46,46,46	0
57	MG	2A	3137	1/1	0.93	0.07	60,60,60,60	0
57	MG	1A	3565	1/1	0.93	0.10	31,31,31,31	0
57	MG	2A	3006	1/1	0.93	0.21	45,45,45,45	0
57	MG	1A	3731	1/1	0.93	0.11	45,45,45,45	0
57	MG	1A	3407	1/1	0.93	0.08	29,29,29,29	0
57	MG	1Q	205	1/1	0.93	0.16	30,30,30,30	0
57	MG	2B	209	1/1	0.93	0.21	58,58,58,58	0
57	MG	1R	201	1/1	0.93	0.11	27,27,27,27	0
57	MG	1A	3103	1/1	0.93	0.25	42,42,42,42	0
57	MG	2a	1763	1/1	0.93	0.20	71,71,71,71	0
57	MG	2A	3495	1/1	0.93	0.08	45,45,45,45	0
57	MG	2D	304	1/1	0.93	0.32	41,41,41,41	0
57	MG	2A	3017	1/1	0.93	0.14	52,52,52,52	0
57	MG	1A	3420	1/1	0.93	0.10	11,11,11,11	0
57	MG	2A	3334	1/1	0.93	0.09	27,27,27,27	0
57	MG	2E	305	1/1	0.93	0.13	30,30,30,30	0
57	MG	2E	306	1/1	0.93	0.12	55,55,55,55	0
57	MG	2A	3502	1/1	0.93	0.09	51,51,51,51	0
57	MG	1A	3089	1/1	0.93	0.12	46,46,46,46	0
57	MG	1A	3361	1/1	0.93	0.20	54,54,54,54	0
57	MG	1A	3030	1/1	0.93	0.21	27,27,27,27	0
57	MG	2A	3160	1/1	0.93	0.18	38,38,38,38	0
57	MG	2A	3162	1/1	0.93	0.21	36,36,36,36	0
57	MG	2A	3028	1/1	0.93	0.28	43,43,43,43	0
57	MG	1W	203	1/1	0.93	0.10	17,17,17,17	0
57	MG	2A	3033	1/1	0.93	0.18	55,55,55,55	0
58	ZN	14	501	1/1	0.93	0.16	119,119,119,119	0
57	MG	15	106	1/1	0.94	0.25	28,28,28,28	0
57	MG	1A	3008	1/1	0.94	0.16	21,21,21,21	0
57	MG	2A	3149	1/1	0.94	0.17	54,54,54,54	0
57	MG	1A	3148	1/1	0.94	0.49	33,33,33,33	0
57	MG	17	105	1/1	0.94	0.20	31,31,31,31	0
57	MG	2A	3153	1/1	0.94	0.24	38,38,38,38	0
57	MG	1A	3734	1/1	0.94	0.09	17,17,17,17	0
57	MG	1A	3493	1/1	0.94	0.05	19,19,19,19	0
57	MG	1A	3395	1/1	0.94	0.10	16,16,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3739	1/1	0.94	0.07	18,18,18,18	0
57	MG	1a	1607	1/1	0.94	0.10	68,68,68,68	0
57	MG	1A	3315	1/1	0.94	0.18	39,39,39,39	0
57	MG	2A	3164	1/1	0.94	0.12	56,56,56,56	0
57	MG	2A	3166	1/1	0.94	0.09	38,38,38,38	0
57	MG	1A	3397	1/1	0.94	0.06	35,35,35,35	0
57	MG	1k	201	1/1	0.94	0.17	55,55,55,55	0
57	MG	1A	3743	1/1	0.94	0.12	35,35,35,35	0
57	MG	1v	102	1/1	0.94	0.12	63,63,63,63	0
57	MG	1A	3628	1/1	0.94	0.08	20,20,20,20	0
57	MG	2A	3655	1/1	0.94	0.17	47,47,47,47	0
57	MG	1a	1614	1/1	0.94	0.20	48,48,48,48	0
57	MG	1A	3119	1/1	0.94	0.06	28,28,28,28	0
57	MG	1A	3241	1/1	0.94	0.10	55,55,55,55	0
57	MG	1A	3633	1/1	0.94	0.07	32,32,32,32	0
57	MG	1A	3244	1/1	0.94	0.11	35,35,35,35	0
57	MG	1A	3186	1/1	0.94	0.14	35,35,35,35	0
57	MG	1A	3249	1/1	0.94	0.15	34,34,34,34	0
57	MG	2A	3185	1/1	0.94	0.14	40,40,40,40	0
57	MG	1x	109	1/1	0.94	0.17	48,48,48,48	0
57	MG	1y	101	1/1	0.94	0.18	34,34,34,34	0
57	MG	2A	3419	1/1	0.94	0.07	24,24,24,24	0
57	MG	2A	3421	1/1	0.94	0.16	45,45,45,45	0
57	MG	1A	3754	1/1	0.94	0.15	34,34,34,34	0
57	MG	1A	3756	1/1	0.94	0.06	32,32,32,32	0
57	MG	1A	3637	1/1	0.94	0.15	36,36,36,36	0
57	MG	1A	3085	1/1	0.94	0.22	41,41,41,41	0
57	MG	1A	3759	1/1	0.94	0.12	44,44,44,44	0
57	MG	1A	3519	1/1	0.94	0.11	43,43,43,43	0
57	MG	1A	3412	1/1	0.94	0.06	13,13,13,13	0
57	MG	2A	3436	1/1	0.94	0.07	38,38,38,38	0
57	MG	2A	3011	1/1	0.94	0.15	41,41,41,41	0
57	MG	2A	3198	1/1	0.94	0.10	66,66,66,66	0
57	MG	2A	3442	1/1	0.94	0.09	35,35,35,35	0
57	MG	2F	305	1/1	0.94	0.15	42,42,42,42	0
57	MG	2A	3012	1/1	0.94	0.06	35,35,35,35	0
57	MG	1A	3413	1/1	0.94	0.09	17,17,17,17	0
57	MG	2Q	203	1/1	0.94	0.23	53,53,53,53	0
57	MG	1A	3418	1/1	0.94	0.08	25,25,25,25	0
57	MG	2A	3447	1/1	0.94	0.18	36,36,36,36	0
57	MG	2U	202	1/1	0.94	0.05	52,52,52,52	0
57	MG	1A	3530	1/1	0.94	0.10	9,9,9,9	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	2V	202	1/1	0.94	0.17	53,53,53,53	0
57	MG	1A	3040	1/1	0.94	0.16	24,24,24,24	0
57	MG	2A	3018	1/1	0.94	0.25	42,42,42,42	0
57	MG	2A	3019	1/1	0.94	0.11	31,31,31,31	0
57	MG	1A	3191	1/1	0.94	0.30	43,43,43,43	0
57	MG	2A	3454	1/1	0.94	0.27	64,64,64,64	0
57	MG	2A	3023	1/1	0.94	0.24	39,39,39,39	0
57	MG	2A	3459	1/1	0.94	0.20	61,61,61,61	0
57	MG	1A	3339	1/1	0.94	0.10	29,29,29,29	0
57	MG	28	101	1/1	0.94	0.09	52,52,52,52	0
57	MG	2a	1602	1/1	0.94	0.09	63,63,63,63	0
57	MG	1a	1639	1/1	0.94	0.08	47,47,47,47	0
57	MG	2A	3212	1/1	0.94	0.18	51,51,51,51	0
57	MG	2A	3213	1/1	0.94	0.26	50,50,50,50	0
57	MG	1A	3541	1/1	0.94	0.11	15,15,15,15	0
57	MG	2A	3465	1/1	0.94	0.17	65,65,65,65	0
57	MG	2A	3217	1/1	0.94	0.23	46,46,46,46	0
57	MG	1A	3654	1/1	0.94	0.23	47,47,47,47	0
57	MG	1A	3778	1/1	0.94	0.15	28,28,28,28	0
57	MG	1A	3542	1/1	0.94	0.10	56,56,56,56	0
57	MG	2a	1613	1/1	0.94	0.17	41,41,41,41	0
57	MG	1A	3192	1/1	0.94	0.18	27,27,27,27	0
57	MG	1A	3661	1/1	0.94	0.13	48,48,48,48	0
57	MG	1A	3428	1/1	0.94	0.09	39,39,39,39	0
57	MG	1A	3342	1/1	0.94	0.07	10,10,10,10	0
57	MG	2a	1622	1/1	0.94	0.22	57,57,57,57	0
57	MG	1a	1653	1/1	0.94	0.14	27,27,27,27	0
57	MG	1A	3054	1/1	0.94	0.16	33,33,33,33	0
57	MG	2A	3480	1/1	0.94	0.10	50,50,50,50	0
57	MG	2A	3041	1/1	0.94	0.26	38,38,38,38	0
57	MG	1A	3557	1/1	0.94	0.07	65,65,65,65	0
57	MG	2A	3234	1/1	0.94	0.13	51,51,51,51	0
57	MG	2a	1631	1/1	0.94	0.26	53,53,53,53	0
57	MG	1A	3669	1/1	0.94	0.12	42,42,42,42	0
57	MG	2a	1634	1/1	0.94	0.17	48,48,48,48	0
57	MG	2A	3237	1/1	0.94	0.22	48,48,48,48	0
57	MG	1A	3155	1/1	0.94	0.10	23,23,23,23	0
57	MG	2A	3239	1/1	0.94	0.09	34,34,34,34	0
57	MG	1A	3561	1/1	0.94	0.10	48,48,48,48	0
57	MG	1a	1663	1/1	0.94	0.14	42,42,42,42	0
57	MG	1A	3201	1/1	0.94	0.22	28,28,28,28	0
57	MG	1A	3069	1/1	0.94	0.30	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	1B	204	1/1	0.94	0.13	31,31,31,31	0
57	MG	1A	3160	1/1	0.94	0.13	29,29,29,29	0
57	MG	1a	1669	1/1	0.94	0.19	53,53,53,53	0
57	MG	1B	206	1/1	0.94	0.07	33,33,33,33	0
57	MG	2A	3499	1/1	0.94	0.16	52,52,52,52	0
57	MG	1A	3269	1/1	0.94	0.17	56,56,56,56	0
57	MG	1A	3570	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3357	1/1	0.94	0.08	35,35,35,35	0
57	MG	2A	3259	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	3164	1/1	0.94	0.13	42,42,42,42	0
57	MG	2A	3506	1/1	0.94	0.09	44,44,44,44	0
57	MG	2A	3507	1/1	0.94	0.14	52,52,52,52	0
57	MG	1A	3095	1/1	0.94	0.20	33,33,33,33	0
57	MG	2A	3265	1/1	0.94	0.12	33,33,33,33	0
57	MG	2a	1659	1/1	0.94	0.08	52,52,52,52	0
57	MG	2A	3267	1/1	0.94	0.09	34,34,34,34	0
57	MG	1A	3214	1/1	0.94	0.18	39,39,39,39	0
57	MG	2A	3520	1/1	0.94	0.09	53,53,53,53	0
57	MG	2A	3521	1/1	0.94	0.12	55,55,55,55	0
57	MG	1a	1679	1/1	0.94	0.16	60,60,60,60	0
57	MG	1D	304	1/1	0.94	0.09	30,30,30,30	0
57	MG	1A	3579	1/1	0.94	0.10	15,15,15,15	0
57	MG	2a	1669	1/1	0.94	0.13	62,62,62,62	0
57	MG	2A	3273	1/1	0.94	0.20	51,51,51,51	0
57	MG	1A	3215	1/1	0.94	0.14	24,24,24,24	0
57	MG	2A	3276	1/1	0.94	0.14	27,27,27,27	0
57	MG	2A	3531	1/1	0.94	0.08	60,60,60,60	0
57	MG	1A	3688	1/1	0.94	0.22	47,47,47,47	0
57	MG	1A	3455	1/1	0.94	0.10	26,26,26,26	0
57	MG	1A	3364	1/1	0.94	0.13	24,24,24,24	0
57	MG	2A	3535	1/1	0.94	0.13	61,61,61,61	0
57	MG	1A	3216	1/1	0.94	0.15	52,52,52,52	0
57	MG	2A	3538	1/1	0.94	0.16	51,51,51,51	0
57	MG	2A	3285	1/1	0.94	0.19	38,38,38,38	0
57	MG	2a	1685	1/1	0.94	0.18	56,56,56,56	0
57	MG	2A	3079	1/1	0.94	0.18	36,36,36,36	0
57	MG	1A	3587	1/1	0.94	0.10	26,26,26,26	0
57	MG	1A	3589	1/1	0.94	0.06	25,25,25,25	0
57	MG	2a	1691	1/1	0.94	0.10	41,41,41,41	0
57	MG	2a	1693	1/1	0.94	0.16	49,49,49,49	0
57	MG	2a	1694	1/1	0.94	0.11	48,48,48,48	0
57	MG	2A	3545	1/1	0.94	0.12	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	2a	1696	1/1	0.94	0.09	42,42,42,42	0
57	MG	1a	1702	1/1	0.94	0.23	36,36,36,36	0
57	MG	1A	3590	1/1	0.94	0.07	43,43,43,43	0
57	MG	2a	1699	1/1	0.94	0.12	59,59,59,59	0
57	MG	1A	3218	1/1	0.94	0.12	28,28,28,28	0
57	MG	2A	3550	1/1	0.94	0.07	62,62,62,62	0
57	MG	1a	1706	1/1	0.94	0.14	48,48,48,48	0
57	MG	2A	3092	1/1	0.94	0.12	58,58,58,58	0
57	MG	1N	201	1/1	0.94	0.12	35,35,35,35	0
57	MG	1a	1710	1/1	0.94	0.12	47,47,47,47	0
57	MG	2A	3097	1/1	0.94	0.14	27,27,27,27	0
57	MG	1A	3459	1/1	0.94	0.07	38,38,38,38	0
57	MG	2A	3309	1/1	0.94	0.15	25,25,25,25	0
57	MG	1a	1712	1/1	0.94	0.22	57,57,57,57	0
57	MG	2A	3311	1/1	0.94	0.12	38,38,38,38	0
57	MG	1A	3594	1/1	0.94	0.08	40,40,40,40	0
57	MG	1A	3130	1/1	0.94	0.35	37,37,37,37	0
57	MG	1a	1715	1/1	0.94	0.19	52,52,52,52	0
57	MG	2A	3316	1/1	0.94	0.10	28,28,28,28	0
57	MG	2A	3320	1/1	0.94	0.09	60,60,60,60	0
57	MG	2a	1720	1/1	0.94	0.14	59,59,59,59	0
57	MG	2A	3567	1/1	0.94	0.10	28,28,28,28	0
57	MG	2A	3324	1/1	0.94	0.09	45,45,45,45	0
57	MG	2A	3326	1/1	0.94	0.09	24,24,24,24	0
57	MG	2A	3571	1/1	0.94	0.13	57,57,57,57	0
57	MG	1a	1716	1/1	0.94	0.17	41,41,41,41	0
57	MG	2A	3328	1/1	0.94	0.13	38,38,38,38	0
57	MG	2A	3329	1/1	0.94	0.07	28,28,28,28	0
57	MG	2A	3330	1/1	0.94	0.07	42,42,42,42	0
57	MG	1A	3596	1/1	0.94	0.06	30,30,30,30	0
57	MG	2A	3577	1/1	0.94	0.12	60,60,60,60	0
57	MG	1Q	202	1/1	0.94	0.16	30,30,30,30	0
57	MG	2A	3109	1/1	0.94	0.12	47,47,47,47	0
57	MG	2A	3338	1/1	0.94	0.12	38,38,38,38	0
57	MG	1A	3706	1/1	0.94	0.10	30,30,30,30	0
57	MG	1a	1722	1/1	0.94	0.14	39,39,39,39	0
57	MG	1A	3371	1/1	0.94	0.11	29,29,29,29	0
57	MG	1a	1724	1/1	0.94	0.19	40,40,40,40	0
57	MG	2A	3114	1/1	0.94	0.10	51,51,51,51	0
57	MG	2A	3588	1/1	0.94	0.33	62,62,62,62	0
57	MG	1A	3303	1/1	0.94	0.09	13,13,13,13	0
57	MG	1a	1728	1/1	0.94	0.15	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1U	201	1/1	0.94	0.18	18,18,18,18	0
57	MG	1A	3710	1/1	0.94	0.09	43,43,43,43	0
57	MG	1A	3607	1/1	0.94	0.09	15,15,15,15	0
57	MG	2A	3353	1/1	0.94	0.11	39,39,39,39	0
57	MG	1A	3712	1/1	0.94	0.36	33,33,33,33	0
57	MG	1A	3713	1/1	0.94	0.36	23,23,23,23	0
57	MG	1W	201	1/1	0.94	0.15	23,23,23,23	0
57	MG	2A	3127	1/1	0.94	0.16	28,28,28,28	0
57	MG	2A	3600	1/1	0.94	0.10	37,37,37,37	0
57	MG	2a	1761	1/1	0.94	0.10	49,49,49,49	0
57	MG	2A	3129	1/1	0.94	0.09	42,42,42,42	0
57	MG	1A	3376	1/1	0.94	0.10	31,31,31,31	0
57	MG	2A	3131	1/1	0.94	0.11	65,65,65,65	0
57	MG	1A	3715	1/1	0.94	0.09	40,40,40,40	0
57	MG	2A	3368	1/1	0.94	0.08	51,51,51,51	0
57	MG	2A	3369	1/1	0.94	0.15	56,56,56,56	0
57	MG	2e	203	1/1	0.94	0.23	55,55,55,55	0
57	MG	1A	3061	1/1	0.94	0.07	40,40,40,40	0
57	MG	1A	3115	1/1	0.94	0.21	33,33,33,33	0
57	MG	1A	3227	1/1	0.94	0.23	46,46,46,46	0
57	MG	2A	3615	1/1	0.94	0.09	53,53,53,53	0
57	MG	1A	3722	1/1	0.94	0.09	31,31,31,31	0
57	MG	1a	1748	1/1	0.94	0.06	52,52,52,52	0
57	MG	1A	3137	1/1	0.94	0.23	29,29,29,29	0
57	MG	1A	3385	1/1	0.94	0.19	36,36,36,36	0
57	MG	15	101	1/1	0.94	0.17	34,34,34,34	0
57	MG	2x	105	1/1	0.94	0.20	40,40,40,40	0
57	MG	1A	3176	1/1	0.94	0.13	36,36,36,36	0
57	MG	1A	3390	1/1	0.94	0.14	36,36,36,36	0
57	MG	2A	3623	1/1	0.94	0.23	48,48,48,48	0
57	MG	2A	3145	1/1	0.94	0.21	44,44,44,44	0
57	MG	2A	3477	1/1	0.95	0.10	33,33,33,33	0
57	MG	2A	3274	1/1	0.95	0.08	26,26,26,26	0
57	MG	2E	307	1/1	0.95	0.17	27,27,27,27	0
57	MG	1a	1738	1/1	0.95	0.24	33,33,33,33	0
57	MG	1A	3333	1/1	0.95	0.10	35,35,35,35	0
57	MG	1A	3001	1/1	0.95	0.11	23,23,23,23	0
57	MG	1a	1743	1/1	0.95	0.13	54,54,54,54	0
57	MG	1A	3532	1/1	0.95	0.09	24,24,24,24	0
57	MG	2P	201	1/1	0.95	0.12	52,52,52,52	0
57	MG	2A	3281	1/1	0.95	0.13	51,51,51,51	0
57	MG	1A	3151	1/1	0.95	0.18	38,38,38,38	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	3194	1/1	0.95	0.22	34,34,34,34	0
57	MG	1A	3086	1/1	0.95	0.22	36,36,36,36	0
57	MG	2A	3115	1/1	0.95	0.19	47,47,47,47	0
57	MG	2A	3116	1/1	0.95	0.26	53,53,53,53	0
57	MG	1A	3257	1/1	0.95	0.16	34,34,34,34	0
57	MG	1A	3020	1/1	0.95	0.20	39,39,39,39	0
57	MG	1A	3015	1/1	0.95	0.12	36,36,36,36	0
57	MG	2Y	201	1/1	0.95	0.10	52,52,52,52	0
57	MG	2A	3295	1/1	0.95	0.07	35,35,35,35	0
57	MG	1A	3655	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	3656	1/1	0.95	0.08	30,30,30,30	0
57	MG	1a	1754	1/1	0.95	0.07	48,48,48,48	0
57	MG	2A	3300	1/1	0.95	0.10	46,46,46,46	0
57	MG	1a	1616	1/1	0.95	0.04	45,45,45,45	0
57	MG	2A	3302	1/1	0.95	0.11	58,58,58,58	0
57	MG	2A	3503	1/1	0.95	0.12	42,42,42,42	0
57	MG	2a	1603	1/1	0.95	0.09	62,62,62,62	0
57	MG	2A	3305	1/1	0.95	0.10	41,41,41,41	0
57	MG	1A	3430	1/1	0.95	0.05	14,14,14,14	0
57	MG	1A	3205	1/1	0.95	0.10	25,25,25,25	0
57	MG	1A	3556	1/1	0.95	0.10	15,15,15,15	0
57	MG	1a	1760	1/1	0.95	0.21	57,57,57,57	0
57	MG	1A	3063	1/1	0.95	0.05	19,19,19,19	0
57	MG	1A	3435	1/1	0.95	0.10	10,10,10,10	0
57	MG	2A	3514	1/1	0.95	0.05	35,35,35,35	0
57	MG	1A	3211	1/1	0.95	0.15	41,41,41,41	0
57	MG	2A	3519	1/1	0.95	0.13	38,38,38,38	0
57	MG	1A	3355	1/1	0.95	0.07	21,21,21,21	0
57	MG	1a	1765	1/1	0.95	0.06	45,45,45,45	0
57	MG	1A	3048	1/1	0.95	0.22	30,30,30,30	0
57	MG	2a	1618	1/1	0.95	0.18	57,57,57,57	0
57	MG	2A	3523	1/1	0.95	0.07	46,46,46,46	0
57	MG	1A	3781	1/1	0.95	0.15	45,45,45,45	0
57	MG	2A	3138	1/1	0.95	0.10	42,42,42,42	0
57	MG	1f	201	1/1	0.95	0.13	52,52,52,52	0
57	MG	1A	3440	1/1	0.95	0.10	21,21,21,21	0
57	MG	2A	3529	1/1	0.95	0.09	49,49,49,49	0
57	MG	2A	3141	1/1	0.95	0.13	39,39,39,39	0
57	MG	1A	3672	1/1	0.95	0.12	48,48,48,48	0
57	MG	1n	101	1/1	0.95	0.12	50,50,50,50	0
57	MG	2A	3332	1/1	0.95	0.15	34,34,34,34	0
57	MG	1A	3035	1/1	0.95	0.27	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	3271	1/1	0.95	0.12	29,29,29,29	0
57	MG	2A	3336	1/1	0.95	0.04	39,39,39,39	0
57	MG	1A	3787	1/1	0.95	0.06	31,31,31,31	0
57	MG	1A	3571	1/1	0.95	0.12	17,17,17,17	0
57	MG	1A	3572	1/1	0.95	0.10	55,55,55,55	0
57	MG	1A	3272	1/1	0.95	0.16	36,36,36,36	0
57	MG	1A	3026	1/1	0.95	0.19	36,36,36,36	0
57	MG	2A	3152	1/1	0.95	0.17	34,34,34,34	0
57	MG	1A	3362	1/1	0.95	0.15	51,51,51,51	0
57	MG	1A	3275	1/1	0.95	0.14	34,34,34,34	0
57	MG	1a	1641	1/1	0.95	0.29	46,46,46,46	0
57	MG	1a	1642	1/1	0.95	0.17	48,48,48,48	0
57	MG	2a	1647	1/1	0.95	0.15	43,43,43,43	0
57	MG	2A	3159	1/1	0.95	0.15	40,40,40,40	0
57	MG	1a	1643	1/1	0.95	0.14	47,47,47,47	0
57	MG	1A	3098	1/1	0.95	0.18	27,27,27,27	0
57	MG	1A	3365	1/1	0.95	0.07	26,26,26,26	0
57	MG	1A	3132	1/1	0.95	0.08	25,25,25,25	0
57	MG	2A	3165	1/1	0.95	0.18	52,52,52,52	0
57	MG	1A	3171	1/1	0.95	0.23	21,21,21,21	0
57	MG	1A	3219	1/1	0.95	0.08	38,38,38,38	0
57	MG	2a	1657	1/1	0.95	0.26	44,44,44,44	0
57	MG	1A	3293	1/1	0.95	0.15	32,32,32,32	0
57	MG	2A	3366	1/1	0.95	0.16	35,35,35,35	0
57	MG	2a	1660	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	3220	1/1	0.95	0.11	32,32,32,32	0
57	MG	1A	3464	1/1	0.95	0.07	18,18,18,18	0
57	MG	1B	214	1/1	0.95	0.06	29,29,29,29	0
57	MG	1B	218	1/1	0.95	0.14	44,44,44,44	0
57	MG	1a	1657	1/1	0.95	0.14	50,50,50,50	0
57	MG	1A	3296	1/1	0.95	0.06	24,24,24,24	0
57	MG	2A	3179	1/1	0.95	0.23	47,47,47,47	0
57	MG	1D	301	1/1	0.95	0.08	25,25,25,25	0
57	MG	2A	3181	1/1	0.95	0.22	51,51,51,51	0
57	MG	1A	3377	1/1	0.95	0.07	49,49,49,49	0
57	MG	1D	303	1/1	0.95	0.15	29,29,29,29	0
57	MG	1A	3016	1/1	0.95	0.08	35,35,35,35	0
57	MG	1D	306	1/1	0.95	0.04	28,28,28,28	0
57	MG	1D	307	1/1	0.95	0.09	30,30,30,30	0
57	MG	1A	3379	1/1	0.95	0.06	30,30,30,30	0
57	MG	2A	3189	1/1	0.95	0.28	50,50,50,50	0
57	MG	1a	1668	1/1	0.95	0.08	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1D	309	1/1	0.95	0.06	16,16,16,16	0
57	MG	1A	3071	1/1	0.95	0.12	38,38,38,38	0
57	MG	2a	1683	1/1	0.95	0.26	48,48,48,48	0
57	MG	2A	3030	1/1	0.95	0.34	38,38,38,38	0
57	MG	1A	3597	1/1	0.95	0.08	43,43,43,43	0
57	MG	1a	1673	1/1	0.95	0.12	42,42,42,42	0
57	MG	2a	1688	1/1	0.95	0.20	56,56,56,56	0
57	MG	1A	3598	1/1	0.95	0.08	30,30,30,30	0
57	MG	1A	3704	1/1	0.95	0.10	51,51,51,51	0
57	MG	1A	3175	1/1	0.95	0.10	37,37,37,37	0
57	MG	1A	3601	1/1	0.95	0.12	54,54,54,54	0
57	MG	1A	3382	1/1	0.95	0.11	35,35,35,35	0
57	MG	1A	3383	1/1	0.95	0.11	46,46,46,46	0
57	MG	1G	202	1/1	0.95	0.09	60,60,60,60	0
57	MG	1A	3072	1/1	0.95	0.11	29,29,29,29	0
57	MG	2A	3596	1/1	0.95	0.09	36,36,36,36	0
57	MG	1A	3138	1/1	0.95	0.11	26,26,26,26	0
57	MG	1A	3612	1/1	0.95	0.11	27,27,27,27	0
57	MG	1A	3484	1/1	0.95	0.07	33,33,33,33	0
57	MG	1P	201	1/1	0.95	0.24	24,24,24,24	0
57	MG	2A	3405	1/1	0.95	0.09	31,31,31,31	0
57	MG	2A	3408	1/1	0.95	0.15	29,29,29,29	0
57	MG	2A	3052	1/1	0.95	0.23	49,49,49,49	0
57	MG	2A	3410	1/1	0.95	0.09	43,43,43,43	0
57	MG	2A	3606	1/1	0.95	0.14	48,48,48,48	0
57	MG	1P	202	1/1	0.95	0.06	15,15,15,15	0
57	MG	2A	3211	1/1	0.95	0.07	37,37,37,37	0
57	MG	2A	3609	1/1	0.95	0.12	40,40,40,40	0
57	MG	1a	1692	1/1	0.95	0.14	60,60,60,60	0
57	MG	1a	1695	1/1	0.95	0.15	70,70,70,70	0
57	MG	2a	1717	1/1	0.95	0.12	46,46,46,46	0
57	MG	1A	3485	1/1	0.95	0.16	37,37,37,37	0
57	MG	1A	3388	1/1	0.95	0.10	34,34,34,34	0
57	MG	2A	3218	1/1	0.95	0.55	42,42,42,42	0
57	MG	1A	3490	1/1	0.95	0.06	37,37,37,37	0
57	MG	1A	3139	1/1	0.95	0.11	40,40,40,40	0
57	MG	1A	3719	1/1	0.95	0.13	29,29,29,29	0
57	MG	1A	3141	1/1	0.95	0.18	28,28,28,28	0
57	MG	2A	3423	1/1	0.95	0.31	52,52,52,52	0
57	MG	1A	3494	1/1	0.95	0.16	31,31,31,31	0
57	MG	1a	1709	1/1	0.95	0.11	37,37,37,37	0
57	MG	2a	1728	1/1	0.95	0.10	49,49,49,49	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	3225	1/1	0.95	0.32	48,48,48,48	0
57	MG	1A	3184	1/1	0.95	0.18	25,25,25,25	0
57	MG	1A	3392	1/1	0.95	0.09	13,13,13,13	0
57	MG	1A	3728	1/1	0.95	0.10	16,16,16,16	0
57	MG	2A	3628	1/1	0.95	0.07	54,54,54,54	0
57	MG	1A	3185	1/1	0.95	0.17	40,40,40,40	0
57	MG	2A	3630	1/1	0.95	0.09	37,37,37,37	0
57	MG	2A	3437	1/1	0.95	0.08	45,45,45,45	0
57	MG	1A	3625	1/1	0.95	0.08	31,31,31,31	0
57	MG	1A	3317	1/1	0.95	0.12	36,36,36,36	0
57	MG	2A	3440	1/1	0.95	0.14	66,66,66,66	0
57	MG	2A	3441	1/1	0.95	0.12	29,29,29,29	0
57	MG	2A	3638	1/1	0.95	0.16	29,29,29,29	0
57	MG	2A	3235	1/1	0.95	0.09	56,56,56,56	0
57	MG	2A	3075	1/1	0.95	0.10	25,25,25,25	0
57	MG	1A	3055	1/1	0.95	0.16	11,11,11,11	0
57	MG	2A	3644	1/1	0.95	0.17	45,45,45,45	0
57	MG	1A	3505	1/1	0.95	0.11	49,49,49,49	0
57	MG	1a	1718	1/1	0.95	0.19	39,39,39,39	0
57	MG	2a	1753	1/1	0.95	0.11	44,44,44,44	0
57	MG	1A	3146	1/1	0.95	0.28	32,32,32,32	0
57	MG	1a	1720	1/1	0.95	0.08	53,53,53,53	0
57	MG	2A	3651	1/1	0.95	0.17	41,41,41,41	0
57	MG	1A	3028	1/1	0.95	0.19	33,33,33,33	0
57	MG	2a	1760	1/1	0.95	0.11	33,33,33,33	0
57	MG	2A	3083	1/1	0.95	0.07	52,52,52,52	0
57	MG	1A	3632	1/1	0.95	0.08	44,44,44,44	0
57	MG	2A	3086	1/1	0.95	0.07	58,58,58,58	0
57	MG	2A	3456	1/1	0.95	0.19	49,49,49,49	0
57	MG	2A	3087	1/1	0.95	0.17	38,38,38,38	0
57	MG	1A	3247	1/1	0.95	0.19	47,47,47,47	0
57	MG	1A	3403	1/1	0.95	0.07	18,18,18,18	0
57	MG	1A	3248	1/1	0.95	0.12	28,28,28,28	0
57	MG	2A	3256	1/1	0.95	0.12	42,42,42,42	0
57	MG	15	102	1/1	0.95	0.44	36,36,36,36	0
57	MG	1A	3744	1/1	0.95	0.25	51,51,51,51	0
57	MG	2A	3096	1/1	0.95	0.14	46,46,46,46	0
57	MG	1A	3329	1/1	0.95	0.09	20,20,20,20	0
57	MG	15	105	1/1	0.95	0.15	39,39,39,39	0
57	MG	1a	1733	1/1	0.95	0.09	50,50,50,50	0
57	MG	1A	3330	1/1	0.95	0.06	34,34,34,34	0
57	MG	1A	3525	1/1	0.95	0.09	12,12,12,12	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	3076	1/1	0.95	0.08	39,39,39,39	0
57	MG	2D	305	1/1	0.95	0.08	34,34,34,34	0
57	MG	2x	107	1/1	0.95	0.06	74,74,74,74	0
57	MG	2A	3474	1/1	0.95	0.08	45,45,45,45	0
57	MG	2A	3103	1/1	0.95	0.11	52,52,52,52	0
57	MG	1A	3641	1/1	0.95	0.07	47,47,47,47	0
57	MG	1a	1604	1/1	0.96	0.15	68,68,68,68	0
57	MG	1a	1606	1/1	0.96	0.11	25,25,25,25	0
57	MG	1A	3408	1/1	0.96	0.06	26,26,26,26	0
57	MG	1a	1608	1/1	0.96	0.17	55,55,55,55	0
57	MG	2A	3304	1/1	0.96	0.14	34,34,34,34	0
57	MG	1A	3513	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3518	1/1	0.96	0.09	37,37,37,37	0
57	MG	2A	3497	1/1	0.96	0.13	34,34,34,34	0
57	MG	1A	3337	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	3258	1/1	0.96	0.14	16,16,16,16	0
57	MG	1A	3521	1/1	0.96	0.11	11,11,11,11	0
57	MG	1A	3522	1/1	0.96	0.09	39,39,39,39	0
57	MG	1A	3760	1/1	0.96	0.15	61,61,61,61	0
57	MG	1A	3259	1/1	0.96	0.15	32,32,32,32	0
57	MG	1A	3416	1/1	0.96	0.07	23,23,23,23	0
57	MG	23	101	1/1	0.96	0.13	40,40,40,40	0
57	MG	1A	3643	1/1	0.96	0.07	44,44,44,44	0
57	MG	1A	3417	1/1	0.96	0.07	18,18,18,18	0
57	MG	2A	3321	1/1	0.96	0.08	28,28,28,28	0
57	MG	1A	3260	1/1	0.96	0.22	40,40,40,40	0
57	MG	1A	3210	1/1	0.96	0.10	40,40,40,40	0
57	MG	2a	1601	1/1	0.96	0.18	33,33,33,33	0
57	MG	2A	3512	1/1	0.96	0.16	50,50,50,50	0
57	MG	2A	3513	1/1	0.96	0.18	54,54,54,54	0
57	MG	1A	3116	1/1	0.96	0.06	34,34,34,34	0
57	MG	1A	3422	1/1	0.96	0.12	35,35,35,35	0
57	MG	2A	3518	1/1	0.96	0.08	41,41,41,41	0
57	MG	1A	3774	1/1	0.96	0.13	35,35,35,35	0
57	MG	1A	3534	1/1	0.96	0.08	26,26,26,26	0
57	MG	1A	3776	1/1	0.96	0.08	46,46,46,46	0
57	MG	1A	3537	1/1	0.96	0.11	15,15,15,15	0
57	MG	1A	3423	1/1	0.96	0.10	15,15,15,15	0
57	MG	1a	1630	1/1	0.96	0.21	49,49,49,49	0
57	MG	1A	3779	1/1	0.96	0.12	38,38,38,38	0
57	MG	1a	1633	1/1	0.96	0.18	52,52,52,52	0
57	MG	1A	3345	1/1	0.96	0.09	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	2a	1616	1/1	0.96	0.10	38,38,38,38	0
57	MG	2A	3528	1/1	0.96	0.09	42,42,42,42	0
57	MG	2A	3341	1/1	0.96	0.19	30,30,30,30	0
57	MG	2A	3342	1/1	0.96	0.08	33,33,33,33	0
57	MG	1A	3140	1/1	0.96	0.16	26,26,26,26	0
57	MG	2A	3155	1/1	0.96	0.12	29,29,29,29	0
57	MG	1A	3080	1/1	0.96	0.08	22,22,22,22	0
57	MG	2A	3157	1/1	0.96	0.14	25,25,25,25	0
57	MG	1A	3544	1/1	0.96	0.10	13,13,13,13	0
57	MG	1x	108	1/1	0.96	0.05	60,60,60,60	0
57	MG	1A	3547	1/1	0.96	0.04	15,15,15,15	0
57	MG	2a	1629	1/1	0.96	0.12	50,50,50,50	0
57	MG	2A	3161	1/1	0.96	0.14	37,37,37,37	0
57	MG	1A	3660	1/1	0.96	0.06	39,39,39,39	0
57	MG	1A	3142	1/1	0.96	0.07	22,22,22,22	0
57	MG	1A	3788	1/1	0.96	0.10	17,17,17,17	0
57	MG	1A	3118	1/1	0.96	0.27	51,51,51,51	0
57	MG	2A	3002	1/1	0.96	0.14	46,46,46,46	0
57	MG	1A	3552	1/1	0.96	0.10	16,16,16,16	0
57	MG	1A	3665	1/1	0.96	0.06	41,41,41,41	0
57	MG	1A	3034	1/1	0.96	0.21	25,25,25,25	0
57	MG	1A	3217	1/1	0.96	0.13	53,53,53,53	0
57	MG	1A	3099	1/1	0.96	0.29	24,24,24,24	0
57	MG	1A	3558	1/1	0.96	0.11	31,31,31,31	0
57	MG	1A	3671	1/1	0.96	0.15	28,28,28,28	0
57	MG	1a	1652	1/1	0.96	0.10	41,41,41,41	0
57	MG	1A	3062	1/1	0.96	0.06	33,33,33,33	0
57	MG	1A	3560	1/1	0.96	0.09	50,50,50,50	0
57	MG	1A	3438	1/1	0.96	0.06	15,15,15,15	0
57	MG	1a	1656	1/1	0.96	0.07	53,53,53,53	0
57	MG	2A	3561	1/1	0.96	0.06	33,33,33,33	0
57	MG	2A	3374	1/1	0.96	0.12	65,65,65,65	0
57	MG	1A	3057	1/1	0.96	0.08	18,18,18,18	0
57	MG	2A	3021	1/1	0.96	0.11	20,20,20,20	0
57	MG	1B	210	1/1	0.96	0.19	48,48,48,48	0
57	MG	1A	3360	1/1	0.96	0.13	11,11,11,11	0
57	MG	2A	3380	1/1	0.96	0.09	46,46,46,46	0
57	MG	2A	3187	1/1	0.96	0.21	48,48,48,48	0
57	MG	1a	1661	1/1	0.96	0.08	56,56,56,56	0
57	MG	1A	3104	1/1	0.96	0.17	48,48,48,48	0
57	MG	1A	3679	1/1	0.96	0.08	22,22,22,22	0
57	MG	1A	3222	1/1	0.96	0.11	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	2A	3386	1/1	0.96	0.11	48,48,48,48	0
57	MG	1B	219	1/1	0.96	0.08	28,28,28,28	0
57	MG	1A	3281	1/1	0.96	0.15	30,30,30,30	0
57	MG	1A	3282	1/1	0.96	0.06	33,33,33,33	0
57	MG	1A	3224	1/1	0.96	0.24	38,38,38,38	0
57	MG	1A	3448	1/1	0.96	0.07	17,17,17,17	0
57	MG	1A	3451	1/1	0.96	0.12	17,17,17,17	0
57	MG	1A	3284	1/1	0.96	0.18	29,29,29,29	0
57	MG	1A	3453	1/1	0.96	0.08	47,47,47,47	0
57	MG	2A	3040	1/1	0.96	0.07	48,48,48,48	0
57	MG	1A	3285	1/1	0.96	0.05	24,24,24,24	0
57	MG	2A	3585	1/1	0.96	0.10	42,42,42,42	0
57	MG	1A	3051	1/1	0.96	0.08	22,22,22,22	0
57	MG	2A	3587	1/1	0.96	0.13	52,52,52,52	0
57	MG	1A	3370	1/1	0.96	0.05	32,32,32,32	0
57	MG	2a	1680	1/1	0.96	0.11	57,57,57,57	0
57	MG	1A	3290	1/1	0.96	0.07	29,29,29,29	0
57	MG	1A	3583	1/1	0.96	0.08	31,31,31,31	0
57	MG	1E	306	1/1	0.96	0.09	11,11,11,11	0
57	MG	2a	1684	1/1	0.96	0.17	38,38,38,38	0
57	MG	2A	3049	1/1	0.96	0.07	40,40,40,40	0
57	MG	2A	3050	1/1	0.96	0.10	48,48,48,48	0
57	MG	1A	3584	1/1	0.96	0.09	63,63,63,63	0
57	MG	1A	3291	1/1	0.96	0.12	40,40,40,40	0
57	MG	2A	3406	1/1	0.96	0.17	35,35,35,35	0
57	MG	2A	3407	1/1	0.96	0.07	25,25,25,25	0
57	MG	1A	3586	1/1	0.96	0.09	46,46,46,46	0
57	MG	1A	3374	1/1	0.96	0.05	37,37,37,37	0
57	MG	1F	308	1/1	0.96	0.11	20,20,20,20	0
57	MG	1A	3702	1/1	0.96	0.11	43,43,43,43	0
57	MG	1G	201	1/1	0.96	0.11	60,60,60,60	0
57	MG	2A	3058	1/1	0.96	0.07	51,51,51,51	0
57	MG	1a	1688	1/1	0.96	0.06	32,32,32,32	0
57	MG	1a	1689	1/1	0.96	0.07	32,32,32,32	0
57	MG	1A	3187	1/1	0.96	0.27	44,44,44,44	0
57	MG	1A	3463	1/1	0.96	0.18	32,32,32,32	0
57	MG	2A	3065	1/1	0.96	0.14	29,29,29,29	0
57	MG	2A	3610	1/1	0.96	0.10	61,61,61,61	0
57	MG	1A	3126	1/1	0.96	0.16	27,27,27,27	0
57	MG	2A	3420	1/1	0.96	0.06	23,23,23,23	0
57	MG	1A	3129	1/1	0.96	0.07	25,25,25,25	0
57	MG	1a	1699	1/1	0.96	0.09	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	1700	1/1	0.96	0.15	60,60,60,60	0
57	MG	2a	1712	1/1	0.96	0.05	58,58,58,58	0
57	MG	1A	3156	1/1	0.96	0.09	22,22,22,22	0
57	MG	2A	3426	1/1	0.96	0.17	22,22,22,22	0
57	MG	1a	1703	1/1	0.96	0.06	33,33,33,33	0
57	MG	2A	3232	1/1	0.96	0.09	41,41,41,41	0
57	MG	1A	3093	1/1	0.96	0.12	41,41,41,41	0
57	MG	2A	3431	1/1	0.96	0.07	45,45,45,45	0
57	MG	1A	3233	1/1	0.96	0.33	37,37,37,37	0
57	MG	1A	3234	1/1	0.96	0.06	24,24,24,24	0
57	MG	2A	3435	1/1	0.96	0.12	34,34,34,34	0
57	MG	1A	3235	1/1	0.96	0.14	15,15,15,15	0
57	MG	1A	3311	1/1	0.96	0.06	16,16,16,16	0
57	MG	2A	3078	1/1	0.96	0.14	44,44,44,44	0
57	MG	1A	3237	1/1	0.96	0.12	23,23,23,23	0
57	MG	1A	3387	1/1	0.96	0.10	41,41,41,41	0
57	MG	1A	3603	1/1	0.96	0.07	57,57,57,57	0
57	MG	1A	3604	1/1	0.96	0.12	34,34,34,34	0
57	MG	2A	3634	1/1	0.96	0.19	51,51,51,51	0
57	MG	2A	3246	1/1	0.96	0.13	54,54,54,54	0
57	MG	1U	203	1/1	0.96	0.10	24,24,24,24	0
57	MG	1A	3605	1/1	0.96	0.14	37,37,37,37	0
57	MG	1U	205	1/1	0.96	0.07	32,32,32,32	0
57	MG	2A	3639	1/1	0.96	0.16	22,22,22,22	0
57	MG	1A	3052	1/1	0.96	0.15	36,36,36,36	0
57	MG	2A	3089	1/1	0.96	0.11	27,27,27,27	0
57	MG	2A	3642	1/1	0.96	0.13	43,43,43,43	0
57	MG	2a	1738	1/1	0.96	0.14	36,36,36,36	0
57	MG	1V	201	1/1	0.96	0.21	18,18,18,18	0
57	MG	2a	1740	1/1	0.96	0.15	40,40,40,40	0
57	MG	1A	3721	1/1	0.96	0.07	31,31,31,31	0
57	MG	1A	3609	1/1	0.96	0.14	30,30,30,30	0
57	MG	2a	1743	1/1	0.96	0.11	48,48,48,48	0
57	MG	1A	3161	1/1	0.96	0.22	42,42,42,42	0
57	MG	2A	3648	1/1	0.96	0.06	25,25,25,25	0
57	MG	2A	3455	1/1	0.96	0.06	40,40,40,40	0
57	MG	2a	1748	1/1	0.96	0.17	50,50,50,50	0
57	MG	2A	3260	1/1	0.96	0.06	24,24,24,24	0
57	MG	2A	3457	1/1	0.96	0.21	47,47,47,47	0
57	MG	1A	3724	1/1	0.96	0.09	34,34,34,34	0
57	MG	1A	3195	1/1	0.96	0.08	28,28,28,28	0
57	MG	1A	3196	1/1	0.96	0.05	38,38,38,38	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	1725	1/1	0.96	0.19	49,49,49,49	0
57	MG	2a	1755	1/1	0.96	0.08	46,46,46,46	0
57	MG	1A	3197	1/1	0.96	0.17	45,45,45,45	0
57	MG	1A	3614	1/1	0.96	0.06	35,35,35,35	0
57	MG	1A	3198	1/1	0.96	0.17	38,38,38,38	0
57	MG	2a	1759	1/1	0.96	0.08	61,61,61,61	0
57	MG	1A	3394	1/1	0.96	0.08	23,23,23,23	0
57	MG	1A	3110	1/1	0.96	0.18	49,49,49,49	0
57	MG	1A	3497	1/1	0.96	0.07	54,54,54,54	0
57	MG	1A	3736	1/1	0.96	0.06	37,37,37,37	0
57	MG	1A	3499	1/1	0.96	0.09	32,32,32,32	0
57	MG	2A	3108	1/1	0.96	0.14	45,45,45,45	0
57	MG	1A	3111	1/1	0.96	0.09	29,29,29,29	0
57	MG	1A	3203	1/1	0.96	0.15	26,26,26,26	0
57	MG	1A	3399	1/1	0.96	0.11	31,31,31,31	0
57	MG	1a	1739	1/1	0.96	0.06	23,23,23,23	0
57	MG	1a	1740	1/1	0.96	0.07	40,40,40,40	0
57	MG	2k	202	1/1	0.96	0.07	61,61,61,61	0
57	MG	1A	3252	1/1	0.96	0.06	39,39,39,39	0
57	MG	1A	3167	1/1	0.96	0.21	46,46,46,46	0
57	MG	1A	3331	1/1	0.96	0.06	33,33,33,33	0
57	MG	1A	3022	1/1	0.96	0.10	16,16,16,16	0
57	MG	2E	301	1/1	0.96	0.13	36,36,36,36	0
57	MG	1A	3508	1/1	0.96	0.10	35,35,35,35	0
57	MG	2E	303	1/1	0.96	0.29	49,49,49,49	0
57	MG	2A	3120	1/1	0.96	0.18	38,38,38,38	0
57	MG	2A	3294	1/1	0.96	0.08	43,43,43,43	0
57	MG	19	101	1/1	0.96	0.11	33,33,33,33	0
57	MG	2A	3296	1/1	0.96	0.07	37,37,37,37	0
57	MG	1A	3078	1/1	0.96	0.06	34,34,34,34	0
57	MG	1A	3209	1/1	0.96	0.19	35,35,35,35	0
58	ZN	24	501	1/1	0.96	0.09	140,140,140,140	0
58	ZN	2n	501	1/1	0.96	0.07	93,93,93,93	0
57	MG	2A	3016	1/1	0.97	0.14	48,48,48,48	0
57	MG	2A	3335	1/1	0.97	0.10	62,62,62,62	0
57	MG	1A	3003	1/1	0.97	0.12	17,17,17,17	0
57	MG	2A	3337	1/1	0.97	0.05	35,35,35,35	0
57	MG	1A	3145	1/1	0.97	0.18	30,30,30,30	0
57	MG	2A	3339	1/1	0.97	0.07	27,27,27,27	0
57	MG	1a	1672	1/1	0.97	0.31	55,55,55,55	0
57	MG	1A	3640	1/1	0.97	0.09	39,39,39,39	0
57	MG	1A	3316	1/1	0.97	0.06	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	1Q	201	1/1	0.97	0.16	41,41,41,41	0
57	MG	1A	3642	1/1	0.97	0.04	44,44,44,44	0
57	MG	2A	3025	1/1	0.97	0.11	39,39,39,39	0
57	MG	2A	3169	1/1	0.97	0.12	43,43,43,43	0
57	MG	1Q	203	1/1	0.97	0.09	16,16,16,16	0
57	MG	1A	3554	1/1	0.97	0.06	40,40,40,40	0
57	MG	1A	3555	1/1	0.97	0.18	46,46,46,46	0
57	MG	2A	3173	1/1	0.97	0.17	43,43,43,43	0
57	MG	1A	3645	1/1	0.97	0.13	33,33,33,33	0
57	MG	2A	3352	1/1	0.97	0.11	40,40,40,40	0
57	MG	1R	202	1/1	0.97	0.30	28,28,28,28	0
57	MG	2A	3031	1/1	0.97	0.07	34,34,34,34	0
57	MG	2a	1619	1/1	0.97	0.16	33,33,33,33	0
57	MG	2A	3178	1/1	0.97	0.07	51,51,51,51	0
57	MG	2a	1621	1/1	0.97	0.11	43,43,43,43	0
57	MG	2A	3541	1/1	0.97	0.06	61,61,61,61	0
57	MG	1A	3178	1/1	0.97	0.07	27,27,27,27	0
57	MG	2A	3358	1/1	0.97	0.10	50,50,50,50	0
57	MG	1U	202	1/1	0.97	0.23	19,19,19,19	0
57	MG	1A	3056	1/1	0.97	0.11	19,19,19,19	0
57	MG	1a	1685	1/1	0.97	0.12	37,37,37,37	0
57	MG	1A	3320	1/1	0.97	0.07	42,42,42,42	0
57	MG	1A	3460	1/1	0.97	0.12	40,40,40,40	0
57	MG	2a	1630	1/1	0.97	0.22	51,51,51,51	0
57	MG	1U	206	1/1	0.97	0.17	32,32,32,32	0
57	MG	1A	3461	1/1	0.97	0.24	41,41,41,41	0
57	MG	1a	1690	1/1	0.97	0.11	39,39,39,39	0
57	MG	2A	3042	1/1	0.97	0.15	41,41,41,41	0
57	MG	1A	3041	1/1	0.97	0.10	16,16,16,16	0
57	MG	1A	3752	1/1	0.97	0.22	26,26,26,26	0
57	MG	2A	3557	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3183	1/1	0.97	0.17	23,23,23,23	0
57	MG	1V	205	1/1	0.97	0.21	28,28,28,28	0
57	MG	1a	1698	1/1	0.97	0.14	54,54,54,54	0
57	MG	1A	3325	1/1	0.97	0.09	41,41,41,41	0
57	MG	1A	3755	1/1	0.97	0.12	38,38,38,38	0
57	MG	1A	3262	1/1	0.97	0.10	39,39,39,39	0
57	MG	1A	3042	1/1	0.97	0.23	33,33,33,33	0
57	MG	1X	103	1/1	0.97	0.10	25,25,25,25	0
57	MG	1A	3004	1/1	0.97	0.10	17,17,17,17	0
57	MG	1A	3012	1/1	0.97	0.05	18,18,18,18	0
57	MG	1a	1707	1/1	0.97	0.18	57,57,57,57	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	102	1/1	0.97	0.17	40,40,40,40	0
57	MG	2a	1651	1/1	0.97	0.14	48,48,48,48	0
57	MG	1A	3473	1/1	0.97	0.13	41,41,41,41	0
57	MG	2A	3059	1/1	0.97	0.17	49,49,49,49	0
57	MG	2A	3060	1/1	0.97	0.06	45,45,45,45	0
57	MG	11	101	1/1	0.97	0.26	31,31,31,31	0
57	MG	1A	3033	1/1	0.97	0.23	19,19,19,19	0
57	MG	1A	3153	1/1	0.97	0.14	34,34,34,34	0
57	MG	1A	3763	1/1	0.97	0.06	40,40,40,40	0
57	MG	1A	3223	1/1	0.97	0.10	35,35,35,35	0
57	MG	1A	3664	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3189	1/1	0.97	0.22	30,30,30,30	0
57	MG	2A	3214	1/1	0.97	0.17	28,28,28,28	0
57	MG	1A	3578	1/1	0.97	0.06	36,36,36,36	0
57	MG	1A	3335	1/1	0.97	0.05	15,15,15,15	0
57	MG	2a	1665	1/1	0.97	0.17	43,43,43,43	0
57	MG	1A	3772	1/1	0.97	0.04	34,34,34,34	0
57	MG	2A	3071	1/1	0.97	0.13	43,43,43,43	0
57	MG	16	101	1/1	0.97	0.13	44,44,44,44	0
57	MG	1A	3668	1/1	0.97	0.10	10,10,10,10	0
57	MG	1A	3398	1/1	0.97	0.07	45,45,45,45	0
57	MG	1A	3336	1/1	0.97	0.10	38,38,38,38	0
57	MG	2a	1672	1/1	0.97	0.16	30,30,30,30	0
57	MG	1A	3102	1/1	0.97	0.16	34,34,34,34	0
57	MG	1A	3013	1/1	0.97	0.15	24,24,24,24	0
57	MG	1A	3274	1/1	0.97	0.04	18,18,18,18	0
57	MG	1a	1602	1/1	0.97	0.08	45,45,45,45	0
57	MG	1A	3491	1/1	0.97	0.08	48,48,48,48	0
57	MG	1A	3128	1/1	0.97	0.46	23,23,23,23	0
57	MG	1a	1605	1/1	0.97	0.21	37,37,37,37	0
57	MG	2A	3231	1/1	0.97	0.11	50,50,50,50	0
57	MG	1A	3341	1/1	0.97	0.06	22,22,22,22	0
57	MG	2A	3233	1/1	0.97	0.12	48,48,48,48	0
57	MG	1A	3157	1/1	0.97	0.15	35,35,35,35	0
57	MG	2A	3085	1/1	0.97	0.17	39,39,39,39	0
57	MG	1A	3496	1/1	0.97	0.05	24,24,24,24	0
57	MG	1A	3083	1/1	0.97	0.32	30,30,30,30	0
57	MG	2A	3088	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3344	1/1	0.97	0.06	13,13,13,13	0
57	MG	2a	1689	1/1	0.97	0.09	43,43,43,43	0
57	MG	1a	1611	1/1	0.97	0.14	37,37,37,37	0
57	MG	1A	3593	1/1	0.97	0.07	18,18,18,18	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	1692	1/1	0.97	0.07	36,36,36,36	0
57	MG	1A	3231	1/1	0.97	0.10	34,34,34,34	0
57	MG	2A	3424	1/1	0.97	0.09	26,26,26,26	0
57	MG	2A	3244	1/1	0.97	0.08	43,43,43,43	0
57	MG	1A	3346	1/1	0.97	0.10	22,22,22,22	0
57	MG	2A	3427	1/1	0.97	0.14	46,46,46,46	0
57	MG	1A	3349	1/1	0.97	0.05	29,29,29,29	0
57	MG	2A	3247	1/1	0.97	0.06	41,41,41,41	0
57	MG	2A	3095	1/1	0.97	0.10	33,33,33,33	0
57	MG	1A	3023	1/1	0.97	0.16	32,32,32,32	0
57	MG	1A	3005	1/1	0.97	0.05	37,37,37,37	0
57	MG	1a	1745	1/1	0.97	0.06	45,45,45,45	0
57	MG	1A	3162	1/1	0.97	0.14	30,30,30,30	0
57	MG	1A	3691	1/1	0.97	0.10	50,50,50,50	0
57	MG	1A	3087	1/1	0.97	0.09	15,15,15,15	0
57	MG	1A	3286	1/1	0.97	0.13	22,22,22,22	0
57	MG	1A	3236	1/1	0.97	0.07	22,22,22,22	0
57	MG	2A	3104	1/1	0.97	0.13	33,33,33,33	0
57	MG	1A	3288	1/1	0.97	0.07	40,40,40,40	0
57	MG	1A	3289	1/1	0.97	0.28	36,36,36,36	0
57	MG	2A	3264	1/1	0.97	0.07	30,30,30,30	0
57	MG	1A	3199	1/1	0.97	0.07	40,40,40,40	0
57	MG	2A	3266	1/1	0.97	0.15	32,32,32,32	0
57	MG	1A	3608	1/1	0.97	0.08	26,26,26,26	0
57	MG	2A	3268	1/1	0.97	0.18	56,56,56,56	0
57	MG	1A	3135	1/1	0.97	0.12	32,32,32,32	0
57	MG	1A	3292	1/1	0.97	0.14	30,30,30,30	0
57	MG	1A	3432	1/1	0.97	0.05	26,26,26,26	0
57	MG	1A	3109	1/1	0.97	0.09	24,24,24,24	0
57	MG	1a	1631	1/1	0.97	0.08	23,23,23,23	0
57	MG	1A	3202	1/1	0.97	0.29	20,20,20,20	0
57	MG	1A	3088	1/1	0.97	0.04	11,11,11,11	0
57	MG	1A	3299	1/1	0.97	0.16	26,26,26,26	0
57	MG	1A	3300	1/1	0.97	0.07	46,46,46,46	0
57	MG	1A	3065	1/1	0.97	0.21	21,21,21,21	0
57	MG	2A	3119	1/1	0.97	0.07	44,44,44,44	0
57	MG	2A	3280	1/1	0.97	0.14	32,32,32,32	0
57	MG	1A	3009	1/1	0.97	0.04	11,11,11,11	0
57	MG	2A	3282	1/1	0.97	0.09	43,43,43,43	0
57	MG	1D	305	1/1	0.97	0.05	24,24,24,24	0
57	MG	1A	3442	1/1	0.97	0.04	20,20,20,20	0
57	MG	2A	3286	1/1	0.97	0.10	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3467	1/1	0.97	0.10	50,50,50,50	0
57	MG	1A	3369	1/1	0.97	0.07	18,18,18,18	0
57	MG	1A	3305	1/1	0.97	0.11	25,25,25,25	0
57	MG	1A	3535	1/1	0.97	0.06	17,17,17,17	0
57	MG	1E	301	1/1	0.97	0.19	28,28,28,28	0
57	MG	2A	3291	1/1	0.97	0.05	47,47,47,47	0
57	MG	2A	3473	1/1	0.97	0.04	40,40,40,40	0
57	MG	1A	3536	1/1	0.97	0.07	29,29,29,29	0
57	MG	2A	3128	1/1	0.97	0.11	48,48,48,48	0
57	MG	1A	3624	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	3114	1/1	0.97	0.16	11,11,11,11	0
57	MG	1A	3538	1/1	0.97	0.07	14,14,14,14	0
57	MG	1x	101	1/1	0.97	0.20	44,44,44,44	0
57	MG	1a	1649	1/1	0.97	0.21	47,47,47,47	0
57	MG	1A	3539	1/1	0.97	0.13	18,18,18,18	0
57	MG	1A	3207	1/1	0.97	0.04	25,25,25,25	0
57	MG	2D	302	1/1	0.97	0.12	22,22,22,22	0
57	MG	1F	302	1/1	0.97	0.15	24,24,24,24	0
57	MG	1F	304	1/1	0.97	0.26	37,37,37,37	0
57	MG	2A	3303	1/1	0.97	0.10	25,25,25,25	0
57	MG	1x	107	1/1	0.97	0.09	47,47,47,47	0
57	MG	1A	3208	1/1	0.97	0.16	21,21,21,21	0
57	MG	1F	306	1/1	0.97	0.10	29,29,29,29	0
57	MG	2A	3307	1/1	0.97	0.05	33,33,33,33	0
57	MG	1x	110	1/1	0.97	0.10	36,36,36,36	0
57	MG	2E	304	1/1	0.97	0.05	46,46,46,46	0
57	MG	1A	3630	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3375	1/1	0.97	0.10	20,20,20,20	0
57	MG	1F	309	1/1	0.97	0.14	28,28,28,28	0
57	MG	2A	3494	1/1	0.97	0.09	42,42,42,42	0
57	MG	1F	310	1/1	0.97	0.08	15,15,15,15	0
57	MG	2A	3313	1/1	0.97	0.11	23,23,23,23	0
57	MG	2A	3146	1/1	0.97	0.21	42,42,42,42	0
57	MG	2j	201	1/1	0.97	0.15	58,58,58,58	0
57	MG	2A	3498	1/1	0.97	0.08	34,34,34,34	0
57	MG	1a	1660	1/1	0.97	0.10	40,40,40,40	0
57	MG	2A	3004	1/1	0.97	0.17	27,27,27,27	0
57	MG	2A	3317	1/1	0.97	0.10	35,35,35,35	0
57	MG	2A	3318	1/1	0.97	0.07	54,54,54,54	0
57	MG	2A	3319	1/1	0.97	0.09	42,42,42,42	0
57	MG	1A	3449	1/1	0.97	0.06	16,16,16,16	0
57	MG	1F	312	1/1	0.97	0.04	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	1F	314	1/1	0.97	0.09	27,27,27,27	0
57	MG	2A	3008	1/1	0.97	0.05	30,30,30,30	0
57	MG	2A	3009	1/1	0.97	0.10	47,47,47,47	0
57	MG	1A	3092	1/1	0.97	0.18	31,31,31,31	0
57	MG	1A	3545	1/1	0.97	0.07	13,13,13,13	0
57	MG	1A	3174	1/1	0.97	0.37	28,28,28,28	0
57	MG	1A	3017	1/1	0.97	0.12	22,22,22,22	0
57	MG	1A	3733	1/1	0.97	0.04	35,35,35,35	0
57	MG	1A	3549	1/1	0.97	0.05	56,56,56,56	0
57	MG	1A	3328	1/1	0.98	0.03	16,16,16,16	0
57	MG	2A	3517	1/1	0.98	0.04	57,57,57,57	0
57	MG	1T	201	1/1	0.98	0.06	39,39,39,39	0
57	MG	1A	3131	1/1	0.98	0.17	25,25,25,25	0
57	MG	1A	3483	1/1	0.98	0.12	28,28,28,28	0
57	MG	2A	3647	1/1	0.98	0.10	32,32,32,32	0
57	MG	1A	3695	1/1	0.98	0.05	29,29,29,29	0
57	MG	1A	3372	1/1	0.98	0.05	48,48,48,48	0
57	MG	1A	3101	1/1	0.98	0.07	35,35,35,35	0
57	MG	1A	3255	1/1	0.98	0.23	31,31,31,31	0
57	MG	1A	3487	1/1	0.98	0.06	22,22,22,22	0
57	MG	1U	208	1/1	0.98	0.04	26,26,26,26	0
57	MG	2A	3175	1/1	0.98	0.05	34,34,34,34	0
57	MG	1a	1758	1/1	0.98	0.06	47,47,47,47	0
57	MG	1A	3133	1/1	0.98	0.06	28,28,28,28	0
57	MG	1A	3701	1/1	0.98	0.04	21,21,21,21	0
57	MG	1V	203	1/1	0.98	0.10	18,18,18,18	0
57	MG	1A	3046	1/1	0.98	0.15	19,19,19,19	0
57	MG	1A	3091	1/1	0.98	0.16	30,30,30,30	0
57	MG	1A	3079	1/1	0.98	0.10	22,22,22,22	0
57	MG	1A	3564	1/1	0.98	0.07	32,32,32,32	0
57	MG	1A	3229	1/1	0.98	0.53	24,24,24,24	0
57	MG	1A	3789	1/1	0.98	0.08	18,18,18,18	0
57	MG	1A	3434	1/1	0.98	0.04	11,11,11,11	0
57	MG	1A	3295	1/1	0.98	0.10	22,22,22,22	0
57	MG	1A	3709	1/1	0.98	0.08	50,50,50,50	0
57	MG	1m	3001	1/1	0.98	0.04	62,62,62,62	0
57	MG	10	101	1/1	0.98	0.22	36,36,36,36	0
57	MG	1A	3569	1/1	0.98	0.08	14,14,14,14	0
57	MG	10	103	1/1	0.98	0.07	36,36,36,36	0
57	MG	1A	3181	1/1	0.98	0.16	25,25,25,25	0
57	MG	2A	3548	1/1	0.98	0.06	24,24,24,24	0
57	MG	1A	3298	1/1	0.98	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	1w	402	1/1	0.98	0.18	36,36,36,36	0
57	MG	1A	3182	1/1	0.98	0.05	20,20,20,20	0
57	MG	11	103	1/1	0.98	0.06	29,29,29,29	0
57	MG	1A	3105	1/1	0.98	0.10	17,17,17,17	0
57	MG	1A	3302	1/1	0.98	0.05	30,30,30,30	0
57	MG	2A	3432	1/1	0.98	0.06	42,42,42,42	0
57	MG	1A	3441	1/1	0.98	0.05	28,28,28,28	0
57	MG	1B	207	1/1	0.98	0.07	42,42,42,42	0
57	MG	2F	302	1/1	0.98	0.04	34,34,34,34	0
57	MG	1A	3717	1/1	0.98	0.14	32,32,32,32	0
57	MG	1A	3576	1/1	0.98	0.09	15,15,15,15	0
57	MG	1A	3386	1/1	0.98	0.04	35,35,35,35	0
57	MG	2a	1706	1/1	0.98	0.08	46,46,46,46	0
57	MG	1A	3158	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3507	1/1	0.98	0.17	27,27,27,27	0
57	MG	17	101	1/1	0.98	0.13	26,26,26,26	0
57	MG	2Q	202	1/1	0.98	0.05	42,42,42,42	0
57	MG	17	102	1/1	0.98	0.12	34,34,34,34	0
57	MG	2A	3322	1/1	0.98	0.11	45,45,45,45	0
57	MG	1B	213	1/1	0.98	0.05	30,30,30,30	0
57	MG	2A	3325	1/1	0.98	0.04	39,39,39,39	0
57	MG	2A	3210	1/1	0.98	0.05	31,31,31,31	0
57	MG	2A	3446	1/1	0.98	0.06	45,45,45,45	0
57	MG	17	104	1/1	0.98	0.08	20,20,20,20	0
57	MG	1A	3070	1/1	0.98	0.06	27,27,27,27	0
57	MG	2A	3003	1/1	0.98	0.10	18,18,18,18	0
57	MG	1a	1691	1/1	0.98	0.06	42,42,42,42	0
57	MG	2A	3215	1/1	0.98	0.13	46,46,46,46	0
57	MG	2A	3452	1/1	0.98	0.08	30,30,30,30	0
57	MG	1B	216	1/1	0.98	0.08	39,39,39,39	0
57	MG	1a	1694	1/1	0.98	0.09	45,45,45,45	0
57	MG	1A	3025	1/1	0.98	0.17	30,30,30,30	0
57	MG	18	102	1/1	0.98	0.07	30,30,30,30	0
57	MG	1A	3306	1/1	0.98	0.11	50,50,50,50	0
57	MG	1A	3347	1/1	0.98	0.04	17,17,17,17	0
57	MG	1A	3726	1/1	0.98	0.06	14,14,14,14	0
57	MG	1A	3348	1/1	0.98	0.10	35,35,35,35	0
57	MG	1A	3514	1/1	0.98	0.08	45,45,45,45	0
57	MG	1A	3516	1/1	0.98	0.07	17,17,17,17	0
57	MG	1A	3084	1/1	0.98	0.09	5,5,5,5	0
57	MG	1A	3588	1/1	0.98	0.04	21,21,21,21	0
57	MG	1A	3450	1/1	0.98	0.06	11,11,11,11	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	3043	1/1	0.98	0.41	25,25,25,25	0
57	MG	1A	3659	1/1	0.98	0.07	67,67,67,67	0
57	MG	1A	3002	1/1	0.98	0.17	35,35,35,35	0
57	MG	1A	3310	1/1	0.98	0.08	33,33,33,33	0
57	MG	2A	3022	1/1	0.98	0.05	35,35,35,35	0
57	MG	1A	3143	1/1	0.98	0.05	23,23,23,23	0
57	MG	1A	3354	1/1	0.98	0.06	10,10,10,10	0
57	MG	1A	3741	1/1	0.98	0.10	22,22,22,22	0
57	MG	2a	1744	1/1	0.98	0.05	53,53,53,53	0
57	MG	1A	3526	1/1	0.98	0.15	35,35,35,35	0
57	MG	1A	3240	1/1	0.98	0.05	29,29,29,29	0
57	MG	1A	3125	1/1	0.98	0.12	19,19,19,19	0
57	MG	2A	3601	1/1	0.98	0.09	37,37,37,37	0
57	MG	2A	3240	1/1	0.98	0.18	38,38,38,38	0
57	MG	1A	3243	1/1	0.98	0.11	24,24,24,24	0
57	MG	1A	3014	1/1	0.98	0.11	19,19,19,19	0
57	MG	1A	3404	1/1	0.98	0.05	10,10,10,10	0
57	MG	2A	3032	1/1	0.98	0.21	39,39,39,39	0
57	MG	1A	3748	1/1	0.98	0.14	33,33,33,33	0
57	MG	1A	3245	1/1	0.98	0.07	32,32,32,32	0
57	MG	1A	3278	1/1	0.98	0.16	11,11,11,11	0
57	MG	1A	3279	1/1	0.98	0.04	17,17,17,17	0
57	MG	1A	3319	1/1	0.98	0.06	10,10,10,10	0
57	MG	2A	3250	1/1	0.98	0.09	33,33,33,33	0
57	MG	2a	1632	1/1	0.98	0.10	48,48,48,48	0
57	MG	1A	3606	1/1	0.98	0.06	37,37,37,37	0
57	MG	1F	313	1/1	0.98	0.08	27,27,27,27	0
57	MG	1a	1727	1/1	0.98	0.11	44,44,44,44	0
57	MG	1A	3675	1/1	0.98	0.07	53,53,53,53	0
57	MG	2A	3255	1/1	0.98	0.04	41,41,41,41	0
57	MG	1A	3409	1/1	0.98	0.11	8,8,8,8	0
57	MG	1A	3169	1/1	0.98	0.19	24,24,24,24	0
57	MG	2A	3378	1/1	0.98	0.11	42,42,42,42	0
57	MG	2A	3258	1/1	0.98	0.07	37,37,37,37	0
57	MG	1A	3321	1/1	0.98	0.07	25,25,25,25	0
57	MG	1A	3468	1/1	0.98	0.07	54,54,54,54	0
57	MG	2A	3046	1/1	0.98	0.24	59,59,59,59	0
57	MG	1A	3469	1/1	0.98	0.06	23,23,23,23	0
57	MG	1A	3127	1/1	0.98	0.19	28,28,28,28	0
57	MG	1a	1636	1/1	0.98	0.05	49,49,49,49	0
57	MG	1O	201	1/1	0.98	0.12	31,31,31,31	0
57	MG	1A	3147	1/1	0.98	0.20	25,25,25,25	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	3112	1/1	0.98	0.21	38,38,38,38	0
57	MG	1A	3546	1/1	0.98	0.07	24,24,24,24	0
57	MG	1A	3764	1/1	0.98	0.05	25,25,25,25	0
57	MG	1A	3068	1/1	0.98	0.11	26,26,26,26	0
57	MG	1A	3477	1/1	0.98	0.07	37,37,37,37	0
57	MG	1A	3419	1/1	0.98	0.03	18,18,18,18	0
57	MG	1A	3550	1/1	0.98	0.05	25,25,25,25	0
57	MG	1A	3690	1/1	0.98	0.12	27,27,27,27	0
58	ZN	1n	102	1/1	0.98	0.05	91,91,91,91	0
58	ZN	2Y	202	1/1	0.98	0.04	92,92,92,92	0
57	MG	1A	3077	1/1	0.98	0.07	32,32,32,32	0
57	MG	2A	3515	1/1	0.98	0.04	51,51,51,51	0
59	SF4	1d	501	8/8	0.98	0.05	54,70,79,79	0
57	MG	1F	303	1/1	0.99	0.12	23,23,23,23	0
57	MG	1A	3410	1/1	0.99	0.10	10,10,10,10	0
57	MG	1A	3783	1/1	0.99	0.08	23,23,23,23	0
57	MG	2A	3355	1/1	0.99	0.09	31,31,31,31	0
57	MG	1A	3737	1/1	0.99	0.07	29,29,29,29	0
57	MG	1A	3528	1/1	0.99	0.04	13,13,13,13	0
57	MG	1A	3651	1/1	0.99	0.06	30,30,30,30	0
57	MG	1A	3529	1/1	0.99	0.06	21,21,21,21	0
57	MG	1A	3081	1/1	0.99	0.05	13,13,13,13	0
57	MG	13	101	1/1	0.99	0.23	31,31,31,31	0
57	MG	2A	3362	1/1	0.99	0.07	24,24,24,24	0
57	MG	2A	3363	1/1	0.99	0.06	28,28,28,28	0
57	MG	2A	3364	1/1	0.99	0.04	33,33,33,33	0
57	MG	1A	3301	1/1	0.99	0.05	28,28,28,28	0
57	MG	1A	3163	1/1	0.99	0.10	11,11,11,11	0
57	MG	1a	1693	1/1	0.99	0.05	50,50,50,50	0
57	MG	1A	3495	1/1	0.99	0.05	38,38,38,38	0
57	MG	2A	3633	1/1	0.99	0.05	31,31,31,31	0
57	MG	1A	3414	1/1	0.99	0.03	19,19,19,19	0
57	MG	1A	3415	1/1	0.99	0.04	13,13,13,13	0
57	MG	1A	3498	1/1	0.99	0.03	46,46,46,46	0
57	MG	1A	3082	1/1	0.99	0.25	25,25,25,25	0
57	MG	1A	3242	1/1	0.99	0.04	22,22,22,22	0
57	MG	1A	3037	1/1	0.99	0.12	26,26,26,26	0
57	MG	2A	3570	1/1	0.99	0.03	38,38,38,38	0
57	MG	1a	1701	1/1	0.99	0.03	29,29,29,29	0
57	MG	1A	3166	1/1	0.99	0.05	27,27,27,27	0
57	MG	1A	3470	1/1	0.99	0.09	30,30,30,30	0
57	MG	1A	3075	1/1	0.99	0.13	21,21,21,21	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	3472	1/1	0.99	0.10	17,17,17,17	0
57	MG	1A	3018	1/1	0.99	0.09	31,31,31,31	0
57	MG	17	107	1/1	0.99	0.05	37,37,37,37	0
57	MG	1A	3047	1/1	0.99	0.13	22,22,22,22	0
57	MG	2A	3511	1/1	0.99	0.12	25,25,25,25	0
57	MG	1A	3475	1/1	0.99	0.04	19,19,19,19	0
57	MG	1A	3509	1/1	0.99	0.06	22,22,22,22	0
57	MG	2A	3262	1/1	0.99	0.08	34,34,34,34	0
57	MG	1A	3401	1/1	0.99	0.04	21,21,21,21	0
57	MG	2A	3323	1/1	0.99	0.07	18,18,18,18	0
57	MG	1A	3053	1/1	0.99	0.06	25,25,25,25	0
57	MG	1B	215	1/1	0.99	0.06	37,37,37,37	0
57	MG	1A	3425	1/1	0.99	0.07	31,31,31,31	0
57	MG	1B	217	1/1	0.99	0.05	35,35,35,35	0
57	MG	1A	3426	1/1	0.99	0.07	11,11,11,11	0
57	MG	1A	3032	1/1	0.99	0.05	21,21,21,21	0
57	MG	1A	3515	1/1	0.99	0.03	25,25,25,25	0
57	MG	1A	3765	1/1	0.99	0.08	21,21,21,21	0
57	MG	1A	3766	1/1	0.99	0.06	32,32,32,32	0
57	MG	1A	3481	1/1	0.99	0.06	25,25,25,25	0
57	MG	1A	3517	1/1	0.99	0.07	32,32,32,32	0
57	MG	1A	3263	1/1	0.99	0.28	26,26,26,26	0
57	MG	1A	3680	1/1	0.99	0.04	42,42,42,42	0
57	MG	2a	1701	1/1	0.99	0.16	32,32,32,32	0
57	MG	1A	3429	1/1	0.99	0.05	18,18,18,18	0
57	MG	1A	3024	1/1	0.99	0.14	11,11,11,11	0
57	MG	1A	3599	1/1	0.99	0.06	16,16,16,16	0
57	MG	1A	3280	1/1	0.99	0.07	17,17,17,17	0
57	MG	1a	1729	1/1	0.99	0.07	33,33,33,33	0
57	MG	1A	3297	1/1	0.99	0.12	17,17,17,17	0
57	MG	2A	3283	1/1	0.99	0.03	43,43,43,43	0
57	MG	2A	3537	1/1	0.99	0.04	42,42,42,42	0
57	MG	1A	3523	1/1	0.99	0.06	27,27,27,27	0
57	MG	1E	304	1/1	0.99	0.07	11,11,11,11	0
57	MG	1A	3562	1/1	0.99	0.07	30,30,30,30	0
57	MG	1A	3265	1/1	0.99	0.07	42,42,42,42	0
58	ZN	1Y	501	1/1	0.99	0.03	58,58,58,58	0
57	MG	1X	102	1/1	0.99	0.07	33,33,33,33	0
58	ZN	15	108	1/1	0.99	0.04	35,35,35,35	0
58	ZN	16	102	1/1	0.99	0.04	37,37,37,37	0
58	ZN	19	102	1/1	0.99	0.04	39,39,39,39	0
57	MG	2A	3611	1/1	0.99	0.07	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	3543	1/1	0.99	0.15	32,32,32,32	0
57	MG	1A	3489	1/1	0.99	0.04	9,9,9,9	0
58	ZN	26	102	1/1	0.99	0.05	64,64,64,64	0
58	ZN	29	501	1/1	0.99	0.04	64,64,64,64	0
57	MG	1A	3251	1/1	0.99	0.25	24,24,24,24	0
57	MG	1A	3566	1/1	0.99	0.07	21,21,21,21	0
59	SF4	2d	501	8/8	0.99	0.04	46,66,70,70	0
57	MG	1A	3727	1/1	1.00	0.07	14,14,14,14	0
57	MG	1A	3323	1/1	1.00	0.02	19,19,19,19	0
58	ZN	25	103	1/1	1.00	0.05	52,52,52,52	0
57	MG	1A	3488	1/1	1.00	0.05	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.