



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 16, 2024 – 12:59 PM EST

PDB ID : 4WQU
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with elongation factor G trapped by the antibiotic dityromycin
Authors : Lin, J.; Gagnon, M.G.; Steitz, T.A.
Deposited on : 2014-10-22
Resolution : 2.80 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

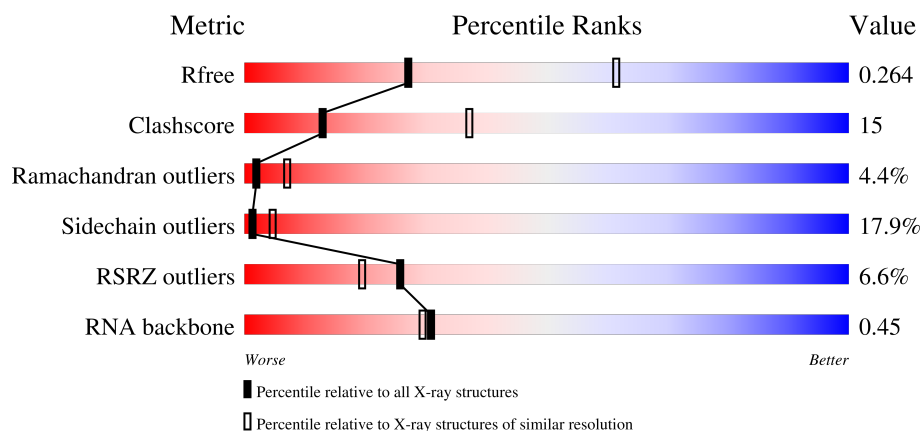
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)
RNA backbone	3690	1037 (3.00-2.60)

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	AA	2915	<div> <div>2%</div> <div>24% 47% 23% . .</div> </div>
1	CA	2915	<div> <div>3%</div> <div>32% 44% 19% . .</div> </div>
2	AB	121	<div> <div>%</div> <div>28% 55% 14% . .</div> </div>
2	CB	121	<div> <div>5%</div> <div>36% 47% 17% .</div> </div>



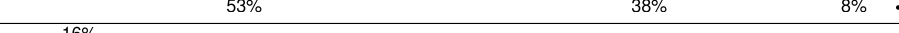

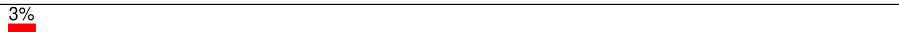
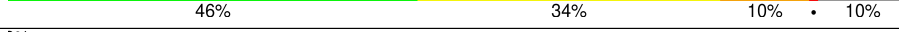

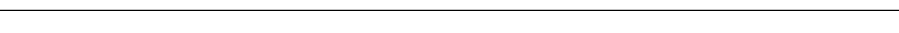





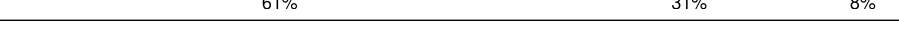

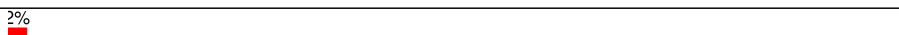


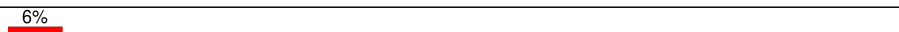


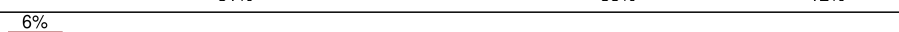


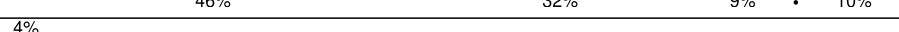
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AC	228	
3	CC	228	
4	AD	276	
4	CD	276	
5	AE	206	
5	CE	206	
6	AF	210	
6	CF	210	
7	AG	182	
7	CG	182	
8	AH	180	
8	CH	180	
9	AK	173	
9	CK	173	
10	AL	147	
10	CL	147	
11	AN	140	
11	CN	140	
12	AO	122	
12	CO	122	
13	AP	150	
13	CP	150	
14	AQ	141	
14	CQ	141	
15	AR	118	

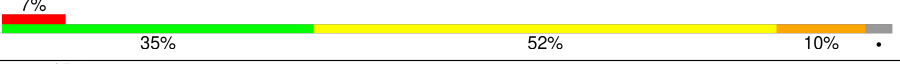
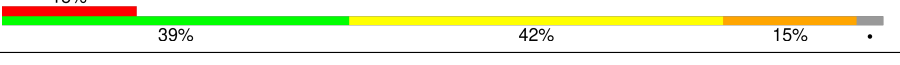



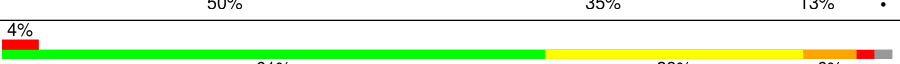
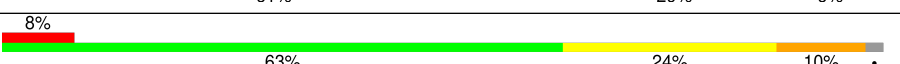
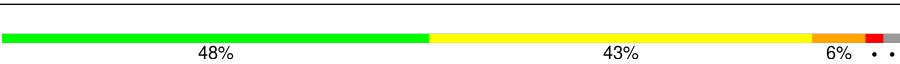


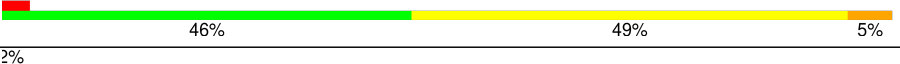
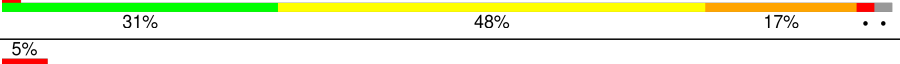

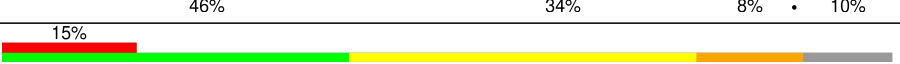

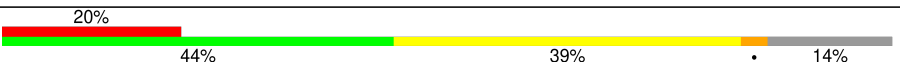


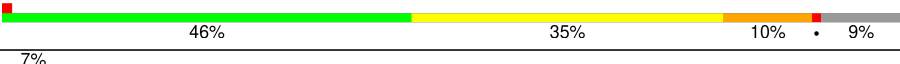






Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	CR	118	
16	AS	112	
16	CS	112	
17	AT	146	
17	CT	146	
18	AU	118	
18	CU	118	
19	AV	101	
19	CV	101	
20	AW	113	
20	CW	113	
21	AX	96	
21	CX	96	
22	AY	110	
22	CY	110	
23	AZ	206	
23	CZ	206	
24	A0	85	
24	C0	85	
25	A1	98	
25	C1	98	
26	A2	72	
26	C2	72	
27	A3	60	
27	C3	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	A4	71	
28	C4	71	
29	A5	60	
29	C5	60	
30	A6	54	
30	C6	54	
31	A7	49	
31	C7	49	
32	A8	65	
32	C8	65	
33	A9	37	
33	C9	37	
34	BA	1521	
34	DA	1521	
35	BB	256	
35	DB	256	
36	BC	239	
36	DC	239	
37	BD	209	
37	DD	209	
38	BE	162	
38	DE	162	
39	BF	101	
39	DF	101	
40	BG	156	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	DG	156	
41	BH	138	
41	DH	138	
42	BI	128	
42	DI	128	
43	BJ	105	
43	DJ	105	
44	BK	129	
44	DK	129	
45	BL	132	
45	DL	132	
46	BM	126	
46	DM	126	
47	BN	61	
47	DN	61	
48	BO	89	
48	DO	89	
49	BP	88	
49	DP	88	
50	BQ	105	
50	DQ	105	
51	BR	88	
51	DR	88	
52	BS	93	
52	DS	93	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	BT	106	
53	DT	106	
54	BU	27	
54	DU	27	
55	BV	18	
55	DV	18	
56	BW	76	
56	BY	76	
56	DW	76	
56	DY	76	
57	BZ	758	
57	DZ	758	
58	BX	10	
58	DX	10	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	2QY	DX	10	-	-	X	-
59	MG	AA	3056	-	-	-	X
59	MG	AA	3093	-	-	-	X
59	MG	AA	3717	-	-	-	X
59	MG	AA	3773	-	-	-	X
59	MG	CA	3093	-	-	-	X
59	MG	DA	1611	-	-	-	X
61	SF4	DD	501	-	-	X	-

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 310038 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	AA	2872	Total	C	N	O	P	0	0	0
			61861	27532	11574	19884	2871			
1	CA	2868	Total	C	N	O	P	0	0	0
			61771	27492	11554	19858	2867			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	137	Total	C	N	O	S	0	0	0
			1063	669	201	192	1			
3	CC	137	Total	C	N	O	S	0	0	0
			1063	669	201	192	1			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AK	130	Total	C	N	O		0	0	0
			641	381	130	130				
9	CK	130	Total	C	N	O		0	0	0
			641	381	130	130				

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AZ	185	Total	C	N	O	S	0	0	0
			1451	927	258	264	2			
23	CZ	185	Total	C	N	O	S	0	0	0
			1451	927	258	264	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
24	C0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	A1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
25	C1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	C2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A3	59	Total	C	N	O		0	0	0
			469	298	90	81				
27	C3	59	Total	C	N	O		0	0	0
			464	296	90	78				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A4	69	Total	C	N	O	S	0	0	0
			558	352	102	99	5			
28	C4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
29	C5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
30	C6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	A7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
31	C7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	A8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
32	C8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	A9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
33	C9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BM	117	Total	C	N	O	S	0	0	0
			923	570	191	160	2			
46	DM	116	Total	C	N	O	S	0	0	0
			907	558	188	159	2			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BR	68	Total	C	N	O	0	0	0
			555	355	108	92			
51	DR	68	Total	C	N	O	0	0	0
			555	355	108	92			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BU	23	Total	C	N	O		0	0	0
			199	122	48	29				
54	DU	23	Total	C	N	O		0	0	0
			199	122	48	29				

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BV	7	Total	C	N	O	P	0	0	0
			148	67	27	47	7			
55	DV	6	Total	C	N	O	P	0	0	0
			123	57	22	39	5			

- Molecule 56 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BW	76	Total	C	N	O	P	S	0	0
			1631	731	290	532	76	2		
56	BY	74	Total	C	N	O	P	S	0	0
			1581	707	285	515	73	1		
56	DW	76	Total	C	N	O	P	S	0	0
			1631	731	290	532	76	2		
56	DY	73	Total	C	N	O	P	S	0	0
			1561	698	283	507	72	1		

- Molecule 57 is a protein called 50S ribosomal protein L9,Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BZ	728	Total	C	N	O	S	0	0	0
			5663	3599	973	1072	19			
57	DZ	730	Total	C	N	O	S	0	0	0
			5682	3611	978	1074	19			

- Molecule 58 is a protein called Dityromycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	BX	10	Total	C	N	O	0	0	0
			93	67	10	16			
58	DX	10	Total	C	N	O	0	0	0
			93	67	10	16			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	821	Total	Mg	0	0
			821	821		
59	AB	23	Total	Mg	0	0
			23	23		
59	AD	12	Total	Mg	0	0
			12	12		
59	AE	5	Total	Mg	0	0
			5	5		
59	AF	8	Total	Mg	0	0
			8	8		
59	AG	2	Total	Mg	0	0
			2	2		
59	AH	1	Total	Mg	0	0
			1	1		
59	AN	3	Total	Mg	0	0
			3	3		
59	AO	1	Total	Mg	0	0
			1	1		
59	AP	4	Total	Mg	0	0
			4	4		
59	AQ	3	Total	Mg	0	0
			3	3		
59	AR	2	Total	Mg	0	0
			2	2		
59	AU	3	Total	Mg	0	0
			3	3		
59	AV	6	Total	Mg	0	0
			6	6		
59	AW	3	Total	Mg	0	0
			3	3		
59	AX	1	Total	Mg	0	0
			1	1		
59	AY	1	Total	Mg	0	0
			1	1		
59	AZ	2	Total	Mg	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	A0	5	Total 5	Mg 5	0	0
59	A2	1	Total 1	Mg 1	0	0
59	A5	1	Total 1	Mg 1	0	0
59	A6	2	Total 2	Mg 2	0	0
59	A7	4	Total 4	Mg 4	0	0
59	A8	1	Total 1	Mg 1	0	0
59	A9	1	Total 1	Mg 1	0	0
59	BA	215	Total 215	Mg 215	0	0
59	BB	1	Total 1	Mg 1	0	0
59	BD	1	Total 1	Mg 1	0	0
59	BE	1	Total 1	Mg 1	0	0
59	BF	1	Total 1	Mg 1	0	0
59	BK	1	Total 1	Mg 1	0	0
59	BL	2	Total 2	Mg 2	0	0
59	BM	1	Total 1	Mg 1	0	0
59	BN	2	Total 2	Mg 2	0	0
59	BS	1	Total 1	Mg 1	0	0
59	BT	1	Total 1	Mg 1	0	0
59	BW	3	Total 3	Mg 3	0	0
59	BZ	1	Total 1	Mg 1	0	0
59	CA	664	Total 664	Mg 664	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	CB	13	Total 13	Mg 13	0	0
59	CD	4	Total 4	Mg 4	0	0
59	CE	5	Total 5	Mg 5	0	0
59	CF	4	Total 4	Mg 4	0	0
59	CG	1	Total 1	Mg 1	0	0
59	CN	1	Total 1	Mg 1	0	0
59	CO	1	Total 1	Mg 1	0	0
59	CP	1	Total 1	Mg 1	0	0
59	CQ	4	Total 4	Mg 4	0	0
59	CR	1	Total 1	Mg 1	0	0
59	CU	1	Total 1	Mg 1	0	0
59	CV	2	Total 2	Mg 2	0	0
59	CW	1	Total 1	Mg 1	0	0
59	CX	1	Total 1	Mg 1	0	0
59	C0	1	Total 1	Mg 1	0	0
59	C1	1	Total 1	Mg 1	0	0
59	C3	1	Total 1	Mg 1	0	0
59	C5	1	Total 1	Mg 1	0	0
59	C7	1	Total 1	Mg 1	0	0
59	C8	1	Total 1	Mg 1	0	0
59	DA	171	Total 171	Mg 171	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	DD	1	Total 1	Mg 1	0	0
59	DE	2	Total 2	Mg 2	0	0
59	DF	1	Total 1	Mg 1	0	0
59	DJ	1	Total 1	Mg 1	0	0
59	DK	1	Total 1	Mg 1	0	0
59	DT	1	Total 1	Mg 1	0	0
59	DW	3	Total 3	Mg 3	0	0
59	DZ	2	Total 2	Mg 2	0	0

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

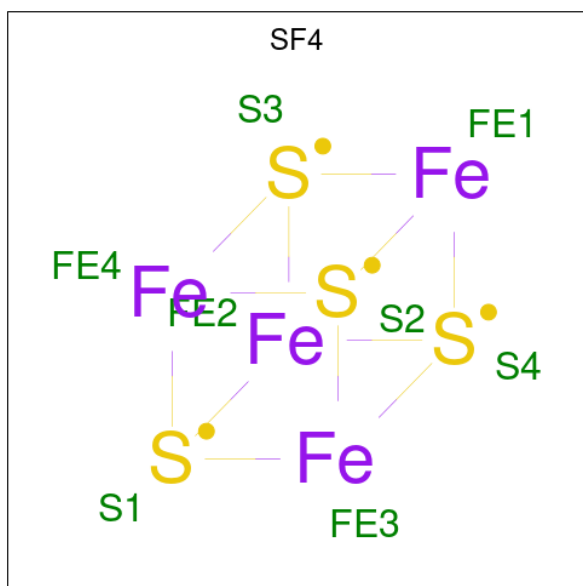
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AY	1	Total 1	Zn 1	0	0
60	A4	1	Total 1	Zn 1	0	0
60	A5	1	Total 1	Zn 1	0	0
60	A6	1	Total 1	Zn 1	0	0
60	A9	1	Total 1	Zn 1	0	0
60	BN	1	Total 1	Zn 1	0	0
60	CY	1	Total 1	Zn 1	0	0
60	C4	1	Total 1	Zn 1	0	0
60	C5	1	Total 1	Zn 1	0	0
60	C6	1	Total 1	Zn 1	0	0
60	C9	1	Total 1	Zn 1	0	0

Continued on next page...

Continued from previous page...

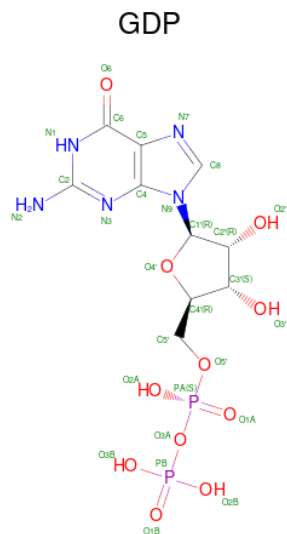
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	DN	1	Total	Zn	0	0
			1	1		

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	BD	1	Total	Fe	S	0	0
			8	4	4		
61	DD	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 63 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	AA	1413	Total O 1413 1413	0	0
63	AB	38	Total O 38 38	0	0
63	AD	10	Total O 10 10	0	0
63	AE	17	Total O 17 17	0	0
63	AF	11	Total O 11 11	0	0
63	AG	3	Total O 3 3	0	0
63	AH	1	Total O 1 1	0	0
63	AN	1	Total O 1 1	0	0
63	AO	3	Total O 3 3	0	0
63	AP	16	Total O 16 16	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AQ	4	Total 4	O 4	0	0
63	AR	2	Total 2	O 2	0	0
63	AS	1	Total 1	O 1	0	0
63	AT	1	Total 1	O 1	0	0
63	AU	4	Total 4	O 4	0	0
63	AV	1	Total 1	O 1	0	0
63	AW	1	Total 1	O 1	0	0
63	AX	3	Total 3	O 3	0	0
63	AZ	1	Total 1	O 1	0	0
63	A0	6	Total 6	O 6	0	0
63	A1	2	Total 2	O 2	0	0
63	A3	2	Total 2	O 2	0	0
63	A5	3	Total 3	O 3	0	0
63	A6	1	Total 1	O 1	0	0
63	A7	2	Total 2	O 2	0	0
63	A8	10	Total 10	O 10	0	0
63	A9	1	Total 1	O 1	0	0
63	BA	213	Total 213	O 213	0	0
63	BD	1	Total 1	O 1	0	0
63	BM	1	Total 1	O 1	0	0
63	BO	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	BP	1	Total	O	0	0
			1	1		
63	BV	1	Total	O	0	0
			1	1		
63	BW	1	Total	O	0	0
			1	1		
63	BZ	2	Total	O	0	0
			2	2		
63	CA	983	Total	O	0	0
			983	983		
63	CB	9	Total	O	0	0
			9	9		
63	CD	15	Total	O	0	0
			15	15		
63	CE	9	Total	O	0	0
			9	9		
63	CF	6	Total	O	0	0
			6	6		
63	CN	1	Total	O	0	0
			1	1		
63	CO	1	Total	O	0	0
			1	1		
63	CP	11	Total	O	0	0
			11	11		
63	CQ	2	Total	O	0	0
			2	2		
63	CT	3	Total	O	0	0
			3	3		
63	CU	2	Total	O	0	0
			2	2		
63	CV	1	Total	O	0	0
			1	1		
63	CW	1	Total	O	0	0
			1	1		
63	CX	1	Total	O	0	0
			1	1		
63	CY	2	Total	O	0	0
			2	2		
63	C0	4	Total	O	0	0
			4	4		
63	C3	2	Total	O	0	0
			2	2		

Continued on next page...

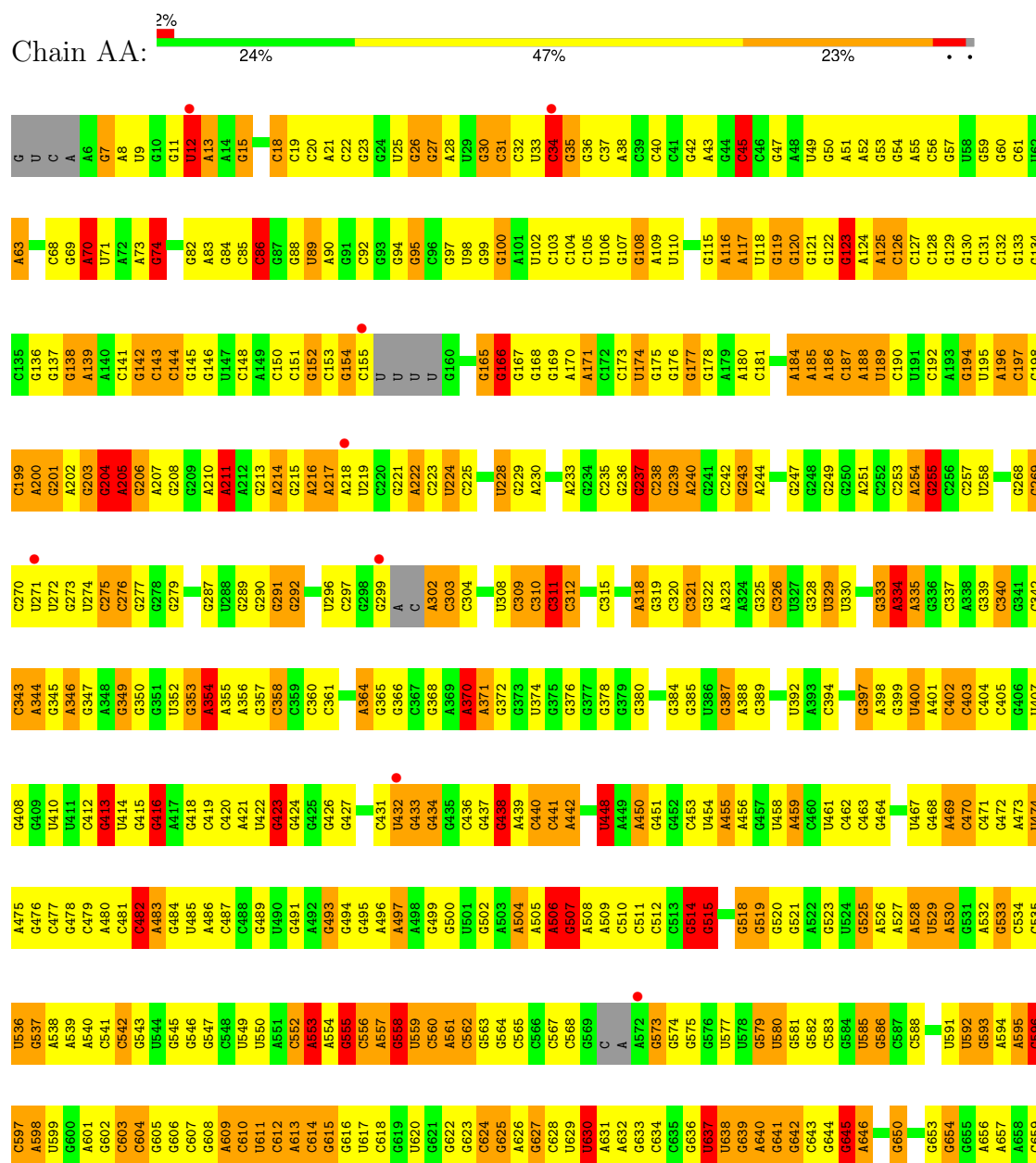
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	C5	1	Total 1	O 1	0	0
63	C7	2	Total 2	O 2	0	0
63	C8	4	Total 4	O 4	0	0
63	DA	157	Total 157	O 157	0	0
63	DD	1	Total 1	O 1	0	0
63	DE	2	Total 2	O 2	0	0
63	DH	1	Total 1	O 1	0	0
63	DJ	1	Total 1	O 1	0	0
63	DK	2	Total 2	O 2	0	0
63	DL	1	Total 1	O 1	0	0
63	DT	1	Total 1	O 1	0	0

3 Residue-property plots

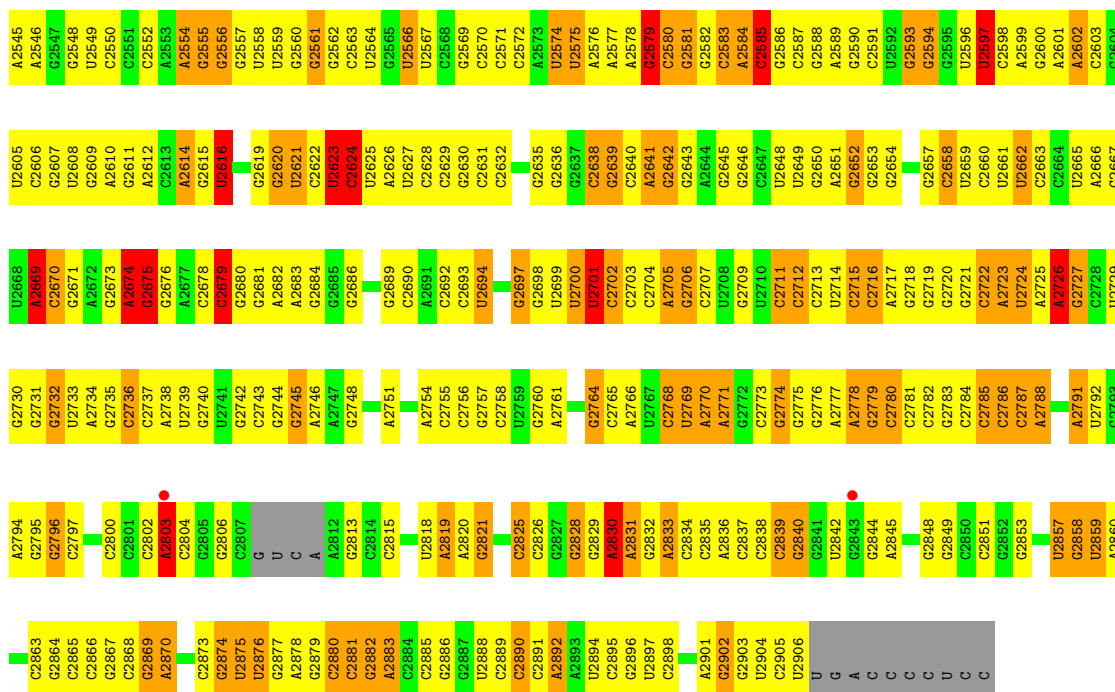
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 23S Ribosomal RNA

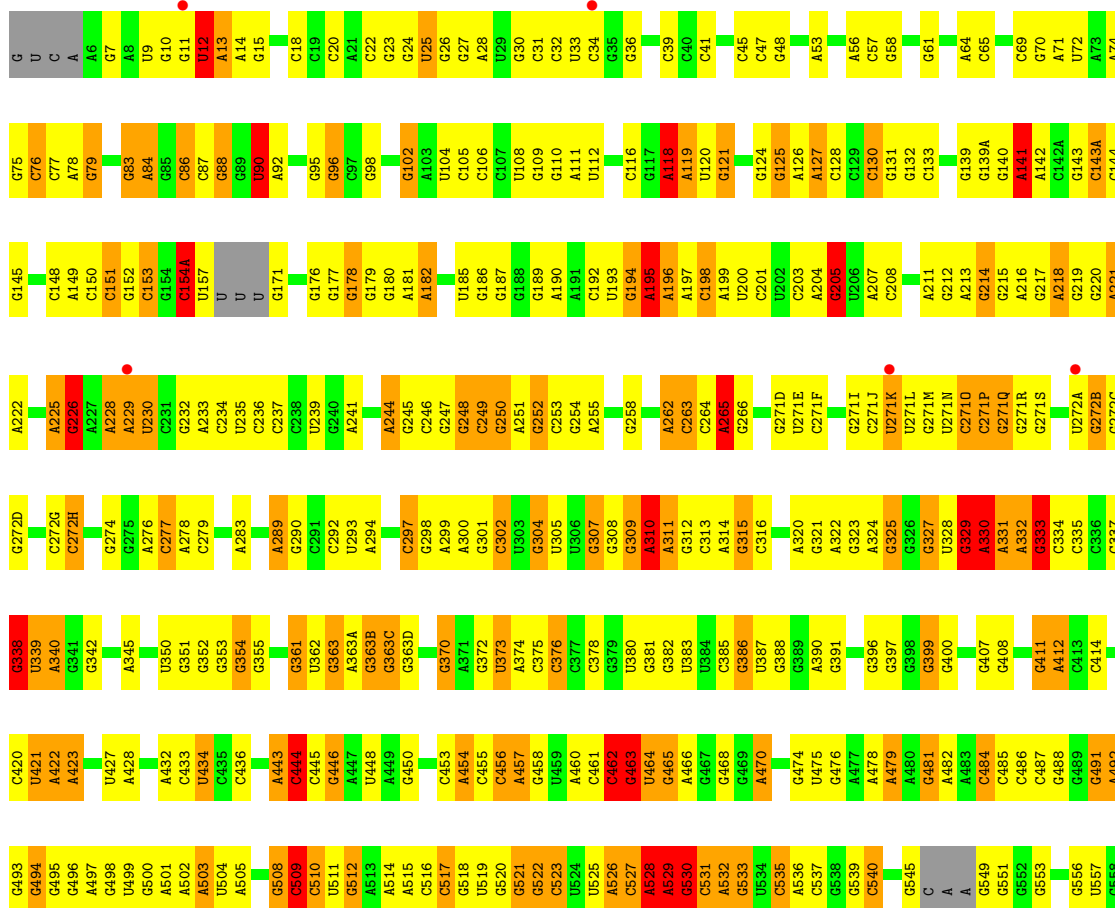
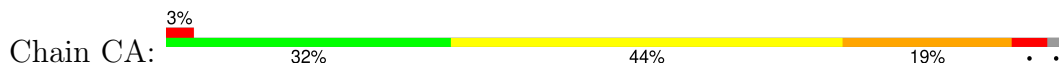


A1557	G1487	C1431	G1296	A1174	G1108	A1047	G987	C914	C852	G790	A724	G660
G1558	C1422	C1422	C1297	A1175	G1109	G1048	G988	G915	C853	G791	A725	G661
C1559	G1423	G1298	A1299	G1176	C1110	G1049	G989	C916	U854	A793	C726	A662
U1560	A1424	A1299	A1299	G1177	U1111	C1050	A990	C1050	G855	A794	C727	G663
C1561	A1425	A1299	A1300	U1178	U1112	C1051	G991	G919	G856	G795	G728	U664
U1562	G1426	U1301	C1302	U1179	U1113	C1052	G992	G920	G857	A798	G729	G665
G1563	A1430	G1302	C1303	C1240	G1114	C1053	G993	G921	U858	A799	C730	G666
G1564	A1431	C1303	C1304	C1241	A1115	C1054	C994	G922	C859	A799	G731	G667
G1565	G1432	C1304	C1305	G1182	A1116	A1055	G995	G927	U860	C800	A732	A668
U1566	A1433	G1306	G1306	G1183	G1117	A1056	C996	C996	C861	C801	A733	A669
G1567	G1370	U1244	U1244	G1184	C1118	G1057	G997	G927	C862	C802	G734	C670
U1568	G1371	C1245	C1245	U1185	A1119	U1058	A998	G932	C863	C803	C734	A671
U1569	U1372	C1246	C1246	U1186	C1122	C1059	G999	C933	C864	U804	U735	G672
G1570	C1373	C1247	C1247	U1187	U1129	U1060	C1000	A934	C865	C805	A736	G673
G1571	G1374	U1248	U1248	U1188	G1061	G1061	G1001	A935	C866	G806	C737	G674
C1572	A1310	A1249	A1249	A1189	G1062	G1062	G1002	C936	U867	C807	C738	
U1573	A1311	U1250	U1250	G1190	G1063	U1069	A1003	A937	C868	C808		
G1574	C1312	G1251	G1251	C1191	C1064	C1064	U1004	G938	C869	C809		
U1575	U1313	C1252	C1252	C1192	U1065	U1065	A1005	C939	U870	U809		
G1576	A1314	C1253	C1253	C1193	A1066	U1072	C1008	G942	C870	A810	U741	A678
U1577	A1315	G1254	G1254	U1194	A1067	U1073	G1007	A942	C871	A811	G742	A
C1578	C1316	U1255	U1255	C1195	U1068	U1074	U1008	G948	C872	A812	G743	G
U1579	A1317	C1260	C1260	A1190	C1069	U1075	C1010	C949	C873	U813	C744	G
U1580	A1318	G1261	G1261	C1191	U1070	U1076	C1015	C954	C874	U814	C745	G
C1581	A1321	U1262	U1262	G1192	C1071	A1077	C1016	A955	C875	U815	A746	G
U1582	A1322	C1263	C1263	C1193	U1072	U1078	G1017	A956	C876	U816	G747	C
G1583	G1323	U1264	U1264	C1194	U1073	U1079	G1018	A957	C877	U817	G748	C
U1584	C1324	A1265	A1265	U1195	U1074	U1080	G1019	A958	C878	U818	G749	G
C1585	G1325	C1266	C1266	C1196	U1075	U1081	C1020	C960	C879	U819	U750	C
U1586	U1326	U1267	U1267	G1197	C1076	U1082	G1021	G961	C880	U820	A752	C
G1587	A1327	G1268	G1268	C1198	A1077	U1083	C1022	A963	C881	A821	A753	G691
U1588	A1328	C1269	C1269	C1199	U1078	U1084	G1023	A964	C882	U822	G760	G692
A1589	U1329	U1270	U1270	C1200	U1079	U1085	G1024	A965	C883	U823	G761	G693
U1590	A1330	C1271	C1271	G1201	U1080	U1086	G1025	A966	C884	A824	G762	G694
A1591	G1331	U1272	U1272	C1202	U1081	U1087	C1026	G967	C885	U825	A763	C696
C1592	U1332	G1273	G1273	G1203	U1082	U1088	G1027	U968	C886	U826	G764	C697
U1593	C1333	C1274	C1274	C1204	U1083	U1089	C1028	C969	C887	U827	A765	G698
G1594	U1334	G1275	G1275	U1205	A1141	U1089	G1029	C970	C888	A828	A766	
C1595	U1335	U1276	U1276	C1206	A1142	U1090	A1030	C971	C889	A829	C766	
U1596	C1336	U1277	U1277	G1207	G1145	U1091	G1031	C972	C890	A830		A701
C1597	U1337	C1278	C1278	C1208	C1146	U1092	G1032	A972	C891	A831	A789	A702
U1598	U1338	U1279	U1279	G1209	C1147	U1093	C1033	G973	C892	U832	G770	G703
G1599	C1339	G1280	G1280	C1210	U1151	C1094	G1034	G974	C893	U833	G771	U704
U1600	U1340	C1281	C1281	U1211	G1152	C1095	G1035	U975	C894	U834	G772	G705
A1601	C1341	U1282	U1282	C1212	C1153	U1096	A1036	G976	C895	U835	G773	C706
G1602	U1342	U1283	U1283	G1213	U1154	U1097	C1037	C977	C896	A836	G774	G707
C1603	C1343	C1284	C1284	C1214	G1155	U1098	G1038	A978	C897	U836	A775	C708
U1604	U1344	U1285	U1285	U1215	C1156	U1099	G1039	G979	C898	U837	G776	G709
G1605	C1345	U1286	U1286	C1216	G1161	C1099	G1040	C980	C899	U838	G777	G710
C1606	U1346	U1287	U1287	C1217	C1162	U1099	G1041	C981	C900	U839	C778	C711
U1607	C1347	U1288	U1288	U1218	U1163	U1099	C1042	U982	C901	U840	C779	G712
G1608	U1348	U1289	U1289	C1219	C1164	U1099	G1043	G983	C902	A841	G780	G713
A1609	C1349	U1290	U1290	C1220	G1165	U1099	G1044	G984	C903	C842	G781	U714
G1610	U1350	U1291	U1291	C1221	C1166	U1100	C1045	G985	C904	U843	A782	U715
C1611	C1351	U1292	U1292	C1222	U1167	A1101	G1046	G986	C905	C844	A783	G716
U1612	G1352	U1293	U1293	C1223	C1168	G1101	C1047	G987	C906	U845	C784	A717
A1613	A1353	U1294	U1294	U1224	U1169	G1102	G1048	G988	C907	U846	G785	C718
G1614	C1354	U1295	U1295	C1225	C1170	G1103	G1049	G989	C908	A847	G786	C719
U1615	U1355	U1296	U1296	C1226	G1171	G1104	C1050	G990	C909	U848	U787	C720
A1616	C1356	U1297	U1297	C1227	C1172	G1105	G1051	G991	C910	C849	G788	U721
G1617	U1357	U1298	U1298	C1228	U1173	G1106	C1052	G992	C911	U850	G789	A722
C1618	A1358	U1299	U1299	C1229	A1174	U1107	G1053	G993	C891	C852		
U1619	C1359	U1300	U1300	C1230	A1175		G1054	G994	C892	C853		
A1620	U1360	U1301	U1301	C1231	A1176		G1055	G995	C893	U854		
G1621	C1361	U1302	U1302	C1232	A1177		G1056	G996	C894	U855		
C1622	A1362	U1303	U1303	C1233	A1178		G1057	G997	C895	U856		
U1623	C1363	U1304	U1304	C1234	A1179		G1058	G998	C896	U857		
A1624	U1364	U1305	U1305	C1235	A1180		G1059	G999	C897	U858		
G1625	C1365	U1306	U1306	C1236	A1181		G1060	G1000	C898	U859		
C1626	A1366	U1307	U1307	C1237	A1182		G1061	G1001	C899	U860		
U1627	C1367	U1308	U1308	C1238	A1183		G1062	G1002	C900	U861		
A1628	U1368	U1309	U1309	C1239	A1184		G1063	G1003	C901	U862		
G1629	C1369	U1310	U1310	C1240	A1185		G1064	G1004	C902	U863		
U1630	A1370	U1311	U1311	C1241	A1186		G1065	G1005	C903	U864		
C1631	C1371	U1312	U1312	C1242	A1187		G1066	G1006	C904	U865		
A1632	U1372	U1313	U1313	C1243	A1188		G1067	G1007	C905	U866		
G1633	C1373	U1314	U1314	C1244	A1189		G1068	G1008	C906	U867		
U1634	A1374	U1315	U1315	C1245	A1190		G1069	G1009	C907	U868		
C1635	C1375	U1316	U1316	C1246	A1191		G1070	G1010	C908	U869		
A1636	U1376	U1317	U1317	C1247	A1192		G1071	G1011	C909	U870		
G1637	C1377	U1318	U1318	C1248	A1193		G1072	G1012	C910	A871		
U1638	A1378	U1319	U1319	C1249	A1194		G1073	G1013	C911	A872		
A1639	C1379	U1320	U1320	C1250	A1195		G1074	G1014	C912	A873		
G1640	U1380	U1321	U1321	C1251	A1196		G1075	G1015	C913	A874		
C1641	C1381	U1322	U1322	C1252	A1197		G1076	G1016	C914	U875		
U1642	A1382	U1323	U1323	C1253	A1198		G1077	G1017	C915	U876		
G1643	C1383	U1324	U1324	C1254	A1199		G1078	G1018	C916	U877		
A1644	U1384	U1325	U1325	C1255	A1200		G1079	G1019	C917	U878		
C1645	C1385	U1326	U1326	C1256	A1201		G1080	G1020	C918	U879		
U1646	U1386	U1327	U1327	C1257	A1202		G1081	G1021	C919	U880		
G1647	C1387	U1328	U1328	C1258	A1203		G1082	G1022	C920	U881		
A1648	U1388	U1329	U1329	C1259	A1204		G1083	G1023	C921	U882		
C1649	C1389	U1330	U1330	C1260	U1205		G1084	G1024	C922	U883		
U1650	U1390	U1331	U1331	C1261	U1206		G1085	G1025	C923	U884		
G1651	C1391	U1332	U1332	C1262	U1207		G1086	G1026	C924	U885		
A1652	U1392	U1333	U1333	C1263	U1208		G1087	G1027	C925	U886		
C1653	C1393	U1334	U1334	C1264	U1209		G1088	G1028	C926	U887		
U1654	U1394	U1335	U1335	C1265	U1210		G1089	G1029	C927	A828		
G1655	C1395	U1336	U1336	C1266	U1211		G1090	G1030	C928	A829		
A1656	U1396	U1337	U1337	C1267	U1212		G1091	G1031	C929	A830		
C1657	C1397	U1338	U1338	C1268	U1213		G1092	G1032	C930	A831		
U1658	U1398	U1339	U1339	C1269	U1214		G1093	G1033	C931	U832		
G1659	C1399	U1340	U1340	C1270	U1215		G1094	G1034	C932	U833		
A1660	U1400	U1341	U1341	C1271	U1216		G1095	G1035	C933	U834		
C1661	C1401	U1342	U1342	C1272	U1217		G1096	G1036	C934	U835		
U1662	U1402	U1343	U1343	C1273	U1218		G1097	G1037	C935	U836		
G1663	C1403	U1344	U1344	C1274	U1219		G1098	G1038	C936	U837		
A1664	U1404	U1345	U1345	C1275	U1220		G1099	G1039	C937			

G2481	G2482	G2483	G2484	A2488	G2489	G2490	G2491	G2492	G2493	G2494	G2495	G2496	A2500	G2501	G2502	G2503	G2504	G2505	G2506	G2507	G2508	A2509	G2510	G2511	G2512	G2513	G2514	G2515	G2516	G2517	G2518	G2519	G2520	G2521	G2522	G2523	G2524	G2525	G2526	G2527	G2528	G2529	G2530	G2531	G2532	G2533	G2534	G2535	G2536	G2537	G2538	G2539	G2540	G2541	G2542	G2543	G2544	
G2419	G2420	G2421	G2422	A2423	A2424	G2425	G2426	C2429	A2430	G2431	G2432	G2433	A2434	G2435	G2436	A2437	A2438	C2439	G2440	G2441	A2442	G2443	A2444	A2445	A2446	A2447	G2448	G2449	G2450	A2451	A2452	C2453	G2454	G2455	G2456	G2457	G2458	G2459	A2460	G2461	A2462	A2463	C2464	G2467	G2468	G2469	G2470	A2471	G2472	G2473	G2474	G2475	G2476	C2477	G2478	G2479	G2480	
C2354	C2355	G2356	G2357	A2358	G2359	U2360	G2361	G2362	G2365	G2366	G2367	G2368	U2369	G2370	G2371	A2372	A2373	G2374	G2375	G2376	G2377	A2378	G2379	C2380	G2383	G2384	G2385	G2386	G2387	A2388	A2389	A2390	G2391	G2392	G2393	G2394	G2395	G2396	G2397	G2398	G2399	G2400	G2401	U2402	G2403	C2406	G2407	G2408	G2409	U2410	G2411	C2415	G2416	G2417	U2418			
C2287	G2288	G2289	A2290	G2291	G2292	C2293	G2294	G2295	G2296	G2297	A2298	G2299	A2300	G2301	G2302	U2303	G2304	G2305	G2306	C2307	G2308	G2309	G2310	G2311	G2312	G2316	G2317	G2318	G2319	G2320	A2321	A2322	A2323	G2324	G2325	G2331	A2332	G2333	A2334	G2335	G2336	G2337	G2338	A2339	A2340	G2341	G2342	G2343	G2344	G2345	G2346	A2347	A2348	G2349	G2350	G2351		
U2225	G2226	G2227	A2228	G2229	G2230	G2231	G2234	G2235	G2236	A2237	G2238	A2239	G2240	G2241	G2242	G2243	U2244	U2245	U2246	G2246	G2247	G2248	G2249	G2250	G2251	G2252	A2253	G2254	U2255	U2256	U2257	G2258	A2259	G2260	U2261	G2262	G2263	G2264	G2265	G2266	G2267	G2268	U2269	C2270	G2271	G2272	G2273	U2274	G2275	G2276	A2279	A2280	G2281	G2282	G2283	U2284	A2285	A2286
C2163	C2164	C2165	U2166	A2167	C2168	G2169	G2170	U2171	U2172	U2173	G2174	G2175	G2176	G2177	G2178	G2179	A2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	G2189	G2190	A2191	U2194	A2195	G2196	G2197	A2198	G2199	G2200	G2201	G2204	G2205	G2206	G2207	G2208	G2209	G2210	U2211	G2212	G2213	G2214	G2215	G2216	G2217	G2218	U2219	A2220	A2221	G2222	G2223	G2224	
U2096	U2097	U2098	A2099	A2100	C2101	G2102	C2103	A2104	G2105	C2106	C2107	U2108	G2112	U2113	U2114	G2115	G2116	C2119	U2120	U2121	U2122	G2123	U2124	G2125	G2126	C2127	G2128	C2129	C2130	U2131	G2132	G2133	G2134	U2135	A2136	G2137	G2138	A2139	U2140	G2141	G2142	G2143	U2144	G2145	G2146	G2147	U2148	G2149	G2153	U2154	G2155	A2156	A2157	G2158	C2162			
U2033	G2034	A2035	A2036	U2037	U2038	U2039	G2040	A2041	A2042	C2043	C2107	U2108	G2046	C2047	G2048	G2049	U2050	G2051	A2052	G2053	G2054	A2055	U2056	G2057	C2058	G2059	C2062	G2063	U2064	G2065	G2066	G2067	G2068	C2072	A2073	G2074	G2075	A2076	G2077	G2078	A2079	A2080	A2081	A2082	G2083	A2084	C2085	C2086	C2087	C2088	G2089	U2090	G2091	G2092	A2093	G2094	C2095	
G1895	G1896	G1900	G1905	C1906	C1908	C1917	G1918	G1919	U1920	G1921	A1922	A1923	G1924	G1925	G1926	G1927	G1928	G1929	C1930	A1934	U1935	C1936	U1937	A1940	A1941	C1942	G1943	G1944	U1945	U1946	C1947	U1948	A1949	A1950	G1951	G1952	U1953	A1954	G1955	C1956	G1957	A1958	A1959	G1960	U1961	U1962	U1963	U1964	U1965	U1966								
G1824	U1825	U1827	U1829	G1830	G1831	G1832	U1833	A1834	U1835	U1836	C1837	G1838	A1841	G1842	A1843	G1844	G1845	A1846	G1847	G1848	U1849	A1850	U1851	A1852	G1853	G1854	G1855	A1856	G1857	C1858	A1859	A1860	G1861	G1862	G1863	G1864	G1870	G1873	A1878	A1879	G1880	G1881	U1882	G1886	G1887	G1888	G1889	A1890	G1891	G1892	G1893	G1894	G1895					
U1753	G1754	C1755	U1765	G1766	A1767	U1768	C1769	C1773	G1776	G1777	G1779	A1780	G1781	C1782	G1783	G1784	G1785	A1786	G1787	U1788	G1789	A1790	A1791	G1792	A1793	G1794	C1795	U1797	A1798	G1799	G1801	C1802	G1803	A1804	C1805	U1806	G1807	U1808	U1809	U1810	A1811	C1812	G1813	A1814	A1815	A1816	G1817	G1818	A1819	A1820	G1821	A1822	G1823					
G1690	C1691	G1692	G1693	G1694	G1695	G1698	A1699	G1700	A1701	G1702	C1703	C1704	C1705	U1706	C1707	G1708	C1709	C1710	A1711	A1712	G1713	G1714	A1715	A1716	C1717	A1718	C1719	G1720	G1721	C1722	A1723	G1724	G1725	U1726	U1727	G1728	G1729	C1730	C1731	C1732	A1736	A1737	C1738	U1739	U1740	C1741	G1742	G1743	G1744	G1745	G1746	A1747	A1748	G1749	G1750	G1751	G1752	
U1626	A1627	G1628	G1629	A1630	C1631	A1632	A1633	C1634	A1635	U1636	G1637	C1638	G1639	G1640	A1643	C1644	C1645	C1646	C1650	G1651	G1652	C1653	A1654	A1655	A1656	C1657	G1658	G1659	A1660	C1663	A1664	G1665	G1666	U1667	G1668	G1669	G1670	C1671	G1672	G1673	G1674	U1675	U1676	C1677	A1678	A1679	G1680	A1681	G1682	C1685	U1686	C1687	G1689					

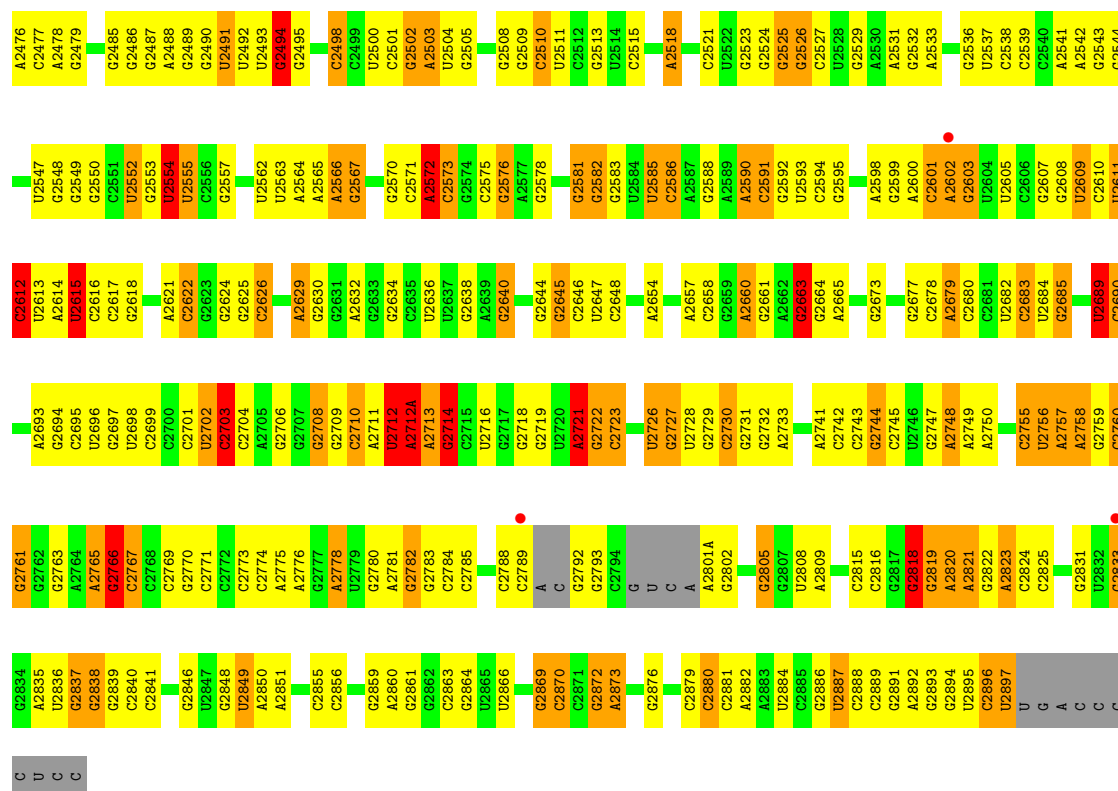


• Molecule 1: 23S Ribosomal RNA

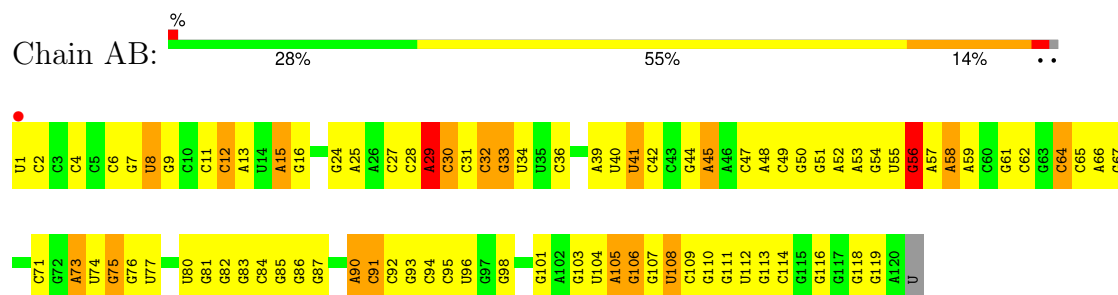


G1401	G1381	G1203	G1131	U1066	G1003	G940	C876	U810	A746	G668	G559
C1402	G1332	A1204	A1132	A1067	C1004	A941	U877	U811	U747	G669	C560
C1403	G1337	U1205	U1133	A1070	C1005	U943	A878	C812	G623	G670	C561
U1405	G1338	G1206	C1135	G1071	C1006	U942	C879	U813	G624	A670	U562
U1406	U1273	C1207	G1136	G1072	C1007	U943	C880	C814	C627	C671	C563
C1407	U1274	C1208	G1137	G1073	C1008	A945	C881	C815	A750	C672	C564
U1408	U1275	G1209	G1138	A1074	C1009	G946	C882	C816	A751	C673	C565
C1409	U1276	A1210	G1139	G1075	A1010	G947	C883	C817	A752	G674	U566
G1410	G1277	U1211	C1140	C1076	G1011	G950	C884	U818	C678	C678	A567
C1411	A1278	A1212	U1141	A1077	C1012	C951	C885	G819	C679	A637	U568
G1412	G1279	G1213	U1142	C1077	C1013	C952	C886	C754	C680	C638	U569
G1413	C1345	A1214	A1143	U1078	U1014	A953	C887	C755	G681	U639	C570
		G1215	C1080	C1079	G1015	G954	C888	C756	C682	C640	A571
		G1216	U1081	C1080	G1016	C955	C889	C757	G683	C641	A572
		C1217	U1082	U1081	U1019	C956	A890	C758	G684	G642	C573
			U1083	U1082	A1020	C957	C892	C759	G685	A643	C574
			U1084	U1083	A1021	A957	C893	C760	G686	A644	A575
			A1085	U1084	U958	A959	C894	C761	G687	C645	U576
			U1086	U1085	G1022	A960	U895	C762	G688	A646	G577
			C1152	U1086	U1023	A961	A896	C763	G689	G647	A578
			U1087	U1087	G1024	C962	C898	C764	G690	C648	C579
			U1088	U1088	G1025	U963	A899	C765	G691	C649	C580
			U1089	U1089	U1026	U964	C900	C766	G692	C650	C581
			A1155	U1090	A1027	C965	A901	C767	G693	C651	G582
			A1156	G1091	A1028	C966	C902	C768	G694	G652	G583
			G1157	C1092	A1028	C967	C903	C769	G695	A652A	C584
						C968	C904	C770	G696	G652B	G585
						U1093	C905	C771	G697	A652C	A586
						U1094	U906	C772	G698	G652D	C587
						A1095	C907	C773	G699	C652E	U588
						U1096	C908	C774	G700	G	C589
						U1097	C909	C775	G701	C	A590
						U1097	C910	C776	G702	C	C591
						U1097	C911	C777	G703	C	G592
						U1097	C912	C778	G704	C	
						U1097	C913	C779	A705	C	
						U1097	C914	C780	A706	C	
						U1097	C915	C781	A707	C	
						U1097	C916	C782	A708	C	
						U1097	C917	C783	A709	C	
						U1097	C918	C784	A710	C	
						U1097	C919	C785	A711	C	
						U1097	C920	C786	A712	C	
						U1097	C921	C787	A713	C	
						U1097	C922	C788	A714	C	
						U1097	C923	C789	A715	C	
						U1097	C924	C790	A716	C	
						U1097	C925	C791	A717	C	
						U1097	C926	C792	A718	C	
						U1097	C927	C793	A719	C	
						U1097	C928	C794	A720	C	
						U1097	C929	C795	A721	C	
						U1097	C930	C796	A722	C	
						U1097	C931	C797	A723	C	
						U1097	C932	C798	A724	C	
						U1097	C933	C799	A725	C	
						U1097	C934	C800	A726	C	
						U1097	C935	C801	A727	C	
						U1097	C936	C802	A728	C	
						U1097	C937	C803	A729	C	
						U1097	C938	C804	A730	C	
						U1097	C939	C805	A731	C	
						U1097	C940	C806	A732	C	
						U1097	C941	C807	A733	C	
						U1097	C942	C808	A734	C	
						U1097	C943	C809	A735	C	
						U1097	C944	C810	A736	C	
						U1097	C945	C811	A737	C	
						U1097	C946	C812	A738	C	
						U1097	C947	C813	A739	C	
						U1097	C948	C814	A740	C	
						U1097	C949	C815	A741	C	
						U1097	C950	C816	A742	C	
						U1097	C951	C817	A743	C	
						U1097	C952	C818	A744	C	
						U1097	C953	C819	A745	C	
						U1097	C954	C820	A746	C	
						U1097	C955	C821	A747	C	
						U1097	C956	C822	A748	C	
						U1097	C957	C823	A749	C	
						U1097	C958	C824	A750	C	
						U1097	C959	C825	A751	C	
						U1097	C960	C826	A752	C	
						U1097	C961	C827	A753	C	
						U1097	C962	C828	A754	C	
						U1097	C963	C829	A755	C	
						U1097	C964	C830	A756	C	
						U1097	C965	C831	A757	C	
						U1097	C966	C832	A758	C	
						U1097	C967	C833	A759	C	
						U1097	C968	C834	A760	C	
						U1097	C969	C835	A761	C	
						U1097	C970	C836	A762	C	
						U1097	C971	C837	A763	C	
						U1097	C972	C838	A764	C	
						U1097	C973	C839	A765	C	
						U1097	C974	C840	A766	C	
						U1097	C975	C841	A767	C	
						U1097	C976	C842	A768	C	
						U1097	C977	C843	A769	C	
						U1097	C978	C844	A770	C	
						U1097	C979	C845	A771	C	
						U1097	C980	C846	A772	C	
						U1097	C981	C847	A773	C	
						U1097	C982	C848	A774	C	
						U1097	C983	C849	A775	C	
						U1097	C984	C850	A776	C	
						U1097	C985	C851	A777	C	
						U1097	C986	C852	A778	C	
						U1097	C987	C853	A779	C	
						U1097	C988	C854	A780	C	
						U1097	C989	C855	A781	C	
						U1097	C990	C856	A782	C	
						U1097	C991	C857	A783	C	
						U1097	C992	C858	A784	C	
						U1097	C993	C859	A785	C	
						U1097	C994	C860	A786	C	
						U1097	C995	C861	A787	C	
						U1097	C996	C862	A788	C	
						U1097	C997	C863	A789	C	
						U1097	C998	C864	A790	C	
						U1097	C999	C865	A791	C	
						U1097	C1000	C866	A792	C	
						U1097	C1001	C867	A793	C	
						U1097	C1002	C868	A794	C	
						U1097	C1003	C869	A795	C	
						U1097	C1004	C870	A796	C	
						U1097	C1005	C871	A797	C	
						U1097	C1006	C872	A798	C	
						U1097	C1007	C873	A799	C	
						U1097	C1008	C874	A800	C	
						U1097	C1009	C875	A801	C	
						U1097	C1010	C876	A802	C	
						U1097	C1011	C877	A803	C	
						U1097	C1012	C878	A804	C	
						U1097	C1013	C879	A805	C	
						U1097	C1014	C880	A806	C	
						U1097	C1015	C881	A807	C	
						U1097	C1016	C882	A808	C	
						U1097	C1017	C883	A809	C	
						U1097	C1018	C884	A810	C	
						U1097	C1019	C885	A811	C	
						U1097	C1020	C886	A812	C	
						U1097	C1021	C887	A813	C	
						U1097	C1022	C888	A814	C	
						U1097	C1023	C889	A815	C	
						U1097	C1024	C890	A816	C	
						U1097	C1025	C891	A817	C	
						U1097	C1026	C892	A818	C	
						U1097	C1027	C893	A819	C	
						U1097	C1028	C894	A820	C	
						U1097	C1029	C895	A821	C	
						U1097	C1030	C896	A822	C	
						U1097	C1031	C897	A823	C	
						U1097	C1032	C898	A824	C	
						U1097	C1033	C899	A825	C	
						U1097	C1034	C900	A826	C	
						U1097	C1035	C901	A827	C	
						U1097	C1036	C902	A828	C	
						U1097	C1037	C903	A829	C	
						U1097	C103				

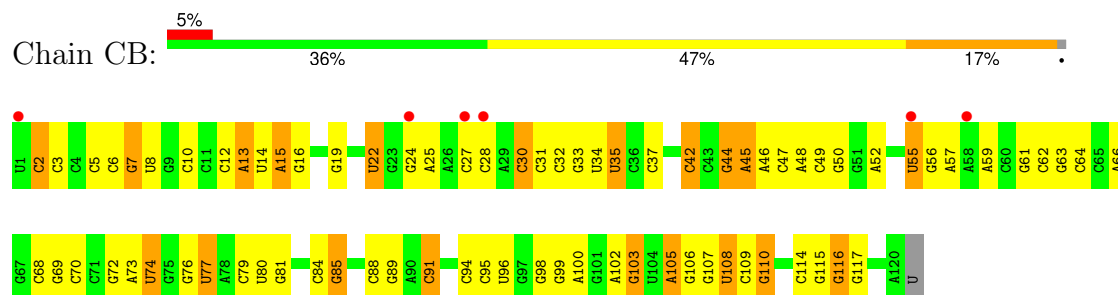
G2405	G2406	G2407	G2408	G2409	G2410	G2414	G2415	G2416	G2417	G2418	A2422	A2423	G2424	A2425	A2426	G2427	G2428	G2429	A2430	G2431	A2434	A2435	G2436	G2437	G2438	G2439	G2440	G2441	G2442	G2443	G2444	G2445	G2446	G2447	A2448	A2451	A2452	A2453	G2454	G2455	G2456	G2457	G2458	G2459	G2460	G2465	G2466	G2467	G2468	G2469	G2470	G2474	G2475																																																																				
C2343	U2344	C2345	C2346	C2347	U2348	C2349	C2350	C2351	C2352	C2353	C2354	C2355	C2356	U2357	C2358	C2359	C2360	C2361	C2362	C2363	C2364	C2365	A2366	C2367	C2368	A2369	C2370	C2371	C2372	C2373	C2374	U2375	C2376	C2377	C2378	C2379	C2380	C2381	C2382	C2383	C2384	C2385	C2386	U2387	C2388	C2389	C2390	C2391	A2392	C2393	C2394	C2395	C2396	C2397	C2398	G2400	U2401	C2404																																																															
G2275	G2276	G2277	A2278	G2279	G2280	C2281	G2282	C2283	C2284	C2285	A2286	A2287	A2288	G2289	G2290	U2291	C2292	C2293	C2294	C2295	U2296	C2297	A2298	G2299	G2302	G2303	C2304	G2305	C2306	G2307	U2312	C2313	C2314	G2315	C2316	C2317	C2318	C2319	A2320	G2321	A2322	G2323	C2324	G2325	C2326	A2327	A2328	G2329	C2330	C2331	U2332	A2333	C2334	A2335	A2336	G2340																																																																	
C2195	C2196	U2197	A2198	C2199	C2200	C2201	C2202	U2203	C2204	C2205	G2206	G2207	A2208	U2218	G2222	A2225	C2226	A2227	C2228	C2229	U2233	G2234	G2235	C2236	C2237	C2238	C2239	U2243	U2244	A2247	C2248	U2249	G2250	G2251	G2252	G2253	C2254	G2255	G2256	U2257	C2258	G2259	C2260	C2261	U2262	C2263	C2264	U2265	A2268	U2269	U2272	A2273	A2274																																																																				
G2133	A2134	C2135	C2136	C2137	C2138	C2139	C2140	C2141	C2142	C2143	U2144	C2145	C2146	C2147	G2148	C2149	U2150	G2151	C2152	C2153	G2154	C2155	G2156	G2157	A2158	C2159	C2160	C2161	C2162	C2163	C2164	G2165	C2166	U2167	C2168	A2169	C2170	A2171	C2172	A2173	C2174	C2175	C2176	C2177	C2178	C2179	U2180	G2181	G2182	C2183	G2187	C2188	U2189	G2190	C2191	C2192	G2193	C2194																																																															
A2057	A2060	C2061	C2062	C2063	C2064	C2065	C2066	G2069	C2070	G2071	C2072	C2073	U2074	U2075	C2078	U2079	G2080	C2081	A2082	U2086	G2087	C2095	U2102	C2103	G2104	C2105	G2106	C2107	C2108	U2109	C2110	C2111	G2112	U2113	A2114	G2115	C2116	A2117	U2118	A2119	G2120	G2121	U2122	G2123	G2124	G2125	A2126	G2127	C2128	C2129	U2130	G2131	U2132																																																																				
G1992	U1993	C1994	U1995	C1996	C1997	C1998	C1999	G2000	A2001	G2002	G2003	C2004	A2005	C2006	C2007	G2010	A2013	A2014	A2015	A2016	A2020	C2021	U2022	G2023	G2024	C2025	C2026	G2027	U2028	G2029	A2030	A2031	G2032	A2033	U2034	G2035	C2036	G2037	C2038	C2039	C2040	U2041	A2042	C2043	C2044	C2045	G2046	U2047	C2050	A2051	C2052	G2053	A2054	C2055	G2056																																																																		
U1833	U1834	C1835	C1836	C1837	C1838	C1839	G1840	U1841	C1842	C1843	C1844	A1847	A1848	C1849	G1850	G1857	G1858	G1859	G1860	G1861	U1864	G1865	C1866	A1867	C1868	C1869	C1870	C1871	C1872	C1873	C1874	C1875	C1876	C1877	C1878	C1879	C1880	C1881	C1882	C1883	C1884	C1885	C1886	C1887	C1888	C1889	A1890	C1892	C1893	C1894	C1895	U1898	C1899	A1900	G1903	G1906	C1907	C1908	C1909	A1913	C1914	U1917	A1918	A1919	C1920																																																								
G1921	G1922	U1923	U1926	U1927	A1928	G1929	G1930	U1931	C1932	C1933	C1934	G1935	A1936	A1937	A1938	U1939	U1943	U1944	G1945	U1946	G1949	G1950	U1951	A1952	A1953	A1954	U1955	U1956	C1957	C1958	C1959	C1962	U1963	A1966	C1967	G1968	A1969	A1970	A1971	A1972	G1973	C1974	C1975	C1979	G1980	A1981	G1984	G1985	C1988	U1991																																																																							
C1774	C1775	G1776	U1777	C1778	U1779	A1780	A1786	C1788	A1789	C1790	A1791	C1792	C1793	U1794	C1795	U1796	C1797	U1798	G1799	C1800	C1801	A1802	C1803	C1804	C1805	C1806	C1807	U1808	A1809	A1810	G1811	C1812	G1813	C1814	C1815	C1816	C1817	C1818	C1819	U1820	A1821	G1822	C1823	G1824	A1825	G1826	C1827	U1828	A1829	C1830	G1831	C1832																																																																					
C1612	G1613	A1614	C1615	A1616	C1617	A1618	G1619	G1620	C1621	U1622	C1623	G1624	G1627	C1632	G1633	A1634	A1637	C1638	U1639	C1640	A1641	C1642	G1643	C1644	C1645	C1646	G1647	C1648	C1651	A1652	C1653	A1654	C1657	C1658	C1659	C1660	G1661	C1662	C1663	A1664	A1665	G1666	G1667	A1668	A1669	C1670	C1671	U1672	C1673	U1674	U1675	C1676	U1677	C1678	C1679	C1680	C1681	C1682	C1683	C1684	C1685	C1686	C1687	C1688	C1689	C1690	C1691	C1692	C1693	C1694	C1695	C1696	C1697	C1698	C1699	C1700	C1701	C1702	C1703	C1704	C1707	C1708	U1709	C1710	C1711	U1720	G1721	C1722	U1729	C1730	C1731	C1732	C1733	C1734	C1735	C1736	C1737	C1738	C1739	C1740	C1741	C1744	G1747A	C1753	C1754	C1755	C1756	U1757	C1758	A1759	A1760	C1761	A1762	C1763	U1764	C1767	U1768	C1769	C1770	C1771	C1772
G1537	G1538	G1539	U1540	G1541	A1542	C1543	C1547	C1548	C1549	C1550	A1553	C1556	C1557	A1558	G1559	G1560	G1561	C1564	C1565	C1566	C1567	C1568	C1569	C1570	A1571	C1572	U1573	C1574	C1575	C1576	C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1599	C1600	G1601	U1602	C1603	C1604	C1605	C1606	A1608	C1609	A1610	C1611																																																										
A1471	A1472	G1473	U1474	G1475	C1476	A1477	C1478	C1479	G1480	C1481	G1482	G1487	G1488	U1489	A1490	G1491	G1492	C1493	A1494	A1495	A1496	U1497	C1498	C1499	G1500	C1501	C1502	U1503	C1504	C1505	C1506	A1507	C1508	C1509	A1509A	A1509B	G1510	C1511	U1512	C1513	U1514	C1515	C1516	C1517	U1518	G1519	C1520	U1523	A1528A	G1529	C1532	G1533	U	A	C1536																																																																		



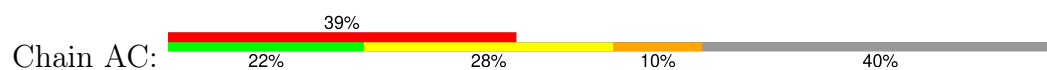
- Molecule 2: 5S Ribosomal RNA

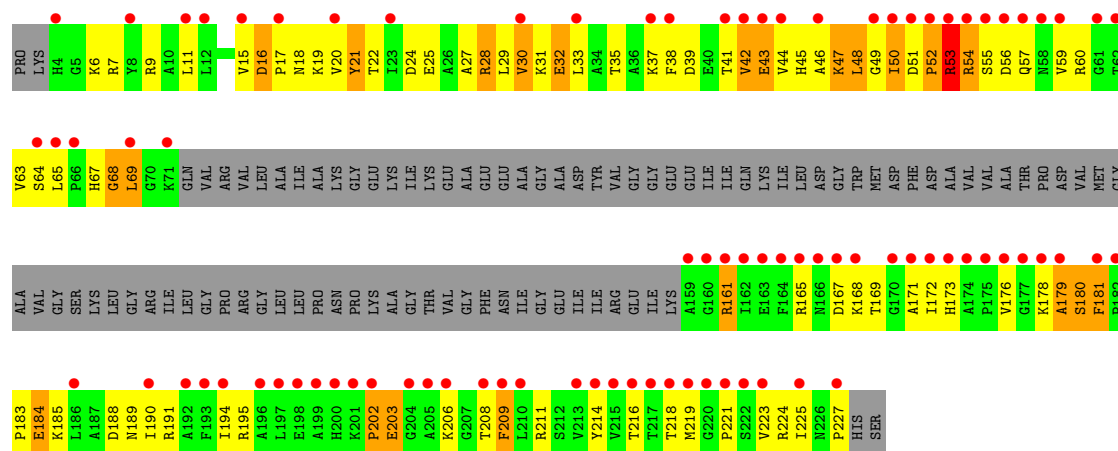


- Molecule 2: 5S Ribosomal RNA

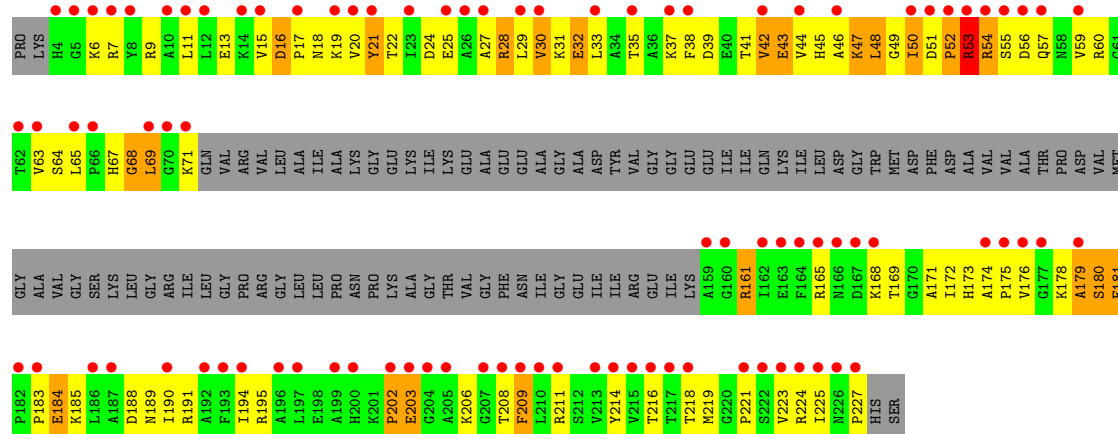
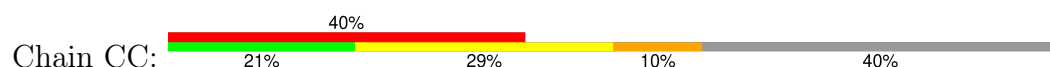


- Molecule 3: 50S ribosomal protein L1

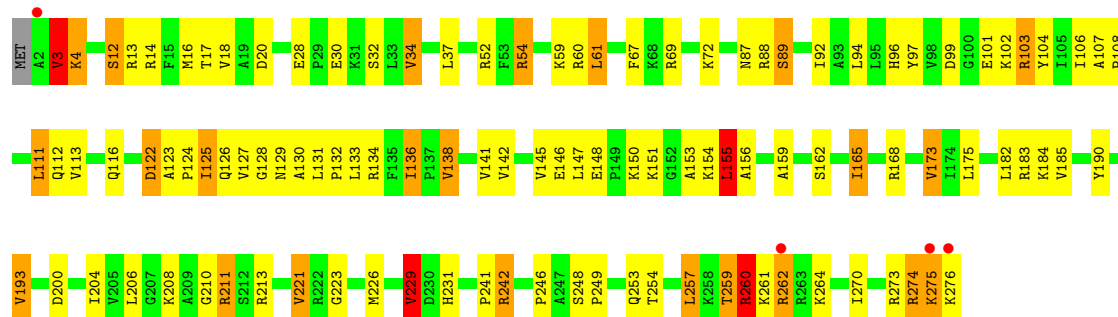




• Molecule 3: 50S ribosomal protein L1

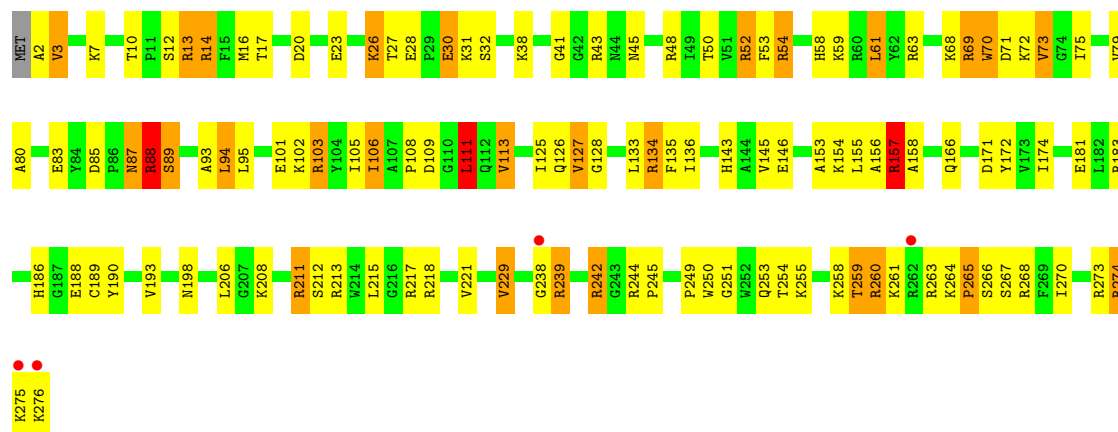


• Molecule 4: 50S ribosomal protein L2



• Molecule 4: 50S ribosomal protein L2





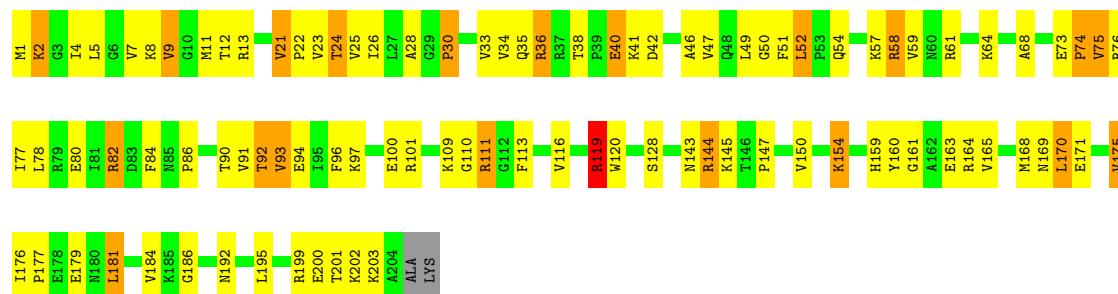
• Molecule 5: 50S ribosomal protein L3

Chain AE: 59% 32% 8%



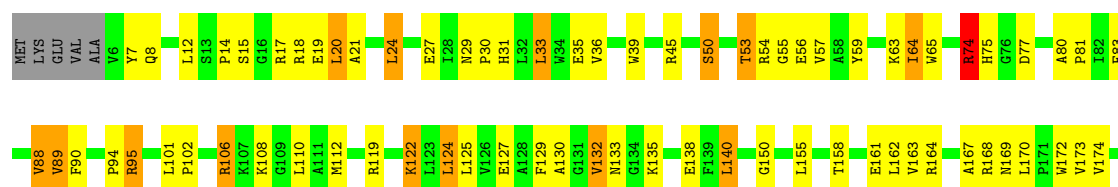
• Molecule 5: 50S ribosomal protein L3

Chain CE: 52% 36% 10%



• Molecule 6: 50S ribosomal protein L4

Chain AF: 54% 33% 9%

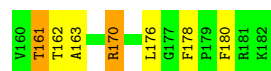
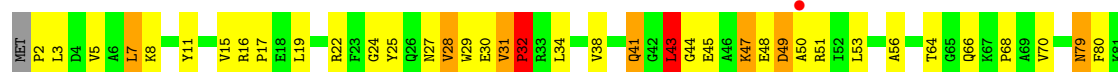




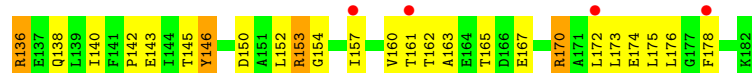
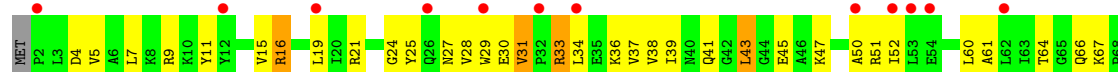
• Molecule 6: 50S ribosomal protein L4



• Molecule 7: 50S ribosomal protein L5

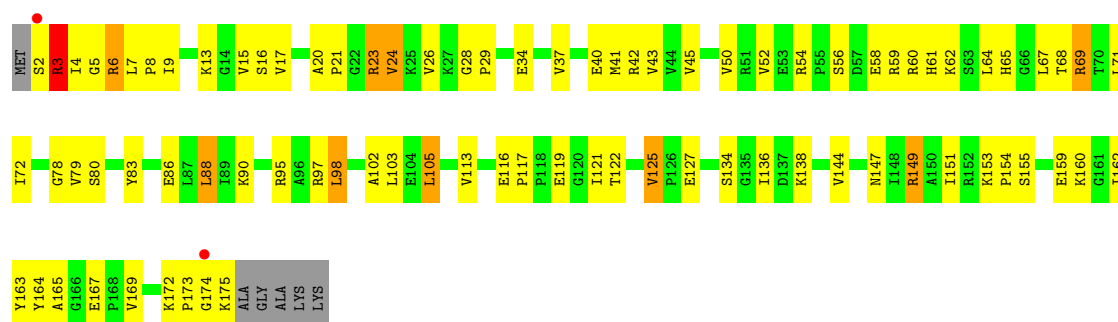


• Molecule 7: 50S ribosomal protein L5

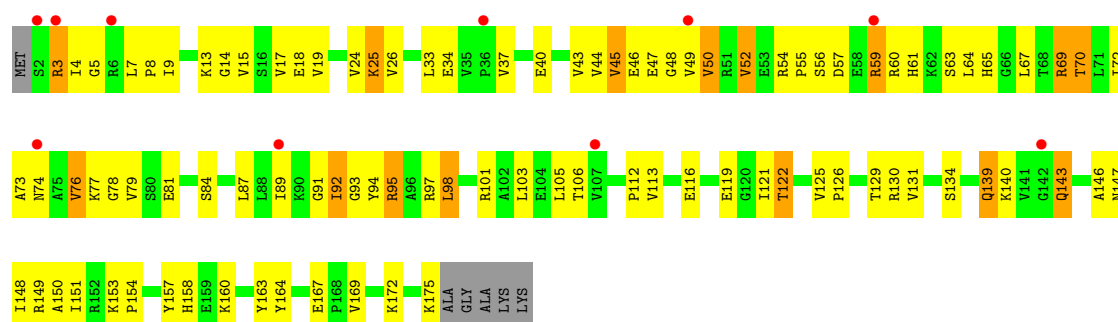


• Molecule 8: 50S ribosomal protein L6

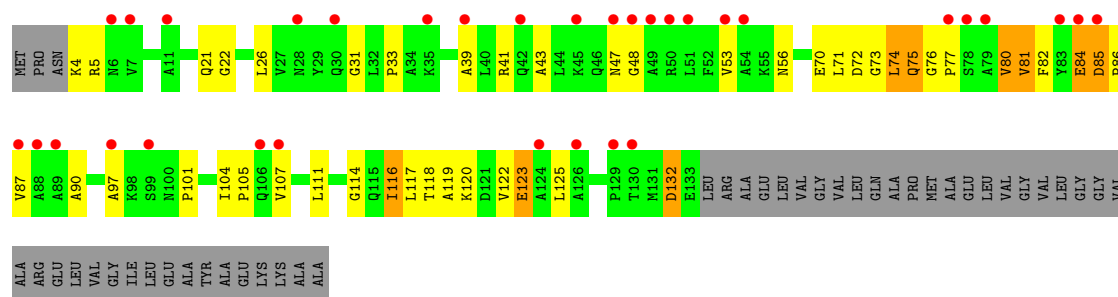




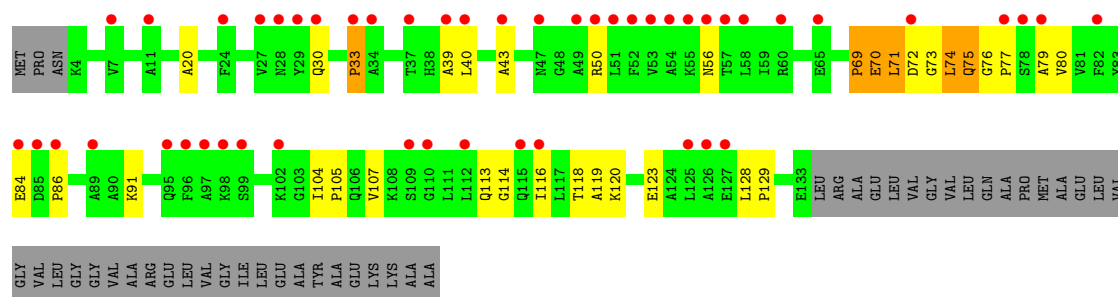
• Molecule 8: 50S ribosomal protein L6



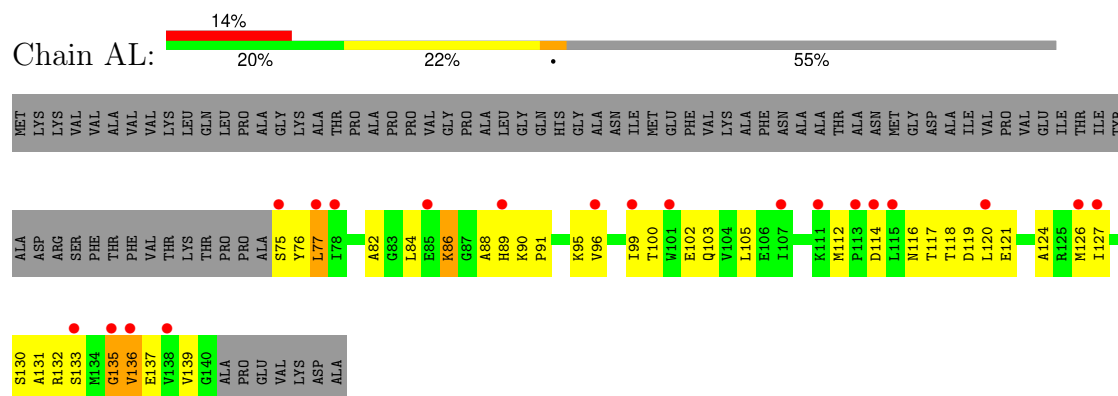
• Molecule 9: 50S ribosomal protein L10



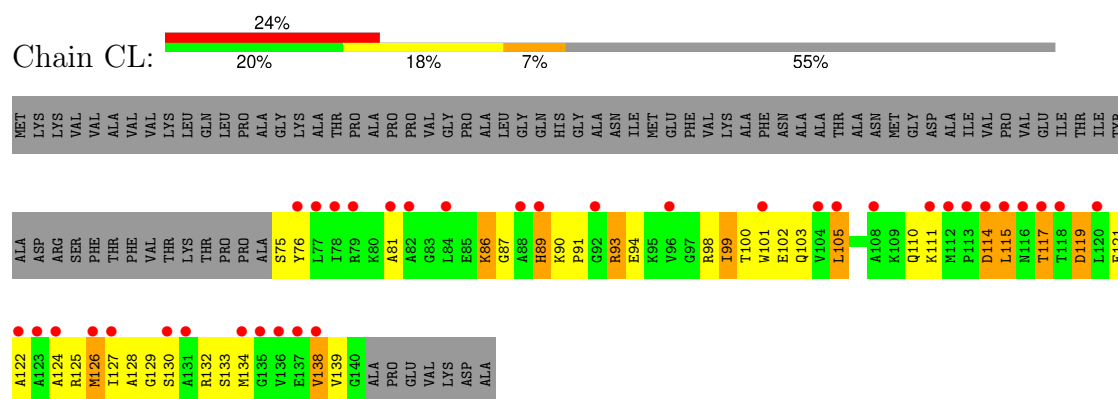
• Molecule 9: 50S ribosomal protein L10



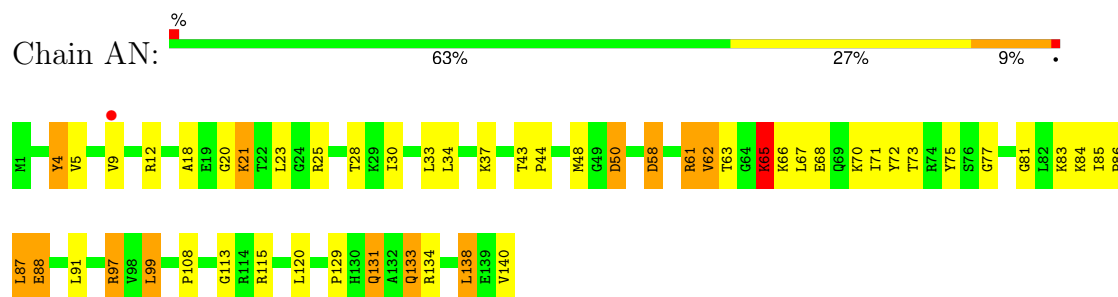
- Molecule 10: 50S ribosomal protein L11



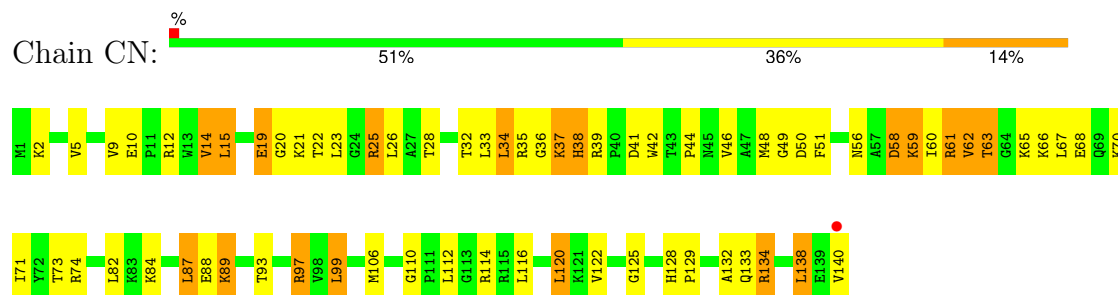
- Molecule 10: 50S ribosomal protein L11



- Molecule 11: 50S ribosomal protein L13

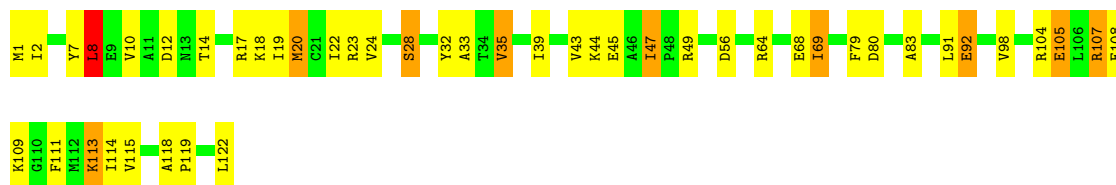


- Molecule 11: 50S ribosomal protein L13



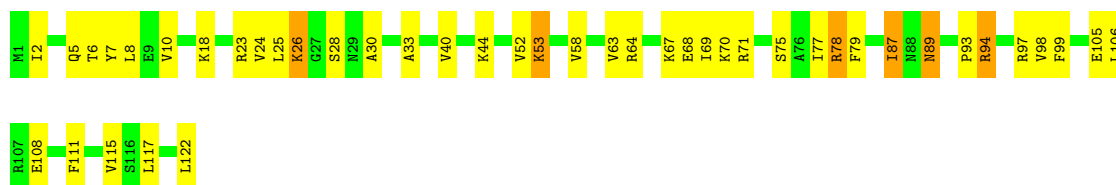
- Molecule 12: 50S ribosomal protein L14

Chain AO:  62% 30% 7%



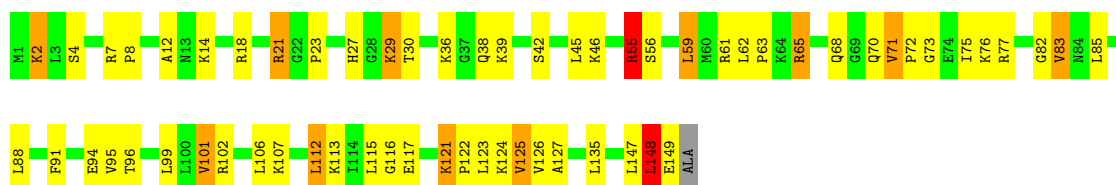
- Molecule 12: 50S ribosomal protein L14

Chain CO:  64% 31% 5%



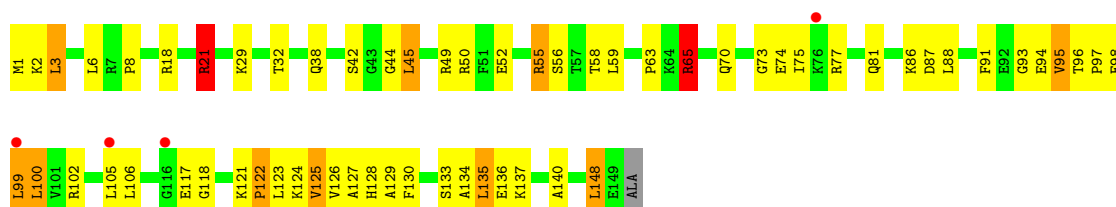
- Molecule 13: 50S ribosomal protein L15

Chain AP:  58% 33% 7%



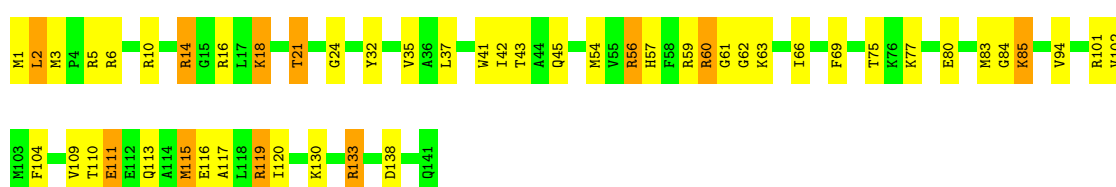
- Molecule 13: 50S ribosomal protein L15

Chain CP:  58% 33% 7%

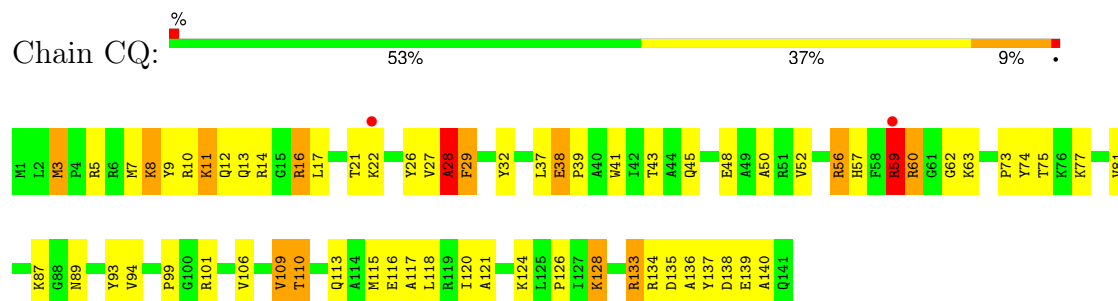


- Molecule 14: 50S ribosomal protein L16

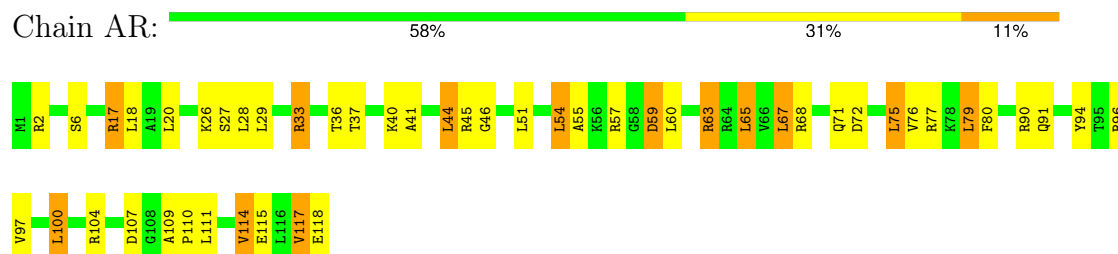
Chain AQ:  65% 28% 8%



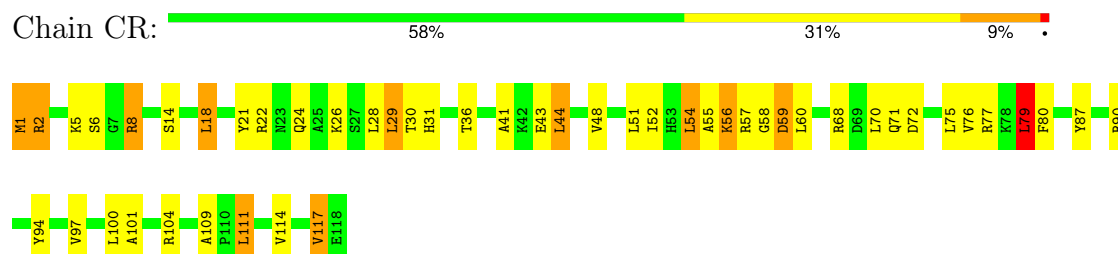
- Molecule 14: 50S ribosomal protein L16



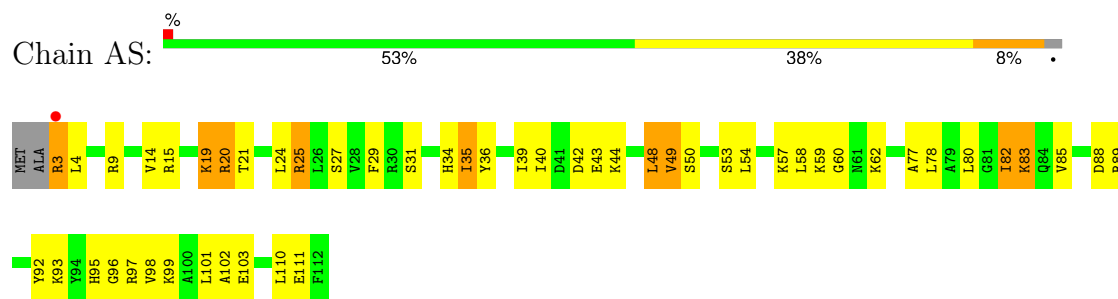
- Molecule 15: 50S ribosomal protein L17



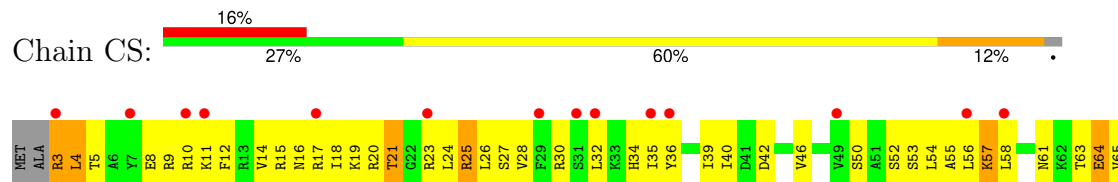
- Molecule 15: 50S ribosomal protein L17

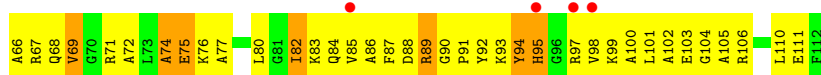


- Molecule 16: 50S ribosomal protein L18

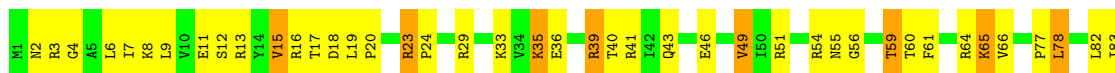


- Molecule 16: 50S ribosomal protein L18

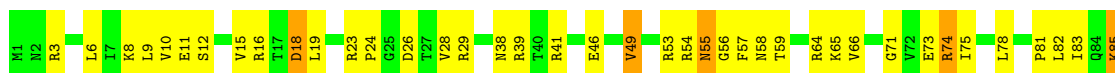




• Molecule 17: 50S ribosomal protein L19



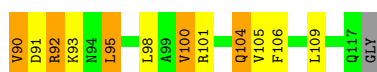
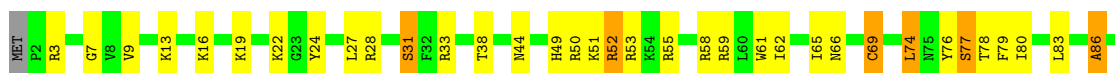
• Molecule 17: 50S ribosomal protein L19



• Molecule 18: 50S ribosomal protein L20

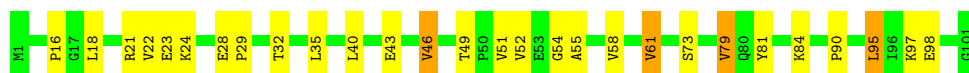


• Molecule 18: 50S ribosomal protein L20

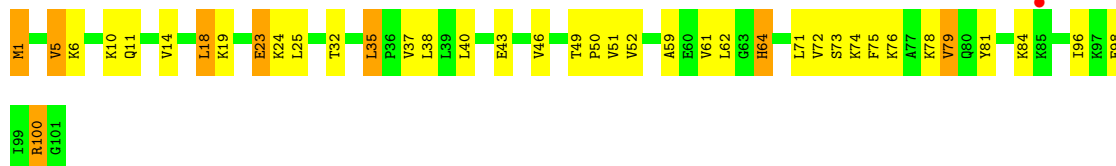


• Molecule 19: 50S ribosomal protein L21





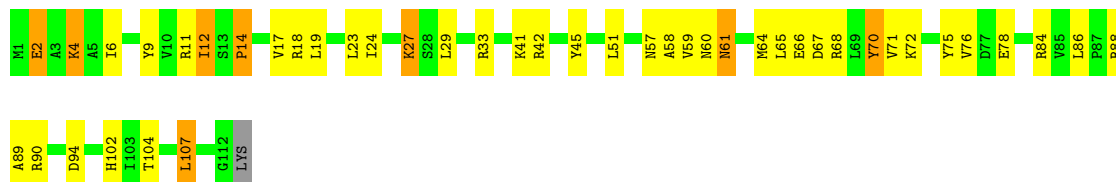
- Molecule 19: 50S ribosomal protein L21



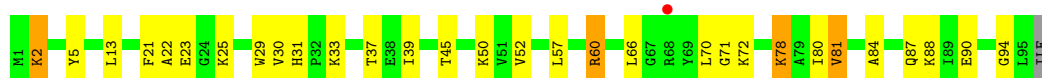
- Molecule 20: 50S ribosomal protein L22



- Molecule 20: 50S ribosomal protein L22



- Molecule 21: 50S ribosomal protein L23



- Molecule 21: 50S ribosomal protein L23

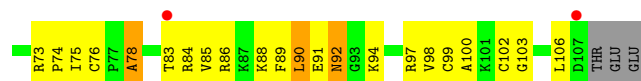
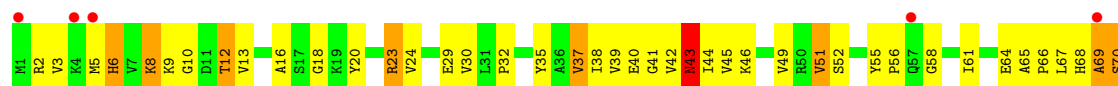
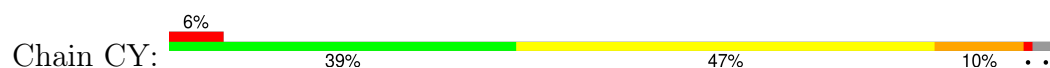




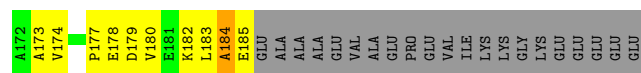
- Molecule 22: 50S ribosomal protein L24



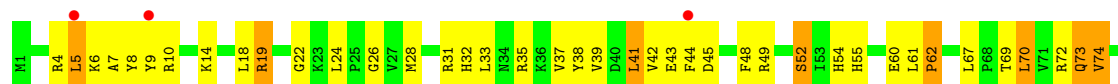
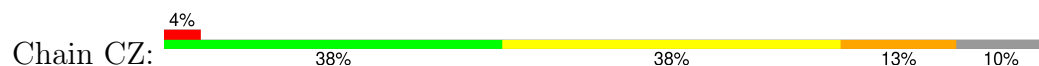
- Molecule 22: 50S ribosomal protein L24

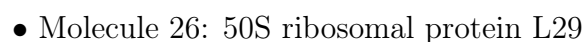


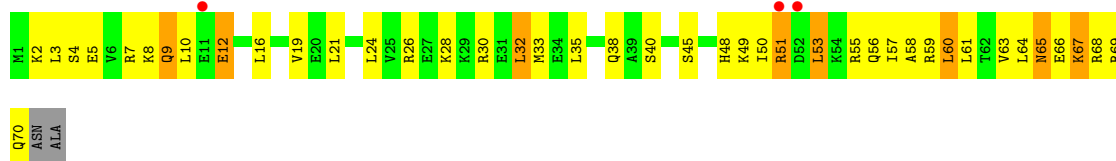
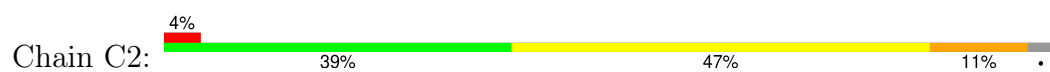
- Molecule 23: 50S ribosomal protein L25



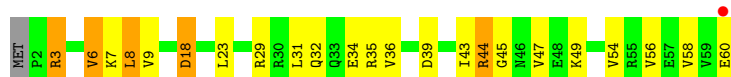
- Molecule 23: 50S ribosomal protein L25



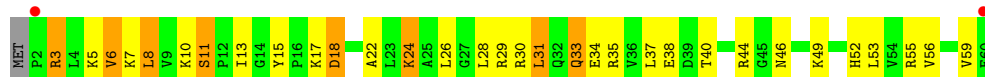




- Molecule 27: 50S ribosomal protein L30



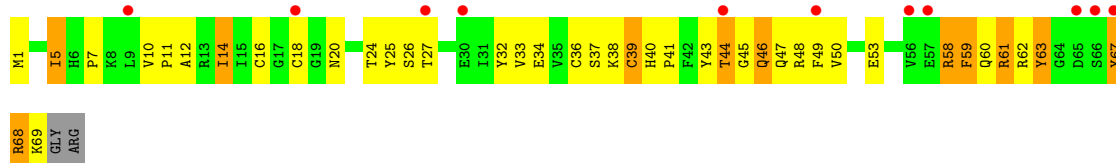
- Molecule 27: 50S ribosomal protein L30



- Molecule 28: 50S ribosomal protein L31



- Molecule 28: 50S ribosomal protein L31



- Molecule 29: 50S ribosomal protein L32

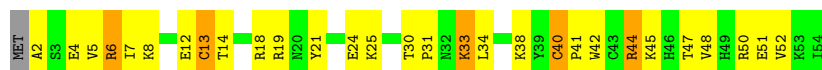


- Molecule 29: 50S ribosomal protein L32





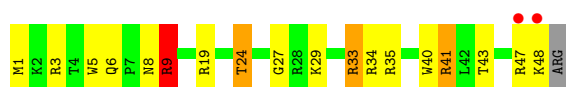
- Molecule 30: 50S ribosomal protein L33



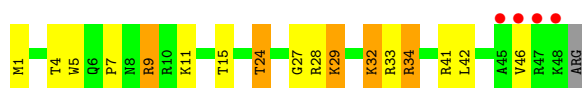
- Molecule 30: 50S ribosomal protein L33



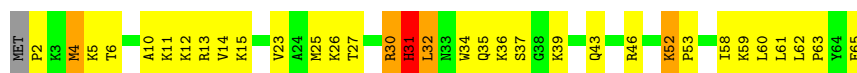
- Molecule 31: 50S ribosomal protein L34



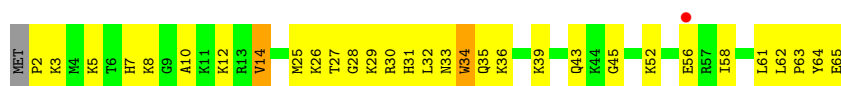
- Molecule 31: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L35



- Molecule 32: 50S ribosomal protein L35

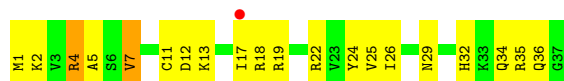


- Molecule 33: 50S ribosomal protein L36

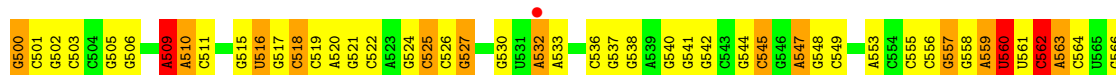
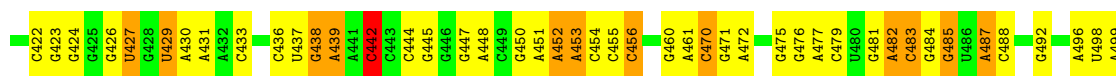
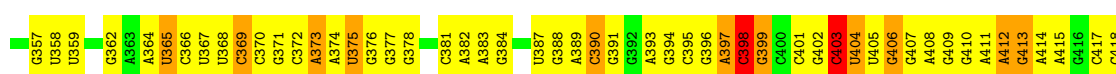
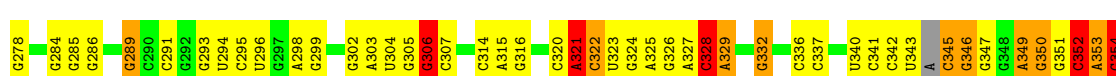
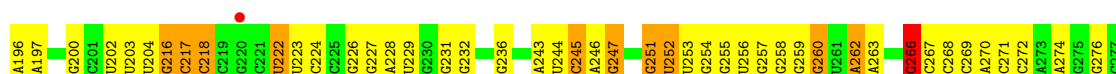
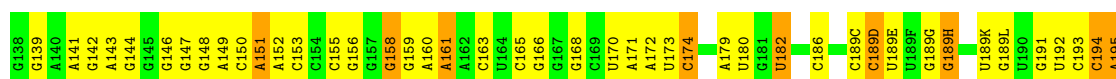
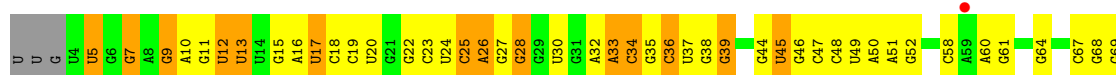




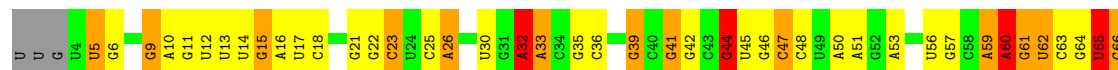
- Molecule 33: 50S ribosomal protein L36



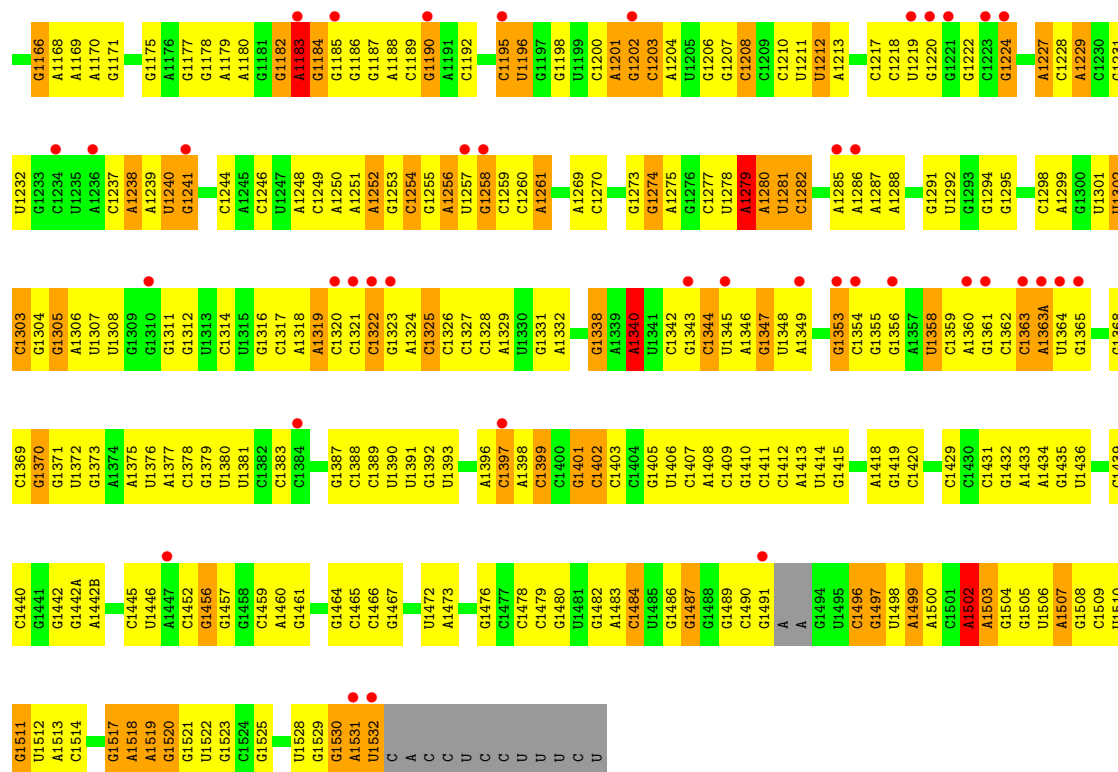
- Molecule 34: 16S Ribosomal RNA



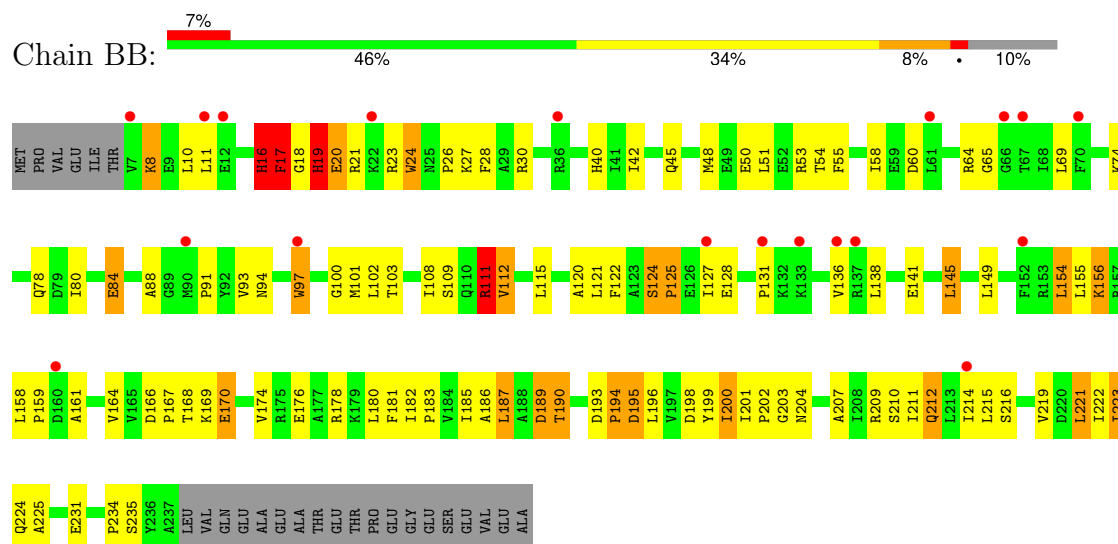
- Molecule 34: 16S Ribosomal RNA



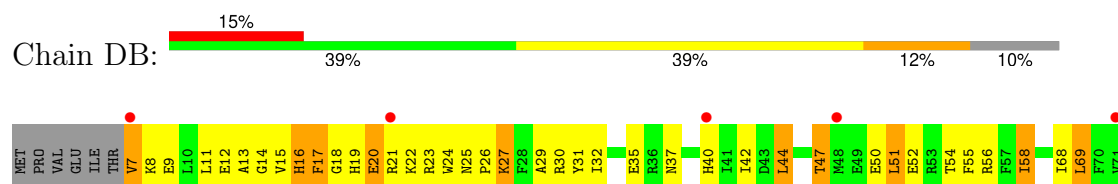
A1101	A1102	C1037	A977	A907	A828	G760	A687	U598	C449	C381	G309	G236	A162	C67
G1103	G1104	U1040	A978	A908	G829	G763	G688	C599	C450	A382	C314	C237	C163	G70
G1105	G1106	U1041	C979	A909	U830	G764	C689	C600	A451	A383	C315	C240	U164	C71
C1107	G1107	G1042	U981	C912	C832	G765	G690	C601	A452	A384	C316	C241	G166	C72
C1108	C1044	A983	A984	A913	U833	A766	U692	A602	C453	G388	C320	C242	A171	G73
G1109	C1045	A985	C984	A914	C834	A767	G693	A607	C454	A389	A321	A243	A172	G79
A1110	U1046	G985	U986	A915	U835	A768	A694	A608	C455	C390	A322	U244	U173	G80
A1111	G1048	A986	A987	A916	G836	G769	A695	A609	C458	G391	C323	C245	C174	U
C1112	U1049	G988	U989	A917	G837	C770	A696	C610	C460	A392	C324	U246	C175	U
C1113	U1050	C989	U990	A918	G838	G771	U697	A611	C461	A393	G325	C247	C176	U
C1114	G1060	U920	C990	A919	C840	G772	G698	C612	C470	G394	A326	G251	C177	U84
C1115	U1062	U921	U991	A920	U841	G773	C701	C613	C471	C395	C327	G252	C178	U88
C1116	G1063	G922	A992	G923	A848	G775	A702	C618	C472	G396	C328	G253	U180	C89
C1117	U1064	A923	G924	G925	G849	A777	G703	U619	C473	A397	C329	G254	U181	G97
C1118	G1065	G926	G927	G928	U850	G778	C707	C620	C474	C398	C330	U255	U182	G98
C1119	U1066	G929	G930	G931	U851	G779	C708	A621	C475	C403	G331	U256	G183	U99
C1120	G1067	G932	G933	G934	G852	A780	C709	C622	U480	U404	G332	G257	U184	C100
U1121	U1068	C932	G935	G936	G853	A781	G713	C623	C481	U405	G333	G258	C186	C101
U1122	C1069	G937	G938	G939	G854	A782	G714	C624	C482	G406	C334	G259	C187	A101
A1123	U1070	G940	G941	G942	G855	C783	A715	U625	C483	G407	C335	G260	C188	G102
C1124	G1061	C935	G936	G937	C856	C784	A716	U626	C484	A408	C336	G261	C189	C103
U1125	U1062	G938	G939	G940	G857	G785	A717	C627	C485	G409	C337	G262	G189	G104
U1126	C1063	A859	A860	A861	G858	G786	C719	C630	C486	G410	C338	G263	C189D	G105
G1127	U1064	A862	A863	A864	G859	A787	C720	U638	C487	A411	C344	G265	U189E	C106
C1128	U1065	G865	G866	G867	G860	A790	G721	C639	C488	A412	C345	G266	U189F	G107
C1129	C1066	G868	G869	G870	G861	G791	A722	U640	C489	G413	C346	G267	U189G	G108
A1130	U1067	G871	G872	G873	G862	G792	A723	U641	C490	A414	C347	G268	G189H	A109
C1131	C1068	G874	G875	G876	G863	G793	G724	C642	C491	A415	C348	G269	C189	C110
C1132	U1070	G877	G878	G879	G864	G794	G725	C643	C492	G416	C350	G270	G189L	G113
G1133	G1010	G880	G881	G882	G865	A795	G726	C644	A496	C417	C351	G271	U190	U114
U1134	U1012	G883	G884	G885	G866	G796	G727	U645	A497	C418	C352	G272	U191	G115
C1135	G1013	G886	G887	G888	G867	G798	A728	C649	C502	C419	C353	G273	U192	U116
C1074	U1014	G889	G890	G891	G868	G799	G730	C650	C503	U420	C354	G274	C193	C193
C1075	A1015	G892	G893	G894	G869	G803	G731	C651	C504	U421	C355	G275	C194	A116
C1076	U1016	G895	G896	G897	G870	G804	C732	U652	C505	C422	C356	G276	A195	G121
C1077	G1017	G898	G899	G900	G871	C805	A733	C656	C506	G425	C357	G277	A196	G122
U1078	G1018	G901	G902	G903	G872	C806	C736	U657	C507	G426	C358	G278	A197	C123
A1080	C1019	G904	G905	G906	G873	A807	A737	C658	C508	U427	C359	G279	G198	G124
G1081	U1020	G907	G908	G909	G874	C810	C738	C659	C509	G428	C360	G280	G199	U125
G1082	U1021	G910	G911	G912	G875	C811	C739	C660	C510	U429	C361	G281	G200	G126
G1083	U1022	G913	G914	G915	G876	C812	C740	C661	C511	A430	C362	G282	G201	G127
G1084	U1023	G916	G917	G918	G877	C813	C741	C662	C512	A431	C363	G283	U202	G128
U1085	C1027	G919	G920	G921	G878	U813	G742	C663	C513	A432	C364	G284	U203	U129
U1086	U1028	G922	G923	G924	G879	A814	G743	C664	C514	C433	C365	G285	U204	G129A
G1089	C1029	G925	G926	G927	G880	A815	U743	C665	C515	U434	C366	G286	G216	A130
U1090	U1030	G928	G929	G930	G881	A816	C747	C670	C516	C435	C367	G287	C221	C131
U1091	G1030A	G931	G932	G933	G882	C817	C748	C671	C517	C436	C368	G288	U222	A134
A1092	U1030B	G934	G935	G936	G883	C818	C749	C672	C518	U437	C369	G289	U223	U143
G1093	G1030C	G937	G938	G939	G884	G818	C750	C673	C519	G438	C370	G290	C224	G144
U1094	A1030D	G940	G941	G942	G885	G821	A753	C674	C520	A439	C371	G291	G227	A143
U1095	G1031	G943	G944	G945	G886	C822	C754	C675	C521	A440	C372	G292	A228	G147
C1096	G1032	G946	G947	G948	G887	C823	C755	C676	C522	A441	C373	G293	G231	G148
C1097	G1033	G949	G950	G951	G888	C824	C756	C677	C523	A442	C374	G294	G232	A149
U1098	U1034	G952	G953	G954	G889	C825	C757	C678	C524	C443	C375	G295	G305	C150
G1099	A1035	G955	G956	G957	G890	G826	C758	C679	C525	C444	C376	G296	C235	A161
U1100	U1036	G958	G959	G960	G891	U827	A759	C684	C526	C445	C377	G297	G308	

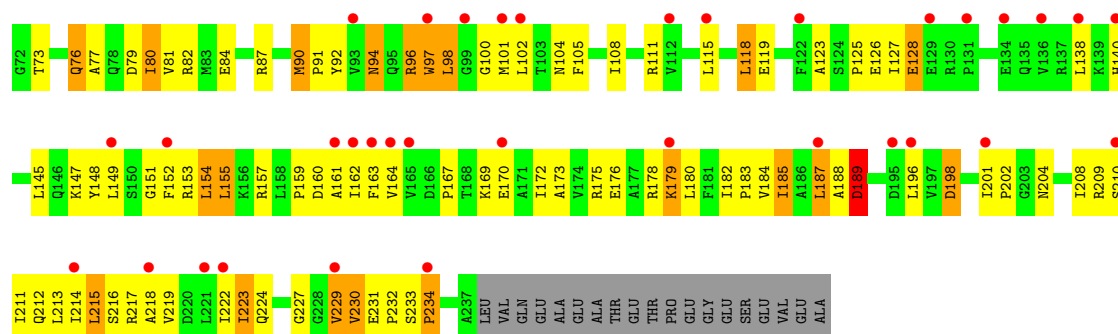


• Molecule 35: 30S ribosomal protein S2

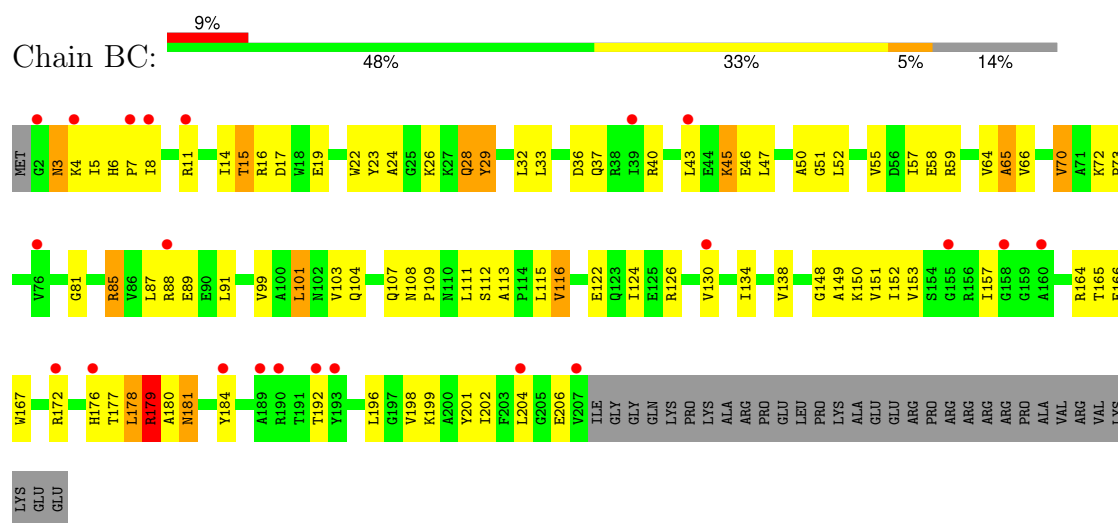


• Molecule 35: 30S ribosomal protein S2

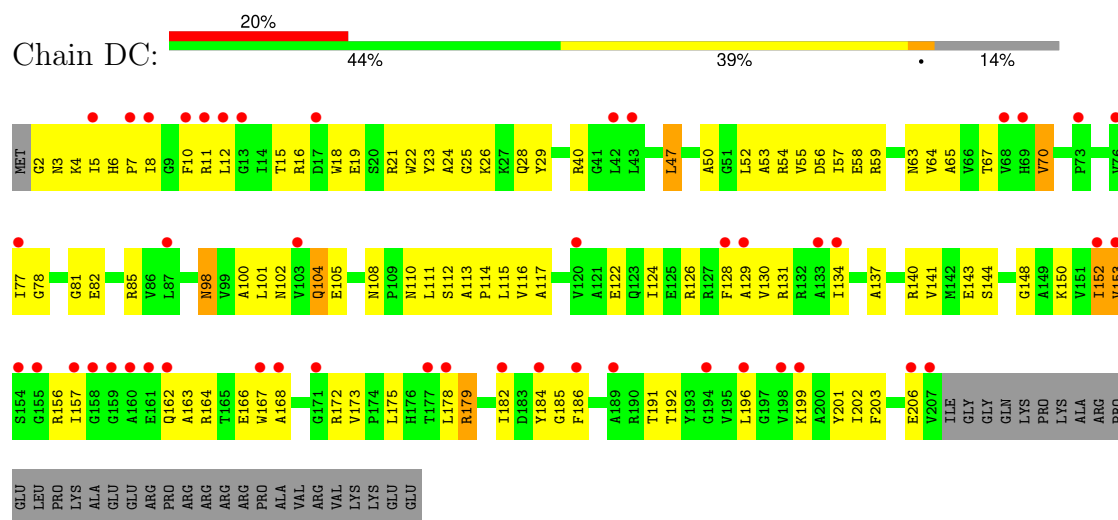




• Molecule 36: 30S ribosomal protein S3

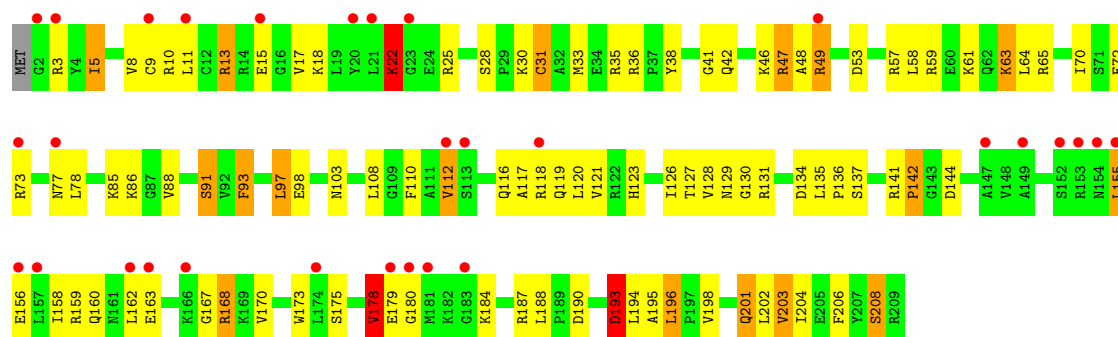


• Molecule 36: 30S ribosomal protein S3

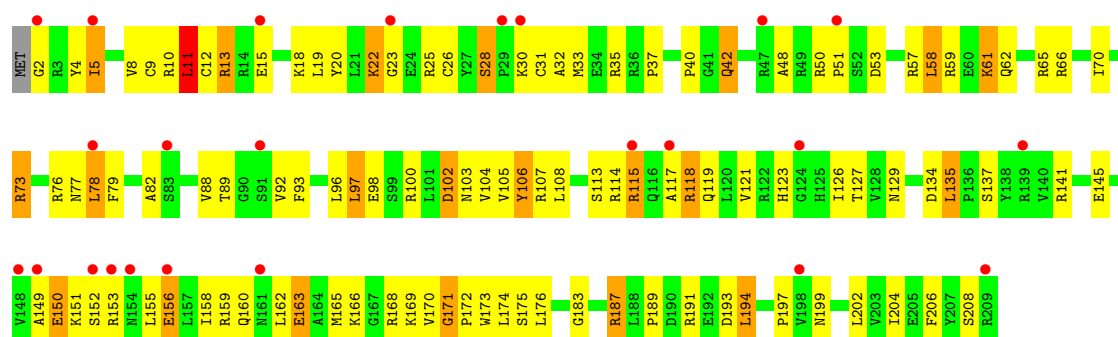


• Molecule 37: 30S ribosomal protein S4

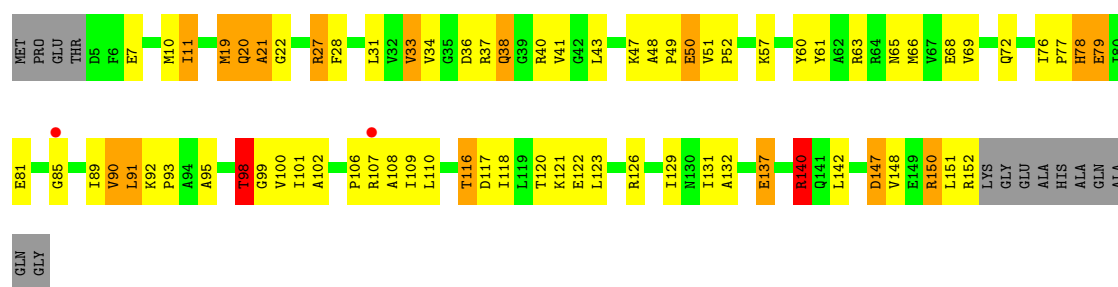




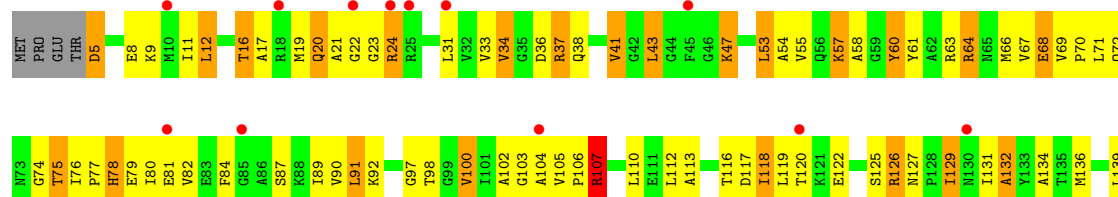
• Molecule 37: 30S ribosomal protein S4

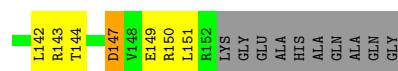


• Molecule 38: 30S ribosomal protein S5

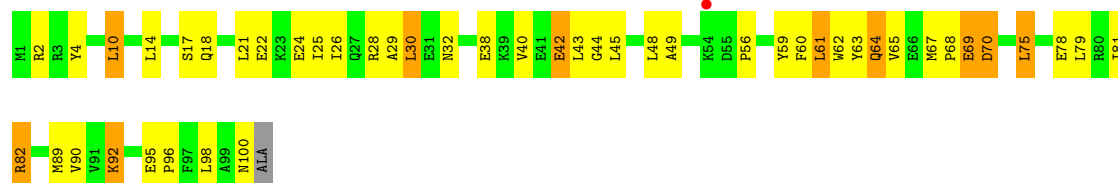


• Molecule 38: 30S ribosomal protein S5

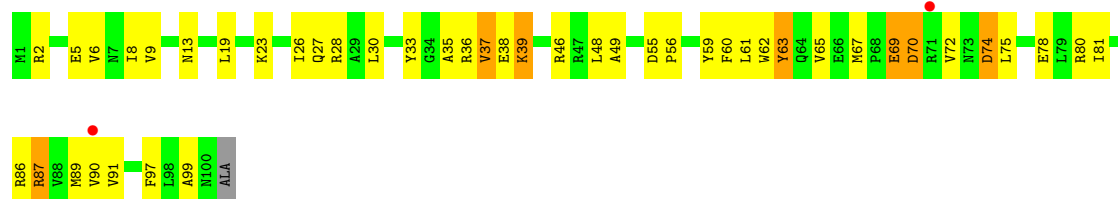




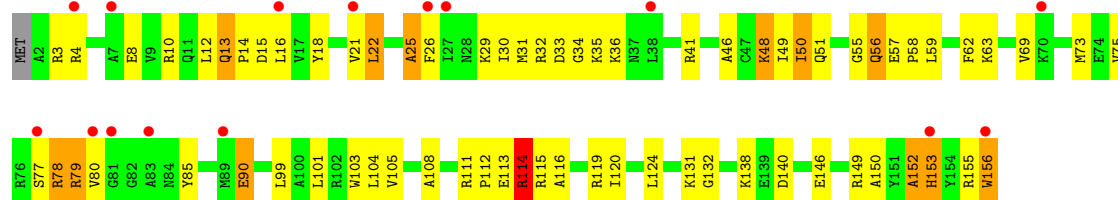
- Molecule 39: 30S ribosomal protein S6



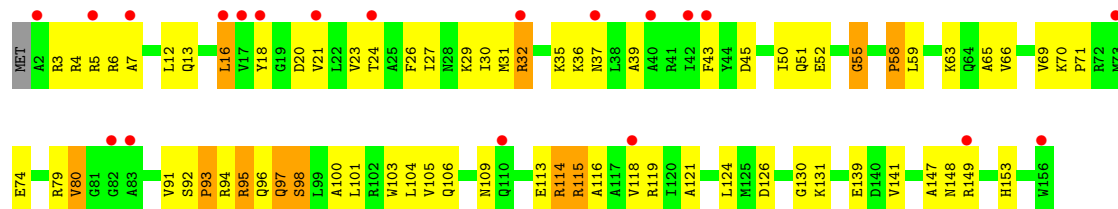
- Molecule 39: 30S ribosomal protein S6



- Molecule 40: 30S ribosomal protein S7

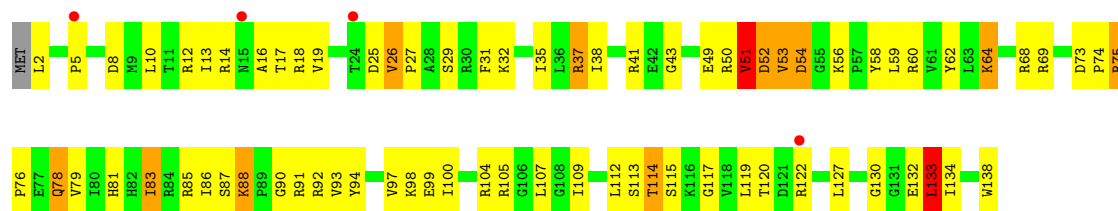


- Molecule 40: 30S ribosomal protein S7

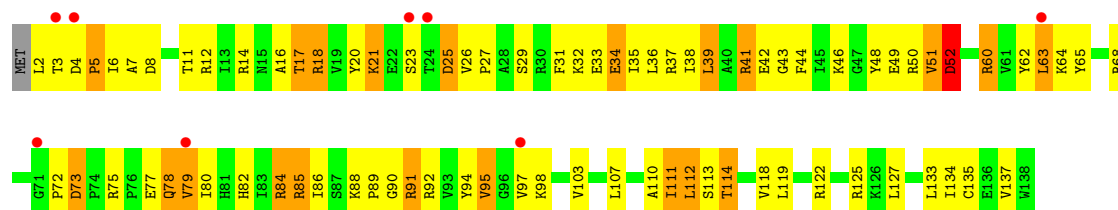


- Molecule 41: 30S ribosomal protein S8

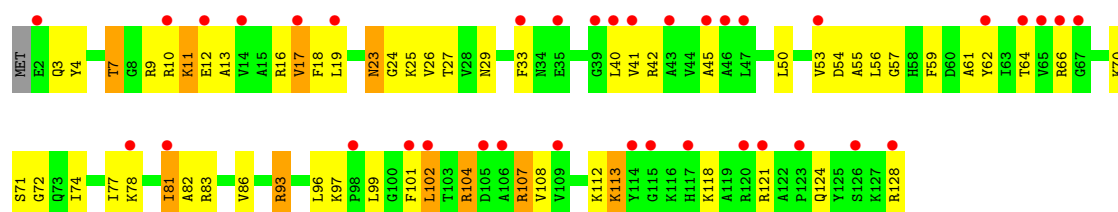




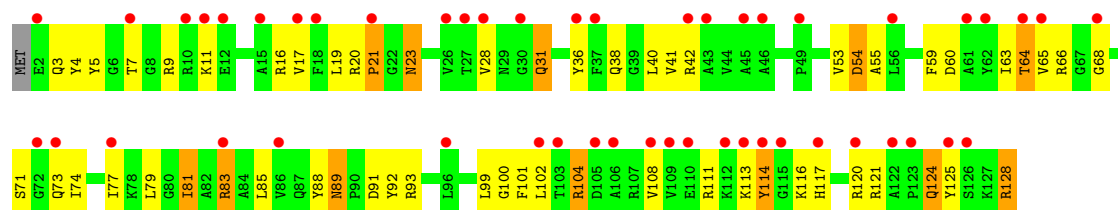
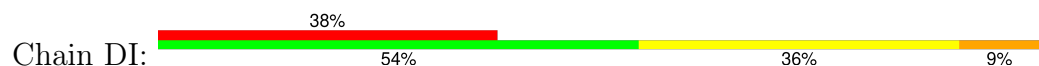
• Molecule 41: 30S ribosomal protein S8



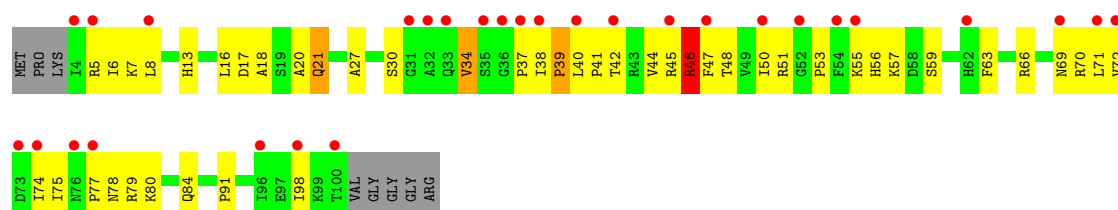
• Molecule 42: 30S ribosomal protein S9



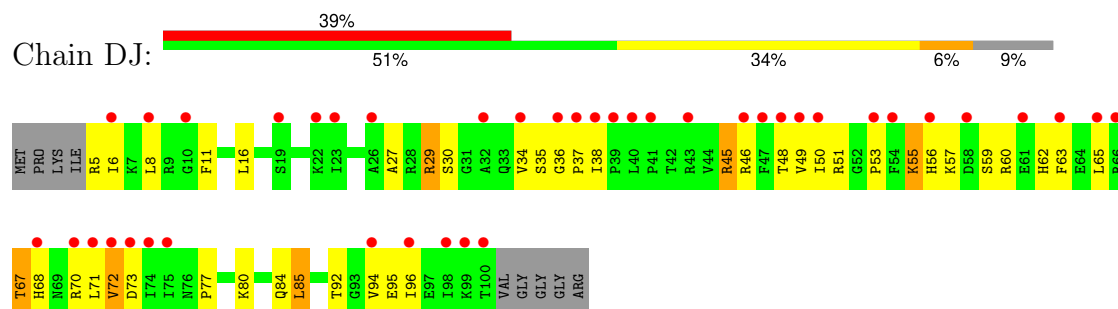
• Molecule 42: 30S ribosomal protein S9



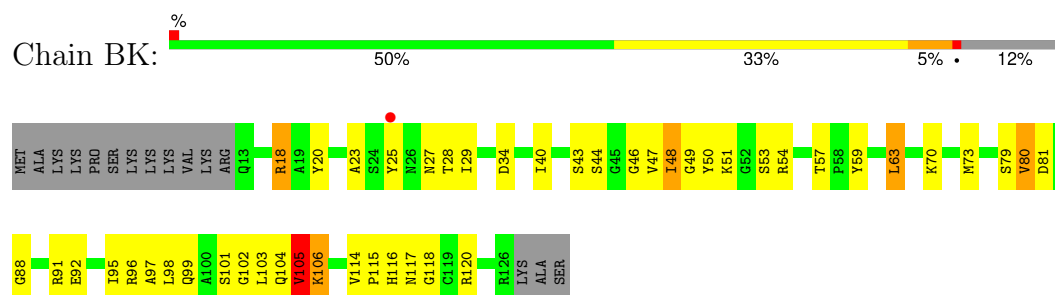
• Molecule 43: 30S ribosomal protein S10



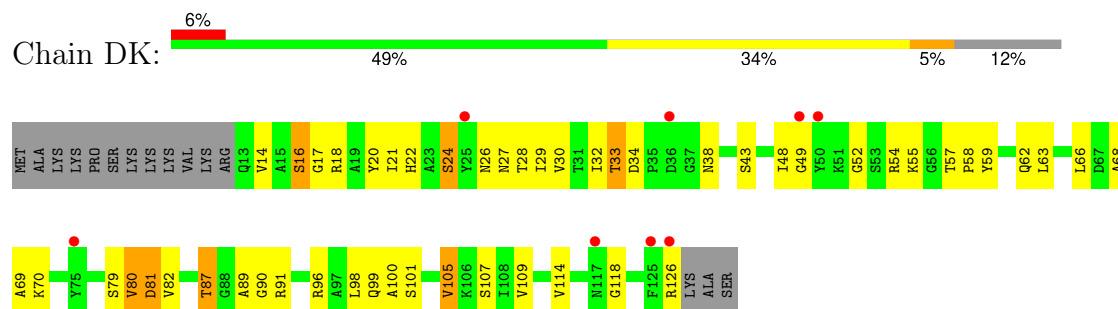
- Molecule 43: 30S ribosomal protein S10



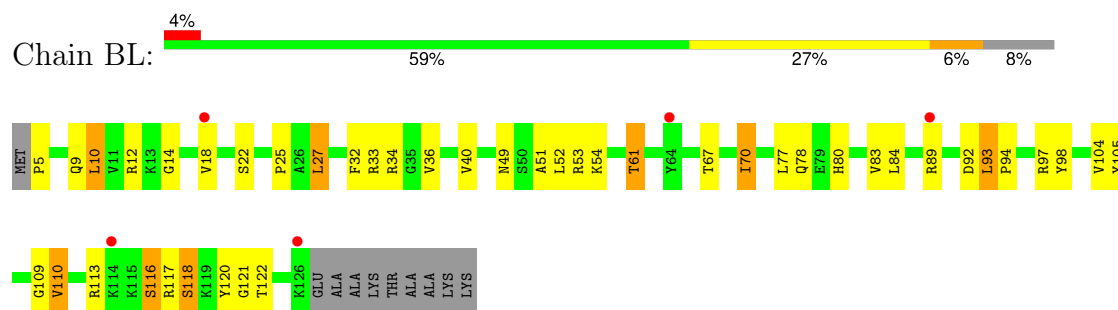
- Molecule 44: 30S ribosomal protein S11



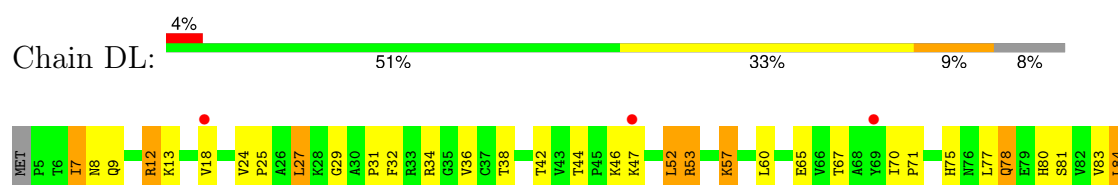
- Molecule 44: 30S ribosomal protein S11



- Molecule 45: 30S ribosomal protein S12

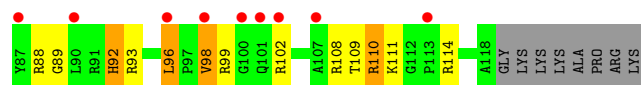


- Molecule 45: 30S ribosomal protein S12

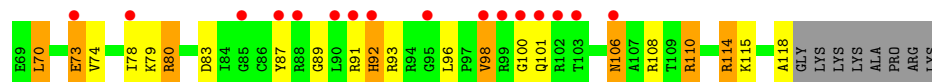
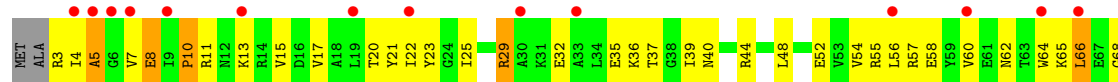




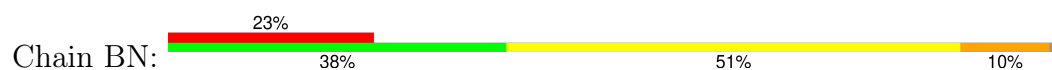
- Molecule 46: 30S ribosomal protein S13



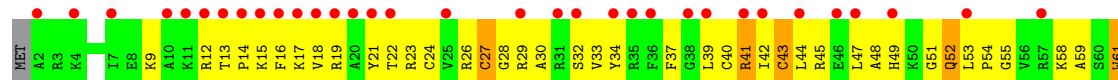
- Molecule 46: 30S ribosomal protein S13



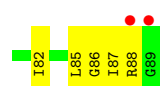
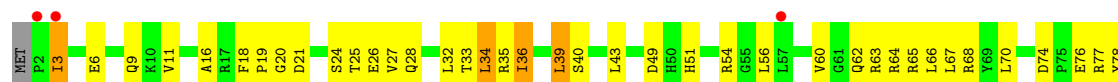
- Molecule 47: 30S ribosomal protein S14 type Z



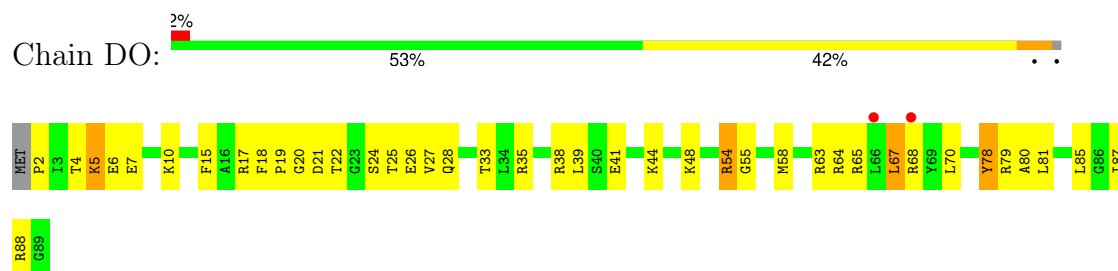
- Molecule 47: 30S ribosomal protein S14 type Z



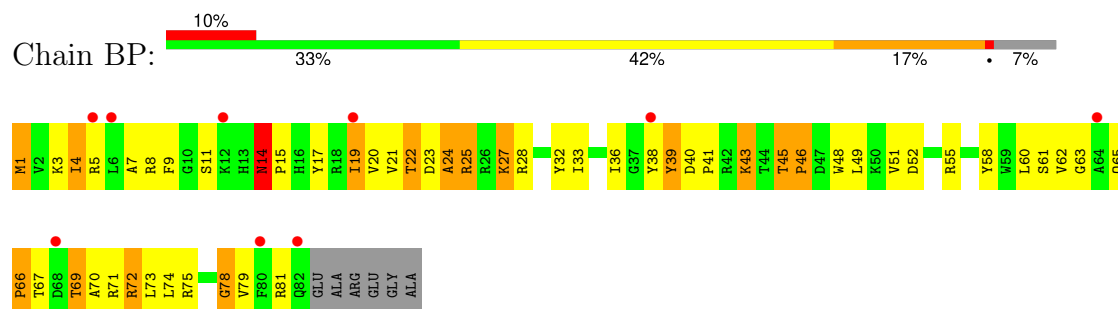
- Molecule 48: 30S ribosomal protein S15



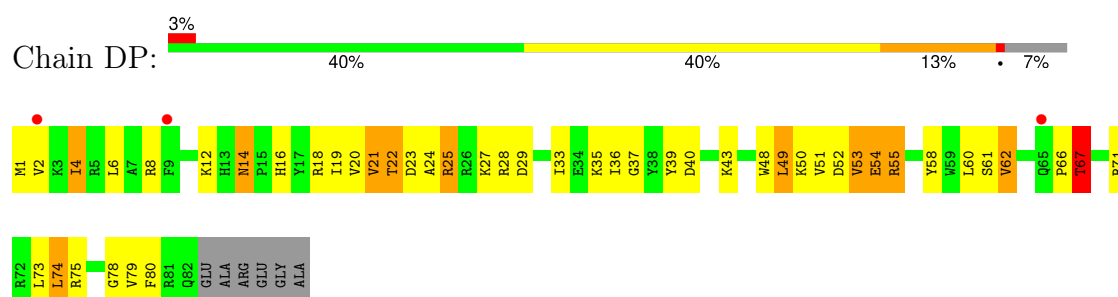
- Molecule 48: 30S ribosomal protein S15



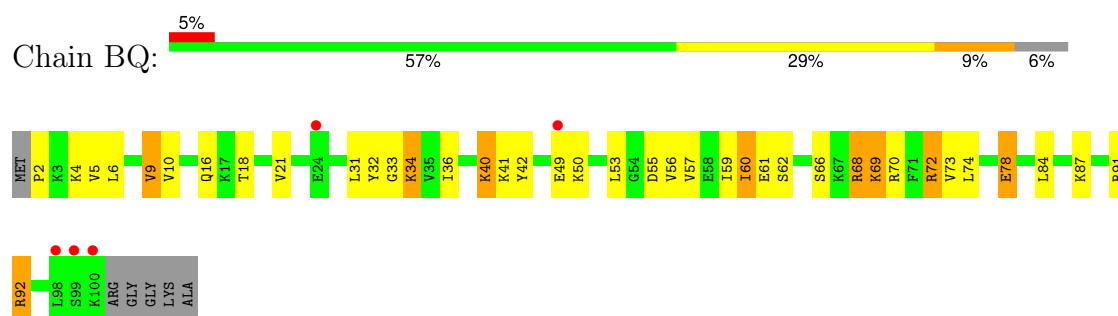
- Molecule 49: 30S ribosomal protein S16



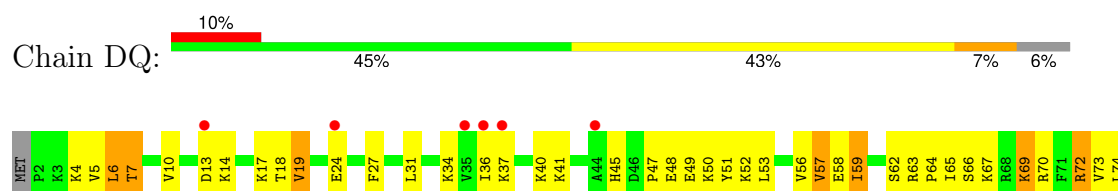
- Molecule 49: 30S ribosomal protein S16

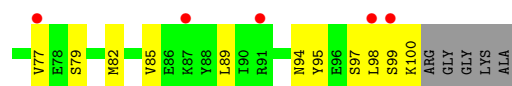


- Molecule 50: 30S ribosomal protein S17

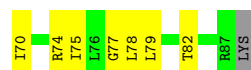
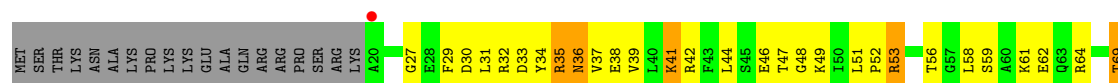


- Molecule 50: 30S ribosomal protein S17

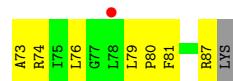
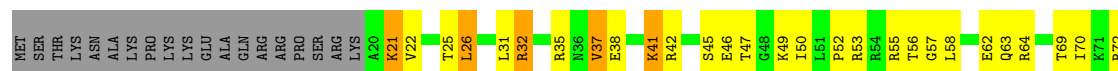




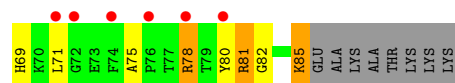
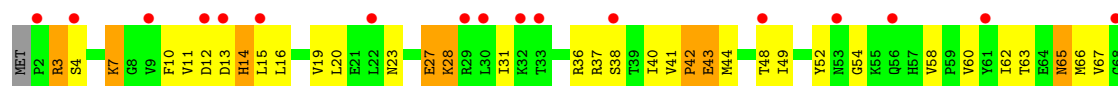
- Molecule 51: 30S ribosomal protein S18



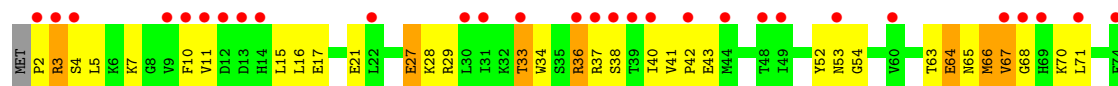
- Molecule 51: 30S ribosomal protein S18



- Molecule 52: 30S ribosomal protein S19

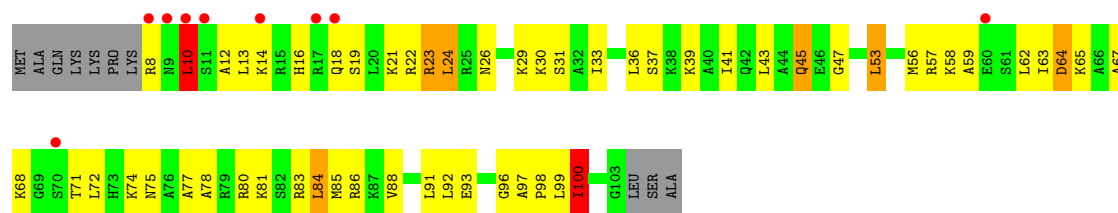


- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20

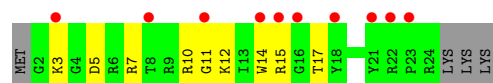
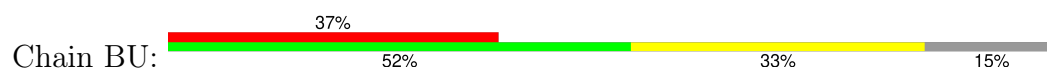




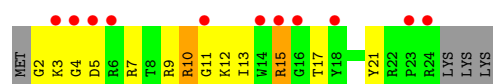
• Molecule 53: 30S ribosomal protein S20



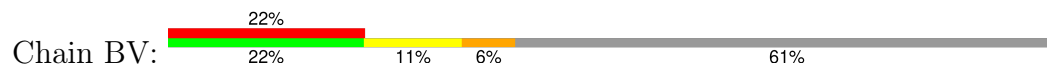
• Molecule 54: 30S ribosomal protein Thx



• Molecule 54: 30S ribosomal protein Thx



• Molecule 55: mRNA

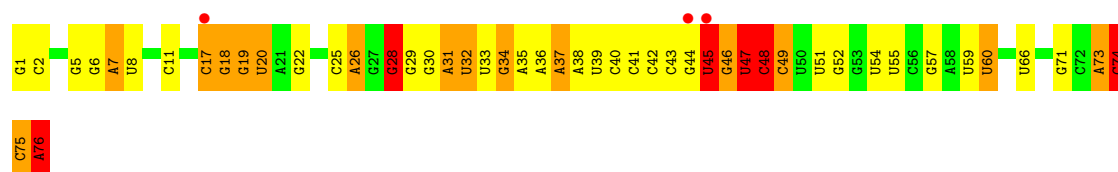


• Molecule 55: mRNA

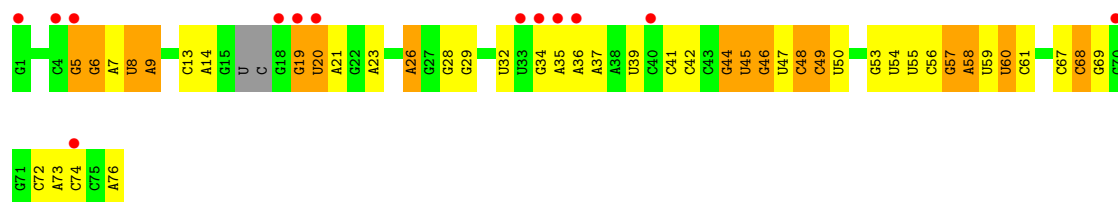


• Molecule 56: P-site tRNA

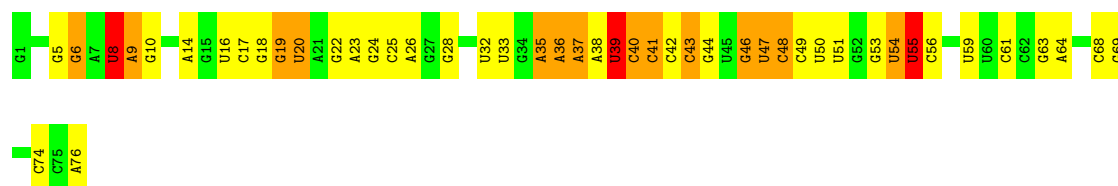




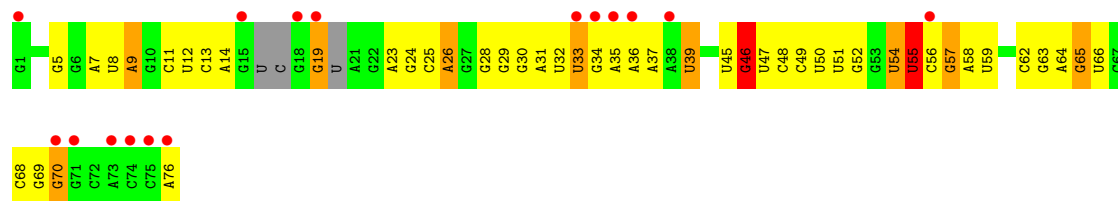
• Molecule 56: P-site tRNA



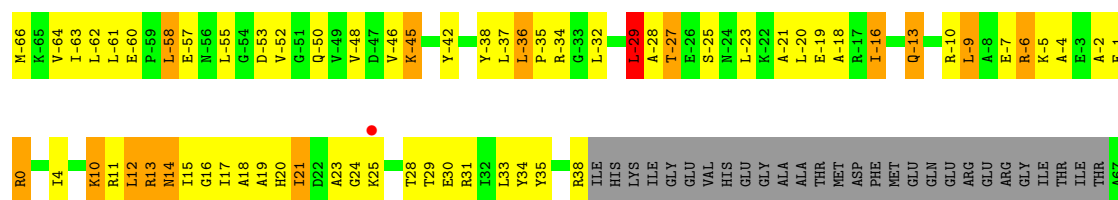
• Molecule 56: P-site tRNA

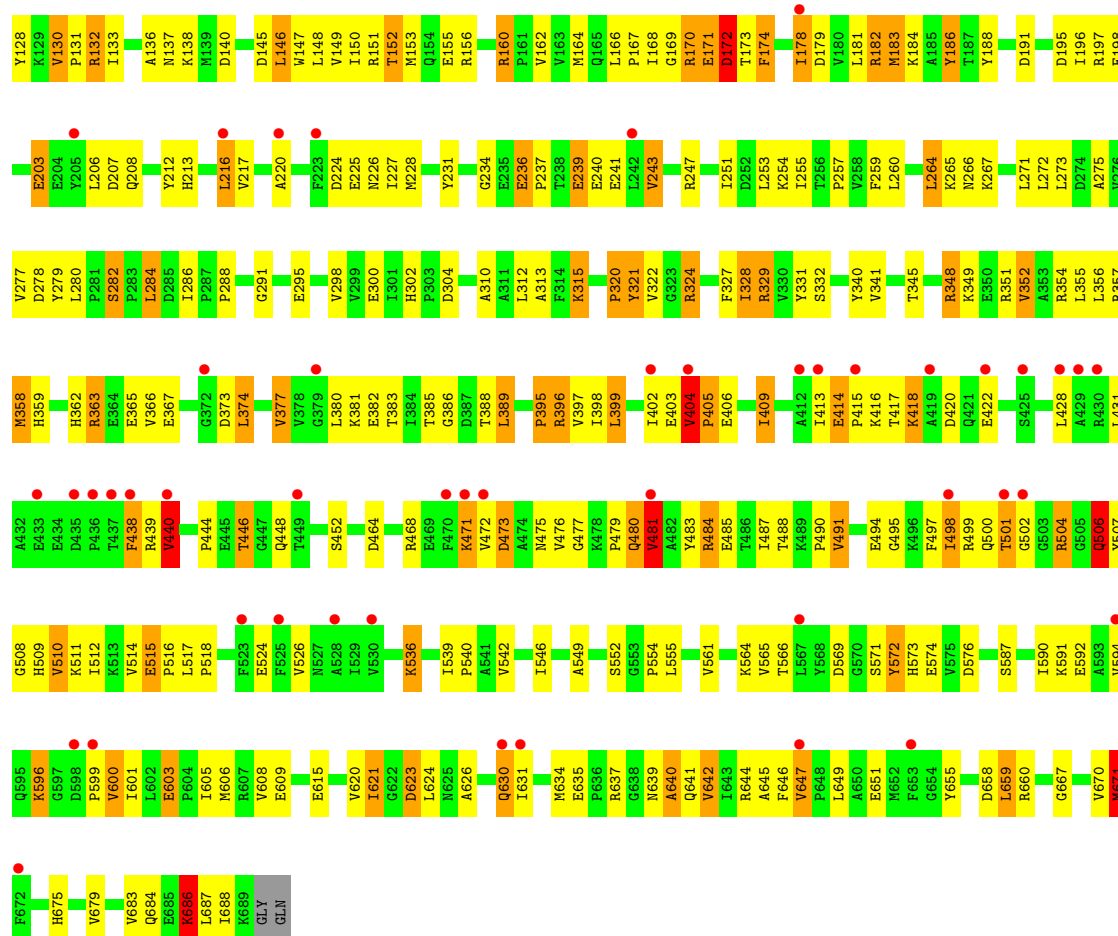


• Molecule 56: P-site tRNA

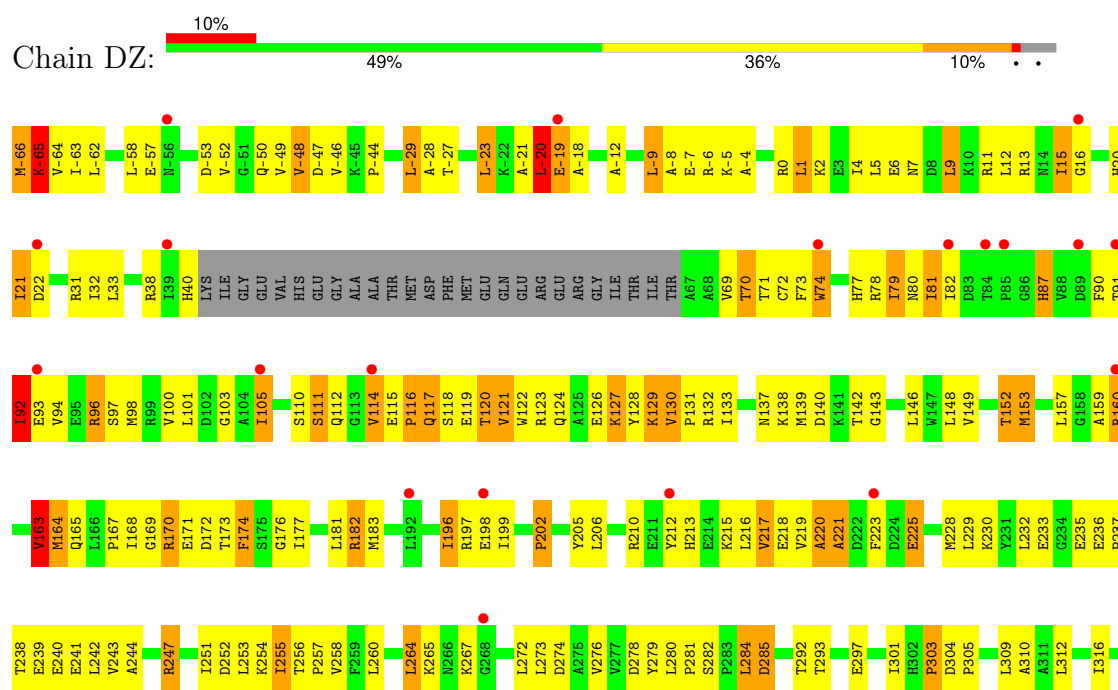


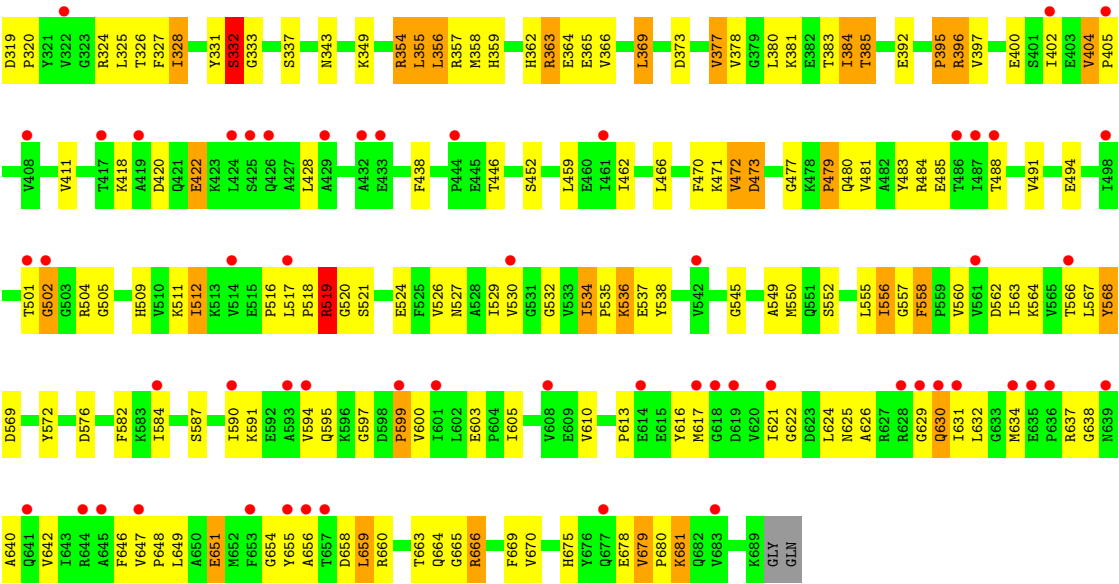
• Molecule 57: 50S ribosomal protein L9,Elongation factor G





• Molecule 57: 50S ribosomal protein L9,Elongation factor G

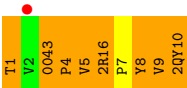




• Molecule 58: Dityromycin



• Molecule 58: Dityromycin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.84Å 450.58Å 623.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 2.80 49.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.5 (49.81-2.80) 94.5 (49.81-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.209 , 0.264 0.210 , 0.264	Depositor DCC
R_{free} test set	67916 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 73.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	310038	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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, PSU, GDP, MVA, 5MU, 2R3, 7MG, MIA, MG, 004, 2QZ, ZN, 4SU, 2QY, 2R1

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	AA	1.41	444/69281 (0.6%)	2.07	3848/108144 (3.6%)
1	CA	1.00	75/69179 (0.1%)	1.66	1653/107984 (1.5%)
2	AB	1.17	7/2878 (0.2%)	1.92	120/4490 (2.7%)
2	CB	0.66	0/2878	1.33	24/4490 (0.5%)
3	AC	0.34	0/1083	0.65	0/1460
3	CC	0.34	0/1083	0.65	0/1460
4	AD	0.94	2/2186 (0.1%)	1.04	5/2944 (0.2%)
4	CD	0.74	0/2192	0.95	6/2951 (0.2%)
5	AE	0.93	0/1592	1.08	2/2149 (0.1%)
5	CE	0.72	0/1592	0.91	1/2149 (0.0%)
6	AF	0.91	2/1619 (0.1%)	1.01	4/2193 (0.2%)
6	CF	0.63	0/1615	0.83	1/2188 (0.0%)
7	AG	0.60	0/1450	0.83	2/1959 (0.1%)
7	CG	0.36	0/1449	0.62	0/1958
8	AH	0.84	0/1356	0.96	1/1834 (0.1%)
8	CH	0.49	0/1356	0.67	0/1834
9	AK	0.34	0/640	0.67	0/889
9	CK	0.28	0/640	0.61	0/889
10	AL	0.31	0/503	0.54	0/673
10	CL	0.34	0/503	0.60	0/673
11	AN	0.95	0/1144	1.01	3/1543 (0.2%)
11	CN	0.61	0/1144	0.81	0/1543
12	AO	0.91	1/943 (0.1%)	1.02	3/1269 (0.2%)
12	CO	0.77	0/943	0.87	0/1269
13	AP	0.85	0/1156	1.03	4/1537 (0.3%)
13	CP	0.57	0/1152	0.87	2/1533 (0.1%)
14	AQ	0.91	0/1143	0.97	2/1527 (0.1%)
14	CQ	0.64	0/1143	0.82	1/1527 (0.1%)
15	AR	0.90	0/982	1.07	4/1312 (0.3%)
15	CR	0.65	0/982	0.88	1/1312 (0.1%)
16	AS	0.76	0/887	0.95	1/1180 (0.1%)
16	CS	0.49	0/880	0.74	0/1172

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.89	0/1105	1.02	3/1477 (0.2%)
17	CT	0.65	0/1097	0.89	1/1468 (0.1%)
18	AU	1.11	3/977 (0.3%)	1.05	1/1301 (0.1%)
18	CU	0.69	1/977 (0.1%)	0.79	0/1301
19	AV	0.98	0/782	1.08	2/1049 (0.2%)
19	CV	0.58	0/782	0.79	0/1049
20	AW	1.10	2/897 (0.2%)	1.09	7/1205 (0.6%)
20	CW	0.80	0/897	0.92	0/1205
21	AX	0.96	0/764	0.99	0/1025
21	CX	0.67	0/764	0.83	1/1025 (0.1%)
22	AY	0.88	0/819	0.97	0/1095
22	CY	0.56	0/819	0.72	0/1095
23	AZ	0.72	1/1483 (0.1%)	0.93	4/2017 (0.2%)
23	CZ	0.45	0/1483	0.73	0/2017
24	A0	0.87	0/616	1.05	1/821 (0.1%)
24	C0	0.60	0/616	0.76	0/821
25	A1	0.87	0/762	0.92	0/1014
25	C1	0.67	0/762	0.89	1/1014 (0.1%)
26	A2	0.79	0/590	0.93	1/781 (0.1%)
26	C2	0.59	0/590	0.73	0/781
27	A3	1.01	0/474	1.06	0/635
27	C3	0.57	0/469	0.81	0/630
28	A4	0.50	0/571	0.72	0/768
28	C4	0.35	0/545	0.59	0/737
29	A5	0.99	0/469	1.05	0/635
29	C5	0.76	1/469 (0.2%)	0.86	0/635
30	A6	0.95	0/460	1.03	1/613 (0.2%)
30	C6	0.71	0/456	0.81	1/608 (0.2%)
31	A7	0.99	0/426	1.11	3/561 (0.5%)
31	C7	0.77	0/426	0.99	1/561 (0.2%)
32	A8	0.95	0/525	0.94	0/691
32	C8	0.63	0/525	0.82	0/691
33	A9	0.98	0/310	1.05	0/407
33	C9	0.64	0/310	0.80	0/407
34	BA	0.77	3/35976 (0.0%)	1.42	439/56145 (0.8%)
34	DA	0.68	1/36119 (0.0%)	1.30	238/56370 (0.4%)
35	BB	0.45	0/1881	0.69	1/2542 (0.0%)
35	DB	0.38	0/1860	0.66	0/2518
36	BC	0.40	0/1576	0.61	0/2130
36	DC	0.35	0/1568	0.55	0/2122
37	BD	0.49	0/1689	0.71	0/2267
37	DD	0.51	0/1708	0.73	1/2289 (0.0%)
38	BE	0.60	0/1145	0.79	0/1543

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DE	0.51	0/1149	0.77	0/1548
39	BF	0.50	0/825	0.77	0/1118
39	DF	0.51	0/833	0.72	0/1128
40	BG	0.43	0/1250	0.60	0/1679
40	DG	0.35	0/1254	0.58	0/1683
41	BH	0.55	0/1108	0.76	0/1494
41	DH	0.45	0/1108	0.75	1/1494 (0.1%)
42	BI	0.44	0/1005	0.64	0/1350
42	DI	0.34	0/997	0.56	0/1343
43	BJ	0.39	0/722	0.71	2/982 (0.2%)
43	DJ	0.34	0/727	0.59	0/988
44	BK	0.56	0/848	0.72	0/1149
44	DK	0.48	0/848	0.63	0/1149
45	BL	0.65	0/946	0.79	0/1274
45	DL	0.64	0/946	0.84	1/1274 (0.1%)
46	BM	0.42	0/933	0.67	0/1253
46	DM	0.30	0/917	0.52	0/1234
47	BN	0.45	0/501	0.67	0/664
47	DN	0.33	0/501	0.60	0/664
48	BO	0.57	0/739	0.74	0/985
48	DO	0.50	0/739	0.70	0/985
49	BP	0.55	0/697	0.81	1/939 (0.1%)
49	DP	0.49	0/693	0.72	0/935
50	BQ	0.58	0/836	0.78	0/1117
50	DQ	0.51	0/836	0.72	0/1117
51	BR	0.55	0/560	0.83	0/746
51	DR	0.48	0/560	0.70	0/746
52	BS	0.34	0/676	0.59	0/911
52	DS	0.31	0/661	0.66	0/893
53	BT	0.50	0/730	0.81	0/965
53	DT	0.46	0/733	0.72	0/969
54	BU	0.42	0/203	0.69	0/266
54	DU	0.38	0/203	0.59	0/266
55	BV	0.64	0/165	1.06	0/254
55	DV	0.54	0/137	1.11	0/211
56	BW	0.86	0/1650	1.64	45/2569 (1.8%)
56	BY	0.42	0/1602	0.95	1/2493 (0.0%)
56	DW	0.65	0/1650	1.29	7/2569 (0.3%)
56	DY	0.35	0/1579	0.86	0/2455
57	BZ	0.49	0/5763	0.72	1/7804 (0.0%)
57	DZ	0.45	0/5784	0.69	1/7835 (0.0%)
58	BX	0.67	0/20	0.66	0/23
58	DX	0.70	0/20	1.43	0/23

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.95	543/329767 (0.2%)	1.50	6455/491645 (1.3%)

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
5	AE	0	1
6	AF	0	1
19	AV	0	1
35	BB	0	1
57	DZ	0	1
58	BX	0	1
All	All	0	6

The worst 5 of 543 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1067	A	N9-C4	-15.28	1.28	1.37
1	AA	354	A	N9-C4	-13.92	1.29	1.37
1	AA	2299	A	N9-C4	-13.50	1.29	1.37
1	AA	1188	A	N9-C4	-13.32	1.29	1.37
1	AA	990	A	N9-C4	-11.81	1.30	1.37

The worst 5 of 6455 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	553	A	N1-C6-N6	26.84	134.71	118.60
1	AA	990	A	N1-C2-N3	21.55	140.07	129.30
1	AA	990	A	C6-C5-N7	-21.18	117.48	132.30
1	AA	354	A	C2-N3-C4	-21.03	100.09	110.60
1	AA	553	A	C6-C5-N7	-20.90	117.67	132.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AE	74	PRO	Peptide
6	AF	194	MET	Peptide
19	AV	54	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
35	BB	93	VAL	Peptide
58	BX	3	004	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	AA	61861	0	31172	849	0
1	CA	61771	0	31146	1165	0
2	AB	2573	0	1306	27	0
2	CB	2573	0	1306	57	0
3	AC	1063	0	1091	153	4
3	CC	1063	0	1090	186	17
4	AD	2136	0	2218	84	0
4	CD	2142	0	2229	85	0
5	AE	1559	0	1618	58	0
5	CE	1559	0	1618	76	0
6	AF	1584	0	1625	62	0
6	CF	1580	0	1619	75	0
7	AG	1425	0	1443	64	0
7	CG	1424	0	1434	82	0
8	AH	1330	0	1407	53	0
8	CH	1330	0	1407	54	0
9	AK	641	0	309	15	0
9	CK	641	0	309	9	0
10	AL	498	0	521	20	0
10	CL	498	0	521	29	0
11	AN	1117	0	1184	31	0
11	CN	1117	0	1184	38	0
12	AO	933	0	996	30	0
12	CO	933	0	996	26	0
13	AP	1139	0	1223	44	0
13	CP	1135	0	1212	57	0
14	AQ	1122	0	1179	37	0
14	CQ	1122	0	1179	54	0
15	AR	968	0	1033	32	0
15	CR	968	0	1033	37	0
16	AS	877	0	938	42	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	CS	870	0	923	67	0
17	AT	1091	0	1151	48	0
17	CT	1083	0	1136	42	0
18	AU	959	0	1019	29	0
18	CU	959	0	1018	40	0
19	AV	771	0	830	11	0
19	CV	771	0	830	24	0
20	AW	886	0	940	23	0
20	CW	886	0	940	40	0
21	AX	750	0	814	24	0
21	CX	750	0	814	28	0
22	AY	806	0	881	37	0
22	CY	806	0	882	45	0
23	AZ	1451	0	1457	61	0
23	CZ	1451	0	1457	72	0
24	A0	608	0	622	20	0
24	C0	608	0	622	27	0
25	A1	755	0	826	29	0
25	C1	755	0	826	23	0
26	A2	588	0	643	16	0
26	C2	588	0	643	28	0
27	A3	469	0	518	12	0
27	C3	464	0	514	25	0
28	A4	558	0	545	31	0
28	C4	532	0	507	28	0
29	A5	455	0	465	15	0
29	C5	455	0	465	16	0
30	A6	453	0	473	17	0
30	C6	449	0	469	20	0
31	A7	418	0	467	16	0
31	C7	418	0	467	12	0
32	A8	517	0	582	25	0
32	C8	517	0	582	24	0
33	A9	307	0	335	11	0
33	C9	307	0	335	13	0
34	BA	32141	0	16224	681	0
34	DA	32268	0	16287	737	0
35	BB	1846	0	1867	78	0
35	DB	1825	0	1828	101	0
36	BC	1552	0	1546	65	0
36	DC	1544	0	1524	63	0
37	BD	1659	0	1679	68	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	DD	1678	0	1719	86	0
38	BE	1129	0	1185	51	0
38	DE	1133	0	1191	69	0
39	BF	812	0	804	29	0
39	DF	820	0	814	37	0
40	BG	1231	0	1238	45	0
40	DG	1235	0	1249	52	0
41	BH	1088	0	1126	53	0
41	DH	1088	0	1126	74	0
42	BI	986	0	995	52	0
42	DI	978	0	966	56	0
43	BJ	709	0	650	32	0
43	DJ	714	0	672	32	0
44	BK	833	0	836	34	0
44	DK	833	0	836	26	0
45	BL	930	0	980	39	0
45	DL	930	0	980	45	0
46	BM	923	0	970	37	0
46	DM	907	0	934	39	0
47	BN	492	0	529	30	0
47	DN	492	0	531	46	0
48	BO	728	0	760	29	0
48	DO	728	0	760	29	0
49	BP	681	0	697	50	0
49	DP	677	0	686	36	0
50	BQ	823	0	891	32	0
50	DQ	823	0	891	35	0
51	BR	555	0	618	24	0
51	DR	555	0	618	30	0
52	BS	661	0	675	36	0
52	DS	646	0	644	34	0
53	BT	728	0	798	36	0
53	DT	731	0	807	27	0
54	BU	199	0	208	7	0
54	DU	199	0	208	9	0
55	BV	148	0	76	3	0
55	DV	123	0	66	1	0
56	BW	1631	0	839	25	0
56	BY	1581	0	805	24	0
56	DW	1631	0	839	33	0
56	DY	1561	0	796	33	0
57	BZ	5663	0	5747	265	17

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DZ	5682	0	5766	236	4
58	BX	93	0	85	14	0
58	DX	93	0	85	15	0
59	A0	5	0	0	0	0
59	A2	1	0	0	0	0
59	A5	1	0	0	0	0
59	A6	2	0	0	0	0
59	A7	4	0	0	0	0
59	A8	1	0	0	0	0
59	A9	1	0	0	0	0
59	AA	821	0	0	0	0
59	AB	23	0	0	0	0
59	AD	12	0	0	0	0
59	AE	5	0	0	0	0
59	AF	8	0	0	0	0
59	AG	2	0	0	0	0
59	AH	1	0	0	0	0
59	AN	3	0	0	0	0
59	AO	1	0	0	0	0
59	AP	4	0	0	0	0
59	AQ	3	0	0	0	0
59	AR	2	0	0	0	0
59	AU	3	0	0	0	0
59	AV	6	0	0	0	0
59	AW	3	0	0	0	0
59	AX	1	0	0	0	0
59	AY	1	0	0	0	0
59	AZ	2	0	0	0	0
59	BA	215	0	0	0	0
59	BB	1	0	0	0	0
59	BD	1	0	0	0	0
59	BE	1	0	0	0	0
59	BF	1	0	0	0	0
59	BK	1	0	0	0	0
59	BL	2	0	0	0	0
59	BM	1	0	0	0	0
59	BN	2	0	0	0	0
59	BS	1	0	0	0	0
59	BT	1	0	0	0	0
59	BW	3	0	0	0	0
59	BZ	1	0	0	0	0
59	C0	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	C1	1	0	0	0	0
59	C3	1	0	0	0	0
59	C5	1	0	0	0	0
59	C7	1	0	0	0	0
59	C8	1	0	0	0	0
59	CA	664	0	0	0	0
59	CB	13	0	0	0	0
59	CD	4	0	0	0	0
59	CE	5	0	0	0	0
59	CF	4	0	0	0	0
59	CG	1	0	0	0	0
59	CN	1	0	0	0	0
59	CO	1	0	0	0	0
59	CP	1	0	0	0	0
59	CQ	4	0	0	0	0
59	CR	1	0	0	0	0
59	CU	1	0	0	0	0
59	CV	2	0	0	0	0
59	CW	1	0	0	0	0
59	CX	1	0	0	0	0
59	DA	171	0	0	0	0
59	DD	1	0	0	0	0
59	DE	2	0	0	0	0
59	DF	1	0	0	0	0
59	DJ	1	0	0	0	0
59	DK	1	0	0	0	0
59	DT	1	0	0	0	0
59	DW	3	0	0	0	0
59	DZ	2	0	0	0	0
60	A4	1	0	0	0	0
60	A5	1	0	0	0	0
60	A6	1	0	0	0	0
60	A9	1	0	0	0	0
60	AY	1	0	0	0	0
60	BN	1	0	0	0	0
60	C4	1	0	0	0	0
60	C5	1	0	0	0	0
60	C6	1	0	0	0	0
60	C9	1	0	0	0	0
60	CY	1	0	0	0	0
60	DN	1	0	0	0	0
61	BD	8	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	DD	8	0	0	2	0
62	BZ	28	0	12	5	0
62	DZ	28	0	12	7	0
63	A0	6	0	0	0	0
63	A1	2	0	0	0	0
63	A3	2	0	0	0	0
63	A5	3	0	0	0	0
63	A6	1	0	0	0	0
63	A7	2	0	0	1	0
63	A8	10	0	0	1	0
63	A9	1	0	0	0	0
63	AA	1413	0	0	66	0
63	AB	38	0	0	3	0
63	AD	10	0	0	2	0
63	AE	17	0	0	4	0
63	AF	11	0	0	1	0
63	AG	3	0	0	1	0
63	AH	1	0	0	0	0
63	AN	1	0	0	0	0
63	AO	3	0	0	0	0
63	AP	16	0	0	1	0
63	AQ	4	0	0	1	0
63	AR	2	0	0	0	0
63	AS	1	0	0	1	0
63	AT	1	0	0	0	0
63	AU	4	0	0	0	0
63	AV	1	0	0	0	0
63	AW	1	0	0	0	0
63	AX	3	0	0	0	0
63	AZ	1	0	0	0	0
63	BA	213	0	0	19	0
63	BD	1	0	0	0	0
63	BM	1	0	0	0	0
63	BO	1	0	0	0	0
63	BP	1	0	0	0	0
63	BV	1	0	0	0	0
63	BW	1	0	0	0	0
63	BZ	2	0	0	0	0
63	C0	4	0	0	0	0
63	C3	2	0	0	0	0
63	C5	1	0	0	0	0
63	C7	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	C8	4	0	0	0	0
63	CA	983	0	0	79	0
63	CB	9	0	0	1	0
63	CD	15	0	0	1	0
63	CE	9	0	0	1	0
63	CF	6	0	0	0	0
63	CN	1	0	0	0	0
63	CO	1	0	0	0	0
63	CP	11	0	0	2	0
63	CQ	2	0	0	1	0
63	CT	3	0	0	0	0
63	CU	2	0	0	0	0
63	CV	1	0	0	1	0
63	CW	1	0	0	0	0
63	CX	1	0	0	0	0
63	CY	2	0	0	1	0
63	DA	157	0	0	13	0
63	DD	1	0	0	0	0
63	DE	2	0	0	2	0
63	DH	1	0	0	0	0
63	DJ	1	0	0	0	0
63	DK	2	0	0	0	0
63	DL	1	0	0	0	0
63	DT	1	0	0	0	0
All	All	310038	0	209219	7350	21

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 15.

The worst 5 of 7350 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:AA:1891:G:H5''	3:AC:206:LYS:CG	1.32	1.59
1:AA:1891:G:C5'	3:AC:206:LYS:HD2	1.36	1.52
1:CA:2128:C:H5''	3:CC:219:MET:CE	1.36	1.51
1:CA:2132:U:C4	3:CC:6:LYS:HE3	1.51	1.41
1:AA:1891:G:C5'	3:AC:206:LYS:CD	2.01	1.37

The worst 5 of 21 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:BZ:502:GLY:CA	3:CC:9:ARG:CD[2_655]	1.16	1.04
3:AC:9:ARG:NH2	57:DZ:504:ARG:NH1[3_654]	1.36	0.84
57:BZ:502:GLY:N	3:CC:9:ARG:CB[2_655]	1.54	0.66
57:BZ:502:GLY:N	3:CC:9:ARG:CD[2_655]	1.69	0.51
57:BZ:573:HIS:CE1	3:CC:13:GLU:OE1[2_655]	1.71	0.49

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	0
3	CC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	0
4	AD	273/276 (99%)	249 (91%)	19 (7%)	5 (2%)	7	24
4	CD	273/276 (99%)	234 (86%)	26 (10%)	13 (5%)	2	6
5	AE	202/206 (98%)	186 (92%)	14 (7%)	2 (1%)	13	39
5	CE	202/206 (98%)	179 (89%)	20 (10%)	3 (2%)	8	29
6	AF	201/210 (96%)	182 (90%)	18 (9%)	1 (0%)	25	56
6	CF	201/210 (96%)	177 (88%)	17 (8%)	7 (4%)	3	10
7	AG	179/182 (98%)	154 (86%)	19 (11%)	6 (3%)	3	11
7	CG	179/182 (98%)	141 (79%)	31 (17%)	7 (4%)	2	9
8	AH	172/180 (96%)	154 (90%)	15 (9%)	3 (2%)	7	26
8	CH	172/180 (96%)	144 (84%)	17 (10%)	11 (6%)	1	3
9	AK	128/173 (74%)	66 (52%)	36 (28%)	26 (20%)	0	0
9	CK	128/173 (74%)	76 (59%)	27 (21%)	25 (20%)	0	0
10	AL	64/147 (44%)	43 (67%)	17 (27%)	4 (6%)	1	3
10	CL	64/147 (44%)	42 (66%)	19 (30%)	3 (5%)	2	6
11	AN	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	19	48
11	CN	138/140 (99%)	120 (87%)	15 (11%)	3 (2%)	5	20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
12	CO	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	4	17
13	AP	147/150 (98%)	130 (88%)	15 (10%)	2 (1%)	9	30
13	CP	147/150 (98%)	119 (81%)	25 (17%)	3 (2%)	6	21
14	AQ	139/141 (99%)	126 (91%)	12 (9%)	1 (1%)	19	48
14	CQ	139/141 (99%)	123 (88%)	14 (10%)	2 (1%)	9	30
15	AR	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
15	CR	116/118 (98%)	102 (88%)	11 (10%)	3 (3%)	4	16
16	AS	108/112 (96%)	88 (82%)	16 (15%)	4 (4%)	2	9
16	CS	108/112 (96%)	83 (77%)	20 (18%)	5 (5%)	2	6
17	AT	129/146 (88%)	114 (88%)	13 (10%)	2 (2%)	8	27
17	CT	129/146 (88%)	116 (90%)	11 (8%)	2 (2%)	8	27
18	AU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
18	CU	114/118 (97%)	100 (88%)	11 (10%)	3 (3%)	4	16
19	AV	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	13	39
19	CV	99/101 (98%)	86 (87%)	10 (10%)	3 (3%)	3	13
20	AW	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
20	CW	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
21	AX	93/96 (97%)	85 (91%)	6 (6%)	2 (2%)	5	20
21	CX	93/96 (97%)	77 (83%)	11 (12%)	5 (5%)	1	5
22	AY	105/110 (96%)	93 (89%)	9 (9%)	3 (3%)	3	13
22	CY	105/110 (96%)	86 (82%)	14 (13%)	5 (5%)	2	6
23	AZ	183/206 (89%)	147 (80%)	24 (13%)	12 (7%)	1	3
23	CZ	183/206 (89%)	134 (73%)	33 (18%)	16 (9%)	0	1
24	A0	75/85 (88%)	70 (93%)	5 (7%)	0	100	100
24	C0	75/85 (88%)	67 (89%)	7 (9%)	1 (1%)	10	32
25	A1	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
25	C1	95/98 (97%)	85 (90%)	7 (7%)	3 (3%)	3	12
26	A2	68/72 (94%)	62 (91%)	6 (9%)	0	100	100
26	C2	68/72 (94%)	60 (88%)	7 (10%)	1 (2%)	8	29
27	A3	57/60 (95%)	51 (90%)	6 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	C3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	3	10
28	A4	67/71 (94%)	46 (69%)	12 (18%)	9 (13%)	0	0
28	C4	67/71 (94%)	43 (64%)	15 (22%)	9 (13%)	0	0
29	A5	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
29	C5	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	7	24
30	A6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
30	C6	51/54 (94%)	42 (82%)	8 (16%)	1 (2%)	6	21
31	A7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
31	C7	46/49 (94%)	41 (89%)	4 (9%)	1 (2%)	5	20
32	A8	62/65 (95%)	60 (97%)	1 (2%)	1 (2%)	8	27
32	C8	62/65 (95%)	54 (87%)	7 (11%)	1 (2%)	8	27
33	A9	35/37 (95%)	35 (100%)	0	0	100	100
33	C9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
35	BB	229/256 (90%)	182 (80%)	33 (14%)	14 (6%)	1	3
35	DB	229/256 (90%)	170 (74%)	41 (18%)	18 (8%)	1	2
36	BC	204/239 (85%)	155 (76%)	38 (19%)	11 (5%)	1	5
36	DC	204/239 (85%)	169 (83%)	29 (14%)	6 (3%)	3	13
37	BD	206/209 (99%)	166 (81%)	28 (14%)	12 (6%)	1	4
37	DD	206/209 (99%)	171 (83%)	27 (13%)	8 (4%)	2	9
38	BE	146/162 (90%)	114 (78%)	24 (16%)	8 (6%)	1	4
38	DE	146/162 (90%)	117 (80%)	22 (15%)	7 (5%)	2	6
39	BF	98/101 (97%)	84 (86%)	11 (11%)	3 (3%)	3	12
39	DF	98/101 (97%)	90 (92%)	5 (5%)	3 (3%)	3	12
40	BG	153/156 (98%)	128 (84%)	13 (8%)	12 (8%)	1	2
40	DG	153/156 (98%)	126 (82%)	22 (14%)	5 (3%)	3	11
41	BH	135/138 (98%)	110 (82%)	22 (16%)	3 (2%)	5	20
41	DH	135/138 (98%)	114 (84%)	14 (10%)	7 (5%)	1	5
42	BI	125/128 (98%)	103 (82%)	15 (12%)	7 (6%)	1	4
42	DI	125/128 (98%)	100 (80%)	21 (17%)	4 (3%)	3	12
43	BJ	95/105 (90%)	76 (80%)	12 (13%)	7 (7%)	1	2
43	DJ	94/105 (90%)	75 (80%)	16 (17%)	3 (3%)	3	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	BK	112/129 (87%)	96 (86%)	14 (12%)	2 (2%)	7	24
44	DK	112/129 (87%)	92 (82%)	16 (14%)	4 (4%)	3	10
45	BL	120/132 (91%)	108 (90%)	11 (9%)	1 (1%)	16	44
45	DL	120/132 (91%)	100 (83%)	16 (13%)	4 (3%)	3	11
46	BM	115/126 (91%)	93 (81%)	18 (16%)	4 (4%)	3	10
46	DM	114/126 (90%)	88 (77%)	17 (15%)	9 (8%)	1	2
47	BN	58/61 (95%)	46 (79%)	9 (16%)	3 (5%)	1	5
47	DN	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	11
48	BO	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	3	10
48	DO	86/89 (97%)	72 (84%)	10 (12%)	4 (5%)	2	6
49	BP	80/88 (91%)	54 (68%)	17 (21%)	9 (11%)	0	1
49	DP	80/88 (91%)	58 (72%)	18 (22%)	4 (5%)	1	5
50	BQ	97/105 (92%)	87 (90%)	7 (7%)	3 (3%)	3	12
50	DQ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
51	BR	66/88 (75%)	57 (86%)	7 (11%)	2 (3%)	3	13
51	DR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
52	BS	82/93 (88%)	64 (78%)	14 (17%)	4 (5%)	2	6
52	DS	81/93 (87%)	63 (78%)	15 (18%)	3 (4%)	2	9
53	BT	94/106 (89%)	78 (83%)	12 (13%)	4 (4%)	2	7
53	DT	94/106 (89%)	75 (80%)	13 (14%)	6 (6%)	1	3
54	BU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
54	DU	21/27 (78%)	17 (81%)	2 (10%)	2 (10%)	0	1
57	BZ	722/758 (95%)	563 (78%)	107 (15%)	52 (7%)	1	2
57	DZ	726/758 (96%)	537 (74%)	132 (18%)	57 (8%)	1	2
58	BX	3/10 (30%)	1 (33%)	0	2 (67%)	0	0
58	DX	3/10 (30%)	0	2 (67%)	1 (33%)	0	0
All	All	13227/14464 (91%)	10975 (83%)	1666 (13%)	586 (4%)	2	7

5 of 586 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	42	VAL
3	AC	47	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	AC	68	GLY
3	AC	180	SER
3	AC	181	PHE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	111/180 (62%)	103 (93%)	8 (7%)	12	34
3	CC	111/180 (62%)	103 (93%)	8 (7%)	12	34
4	AD	215/218 (99%)	173 (80%)	42 (20%)	1	3
4	CD	216/218 (99%)	178 (82%)	38 (18%)	1	5
5	AE	164/166 (99%)	138 (84%)	26 (16%)	2	7
5	CE	164/166 (99%)	137 (84%)	27 (16%)	2	6
6	AF	160/166 (96%)	132 (82%)	28 (18%)	1	5
6	CF	159/166 (96%)	126 (79%)	33 (21%)	1	3
7	AG	143/156 (92%)	115 (80%)	28 (20%)	1	3
7	CG	142/156 (91%)	114 (80%)	28 (20%)	1	3
8	AH	144/148 (97%)	120 (83%)	24 (17%)	2	6
8	CH	144/148 (97%)	118 (82%)	26 (18%)	1	4
10	AL	50/111 (45%)	39 (78%)	11 (22%)	1	2
10	CL	50/111 (45%)	35 (70%)	15 (30%)	0	1
11	AN	118/119 (99%)	93 (79%)	25 (21%)	1	3
11	CN	118/119 (99%)	85 (72%)	33 (28%)	0	1
12	AO	100/100 (100%)	87 (87%)	13 (13%)	3	11
12	CO	100/100 (100%)	86 (86%)	14 (14%)	3	9
13	AP	116/116 (100%)	97 (84%)	19 (16%)	2	6
13	CP	115/116 (99%)	95 (83%)	20 (17%)	1	5
14	AQ	111/111 (100%)	94 (85%)	17 (15%)	2	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	CQ	111/111 (100%)	83 (75%)	28 (25%)	0	1
15	AR	101/101 (100%)	80 (79%)	21 (21%)	1	3
15	CR	101/101 (100%)	87 (86%)	14 (14%)	3	9
16	AS	87/88 (99%)	71 (82%)	16 (18%)	1	4
16	CS	85/88 (97%)	68 (80%)	17 (20%)	1	3
17	AT	115/127 (91%)	96 (84%)	19 (16%)	2	6
17	CT	113/127 (89%)	98 (87%)	15 (13%)	3	10
18	AU	93/94 (99%)	77 (83%)	16 (17%)	1	5
18	CU	93/94 (99%)	81 (87%)	12 (13%)	3	11
19	AV	80/82 (98%)	67 (84%)	13 (16%)	2	6
19	CV	80/82 (98%)	65 (81%)	15 (19%)	1	4
20	AW	90/92 (98%)	76 (84%)	14 (16%)	2	7
20	CW	90/92 (98%)	75 (83%)	15 (17%)	2	6
21	AX	77/78 (99%)	67 (87%)	10 (13%)	3	11
21	CX	77/78 (99%)	66 (86%)	11 (14%)	2	9
22	AY	85/91 (93%)	66 (78%)	19 (22%)	1	2
22	CY	85/91 (93%)	66 (78%)	19 (22%)	1	2
23	AZ	156/179 (87%)	120 (77%)	36 (23%)	0	2
23	CZ	156/179 (87%)	125 (80%)	31 (20%)	1	3
24	A0	61/67 (91%)	55 (90%)	6 (10%)	6	21
24	C0	61/67 (91%)	50 (82%)	11 (18%)	1	4
25	A1	80/83 (96%)	66 (82%)	14 (18%)	1	5
25	C1	80/83 (96%)	66 (82%)	14 (18%)	1	5
26	A2	65/67 (97%)	56 (86%)	9 (14%)	3	10
26	C2	65/67 (97%)	51 (78%)	14 (22%)	1	2
27	A3	51/52 (98%)	41 (80%)	10 (20%)	1	3
27	C3	50/52 (96%)	38 (76%)	12 (24%)	0	2
28	A4	60/63 (95%)	52 (87%)	8 (13%)	3	10
28	C4	53/63 (84%)	39 (74%)	14 (26%)	0	1
29	A5	50/52 (96%)	43 (86%)	7 (14%)	3	9
29	C5	50/52 (96%)	42 (84%)	8 (16%)	2	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	A6	51/52 (98%)	37 (72%)	14 (28%)	0	1
30	C6	50/52 (96%)	43 (86%)	7 (14%)	3	9
31	A7	41/42 (98%)	35 (85%)	6 (15%)	2	8
31	C7	41/42 (98%)	35 (85%)	6 (15%)	2	8
32	A8	54/55 (98%)	43 (80%)	11 (20%)	1	3
32	C8	54/55 (98%)	48 (89%)	6 (11%)	5	16
33	A9	34/34 (100%)	30 (88%)	4 (12%)	4	14
33	C9	34/34 (100%)	30 (88%)	4 (12%)	4	14
35	BB	192/220 (87%)	157 (82%)	35 (18%)	1	4
35	DB	187/220 (85%)	148 (79%)	39 (21%)	1	3
36	BC	143/188 (76%)	127 (89%)	16 (11%)	5	16
36	DC	141/188 (75%)	113 (80%)	28 (20%)	1	3
37	BD	170/181 (94%)	136 (80%)	34 (20%)	1	3
37	DD	174/181 (96%)	143 (82%)	31 (18%)	1	5
38	BE	113/123 (92%)	86 (76%)	27 (24%)	0	2
38	DE	114/123 (93%)	82 (72%)	32 (28%)	0	1
39	BF	84/90 (93%)	70 (83%)	14 (17%)	2	6
39	DF	86/90 (96%)	74 (86%)	12 (14%)	3	9
40	BG	119/127 (94%)	99 (83%)	20 (17%)	1	6
40	DG	120/127 (94%)	104 (87%)	16 (13%)	3	10
41	BH	114/119 (96%)	90 (79%)	24 (21%)	1	3
41	DH	114/119 (96%)	86 (75%)	28 (25%)	0	2
42	BI	91/99 (92%)	78 (86%)	13 (14%)	2	9
42	DI	89/99 (90%)	73 (82%)	16 (18%)	1	4
43	BJ	66/92 (72%)	58 (88%)	8 (12%)	4	13
43	DJ	69/92 (75%)	58 (84%)	11 (16%)	2	7
44	BK	83/99 (84%)	65 (78%)	18 (22%)	1	2
44	DK	83/99 (84%)	64 (77%)	19 (23%)	0	2
45	BL	97/109 (89%)	83 (86%)	14 (14%)	2	8
45	DL	97/109 (89%)	74 (76%)	23 (24%)	0	2
46	BM	91/101 (90%)	80 (88%)	11 (12%)	4	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	DM	88/101 (87%)	75 (85%)	13 (15%)	2	8
47	BN	49/50 (98%)	38 (78%)	11 (22%)	1	2
47	DN	49/50 (98%)	42 (86%)	7 (14%)	2	9
48	BO	78/80 (98%)	70 (90%)	8 (10%)	6	19
48	DO	78/80 (98%)	66 (85%)	12 (15%)	2	7
49	BP	69/74 (93%)	54 (78%)	15 (22%)	1	2
49	DP	68/74 (92%)	51 (75%)	17 (25%)	0	1
50	BQ	94/97 (97%)	82 (87%)	12 (13%)	3	12
50	DQ	94/97 (97%)	80 (85%)	14 (15%)	2	8
51	BR	59/77 (77%)	49 (83%)	10 (17%)	1	5
51	DR	59/77 (77%)	52 (88%)	7 (12%)	4	14
52	BS	70/80 (88%)	59 (84%)	11 (16%)	2	7
52	DS	67/80 (84%)	55 (82%)	12 (18%)	1	5
53	BT	70/82 (85%)	53 (76%)	17 (24%)	0	2
53	DT	71/82 (87%)	59 (83%)	12 (17%)	1	5
54	BU	18/22 (82%)	17 (94%)	1 (6%)	17	47
54	DU	18/22 (82%)	16 (89%)	2 (11%)	5	16
57	BZ	604/636 (95%)	477 (79%)	127 (21%)	1	3
57	DZ	607/636 (95%)	509 (84%)	98 (16%)	2	6
58	BX	3/3 (100%)	3 (100%)	0	100	100
58	DX	3/3 (100%)	3 (100%)	0	100	100
All	All	10664/11678 (91%)	8760 (82%)	1904 (18%)	1	5

5 of 1904 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
57	BZ	623	ASP
51	DR	21	LYS
11	CN	138	LEU
49	DP	60	LEU
57	DZ	624	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 172 such sidechains are listed below:

Mol	Chain	Res	Type
24	C0	70	GLN
42	DI	89	ASN
35	DB	40	HIS
37	DD	160	GLN
44	DK	93	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2865/2915 (98%)	526 (18%)	51 (1%)
1	CA	2860/2915 (98%)	611 (21%)	39 (1%)
2	AB	119/121 (98%)	15 (12%)	0
2	CB	119/121 (98%)	27 (22%)	0
34	BA	1491/1521 (98%)	331 (22%)	20 (1%)
34	DA	1498/1521 (98%)	350 (23%)	22 (1%)
55	BV	6/18 (33%)	2 (33%)	0
55	DV	5/18 (27%)	1 (20%)	0
56	BW	74/76 (97%)	16 (21%)	1 (1%)
56	BY	71/76 (93%)	23 (32%)	2 (2%)
56	DW	74/76 (97%)	23 (31%)	2 (2%)
56	DY	69/76 (90%)	21 (30%)	1 (1%)
All	All	9251/9454 (97%)	1946 (21%)	138 (1%)

5 of 1946 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	U
1	AA	13	A
1	AA	15	G
1	AA	34	C
1	AA	45	C

5 of 138 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	DA	115	G
34	DA	428	G
34	DA	1065	U
1	AA	2769	U
1	AA	2739	U

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

42 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$
56	MIA	BW	37	56	24,31,32	2.37	5 (20%)	22,44,47	2.29	7 (31%)
56	PSU	DW	39	56	18,21,22	1.35	2 (11%)	21,30,33	2.08	4 (19%)
56	5MU	DW	54	56	19,22,23	1.49	4 (21%)	27,32,35	2.07	7 (25%)
58	MVA	DX	5	58	6,7,8	1.06	0	6,8,10	1.57	1 (16%)
58	004	DX	3	58	9,10,11	1.53	1 (11%)	9,12,14	1.28	1 (11%)
56	7MG	BW	46	56	23,26,27	1.29	4 (17%)	27,39,42	2.77	7 (25%)
56	PSU	BW	32	56	18,21,22	1.34	3 (16%)	21,30,33	1.83	5 (23%)
58	2R3	DX	8	58	12,14,15	0.60	0	16,18,20	1.77	5 (31%)
58	MVA	DX	9	58	6,7,8	1.14	1 (16%)	6,8,10	1.58	1 (16%)
58	2R1	BX	6	58	10,10,11	2.35	3 (30%)	8,13,15	3.80	3 (37%)
56	4SU	DY	8	56	18,21,22	1.84	4 (22%)	25,30,33	2.35	6 (24%)
56	MIA	DY	37	56	17,24,32	0.93	1 (5%)	16,35,47	1.32	2 (12%)
56	PSU	BW	55	56	18,21,22	1.37	1 (5%)	21,30,33	1.95	3 (14%)
56	PSU	DW	55	56	18,21,22	1.40	2 (11%)	21,30,33	2.01	5 (23%)
56	7MG	DW	46	56	23,26,27	1.30	3 (13%)	27,39,42	2.71	7 (25%)
58	2QZ	DX	1	58	7,8,9	0.55	0	7,10,12	4.52	3 (42%)
58	2R3	BX	8	58	12,14,15	0.70	0	16,18,20	2.13	9 (56%)
56	5MU	BY	54	56	19,22,23	1.53	5 (26%)	27,32,35	2.21	8 (29%)
56	7MG	DY	46	56	23,26,27	1.24	3 (13%)	27,39,42	2.76	7 (25%)
56	PSU	DY	32	56	18,21,22	1.36	2 (11%)	21,30,33	1.95	4 (19%)
56	PSU	DY	55	56	18,21,22	1.42	2 (11%)	21,30,33	2.01	3 (14%)
56	PSU	DY	39	56	18,21,22	1.43	2 (11%)	21,30,33	1.97	3 (14%)
58	2QY	DX	10	58	12,13,14	1.66	1 (8%)	14,16,18	3.67	6 (42%)
56	PSU	BY	55	56	18,21,22	1.39	2 (11%)	21,30,33	1.98	3 (14%)
58	004	BX	3	58	9,10,11	1.39	1 (11%)	9,12,14	1.32	1 (11%)
56	5MU	BW	54	56	19,22,23	1.44	4 (21%)	27,32,35	1.98	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PSU	BY	39	56	18,21,22	1.39	2 (11%)	21,30,33	1.93	3 (14%)
58	2QZ	BX	1	58	7,8,9	0.67	0	7,10,12	4.73	4 (57%)
56	MIA	DW	37	56	24,31,32	2.18	4 (16%)	22,44,47	2.17	6 (27%)
58	MVA	BX	5	58	6,7,8	0.52	0	6,8,10	1.39	1 (16%)
56	5MU	DY	54	56	19,22,23	1.44	6 (31%)	27,32,35	2.07	5 (18%)
58	2R1	DX	6	58	10,10,11	1.65	2 (20%)	8,13,15	2.10	3 (37%)
56	PSU	BY	32	56	18,21,22	1.40	2 (11%)	21,30,33	1.94	3 (14%)
56	4SU	BY	8	56	18,21,22	1.75	4 (22%)	25,30,33	2.14	6 (24%)
56	MIA	BY	37	56	17,24,32	1.02	1 (5%)	16,35,47	1.37	2 (12%)
56	PSU	DW	32	56	18,21,22	1.43	3 (16%)	21,30,33	2.14	4 (19%)
58	MVA	BX	9	58	6,7,8	0.77	0	6,8,10	1.50	1 (16%)
56	PSU	BW	39	56	18,21,22	1.37	2 (11%)	21,30,33	2.02	5 (23%)
56	7MG	BY	46	56	23,26,27	1.30	3 (13%)	27,39,42	2.71	7 (25%)
58	2QY	BX	10	58	12,13,14	1.73	2 (16%)	14,16,18	4.12	6 (42%)
56	4SU	DW	8	56	18,21,22	1.83	5 (27%)	25,30,33	2.31	4 (16%)
56	4SU	BW	8	56	18,21,22	1.49	3 (16%)	25,30,33	2.18	5 (20%)

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
56	MIA	BW	37	56	-	5/11/33/34	0/3/3/3
56	PSU	DW	39	56	-	1/7/25/26	0/2/2/2
56	5MU	DW	54	56	-	0/7/25/26	0/2/2/2
58	MVA	DX	5	58	-	4/6/8/10	-
58	004	DX	3	58	-	0/4/6/8	0/1/1/1
56	7MG	BW	46	56	-	1/7/37/38	0/3/3/3
56	PSU	BW	32	56	-	4/7/25/26	0/2/2/2
58	2R3	DX	8	58	-	6/11/12/14	0/1/1/1
58	MVA	DX	9	58	-	4/6/8/10	-
58	2R1	BX	6	58	-	0/2/14/16	0/1/1/1
56	4SU	DY	8	56	-	1/7/25/26	0/2/2/2
56	MIA	DY	37	56	-	3/3/25/34	0/3/3/3
56	PSU	BW	55	56	-	2/7/25/26	0/2/2/2
56	PSU	DW	55	56	-	2/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	7MG	DW	46	56	-	4/7/37/38	0/3/3/3
58	2QZ	DX	1	58	-	1/8/10/12	-
58	2R3	BX	8	58	-	6/11/12/14	0/1/1/1
56	5MU	BY	54	56	-	2/7/25/26	0/2/2/2
56	7MG	DY	46	56	-	3/7/37/38	0/3/3/3
56	PSU	DY	32	56	-	0/7/25/26	0/2/2/2
56	PSU	DY	55	56	-	3/7/25/26	0/2/2/2
56	PSU	DY	39	56	-	2/7/25/26	0/2/2/2
58	2QY	DX	10	58	-	3/5/8/10	0/1/1/1
56	PSU	BY	55	56	-	2/7/25/26	0/2/2/2
58	004	BX	3	58	-	0/4/6/8	0/1/1/1
56	5MU	BW	54	56	-	1/7/25/26	0/2/2/2
56	PSU	BY	39	56	-	0/7/25/26	0/2/2/2
58	2QZ	BX	1	58	-	1/8/10/12	-
56	MIA	DW	37	56	-	7/11/33/34	0/3/3/3
58	MVA	BX	5	58	-	4/6/8/10	-
56	5MU	DY	54	56	-	2/7/25/26	0/2/2/2
58	2R1	DX	6	58	-	2/2/14/16	0/1/1/1
56	PSU	BY	32	56	-	0/7/25/26	0/2/2/2
56	4SU	BY	8	56	-	1/7/25/26	0/2/2/2
56	MIA	BY	37	56	-	2/3/25/34	0/3/3/3
56	PSU	DW	32	56	-	2/7/25/26	0/2/2/2
58	MVA	BX	9	58	-	2/6/8/10	-
56	PSU	BW	39	56	-	0/7/25/26	0/2/2/2
56	7MG	BY	46	56	-	4/7/37/38	0/3/3/3
58	2QY	BX	10	58	-	3/5/8/10	0/1/1/1
56	4SU	DW	8	56	-	0/7/25/26	0/2/2/2
56	4SU	BW	8	56	-	0/7/25/26	0/2/2/2

The worst 5 of 95 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BW	37	MIA	C13-C14	7.51	1.54	1.32
56	DW	37	MIA	C13-C14	7.11	1.53	1.32
56	BW	37	MIA	C2-S10	-7.10	1.69	1.75
56	DW	37	MIA	C2-S10	-5.65	1.71	1.75
58	DX	10	2QY	C-CA	5.23	1.52	1.43

The worst 5 of 183 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BX	1	2QZ	OG1-CB-CG2	11.46	143.95	109.68
58	DX	1	2QZ	OG1-CB-CG2	11.15	143.03	109.68
58	BX	10	2QY	CN-N-CA	-11.03	107.25	123.98
56	BW	46	7MG	N9-C4-N3	9.66	139.62	125.46
56	DY	46	7MG	N9-C4-N3	9.62	139.55	125.46

There are no chirality outliers.

5 of 90 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	BW	32	PSU	C2'-C1'-C5-C4
56	BW	32	PSU	O4'-C1'-C5-C4
56	BW	32	PSU	O4'-C1'-C5-C6
56	BW	37	MIA	N6-C12-C13-C14
56	BW	37	MIA	C12-C13-C14-C15

There are no ring outliers.

23 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	BW	37	MIA	2	0
56	DW	39	PSU	6	0
56	DW	54	5MU	1	0
58	DX	5	MVA	2	0
58	DX	3	004	1	0
56	BW	32	PSU	1	0
58	DX	8	2R3	2	0
58	DX	9	MVA	4	0
58	BX	6	2R1	5	0
56	DW	55	PSU	1	0
58	DX	1	2QZ	2	0
58	BX	8	2R3	2	0
56	DY	46	7MG	2	0
56	DY	55	PSU	2	0
58	DX	10	2QY	9	0
58	BX	3	004	4	0
56	DW	37	MIA	2	0
58	BX	5	MVA	2	0
58	DX	6	2R1	2	0
56	BY	8	4SU	1	0
58	BX	9	MVA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	BX	10	2QY	1	0
56	DW	8	4SU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2056 ligands modelled in this entry, 2052 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	SF4	BD	501	-	0,12,12	-	-	-		
61	SF4	DD	501	37	0,12,12	-	-	-		
62	GDP	BZ	702	59	25,30,30	0.95	0	30,47,47	1.33	4 (13%)
62	GDP	DZ	703	59	25,30,30	1.04	0	30,47,47	1.01	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	GDP	BZ	702	59	-	3/12/32/32	0/3/3/3
61	SF4	BD	501	-	-	-	0/6/5/5
61	SF4	DD	501	37	-	-	0/6/5/5
62	GDP	DZ	703	59	-	1/12/32/32	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	BZ	702	GDP	C8-N7-C5	3.34	108.23	102.55
62	BZ	702	GDP	C4'-O4'-C1'	-2.78	107.38	109.92
62	BZ	702	GDP	O3B-PB-O2B	2.24	116.22	107.80
62	BZ	702	GDP	O3'-C3'-C2'	-2.07	105.17	111.82
62	DZ	703	GDP	C8-N7-C5	2.07	106.07	102.55

There are no chirality outliers.

All (4) torsion outliers are listed below:

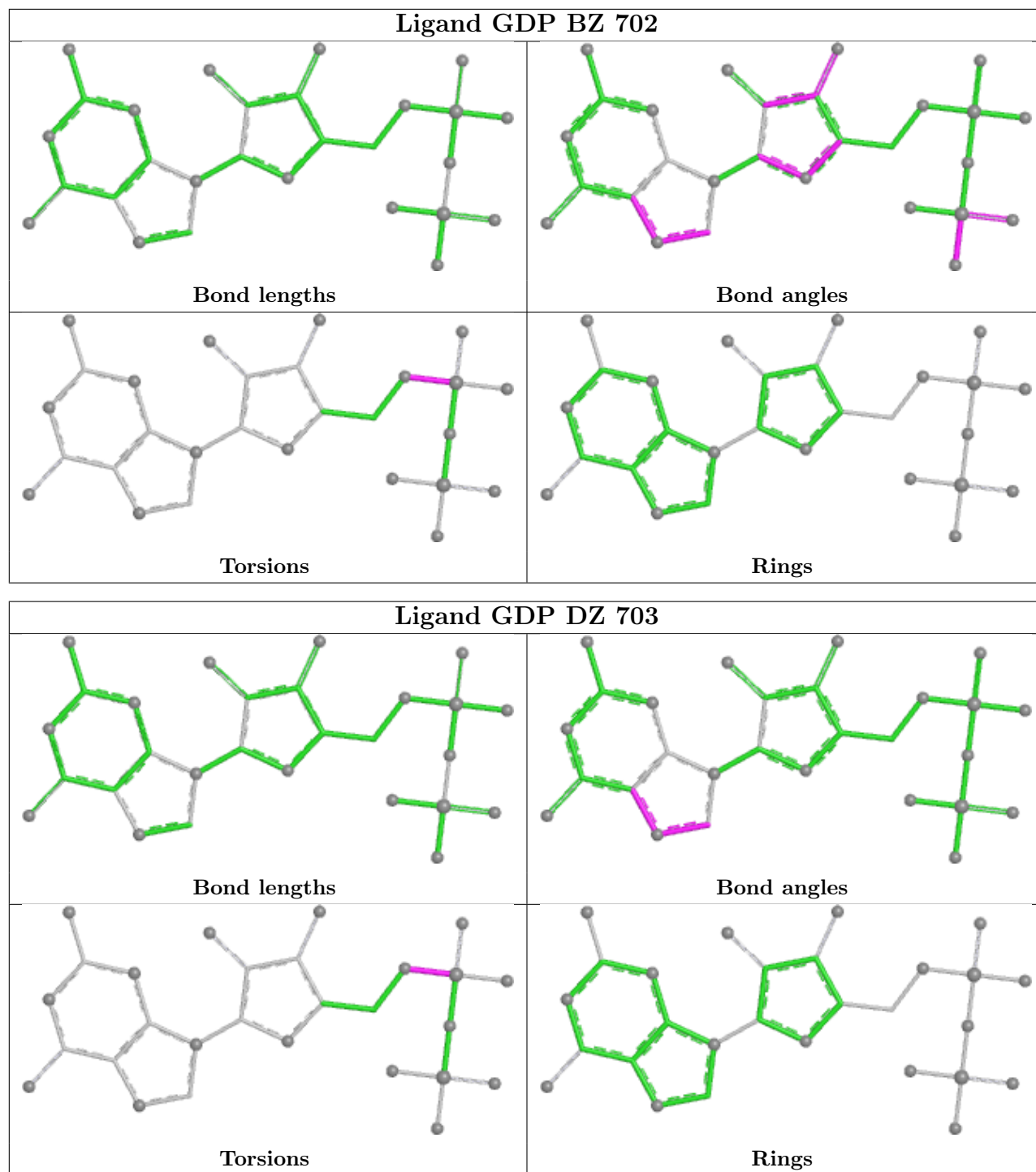
Mol	Chain	Res	Type	Atoms
62	BZ	702	GDP	C5'-O5'-PA-O3A
62	BZ	702	GDP	C5'-O5'-PA-O1A
62	BZ	702	GDP	C5'-O5'-PA-O2A
62	DZ	703	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	BD	501	SF4	1	0
61	DD	501	SF4	2	0
62	BZ	702	GDP	5	0
62	DZ	703	GDP	7	0

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



5.7 Other polymers [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	AA	2872/2915 (98%)	-0.80	45 (1%) 70 63	13, 31, 166, 310	0
1	CA	2868/2915 (98%)	-0.28	74 (2%) 57 49	23, 54, 175, 327	0
2	AB	120/121 (99%)	-0.67	1 (0%) 82 77	23, 46, 65, 111	0
2	CB	120/121 (99%)	0.64	6 (5%) 35 28	54, 103, 145, 177	0
3	AC	137/228 (60%)	2.58	88 (64%) 0 0	89, 187, 231, 259	0
3	CC	137/228 (60%)	2.74	91 (66%) 0 0	142, 205, 249, 270	0
4	AD	275/276 (99%)	-0.75	4 (1%) 71 64	8, 30, 56, 122	0
4	CD	275/276 (99%)	-0.40	4 (1%) 71 64	13, 43, 76, 133	0
5	AE	204/206 (99%)	-0.80	0 100 100	7, 30, 60, 99	0
5	CE	204/206 (99%)	-0.38	0 100 100	15, 51, 85, 143	0
6	AF	203/210 (96%)	-0.76	0 100 100	5, 31, 75, 140	0
6	CF	203/210 (96%)	-0.01	3 (1%) 71 64	20, 66, 122, 158	0
7	AG	181/182 (99%)	-0.01	1 (0%) 85 81	33, 66, 114, 178	0
7	CG	181/182 (99%)	1.08	21 (11%) 11 9	73, 124, 181, 208	0
8	AH	174/180 (96%)	-0.46	2 (1%) 77 71	21, 45, 72, 198	0
8	CH	174/180 (96%)	0.59	10 (5%) 30 24	51, 90, 139, 171	0
9	AK	130/173 (75%)	1.47	33 (25%) 2 2	65, 130, 195, 217	0
9	CK	130/173 (75%)	1.87	49 (37%) 1 1	84, 161, 205, 230	0
10	AL	66/147 (44%)	1.80	20 (30%) 1 1	109, 180, 227, 243	0
10	CL	66/147 (44%)	2.40	36 (54%) 0 0	104, 180, 226, 260	0
11	AN	140/140 (100%)	-0.84	1 (0%) 84 79	11, 27, 54, 96	0
11	CN	140/140 (100%)	-0.11	1 (0%) 84 79	35, 58, 92, 142	0
12	AO	122/122 (100%)	-0.82	0 100 100	16, 35, 64, 91	0
12	CO	122/122 (100%)	-0.43	0 100 100	28, 48, 80, 94	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	149/150 (99%)	-0.65	0 100 100	8, 37, 77, 126	0
13	CP	149/150 (99%)	0.23	4 (2%) 56 47	26, 73, 123, 155	0
14	AQ	141/141 (100%)	-0.74	0 100 100	9, 31, 53, 97	0
14	CQ	141/141 (100%)	0.09	2 (1%) 73 66	18, 62, 94, 145	0
15	AR	118/118 (100%)	-0.93	0 100 100	13, 27, 51, 75	0
15	CR	118/118 (100%)	-0.38	0 100 100	25, 49, 73, 106	0
16	AS	110/112 (98%)	-0.40	1 (0%) 81 75	24, 46, 74, 86	0
16	CS	110/112 (98%)	1.25	18 (16%) 5 5	59, 95, 139, 166	0
17	AT	131/146 (89%)	-0.40	4 (3%) 51 43	20, 39, 93, 218	0
17	CT	131/146 (89%)	-0.08	3 (2%) 61 52	35, 56, 103, 151	0
18	AU	116/118 (98%)	-1.04	0 100 100	7, 22, 38, 87	0
18	CU	116/118 (98%)	-0.05	0 100 100	31, 55, 88, 107	0
19	AV	101/101 (100%)	-1.05	0 100 100	10, 27, 56, 76	0
19	CV	101/101 (100%)	-0.10	1 (0%) 79 73	28, 68, 101, 162	0
20	AW	112/113 (99%)	-0.93	0 100 100	10, 23, 47, 145	0
20	CW	112/113 (99%)	-0.34	0 100 100	26, 44, 74, 159	0
21	AX	95/96 (98%)	-0.61	1 (1%) 77 71	12, 33, 63, 107	0
21	CX	95/96 (98%)	0.23	6 (6%) 27 21	36, 62, 97, 173	0
22	AY	107/110 (97%)	-0.44	2 (1%) 66 58	18, 42, 88, 117	0
22	CY	107/110 (97%)	0.50	7 (6%) 26 20	48, 80, 124, 170	0
23	AZ	185/206 (89%)	-0.21	3 (1%) 70 63	27, 55, 94, 136	0
23	CZ	185/206 (89%)	0.68	8 (4%) 40 32	52, 97, 144, 173	0
24	A0	77/85 (90%)	-0.73	0 100 100	9, 31, 53, 82	0
24	C0	77/85 (90%)	0.52	7 (9%) 16 12	27, 67, 104, 127	0
25	A1	97/98 (98%)	-0.55	1 (1%) 79 73	15, 38, 79, 97	0
25	C1	97/98 (98%)	0.03	3 (3%) 51 43	30, 55, 94, 139	0
26	A2	70/72 (97%)	-0.31	2 (2%) 54 45	14, 43, 63, 135	0
26	C2	70/72 (97%)	0.51	3 (4%) 40 32	47, 78, 109, 151	0
27	A3	59/60 (98%)	-0.78	1 (1%) 69 61	10, 26, 50, 110	0
27	C3	59/60 (98%)	0.16	2 (3%) 48 40	31, 62, 102, 162	0
28	A4	69/71 (97%)	0.64	5 (7%) 23 17	47, 101, 187, 216	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	C4	69/71 (97%)	1.14	11 (15%) 6 5	86, 158, 194, 226	0
29	A5	59/60 (98%)	-0.95	0 100 100	11, 22, 48, 66	0
29	C5	59/60 (98%)	-0.44	0 100 100	16, 46, 81, 120	0
30	A6	53/54 (98%)	-0.64	0 100 100	17, 35, 61, 75	0
30	C6	53/54 (98%)	0.07	0 100 100	40, 62, 85, 101	0
31	A7	48/49 (97%)	-0.68	2 (4%) 41 33	11, 20, 52, 99	0
31	C7	48/49 (97%)	-0.17	4 (8%) 19 14	23, 35, 95, 120	0
32	A8	64/65 (98%)	-0.88	0 100 100	13, 26, 39, 61	0
32	C8	64/65 (98%)	-0.09	1 (1%) 70 63	26, 53, 71, 93	0
33	A9	37/37 (100%)	-0.57	1 (2%) 56 47	19, 32, 61, 65	0
33	C9	37/37 (100%)	0.25	1 (2%) 56 47	43, 61, 90, 101	0
34	BA	1495/1521 (98%)	0.27	24 (1%) 70 63	23, 81, 179, 326	0
34	DA	1501/1521 (98%)	0.52	77 (5%) 34 27	39, 93, 206, 304	0
35	BB	231/256 (90%)	0.75	19 (8%) 19 14	52, 103, 165, 193	0
35	DB	231/256 (90%)	1.21	39 (16%) 5 5	66, 134, 196, 226	0
36	BC	206/239 (86%)	0.90	22 (10%) 12 10	72, 113, 168, 187	0
36	DC	206/239 (86%)	1.35	47 (22%) 2 3	88, 150, 194, 221	0
37	BD	208/209 (99%)	1.00	30 (14%) 7 6	53, 90, 140, 180	0
37	DD	208/209 (99%)	0.82	24 (11%) 11 9	52, 87, 132, 197	0
38	BE	148/162 (91%)	0.19	2 (1%) 73 66	36, 71, 108, 150	0
38	DE	148/162 (91%)	0.66	12 (8%) 19 15	42, 88, 131, 177	0
39	BF	100/101 (99%)	0.30	1 (1%) 79 73	42, 80, 123, 144	0
39	DF	100/101 (99%)	0.42	2 (2%) 64 56	48, 90, 133, 146	0
40	BG	155/156 (99%)	0.66	15 (9%) 15 11	65, 100, 155, 193	0
40	DG	155/156 (99%)	0.98	20 (12%) 9 7	79, 130, 177, 212	0
41	BH	137/138 (99%)	0.44	4 (2%) 54 45	44, 72, 105, 119	0
41	DH	137/138 (99%)	0.71	8 (5%) 30 23	51, 90, 124, 159	0
42	BI	127/128 (99%)	1.46	37 (29%) 1 2	58, 114, 168, 190	0
42	DI	127/128 (99%)	1.92	49 (38%) 1 1	78, 153, 189, 243	0
43	BJ	97/105 (92%)	1.55	29 (29%) 1 1	74, 121, 172, 194	0
43	DJ	96/105 (91%)	1.84	41 (42%) 1 1	75, 158, 198, 215	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BK	114/129 (88%)	0.11	1 (0%) 81 75	29, 73, 115, 125	0
44	DK	114/129 (88%)	0.53	8 (7%) 24 18	59, 92, 138, 168	0
45	BL	122/132 (92%)	0.10	5 (4%) 42 34	26, 60, 88, 110	0
45	DL	122/132 (92%)	0.42	5 (4%) 42 34	40, 70, 99, 142	0
46	BM	117/126 (92%)	0.79	12 (10%) 13 10	62, 107, 151, 187	0
46	DM	116/126 (92%)	1.52	30 (25%) 2 2	64, 154, 201, 235	0
47	BN	60/61 (98%)	1.44	14 (23%) 2 3	59, 109, 151, 171	0
47	DN	60/61 (98%)	2.16	33 (55%) 0 0	94, 141, 190, 208	0
48	BO	88/89 (98%)	0.21	5 (5%) 30 24	34, 68, 106, 139	0
48	DO	88/89 (98%)	0.44	2 (2%) 61 52	49, 81, 115, 139	0
49	BP	82/88 (93%)	0.81	9 (10%) 12 9	45, 80, 125, 150	0
49	DP	82/88 (93%)	0.61	3 (3%) 45 37	48, 76, 108, 120	0
50	BQ	99/105 (94%)	0.20	5 (5%) 34 27	43, 71, 103, 118	0
50	DQ	99/105 (94%)	0.66	11 (11%) 12 9	46, 79, 116, 148	0
51	BR	68/88 (77%)	0.12	1 (1%) 71 64	44, 71, 115, 135	0
51	DR	68/88 (77%)	0.40	1 (1%) 71 64	57, 89, 127, 146	0
52	BS	84/93 (90%)	1.51	23 (27%) 2 2	64, 126, 168, 222	0
52	DS	83/93 (89%)	1.89	33 (39%) 1 1	98, 162, 210, 220	0
53	BT	96/106 (90%)	0.69	9 (9%) 15 12	49, 84, 117, 159	0
53	DT	96/106 (90%)	0.63	8 (8%) 19 14	47, 81, 126, 145	0
54	BU	23/27 (85%)	1.82	10 (43%) 1 1	59, 99, 112, 154	0
54	DU	23/27 (85%)	2.32	11 (47%) 0 1	78, 132, 157, 179	0
55	BV	7/18 (38%)	1.56	4 (57%) 0 0	60, 68, 174, 188	0
55	DV	6/18 (33%)	2.06	3 (50%) 0 1	87, 94, 180, 202	0
56	BW	69/76 (90%)	-0.10	3 (4%) 40 32	37, 69, 117, 208	0
56	BY	67/76 (88%)	1.20	13 (19%) 4 4	74, 230, 278, 300	0
56	DW	69/76 (90%)	0.34	0 100 100	46, 106, 150, 254	0
56	DY	66/76 (86%)	1.43	16 (24%) 2 2	141, 280, 312, 332	0
57	BZ	728/758 (96%)	0.57	54 (7%) 22 17	37, 96, 187, 244	0
57	DZ	730/758 (96%)	0.76	76 (10%) 13 10	27, 112, 210, 259	0
58	BX	3/10 (30%)	0.56	0 100 100	81, 81, 81, 82	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
58	DX	3/10 (30%)	0.98	1 (33%) 1 1	78, 78, 80, 81	0
All	All	22705/23918 (94%)	0.14	1505 (6%) 26 19	5, 69, 187, 332	0

The worst 5 of 1505 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
42	DI	106	ALA	11.2
25	C1	2	SER	10.4
3	CC	213	VAL	7.5
36	BC	2	GLY	7.3
10	CL	127	ILE	7.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	PSU	DY	39	20/21	0.37	0.15	291,291,291,291	0
56	5MU	DY	54	21/22	0.38	0.15	303,303,303,303	0
56	PSU	BY	32	20/21	0.45	0.14	226,226,226,226	0
56	PSU	DY	32	20/21	0.51	0.19	275,275,275,275	0
56	7MG	BY	46	24/25	0.55	0.13	276,276,276,276	0
56	PSU	BY	55	20/21	0.57	0.13	243,243,243,243	0
56	PSU	BY	39	20/21	0.61	0.15	197,197,197,197	0
56	PSU	DY	55	20/21	0.61	0.16	252,252,252,252	0
56	MIA	DY	37	22/30	0.62	0.19	271,271,271,271	0
56	5MU	BY	54	21/22	0.64	0.14	246,246,246,246	0
56	MIA	BY	37	22/30	0.70	0.15	186,186,186,186	0
58	MVA	BX	5	8/9	0.72	0.17	82,82,82,82	0
56	4SU	BY	8	20/21	0.74	0.09	239,239,239,239	0
58	2R1	DX	6	10/11	0.76	0.12	81,81,81,81	0
56	4SU	DY	8	20/21	0.78	0.09	277,277,277,277	0
56	7MG	DW	46	24/25	0.78	0.13	124,124,124,124	0
58	2R1	BX	6	10/11	0.79	0.14	82,82,82,82	1
56	7MG	DY	46	24/25	0.79	0.12	266,266,266,266	0
56	5MU	DW	54	21/22	0.81	0.11	95,95,95,95	1
58	004	DX	3	10/11	0.82	0.13	81,81,81,81	0
56	PSU	DW	32	20/21	0.82	0.15	126,126,126,126	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	PSU	DW	55	20/21	0.84	0.09	92,92,92,92	0
56	PSU	DW	39	20/21	0.84	0.15	112,112,112,112	1
58	MVA	BX	9	8/9	0.85	0.16	82,82,82,82	0
56	7MG	BW	46	24/25	0.86	0.12	76,76,76,76	3
58	004	BX	3	10/11	0.87	0.12	82,82,82,82	0
56	PSU	BW	55	20/21	0.88	0.08	79,79,79,79	0
56	4SU	DW	8	20/21	0.88	0.09	103,103,103,103	0
58	2QY	BX	10	13/14	0.88	0.12	82,82,82,82	0
58	2QY	DX	10	13/14	0.88	0.10	81,81,81,81	0
58	2R3	BX	8	14/15	0.89	0.10	82,82,82,82	0
58	MVA	DX	5	8/9	0.89	0.11	81,81,81,81	0
56	5MU	BW	54	21/22	0.89	0.09	80,80,80,80	0
56	MIA	DW	37	29/30	0.89	0.14	109,109,109,109	0
56	MIA	BW	37	29/30	0.91	0.11	79,79,79,79	0
58	MVA	DX	9	8/9	0.91	0.10	81,81,81,81	0
58	2QZ	BX	1	9/10	0.91	0.12	82,82,82,82	0
56	PSU	BW	32	20/21	0.91	0.10	73,73,73,73	1
58	2QZ	DX	1	9/10	0.93	0.13	81,81,81,81	0
56	4SU	BW	8	20/21	0.94	0.07	60,60,60,60	1
58	2R3	DX	8	14/15	0.94	0.09	81,81,81,81	0
56	PSU	BW	39	20/21	0.95	0.09	65,65,65,65	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	1776	1/1	0.21	0.20	97,97,97,97	0
59	MG	DA	1718	1/1	0.24	0.21	101,101,101,101	0
59	MG	CB	3013	1/1	0.32	0.16	100,100,100,100	0
59	MG	BA	1790	1/1	0.43	0.17	96,96,96,96	0
59	MG	DA	1754	1/1	0.50	0.28	120,120,120,120	0
59	MG	DA	1757	1/1	0.52	0.27	111,111,111,111	0
59	MG	AA	3056	1/1	0.53	0.48	96,96,96,96	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3363	1/1	0.54	0.14	88,88,88,88	0
59	MG	BA	1616	1/1	0.55	0.22	122,122,122,122	0
59	MG	AA	3277	1/1	0.55	0.25	99,99,99,99	0
59	MG	BA	1691	1/1	0.56	0.26	86,86,86,86	0
59	MG	CA	3624	1/1	0.56	0.24	118,118,118,118	0
59	MG	BB	3001	1/1	0.56	0.26	91,91,91,91	0
59	MG	CA	3620	1/1	0.59	0.25	96,96,96,96	0
59	MG	CA	3488	1/1	0.59	0.28	88,88,88,88	0
59	MG	AA	3773	1/1	0.61	0.62	35,35,35,35	1
59	MG	AA	3296	1/1	0.61	0.20	67,67,67,67	0
59	MG	AA	3418	1/1	0.62	0.13	74,74,74,74	0
59	MG	DA	1609	1/1	0.63	0.13	89,89,89,89	0
59	MG	BA	1786	1/1	0.63	0.16	82,82,82,82	0
59	MG	BL	201	1/1	0.65	0.13	84,84,84,84	0
59	MG	CA	3289	1/1	0.65	0.15	65,65,65,65	0
59	MG	CA	3304	1/1	0.65	0.14	67,67,67,67	0
59	MG	AA	3717	1/1	0.66	0.52	68,68,68,68	0
59	MG	CA	3545	1/1	0.66	0.21	86,86,86,86	0
59	MG	BA	1707	1/1	0.66	0.14	72,72,72,72	0
59	MG	AA	3464	1/1	0.67	0.19	66,66,66,66	0
59	MG	DA	1710	1/1	0.67	0.11	104,104,104,104	0
59	MG	AA	3643	1/1	0.67	0.23	84,84,84,84	0
59	MG	AA	3347	1/1	0.67	0.13	88,88,88,88	0
59	MG	CA	3096	1/1	0.67	0.38	125,125,125,125	0
59	MG	BA	1660	1/1	0.68	0.25	82,82,82,82	0
59	MG	CA	3485	1/1	0.68	0.10	85,85,85,85	0
59	MG	CA	3546	1/1	0.68	0.14	88,88,88,88	0
59	MG	CA	3560	1/1	0.68	0.24	79,79,79,79	0
59	MG	DA	1611	1/1	0.69	0.41	89,89,89,89	0
59	MG	AA	3040	1/1	0.69	0.23	113,113,113,113	0
59	MG	BA	1673	1/1	0.69	0.15	80,80,80,80	0
59	MG	DA	1738	1/1	0.69	0.13	95,95,95,95	0
59	MG	DA	1749	1/1	0.69	0.13	77,77,77,77	0
59	MG	AA	3747	1/1	0.69	0.17	85,85,85,85	0
59	MG	CA	3579	1/1	0.69	0.15	65,65,65,65	0
59	MG	CQ	202	1/1	0.70	0.28	74,74,74,74	0
59	MG	BA	1741	1/1	0.70	0.10	88,88,88,88	0
59	MG	AA	3242	1/1	0.70	0.22	85,85,85,85	0
59	MG	DA	1631	1/1	0.70	0.11	74,74,74,74	0
59	MG	CA	3444	1/1	0.70	0.10	67,67,67,67	0
59	MG	CA	3460	1/1	0.71	0.33	104,104,104,104	0
59	MG	AA	3629	1/1	0.71	0.19	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3350	1/1	0.72	0.14	82,82,82,82	0
59	MG	CA	3237	1/1	0.72	0.17	94,94,94,94	0
59	MG	AA	3617	1/1	0.72	0.11	77,77,77,77	0
59	MG	CA	3127	1/1	0.72	0.23	94,94,94,94	0
59	MG	CA	3557	1/1	0.72	0.20	76,76,76,76	0
59	MG	CA	3066	1/1	0.73	0.16	69,69,69,69	0
59	MG	BA	1675	1/1	0.73	0.20	100,100,100,100	0
59	MG	CA	3535	1/1	0.73	0.22	77,77,77,77	0
59	MG	BA	1812	1/1	0.73	0.19	79,79,79,79	0
59	MG	CA	3149	1/1	0.73	0.26	100,100,100,100	0
59	MG	CA	3172	1/1	0.73	0.25	81,81,81,81	0
59	MG	CA	3055	1/1	0.73	0.16	77,77,77,77	0
59	MG	AA	3780	1/1	0.74	0.12	72,72,72,72	0
59	MG	AA	3619	1/1	0.74	0.12	47,47,47,47	0
59	MG	CA	3244	1/1	0.74	0.26	89,89,89,89	0
59	MG	CA	3139	1/1	0.74	0.22	126,126,126,126	0
59	MG	DA	1756	1/1	0.74	0.22	86,86,86,86	0
59	MG	CA	3089	1/1	0.74	0.25	87,87,87,87	0
59	MG	DA	1769	1/1	0.74	0.22	74,74,74,74	0
59	MG	CA	3100	1/1	0.75	0.29	81,81,81,81	0
59	MG	AA	3219	1/1	0.75	0.18	61,61,61,61	0
59	MG	AA	3781	1/1	0.75	0.17	72,72,72,72	0
59	MG	AA	3480	1/1	0.75	0.22	88,88,88,88	0
59	MG	BA	1657	1/1	0.75	0.26	78,78,78,78	0
59	MG	AA	3678	1/1	0.75	0.16	77,77,77,77	0
59	MG	DT	3001	1/1	0.75	0.24	60,60,60,60	0
59	MG	DA	1663	1/1	0.76	0.23	91,91,91,91	0
59	MG	DA	1668	1/1	0.76	0.33	65,65,65,65	0
59	MG	BA	1775	1/1	0.76	0.18	90,90,90,90	0
59	MG	CA	3093	1/1	0.76	0.41	75,75,75,75	0
59	MG	CA	3646	1/1	0.76	0.16	91,91,91,91	0
59	MG	AA	3269	1/1	0.76	0.23	63,63,63,63	0
59	MG	A0	101	1/1	0.76	0.13	69,69,69,69	0
59	MG	CA	3108	1/1	0.76	0.22	78,78,78,78	0
59	MG	CA	3240	1/1	0.76	0.27	71,71,71,71	0
59	MG	CA	3125	1/1	0.76	0.39	78,78,78,78	0
59	MG	DA	1655	1/1	0.76	0.24	83,83,83,83	0
59	MG	CA	3583	1/1	0.77	0.14	80,80,80,80	0
59	MG	CA	3586	1/1	0.77	0.31	93,93,93,93	0
59	MG	CA	3587	1/1	0.77	0.10	70,70,70,70	0
59	MG	AA	3481	1/1	0.77	0.19	78,78,78,78	0
59	MG	AA	3016	1/1	0.77	0.21	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	DA	1727	1/1	0.77	0.09	61,61,61,61	0
59	MG	DA	1732	1/1	0.77	0.12	85,85,85,85	0
59	MG	CA	3032	1/1	0.77	0.30	100,100,100,100	0
59	MG	DA	1740	1/1	0.77	0.17	68,68,68,68	0
59	MG	CA	3235	1/1	0.77	0.17	78,78,78,78	0
59	MG	BA	1697	1/1	0.77	0.34	99,99,99,99	0
59	MG	AA	3232	1/1	0.77	0.20	58,58,58,58	0
59	MG	CA	3566	1/1	0.77	0.17	30,30,30,30	1
59	MG	AA	3275	1/1	0.77	0.39	89,89,89,89	0
59	MG	DA	1635	1/1	0.77	0.22	75,75,75,75	0
59	MG	DW	503	1/1	0.77	0.19	85,85,85,85	0
59	MG	CA	3608	1/1	0.78	0.25	50,50,50,50	1
59	MG	CA	3007	1/1	0.78	0.26	92,92,92,92	0
59	MG	CA	3467	1/1	0.78	0.33	77,77,77,77	0
59	MG	BA	1758	1/1	0.78	0.26	76,76,76,76	0
59	MG	AA	3122	1/1	0.78	0.34	99,99,99,99	0
59	MG	CA	3376	1/1	0.78	0.12	78,78,78,78	0
59	MG	CQ	204	1/1	0.78	0.16	74,74,74,74	0
59	MG	CA	3395	1/1	0.78	0.26	50,50,50,50	0
59	MG	CA	3236	1/1	0.78	0.36	81,81,81,81	0
59	MG	DA	1708	1/1	0.79	0.20	77,77,77,77	0
59	MG	BA	1719	1/1	0.79	0.15	62,62,62,62	0
59	MG	DA	1715	1/1	0.79	0.19	79,79,79,79	0
59	MG	CA	3506	1/1	0.79	0.12	63,63,63,63	0
59	MG	AA	3093	1/1	0.79	0.68	92,92,92,92	0
59	MG	BA	1670	1/1	0.79	0.13	69,69,69,69	0
59	MG	CA	3323	1/1	0.79	0.20	87,87,87,87	0
59	MG	CA	3044	1/1	0.79	0.21	89,89,89,89	0
59	MG	AA	3583	1/1	0.79	0.13	63,63,63,63	0
59	MG	CA	3155	1/1	0.79	0.28	112,112,112,112	0
59	MG	BA	1625	1/1	0.79	0.20	86,86,86,86	0
59	MG	BA	1628	1/1	0.79	0.21	87,87,87,87	0
59	MG	DA	1762	1/1	0.79	0.20	61,61,61,61	0
59	MG	BA	1694	1/1	0.79	0.31	83,83,83,83	0
59	MG	BA	1634	1/1	0.79	0.27	64,64,64,64	0
59	MG	AA	3267	1/1	0.79	0.12	53,53,53,53	0
59	MG	BA	1800	1/1	0.80	0.18	77,77,77,77	0
59	MG	CA	3638	1/1	0.80	0.28	76,76,76,76	0
59	MG	AA	3642	1/1	0.80	0.18	71,71,71,71	0
59	MG	DA	1724	1/1	0.80	0.16	70,70,70,70	0
59	MG	AA	3708	1/1	0.80	0.30	61,61,61,61	0
59	MG	AA	3202	1/1	0.80	0.17	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3124	1/1	0.80	0.23	65,65,65,65	0
59	MG	DA	1604	1/1	0.80	0.20	80,80,80,80	0
59	MG	CA	3565	1/1	0.80	0.12	95,95,95,95	0
59	MG	CA	3465	1/1	0.80	0.27	70,70,70,70	0
59	MG	CA	3184	1/1	0.80	0.27	77,77,77,77	0
59	MG	CA	3186	1/1	0.80	0.20	77,77,77,77	0
59	MG	AA	3660	1/1	0.80	0.16	61,61,61,61	0
59	MG	CA	3492	1/1	0.80	0.15	59,59,59,59	0
59	MG	CA	3494	1/1	0.80	0.14	97,97,97,97	0
59	MG	CA	3357	1/1	0.80	0.14	66,66,66,66	0
59	MG	BA	1767	1/1	0.81	0.11	96,96,96,96	0
59	MG	CA	3518	1/1	0.81	0.12	65,65,65,65	0
59	MG	BA	1662	1/1	0.81	0.28	70,70,70,70	0
59	MG	CA	3246	1/1	0.81	0.27	57,57,57,57	0
59	MG	AA	3323	1/1	0.81	0.10	64,64,64,64	0
59	MG	CA	3295	1/1	0.81	0.19	66,66,66,66	0
59	MG	BA	1671	1/1	0.81	0.35	101,101,101,101	0
59	MG	AA	3157	1/1	0.81	0.22	91,91,91,91	0
59	MG	DA	1704	1/1	0.81	0.11	49,49,49,49	0
59	MG	AA	3622	1/1	0.81	0.18	60,60,60,60	0
59	MG	AA	3108	1/1	0.81	0.43	101,101,101,101	0
59	MG	BA	1693	1/1	0.81	0.19	76,76,76,76	0
59	MG	AA	3571	1/1	0.81	0.20	94,94,94,94	0
59	MG	BS	101	1/1	0.81	0.11	79,79,79,79	0
59	MG	CA	3605	1/1	0.81	0.22	70,70,70,70	0
59	MG	AA	3441	1/1	0.81	0.19	58,58,58,58	0
59	MG	DA	1733	1/1	0.81	0.19	92,92,92,92	0
59	MG	CA	3164	1/1	0.81	0.23	64,64,64,64	0
59	MG	CA	3622	1/1	0.81	0.15	50,50,50,50	0
59	MG	DA	1746	1/1	0.81	0.13	81,81,81,81	0
59	MG	BA	1648	1/1	0.81	0.09	74,74,74,74	0
59	MG	AA	3776	1/1	0.81	0.11	69,69,69,69	0
59	MG	CA	3643	1/1	0.81	0.10	79,79,79,79	0
59	MG	BA	1659	1/1	0.81	0.21	67,67,67,67	0
59	MG	CB	3001	1/1	0.81	0.16	72,72,72,72	0
59	MG	CA	3065	1/1	0.81	0.24	56,56,56,56	0
59	MG	AA	3644	1/1	0.81	0.22	56,56,56,56	0
59	MG	CA	3067	1/1	0.81	0.16	63,63,63,63	0
59	MG	CA	3530	1/1	0.82	0.24	71,71,71,71	0
59	MG	CA	3111	1/1	0.82	0.23	79,79,79,79	0
59	MG	CA	3539	1/1	0.82	0.16	90,90,90,90	0
59	MG	CA	3204	1/1	0.82	0.11	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3222	1/1	0.82	0.17	57,57,57,57	0
59	MG	CA	3379	1/1	0.82	0.11	83,83,83,83	0
59	MG	CA	3389	1/1	0.82	0.17	59,59,59,59	0
59	MG	DA	1662	1/1	0.82	0.24	75,75,75,75	0
59	MG	AA	3206	1/1	0.82	0.25	106,106,106,106	0
59	MG	CA	3408	1/1	0.82	0.12	58,58,58,58	0
59	MG	DA	1674	1/1	0.82	0.21	77,77,77,77	0
59	MG	CA	3420	1/1	0.82	0.20	69,69,69,69	0
59	MG	CA	3581	1/1	0.82	0.13	38,38,38,38	0
59	MG	CA	3433	1/1	0.82	0.12	82,82,82,82	0
59	MG	AA	3625	1/1	0.82	0.19	51,51,51,51	0
59	MG	CA	3456	1/1	0.82	0.13	54,54,54,54	0
59	MG	CA	3594	1/1	0.82	0.08	73,73,73,73	0
59	MG	BA	1782	1/1	0.82	0.12	47,47,47,47	0
59	MG	CA	3129	1/1	0.82	0.15	64,64,64,64	0
59	MG	CA	3612	1/1	0.82	0.29	83,83,83,83	0
59	MG	DA	1737	1/1	0.82	0.15	69,69,69,69	0
59	MG	CA	3619	1/1	0.82	0.17	40,40,40,40	0
59	MG	CA	3078	1/1	0.82	0.23	57,57,57,57	0
59	MG	CA	3146	1/1	0.82	0.32	82,82,82,82	0
59	MG	BA	1612	1/1	0.82	0.18	92,92,92,92	0
59	MG	DA	1753	1/1	0.82	0.31	79,79,79,79	0
59	MG	BA	1748	1/1	0.82	0.09	63,63,63,63	0
59	MG	DA	1755	1/1	0.82	0.32	88,88,88,88	0
59	MG	AA	3719	1/1	0.82	0.18	59,59,59,59	0
59	MG	CA	3502	1/1	0.82	0.28	90,90,90,90	0
59	MG	CA	3050	1/1	0.82	0.22	75,75,75,75	0
59	MG	CA	3510	1/1	0.82	0.17	95,95,95,95	0
59	MG	CQ	201	1/1	0.82	0.19	72,72,72,72	0
59	MG	AA	3737	1/1	0.82	0.10	54,54,54,54	0
59	MG	DA	1629	1/1	0.83	0.20	59,59,59,59	0
59	MG	AA	3611	1/1	0.83	0.15	47,47,47,47	0
59	MG	CA	3428	1/1	0.83	0.14	58,58,58,58	0
59	MG	DA	1639	1/1	0.83	0.14	69,69,69,69	0
59	MG	BA	1610	1/1	0.83	0.15	78,78,78,78	0
59	MG	AA	3198	1/1	0.83	0.20	63,63,63,63	0
59	MG	AA	3212	1/1	0.83	0.24	81,81,81,81	0
59	MG	CA	3117	1/1	0.83	0.21	67,67,67,67	0
59	MG	BA	1755	1/1	0.83	0.10	86,86,86,86	0
59	MG	DA	1675	1/1	0.83	0.51	70,70,70,70	0
59	MG	DA	1676	1/1	0.83	0.15	74,74,74,74	0
59	MG	AA	3653	1/1	0.83	0.11	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3126	1/1	0.83	0.15	62,62,62,62	0
59	MG	CA	3035	1/1	0.83	0.38	69,69,69,69	0
59	MG	AA	3367	1/1	0.83	0.14	60,60,60,60	0
59	MG	CA	3135	1/1	0.83	0.24	59,59,59,59	0
59	MG	DA	1722	1/1	0.83	0.11	77,77,77,77	0
59	MG	CA	3501	1/1	0.83	0.21	74,74,74,74	0
59	MG	CA	3314	1/1	0.83	0.12	57,57,57,57	0
59	MG	BA	1772	1/1	0.83	0.11	66,66,66,66	0
59	MG	CA	3507	1/1	0.83	0.18	83,83,83,83	0
59	MG	BA	1679	1/1	0.83	0.21	59,59,59,59	0
59	MG	CA	3644	1/1	0.83	0.20	66,66,66,66	0
59	MG	AA	3266	1/1	0.83	0.50	90,90,90,90	0
59	MG	AA	3128	1/1	0.83	0.34	89,89,89,89	0
59	MG	CA	3157	1/1	0.83	0.21	81,81,81,81	0
59	MG	CA	3538	1/1	0.83	0.14	72,72,72,72	0
59	MG	AA	3715	1/1	0.83	0.23	33,33,33,33	1
59	MG	BA	1695	1/1	0.83	0.10	83,83,83,83	0
59	MG	AB	3017	1/1	0.83	0.11	59,59,59,59	0
59	MG	BA	1811	1/1	0.83	0.13	77,77,77,77	0
59	MG	DA	1610	1/1	0.83	0.23	71,71,71,71	0
59	MG	CA	3411	1/1	0.83	0.15	57,57,57,57	0
59	MG	DA	1618	1/1	0.83	0.29	91,91,91,91	0
59	MG	DA	1626	1/1	0.83	0.16	71,71,71,71	0
59	MG	DA	1638	1/1	0.84	0.15	80,80,80,80	0
59	MG	CA	3216	1/1	0.84	0.21	79,79,79,79	0
59	MG	DA	1644	1/1	0.84	0.16	94,94,94,94	0
59	MG	DA	1652	1/1	0.84	0.15	80,80,80,80	0
59	MG	AA	3141	1/1	0.84	0.09	68,68,68,68	0
59	MG	CA	3591	1/1	0.84	0.10	60,60,60,60	0
59	MG	AA	3018	1/1	0.84	0.61	67,67,67,67	0
59	MG	CA	3598	1/1	0.84	0.09	65,65,65,65	0
59	MG	AA	3235	1/1	0.84	0.27	93,93,93,93	0
59	MG	BA	1792	1/1	0.84	0.18	80,80,80,80	0
59	MG	CA	3610	1/1	0.84	0.12	69,69,69,69	0
59	MG	DA	1677	1/1	0.84	0.15	78,78,78,78	0
59	MG	CA	3239	1/1	0.84	0.12	69,69,69,69	0
59	MG	BA	1619	1/1	0.84	0.12	59,59,59,59	0
59	MG	AA	3542	1/1	0.84	0.14	58,58,58,58	0
59	MG	AA	3274	1/1	0.84	0.15	75,75,75,75	0
59	MG	AA	3754	1/1	0.84	0.17	64,64,64,64	0
59	MG	BA	1638	1/1	0.84	0.18	66,66,66,66	0
59	MG	BA	1644	1/1	0.84	0.16	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	1721	1/1	0.84	0.10	66,66,66,66	0
59	MG	BA	1727	1/1	0.84	0.13	77,77,77,77	0
59	MG	BA	1733	1/1	0.84	0.21	78,78,78,78	0
59	MG	DA	1736	1/1	0.84	0.09	78,78,78,78	0
59	MG	AA	3756	1/1	0.84	0.10	49,49,49,49	0
59	MG	AA	3758	1/1	0.84	0.25	43,43,43,43	1
59	MG	AA	3582	1/1	0.84	0.23	76,76,76,76	0
59	MG	CA	3378	1/1	0.84	0.17	97,97,97,97	0
59	MG	DA	1748	1/1	0.84	0.13	70,70,70,70	0
59	MG	AA	3138	1/1	0.84	0.09	38,38,38,38	0
59	MG	AA	3425	1/1	0.84	0.17	77,77,77,77	0
59	MG	AA	3246	1/1	0.84	0.12	52,52,52,52	0
59	MG	CA	3398	1/1	0.84	0.14	67,67,67,67	0
59	MG	CA	3070	1/1	0.84	0.13	60,60,60,60	0
59	MG	DA	1623	1/1	0.84	0.14	72,72,72,72	0
59	MG	AA	3706	1/1	0.84	0.24	41,41,41,41	1
59	MG	CA	3193	1/1	0.84	0.17	89,89,89,89	0
59	MG	CA	3203	1/1	0.84	0.11	73,73,73,73	0
59	MG	AA	3453	1/1	0.84	0.15	39,39,39,39	0
59	MG	AA	3740	1/1	0.85	0.17	61,61,61,61	0
59	MG	CA	3511	1/1	0.85	0.10	81,81,81,81	0
59	MG	DA	1622	1/1	0.85	0.15	60,60,60,60	0
59	MG	CA	3516	1/1	0.85	0.17	79,79,79,79	0
59	MG	CA	3076	1/1	0.85	0.25	64,64,64,64	0
59	MG	BA	1764	1/1	0.85	0.10	71,71,71,71	0
59	MG	AB	3021	1/1	0.85	0.22	65,65,65,65	0
59	MG	AD	301	1/1	0.85	0.19	57,57,57,57	0
59	MG	AD	308	1/1	0.85	0.14	65,65,65,65	0
59	MG	CA	3542	1/1	0.85	0.15	87,87,87,87	0
59	MG	DA	1640	1/1	0.85	0.27	77,77,77,77	0
59	MG	AE	305	1/1	0.85	0.19	48,48,48,48	0
59	MG	DA	1649	1/1	0.85	0.27	69,69,69,69	0
59	MG	CA	3107	1/1	0.85	0.20	77,77,77,77	0
59	MG	BA	1778	1/1	0.85	0.10	54,54,54,54	0
59	MG	DA	1659	1/1	0.85	0.27	78,78,78,78	0
59	MG	CA	3341	1/1	0.85	0.12	73,73,73,73	0
59	MG	BA	1780	1/1	0.85	0.11	60,60,60,60	0
59	MG	AZ	302	1/1	0.85	0.12	55,55,55,55	0
59	MG	AA	3630	1/1	0.85	0.35	72,72,72,72	0
59	MG	A2	3001	1/1	0.85	0.13	53,53,53,53	0
59	MG	BA	1601	1/1	0.85	0.14	95,95,95,95	0
59	MG	BA	1797	1/1	0.85	0.15	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3700	1/1	0.85	0.12	70,70,70,70	0
59	MG	CA	3392	1/1	0.85	0.11	43,43,43,43	0
59	MG	DA	1709	1/1	0.85	0.13	70,70,70,70	0
59	MG	AA	3755	1/1	0.85	0.31	78,78,78,78	0
59	MG	AA	3314	1/1	0.85	0.14	57,57,57,57	0
59	MG	AA	3181	1/1	0.85	0.26	79,79,79,79	0
59	MG	BA	1699	1/1	0.85	0.07	72,72,72,72	0
59	MG	BA	1704	1/1	0.85	0.20	71,71,71,71	0
59	MG	CA	3001	1/1	0.85	0.18	64,64,64,64	0
59	MG	DA	1730	1/1	0.85	0.17	71,71,71,71	0
59	MG	CA	3614	1/1	0.85	0.12	62,62,62,62	0
59	MG	CA	3432	1/1	0.85	0.17	32,32,32,32	0
59	MG	AA	3769	1/1	0.85	0.15	63,63,63,63	0
59	MG	AA	3516	1/1	0.85	0.17	65,65,65,65	0
59	MG	BA	1631	1/1	0.85	0.13	71,71,71,71	0
59	MG	CA	3041	1/1	0.85	0.25	61,61,61,61	0
59	MG	AA	3651	1/1	0.85	0.17	77,77,77,77	0
59	MG	CA	3202	1/1	0.85	0.24	73,73,73,73	0
59	MG	CA	3470	1/1	0.85	0.18	74,74,74,74	0
59	MG	DA	1750	1/1	0.85	0.15	67,67,67,67	0
59	MG	CA	3047	1/1	0.85	0.19	84,84,84,84	0
59	MG	AA	3607	1/1	0.85	0.14	60,60,60,60	1
59	MG	CE	301	1/1	0.85	0.17	53,53,53,53	0
59	MG	AA	3427	1/1	0.85	0.07	61,61,61,61	0
59	MG	BA	1744	1/1	0.85	0.14	57,57,57,57	0
59	MG	CA	3226	1/1	0.85	0.24	52,52,52,52	0
59	MG	AA	3787	1/1	0.85	0.14	82,82,82,82	0
59	MG	DJ	5001	1/1	0.85	0.10	82,82,82,82	0
59	MG	AA	3796	1/1	0.85	0.19	78,78,78,78	0
59	MG	CA	3069	1/1	0.85	0.45	81,81,81,81	0
59	MG	CA	3134	1/1	0.86	0.17	71,71,71,71	0
59	MG	AA	3680	1/1	0.86	0.21	79,79,79,79	0
59	MG	CA	3038	1/1	0.86	0.31	97,97,97,97	0
59	MG	DA	1632	1/1	0.86	0.20	57,57,57,57	0
59	MG	DA	1634	1/1	0.86	0.23	66,66,66,66	0
59	MG	CA	3367	1/1	0.86	0.14	63,63,63,63	0
59	MG	CA	3555	1/1	0.86	0.08	71,71,71,71	0
59	MG	AA	3694	1/1	0.86	0.08	53,53,53,53	0
59	MG	CA	3148	1/1	0.86	0.26	62,62,62,62	0
59	MG	DA	1643	1/1	0.86	0.18	79,79,79,79	0
59	MG	CA	3042	1/1	0.86	0.28	65,65,65,65	0
59	MG	CA	3388	1/1	0.86	0.11	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3154	1/1	0.86	0.20	64,64,64,64	0
59	MG	AA	3536	1/1	0.86	0.18	66,66,66,66	0
59	MG	BA	1614	1/1	0.86	0.19	72,72,72,72	0
59	MG	BA	1687	1/1	0.86	0.23	52,52,52,52	0
59	MG	AA	3170	1/1	0.86	0.16	54,54,54,54	0
59	MG	AA	3315	1/1	0.86	0.23	65,65,65,65	0
59	MG	AA	3133	1/1	0.86	0.20	50,50,50,50	0
59	MG	BA	1781	1/1	0.86	0.09	63,63,63,63	0
59	MG	AA	3344	1/1	0.86	0.13	22,22,22,22	0
59	MG	CA	3606	1/1	0.86	0.30	73,73,73,73	0
59	MG	DA	1678	1/1	0.86	0.21	66,66,66,66	0
59	MG	DA	1690	1/1	0.86	0.19	73,73,73,73	0
59	MG	DA	1692	1/1	0.86	0.12	53,53,53,53	0
59	MG	DA	1694	1/1	0.86	0.13	106,106,106,106	0
59	MG	DA	1698	1/1	0.86	0.20	97,97,97,97	0
59	MG	BA	1783	1/1	0.86	0.15	57,57,57,57	0
59	MG	AA	3586	1/1	0.86	0.19	74,74,74,74	0
59	MG	CA	3212	1/1	0.86	0.29	84,84,84,84	0
59	MG	BA	1788	1/1	0.86	0.37	79,79,79,79	0
59	MG	DA	1713	1/1	0.86	0.09	49,49,49,49	0
59	MG	CA	3083	1/1	0.86	0.21	61,61,61,61	0
59	MG	CA	3223	1/1	0.86	0.09	59,59,59,59	0
59	MG	AA	3189	1/1	0.86	0.20	62,62,62,62	0
59	MG	CA	3481	1/1	0.86	0.12	64,64,64,64	0
59	MG	CA	3626	1/1	0.86	0.16	61,61,61,61	0
59	MG	CA	3633	1/1	0.86	0.12	68,68,68,68	0
59	MG	CA	3634	1/1	0.86	0.13	82,82,82,82	0
59	MG	AA	3195	1/1	0.86	0.26	69,69,69,69	0
59	MG	BA	1795	1/1	0.86	0.07	59,59,59,59	0
59	MG	AA	3614	1/1	0.86	0.14	50,50,50,50	1
59	MG	CA	3104	1/1	0.86	0.18	80,80,80,80	0
59	MG	CA	3647	1/1	0.86	0.10	85,85,85,85	0
59	MG	CA	3649	1/1	0.86	0.18	51,51,51,51	0
59	MG	CA	3499	1/1	0.86	0.19	62,62,62,62	0
59	MG	BA	1718	1/1	0.86	0.07	63,63,63,63	0
59	MG	BA	1646	1/1	0.86	0.25	66,66,66,66	0
59	MG	AA	3409	1/1	0.86	0.14	60,60,60,60	0
59	MG	CA	3273	1/1	0.86	0.13	58,58,58,58	0
59	MG	CA	3508	1/1	0.86	0.11	52,52,52,52	0
59	MG	AF	307	1/1	0.86	0.21	76,76,76,76	0
59	MG	AG	202	1/1	0.86	0.08	54,54,54,54	0
59	MG	AA	3675	1/1	0.86	0.12	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3307	1/1	0.86	0.13	60,60,60,60	0
59	MG	DE	201	1/1	0.86	0.17	84,84,84,84	0
59	MG	AA	3676	1/1	0.86	0.10	26,26,26,26	0
59	MG	DK	5001	1/1	0.86	0.11	76,76,76,76	0
59	MG	BA	1665	1/1	0.86	0.21	73,73,73,73	0
59	MG	AA	3068	1/1	0.86	0.33	73,73,73,73	0
59	MG	AA	3495	1/1	0.87	0.17	35,35,35,35	0
59	MG	CA	3230	1/1	0.87	0.25	49,49,49,49	0
59	MG	CA	3233	1/1	0.87	0.13	59,59,59,59	0
59	MG	DA	1614	1/1	0.87	0.09	65,65,65,65	0
59	MG	CA	3504	1/1	0.87	0.13	79,79,79,79	0
59	MG	BA	1664	1/1	0.87	0.11	56,56,56,56	0
59	MG	CA	3080	1/1	0.87	0.16	75,75,75,75	0
59	MG	DA	1624	1/1	0.87	0.07	82,82,82,82	0
59	MG	AA	3096	1/1	0.87	0.18	59,59,59,59	0
59	MG	CA	3238	1/1	0.87	0.18	69,69,69,69	0
59	MG	BA	1669	1/1	0.87	0.21	66,66,66,66	0
59	MG	AA	3357	1/1	0.87	0.14	55,55,55,55	0
59	MG	AA	3098	1/1	0.87	0.27	51,51,51,51	0
59	MG	AA	3213	1/1	0.87	0.33	76,76,76,76	0
59	MG	CA	3532	1/1	0.87	0.15	49,49,49,49	0
59	MG	CA	3534	1/1	0.87	0.08	73,73,73,73	0
59	MG	AA	3186	1/1	0.87	0.13	48,48,48,48	0
59	MG	DA	1641	1/1	0.87	0.10	74,74,74,74	0
59	MG	CA	3288	1/1	0.87	0.14	49,49,49,49	0
59	MG	BA	1676	1/1	0.87	0.25	61,61,61,61	0
59	MG	CA	3294	1/1	0.87	0.07	72,72,72,72	0
59	MG	AA	3055	1/1	0.87	0.26	65,65,65,65	0
59	MG	CA	3298	1/1	0.87	0.23	57,57,57,57	0
59	MG	AA	3659	1/1	0.87	0.16	73,73,73,73	0
59	MG	CA	3112	1/1	0.87	0.21	69,69,69,69	0
59	MG	CA	3115	1/1	0.87	0.29	67,67,67,67	0
59	MG	A7	104	1/1	0.87	0.09	55,55,55,55	0
59	MG	CA	3333	1/1	0.87	0.17	68,68,68,68	0
59	MG	CA	3573	1/1	0.87	0.12	65,65,65,65	0
59	MG	CA	3340	1/1	0.87	0.17	66,66,66,66	0
59	MG	AA	3288	1/1	0.87	0.14	39,39,39,39	0
59	MG	BA	1602	1/1	0.87	0.20	79,79,79,79	0
59	MG	AA	3435	1/1	0.87	0.11	52,52,52,52	0
59	MG	AA	3761	1/1	0.87	0.43	92,92,92,92	0
59	MG	AA	3608	1/1	0.87	0.13	60,60,60,60	0
59	MG	CA	3133	1/1	0.87	0.14	85,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3595	1/1	0.87	0.14	70,70,70,70	0
59	MG	CA	3596	1/1	0.87	0.11	51,51,51,51	0
59	MG	AA	3771	1/1	0.87	0.18	60,60,60,60	0
59	MG	CA	3603	1/1	0.87	0.16	49,49,49,49	0
59	MG	AA	3677	1/1	0.87	0.22	69,69,69,69	0
59	MG	BA	1714	1/1	0.87	0.21	74,74,74,74	0
59	MG	DA	1717	1/1	0.87	0.20	95,95,95,95	0
59	MG	BA	1623	1/1	0.87	0.17	67,67,67,67	0
59	MG	CA	3022	1/1	0.87	0.30	69,69,69,69	0
59	MG	AA	3194	1/1	0.87	0.21	82,82,82,82	0
59	MG	CA	3034	1/1	0.87	0.27	77,77,77,77	0
59	MG	AA	3241	1/1	0.87	0.18	65,65,65,65	0
59	MG	BA	1724	1/1	0.87	0.12	67,67,67,67	0
59	MG	CA	3621	1/1	0.87	0.12	61,61,61,61	0
59	MG	CA	3414	1/1	0.87	0.14	34,34,34,34	1
59	MG	AA	3063	1/1	0.87	0.15	54,54,54,54	0
59	MG	CA	3165	1/1	0.87	0.20	57,57,57,57	0
59	MG	DA	1739	1/1	0.87	0.14	73,73,73,73	0
59	MG	AA	3124	1/1	0.87	0.30	62,62,62,62	0
59	MG	DA	1742	1/1	0.87	0.11	72,72,72,72	0
59	MG	CA	3180	1/1	0.87	0.20	62,62,62,62	0
59	MG	CA	3442	1/1	0.87	0.31	74,74,74,74	0
59	MG	AA	3792	1/1	0.87	0.09	48,48,48,48	0
59	MG	AA	3169	1/1	0.87	0.19	35,35,35,35	0
59	MG	CA	3190	1/1	0.87	0.16	66,66,66,66	0
59	MG	AA	3814	1/1	0.87	0.26	72,72,72,72	0
59	MG	AA	3817	1/1	0.87	0.10	75,75,75,75	0
59	MG	CA	3057	1/1	0.87	0.19	60,60,60,60	0
59	MG	CA	3480	1/1	0.87	0.12	50,50,50,50	0
59	MG	AA	3493	1/1	0.87	0.09	77,77,77,77	0
59	MG	CE	305	1/1	0.87	0.06	58,58,58,58	0
59	MG	BA	1658	1/1	0.87	0.32	66,66,66,66	0
59	MG	AB	3020	1/1	0.87	0.16	62,62,62,62	0
59	MG	AA	3711	1/1	0.87	0.27	43,43,43,43	1
59	MG	BA	1774	1/1	0.87	0.14	50,50,50,50	0
59	MG	DA	1605	1/1	0.87	0.15	105,105,105,105	0
59	MG	DZ	701	1/1	0.87	0.11	72,72,72,72	0
59	MG	CA	3219	1/1	0.88	0.15	42,42,42,42	0
59	MG	BA	1713	1/1	0.88	0.24	68,68,68,68	0
59	MG	BA	1656	1/1	0.88	0.20	75,75,75,75	0
59	MG	CA	3225	1/1	0.88	0.17	64,64,64,64	0
59	MG	BA	1803	1/1	0.88	0.11	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	1810	1/1	0.88	0.09	82,82,82,82	0
59	MG	DA	1654	1/1	0.88	0.27	63,63,63,63	0
59	MG	BA	1716	1/1	0.88	0.15	86,86,86,86	0
59	MG	AA	3281	1/1	0.88	0.25	75,75,75,75	0
59	MG	AA	3705	1/1	0.88	0.24	53,53,53,53	1
59	MG	BE	3001	1/1	0.88	0.08	78,78,78,78	0
59	MG	DA	1665	1/1	0.88	0.12	63,63,63,63	0
59	MG	AA	3775	1/1	0.88	0.28	25,25,25,25	1
59	MG	AA	3365	1/1	0.88	0.20	77,77,77,77	0
59	MG	CA	3474	1/1	0.88	0.15	59,59,59,59	0
59	MG	AA	3601	1/1	0.88	0.10	61,61,61,61	0
59	MG	BA	1663	1/1	0.88	0.14	43,43,43,43	0
59	MG	BA	1739	1/1	0.88	0.11	62,62,62,62	0
59	MG	DA	1679	1/1	0.88	0.12	70,70,70,70	0
59	MG	DA	1683	1/1	0.88	0.13	58,58,58,58	0
59	MG	CA	3254	1/1	0.88	0.15	85,85,85,85	0
59	MG	CA	3256	1/1	0.88	0.20	65,65,65,65	0
59	MG	CA	3023	1/1	0.88	0.14	68,68,68,68	0
59	MG	CA	3278	1/1	0.88	0.09	58,58,58,58	0
59	MG	CA	3628	1/1	0.88	0.10	54,54,54,54	0
59	MG	CA	3500	1/1	0.88	0.14	75,75,75,75	0
59	MG	CA	3284	1/1	0.88	0.19	75,75,75,75	0
59	MG	AA	3603	1/1	0.88	0.24	76,76,76,76	0
59	MG	AA	3712	1/1	0.88	0.28	70,70,70,70	0
59	MG	AA	3649	1/1	0.88	0.15	62,62,62,62	0
59	MG	CA	3037	1/1	0.88	0.33	57,57,57,57	0
59	MG	AA	3010	1/1	0.88	0.18	46,46,46,46	0
59	MG	CA	3509	1/1	0.88	0.09	83,83,83,83	0
59	MG	CA	3656	1/1	0.88	0.23	63,63,63,63	0
59	MG	AA	3800	1/1	0.88	0.10	35,35,35,35	0
59	MG	CB	3005	1/1	0.88	0.19	63,63,63,63	0
59	MG	CB	3011	1/1	0.88	0.21	56,56,56,56	0
59	MG	AA	3486	1/1	0.88	0.13	67,67,67,67	0
59	MG	CA	3043	1/1	0.88	0.19	61,61,61,61	0
59	MG	AA	3027	1/1	0.88	0.38	75,75,75,75	0
59	MG	AA	3158	1/1	0.88	0.23	68,68,68,68	0
59	MG	AA	3273	1/1	0.88	0.09	90,90,90,90	0
59	MG	BA	1682	1/1	0.88	0.32	70,70,70,70	0
59	MG	BA	1683	1/1	0.88	0.23	71,71,71,71	0
59	MG	DA	1743	1/1	0.88	0.11	59,59,59,59	0
59	MG	CA	3171	1/1	0.88	0.18	56,56,56,56	0
59	MG	BA	1630	1/1	0.88	0.17	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3118	1/1	0.88	0.25	76,76,76,76	0
59	MG	BA	1633	1/1	0.88	0.26	63,63,63,63	0
59	MG	AA	3337	1/1	0.88	0.12	75,75,75,75	0
59	MG	CA	3553	1/1	0.88	0.14	90,90,90,90	0
59	MG	AA	3066	1/1	0.88	0.14	51,51,51,51	0
59	MG	CA	3075	1/1	0.88	0.16	90,90,90,90	0
59	MG	AA	3627	1/1	0.88	0.11	76,76,76,76	0
59	MG	CA	3563	1/1	0.88	0.13	75,75,75,75	0
59	MG	BA	1698	1/1	0.88	0.18	63,63,63,63	0
59	MG	DA	1771	1/1	0.88	0.09	60,60,60,60	0
59	MG	BA	1645	1/1	0.88	0.12	74,74,74,74	0
59	MG	DE	202	1/1	0.88	0.09	100,100,100,100	0
59	MG	AA	3215	1/1	0.88	0.20	59,59,59,59	0
59	MG	CA	3577	1/1	0.88	0.10	51,51,51,51	1
59	MG	CA	3406	1/1	0.88	0.10	77,77,77,77	0
59	MG	AA	3699	1/1	0.88	0.17	71,71,71,71	0
59	MG	CA	3217	1/1	0.88	0.18	62,62,62,62	0
59	MG	CA	3270	1/1	0.89	0.20	76,76,76,76	0
59	MG	DA	1608	1/1	0.89	0.10	57,57,57,57	0
59	MG	CA	3020	1/1	0.89	0.12	47,47,47,47	0
59	MG	AA	3251	1/1	0.89	0.21	56,56,56,56	0
59	MG	AA	3339	1/1	0.89	0.13	49,49,49,49	0
59	MG	CA	3515	1/1	0.89	0.07	54,54,54,54	0
59	MG	CA	3030	1/1	0.89	0.20	59,59,59,59	0
59	MG	CA	3517	1/1	0.89	0.11	62,62,62,62	0
59	MG	BA	1672	1/1	0.89	0.24	65,65,65,65	0
59	MG	CA	3524	1/1	0.89	0.09	52,52,52,52	0
59	MG	CA	3529	1/1	0.89	0.08	68,68,68,68	0
59	MG	CA	3291	1/1	0.89	0.17	48,48,48,48	0
59	MG	BA	1756	1/1	0.89	0.07	85,85,85,85	0
59	MG	BA	1615	1/1	0.89	0.08	62,62,62,62	0
59	MG	DA	1633	1/1	0.89	0.22	55,55,55,55	0
59	MG	CA	3296	1/1	0.89	0.08	79,79,79,79	0
59	MG	CA	3536	1/1	0.89	0.13	84,84,84,84	0
59	MG	CA	3537	1/1	0.89	0.17	59,59,59,59	0
59	MG	AA	3664	1/1	0.89	0.14	62,62,62,62	0
59	MG	AA	3736	1/1	0.89	0.10	59,59,59,59	0
59	MG	CA	3040	1/1	0.89	0.30	79,79,79,79	0
59	MG	AA	3530	1/1	0.89	0.14	20,20,20,20	1
59	MG	AA	3278	1/1	0.89	0.17	60,60,60,60	0
59	MG	AA	3819	1/1	0.89	0.15	35,35,35,35	1
59	MG	CA	3335	1/1	0.89	0.19	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3041	1/1	0.89	0.12	37,37,37,37	0
59	MG	CA	3559	1/1	0.89	0.10	75,75,75,75	0
59	MG	BA	1689	1/1	0.89	0.37	71,71,71,71	0
59	MG	CA	3344	1/1	0.89	0.06	68,68,68,68	0
59	MG	AA	3565	1/1	0.89	0.12	44,44,44,44	0
59	MG	AA	3450	1/1	0.89	0.08	58,58,58,58	0
59	MG	AA	3692	1/1	0.89	0.11	36,36,36,36	1
59	MG	DA	1669	1/1	0.89	0.13	65,65,65,65	0
59	MG	CA	3576	1/1	0.89	0.08	71,71,71,71	0
59	MG	AA	3051	1/1	0.89	0.31	48,48,48,48	0
59	MG	AA	3698	1/1	0.89	0.07	41,41,41,41	0
59	MG	AA	3767	1/1	0.89	0.20	67,67,67,67	0
59	MG	CA	3189	1/1	0.89	0.14	50,50,50,50	0
59	MG	BA	1789	1/1	0.89	0.14	72,72,72,72	0
59	MG	AA	3209	1/1	0.89	0.17	62,62,62,62	0
59	MG	CA	3589	1/1	0.89	0.14	71,71,71,71	0
59	MG	CA	3194	1/1	0.89	0.11	52,52,52,52	0
59	MG	CA	3200	1/1	0.89	0.12	51,51,51,51	0
59	MG	DA	1695	1/1	0.89	0.15	63,63,63,63	0
59	MG	CA	3072	1/1	0.89	0.12	66,66,66,66	0
59	MG	AA	3466	1/1	0.89	0.20	76,76,76,76	0
59	MG	AA	3139	1/1	0.89	0.17	60,60,60,60	0
59	MG	CA	3205	1/1	0.89	0.12	81,81,81,81	0
59	MG	CA	3207	1/1	0.89	0.22	75,75,75,75	0
59	MG	CA	3208	1/1	0.89	0.19	74,74,74,74	0
59	MG	AA	3140	1/1	0.89	0.23	62,62,62,62	0
59	MG	A6	103	1/1	0.89	0.27	72,72,72,72	0
59	MG	CA	3081	1/1	0.89	0.15	63,63,63,63	0
59	MG	CA	3441	1/1	0.89	0.17	56,56,56,56	0
59	MG	AA	3604	1/1	0.89	0.18	81,81,81,81	0
59	MG	BA	1805	1/1	0.89	0.13	71,71,71,71	0
59	MG	CA	3454	1/1	0.89	0.08	81,81,81,81	0
59	MG	BA	1808	1/1	0.89	0.10	54,54,54,54	0
59	MG	CA	3224	1/1	0.89	0.22	59,59,59,59	0
59	MG	BA	1717	1/1	0.89	0.13	78,78,78,78	0
59	MG	CA	3098	1/1	0.89	0.11	70,70,70,70	0
59	MG	AA	3415	1/1	0.89	0.19	62,62,62,62	0
59	MG	CA	3101	1/1	0.89	0.22	84,84,84,84	0
59	MG	CA	3477	1/1	0.89	0.14	69,69,69,69	0
59	MG	CA	3478	1/1	0.89	0.13	65,65,65,65	0
59	MG	AA	3017	1/1	0.89	0.11	61,61,61,61	0
59	MG	CA	3645	1/1	0.89	0.10	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	1603	1/1	0.89	0.20	61,61,61,61	0
59	MG	BA	1609	1/1	0.89	0.08	62,62,62,62	0
59	MG	CA	3486	1/1	0.89	0.13	81,81,81,81	0
59	MG	DA	1752	1/1	0.89	0.20	52,52,52,52	0
59	MG	AA	3786	1/1	0.89	0.09	53,53,53,53	0
59	MG	CA	3490	1/1	0.89	0.09	50,50,50,50	0
59	MG	CB	3003	1/1	0.89	0.09	65,65,65,65	0
59	MG	BN	503	1/1	0.89	0.07	62,62,62,62	0
59	MG	CA	3114	1/1	0.89	0.26	66,66,66,66	0
59	MG	DA	1761	1/1	0.89	0.12	72,72,72,72	0
59	MG	CB	3012	1/1	0.89	0.15	62,62,62,62	0
59	MG	DA	1767	1/1	0.89	0.09	74,74,74,74	0
59	MG	CA	3241	1/1	0.89	0.19	72,72,72,72	0
59	MG	DA	1770	1/1	0.89	0.09	63,63,63,63	0
59	MG	BA	1666	1/1	0.89	0.19	61,61,61,61	0
59	MG	CA	3116	1/1	0.89	0.21	52,52,52,52	0
59	MG	CF	301	1/1	0.89	0.19	61,61,61,61	0
59	MG	CA	3249	1/1	0.89	0.09	61,61,61,61	0
59	MG	BA	1667	1/1	0.89	0.17	74,74,74,74	0
59	MG	CQ	203	1/1	0.89	0.15	54,54,54,54	0
59	MG	BA	1611	1/1	0.89	0.08	31,31,31,31	0
59	MG	CA	3268	1/1	0.89	0.20	52,52,52,52	0
59	MG	CA	3140	1/1	0.90	0.26	63,63,63,63	0
59	MG	CA	3520	1/1	0.90	0.11	73,73,73,73	0
59	MG	DA	1606	1/1	0.90	0.06	85,85,85,85	0
59	MG	CA	3521	1/1	0.90	0.17	74,74,74,74	0
59	MG	CA	3141	1/1	0.90	0.22	68,68,68,68	0
59	MG	CA	3526	1/1	0.90	0.14	58,58,58,58	0
59	MG	CA	3145	1/1	0.90	0.09	76,76,76,76	0
59	MG	AA	3556	1/1	0.90	0.13	66,66,66,66	0
59	MG	AA	3356	1/1	0.90	0.14	80,80,80,80	0
59	MG	AF	308	1/1	0.90	0.13	57,57,57,57	0
59	MG	AA	3765	1/1	0.90	0.15	60,60,60,60	0
59	MG	AR	202	1/1	0.90	0.08	28,28,28,28	0
59	MG	AA	3626	1/1	0.90	0.12	35,35,35,35	0
59	MG	CA	3159	1/1	0.90	0.17	69,69,69,69	0
59	MG	BA	1754	1/1	0.90	0.14	49,49,49,49	0
59	MG	CA	3540	1/1	0.90	0.08	54,54,54,54	0
59	MG	AA	3180	1/1	0.90	0.22	69,69,69,69	0
59	MG	AA	3628	1/1	0.90	0.13	70,70,70,70	0
59	MG	CA	3343	1/1	0.90	0.08	32,32,32,32	0
59	MG	CA	3548	1/1	0.90	0.08	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	A6	101	1/1	0.90	0.16	60,60,60,60	0
59	MG	CA	3176	1/1	0.90	0.26	60,60,60,60	0
59	MG	CA	3354	1/1	0.90	0.12	49,49,49,49	0
59	MG	CA	3558	1/1	0.90	0.09	64,64,64,64	0
59	MG	AA	3772	1/1	0.90	0.27	61,61,61,61	1
59	MG	DA	1646	1/1	0.90	0.08	57,57,57,57	0
59	MG	A7	103	1/1	0.90	0.17	55,55,55,55	0
59	MG	BA	1668	1/1	0.90	0.09	69,69,69,69	0
59	MG	CA	3061	1/1	0.90	0.15	68,68,68,68	0
59	MG	AA	3143	1/1	0.90	0.10	48,48,48,48	0
59	MG	DA	1658	1/1	0.90	0.23	51,51,51,51	0
59	MG	CA	3571	1/1	0.90	0.08	45,45,45,45	0
59	MG	DA	1660	1/1	0.90	0.07	80,80,80,80	0
59	MG	DA	1661	1/1	0.90	0.13	66,66,66,66	0
59	MG	AA	3070	1/1	0.90	0.35	81,81,81,81	0
59	MG	AA	3632	1/1	0.90	0.13	54,54,54,54	0
59	MG	CA	3196	1/1	0.90	0.34	68,68,68,68	0
59	MG	CA	3199	1/1	0.90	0.16	55,55,55,55	0
59	MG	AA	3640	1/1	0.90	0.12	68,68,68,68	0
59	MG	DA	1672	1/1	0.90	0.10	77,77,77,77	0
59	MG	BA	1779	1/1	0.90	0.12	85,85,85,85	0
59	MG	CA	3585	1/1	0.90	0.11	36,36,36,36	1
59	MG	AA	3253	1/1	0.90	0.13	64,64,64,64	0
59	MG	AA	3061	1/1	0.90	0.18	59,59,59,59	0
59	MG	AA	3161	1/1	0.90	0.07	43,43,43,43	0
59	MG	AA	3646	1/1	0.90	0.14	53,53,53,53	0
59	MG	AA	3218	1/1	0.90	0.17	67,67,67,67	0
59	MG	CA	3210	1/1	0.90	0.19	62,62,62,62	0
59	MG	AA	3166	1/1	0.90	0.18	40,40,40,40	0
59	MG	AA	3802	1/1	0.90	0.14	86,86,86,86	0
59	MG	AA	3109	1/1	0.90	0.13	56,56,56,56	0
59	MG	CA	3604	1/1	0.90	0.07	62,62,62,62	0
59	MG	BA	1620	1/1	0.90	0.09	52,52,52,52	0
59	MG	CA	3221	1/1	0.90	0.19	65,65,65,65	0
59	MG	CA	3451	1/1	0.90	0.14	62,62,62,62	0
59	MG	AA	3816	1/1	0.90	0.26	66,66,66,66	0
59	MG	CA	3455	1/1	0.90	0.22	49,49,49,49	0
59	MG	AA	3610	1/1	0.90	0.17	59,59,59,59	0
59	MG	CA	3615	1/1	0.90	0.12	28,28,28,28	0
59	MG	AA	3739	1/1	0.90	0.09	38,38,38,38	0
59	MG	DA	1721	1/1	0.90	0.07	80,80,80,80	0
59	MG	BA	1696	1/1	0.90	0.10	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AB	3003	1/1	0.90	0.16	60,60,60,60	0
59	MG	CA	3229	1/1	0.90	0.12	53,53,53,53	0
59	MG	AB	3004	1/1	0.90	0.25	69,69,69,69	0
59	MG	AA	3035	1/1	0.90	0.09	48,48,48,48	0
59	MG	AA	3541	1/1	0.90	0.10	74,74,74,74	0
59	MG	BA	1706	1/1	0.90	0.10	63,63,63,63	0
59	MG	CA	3113	1/1	0.90	0.16	38,38,38,38	0
59	MG	CA	3636	1/1	0.90	0.10	64,64,64,64	0
59	MG	AA	3615	1/1	0.90	0.17	43,43,43,43	0
59	MG	BA	1708	1/1	0.90	0.08	64,64,64,64	0
59	MG	BA	1711	1/1	0.90	0.10	61,61,61,61	0
59	MG	BA	1640	1/1	0.90	0.18	52,52,52,52	0
59	MG	CA	3242	1/1	0.90	0.24	82,82,82,82	0
59	MG	CA	3118	1/1	0.90	0.14	65,65,65,65	0
59	MG	CA	3119	1/1	0.90	0.32	55,55,55,55	0
59	MG	CA	3654	1/1	0.90	0.20	90,90,90,90	0
59	MG	DA	1751	1/1	0.90	0.12	64,64,64,64	0
59	MG	CA	3247	1/1	0.90	0.16	39,39,39,39	0
59	MG	CA	3660	1/1	0.90	0.22	60,60,60,60	0
59	MG	CA	3120	1/1	0.90	0.17	42,42,42,42	0
59	MG	CB	3002	1/1	0.90	0.08	63,63,63,63	0
59	MG	BA	1643	1/1	0.90	0.18	66,66,66,66	0
59	MG	AA	3203	1/1	0.90	0.07	59,59,59,59	0
59	MG	CA	3257	1/1	0.90	0.11	35,35,35,35	0
59	MG	CA	3264	1/1	0.90	0.16	60,60,60,60	0
59	MG	DA	1765	1/1	0.90	0.07	64,64,64,64	0
59	MG	CA	3003	1/1	0.90	0.23	62,62,62,62	0
59	MG	AD	302	1/1	0.90	0.27	85,85,85,85	0
59	MG	AA	3551	1/1	0.90	0.09	39,39,39,39	0
59	MG	AE	302	1/1	0.90	0.11	57,57,57,57	0
59	MG	CG	3001	1/1	0.90	0.08	65,65,65,65	0
59	MG	CN	5001	1/1	0.90	0.09	65,65,65,65	0
59	MG	CA	3514	1/1	0.90	0.23	64,64,64,64	0
59	MG	BA	1654	1/1	0.90	0.14	76,76,76,76	0
59	MG	BA	1655	1/1	0.90	0.07	59,59,59,59	0
59	MG	DW	502	1/1	0.90	0.08	58,58,58,58	0
59	MG	BA	1726	1/1	0.90	0.10	46,46,46,46	0
59	MG	DA	1601	1/1	0.90	0.16	74,74,74,74	0
60	ZN	C4	501	1/1	0.90	0.07	194,194,194,194	0
59	MG	AA	3783	1/1	0.91	0.26	53,53,53,53	1
59	MG	AA	3184	1/1	0.91	0.16	75,75,75,75	0
59	MG	AA	3160	1/1	0.91	0.08	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3101	1/1	0.91	0.43	68,68,68,68	0
59	MG	BW	502	1/1	0.91	0.13	59,59,59,59	0
59	MG	BA	1700	1/1	0.91	0.22	52,52,52,52	0
59	MG	BA	1703	1/1	0.91	0.18	51,51,51,51	0
59	MG	AA	3794	1/1	0.91	0.19	60,60,60,60	0
59	MG	CA	3150	1/1	0.91	0.15	57,57,57,57	0
59	MG	AA	3165	1/1	0.91	0.14	52,52,52,52	0
59	MG	AA	3440	1/1	0.91	0.10	63,63,63,63	0
59	MG	AA	3635	1/1	0.91	0.07	49,49,49,49	0
59	MG	CA	3024	1/1	0.91	0.19	100,100,100,100	0
59	MG	CA	3348	1/1	0.91	0.14	44,44,44,44	0
59	MG	BA	1624	1/1	0.91	0.10	58,58,58,58	0
59	MG	AA	3803	1/1	0.91	0.15	45,45,45,45	0
59	MG	DA	1637	1/1	0.91	0.18	68,68,68,68	0
59	MG	AA	3810	1/1	0.91	0.23	67,67,67,67	0
59	MG	AA	3102	1/1	0.91	0.24	47,47,47,47	0
59	MG	CA	3366	1/1	0.91	0.15	49,49,49,49	0
59	MG	AA	3447	1/1	0.91	0.11	56,56,56,56	0
59	MG	DA	1642	1/1	0.91	0.10	62,62,62,62	0
59	MG	CA	3368	1/1	0.91	0.12	44,44,44,44	0
59	MG	AA	3716	1/1	0.91	0.15	66,66,66,66	0
59	MG	CA	3182	1/1	0.91	0.17	38,38,38,38	0
59	MG	CA	3572	1/1	0.91	0.19	70,70,70,70	0
59	MG	AA	3224	1/1	0.91	0.20	56,56,56,56	0
59	MG	CA	3380	1/1	0.91	0.15	59,59,59,59	0
59	MG	BA	1635	1/1	0.91	0.34	65,65,65,65	0
59	MG	DA	1656	1/1	0.91	0.14	63,63,63,63	0
59	MG	AA	3451	1/1	0.91	0.14	57,57,57,57	0
59	MG	AA	3722	1/1	0.91	0.12	37,37,37,37	0
59	MG	AA	3724	1/1	0.91	0.11	47,47,47,47	0
59	MG	CA	3046	1/1	0.91	0.15	68,68,68,68	0
59	MG	AA	3135	1/1	0.91	0.14	55,55,55,55	0
59	MG	AA	3153	1/1	0.91	0.17	59,59,59,59	0
59	MG	AA	3240	1/1	0.91	0.15	69,69,69,69	0
59	MG	DA	1667	1/1	0.91	0.08	66,66,66,66	0
59	MG	CA	3412	1/1	0.91	0.13	59,59,59,59	0
59	MG	CA	3593	1/1	0.91	0.21	61,61,61,61	0
59	MG	AA	3652	1/1	0.91	0.10	53,53,53,53	0
59	MG	CA	3059	1/1	0.91	0.13	58,58,58,58	0
59	MG	AD	307	1/1	0.91	0.21	86,86,86,86	0
59	MG	CA	3431	1/1	0.91	0.13	75,75,75,75	0
59	MG	BA	1749	1/1	0.91	0.12	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3742	1/1	0.91	0.16	68,68,68,68	0
59	MG	CA	3435	1/1	0.91	0.07	55,55,55,55	0
59	MG	CA	3436	1/1	0.91	0.14	64,64,64,64	0
59	MG	AA	3467	1/1	0.91	0.14	49,49,49,49	0
59	MG	AA	3657	1/1	0.91	0.10	63,63,63,63	0
59	MG	AF	302	1/1	0.91	0.14	47,47,47,47	0
59	MG	BA	1759	1/1	0.91	0.17	63,63,63,63	0
59	MG	BA	1763	1/1	0.91	0.12	76,76,76,76	0
59	MG	DA	1700	1/1	0.91	0.13	61,61,61,61	0
59	MG	DA	1703	1/1	0.91	0.10	89,89,89,89	0
59	MG	CA	3616	1/1	0.91	0.23	74,74,74,74	0
59	MG	DA	1705	1/1	0.91	0.10	68,68,68,68	0
59	MG	AA	3468	1/1	0.91	0.07	55,55,55,55	0
59	MG	AA	3174	1/1	0.91	0.22	59,59,59,59	0
59	MG	BA	1661	1/1	0.91	0.25	63,63,63,63	0
59	MG	AA	3363	1/1	0.91	0.10	82,82,82,82	0
59	MG	AN	3003	1/1	0.91	0.07	55,55,55,55	0
59	MG	AP	204	1/1	0.91	0.08	59,59,59,59	0
59	MG	CA	3092	1/1	0.91	0.37	79,79,79,79	0
59	MG	CA	3630	1/1	0.91	0.10	65,65,65,65	0
59	MG	CA	3228	1/1	0.91	0.28	59,59,59,59	0
59	MG	AQ	203	1/1	0.91	0.10	32,32,32,32	0
59	MG	CA	3635	1/1	0.91	0.10	48,48,48,48	0
59	MG	DA	1728	1/1	0.91	0.10	71,71,71,71	0
59	MG	CA	3095	1/1	0.91	0.15	58,58,58,58	0
59	MG	AA	3485	1/1	0.91	0.07	48,48,48,48	0
59	MG	CA	3483	1/1	0.91	0.15	64,64,64,64	0
59	MG	AX	3001	1/1	0.91	0.12	52,52,52,52	0
59	MG	AY	502	1/1	0.91	0.19	60,60,60,60	0
59	MG	AA	3763	1/1	0.91	0.10	47,47,47,47	0
59	MG	AA	3106	1/1	0.91	0.09	33,33,33,33	0
59	MG	CA	3106	1/1	0.91	0.18	66,66,66,66	0
59	MG	A0	105	1/1	0.91	0.06	30,30,30,30	0
59	MG	CA	3495	1/1	0.91	0.14	70,70,70,70	0
59	MG	AA	3012	1/1	0.91	0.15	49,49,49,49	0
59	MG	CA	3663	1/1	0.91	0.12	64,64,64,64	0
59	MG	AA	3289	1/1	0.91	0.12	53,53,53,53	0
59	MG	AA	3496	1/1	0.91	0.18	31,31,31,31	0
59	MG	CA	3245	1/1	0.91	0.25	62,62,62,62	0
59	MG	BA	1791	1/1	0.91	0.11	72,72,72,72	0
59	MG	CB	3007	1/1	0.91	0.16	52,52,52,52	0
59	MG	AA	3683	1/1	0.91	0.12	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	1678	1/1	0.91	0.13	54,54,54,54	0
59	MG	AA	3687	1/1	0.91	0.20	52,52,52,52	0
59	MG	CD	302	1/1	0.91	0.21	56,56,56,56	0
59	MG	DA	1758	1/1	0.91	0.15	75,75,75,75	0
59	MG	DA	1759	1/1	0.91	0.08	53,53,53,53	0
59	MG	AA	3508	1/1	0.91	0.15	43,43,43,43	0
59	MG	BA	1802	1/1	0.91	0.17	76,76,76,76	0
59	MG	AA	3693	1/1	0.91	0.17	69,69,69,69	0
59	MG	AA	3414	1/1	0.91	0.06	37,37,37,37	0
59	MG	BA	1604	1/1	0.91	0.16	63,63,63,63	0
59	MG	CP	201	1/1	0.91	0.09	62,62,62,62	1
59	MG	BA	1605	1/1	0.91	0.13	73,73,73,73	0
59	MG	BA	1606	1/1	0.91	0.22	126,126,126,126	0
59	MG	AA	3290	1/1	0.91	0.09	64,64,64,64	0
59	MG	BA	1814	1/1	0.91	0.10	69,69,69,69	0
59	MG	CA	3130	1/1	0.91	0.07	55,55,55,55	0
59	MG	DA	1602	1/1	0.91	0.08	45,45,45,45	0
59	MG	AA	3782	1/1	0.91	0.09	44,44,44,44	0
59	MG	CA	3293	1/1	0.91	0.12	60,60,60,60	0
59	MG	BD	502	1/1	0.91	0.24	64,64,64,64	0
59	MG	DA	1607	1/1	0.91	0.08	86,86,86,86	0
59	MG	CA	3086	1/1	0.92	0.38	85,85,85,85	0
59	MG	CA	3087	1/1	0.92	0.36	68,68,68,68	0
59	MG	CA	3503	1/1	0.92	0.19	52,52,52,52	0
59	MG	CA	3088	1/1	0.92	0.18	67,67,67,67	0
59	MG	CX	5001	1/1	0.92	0.11	65,65,65,65	0
59	MG	BA	1771	1/1	0.92	0.11	65,65,65,65	0
59	MG	AP	203	1/1	0.92	0.09	44,44,44,44	0
59	MG	CA	3243	1/1	0.92	0.12	58,58,58,58	0
59	MG	AA	3280	1/1	0.92	0.12	53,53,53,53	0
59	MG	CA	3094	1/1	0.92	0.13	59,59,59,59	0
59	MG	AA	3175	1/1	0.92	0.26	63,63,63,63	0
59	MG	AR	201	1/1	0.92	0.14	63,63,63,63	0
59	MG	AA	3695	1/1	0.92	0.10	67,67,67,67	0
59	MG	AW	3002	1/1	0.92	0.12	47,47,47,47	0
59	MG	AA	3371	1/1	0.92	0.09	53,53,53,53	0
59	MG	AA	3375	1/1	0.92	0.17	48,48,48,48	0
59	MG	AA	3378	1/1	0.92	0.19	56,56,56,56	0
59	MG	DA	1619	1/1	0.92	0.17	59,59,59,59	0
59	MG	AA	3701	1/1	0.92	0.14	81,81,81,81	0
59	MG	A0	102	1/1	0.92	0.07	56,56,56,56	0
59	MG	AA	3283	1/1	0.92	0.25	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	DA	1625	1/1	0.92	0.09	50,50,50,50	0
59	MG	CA	3274	1/1	0.92	0.14	52,52,52,52	0
59	MG	DA	1627	1/1	0.92	0.05	77,77,77,77	0
59	MG	CA	3276	1/1	0.92	0.08	44,44,44,44	0
59	MG	AA	3785	1/1	0.92	0.10	61,61,61,61	0
59	MG	CA	3280	1/1	0.92	0.07	48,48,48,48	0
59	MG	AA	3285	1/1	0.92	0.22	51,51,51,51	0
59	MG	CA	3287	1/1	0.92	0.13	45,45,45,45	0
59	MG	AA	3286	1/1	0.92	0.29	40,40,40,40	0
59	MG	DA	1636	1/1	0.92	0.24	62,62,62,62	0
59	MG	AA	3019	1/1	0.92	0.16	70,70,70,70	0
59	MG	BA	1793	1/1	0.92	0.09	65,65,65,65	0
59	MG	AA	3249	1/1	0.92	0.17	59,59,59,59	0
59	MG	BA	1796	1/1	0.92	0.16	57,57,57,57	0
59	MG	AA	3636	1/1	0.92	0.13	86,86,86,86	0
59	MG	BA	1798	1/1	0.92	0.11	73,73,73,73	0
59	MG	CA	3547	1/1	0.92	0.12	69,69,69,69	0
59	MG	AA	3544	1/1	0.92	0.09	26,26,26,26	0
59	MG	DA	1645	1/1	0.92	0.07	58,58,58,58	0
59	MG	CA	3551	1/1	0.92	0.09	63,63,63,63	0
59	MG	BA	1801	1/1	0.92	0.07	65,65,65,65	0
59	MG	AA	3550	1/1	0.92	0.10	38,38,38,38	0
59	MG	AA	3718	1/1	0.92	0.14	42,42,42,42	0
59	MG	CA	3128	1/1	0.92	0.18	50,50,50,50	0
59	MG	CA	3325	1/1	0.92	0.08	38,38,38,38	0
59	MG	BA	1684	1/1	0.92	0.18	61,61,61,61	0
59	MG	AA	3804	1/1	0.92	0.07	50,50,50,50	0
59	MG	AA	3250	1/1	0.92	0.15	123,123,123,123	0
59	MG	BA	1607	1/1	0.92	0.08	64,64,64,64	0
59	MG	BA	1608	1/1	0.92	0.25	57,57,57,57	0
59	MG	AA	3293	1/1	0.92	0.07	27,27,27,27	0
59	MG	AA	3208	1/1	0.92	0.29	54,54,54,54	0
59	MG	DA	1666	1/1	0.92	0.19	53,53,53,53	0
59	MG	CA	3575	1/1	0.92	0.09	71,71,71,71	0
59	MG	AA	3313	1/1	0.92	0.13	39,39,39,39	0
59	MG	CA	3352	1/1	0.92	0.10	79,79,79,79	0
59	MG	DA	1670	1/1	0.92	0.10	49,49,49,49	0
59	MG	DA	1671	1/1	0.92	0.21	56,56,56,56	0
59	MG	AA	3818	1/1	0.92	0.12	61,61,61,61	0
59	MG	AA	3577	1/1	0.92	0.07	42,42,42,42	0
59	MG	CA	3147	1/1	0.92	0.13	55,55,55,55	0
59	MG	BL	202	1/1	0.92	0.10	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AB	3002	1/1	0.92	0.13	52,52,52,52	0
59	MG	AA	3252	1/1	0.92	0.09	44,44,44,44	0
59	MG	BA	1617	1/1	0.92	0.12	118,118,118,118	0
59	MG	BW	503	1/1	0.92	0.21	60,60,60,60	0
59	MG	DA	1684	1/1	0.92	0.12	69,69,69,69	0
59	MG	DA	1688	1/1	0.92	0.13	51,51,51,51	0
59	MG	AA	3448	1/1	0.92	0.07	62,62,62,62	0
59	MG	AB	3006	1/1	0.92	0.11	57,57,57,57	0
59	MG	AB	3009	1/1	0.92	0.07	50,50,50,50	0
59	MG	CA	3015	1/1	0.92	0.15	51,51,51,51	0
59	MG	AA	3225	1/1	0.92	0.18	73,73,73,73	0
59	MG	CA	3600	1/1	0.92	0.13	86,86,86,86	0
59	MG	DA	1701	1/1	0.92	0.14	68,68,68,68	0
59	MG	CA	3394	1/1	0.92	0.17	69,69,69,69	0
59	MG	AB	3018	1/1	0.92	0.09	69,69,69,69	0
59	MG	BA	1627	1/1	0.92	0.07	51,51,51,51	0
59	MG	DA	1706	1/1	0.92	0.14	66,66,66,66	0
59	MG	AA	3596	1/1	0.92	0.12	65,65,65,65	0
59	MG	AA	3752	1/1	0.92	0.10	42,42,42,42	0
59	MG	CA	3031	1/1	0.92	0.20	68,68,68,68	0
59	MG	AA	3229	1/1	0.92	0.27	67,67,67,67	0
59	MG	CA	3413	1/1	0.92	0.10	39,39,39,39	0
59	MG	CA	3033	1/1	0.92	0.22	55,55,55,55	0
59	MG	CA	3419	1/1	0.92	0.08	59,59,59,59	0
59	MG	BA	1632	1/1	0.92	0.09	48,48,48,48	0
59	MG	CA	3421	1/1	0.92	0.15	57,57,57,57	0
59	MG	AA	3231	1/1	0.92	0.15	64,64,64,64	0
59	MG	DA	1725	1/1	0.92	0.12	58,58,58,58	0
59	MG	CA	3430	1/1	0.92	0.19	41,41,41,41	0
59	MG	BA	1720	1/1	0.92	0.09	61,61,61,61	0
59	MG	AD	303	1/1	0.92	0.25	58,58,58,58	0
59	MG	CA	3198	1/1	0.92	0.11	34,34,34,34	0
59	MG	AD	305	1/1	0.92	0.11	50,50,50,50	0
59	MG	CA	3631	1/1	0.92	0.10	65,65,65,65	0
59	MG	AA	3150	1/1	0.92	0.20	45,45,45,45	0
59	MG	BA	1639	1/1	0.92	0.23	61,61,61,61	0
59	MG	BA	1729	1/1	0.92	0.11	53,53,53,53	0
59	MG	BA	1730	1/1	0.92	0.11	53,53,53,53	0
59	MG	DA	1741	1/1	0.92	0.21	67,67,67,67	0
59	MG	CA	3637	1/1	0.92	0.39	61,61,61,61	0
59	MG	CA	3447	1/1	0.92	0.13	73,73,73,73	0
59	MG	CA	3639	1/1	0.92	0.23	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	1732	1/1	0.92	0.07	70,70,70,70	0
59	MG	AA	3057	1/1	0.92	0.11	46,46,46,46	0
59	MG	BA	1737	1/1	0.92	0.24	79,79,79,79	0
59	MG	CA	3051	1/1	0.92	0.23	57,57,57,57	0
59	MG	AE	301	1/1	0.92	0.10	69,69,69,69	0
59	MG	CA	3213	1/1	0.92	0.19	51,51,51,51	0
59	MG	CA	3652	1/1	0.92	0.07	23,23,23,23	0
59	MG	AA	3237	1/1	0.92	0.17	76,76,76,76	0
59	MG	AA	3238	1/1	0.92	0.17	76,76,76,76	0
59	MG	BA	1747	1/1	0.92	0.09	65,65,65,65	0
59	MG	CA	3662	1/1	0.92	0.14	33,33,33,33	0
59	MG	AA	3474	1/1	0.92	0.06	18,18,18,18	1
59	MG	BA	1647	1/1	0.92	0.26	57,57,57,57	0
59	MG	BA	1752	1/1	0.92	0.16	59,59,59,59	0
59	MG	DA	1763	1/1	0.92	0.10	76,76,76,76	0
59	MG	AF	304	1/1	0.92	0.18	41,41,41,41	0
59	MG	BA	1651	1/1	0.92	0.16	55,55,55,55	0
59	MG	CA	3484	1/1	0.92	0.11	78,78,78,78	0
59	MG	CB	3008	1/1	0.92	0.14	66,66,66,66	0
59	MG	BA	1652	1/1	0.92	0.09	59,59,59,59	0
59	MG	AA	3199	1/1	0.92	0.14	41,41,41,41	0
59	MG	AA	3768	1/1	0.92	0.07	58,58,58,58	0
59	MG	CA	3077	1/1	0.92	0.12	42,42,42,42	0
59	MG	CA	3231	1/1	0.92	0.23	60,60,60,60	0
59	MG	CA	3493	1/1	0.92	0.17	65,65,65,65	0
59	MG	BA	1762	1/1	0.92	0.08	74,74,74,74	0
59	MG	AA	3361	1/1	0.92	0.16	53,53,53,53	0
59	MG	AN	3001	1/1	0.92	0.13	58,58,58,58	0
59	MG	DZ	702	1/1	0.92	0.13	57,57,57,57	0
59	MG	AA	3065	1/1	0.92	0.22	62,62,62,62	0
59	MG	BK	201	1/1	0.93	0.10	44,44,44,44	0
59	MG	AB	3008	1/1	0.93	0.17	52,52,52,52	0
59	MG	BA	1712	1/1	0.93	0.34	57,57,57,57	0
59	MG	AA	3492	1/1	0.93	0.08	26,26,26,26	0
59	MG	AA	3374	1/1	0.93	0.14	49,49,49,49	0
59	MG	AA	3080	1/1	0.93	0.32	61,61,61,61	0
59	MG	AA	3086	1/1	0.93	0.12	55,55,55,55	0
59	MG	DA	1616	1/1	0.93	0.19	51,51,51,51	0
59	MG	BZ	701	1/1	0.93	0.11	49,49,49,49	0
59	MG	AA	3499	1/1	0.93	0.07	48,48,48,48	0
59	MG	DA	1620	1/1	0.93	0.17	57,57,57,57	0
59	MG	CA	3310	1/1	0.93	0.09	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3313	1/1	0.93	0.18	38,38,38,38	0
59	MG	CA	3137	1/1	0.93	0.15	69,69,69,69	0
59	MG	CA	3319	1/1	0.93	0.08	65,65,65,65	0
59	MG	CA	3543	1/1	0.93	0.09	71,71,71,71	0
59	MG	AB	3023	1/1	0.93	0.19	54,54,54,54	0
59	MG	CA	3005	1/1	0.93	0.12	48,48,48,48	0
59	MG	CA	3331	1/1	0.93	0.12	52,52,52,52	0
59	MG	AA	3088	1/1	0.93	0.14	39,39,39,39	0
59	MG	CA	3549	1/1	0.93	0.11	70,70,70,70	0
59	MG	CA	3011	1/1	0.93	0.15	63,63,63,63	0
59	MG	CA	3336	1/1	0.93	0.10	64,64,64,64	0
59	MG	CA	3554	1/1	0.93	0.08	66,66,66,66	0
59	MG	AA	3732	1/1	0.93	0.15	70,70,70,70	0
59	MG	CA	3016	1/1	0.93	0.17	52,52,52,52	0
59	MG	AA	3633	1/1	0.93	0.12	48,48,48,48	0
59	MG	BA	1725	1/1	0.93	0.07	54,54,54,54	0
59	MG	BA	1637	1/1	0.93	0.23	72,72,72,72	0
59	MG	AA	3258	1/1	0.93	0.16	68,68,68,68	0
59	MG	CA	3026	1/1	0.93	0.12	32,32,32,32	1
59	MG	CA	3028	1/1	0.93	0.20	51,51,51,51	0
59	MG	CA	3569	1/1	0.93	0.09	41,41,41,41	0
59	MG	AA	3520	1/1	0.93	0.08	17,17,17,17	0
59	MG	DA	1647	1/1	0.93	0.15	51,51,51,51	0
59	MG	AA	3298	1/1	0.93	0.09	58,58,58,58	0
59	MG	DA	1650	1/1	0.93	0.16	50,50,50,50	0
59	MG	BA	1641	1/1	0.93	0.12	54,54,54,54	0
59	MG	CA	3166	1/1	0.93	0.16	27,27,27,27	0
59	MG	BA	1642	1/1	0.93	0.11	60,60,60,60	0
59	MG	CA	3373	1/1	0.93	0.18	58,58,58,58	0
59	MG	CA	3375	1/1	0.93	0.16	68,68,68,68	0
59	MG	AD	309	1/1	0.93	0.10	56,56,56,56	0
59	MG	AA	3641	1/1	0.93	0.10	51,51,51,51	0
59	MG	CA	3177	1/1	0.93	0.12	29,29,29,29	0
59	MG	CA	3178	1/1	0.93	0.10	54,54,54,54	0
59	MG	AA	3746	1/1	0.93	0.14	73,73,73,73	0
59	MG	DA	1664	1/1	0.93	0.05	66,66,66,66	0
59	MG	BA	1742	1/1	0.93	0.09	48,48,48,48	0
59	MG	CA	3590	1/1	0.93	0.11	59,59,59,59	0
59	MG	CA	3390	1/1	0.93	0.06	80,80,80,80	0
59	MG	AA	3300	1/1	0.93	0.09	22,22,22,22	0
59	MG	BA	1745	1/1	0.93	0.05	46,46,46,46	0
59	MG	CA	3188	1/1	0.93	0.14	94,94,94,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3751	1/1	0.93	0.24	61,61,61,61	0
59	MG	CA	3402	1/1	0.93	0.10	66,66,66,66	0
59	MG	AA	3420	1/1	0.93	0.07	25,25,25,25	1
59	MG	CA	3602	1/1	0.93	0.09	84,84,84,84	0
59	MG	AA	3307	1/1	0.93	0.17	61,61,61,61	0
59	MG	AA	3026	1/1	0.93	0.07	47,47,47,47	0
59	MG	AA	3196	1/1	0.93	0.16	55,55,55,55	0
59	MG	CA	3048	1/1	0.93	0.05	47,47,47,47	0
59	MG	AA	3067	1/1	0.93	0.21	61,61,61,61	0
59	MG	CA	3609	1/1	0.93	0.10	52,52,52,52	0
59	MG	AA	3555	1/1	0.93	0.07	45,45,45,45	0
59	MG	DA	1689	1/1	0.93	0.08	56,56,56,56	0
59	MG	CA	3201	1/1	0.93	0.21	45,45,45,45	0
59	MG	CA	3054	1/1	0.93	0.15	36,36,36,36	0
59	MG	CA	3426	1/1	0.93	0.15	38,38,38,38	0
59	MG	AA	3322	1/1	0.93	0.14	61,61,61,61	0
59	MG	AA	3655	1/1	0.93	0.12	55,55,55,55	0
59	MG	DA	1699	1/1	0.93	0.11	74,74,74,74	0
59	MG	AQ	201	1/1	0.93	0.12	48,48,48,48	0
59	MG	AA	3558	1/1	0.93	0.07	48,48,48,48	0
59	MG	CA	3062	1/1	0.93	0.13	38,38,38,38	0
59	MG	CA	3623	1/1	0.93	0.09	64,64,64,64	0
59	MG	CA	3209	1/1	0.93	0.14	73,73,73,73	0
59	MG	AA	3563	1/1	0.93	0.12	34,34,34,34	0
59	MG	DA	1707	1/1	0.93	0.11	61,61,61,61	0
59	MG	AA	3446	1/1	0.93	0.17	59,59,59,59	0
59	MG	AV	201	1/1	0.93	0.13	38,38,38,38	0
59	MG	CA	3068	1/1	0.93	0.31	66,66,66,66	0
59	MG	AA	3050	1/1	0.93	0.14	28,28,28,28	0
59	MG	DA	1714	1/1	0.93	0.08	68,68,68,68	0
59	MG	AA	3329	1/1	0.93	0.07	40,40,40,40	1
59	MG	AA	3234	1/1	0.93	0.19	36,36,36,36	0
59	MG	CA	3073	1/1	0.93	0.10	49,49,49,49	0
59	MG	DA	1719	1/1	0.93	0.18	61,61,61,61	0
59	MG	AZ	301	1/1	0.93	0.14	86,86,86,86	0
59	MG	AA	3148	1/1	0.93	0.24	29,29,29,29	1
59	MG	AA	3127	1/1	0.93	0.15	57,57,57,57	0
59	MG	CA	3642	1/1	0.93	0.21	52,52,52,52	0
59	MG	DA	1726	1/1	0.93	0.14	60,60,60,60	0
59	MG	AA	3593	1/1	0.93	0.20	15,15,15,15	1
59	MG	AA	3682	1/1	0.93	0.09	31,31,31,31	0
59	MG	CA	3472	1/1	0.93	0.23	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3455	1/1	0.93	0.14	32,32,32,32	1
59	MG	AA	3684	1/1	0.93	0.13	51,51,51,51	0
59	MG	DA	1734	1/1	0.93	0.05	65,65,65,65	0
59	MG	DA	1735	1/1	0.93	0.07	73,73,73,73	0
59	MG	AA	3461	1/1	0.93	0.12	62,62,62,62	0
59	MG	AA	3688	1/1	0.93	0.10	25,25,25,25	0
59	MG	AA	3346	1/1	0.93	0.18	59,59,59,59	0
59	MG	AA	3791	1/1	0.93	0.14	51,51,51,51	0
59	MG	CA	3659	1/1	0.93	0.07	55,55,55,55	0
59	MG	AA	3177	1/1	0.93	0.15	59,59,59,59	0
59	MG	AA	3606	1/1	0.93	0.09	34,34,34,34	0
59	MG	AA	3179	1/1	0.93	0.16	45,45,45,45	1
59	MG	BA	1794	1/1	0.93	0.06	38,38,38,38	0
59	MG	AA	3028	1/1	0.93	0.10	39,39,39,39	0
59	MG	AA	3471	1/1	0.93	0.08	56,56,56,56	0
59	MG	CB	3004	1/1	0.93	0.10	55,55,55,55	0
59	MG	AA	3473	1/1	0.93	0.07	53,53,53,53	0
59	MG	AA	3282	1/1	0.93	0.13	33,33,33,33	0
59	MG	AA	3703	1/1	0.93	0.15	56,56,56,56	0
59	MG	AA	3704	1/1	0.93	0.09	49,49,49,49	0
59	MG	AA	3210	1/1	0.93	0.18	59,59,59,59	1
59	MG	AA	3079	1/1	0.93	0.08	27,27,27,27	0
59	MG	CD	301	1/1	0.93	0.13	43,43,43,43	0
59	MG	CA	3253	1/1	0.93	0.10	70,70,70,70	0
59	MG	CA	3110	1/1	0.93	0.12	56,56,56,56	0
59	MG	CE	304	1/1	0.93	0.16	75,75,75,75	0
59	MG	BA	1613	1/1	0.93	0.06	76,76,76,76	0
59	MG	BA	1807	1/1	0.93	0.12	61,61,61,61	0
59	MG	AA	3618	1/1	0.93	0.10	72,72,72,72	0
59	MG	AA	3710	1/1	0.93	0.21	29,29,29,29	1
59	MG	AB	3001	1/1	0.93	0.16	74,74,74,74	0
59	MG	AA	3134	1/1	0.93	0.13	62,62,62,62	0
59	MG	BA	1705	1/1	0.93	0.14	53,53,53,53	0
59	MG	BA	1815	1/1	0.93	0.18	53,53,53,53	0
59	MG	AA	3185	1/1	0.93	0.17	76,76,76,76	0
59	MG	CV	201	1/1	0.93	0.18	117,117,117,117	0
59	MG	AA	3714	1/1	0.93	0.14	70,70,70,70	0
59	MG	C5	101	1/1	0.93	0.21	66,66,66,66	0
59	MG	CA	3121	1/1	0.93	0.07	49,49,49,49	0
59	MG	CA	3285	1/1	0.93	0.09	63,63,63,63	0
59	MG	DA	1603	1/1	0.93	0.08	72,72,72,72	0
59	MG	CA	3122	1/1	0.93	0.15	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3490	1/1	0.93	0.12	27,27,27,27	0
62	GDP	DZ	703	28/28	0.93	0.08	66,66,66,66	1
59	MG	AA	3226	1/1	0.94	0.11	46,46,46,46	0
59	MG	CA	3550	1/1	0.94	0.07	62,62,62,62	1
59	MG	CA	3360	1/1	0.94	0.09	38,38,38,38	0
59	MG	AA	3002	1/1	0.94	0.13	57,57,57,57	0
59	MG	CA	3365	1/1	0.94	0.07	55,55,55,55	0
59	MG	CA	3183	1/1	0.94	0.08	49,49,49,49	0
59	MG	CA	3556	1/1	0.94	0.13	62,62,62,62	0
59	MG	AA	3325	1/1	0.94	0.11	70,70,70,70	0
59	MG	CA	3185	1/1	0.94	0.12	48,48,48,48	0
59	MG	DA	1630	1/1	0.94	0.28	62,62,62,62	0
59	MG	CA	3370	1/1	0.94	0.07	41,41,41,41	0
59	MG	AA	3443	1/1	0.94	0.09	33,33,33,33	0
59	MG	CA	3561	1/1	0.94	0.08	41,41,41,41	1
59	MG	AA	3444	1/1	0.94	0.12	66,66,66,66	0
59	MG	AA	3445	1/1	0.94	0.07	23,23,23,23	0
59	MG	AA	3743	1/1	0.94	0.16	67,67,67,67	0
59	MG	AD	311	1/1	0.94	0.13	37,37,37,37	0
59	MG	AA	3645	1/1	0.94	0.11	58,58,58,58	0
59	MG	AA	3142	1/1	0.94	0.14	64,64,64,64	0
59	MG	CA	3056	1/1	0.94	0.08	63,63,63,63	0
59	MG	AE	304	1/1	0.94	0.08	52,52,52,52	0
59	MG	CA	3391	1/1	0.94	0.12	51,51,51,51	0
59	MG	AA	3748	1/1	0.94	0.08	45,45,45,45	0
59	MG	AA	3162	1/1	0.94	0.21	67,67,67,67	0
59	MG	AA	3204	1/1	0.94	0.14	54,54,54,54	0
59	MG	CA	3582	1/1	0.94	0.08	99,99,99,99	0
59	MG	CA	3396	1/1	0.94	0.06	39,39,39,39	0
59	MG	AA	3753	1/1	0.94	0.08	30,30,30,30	0
59	MG	CA	3399	1/1	0.94	0.07	57,57,57,57	0
59	MG	DA	1651	1/1	0.94	0.10	63,63,63,63	0
59	MG	AA	3559	1/1	0.94	0.09	46,46,46,46	0
59	MG	AG	201	1/1	0.94	0.07	38,38,38,38	0
59	MG	BA	1770	1/1	0.94	0.06	54,54,54,54	0
59	MG	CA	3409	1/1	0.94	0.14	42,42,42,42	0
59	MG	AA	3562	1/1	0.94	0.08	56,56,56,56	0
59	MG	AA	3205	1/1	0.94	0.10	42,42,42,42	0
59	MG	AA	3025	1/1	0.94	0.12	68,68,68,68	0
59	MG	AA	3760	1/1	0.94	0.14	55,55,55,55	0
59	MG	CA	3417	1/1	0.94	0.10	56,56,56,56	0
59	MG	CA	3599	1/1	0.94	0.07	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3207	1/1	0.94	0.14	60,60,60,60	0
59	MG	AA	3575	1/1	0.94	0.09	35,35,35,35	0
59	MG	AA	3352	1/1	0.94	0.17	47,47,47,47	0
59	MG	AA	3667	1/1	0.94	0.12	41,41,41,41	0
59	MG	AA	3669	1/1	0.94	0.10	81,81,81,81	0
59	MG	AA	3670	1/1	0.94	0.08	54,54,54,54	0
59	MG	AV	206	1/1	0.94	0.09	33,33,33,33	0
59	MG	AW	3001	1/1	0.94	0.22	54,54,54,54	0
59	MG	AA	3456	1/1	0.94	0.09	56,56,56,56	0
59	MG	CA	3611	1/1	0.94	0.10	59,59,59,59	0
59	MG	CA	3434	1/1	0.94	0.09	32,32,32,32	0
59	MG	AA	3145	1/1	0.94	0.11	44,44,44,44	0
59	MG	AA	3584	1/1	0.94	0.06	17,17,17,17	0
59	MG	AA	3046	1/1	0.94	0.11	35,35,35,35	0
59	MG	AA	3187	1/1	0.94	0.28	56,56,56,56	0
59	MG	AA	3594	1/1	0.94	0.10	56,56,56,56	0
59	MG	CA	3232	1/1	0.94	0.21	54,54,54,54	0
59	MG	DA	1685	1/1	0.94	0.07	46,46,46,46	0
59	MG	AA	3362	1/1	0.94	0.07	46,46,46,46	0
59	MG	AA	3599	1/1	0.94	0.07	59,59,59,59	0
59	MG	AA	3686	1/1	0.94	0.13	61,61,61,61	0
59	MG	CA	3625	1/1	0.94	0.13	64,64,64,64	0
59	MG	CA	3099	1/1	0.94	0.19	58,58,58,58	0
59	MG	BA	1681	1/1	0.94	0.06	53,53,53,53	0
59	MG	CA	3464	1/1	0.94	0.08	36,36,36,36	0
59	MG	A5	502	1/1	0.94	0.11	51,51,51,51	0
59	MG	CA	3632	1/1	0.94	0.10	74,74,74,74	0
59	MG	AA	3244	1/1	0.94	0.20	52,52,52,52	0
59	MG	CA	3469	1/1	0.94	0.14	61,61,61,61	0
59	MG	AA	3602	1/1	0.94	0.11	51,51,51,51	0
59	MG	BA	1685	1/1	0.94	0.08	50,50,50,50	0
59	MG	A7	102	1/1	0.94	0.12	37,37,37,37	0
59	MG	BA	1688	1/1	0.94	0.19	61,61,61,61	0
59	MG	AA	3287	1/1	0.94	0.22	43,43,43,43	0
59	MG	AA	3211	1/1	0.94	0.11	56,56,56,56	0
59	MG	BA	1692	1/1	0.94	0.19	55,55,55,55	0
59	MG	AA	3370	1/1	0.94	0.08	47,47,47,47	0
59	MG	CA	3251	1/1	0.94	0.13	82,82,82,82	0
59	MG	AA	3479	1/1	0.94	0.07	55,55,55,55	0
59	MG	BA	1813	1/1	0.94	0.10	55,55,55,55	0
59	MG	CA	3487	1/1	0.94	0.16	60,60,60,60	0
59	MG	CA	3651	1/1	0.94	0.29	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3099	1/1	0.94	0.16	53,53,53,53	0
59	MG	AA	3609	1/1	0.94	0.07	58,58,58,58	0
59	MG	AA	3193	1/1	0.94	0.21	40,40,40,40	0
59	MG	CA	3658	1/1	0.94	0.17	64,64,64,64	0
59	MG	AA	3073	1/1	0.94	0.06	31,31,31,31	0
59	MG	CA	3269	1/1	0.94	0.18	81,81,81,81	0
59	MG	AA	3090	1/1	0.94	0.12	53,53,53,53	0
59	MG	CA	3498	1/1	0.94	0.07	49,49,49,49	0
59	MG	AA	3805	1/1	0.94	0.12	58,58,58,58	0
59	MG	AA	3808	1/1	0.94	0.13	72,72,72,72	0
59	MG	AA	3381	1/1	0.94	0.06	16,16,16,16	0
59	MG	AA	3813	1/1	0.94	0.07	29,29,29,29	1
59	MG	AA	3616	1/1	0.94	0.09	57,57,57,57	0
59	MG	CA	3281	1/1	0.94	0.07	21,21,21,21	0
59	MG	AA	3385	1/1	0.94	0.09	49,49,49,49	0
59	MG	CB	3010	1/1	0.94	0.09	51,51,51,51	0
59	MG	AA	3400	1/1	0.94	0.07	13,13,13,13	0
59	MG	BA	1710	1/1	0.94	0.09	81,81,81,81	0
59	MG	AA	3709	1/1	0.94	0.21	23,23,23,23	1
59	MG	AA	3104	1/1	0.94	0.13	54,54,54,54	0
59	MG	AA	3256	1/1	0.94	0.10	49,49,49,49	0
59	MG	CA	3513	1/1	0.94	0.10	70,70,70,70	0
59	MG	BA	1618	1/1	0.94	0.16	52,52,52,52	0
59	MG	AA	3497	1/1	0.94	0.10	44,44,44,44	0
59	MG	CA	3012	1/1	0.94	0.10	65,65,65,65	0
59	MG	AA	3220	1/1	0.94	0.08	62,62,62,62	0
59	MG	CA	3142	1/1	0.94	0.17	61,61,61,61	0
59	MG	BA	1621	1/1	0.94	0.06	51,51,51,51	0
59	MG	BA	1622	1/1	0.94	0.17	65,65,65,65	0
59	MG	AA	3501	1/1	0.94	0.07	49,49,49,49	0
59	MG	AA	3264	1/1	0.94	0.23	51,51,51,51	0
59	MG	CA	3527	1/1	0.94	0.16	76,76,76,76	0
59	MG	CR	201	1/1	0.94	0.07	34,34,34,34	0
59	MG	CU	201	1/1	0.94	0.14	74,74,74,74	0
59	MG	CA	3528	1/1	0.94	0.08	38,38,38,38	0
59	MG	BA	1722	1/1	0.94	0.15	51,51,51,51	0
59	MG	AA	3197	1/1	0.94	0.08	45,45,45,45	0
59	MG	DA	1766	1/1	0.94	0.07	74,74,74,74	0
59	MG	CA	3153	1/1	0.94	0.20	73,73,73,73	0
59	MG	DA	1768	1/1	0.94	0.06	59,59,59,59	0
59	MG	AA	3178	1/1	0.94	0.19	48,48,48,48	0
59	MG	AB	3013	1/1	0.94	0.09	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	1629	1/1	0.94	0.12	61,61,61,61	0
59	MG	AB	3014	1/1	0.94	0.09	56,56,56,56	0
59	MG	CA	3161	1/1	0.94	0.17	57,57,57,57	0
59	MG	AA	3521	1/1	0.94	0.08	19,19,19,19	0
59	MG	BA	1731	1/1	0.94	0.10	45,45,45,45	0
59	MG	AA	3321	1/1	0.94	0.11	61,61,61,61	0
59	MG	CA	3036	1/1	0.94	0.16	32,32,32,32	0
59	MG	AA	3535	1/1	0.94	0.06	48,48,48,48	0
59	MG	AA	3730	1/1	0.94	0.09	75,75,75,75	0
59	MG	DA	1615	1/1	0.94	0.07	58,58,58,58	0
59	MG	BA	1738	1/1	0.94	0.05	66,66,66,66	0
59	MG	AA	3731	1/1	0.94	0.10	51,51,51,51	0
59	MG	AA	3762	1/1	0.95	0.07	23,23,23,23	0
59	MG	AA	3144	1/1	0.95	0.14	50,50,50,50	0
59	MG	CB	3006	1/1	0.95	0.08	71,71,71,71	0
59	MG	CA	3197	1/1	0.95	0.13	45,45,45,45	0
59	MG	AA	3082	1/1	0.95	0.17	60,60,60,60	0
59	MG	CA	3448	1/1	0.95	0.09	37,37,37,37	0
59	MG	AA	3373	1/1	0.95	0.10	48,48,48,48	0
59	MG	AA	3114	1/1	0.95	0.09	26,26,26,26	0
59	MG	AA	3230	1/1	0.95	0.15	69,69,69,69	0
59	MG	AA	3377	1/1	0.95	0.07	20,20,20,20	0
59	MG	AA	3650	1/1	0.95	0.09	49,49,49,49	0
59	MG	CA	3462	1/1	0.95	0.10	63,63,63,63	0
59	MG	CE	302	1/1	0.95	0.06	64,64,64,64	0
59	MG	AA	3532	1/1	0.95	0.12	20,20,20,20	0
59	MG	AA	3116	1/1	0.95	0.24	35,35,35,35	0
59	MG	AA	3188	1/1	0.95	0.15	31,31,31,31	0
59	MG	CF	304	1/1	0.95	0.08	65,65,65,65	0
59	MG	CA	3468	1/1	0.95	0.05	53,53,53,53	0
59	MG	CA	3039	1/1	0.95	0.22	37,37,37,37	0
59	MG	AA	3233	1/1	0.95	0.15	46,46,46,46	0
59	MG	AA	3656	1/1	0.95	0.18	80,80,80,80	0
59	MG	AA	3389	1/1	0.95	0.07	25,25,25,25	0
59	MG	AA	3658	1/1	0.95	0.08	42,42,42,42	0
59	MG	CA	3215	1/1	0.95	0.13	54,54,54,54	0
59	MG	AA	3049	1/1	0.95	0.12	35,35,35,35	0
59	MG	AA	3547	1/1	0.95	0.13	60,60,60,60	0
59	MG	AA	3549	1/1	0.95	0.05	66,66,66,66	0
59	MG	AA	3788	1/1	0.95	0.15	61,61,61,61	0
59	MG	C3	3001	1/1	0.95	0.09	72,72,72,72	0
59	MG	AA	3789	1/1	0.95	0.10	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3790	1/1	0.95	0.23	57,57,57,57	0
59	MG	AA	3403	1/1	0.95	0.09	42,42,42,42	0
59	MG	AA	3405	1/1	0.95	0.15	44,44,44,44	0
59	MG	CA	3489	1/1	0.95	0.09	39,39,39,39	0
59	MG	BA	1734	1/1	0.95	0.09	61,61,61,61	0
59	MG	CA	3227	1/1	0.95	0.15	41,41,41,41	0
59	MG	BA	1736	1/1	0.95	0.10	67,67,67,67	0
59	MG	CA	3058	1/1	0.95	0.19	67,67,67,67	0
59	MG	AA	3155	1/1	0.95	0.18	93,93,93,93	0
59	MG	CA	3060	1/1	0.95	0.29	72,72,72,72	0
59	MG	AA	3671	1/1	0.95	0.11	19,19,19,19	0
59	MG	DA	1612	1/1	0.95	0.10	57,57,57,57	0
59	MG	DA	1613	1/1	0.95	0.22	48,48,48,48	0
59	MG	AA	3798	1/1	0.95	0.09	25,25,25,25	0
59	MG	CA	3063	1/1	0.95	0.09	34,34,34,34	0
59	MG	AA	3673	1/1	0.95	0.07	38,38,38,38	0
59	MG	DA	1617	1/1	0.95	0.14	64,64,64,64	0
59	MG	AA	3674	1/1	0.95	0.10	30,30,30,30	0
59	MG	AA	3119	1/1	0.95	0.10	47,47,47,47	0
59	MG	AA	3120	1/1	0.95	0.11	33,33,33,33	0
59	MG	AA	3294	1/1	0.95	0.09	37,37,37,37	0
59	MG	AA	3807	1/1	0.95	0.16	77,77,77,77	0
59	MG	AA	3033	1/1	0.95	0.13	55,55,55,55	0
59	MG	AA	3809	1/1	0.95	0.17	57,57,57,57	0
59	MG	CA	3074	1/1	0.95	0.06	49,49,49,49	0
59	MG	AA	3001	1/1	0.95	0.09	25,25,25,25	0
59	MG	AA	3299	1/1	0.95	0.19	47,47,47,47	0
59	MG	AA	3570	1/1	0.95	0.06	14,14,14,14	0
59	MG	AA	3431	1/1	0.95	0.10	25,25,25,25	0
59	MG	CA	3079	1/1	0.95	0.07	41,41,41,41	0
59	MG	CA	3252	1/1	0.95	0.16	62,62,62,62	0
59	MG	CA	3519	1/1	0.95	0.14	48,48,48,48	0
59	MG	AA	3685	1/1	0.95	0.08	72,72,72,72	0
59	MG	AA	3573	1/1	0.95	0.07	12,12,12,12	0
59	MG	AA	3432	1/1	0.95	0.15	42,42,42,42	0
59	MG	CA	3084	1/1	0.95	0.10	56,56,56,56	0
59	MG	CA	3258	1/1	0.95	0.25	51,51,51,51	0
59	MG	CA	3259	1/1	0.95	0.12	80,80,80,80	0
59	MG	AA	3006	1/1	0.95	0.09	52,52,52,52	0
59	MG	CA	3265	1/1	0.95	0.14	61,61,61,61	0
59	MG	CA	3531	1/1	0.95	0.06	47,47,47,47	0
59	MG	BA	1766	1/1	0.95	0.08	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3579	1/1	0.95	0.11	54,54,54,54	0
59	MG	AA	3580	1/1	0.95	0.16	54,54,54,54	0
59	MG	CA	3090	1/1	0.95	0.15	77,77,77,77	0
59	MG	AA	3302	1/1	0.95	0.09	51,51,51,51	0
59	MG	AB	3005	1/1	0.95	0.16	44,44,44,44	0
59	MG	CA	3277	1/1	0.95	0.16	55,55,55,55	0
59	MG	AA	3306	1/1	0.95	0.12	52,52,52,52	0
59	MG	CA	3541	1/1	0.95	0.12	63,63,63,63	0
59	MG	CA	3279	1/1	0.95	0.07	26,26,26,26	0
59	MG	AA	3163	1/1	0.95	0.14	72,72,72,72	0
59	MG	CA	3544	1/1	0.95	0.11	60,60,60,60	0
59	MG	AA	3309	1/1	0.95	0.15	46,46,46,46	0
59	MG	CA	3097	1/1	0.95	0.17	66,66,66,66	0
59	MG	AA	3588	1/1	0.95	0.09	47,47,47,47	0
59	MG	AA	3164	1/1	0.95	0.20	71,71,71,71	0
59	MG	AB	3015	1/1	0.95	0.07	28,28,28,28	0
59	MG	AB	3016	1/1	0.95	0.07	34,34,34,34	0
59	MG	CA	3290	1/1	0.95	0.15	34,34,34,34	0
59	MG	CA	3102	1/1	0.95	0.14	62,62,62,62	0
59	MG	AA	3094	1/1	0.95	0.25	80,80,80,80	0
59	MG	CA	3105	1/1	0.95	0.08	39,39,39,39	0
59	MG	AA	3014	1/1	0.95	0.12	31,31,31,31	0
59	MG	BA	1784	1/1	0.95	0.08	68,68,68,68	0
59	MG	BA	1785	1/1	0.95	0.08	62,62,62,62	0
59	MG	CA	3299	1/1	0.95	0.08	64,64,64,64	0
59	MG	AB	3019	1/1	0.95	0.13	70,70,70,70	0
59	MG	AA	3319	1/1	0.95	0.11	58,58,58,58	0
59	MG	AA	3449	1/1	0.95	0.11	50,50,50,50	0
59	MG	AA	3167	1/1	0.95	0.07	45,45,45,45	0
59	MG	AA	3044	1/1	0.95	0.19	52,52,52,52	0
59	MG	AA	3059	1/1	0.95	0.20	40,40,40,40	0
59	MG	DA	1681	1/1	0.95	0.20	70,70,70,70	0
59	MG	CA	3322	1/1	0.95	0.14	40,40,40,40	0
59	MG	AA	3605	1/1	0.95	0.17	45,45,45,45	0
59	MG	AA	3454	1/1	0.95	0.12	61,61,61,61	0
59	MG	DA	1686	1/1	0.95	0.16	56,56,56,56	0
59	MG	DA	1687	1/1	0.95	0.25	56,56,56,56	0
59	MG	AD	306	1/1	0.95	0.21	41,41,41,41	0
59	MG	CA	3332	1/1	0.95	0.09	29,29,29,29	0
59	MG	AA	3171	1/1	0.95	0.14	54,54,54,54	0
59	MG	CA	3334	1/1	0.95	0.12	47,47,47,47	0
59	MG	AA	3136	1/1	0.95	0.15	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3458	1/1	0.95	0.09	40,40,40,40	0
59	MG	CA	3338	1/1	0.95	0.10	64,64,64,64	0
59	MG	BA	1799	1/1	0.95	0.11	64,64,64,64	0
59	MG	AA	3331	1/1	0.95	0.07	15,15,15,15	0
59	MG	AA	3261	1/1	0.95	0.11	25,25,25,25	0
59	MG	DA	1702	1/1	0.95	0.09	63,63,63,63	0
59	MG	AA	3613	1/1	0.95	0.07	48,48,48,48	0
59	MG	CA	3347	1/1	0.95	0.07	45,45,45,45	0
59	MG	AA	3263	1/1	0.95	0.17	24,24,24,24	1
59	MG	AA	3723	1/1	0.95	0.07	49,49,49,49	0
59	MG	CA	3351	1/1	0.95	0.08	46,46,46,46	0
59	MG	BA	1806	1/1	0.95	0.12	55,55,55,55	0
59	MG	AA	3342	1/1	0.95	0.13	51,51,51,51	0
59	MG	CA	3597	1/1	0.95	0.10	58,58,58,58	0
59	MG	CA	3131	1/1	0.95	0.11	26,26,26,26	0
59	MG	CA	3358	1/1	0.95	0.13	36,36,36,36	0
59	MG	AF	303	1/1	0.95	0.15	39,39,39,39	0
59	MG	DA	1716	1/1	0.95	0.05	57,57,57,57	0
59	MG	CA	3601	1/1	0.95	0.06	57,57,57,57	0
59	MG	CA	3362	1/1	0.95	0.08	43,43,43,43	0
59	MG	AA	3077	1/1	0.95	0.19	43,43,43,43	0
59	MG	DA	1720	1/1	0.95	0.10	60,60,60,60	0
59	MG	AA	3176	1/1	0.95	0.16	70,70,70,70	0
59	MG	AA	3472	1/1	0.95	0.09	42,42,42,42	0
59	MG	DA	1723	1/1	0.95	0.06	53,53,53,53	0
59	MG	CA	3138	1/1	0.95	0.08	86,86,86,86	0
59	MG	CA	3607	1/1	0.95	0.08	64,64,64,64	0
59	MG	AA	3733	1/1	0.95	0.08	49,49,49,49	0
59	MG	AA	3078	1/1	0.95	0.26	70,70,70,70	0
59	MG	CA	3371	1/1	0.95	0.12	52,52,52,52	0
59	MG	DA	1729	1/1	0.95	0.14	49,49,49,49	0
59	MG	AA	3620	1/1	0.95	0.05	22,22,22,22	0
59	MG	AA	3349	1/1	0.95	0.08	47,47,47,47	0
59	MG	AO	5001	1/1	0.95	0.06	34,34,34,34	0
59	MG	AA	3623	1/1	0.95	0.06	28,28,28,28	0
59	MG	BF	3001	1/1	0.95	0.07	49,49,49,49	0
59	MG	AA	3624	1/1	0.95	0.07	42,42,42,42	0
59	MG	CA	3381	1/1	0.95	0.07	50,50,50,50	0
59	MG	CA	3384	1/1	0.95	0.12	55,55,55,55	0
59	MG	CA	3385	1/1	0.95	0.27	61,61,61,61	0
59	MG	AA	3350	1/1	0.95	0.06	36,36,36,36	0
59	MG	AQ	202	1/1	0.95	0.15	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3152	1/1	0.95	0.14	64,64,64,64	0
59	MG	BN	502	1/1	0.95	0.09	87,87,87,87	0
59	MG	DA	1745	1/1	0.95	0.20	50,50,50,50	0
59	MG	AA	3744	1/1	0.95	0.08	34,34,34,34	0
59	MG	AA	3060	1/1	0.95	0.13	20,20,20,20	0
59	MG	BW	501	1/1	0.95	0.21	47,47,47,47	0
59	MG	AA	3355	1/1	0.95	0.12	57,57,57,57	0
59	MG	AA	3270	1/1	0.95	0.23	55,55,55,55	0
59	MG	CA	3162	1/1	0.95	0.23	31,31,31,31	0
59	MG	CA	3400	1/1	0.95	0.11	57,57,57,57	0
59	MG	AA	3750	1/1	0.95	0.17	51,51,51,51	0
59	MG	AA	3105	1/1	0.95	0.14	52,52,52,52	0
59	MG	CA	3002	1/1	0.95	0.16	28,28,28,28	0
59	MG	CA	3167	1/1	0.95	0.07	50,50,50,50	0
59	MG	AA	3015	1/1	0.95	0.27	57,57,57,57	0
59	MG	CA	3004	1/1	0.95	0.15	49,49,49,49	0
59	MG	AA	3081	1/1	0.95	0.12	56,56,56,56	0
59	MG	AA	3276	1/1	0.95	0.12	67,67,67,67	0
59	MG	CA	3008	1/1	0.95	0.11	46,46,46,46	0
59	MG	CA	3418	1/1	0.95	0.12	34,34,34,34	0
59	MG	CA	3648	1/1	0.95	0.17	52,52,52,52	0
59	MG	CA	3010	1/1	0.95	0.07	43,43,43,43	0
59	MG	AA	3182	1/1	0.95	0.17	46,46,46,46	0
59	MG	AA	3366	1/1	0.95	0.06	35,35,35,35	1
59	MG	CA	3013	1/1	0.95	0.09	42,42,42,42	0
59	MG	CA	3655	1/1	0.95	0.21	52,52,52,52	0
59	MG	BA	1701	1/1	0.95	0.08	54,54,54,54	0
59	MG	CA	3657	1/1	0.95	0.16	41,41,41,41	0
59	MG	BA	1702	1/1	0.95	0.14	46,46,46,46	0
59	MG	CA	3187	1/1	0.95	0.11	37,37,37,37	0
59	MG	AA	3638	1/1	0.95	0.12	71,71,71,71	0
59	MG	AA	3183	1/1	0.95	0.10	58,58,58,58	0
59	MG	A0	103	1/1	0.95	0.07	70,70,70,70	0
59	MG	CA	3664	1/1	0.95	0.10	48,48,48,48	0
59	MG	CA	3191	1/1	0.95	0.16	46,46,46,46	0
59	MG	AA	3368	1/1	0.95	0.14	49,49,49,49	0
62	GDP	BZ	702	28/28	0.95	0.07	57,57,57,57	0
59	MG	CA	3440	1/1	0.95	0.17	49,49,49,49	0
59	MG	AA	3034	1/1	0.96	0.14	49,49,49,49	0
59	MG	AA	3058	1/1	0.96	0.04	22,22,22,22	0
59	MG	AA	3672	1/1	0.96	0.06	48,48,48,48	0
59	MG	AA	3091	1/1	0.96	0.32	47,47,47,47	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3779	1/1	0.96	0.05	22,22,22,22	0
59	MG	BA	1690	1/1	0.96	0.17	71,71,71,71	0
59	MG	C1	101	1/1	0.96	0.10	57,57,57,57	0
59	MG	AA	3460	1/1	0.96	0.07	27,27,27,27	0
59	MG	CA	3505	1/1	0.96	0.05	67,67,67,67	0
59	MG	C7	101	1/1	0.96	0.11	56,56,56,56	0
59	MG	C8	5001	1/1	0.96	0.11	37,37,37,37	0
59	MG	AA	3201	1/1	0.96	0.11	53,53,53,53	0
59	MG	AA	3168	1/1	0.96	0.07	47,47,47,47	0
59	MG	AA	3587	1/1	0.96	0.12	28,28,28,28	0
59	MG	CA	3286	1/1	0.96	0.08	58,58,58,58	0
59	MG	AA	3111	1/1	0.96	0.06	24,24,24,24	0
59	MG	A0	104	1/1	0.96	0.13	51,51,51,51	0
59	MG	AA	3590	1/1	0.96	0.09	60,60,60,60	0
59	MG	AA	3291	1/1	0.96	0.07	45,45,45,45	0
59	MG	AA	3112	1/1	0.96	0.16	61,61,61,61	0
59	MG	AA	3113	1/1	0.96	0.11	45,45,45,45	0
59	MG	AA	3372	1/1	0.96	0.11	37,37,37,37	0
59	MG	AA	3247	1/1	0.96	0.20	55,55,55,55	0
59	MG	CA	3132	1/1	0.96	0.07	48,48,48,48	0
59	MG	AA	3172	1/1	0.96	0.15	47,47,47,47	0
59	MG	AA	3092	1/1	0.96	0.18	39,39,39,39	0
59	MG	CA	3522	1/1	0.96	0.10	54,54,54,54	0
59	MG	A8	5001	1/1	0.96	0.06	30,30,30,30	0
59	MG	CA	3305	1/1	0.96	0.11	48,48,48,48	0
59	MG	AA	3689	1/1	0.96	0.05	35,35,35,35	0
59	MG	AA	3797	1/1	0.96	0.08	52,52,52,52	0
59	MG	DA	1621	1/1	0.96	0.06	42,42,42,42	0
59	MG	CA	3312	1/1	0.96	0.09	38,38,38,38	0
59	MG	AA	3690	1/1	0.96	0.11	50,50,50,50	0
59	MG	AA	3799	1/1	0.96	0.10	42,42,42,42	0
59	MG	CA	3315	1/1	0.96	0.09	47,47,47,47	0
59	MG	CA	3316	1/1	0.96	0.08	43,43,43,43	0
59	MG	CA	3317	1/1	0.96	0.06	49,49,49,49	0
59	MG	AA	3030	1/1	0.96	0.19	24,24,24,24	1
59	MG	AA	3047	1/1	0.96	0.04	29,29,29,29	0
59	MG	CA	3144	1/1	0.96	0.14	40,40,40,40	0
59	MG	CA	3009	1/1	0.96	0.05	27,27,27,27	0
59	MG	CA	3326	1/1	0.96	0.08	28,28,28,28	0
59	MG	CA	3330	1/1	0.96	0.08	36,36,36,36	0
59	MG	AA	3483	1/1	0.96	0.07	46,46,46,46	0
59	MG	AA	3095	1/1	0.96	0.12	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	1715	1/1	0.96	0.08	60,60,60,60	0
59	MG	AA	3696	1/1	0.96	0.08	66,66,66,66	0
59	MG	CA	3014	1/1	0.96	0.10	50,50,50,50	0
59	MG	AA	3697	1/1	0.96	0.08	40,40,40,40	0
59	MG	AA	3254	1/1	0.96	0.14	52,52,52,52	0
59	MG	CA	3018	1/1	0.96	0.06	41,41,41,41	0
59	MG	AA	3488	1/1	0.96	0.06	36,36,36,36	0
59	MG	CA	3021	1/1	0.96	0.15	69,69,69,69	0
59	MG	CA	3158	1/1	0.96	0.17	54,54,54,54	0
59	MG	CA	3345	1/1	0.96	0.07	46,46,46,46	0
59	MG	AA	3386	1/1	0.96	0.09	45,45,45,45	0
59	MG	CA	3160	1/1	0.96	0.17	57,57,57,57	0
59	MG	AA	3036	1/1	0.96	0.08	25,25,25,25	0
59	MG	AA	3390	1/1	0.96	0.06	23,23,23,23	0
59	MG	CA	3025	1/1	0.96	0.16	59,59,59,59	0
59	MG	BA	1723	1/1	0.96	0.06	70,70,70,70	0
59	MG	AA	3391	1/1	0.96	0.07	19,19,19,19	0
59	MG	CA	3029	1/1	0.96	0.11	56,56,56,56	0
59	MG	CA	3564	1/1	0.96	0.14	80,80,80,80	0
59	MG	CA	3168	1/1	0.96	0.21	58,58,58,58	0
59	MG	AA	3395	1/1	0.96	0.07	54,54,54,54	0
59	MG	AA	3398	1/1	0.96	0.13	31,31,31,31	0
59	MG	CA	3173	1/1	0.96	0.21	61,61,61,61	0
59	MG	CA	3174	1/1	0.96	0.28	50,50,50,50	0
59	MG	AA	3257	1/1	0.96	0.19	54,54,54,54	0
59	MG	AA	3820	1/1	0.96	0.06	25,25,25,25	0
59	MG	AA	3500	1/1	0.96	0.11	59,59,59,59	0
59	MG	CA	3179	1/1	0.96	0.15	60,60,60,60	0
59	MG	AA	3149	1/1	0.96	0.08	51,51,51,51	0
59	MG	CA	3374	1/1	0.96	0.09	60,60,60,60	0
59	MG	AA	3503	1/1	0.96	0.05	54,54,54,54	0
59	MG	AA	3621	1/1	0.96	0.04	17,17,17,17	0
59	MG	CA	3377	1/1	0.96	0.07	52,52,52,52	0
59	MG	DA	1673	1/1	0.96	0.06	82,82,82,82	0
59	MG	AA	3713	1/1	0.96	0.21	27,27,27,27	0
59	MG	BA	1626	1/1	0.96	0.12	41,41,41,41	0
59	MG	AA	3507	1/1	0.96	0.07	50,50,50,50	0
59	MG	AA	3121	1/1	0.96	0.09	53,53,53,53	0
59	MG	AA	3152	1/1	0.96	0.11	10,10,10,10	0
59	MG	CA	3592	1/1	0.96	0.09	64,64,64,64	0
59	MG	DA	1680	1/1	0.96	0.10	56,56,56,56	0
59	MG	AB	3012	1/1	0.96	0.06	23,23,23,23	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	DA	1682	1/1	0.96	0.17	52,52,52,52	0
59	MG	CA	3387	1/1	0.96	0.06	50,50,50,50	0
59	MG	AA	3216	1/1	0.96	0.25	38,38,38,38	0
59	MG	CA	3045	1/1	0.96	0.21	60,60,60,60	0
59	MG	CA	3192	1/1	0.96	0.04	45,45,45,45	0
59	MG	BA	1743	1/1	0.96	0.04	41,41,41,41	0
59	MG	AA	3217	1/1	0.96	0.18	29,29,29,29	1
59	MG	AA	3524	1/1	0.96	0.07	41,41,41,41	0
59	MG	CA	3049	1/1	0.96	0.19	46,46,46,46	0
59	MG	AA	3529	1/1	0.96	0.13	30,30,30,30	0
59	MG	AA	3417	1/1	0.96	0.06	25,25,25,25	0
59	MG	BA	1636	1/1	0.96	0.21	57,57,57,57	0
59	MG	DA	1696	1/1	0.96	0.12	53,53,53,53	0
59	MG	BA	1751	1/1	0.96	0.08	48,48,48,48	0
59	MG	AA	3039	1/1	0.96	0.20	34,34,34,34	1
59	MG	CA	3403	1/1	0.96	0.06	70,70,70,70	0
59	MG	CA	3404	1/1	0.96	0.08	65,65,65,65	0
59	MG	CA	3405	1/1	0.96	0.08	55,55,55,55	0
59	MG	AA	3725	1/1	0.96	0.06	13,13,13,13	0
59	MG	AA	3729	1/1	0.96	0.10	41,41,41,41	0
59	MG	AA	3268	1/1	0.96	0.11	66,66,66,66	0
59	MG	CA	3613	1/1	0.96	0.11	57,57,57,57	0
59	MG	CA	3410	1/1	0.96	0.08	25,25,25,25	0
59	MG	CA	3206	1/1	0.96	0.16	44,44,44,44	0
59	MG	AB	3022	1/1	0.96	0.11	61,61,61,61	0
59	MG	AA	3424	1/1	0.96	0.08	14,14,14,14	0
59	MG	DA	1711	1/1	0.96	0.14	60,60,60,60	0
59	MG	BA	1761	1/1	0.96	0.10	62,62,62,62	0
59	MG	CA	3416	1/1	0.96	0.07	44,44,44,44	0
59	MG	AA	3634	1/1	0.96	0.17	76,76,76,76	0
59	MG	AA	3154	1/1	0.96	0.09	57,57,57,57	0
59	MG	AA	3123	1/1	0.96	0.12	54,54,54,54	0
59	MG	AA	3637	1/1	0.96	0.18	17,17,17,17	1
59	MG	AA	3334	1/1	0.96	0.09	63,63,63,63	0
59	MG	CA	3422	1/1	0.96	0.10	43,43,43,43	0
59	MG	BA	1768	1/1	0.96	0.08	64,64,64,64	0
59	MG	CA	3218	1/1	0.96	0.27	40,40,40,40	0
59	MG	CA	3429	1/1	0.96	0.07	59,59,59,59	0
59	MG	AA	3546	1/1	0.96	0.07	60,60,60,60	0
59	MG	CA	3071	1/1	0.96	0.08	45,45,45,45	0
59	MG	BA	1649	1/1	0.96	0.11	35,35,35,35	0
59	MG	BA	1650	1/1	0.96	0.10	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	1773	1/1	0.96	0.07	40,40,40,40	0
59	MG	AA	3271	1/1	0.96	0.15	34,34,34,34	0
59	MG	AA	3338	1/1	0.96	0.07	28,28,28,28	0
59	MG	CA	3640	1/1	0.96	0.10	43,43,43,43	0
59	MG	BA	1653	1/1	0.96	0.13	56,56,56,56	0
59	MG	AA	3272	1/1	0.96	0.06	55,55,55,55	0
59	MG	AD	312	1/1	0.96	0.18	78,78,78,78	0
59	MG	AA	3156	1/1	0.96	0.17	49,49,49,49	0
59	MG	CA	3445	1/1	0.96	0.07	22,22,22,22	0
59	MG	CA	3446	1/1	0.96	0.05	33,33,33,33	0
59	MG	AA	3442	1/1	0.96	0.09	23,23,23,23	0
59	MG	AA	3064	1/1	0.96	0.05	32,32,32,32	0
59	MG	CA	3450	1/1	0.96	0.05	54,54,54,54	0
59	MG	AA	3648	1/1	0.96	0.07	41,41,41,41	0
59	MG	CA	3234	1/1	0.96	0.18	50,50,50,50	0
59	MG	AA	3031	1/1	0.96	0.14	63,63,63,63	0
59	MG	AA	3228	1/1	0.96	0.08	32,32,32,32	0
59	MG	DA	1747	1/1	0.96	0.07	48,48,48,48	0
59	MG	AA	3348	1/1	0.96	0.05	53,53,53,53	0
59	MG	CA	3461	1/1	0.96	0.09	34,34,34,34	0
59	MG	BA	1787	1/1	0.96	0.13	55,55,55,55	0
59	MG	AA	3159	1/1	0.96	0.16	55,55,55,55	0
59	MG	CA	3091	1/1	0.96	0.16	69,69,69,69	0
59	MG	AA	3564	1/1	0.96	0.06	44,44,44,44	0
59	MG	AA	3654	1/1	0.96	0.05	67,67,67,67	0
59	MG	AA	3005	1/1	0.96	0.13	64,64,64,64	0
59	MG	AA	3566	1/1	0.96	0.06	56,56,56,56	0
59	MG	AA	3567	1/1	0.96	0.07	26,26,26,26	0
59	MG	CA	3473	1/1	0.96	0.10	51,51,51,51	0
59	MG	AA	3129	1/1	0.96	0.08	34,34,34,34	1
59	MG	DA	1760	1/1	0.96	0.07	61,61,61,61	0
59	MG	AP	201	1/1	0.96	0.20	72,72,72,72	0
59	MG	AA	3131	1/1	0.96	0.12	63,63,63,63	0
59	MG	CA	3479	1/1	0.96	0.08	50,50,50,50	0
59	MG	AA	3764	1/1	0.96	0.07	73,73,73,73	0
59	MG	AA	3083	1/1	0.96	0.14	61,61,61,61	0
59	MG	BA	1674	1/1	0.96	0.20	48,48,48,48	0
59	MG	CA	3103	1/1	0.96	0.17	53,53,53,53	0
59	MG	AA	3766	1/1	0.96	0.10	54,54,54,54	0
59	MG	AA	3042	1/1	0.96	0.09	32,32,32,32	0
59	MG	CD	303	1/1	0.96	0.08	70,70,70,70	0
59	MG	DD	502	1/1	0.96	0.18	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	1677	1/1	0.96	0.09	28,28,28,28	0
59	MG	AA	3576	1/1	0.96	0.08	52,52,52,52	0
59	MG	CA	3260	1/1	0.96	0.07	35,35,35,35	0
59	MG	AA	3668	1/1	0.96	0.10	54,54,54,54	0
59	MG	CA	3491	1/1	0.96	0.04	44,44,44,44	0
59	MG	DW	501	1/1	0.96	0.14	44,44,44,44	0
59	MG	CF	303	1/1	0.96	0.11	51,51,51,51	0
59	MG	CA	3109	1/1	0.96	0.07	35,35,35,35	0
59	MG	AU	201	1/1	0.96	0.11	46,46,46,46	0
59	MG	AA	3359	1/1	0.96	0.06	31,31,31,31	0
60	ZN	A4	501	1/1	0.96	0.04	117,117,117,117	0
59	MG	AV	203	1/1	0.96	0.08	47,47,47,47	0
59	MG	CA	3496	1/1	0.96	0.10	56,56,56,56	0
59	MG	CA	3497	1/1	0.96	0.07	45,45,45,45	0
59	MG	AA	3511	1/1	0.97	0.06	14,14,14,14	0
59	MG	CA	3181	1/1	0.97	0.14	40,40,40,40	0
59	MG	CA	3349	1/1	0.97	0.07	23,23,23,23	0
59	MG	AA	3514	1/1	0.97	0.07	42,42,42,42	0
59	MG	AA	3089	1/1	0.97	0.10	49,49,49,49	0
59	MG	AA	3422	1/1	0.97	0.09	23,23,23,23	0
59	MG	CA	3533	1/1	0.97	0.08	45,45,45,45	0
59	MG	CA	3353	1/1	0.97	0.06	45,45,45,45	0
59	MG	AB	3010	1/1	0.97	0.04	62,62,62,62	0
59	MG	CA	3355	1/1	0.97	0.08	35,35,35,35	0
59	MG	AA	3146	1/1	0.97	0.05	29,29,29,29	0
59	MG	AA	3071	1/1	0.97	0.14	40,40,40,40	0
59	MG	CA	3359	1/1	0.97	0.04	33,33,33,33	0
59	MG	AA	3527	1/1	0.97	0.06	27,27,27,27	0
59	MG	CA	3053	1/1	0.97	0.14	32,32,32,32	0
59	MG	AA	3720	1/1	0.97	0.08	55,55,55,55	0
59	MG	CA	3364	1/1	0.97	0.04	22,22,22,22	0
59	MG	BA	1757	1/1	0.97	0.12	43,43,43,43	0
59	MG	AA	3721	1/1	0.97	0.12	40,40,40,40	0
59	MG	AA	3221	1/1	0.97	0.05	30,30,30,30	0
59	MG	AA	3430	1/1	0.97	0.05	39,39,39,39	0
59	MG	CA	3195	1/1	0.97	0.18	47,47,47,47	0
59	MG	AA	3222	1/1	0.97	0.06	4,4,4,4	0
59	MG	AA	3533	1/1	0.97	0.09	22,22,22,22	0
59	MG	AA	3726	1/1	0.97	0.06	12,12,12,12	0
59	MG	DA	1628	1/1	0.97	0.04	39,39,39,39	0
59	MG	CA	3552	1/1	0.97	0.09	30,30,30,30	0
59	MG	BA	1765	1/1	0.97	0.12	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3728	1/1	0.97	0.12	29,29,29,29	0
59	MG	CA	3064	1/1	0.97	0.07	48,48,48,48	0
59	MG	AA	3255	1/1	0.97	0.09	38,38,38,38	0
59	MG	AA	3631	1/1	0.97	0.13	46,46,46,46	0
59	MG	AA	3433	1/1	0.97	0.10	37,37,37,37	0
59	MG	AA	3539	1/1	0.97	0.11	34,34,34,34	0
59	MG	AD	304	1/1	0.97	0.06	17,17,17,17	0
59	MG	AA	3434	1/1	0.97	0.07	17,17,17,17	0
59	MG	CA	3386	1/1	0.97	0.09	50,50,50,50	0
59	MG	AA	3735	1/1	0.97	0.05	25,25,25,25	0
59	MG	AA	3351	1/1	0.97	0.08	29,29,29,29	0
59	MG	AA	3126	1/1	0.97	0.14	79,79,79,79	0
59	MG	CA	3567	1/1	0.97	0.05	26,26,26,26	0
59	MG	AA	3545	1/1	0.97	0.09	43,43,43,43	0
59	MG	AA	3292	1/1	0.97	0.07	24,24,24,24	0
59	MG	AA	3741	1/1	0.97	0.05	21,21,21,21	0
59	MG	AA	3107	1/1	0.97	0.06	49,49,49,49	0
59	MG	AA	3009	1/1	0.97	0.04	22,22,22,22	0
59	MG	AA	3358	1/1	0.97	0.04	45,45,45,45	0
59	MG	AA	3745	1/1	0.97	0.10	68,68,68,68	0
59	MG	CA	3220	1/1	0.97	0.05	59,59,59,59	0
59	MG	DA	1653	1/1	0.97	0.19	55,55,55,55	0
59	MG	CA	3580	1/1	0.97	0.09	76,76,76,76	0
59	MG	AF	301	1/1	0.97	0.11	38,38,38,38	0
59	MG	CA	3082	1/1	0.97	0.14	76,76,76,76	0
59	MG	AA	3259	1/1	0.97	0.12	41,41,41,41	1
59	MG	AA	3552	1/1	0.97	0.10	63,63,63,63	0
59	MG	AA	3553	1/1	0.97	0.04	43,43,43,43	0
59	MG	AA	3749	1/1	0.97	0.08	73,73,73,73	0
59	MG	CA	3407	1/1	0.97	0.08	36,36,36,36	0
59	MG	AA	3554	1/1	0.97	0.09	40,40,40,40	0
59	MG	AA	3360	1/1	0.97	0.09	22,22,22,22	0
59	MG	AA	3297	1/1	0.97	0.09	27,27,27,27	0
59	MG	AH	201	1/1	0.97	0.18	64,64,64,64	0
59	MG	AA	3557	1/1	0.97	0.08	37,37,37,37	0
59	MG	AA	3227	1/1	0.97	0.04	22,22,22,22	0
59	MG	AA	3075	1/1	0.97	0.10	49,49,49,49	0
59	MG	CA	3415	1/1	0.97	0.10	34,34,34,34	0
59	MG	AA	3110	1/1	0.97	0.14	52,52,52,52	0
59	MG	AA	3265	1/1	0.97	0.13	43,43,43,43	0
59	MG	AA	3452	1/1	0.97	0.04	14,14,14,14	0
59	MG	AA	3305	1/1	0.97	0.06	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3132	1/1	0.97	0.08	41,41,41,41	0
59	MG	BA	1680	1/1	0.97	0.10	40,40,40,40	0
59	MG	AA	3369	1/1	0.97	0.05	47,47,47,47	0
59	MG	CA	3424	1/1	0.97	0.09	66,66,66,66	0
59	MG	CA	3425	1/1	0.97	0.07	50,50,50,50	0
59	MG	BA	1804	1/1	0.97	0.06	45,45,45,45	0
59	MG	CA	3427	1/1	0.97	0.11	37,37,37,37	0
59	MG	AA	3062	1/1	0.97	0.11	47,47,47,47	0
59	MG	AA	3021	1/1	0.97	0.08	33,33,33,33	0
59	MG	AA	3661	1/1	0.97	0.09	41,41,41,41	1
59	MG	AU	203	1/1	0.97	0.11	25,25,25,25	0
59	MG	BA	1809	1/1	0.97	0.09	61,61,61,61	0
59	MG	BA	1686	1/1	0.97	0.12	36,36,36,36	0
59	MG	CA	3248	1/1	0.97	0.10	53,53,53,53	0
59	MG	AA	3662	1/1	0.97	0.05	60,60,60,60	0
59	MG	CA	3250	1/1	0.97	0.06	38,38,38,38	0
59	MG	CA	3437	1/1	0.97	0.08	64,64,64,64	0
59	MG	DA	1693	1/1	0.97	0.06	67,67,67,67	0
59	MG	AA	3572	1/1	0.97	0.10	17,17,17,17	0
59	MG	AA	3665	1/1	0.97	0.17	40,40,40,40	0
59	MG	AA	3666	1/1	0.97	0.14	41,41,41,41	0
59	MG	DA	1697	1/1	0.97	0.04	48,48,48,48	0
59	MG	AA	3459	1/1	0.97	0.11	53,53,53,53	0
59	MG	AW	3003	1/1	0.97	0.06	28,28,28,28	0
59	MG	AA	3310	1/1	0.97	0.08	56,56,56,56	0
59	MG	CA	3627	1/1	0.97	0.09	60,60,60,60	0
59	MG	AA	3043	1/1	0.97	0.16	45,45,45,45	0
59	MG	CA	3629	1/1	0.97	0.05	55,55,55,55	0
59	MG	AA	3462	1/1	0.97	0.04	54,54,54,54	0
59	MG	AA	3777	1/1	0.97	0.06	41,41,41,41	0
59	MG	CA	3263	1/1	0.97	0.07	64,64,64,64	0
59	MG	CA	3453	1/1	0.97	0.06	35,35,35,35	0
59	MG	AA	3578	1/1	0.97	0.06	28,28,28,28	0
59	MG	AA	3023	1/1	0.97	0.17	53,53,53,53	0
59	MG	BM	201	1/1	0.97	0.04	62,62,62,62	0
59	MG	CA	3457	1/1	0.97	0.09	43,43,43,43	0
59	MG	DA	1712	1/1	0.97	0.13	53,53,53,53	0
59	MG	CA	3458	1/1	0.97	0.05	54,54,54,54	0
59	MG	AA	3137	1/1	0.97	0.28	53,53,53,53	0
59	MG	AA	3376	1/1	0.97	0.11	35,35,35,35	0
59	MG	CA	3641	1/1	0.97	0.04	46,46,46,46	0
59	MG	AA	3316	1/1	0.97	0.10	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3463	1/1	0.97	0.10	56,56,56,56	0
59	MG	BT	3001	1/1	0.97	0.05	46,46,46,46	0
59	MG	CA	3275	1/1	0.97	0.07	61,61,61,61	0
59	MG	AA	3470	1/1	0.97	0.05	39,39,39,39	0
59	MG	AA	3585	1/1	0.97	0.08	35,35,35,35	0
59	MG	AA	3318	1/1	0.97	0.09	23,23,23,23	0
59	MG	AA	3380	1/1	0.97	0.04	18,18,18,18	0
59	MG	AA	3236	1/1	0.97	0.10	57,57,57,57	0
59	MG	AA	3384	1/1	0.97	0.06	22,22,22,22	0
59	MG	AA	3592	1/1	0.97	0.05	26,26,26,26	0
59	MG	CA	3475	1/1	0.97	0.18	50,50,50,50	0
59	MG	CA	3476	1/1	0.97	0.05	38,38,38,38	0
59	MG	BA	1709	1/1	0.97	0.15	50,50,50,50	0
59	MG	DA	1731	1/1	0.97	0.08	49,49,49,49	0
59	MG	AA	3115	1/1	0.97	0.09	44,44,44,44	0
59	MG	A9	502	1/1	0.97	0.13	41,41,41,41	0
59	MG	AA	3045	1/1	0.97	0.12	55,55,55,55	0
59	MG	AA	3795	1/1	0.97	0.13	22,22,22,22	0
59	MG	AA	3595	1/1	0.97	0.07	42,42,42,42	0
59	MG	AA	3387	1/1	0.97	0.05	29,29,29,29	0
59	MG	AA	3598	1/1	0.97	0.12	51,51,51,51	0
59	MG	CA	3143	1/1	0.97	0.20	41,41,41,41	0
59	MG	AA	3029	1/1	0.97	0.10	28,28,28,28	0
59	MG	AA	3691	1/1	0.97	0.06	62,62,62,62	0
59	MG	CA	3297	1/1	0.97	0.10	36,36,36,36	0
59	MG	AA	3600	1/1	0.97	0.07	25,25,25,25	0
59	MG	DA	1744	1/1	0.97	0.07	66,66,66,66	0
59	MG	AA	3100	1/1	0.97	0.10	29,29,29,29	0
59	MG	CA	3300	1/1	0.97	0.05	47,47,47,47	0
59	MG	CB	3009	1/1	0.97	0.12	67,67,67,67	0
59	MG	CA	3301	1/1	0.97	0.07	60,60,60,60	0
59	MG	CA	3017	1/1	0.97	0.06	30,30,30,30	0
59	MG	AA	3024	1/1	0.97	0.12	48,48,48,48	0
59	MG	CA	3306	1/1	0.97	0.04	24,24,24,24	0
59	MG	AA	3394	1/1	0.97	0.07	39,39,39,39	0
59	MG	AA	3806	1/1	0.97	0.13	42,42,42,42	0
59	MG	AA	3330	1/1	0.97	0.05	66,66,66,66	0
59	MG	CD	304	1/1	0.97	0.13	28,28,28,28	0
59	MG	AA	3069	1/1	0.97	0.03	28,28,28,28	0
59	MG	AA	3245	1/1	0.97	0.07	11,11,11,11	0
59	MG	CE	303	1/1	0.97	0.20	51,51,51,51	0
59	MG	CA	3156	1/1	0.97	0.14	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3336	1/1	0.97	0.08	51,51,51,51	0
59	MG	BA	1728	1/1	0.97	0.12	47,47,47,47	0
59	MG	CF	302	1/1	0.97	0.22	69,69,69,69	0
59	MG	CA	3027	1/1	0.97	0.04	31,31,31,31	0
59	MG	DA	1764	1/1	0.97	0.05	71,71,71,71	0
59	MG	AA	3811	1/1	0.97	0.08	56,56,56,56	0
59	MG	AA	3812	1/1	0.97	0.06	41,41,41,41	0
59	MG	AA	3004	1/1	0.97	0.09	21,21,21,21	0
59	MG	CO	5001	1/1	0.97	0.08	50,50,50,50	0
59	MG	AA	3408	1/1	0.97	0.11	41,41,41,41	0
59	MG	CA	3328	1/1	0.97	0.05	35,35,35,35	0
59	MG	AA	3815	1/1	0.97	0.08	30,30,30,30	0
59	MG	AA	3498	1/1	0.97	0.13	47,47,47,47	0
59	MG	BA	1735	1/1	0.97	0.13	41,41,41,41	0
59	MG	AA	3190	1/1	0.97	0.04	24,24,24,24	0
59	MG	DF	3001	1/1	0.97	0.11	54,54,54,54	0
59	MG	AA	3612	1/1	0.97	0.05	68,68,68,68	0
59	MG	AA	3413	1/1	0.97	0.07	25,25,25,25	0
59	MG	CW	201	1/1	0.97	0.13	46,46,46,46	0
59	MG	AA	3191	1/1	0.97	0.03	16,16,16,16	0
59	MG	C0	101	1/1	0.97	0.11	59,59,59,59	0
59	MG	BA	1740	1/1	0.97	0.10	50,50,50,50	0
59	MG	CA	3175	1/1	0.97	0.10	31,31,31,31	0
59	MG	AA	3340	1/1	0.97	0.05	3,3,3,3	0
59	MG	AA	3341	1/1	0.97	0.06	25,25,25,25	0
60	ZN	BN	501	1/1	0.97	0.04	132,132,132,132	0
59	MG	CA	3523	1/1	0.97	0.10	37,37,37,37	0
61	SF4	DD	501	8/8	0.97	0.05	82,82,82,82	1
59	MG	AA	3284	1/1	0.97	0.21	60,60,60,60	0
59	MG	AA	3509	1/1	0.97	0.08	40,40,40,40	0
59	MG	CA	3452	1/1	0.98	0.05	36,36,36,36	0
59	MG	AA	3008	1/1	0.98	0.06	26,26,26,26	0
59	MG	AA	3548	1/1	0.98	0.04	7,7,7,7	0
59	MG	A7	101	1/1	0.98	0.08	47,47,47,47	0
59	MG	CA	3308	1/1	0.98	0.04	39,39,39,39	0
59	MG	CA	3309	1/1	0.98	0.10	22,22,22,22	0
59	MG	AA	3311	1/1	0.98	0.07	2,2,2,2	0
59	MG	CA	3459	1/1	0.98	0.04	28,28,28,28	0
59	MG	AA	3353	1/1	0.98	0.07	39,39,39,39	0
59	MG	AA	3399	1/1	0.98	0.03	16,16,16,16	0
59	MG	DA	1648	1/1	0.98	0.10	40,40,40,40	0
59	MG	AA	3354	1/1	0.98	0.04	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3402	1/1	0.98	0.04	27,27,27,27	0
59	MG	AA	3048	1/1	0.98	0.04	28,28,28,28	0
59	MG	AA	3404	1/1	0.98	0.09	27,27,27,27	0
59	MG	CA	3466	1/1	0.98	0.21	56,56,56,56	0
59	MG	CA	3318	1/1	0.98	0.05	24,24,24,24	0
59	MG	AA	3032	1/1	0.98	0.12	59,59,59,59	0
59	MG	CA	3320	1/1	0.98	0.07	36,36,36,36	0
59	MG	DA	1657	1/1	0.98	0.05	23,23,23,23	0
59	MG	AA	3469	1/1	0.98	0.03	32,32,32,32	0
59	MG	CA	3617	1/1	0.98	0.07	41,41,41,41	0
59	MG	CA	3618	1/1	0.98	0.17	40,40,40,40	0
59	MG	CA	3471	1/1	0.98	0.10	33,33,33,33	0
59	MG	AA	3406	1/1	0.98	0.04	20,20,20,20	0
59	MG	CA	3324	1/1	0.98	0.06	26,26,26,26	0
59	MG	AA	3639	1/1	0.98	0.07	18,18,18,18	0
59	MG	AA	3262	1/1	0.98	0.03	15,15,15,15	0
59	MG	CA	3327	1/1	0.98	0.05	38,38,38,38	0
59	MG	AA	3560	1/1	0.98	0.05	29,29,29,29	0
59	MG	CA	3085	1/1	0.98	0.07	25,25,25,25	0
59	MG	AA	3561	1/1	0.98	0.07	21,21,21,21	0
59	MG	AA	3037	1/1	0.98	0.04	4,4,4,4	0
59	MG	AA	3410	1/1	0.98	0.10	57,57,57,57	0
59	MG	CA	3482	1/1	0.98	0.10	61,61,61,61	0
59	MG	AA	3411	1/1	0.98	0.04	12,12,12,12	0
59	MG	AA	3475	1/1	0.98	0.08	45,45,45,45	0
59	MG	AB	3007	1/1	0.98	0.04	39,39,39,39	0
59	MG	CA	3337	1/1	0.98	0.05	20,20,20,20	0
59	MG	AA	3734	1/1	0.98	0.09	26,26,26,26	0
59	MG	AA	3647	1/1	0.98	0.04	43,43,43,43	0
59	MG	AA	3412	1/1	0.98	0.10	39,39,39,39	0
59	MG	AB	3011	1/1	0.98	0.05	29,29,29,29	0
59	MG	AA	3317	1/1	0.98	0.07	24,24,24,24	0
59	MG	AA	3568	1/1	0.98	0.04	15,15,15,15	0
59	MG	AA	3097	1/1	0.98	0.10	22,22,22,22	0
59	MG	AA	3200	1/1	0.98	0.15	30,30,30,30	0
59	MG	AA	3484	1/1	0.98	0.08	53,53,53,53	0
59	MG	CA	3214	1/1	0.98	0.07	22,22,22,22	0
59	MG	AA	3084	1/1	0.98	0.07	23,23,23,23	0
59	MG	AA	3574	1/1	0.98	0.05	12,12,12,12	0
59	MG	AA	3243	1/1	0.98	0.10	43,43,43,43	0
59	MG	AA	3364	1/1	0.98	0.08	23,23,23,23	0
59	MG	AA	3421	1/1	0.98	0.07	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3491	1/1	0.98	0.04	46,46,46,46	0
59	MG	AA	3130	1/1	0.98	0.08	34,34,34,34	0
59	MG	CA	3653	1/1	0.98	0.06	32,32,32,32	0
59	MG	AA	3423	1/1	0.98	0.10	16,16,16,16	0
59	MG	AA	3581	1/1	0.98	0.07	52,52,52,52	0
59	MG	CA	3361	1/1	0.98	0.14	43,43,43,43	0
59	MG	AA	3494	1/1	0.98	0.06	34,34,34,34	0
59	MG	AA	3223	1/1	0.98	0.04	15,15,15,15	0
59	MG	CA	3006	1/1	0.98	0.03	22,22,22,22	0
59	MG	AA	3326	1/1	0.98	0.05	36,36,36,36	1
59	MG	CA	3661	1/1	0.98	0.09	27,27,27,27	0
59	MG	AA	3426	1/1	0.98	0.07	20,20,20,20	0
59	MG	CA	3512	1/1	0.98	0.07	53,53,53,53	0
59	MG	AA	3327	1/1	0.98	0.04	31,31,31,31	0
59	MG	AA	3757	1/1	0.98	0.03	14,14,14,14	0
59	MG	CA	3369	1/1	0.98	0.07	48,48,48,48	0
59	MG	AA	3429	1/1	0.98	0.09	31,31,31,31	0
59	MG	AD	310	1/1	0.98	0.07	46,46,46,46	0
59	MG	AA	3759	1/1	0.98	0.05	57,57,57,57	0
59	MG	AA	3147	1/1	0.98	0.22	40,40,40,40	1
59	MG	AA	3589	1/1	0.98	0.04	55,55,55,55	0
59	MG	AA	3085	1/1	0.98	0.11	46,46,46,46	0
59	MG	CA	3123	1/1	0.98	0.04	29,29,29,29	0
59	MG	AA	3591	1/1	0.98	0.11	52,52,52,52	0
59	MG	AA	3502	1/1	0.98	0.04	29,29,29,29	1
59	MG	CA	3525	1/1	0.98	0.10	23,23,23,23	0
59	MG	CA	3019	1/1	0.98	0.03	22,22,22,22	0
59	MG	AA	3295	1/1	0.98	0.07	57,57,57,57	0
59	MG	AA	3333	1/1	0.98	0.06	11,11,11,11	0
59	MG	AA	3038	1/1	0.98	0.17	29,29,29,29	1
59	MG	AA	3087	1/1	0.98	0.15	55,55,55,55	0
59	MG	BA	1750	1/1	0.98	0.05	55,55,55,55	0
59	MG	AA	3597	1/1	0.98	0.04	33,33,33,33	0
59	MG	AA	3770	1/1	0.98	0.08	43,43,43,43	0
59	MG	BA	1753	1/1	0.98	0.06	48,48,48,48	0
59	MG	AA	3681	1/1	0.98	0.04	42,42,42,42	0
59	MG	CA	3136	1/1	0.98	0.04	63,63,63,63	0
59	MG	AA	3510	1/1	0.98	0.05	17,17,17,17	0
59	MG	AA	3437	1/1	0.98	0.05	17,17,17,17	0
59	MG	AA	3774	1/1	0.98	0.22	25,25,25,25	1
59	MG	CA	3397	1/1	0.98	0.08	57,57,57,57	0
59	MG	AN	3002	1/1	0.98	0.09	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3255	1/1	0.98	0.09	28,28,28,28	0
59	MG	AA	3512	1/1	0.98	0.05	38,38,38,38	0
59	MG	BA	1760	1/1	0.98	0.07	53,53,53,53	0
59	MG	AA	3439	1/1	0.98	0.08	37,37,37,37	0
59	MG	AA	3515	1/1	0.98	0.07	12,12,12,12	0
59	MG	AP	202	1/1	0.98	0.21	21,21,21,21	1
59	MG	CA	3261	1/1	0.98	0.07	47,47,47,47	0
59	MG	AA	3778	1/1	0.98	0.04	43,43,43,43	0
59	MG	AA	3117	1/1	0.98	0.22	25,25,25,25	1
59	MG	CV	202	1/1	0.98	0.09	38,38,38,38	0
59	MG	AA	3052	1/1	0.98	0.07	11,11,11,11	0
59	MG	CA	3267	1/1	0.98	0.04	38,38,38,38	0
59	MG	AA	3053	1/1	0.98	0.12	19,19,19,19	0
59	MG	AA	3522	1/1	0.98	0.06	30,30,30,30	0
59	MG	AA	3523	1/1	0.98	0.03	13,13,13,13	0
59	MG	CA	3271	1/1	0.98	0.07	48,48,48,48	0
59	MG	CA	3272	1/1	0.98	0.14	49,49,49,49	0
59	MG	AA	3301	1/1	0.98	0.05	39,39,39,39	0
59	MG	AA	3525	1/1	0.98	0.07	35,35,35,35	0
59	MG	AU	202	1/1	0.98	0.06	31,31,31,31	0
59	MG	AA	3379	1/1	0.98	0.11	23,23,23,23	0
59	MG	CA	3562	1/1	0.98	0.04	29,29,29,29	0
59	MG	AA	3528	1/1	0.98	0.06	19,19,19,19	0
59	MG	AV	202	1/1	0.98	0.08	38,38,38,38	0
59	MG	BA	1777	1/1	0.98	0.13	71,71,71,71	0
59	MG	AA	3054	1/1	0.98	0.06	21,21,21,21	0
59	MG	CA	3052	1/1	0.98	0.10	44,44,44,44	0
59	MG	CA	3568	1/1	0.98	0.04	39,39,39,39	0
59	MG	CA	3283	1/1	0.98	0.03	31,31,31,31	0
59	MG	CA	3570	1/1	0.98	0.04	36,36,36,36	0
59	MG	AV	204	1/1	0.98	0.09	45,45,45,45	0
59	MG	AA	3303	1/1	0.98	0.06	24,24,24,24	0
59	MG	AA	3531	1/1	0.98	0.06	24,24,24,24	0
59	MG	AA	3382	1/1	0.98	0.05	37,37,37,37	0
59	MG	AA	3383	1/1	0.98	0.05	20,20,20,20	0
59	MG	AA	3534	1/1	0.98	0.10	14,14,14,14	0
59	MG	CA	3169	1/1	0.98	0.10	34,34,34,34	0
59	MG	CA	3170	1/1	0.98	0.04	32,32,32,32	0
59	MG	CA	3292	1/1	0.98	0.03	12,12,12,12	0
59	MG	AA	3702	1/1	0.98	0.10	14,14,14,14	0
59	MG	AA	3343	1/1	0.98	0.06	46,46,46,46	0
59	MG	CA	3584	1/1	0.98	0.05	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3439	1/1	0.98	0.08	32,32,32,32	0
59	MG	AA	3304	1/1	0.98	0.07	47,47,47,47	0
59	MG	AA	3173	1/1	0.98	0.07	46,46,46,46	0
59	MG	CA	3588	1/1	0.98	0.04	32,32,32,32	0
59	MG	AA	3279	1/1	0.98	0.09	34,34,34,34	0
59	MG	AA	3007	1/1	0.98	0.03	12,12,12,12	0
59	MG	AA	3543	1/1	0.98	0.06	32,32,32,32	0
59	MG	AA	3308	1/1	0.98	0.09	18,18,18,18	0
59	MG	AA	3013	1/1	0.98	0.05	28,28,28,28	0
59	MG	CA	3302	1/1	0.98	0.07	37,37,37,37	0
60	ZN	DN	501	1/1	0.98	0.04	117,117,117,117	0
61	SF4	BD	501	8/8	0.98	0.04	78,78,78,78	0
59	MG	CA	3449	1/1	0.98	0.04	55,55,55,55	0
59	MG	CA	3303	1/1	0.98	0.10	43,43,43,43	0
59	MG	AA	3392	1/1	0.98	0.07	17,17,17,17	0
59	MG	AA	3312	1/1	0.99	0.02	23,23,23,23	0
59	MG	AA	3393	1/1	0.99	0.07	23,23,23,23	0
59	MG	CA	3393	1/1	0.99	0.05	68,68,68,68	0
59	MG	AA	3727	1/1	0.99	0.03	23,23,23,23	0
59	MG	AA	3074	1/1	0.99	0.06	14,14,14,14	0
59	MG	AA	3332	1/1	0.99	0.04	17,17,17,17	0
59	MG	AA	3487	1/1	0.99	0.03	49,49,49,49	0
59	MG	AA	3784	1/1	0.99	0.07	59,59,59,59	0
59	MG	CA	3650	1/1	0.99	0.08	14,14,14,14	0
59	MG	AA	3679	1/1	0.99	0.04	36,36,36,36	0
59	MG	CA	3321	1/1	0.99	0.06	28,28,28,28	0
59	MG	CA	3401	1/1	0.99	0.04	28,28,28,28	0
59	MG	AA	3003	1/1	0.99	0.02	8,8,8,8	0
59	MG	BA	1769	1/1	0.99	0.05	58,58,58,58	0
59	MG	AA	3489	1/1	0.99	0.04	15,15,15,15	0
59	MG	AA	3022	1/1	0.99	0.02	5,5,5,5	0
59	MG	AA	3192	1/1	0.99	0.05	30,30,30,30	0
59	MG	AA	3537	1/1	0.99	0.10	20,20,20,20	0
59	MG	CA	3574	1/1	0.99	0.04	37,37,37,37	0
59	MG	AA	3538	1/1	0.99	0.05	15,15,15,15	0
59	MG	CA	3329	1/1	0.99	0.04	21,21,21,21	0
59	MG	AA	3738	1/1	0.99	0.07	24,24,24,24	0
59	MG	CA	3578	1/1	0.99	0.05	38,38,38,38	0
59	MG	AA	3793	1/1	0.99	0.07	7,7,7,7	0
59	MG	AA	3401	1/1	0.99	0.04	21,21,21,21	0
59	MG	CA	3262	1/1	0.99	0.03	11,11,11,11	0
59	MG	AA	3540	1/1	0.99	0.03	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3428	1/1	0.99	0.04	18,18,18,18	0
59	MG	AA	3457	1/1	0.99	0.05	30,30,30,30	0
59	MG	CA	3266	1/1	0.99	0.07	36,36,36,36	0
59	MG	AA	3260	1/1	0.99	0.06	21,21,21,21	0
59	MG	CA	3339	1/1	0.99	0.04	24,24,24,24	0
59	MG	AA	3011	1/1	0.99	0.04	16,16,16,16	0
59	MG	AA	3248	1/1	0.99	0.08	22,22,22,22	0
59	MG	CA	3342	1/1	0.99	0.03	33,33,33,33	0
59	MG	CA	3423	1/1	0.99	0.10	46,46,46,46	0
59	MG	AA	3320	1/1	0.99	0.09	37,37,37,37	0
59	MG	AE	303	1/1	0.99	0.09	19,19,19,19	0
59	MG	AA	3214	1/1	0.99	0.22	58,58,58,58	1
59	MG	CA	3346	1/1	0.99	0.06	30,30,30,30	0
59	MG	AA	3463	1/1	0.99	0.02	15,15,15,15	0
59	MG	AA	3407	1/1	0.99	0.04	10,10,10,10	0
59	MG	AA	3465	1/1	0.99	0.06	42,42,42,42	0
59	MG	AA	3103	1/1	0.99	0.02	5,5,5,5	0
59	MG	AA	3504	1/1	0.99	0.03	29,29,29,29	0
59	MG	CA	3211	1/1	0.99	0.04	29,29,29,29	0
59	MG	AF	305	1/1	0.99	0.08	19,19,19,19	0
59	MG	AF	306	1/1	0.99	0.06	36,36,36,36	0
59	MG	AA	3505	1/1	0.99	0.04	30,30,30,30	0
59	MG	CA	3356	1/1	0.99	0.07	44,44,44,44	0
59	MG	CA	3438	1/1	0.99	0.04	24,24,24,24	0
59	MG	CA	3282	1/1	0.99	0.05	36,36,36,36	0
59	MG	AA	3506	1/1	0.99	0.03	48,48,48,48	0
59	MG	CA	3151	1/1	0.99	0.03	38,38,38,38	0
59	MG	AA	3436	1/1	0.99	0.03	12,12,12,12	0
59	MG	CA	3443	1/1	0.99	0.04	28,28,28,28	0
59	MG	AA	3125	1/1	0.99	0.06	22,22,22,22	1
59	MG	AA	3438	1/1	0.99	0.06	17,17,17,17	0
59	MG	AA	3324	1/1	0.99	0.02	15,15,15,15	0
59	MG	AA	3345	1/1	0.99	0.07	6,6,6,6	0
59	MG	AA	3707	1/1	0.99	0.04	59,59,59,59	0
59	MG	AA	3239	1/1	0.99	0.14	25,25,25,25	1
59	MG	AA	3513	1/1	0.99	0.04	41,41,41,41	0
59	MG	AA	3072	1/1	0.99	0.03	19,19,19,19	0
59	MG	AA	3388	1/1	0.99	0.02	28,28,28,28	0
59	MG	AA	3821	1/1	0.99	0.09	82,82,82,82	0
59	MG	CA	3163	1/1	0.99	0.13	30,30,30,30	0
59	MG	CA	3372	1/1	0.99	0.08	35,35,35,35	0
59	MG	AA	3151	1/1	0.99	0.08	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	1746	1/1	0.99	0.04	33,33,33,33	0
59	MG	AA	3517	1/1	0.99	0.03	23,23,23,23	0
59	MG	AA	3663	1/1	0.99	0.05	11,11,11,11	0
59	MG	AA	3518	1/1	0.99	0.04	14,14,14,14	0
59	MG	DA	1691	1/1	0.99	0.06	63,63,63,63	0
59	MG	AA	3519	1/1	0.99	0.12	27,27,27,27	0
59	MG	AA	3476	1/1	0.99	0.03	28,28,28,28	0
59	MG	AA	3477	1/1	0.99	0.03	14,14,14,14	0
59	MG	AA	3478	1/1	0.99	0.04	33,33,33,33	0
59	MG	CA	3382	1/1	0.99	0.06	38,38,38,38	0
59	MG	CA	3383	1/1	0.99	0.04	30,30,30,30	0
59	MG	AA	3328	1/1	0.99	0.06	42,42,42,42	0
60	ZN	CY	501	1/1	0.99	0.03	101,101,101,101	0
59	MG	AA	3020	1/1	0.99	0.04	11,11,11,11	0
60	ZN	C5	102	1/1	0.99	0.04	66,66,66,66	0
60	ZN	C6	501	1/1	0.99	0.03	66,66,66,66	0
60	ZN	C9	501	1/1	0.99	0.03	75,75,75,75	0
59	MG	AA	3419	1/1	0.99	0.06	20,20,20,20	0
59	MG	AA	3526	1/1	0.99	0.11	19,19,19,19	0
59	MG	AV	205	1/1	0.99	0.04	42,42,42,42	0
59	MG	CA	3311	1/1	0.99	0.05	50,50,50,50	0
59	MG	AA	3482	1/1	0.99	0.03	41,41,41,41	0
59	MG	AA	3397	1/1	1.00	0.05	13,13,13,13	0
59	MG	AA	3569	1/1	1.00	0.04	17,17,17,17	0
59	MG	AA	3076	1/1	1.00	0.03	0,0,0,0	0
59	MG	AA	3335	1/1	1.00	0.08	15,15,15,15	0
59	MG	AA	3416	1/1	1.00	0.03	14,14,14,14	0
59	MG	AA	3801	1/1	1.00	0.05	27,27,27,27	0
60	ZN	AY	501	1/1	1.00	0.01	61,61,61,61	0
59	MG	AA	3396	1/1	1.00	0.07	16,16,16,16	0
60	ZN	A5	501	1/1	1.00	0.01	30,30,30,30	0
60	ZN	A6	102	1/1	1.00	0.03	40,40,40,40	0
60	ZN	A9	501	1/1	1.00	0.02	42,42,42,42	0

6.5 Other polymers

There are no such residues in this entry.