



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 12:04 pm BST

PDB ID : 4WPO  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with elongation factor G in the pre-translocational state  
Authors : Lin, J.; Gagnon, M.G.; Steitz, T.A.  
Deposited on : 2014-10-20  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11



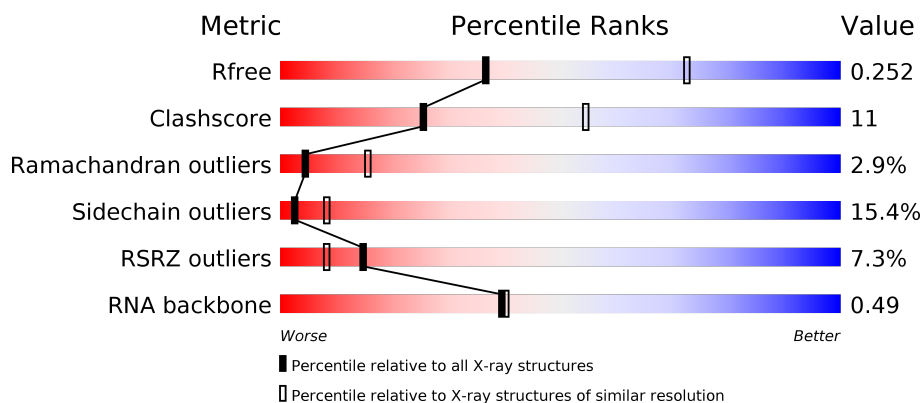
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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

Mol	Chain	Length	Quality of chain
1	AA	2915	<div> <div>2%</div> <div>39% 41% 16%</div> </div>
1	CA	2915	<div> <div>4%</div> <div>48% 37% 12%</div> </div>
2	AB	121	<div> <div>56% 35% 8%</div> </div>
2	CB	121	<div> <div>58% 31% 10%</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	24	
55	DV	24	
56	BW	76	
56	DW	76	
57	BX	77	
57	DX	77	
58	BY	76	
58	DY	76	
59	BZ	758	
59	DZ	758	

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
56	PSU	DW	55	-	-	-	X
56	4SU	DW	8	-	-	-	X
58	PSU	DY	55	-	-	-	X
60	MG	A0	104	-	-	-	X
60	MG	AA	3015	-	-	-	X
60	MG	AA	3051	-	-	-	X
60	MG	AA	3059	-	-	-	X
60	MG	AA	3088	-	-	-	X
60	MG	AA	3093	-	-	-	X
60	MG	AA	3108	-	-	-	X
60	MG	AA	3110	-	-	-	X
60	MG	AA	3136	-	-	-	X
60	MG	AA	3152	-	-	-	X

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	AA	3159	-	-	-	X
60	MG	AA	3161	-	-	-	X
60	MG	AA	3183	-	-	-	X
60	MG	AA	3192	-	-	-	X
60	MG	AA	3203	-	-	-	X
60	MG	AA	3210	-	-	-	X
60	MG	AA	3225	-	-	-	X
60	MG	AA	3234	-	-	-	X
60	MG	AA	3246	-	-	-	X
60	MG	AA	3249	-	-	-	X
60	MG	AA	3263	-	-	-	X
60	MG	AA	3490	-	-	-	X
60	MG	AA	3599	-	-	-	X
60	MG	AA	3640	-	-	-	X
60	MG	AA	3692	-	-	-	X
60	MG	AA	3702	-	-	-	X
60	MG	AA	3713	-	-	-	X
60	MG	AA	3739	-	-	-	X
60	MG	AA	3770	-	-	-	X
60	MG	AA	3805	-	-	-	X
60	MG	AA	3828	-	-	-	X
60	MG	AF	304	-	-	-	X
60	MG	BA	1621	-	-	-	X
60	MG	BA	1646	-	-	-	X
60	MG	BA	1657	-	-	-	X
60	MG	BA	1800	-	-	-	X
60	MG	BA	1804	-	-	-	X
60	MG	BK	3101	-	-	-	X
60	MG	BW	101	-	-	-	X
60	MG	CA	3015	-	-	-	X
60	MG	CA	3016	-	-	-	X
60	MG	CA	3031	-	-	-	X
60	MG	CA	3032	-	-	-	X
60	MG	CA	3042	-	-	-	X
60	MG	CA	3057	-	-	-	X
60	MG	CA	3063	-	-	-	X
60	MG	CA	3067	-	-	-	X
60	MG	CA	3070	-	-	-	X
60	MG	CA	3073	-	-	-	X
60	MG	CA	3079	-	-	-	X
60	MG	CA	3080	-	-	-	X
60	MG	CA	3085	-	-	-	X

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	CA	3087	-	-	-	X
60	MG	CA	3089	-	-	-	X
60	MG	CA	3090	-	-	-	X
60	MG	CA	3092	-	-	-	X
60	MG	CA	3098	-	-	-	X
60	MG	CA	3113	-	-	-	X
60	MG	CA	3139	-	-	-	X
60	MG	CA	3155	-	-	-	X
60	MG	CA	3177	-	-	-	X
60	MG	CA	3183	-	-	-	X
60	MG	CA	3194	-	-	-	X
60	MG	CA	3199	-	-	-	X
60	MG	CA	3206	-	-	-	X
60	MG	CA	3222	-	-	-	X
60	MG	CA	3467	-	-	-	X
60	MG	CA	3491	-	-	-	X
60	MG	CA	3543	-	-	-	X
60	MG	CA	3575	-	-	-	X
60	MG	CA	3590	-	-	-	X
60	MG	CA	3597	-	-	-	X
60	MG	CA	3653	-	-	-	X
60	MG	CF	306	-	-	-	X
60	MG	CQ	201	-	-	-	X
60	MG	DA	1608	-	-	-	X
60	MG	DA	1615	-	-	-	X
60	MG	DA	1671	-	-	-	X
60	MG	DA	1715	-	-	-	X
60	MG	DA	1739	-	-	-	X
60	MG	DA	1764	-	-	-	X
60	MG	DW	3001	-	-	-	X
60	MG	DX	3001	-	-	-	X



## 2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 313372 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	171	Total	C	N	O	S	0	0	0
			1349	862	243	242	2			
23	CZ	174	Total	C	N	O	S	0	0	0
			1360	870	243	245	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
24	C0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	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	1497	Total	C	N	O	P	0	0	0
			32185	14324	5968	10396	1497			
34	DA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

- 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	123	Total	C	N	O	S	0	0	0
			966	598	200	166	2			
46	DM	122	Total	C	N	O	S	0	0	0
			950	586	197	165	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	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
55	DV	12	Total	C	N	O	P	0	0	0
			252	115	46	80	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BW	74	Total	C	N	O	P	0	0	0
			1599	722	287	515	73			
56	DW	72	Total	C	N	O	P	0	0	0
			1552	697	280	502	72			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BX	76	Total	C	N	O	P	0	0	0
			1635	731	296	530	76			
57	DX	76	Total	C	N	O	P	0	0	0
			1635	731	296	530	76			

- Molecule 58 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BY	74	Total	C	N	O	P	0	0	0
			1581	707	285	515	73			

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
58	DY	73	Total	C	N	O	P	S	0	0	0
			1561	698	283	507	72	1			

- Molecule 59 is a protein called 50S ribosomal protein L9,Elongation factor G.

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

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AP	2	Total	Mg	0	0
			2	2		
60	CR	2	Total	Mg	0	0
			2	2		
60	BA	213	Total	Mg	0	0
			213	213		
60	CA	664	Total	Mg	0	0
			664	664		
60	C8	1	Total	Mg	0	0
			1	1		
60	C5	1	Total	Mg	0	0
			1	1		
60	AB	23	Total	Mg	0	0
			23	23		
60	BL	2	Total	Mg	0	0
			2	2		
60	CV	2	Total	Mg	0	0
			2	2		
60	A6	1	Total	Mg	0	0
			1	1		
60	BE	1	Total	Mg	0	0
			1	1		
60	AW	4	Total	Mg	0	0
			4	4		
60	AN	3	Total	Mg	0	0
			3	3		
60	DZ	1	Total	Mg	0	0
			1	1		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AX	2	Total 2	Mg 2	0	0
60	CN	1	Total 1	Mg 1	0	0
60	A2	1	Total 1	Mg 1	0	0
60	DX	1	Total 1	Mg 1	0	0
60	CY	1	Total 1	Mg 1	0	0
60	DD	1	Total 1	Mg 1	0	0
60	BB	1	Total 1	Mg 1	0	0
60	BT	1	Total 1	Mg 1	0	0
60	AE	5	Total 5	Mg 5	0	0
60	BM	1	Total 1	Mg 1	0	0
60	CU	1	Total 1	Mg 1	0	0
60	BF	1	Total 1	Mg 1	0	0
60	AV	1	Total 1	Mg 1	0	0
60	BX	15	Total 15	Mg 15	0	0
60	DA	168	Total 168	Mg 168	0	0
60	CB	13	Total 13	Mg 13	0	0
60	C0	2	Total 2	Mg 2	0	0
60	AA	834	Total 834	Mg 834	0	0
60	DF	1	Total 1	Mg 1	0	0
60	CQ	4	Total 4	Mg 4	0	0
60	A5	1	Total 1	Mg 1	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AR	1	Total 1	Mg 1	0	0
60	CG	1	Total 1	Mg 1	0	0
60	DK	2	Total 2	Mg 2	0	0
60	A1	2	Total 2	Mg 2	0	0
60	AD	10	Total 10	Mg 10	0	0
60	BN	2	Total 2	Mg 2	0	0
60	DJ	1	Total 1	Mg 1	0	0
60	BY	2	Total 2	Mg 2	0	0
60	C7	1	Total 1	Mg 1	0	0
60	C3	1	Total 1	Mg 1	0	0
60	AZ	1	Total 1	Mg 1	0	0
60	A4	1	Total 1	Mg 1	0	0
60	BK	1	Total 1	Mg 1	0	0
60	AU	4	Total 4	Mg 4	0	0
60	DW	1	Total 1	Mg 1	0	0
60	A9	1	Total 1	Mg 1	0	0
60	CF	6	Total 6	Mg 6	0	0
60	BV	1	Total 1	Mg 1	0	0
60	A0	5	Total 5	Mg 5	0	0
60	AG	2	Total 2	Mg 2	0	0
60	DE	2	Total 2	Mg 2	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AQ	3	Total 3	Mg 3	0	0
60	CE	6	Total 6	Mg 6	0	0
60	AH	1	Total 1	Mg 1	0	0
60	BZ	1	Total 1	Mg 1	0	0
60	CO	2	Total 2	Mg 2	0	0
60	CP	1	Total 1	Mg 1	0	0
60	A7	1	Total 1	Mg 1	0	0
60	CD	4	Total 4	Mg 4	0	0
60	BD	1	Total 1	Mg 1	0	0
60	DT	1	Total 1	Mg 1	0	0
60	A8	2	Total 2	Mg 2	0	0
60	AO	1	Total 1	Mg 1	0	0
60	BW	2	Total 2	Mg 2	0	0
60	AY	1	Total 1	Mg 1	0	0
60	AF	5	Total 5	Mg 5	0	0

- Molecule 61 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	1	Total 1	K 1	0	0

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	AY	1	Total 1	Zn 1	0	0

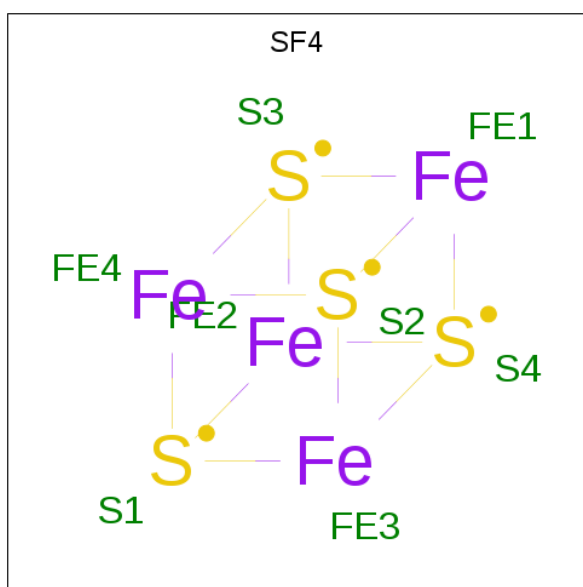
*Continued on next page...*



*Continued from previous page...*

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

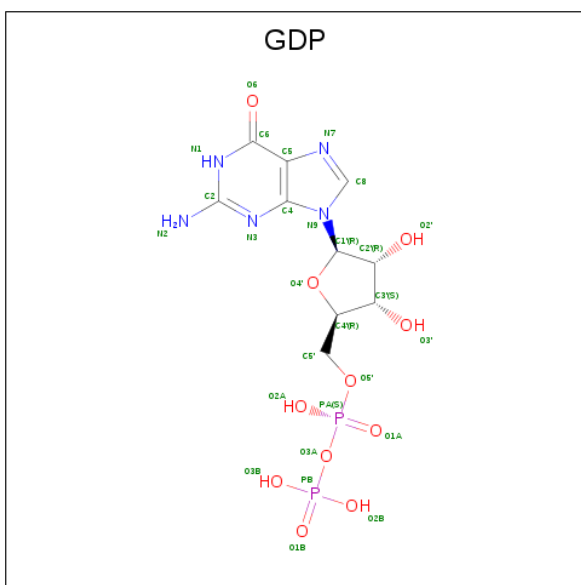
- Molecule 63 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).





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

- Molecule 64 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



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

- Molecule 65 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	AA	1408	Total	O	0	0
			1408	1408		
65	AB	36	Total	O	0	0
			36	36		
65	AD	15	Total	O	0	0
			15	15		
65	AE	19	Total	O	0	0
			19	19		
65	AF	7	Total	O	0	0
			7	7		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	AG	3	Total 3	O 3	0	0
65	AH	1	Total 1	O 1	0	0
65	AN	2	Total 2	O 2	0	0
65	AO	1	Total 1	O 1	0	0
65	AP	15	Total 15	O 15	0	0
65	AQ	4	Total 4	O 4	0	0
65	AR	2	Total 2	O 2	0	0
65	AS	1	Total 1	O 1	0	0
65	AT	2	Total 2	O 2	0	0
65	AU	5	Total 5	O 5	0	0
65	AV	2	Total 2	O 2	0	0
65	AW	2	Total 2	O 2	0	0
65	AX	3	Total 3	O 3	0	0
65	AZ	1	Total 1	O 1	0	0
65	A0	6	Total 6	O 6	0	0
65	A1	1	Total 1	O 1	0	0
65	A3	1	Total 1	O 1	0	0
65	A5	3	Total 3	O 3	0	0
65	A6	2	Total 2	O 2	0	0
65	A7	4	Total 4	O 4	0	0
65	A8	10	Total 10	O 10	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	BA	212	Total 212	O 212	0	0
65	BD	2	Total 2	O 2	0	0
65	BE	2	Total 2	O 2	0	0
65	BL	1	Total 1	O 1	0	0
65	BM	1	Total 1	O 1	0	0
65	BV	2	Total 2	O 2	0	0
65	BW	3	Total 3	O 3	0	0
65	BX	8	Total 8	O 8	0	0
65	BY	1	Total 1	O 1	0	0
65	BZ	2	Total 2	O 2	0	0
65	CA	985	Total 985	O 985	0	0
65	CB	9	Total 9	O 9	0	0
65	CD	14	Total 14	O 14	0	0
65	CE	13	Total 13	O 13	0	0
65	CF	7	Total 7	O 7	0	0
65	CN	2	Total 2	O 2	0	0
65	CP	10	Total 10	O 10	0	0
65	CQ	1	Total 1	O 1	0	0
65	CR	1	Total 1	O 1	0	0
65	CT	3	Total 3	O 3	0	0
65	CU	2	Total 2	O 2	0	0

*Continued on next page...*



*Continued from previous page...*

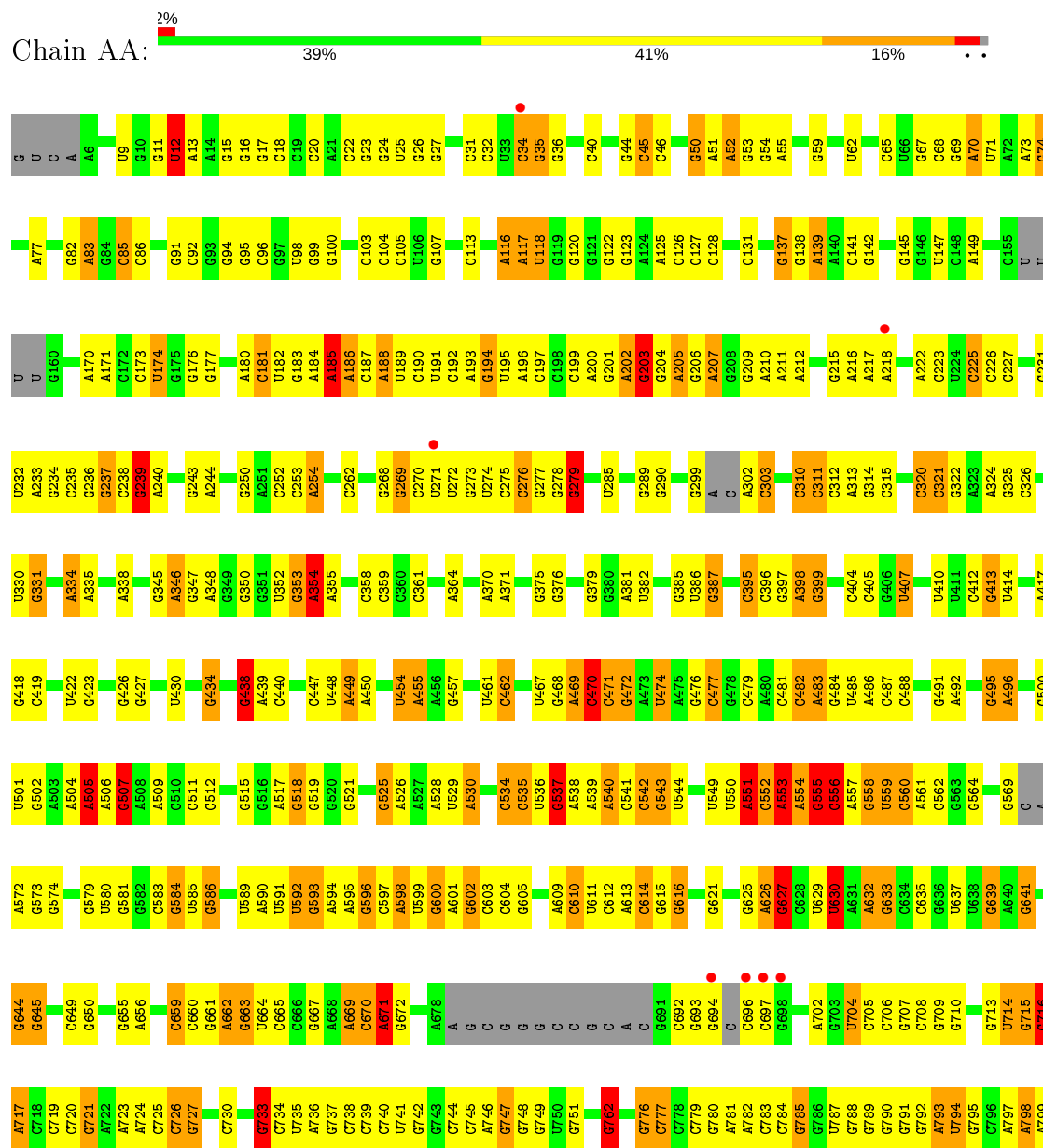
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	CV	1	Total	O	0	0
			1	1		
65	CY	1	Total	O	0	0
			1	1		
65	C0	6	Total	O	0	0
			6	6		
65	C1	2	Total	O	0	0
			2	2		
65	C3	2	Total	O	0	0
			2	2		
65	C6	1	Total	O	0	0
			1	1		
65	C7	1	Total	O	0	0
			1	1		
65	C8	3	Total	O	0	0
			3	3		
65	DA	155	Total	O	0	0
			155	155		
65	DE	4	Total	O	0	0
			4	4		
65	DJ	1	Total	O	0	0
			1	1		
65	DK	2	Total	O	0	0
			2	2		
65	DL	1	Total	O	0	0
			1	1		
65	DW	2	Total	O	0	0
			2	2		
65	DX	1	Total	O	0	0
			1	1		



### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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



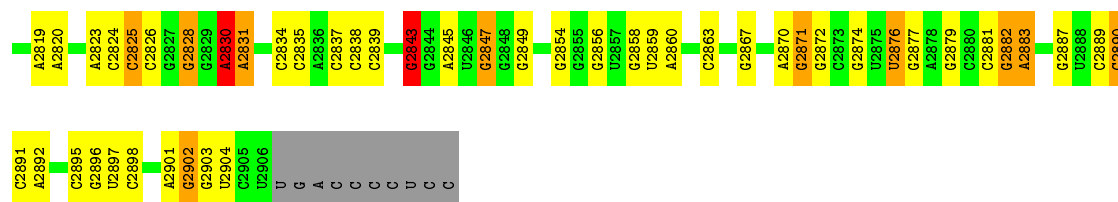


G1754	A1678	C1595	G1513	C1366	G1290	G1214	G1139	A1073	G1007	C935	C864	C800
G1755	A1679	C1596	C1514	A1367	G1291	G1217	U1140	A1074	U1008	C936	G865	C801
U1756	C1683	C1597	C1515	A1368	A1292	G1218	A1141	A1075	C1009	A937	A866	C802
G1757		C1598	A1518	A1369	A1293	G1219	A1142	G1076	C1010	G938	A867	G806
G1764	U1686	C1604	G1522	G1370	U1295	A1220	U1143	G1077	G1011	C939	U868	G807
U1765	A1687	A1605		G1371	U1296	G1221	A1144	A1078	U1014	C940	U869	A808
G1766	A1688	G1606	G1525	G1374	G1297	A1222	U1147	U1079	C1015	U941	C870	
A1767	G1689	G1607	G1526	U1375	G1298	A1223		G1080	C1016	A942	A871	A811
U1768			G1528	A1376	A1299	G1224	C1150	C1084	G1017	C944	C872	C813
G1769	C1691	C1611		A1377	A1300	G1231	U1151		A1018	A945	U875	U814
G1770	G1692	C1612		G1378	U1301	G1232	G1152	C1087	G1019	U876	U877	G816
C1693	C1693	A1613		C1379	G1302	A1233	G1153		G1022	G878	G879	G817
G1772	A1694		U1535	G1380	C1303	A1234	U1154	G1090	G1021	C954	U880	G818
C1695		A1616	C1539	U1381	G1304	G1235	C1155	A1091	G1022	A955	U881	
G1696	A1617	A1617		A1382	C1305	G1236	G1156	A1092	G1023	G879	U882	
G1697	A1618	A1618		G1383	G1306	G1237	A1157	G1093	G1024	A956	U883	
			A1542	G1384			G1158	A1094	G1025	A957	C881	U820
A1701	U1623	U1623		G1385	A1311	G1240	U1159	A1095	A1026	C958	A882	A821
A1702	C1624	C1624	U1543	U1386	G1312	G1241	G1160	A1096	A1027	U859	U883	G822
U1703	U1625	U1625	C1544	G1387	U1313	G1242		G1097	G1028	C960	C884	G823
C1704	A1626	A1626	G1545	A1388	A1314	U1243	C1169	C1098	A1029	C961	U885	U826
C1705	A1627	A1627	G1546	A1389	A1315	U1244	C1170	C1099	A1030	G962	U886	G827
					G1316	G1245	G1171	A1100	G1031	C887	U887	A828
C1709	G1628	G1628	U1549	G1391	G1317	G1246	A1172	G1101	C1032	A963	A888	A829
C1710	A1630	A1630	C1550	G1392	G1318	G1247	A1173	G1102	G1033	C969	C891	A830
A1711	C1631	C1631	C1551	G1393			A1174	A1103	A1036	C970	G892	A831
A1712	A1632	A1632	C1552	C1397	A1321	A1248	A1175	G1104	C1037	C971	U907	C842
C1713	A1633	A1633	A1553	U1398	A1322	G1249	U1176	G1105	G1038	A972	C843	C844
G1714	G1634	G1634	A1554	A1399	G1323	G1252	G1177	U1106	G1039	U894	C833	U834
A1715	C1635	C1635	A1556	A1400	A1324	C1253	U1178	U1107	G1040	G974	G895	A835
A1716	U1636	U1636		G1401		G1254	U1179	G1108	C1041	U895	A896	A836
A1804	G1637	G1637	C1561	G1402	G1329	A1255	C1180	G1109	G1042	G976	C897	C837
C1805	A1643	A1643	U1566	U1403	A1332	U1256	G1181	G1110	A1043	G977	U898	C838
G1718	C1644	C1644	G1567	G1404		G1257	G1182	U1111	G1044	G978	G839	A840
U1720	G1645	G1645		A1405		A1258	G1183	U1112		C980	U905	G841
G1721	C1646	C1646		A1406		A1259	G1184	U1113	G1048	C981	C906	G842
C1722	U1647	U1647	G1571	A1407	G1336	G1260	G1185	A1115	G1049	A986	U907	C843
A1723	G1648	G1648	G1572	G1410	C1337	G1261	U1186	C1050	C1051	C987	C908	G844
A1811	U1648	U1648	G1573	A1411	C1339	G1262	U1187	G1117	C1052	U988	U858	G845
G1725			A1574	A1412		G1265	A1188	C1118	C1053	C989	C912	A846
			A1575	G1415	G1342		A1189		C1054	A990	A913	A847
A1813	C1653	C1653	A1576		C1343	G1270	C1190	G1121	C1055	C991	U924	C853
A1814	A1654	A1654	G1577	U1418	G1344	G1271	C1196	C1122	C1056	G992	A925	U854
A1815	A1655	A1655	C1578	A1419	G1345	A1272	G1197	A1123	A1057	G993	A926	G855
A1817	A1656	A1656		G1420	A1347	G1273	C1198	U1124	G1058	G994	G927	G856
	C1657	C1657	G	C1421	A1348	G1274	C1199	U1125	U1059	C995	G928	U857
A1820	G1658	G1658	U	G1422	G1349	G1275	G1200	C1126	C1060	G996	U929	U858
C1821	A1660	A1660	A	G1423			A1201	U1127	G1061	C997	G930	C859
A1822			C	A1424	A1354	G1278		U1128	A1062	G998	G931	U860
G1823	A1664	A1664	G1584	A1425	G1355		C1204	U1129	A1067	A999	C932	C861
G1744	G1665	G1665	G1585	G1426	G1356	G1281	C1207	A1130	A1068	G999	C933	C862
A1745	A1666	A1666	G1586	G1427	G1357	G1282	G1208	A1131	G1069	C1000	A1004	C863
G1746	U1667	U1667	U1587	G1428	G1358	G1283	G1209	A1134	U1070	G1001	G934	
A1747			G1588	A1430	U1359	G1285	G1210	G1135	A1003	G1002	U935	
	C1671	C1671	A1589	A1431	C1360	U1286	G1211	G1136	A1004	A1005	U936	
G1750	G1672	G1672	C1590	G1432	C1361	A1287	G1212	G1137	G1071	A1006	A934	
A1751	G1673	G1673		C1433	C1362	A1288	U1213	C1138				
G1752	G1674	G1674	C1593	G1434	G1365	G1289						
U1753			C1594									



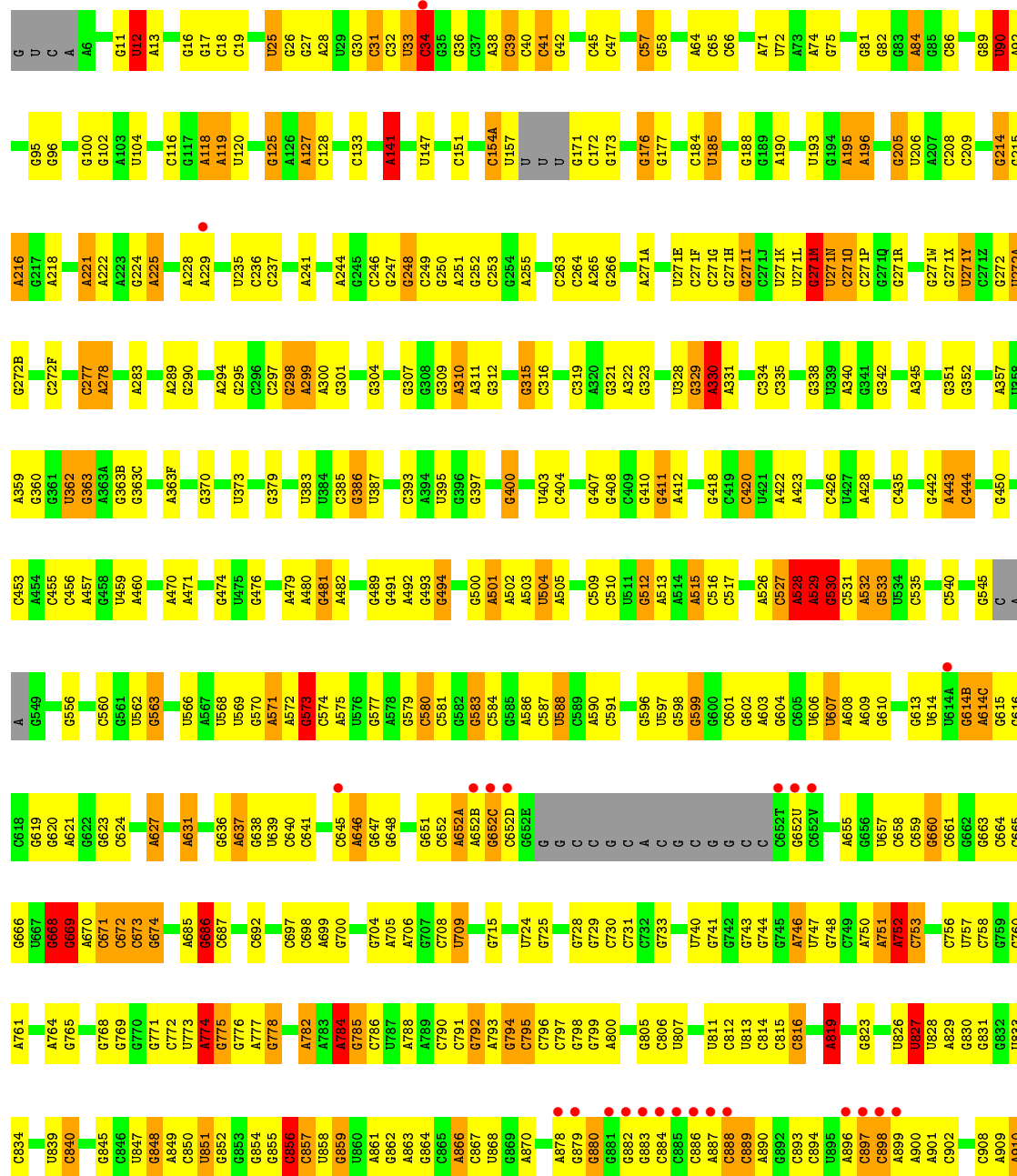
G2744	G2745	A2746	A2674	G2675	G2676	A2677	A2682	G2683	G2684	G2685	G2686	C2690	C2693	G2694	G2695	G2696	G2697	G2698	G2699	G2700	G2701	G2702	G2703	G2704	G2705	G2706	G2707	G2708	G2709	G2710	G2711	G2712	G2713	G2714	G2715	G2720	G2721	G2722	G2723	G2724	G2725	A2726	G2727	G2728	G2729	G2732	G2733	G2734	G2735	G2736	G2737	G2738	G2739	G2740	G2743																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
C2603	G2604	U2605	C2606	G2607	G2608	G2609	A2610	G2611	A2612	G2613	G2614	U2615	U2616	U2617	G2619	G2620	U2621	C2622	C2623	C2624	C2625	U2626	G2627	G2628	C2629	G2630	C2631	C2632	A2633	G2636	G2637	C2638	G2639	C2640	A2641	G2642	G2643	A2644	U2649	G2650	A2651	G2652	G2653	G2654	G2655	G2656	G2657	C2658	G2659	G2660	U2661	U2662	C2663	A2666	G2667																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
G2539	U2540	G2541	A2542	G2543	G2544	G2547	C2550	C2551	C2552	A2553	A2554	G2555	G2556	G2557	G2558	U2559	C2560	G2561	U2564	G2565	U2566	U2567	C2568	C2569	G2570	G2571	C2572	A2573	U2574	U2575	A2576	G2577	A2578	C2579	G2580	G2581	G2582	C2583	A2584	C2585	G2586	C2587	A2588	A2589	G2590	C2591	G2594	G2595	U2596	U2597	C2598	A2599	G2600	A2601	A2602																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
C2477	C2478	C2479	C2480	A2481	G2482	C2483	G2484	C2485	G2486	A2487	G2488	C2489	G2490	G2491	G2492	G2493	G2494	G2495	G2496	G2497	G2498	C2499	A2500	A2501	G2502	U2503	U2504	U2505	G2506	A2509	C2510	U2511	U2512	C2513	G2514	A2515	U2516	U2517	U2518	C2519	G2520	G2521	C2522	U2523	C2524	U2525	C2526	C2527	C2528	C2529	A2530	U2531	C2532	C2533	G2534	U2535	U2536	G2537	G2538	G2539	G2540	G2541	G2542	G2543	G2544	G2545	G2546	G2547	G2548	G2549	G2550	G2551	G2552	G2553	G2554	G2555	G2556	G2557	G2558	G2559	G2560	G2561	G2562	G2563	G2564	G2565	G2566	G2567	G2568	G2569	G2570	G2571	G2572	G2573	G2574	G2575	G2576	G2577	G2578	G2579	G2580	G2581	G2582	G2583	G2584	G2585	G2586	G2587	G2588	G2589	G2590	G2591	G2592	G2593	G2594	G2595	G2596	G2597	G2598	G2599	G2600	G2601	G2602	G2603	G2604	G2605	G2606	G2607	G2608	G2609	G2610	G2611	G2612	G2613	G2614	G2615	G2616	G2617	G2618	G2619	G2620	G2621	G2622	G2623	G2624	G2625	G2626	G2627	G2628	G2629	G2630	G2631	G2632	G2633	G2634	G2635	G2636	G2637	G2638	G2639	G2640	G2641	G2642	G2643	G2644	G2645	G2646	G2647	G2648	G2649	G2650	G2651	G2652	G2653	G2654	G2655	G2656	G2657	G2658	G2659	G2660	G2661	G2662	G2663	G2664	G2665	G2666	G2667	G2668	G2669	G2670	G2671	G2672	G2673	G2674	G2675	G2676	G2677	G2678	G2679	G2680	G2681	G2682	G2683	G2684	G2685	G2686	G2687	G2688	G2689	G2690	G2691	G2692	G2693	G2694	G2695	G2696	G2697	G2698	G2699	G2700	G2701	G2702	G2703	G2704	G2705	G2706	G2707	G2708	G2709	G2710	G2711	G2712	G2713	G2714	G2715	G2716	G2717	G2718	G2719	G2720	G2721	G2722	G2723	G2724	G2725	G2726	G2727	G2728	G2729	G2730	G2731	G2732	G2733	G2734	G2735	G2736	G2737	G2738	G2739	G2740	G2741	G2742	G2743	G2744	G2745	G2746	G2747	G2748	G2749	G2750	G2751	G2752	G2753	G2754	G2755	G2756	G2757	G2758	G2759	G2760	G2761	G2762	G2763	G2764	G2765	G2766	G2767	G2768	G2769	G2770	G2771	G2772	G2773	G2774	G2775	G2776	G2777	G2778	G2779	G2780	G2781	G2782	G2783	G2784	G2785	G2786	G2787	G2788	G2789	G2790	G2791	G2792	G2793	G2794	G2795	G2796	G2797	G2798	G2799	G2800	G2801	G2802	G2803	G2804	G2805	G2806	G2807	G2808	G2809	G2810	G2811	G2812	G2813	G2814	G2815	G2816	G2817	G2818	G2819	G2820	G2821	G2822	G2823	G2824	G2825	G2826	G2827	G2828	G2829	G2830	G2831	G2832	G2833	G2834	G2835	G2836	G2837	G2838	G2839	G2840	G2841	G2842	G2843	G2844	G2845	G2846	G2847	G2848	G2849	G2850	G2851	G2852	G2853	G2854	G2855	G2856	G2857	G2858	G2859	G2860	G2861	G2862	G2863	G2864	G2865	G2866	G2867	G2868	G2869	G2870	G2871	G2872	G2873	G2874	G2875	G2876	G2877	G2878	G2879	G2880	G2881	G2882	G2883	G2884	G2885	G2886	G2887	G2888	G2889	G2890	G2891	G2892	G2893	G2894	G2895	G2896	G2897	G2898	G2899	G2900	G2901	G2902	G2903	G2904	G2905	G2906	G2907	G2908	G2909	G2910	G2911	G2912	G2913	G2914	G2915	G2916	G2917	G2918	G2919	G2920	G2921	G2922	G2923	G2924	G2925	G2926	G2927	G2928	G2929	G2930	G2931	G2932	G2933	G2934	G2935	G2936	G2937	G2938	G2939	G2940	G2941	G2942	G2943	G2944	G2945	G2946	G2947	G2948	G2949	G2950	G2951	G2952	G2953	G2954	G2955	G2956	G2957	G2958	G2959	G2960	G2961	G2962	G2963	G2964	G2965	G2966	G2967	G2968	G2969	G2970	G2971	G2972	G2973	G2974	G2975	G2976	G2977	G2978	G2979	G2980	G2981	G2982	G2983	G2984	G2985	G2986	G2987	G2988	G2989	G2990	G2991	G2992	G2993	G2994	G2995	G2996	G2997	G2998	G2999	G3000	G3001	G3002	G3003	G3004	G3005	G3006	G3007	G3008	G3009	G3010	G3011	G3012	G3013	G3014	G3015	G3016	G3017	G3018	G3019	G3020	G3021	G3022	G3023	G3024	G3025	G3026	G3027	G3028	G3029	G3030	G3031	G3032	G3033	G3034	G3035	G3036	G3037	G3038	G3039	G3040	G3041	G3042	G3043	G3044	G3045	G3046	G3047	G3048	G3049	G3050	G3051	G3052	G3053	G3054	G3055	G3056	G3057	G3058	G3059	G3060	G3061	G3062	G3063	G3064	G3065	G3066	G3067	G3068	G3069	G3070	G3071	G3072	G3073	G3074	G3075	G3076	G3077	G3078	G3079	G3080	G3081	G3082	G3083	G3084	G3085	G3086	G3087	G3088	G3089	G3090	G3091	G3092	G3093	G3094	G3095	G3096	G3097	G3098	G3099	G3100	G3101	G3102	G3103	G3104	G3105	G3106	G3107	G3108	G3109	G3110	G3111	G3112	G3113	G3114	G3115	G3116	G3117	G3118	G3119	G3120	G3121	G3122	G3123	G3124	G3125	G3126	G3127	G3128	G3129	G3130	G3131	G3132	G3133	G3134	G3135	G3136	G3137	G3138	G3139	G3140	G3141	G3142	G3143	G3144	G3145	G3146	G3147	G3148	G3149	G3150	G3151	G3152	G3153	G3154	G3155	G3156	G3157	G3158	G3159	G3160	G3161	G3162	G3163	G3164	G3165	G3166	G3167	G3168	G3169	G3170	G3171	G3172	G3173	G3174	G3175	G3176	G3177	G3178	G3179	G3180	G3181	G3182	G3183	G3184	G3185	G3186	G3187	G3188	G3189	G3190	G3191	G3192	G3193	G3194	G3195	G3196	G3197	G3198	G3199	G3200	G3201	G3202	G3203	G3204	G3205	G3206	G3207	G3208	G3209	G3210	G3211	G3212	G3213	G3214	G3215	G3216	G3217	G3218	G3219	G3220	G3221	G3222	G3223	G3224	G3225	G3226	G3227	G3228	G3229	G3230	G3231	G3232	G3233	G3234	G3235	G3236	G3237	G3238	G3239	G3240	G3241	G3242	G3243	G3244	G3245	G3246	G3247	G3248	G3249	G3250	G3251	G3252	G3253	G3254	G3255	G3256	G3257	G3258	G3259	G3260	G3261	G3262	G3263	G3264	G3265	G3266	G3267	G3268	G3269	G3270	G3271	G3272	G3273	G3274	G3275	G3276	G3277	G3278	G3279	G3280	G3281	G3282	G3283	G3284	G3285	G3286	G3287	G3288	G3289	G3290	G3291	G3292	G3293	G3294	G3295	G3296	G3297	G3298	G3299	G3300	G3301	G3302	G3303	G3304	G3305	G3306	G3307	G3308	G3309	G3310	G3311	G3312	G3313	G3314	G3315	G3316	G3317	G3318	G3319	G3320	G3321	G3322	G3323	G3324	G3325	G3326	G3327	G3328	G3329	G3330	G3331	G3332	G3333	G3334	G3335	G3336	G3337	G3338	G3339	G3340	G3341	G3342	G3343	G3344	G3345	G3346	G3347	G3348	G3349	G3350	G3351	G3352	G3353	G3354	G3355	G3356	G3357	G3358	G3359	G3360	G3361	G3362	G3363	G3364	G3365	G3366	G3367	G3368	G3369	G3370	G3371	G3372	G3373	G3374	G3375	G3376	G3377	G3378	G3379	G3380	G3381	G3382	G3383	G3384	G3385	G3386	G3387	G3388	G3389	G3390	G3391	G3392	G3393	G3394	G3395	G3396	G3397	G3398	G3399	G3400	G3401	G3402	G3403	G3404	G3405	G3406	G3407	G3408	G3409	G3410	G3411	G3412	G3413	G3414	G3415	G3416	G3417	G3418	G3419	G3420	G3421	G3422	G3423	G3424	G3425	G3426	G3427	G3428	G3429	G3430	G3431	G3432	G3433	G3434	G3435	G3436	G3437	G3438	G3439	G3440	G3441	G3442	G3443	G3444	G3445	G3446	G3447	G3448	G3449	G3450	G3451	G3452	G3453	G3454	G3455	G3456	G3457	G3458	G3459	G3460	G3461	G3462	G3463	G3464	G3465	G3466	G3467	G3468	G3469	G3470	G3471	G3472	G3473	G3474	G3475	G3476	G3477	G3478	G3479	G3480	G3481	G3482	G3483	G3484	G3485	G3486	G3487	G3488	G3489	G3490	G3491	G3492	G3493	G3494	G3495	G3496	G3497	G3498	G3499	G3500	G3501	G3502	G3503	G3504	G3505	G3506	G3507	G3508	G3509	G3510	G3511	G3512	G3513	G3514	G3515	G3516	G3517	G3518	G3519	G3520	G3521	G3522	G3523	G3524	G3525	G3526	G3527	G3528	G3529	G3530	G3531	G3532	G3533	G3534	G3535	G3536	G3537	G3538	G3539	G3540	G3541	G3542	G3543	G3544	G3545	G3546	G3547	G3548	G3549	G3550	G3551	G3552	G3553	G3554	G3555	G3556	G3557	G3558	G3559	G3560	G3561	G3562	G3563	G3564	G3565	G3566	G3567	G3568	G3569	G3570	G3571	G3572	G3573	G3574	G3575	G3576	G3577	G3578	G3579	G3580	G3581	G3582	G3583	G3584	G3585	G3586	G3587	G3588	G3589	G3590	G3591	G3592	G3593	G3594	G3595	G3596	G3597	G3598	G3599	G3600	G3601	G3602	G3603	G3604	G3605	G3606	G3607	G3608	G3609	G3610	G3611	G3612	G3613	G3614	G3615	G3616	G3617	G3618	G3619	G3620	G3621	G3622	G3623	G3624	G3625	G3626	G3627	G3628	G3629	G3630	G3631	G3632	G3633	G3634	G3635	G3636	G3637	G3638	G3639	G3640	G3641	G3642	G3643	G3644	G3645	G3646	G3647	G3648	G3649	G3650	G3651	G3652	G3653	G3654	G3655	G3656	G3657	G3658	G3659	G3660	G3661	G3662	G3663	G3664	G3665	G3666	G3667</





# Molecule 1: 23S Ribosomal RNA

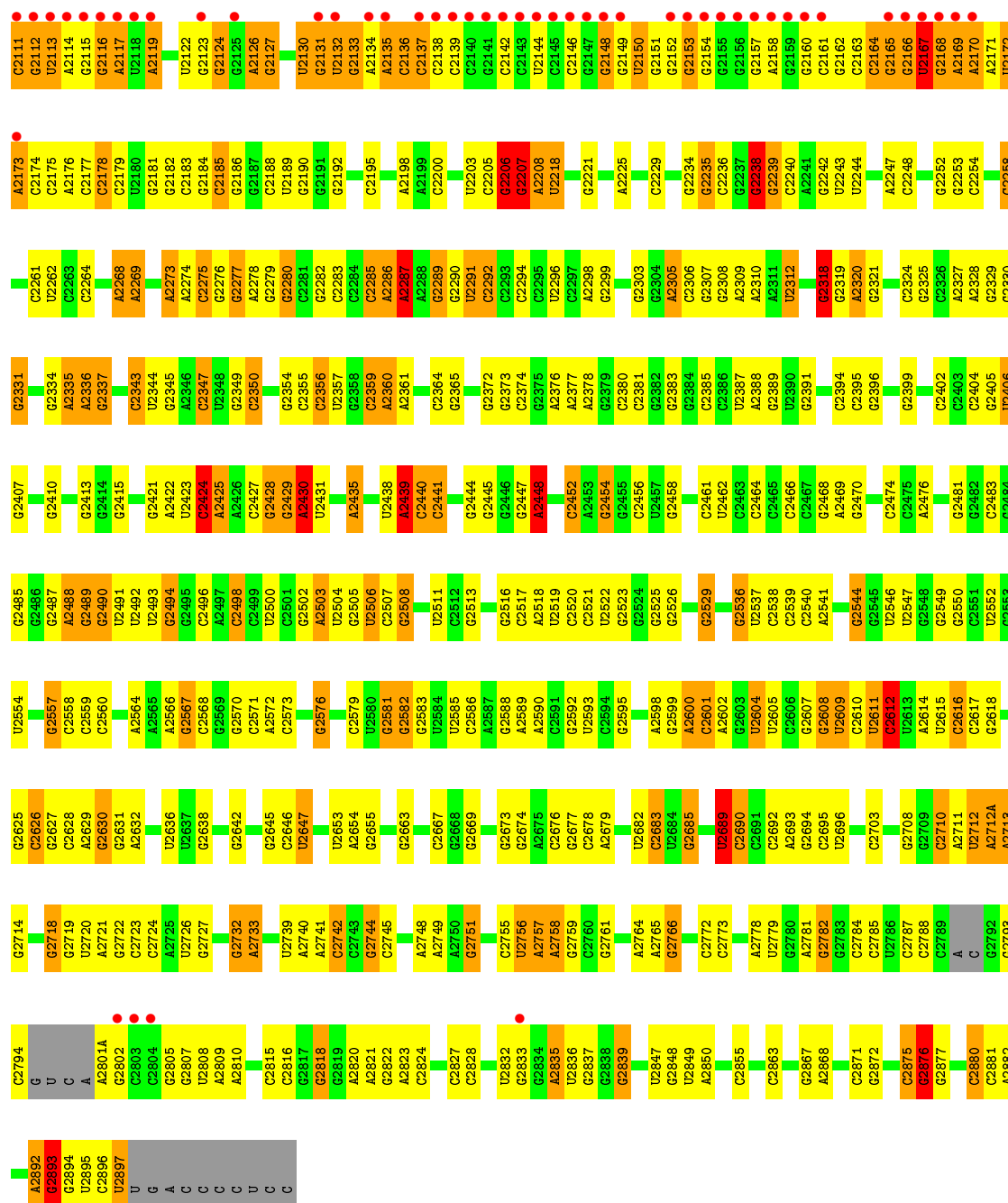
Chain CA: 4% 48% 37% 12% ..



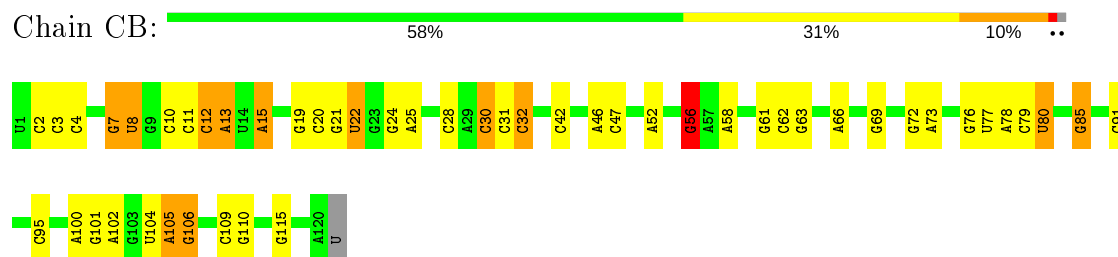


G2032	A1937	G1828	A1755	G1651	C1565	G1480	G1310	A1220	C1135	A1067	G997	C915
A2033	A1938	A1829	G1756	A1652	A1566	U1481	G1311	G1232	G1136	G1068	A1000	G916
	U1939	G1830	G1567	G1653	A1567	G1482	U1312	G1233	G1139	A1069	A1001	A917
C2036		G1831	A1762	A1654	G1568	G1484	U1313	G1234	C1140	G1071	G1003	A918
G2038	G1945	G1832	G1763	A1655	A1569	U1485	C1314	G1235	C1141	G1072	G1002	G919
G2039	U1946		G1764	A1656	A1570	A1486	C1315	U1236	U1142	A1073	C1004	
C2040	G1947	G1835	G1765	C1657	A1571	G1487	G1319	G1237	A1142A	G1074	C1005	U922
C2041	A1952	G1836	U1768	G1658		G1488	C1320	A1238	A1143	G1075	C1006	C923
A2042	U1955	G1837	C1771	U1489	C1577	U1489	G1321	G1239	C1144	C1076		C924
C2043		U1841	G1772	A1490	A1578	A1490	C1327	U1240	C1145	U1077	U1012	C925
		G1842	A1773		A1579			G1241		C1078	C1013	
G2045	U1963		C1774	G1494	C1582	G1494	A1331		G1149	U1079		G928
G1964	G1964	A1847	A1778	A1495	A1583	A1495	G1332	A1247	C1150	C1080	G1016	U930
A1966	A1966	A1848	U1779	A1496	A1586	G1497	A1336		G1151	U1081		G931
G1967	G1967	G1850	A1780	C1670	A1586	C1498	G1337	G1250	C1152	U1082	U1019	G932
G1968	G1968		C1781	C1671		C1499	G1338	G1251	C1153	U1083	A1020	A933
A1969	A1969	G1855	C1782	C1672	C1589	G1499	G1339	G1252	G1154	A1084	A1021	G934
A1970	A1970	G1856	A1783	G1674	U1590	G1500	U1340	A1253	A1155	A1085	G1022	
A1971	A1971	G1857	A1784	C1675	G1425	C1501	U1341	G1256	C1158	U1086	U1023	G938
A1972	A1972	A1858	A1785	A1676	A1426		A1342			G1087	G1024	
A1859	A1859	G1859	A1786	A1677	A1427	C1505	G1343	G1259	U1165	A1088	U1025	A941
G1860	G1860		U1680	U1678	C1604	G1509	G1344		C1166	U1090	U1026	G942
			G1681	G1681		A1509A		G1266		U1091	A1027	
C1866	C1866				C1607		G1348	U1267	G1169	C1082	A1029	G946
A1876	A1876	G1790	C1684	U1514	A1608	U1514	A1349	A1268	G1170	G1093	G1030	G947
A1877	A1877	A1791	A1609	G1515	A1609	G1515	C1350	A1269	G1171	U1094	G1031	G948
G1878	G1878	G1792	G1687	C1516	A1610	C1516	C1351	G1271	G	A1095	A1032	C949
		G1793	U1688	G1517	C1611	G1517	A1354	A1272	U	U1097	U1033	
G1883	G1883	U1794	A1689	U1518	C1612	U1518	G1355	A1273	A	A1098	G1034	G954
A1884	A1884	C1795	A1692	G1519	C1613	G1519	G1356	U1274	C1178	G1099	U1035	G955
A1885	A1885	U1796	U1693	A1614	A1614		A1359		C1179	C1100	G1036	G956
A1889	A1889	G1797	C1694	C1615	A1616	G1525	A1360	A1278	C1179	C1101	G1037	A957
A1890	A1890	U1798	G1695	A1616			C1180	G1279	C1180	U108	U958	A959
G1891	G1891	G1799	G1696	C1617		A1528	G1364		C1181	C1102	G1039	A960
		G1800	G1697		G1622		A1365	U1282		C1104		G961
G1801	G1801	A1698	C1697		G1623	C1532		G1283	G1184	U105	G1042	G962
A1802	A1802	G1699	A1698	C1532	G1623	U1532	G1368	A1284	G1106	G1107	G1043	U963
A1803	A1803	G1699	C1699	C1533			G1369	G1285	U1188	A1045	C1044	
C1804	C1804	A1700	G1700	A	G1626	U	C1370	A1286	A1189	U108	A1046	
U1805	U1805	G1701	A1701		G1627		G1371	A1287	U1189	C1109	G1047	G968
G1806	G1806	G1702	G1702	C1536	G1628	C1536	U1372	U1288	C1200	G1110	A1048	G971
G1807	G1807	G1703	G1703		U1629		A1373	C1289	C1201	A1111	G972	
U1808	U1808						G1374	C1290	G1202	U1112	C1052	A973
A1809	A1809	U1709	U1709	A1542	G1633	A1542	A1379	U1292	U1205	G1116	A1054	C975
A1810	A1810	C1710	A1634	C1546	A1634	C1546				C1119	G1055	A981
G1811	G1811			G1547	A1637	G1547		G1296	C1208	A1057	A1056	G982
A1812	A1812	U1713	G1714	C1548	C1638	C1548	A1384	C1297	G1209	G1058	G983	
G1813	G1813	G1714					G1385	C1298	G1209	U1122	G1059	
A1814	A1814	G1719		G1552	A1641	A1469	C1386	G1299	U1210	G1122	U1060	G987
G1815	G1815	U1720	U1720	A1553	G1642	G1470	C1387	A1301	U1211	G1125	U1061	
G1816	G1816	G1721	G1721	A1554	G1643	A1472		A1302	G1212	A1128	G1062	C991
G1817	G1817	A1722	A1722	A1554	G1644	G1473	U1394	A1303	G1215	A1129	G1063	C992
U1723	U1723	G1723	G1723	C1557	G1645	C1474	A1395	G1303	G1216	U1130	C1064	G993
U1739	U1739	U1739	U1739	A1558	G1646		U1396		C1217		U1066	
G1740	G1740	A1741	A1741	G1559	G1647	A1477	U1397	A1308				
				G1560	G1648	G1478		G1309				A996
						G1479	G1400					

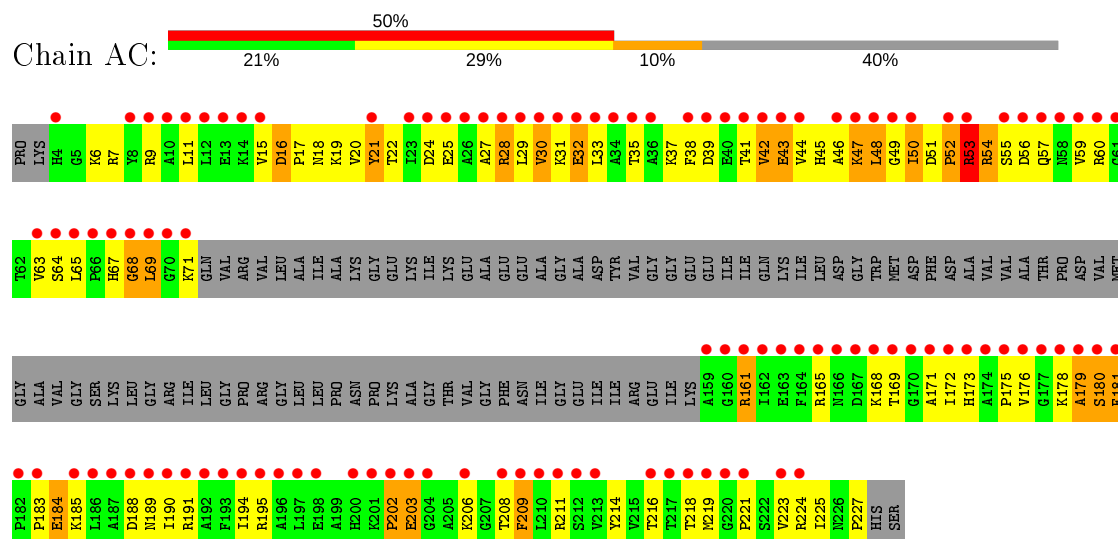




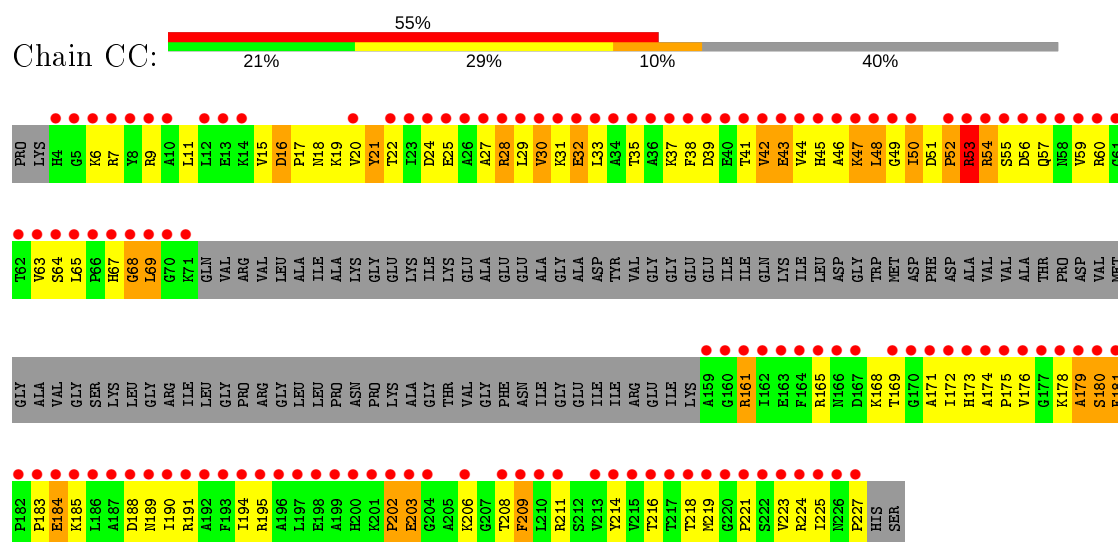




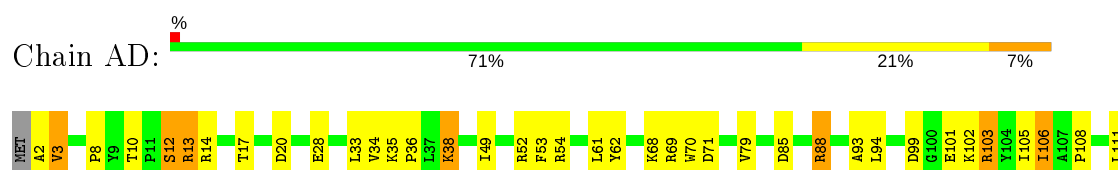
- Molecule 3: 50S ribosomal protein L1



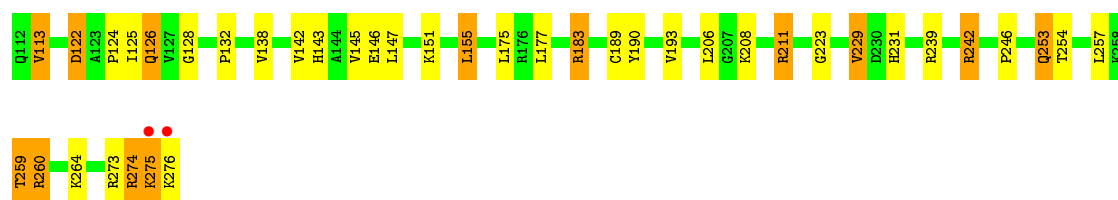
- Molecule 3: 50S ribosomal protein L1



- Molecule 4: 50S ribosomal protein L2

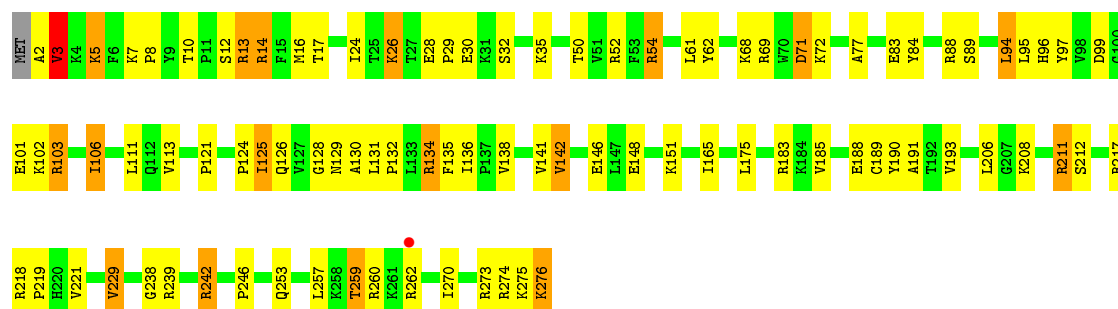






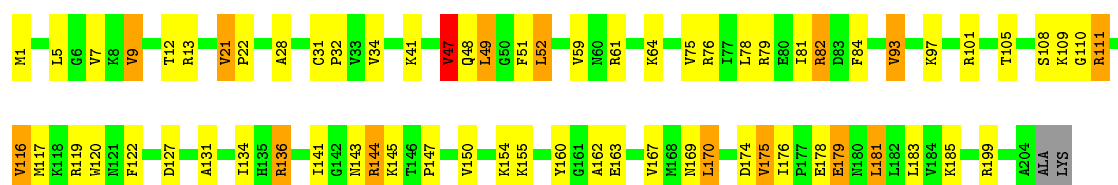
• Molecule 4: 50S ribosomal protein L2

Chain CD: 66% 27% 6%



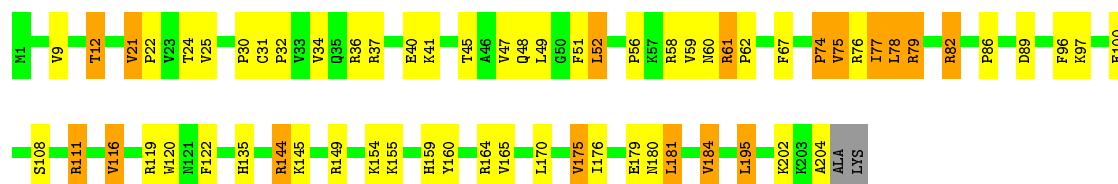
• Molecule 5: 50S ribosomal protein L3

Chain AE: 66% 26% 7%



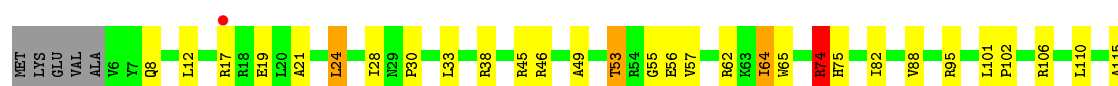
• Molecule 5: 50S ribosomal protein L3

Chain CE: 67% 23% 8%

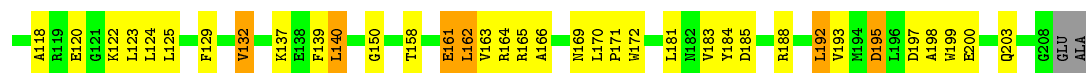


• Molecule 6: 50S ribosomal protein L4

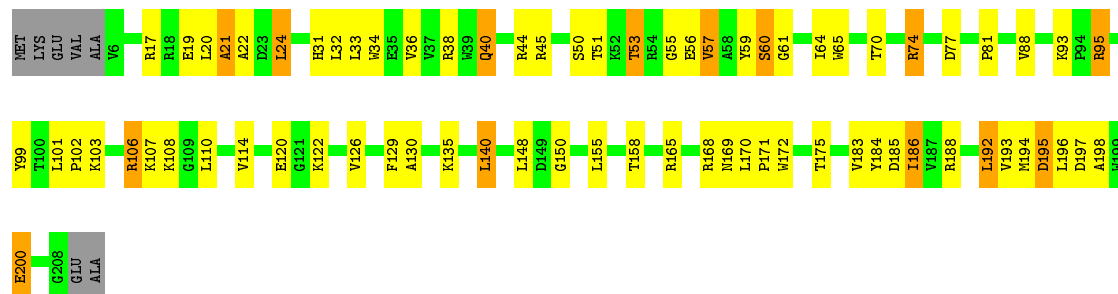
Chain AF: 65% 27% 8%



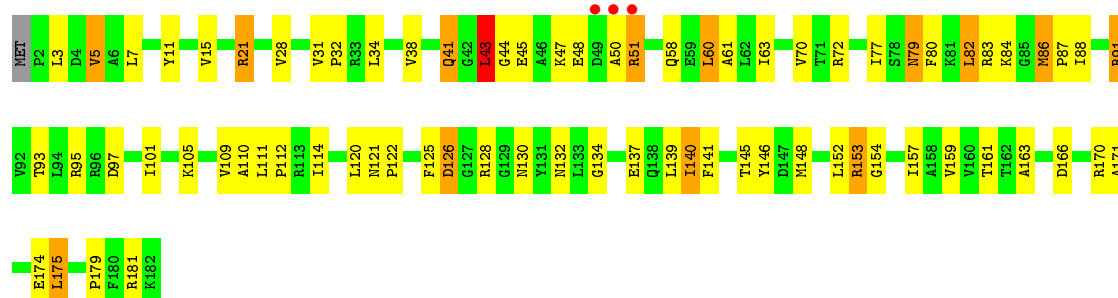




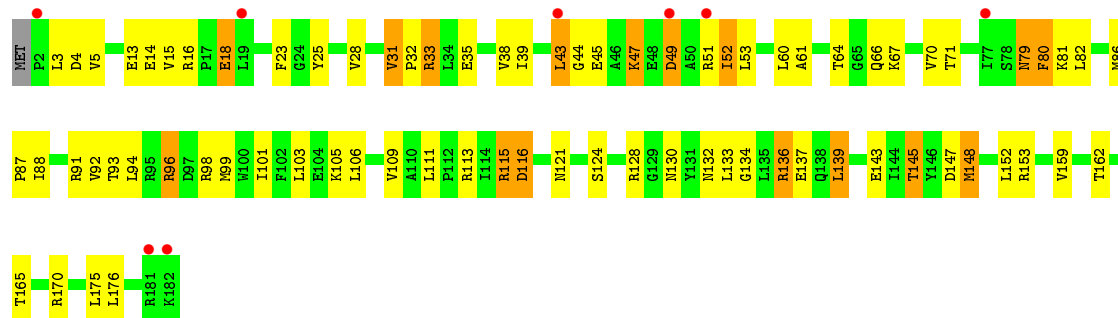
• Molecule 6: 50S ribosomal protein L4



• Molecule 7: 50S ribosomal protein L5



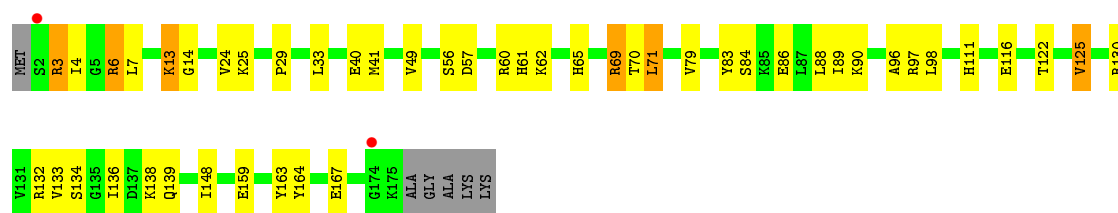
• Molecule 7: 50S ribosomal protein L5



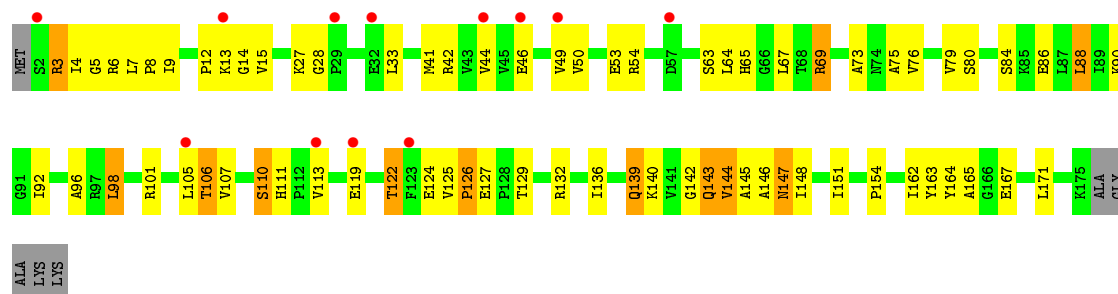
• Molecule 8: 50S ribosomal protein L6



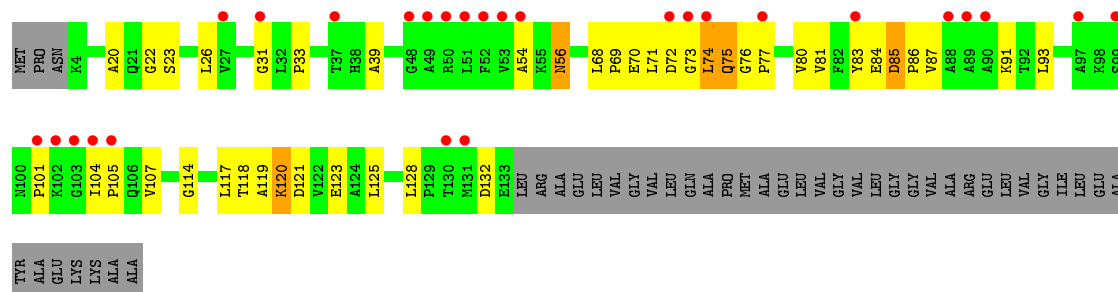




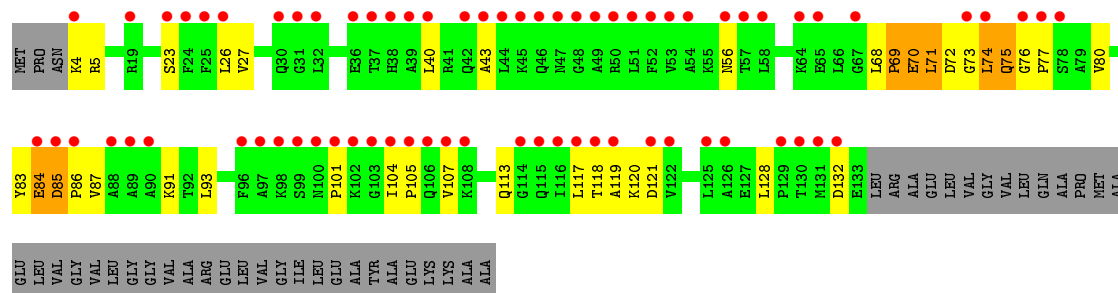
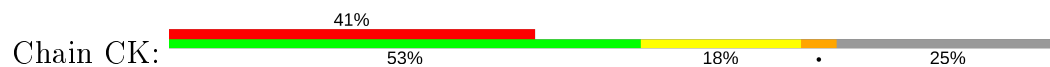
• Molecule 8: 50S ribosomal protein L6



• Molecule 9: 50S ribosomal protein L10



• Molecule 9: 50S ribosomal protein L10



• Molecule 10: 50S ribosomal protein L11



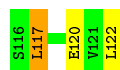
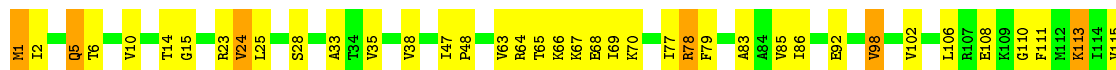




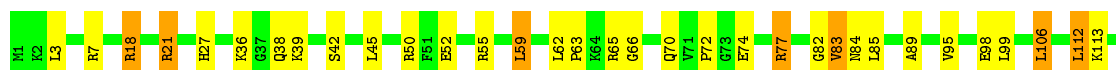




- Molecule 12: 50S ribosomal protein L14



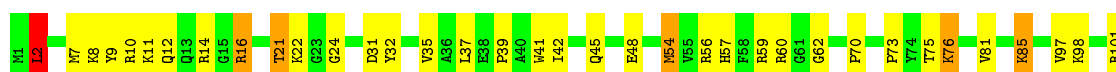
- Molecule 13: 50S ribosomal protein L15



- Molecule 13: 50S ribosomal protein L15



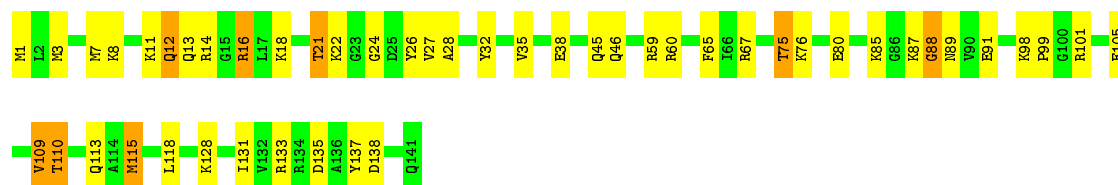
- Molecule 14: 50S ribosomal protein L16



- Molecule 14: 50S ribosomal protein L16

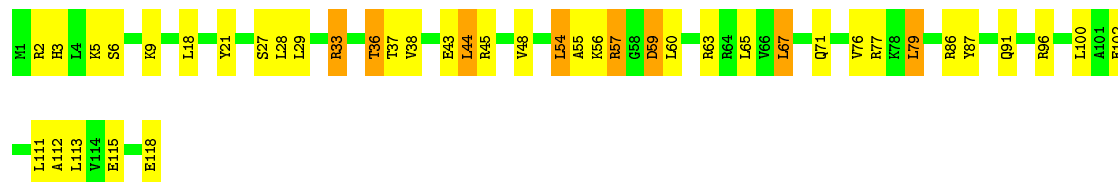






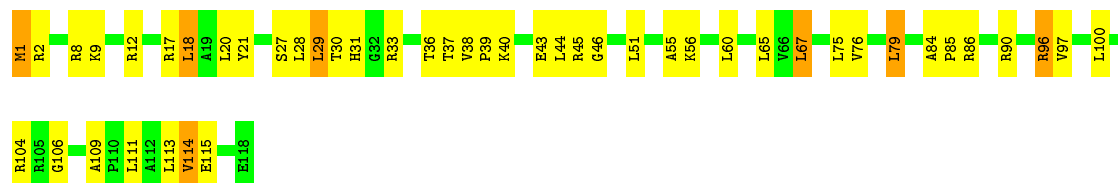
- Molecule 15: 50S ribosomal protein L17

Chain AR: 64% 29% 7%



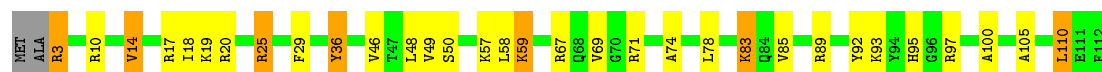
- Molecule 15: 50S ribosomal protein L17

Chain CR: 60% 34% 6%



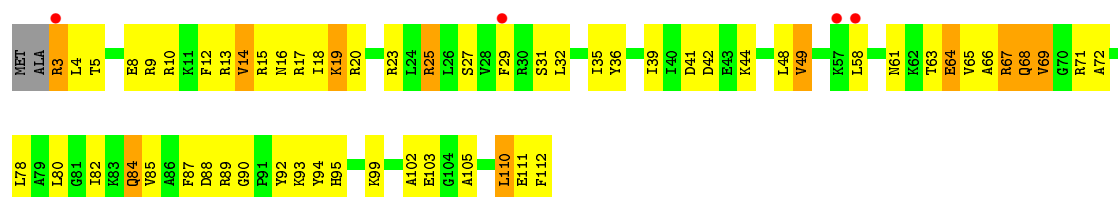
- Molecule 16: 50S ribosomal protein L18

Chain AS: 70% 22% 6%



- Molecule 16: 50S ribosomal protein L18

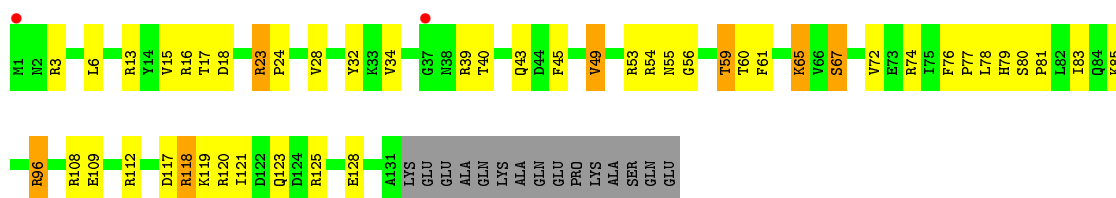
Chain CS: 45% 44% 10%



- Molecule 17: 50S ribosomal protein L19

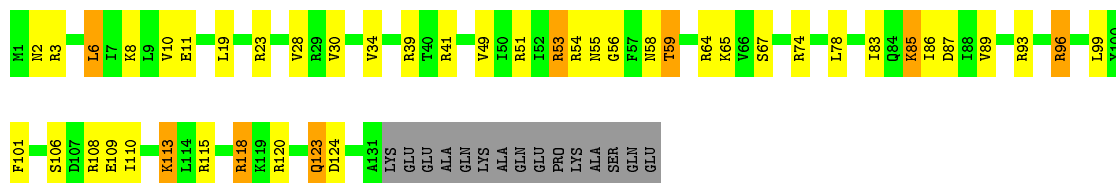
Chain AT: 57% 28% 5% 10%





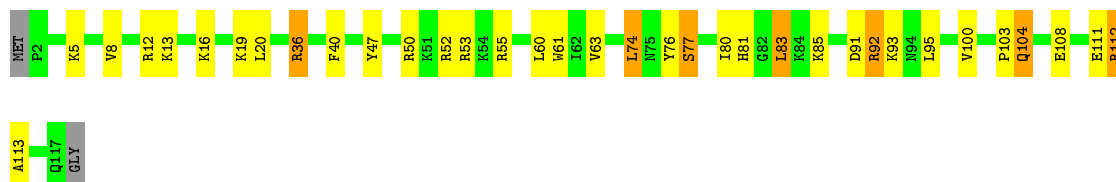
- Molecule 17: 50S ribosomal protein L19

Chain CT: 59% 25% 5% 10%



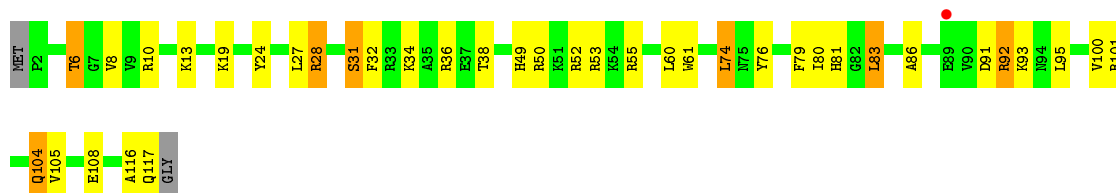
- Molecule 18: 50S ribosomal protein L20

Chain AU: 69% 24% 6%



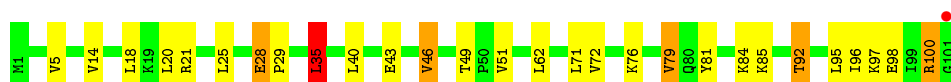
- Molecule 18: 50S ribosomal protein L20

Chain CU: 66% 26% 6%



- Molecule 19: 50S ribosomal protein L21

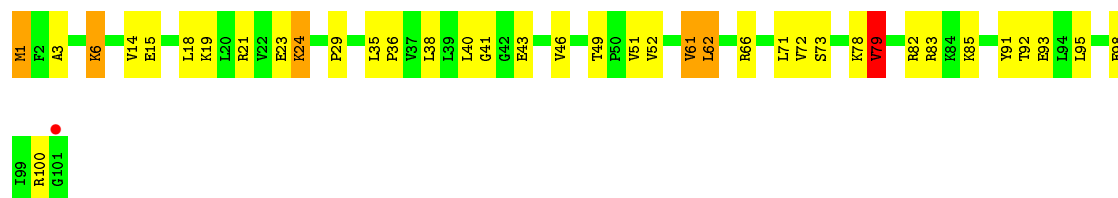
Chain AV: 72% 22% 5%



- Molecule 19: 50S ribosomal protein L21

Chain CV: 62% 32% 5%





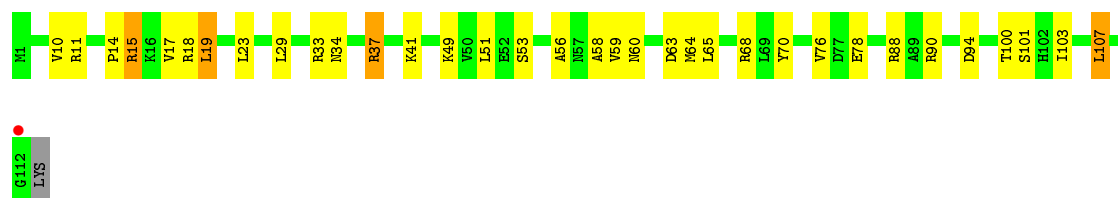
- Molecule 20: 50S ribosomal protein L22

Chain AW: 76% 18% 5% •



- Molecule 20: 50S ribosomal protein L22

Chain CW: 69% 27% • •



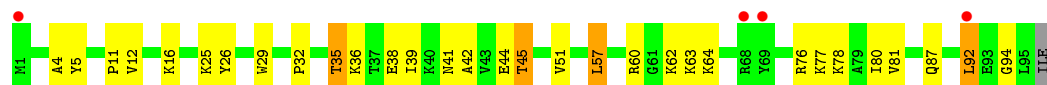
- Molecule 21: 50S ribosomal protein L23

Chain AX: 69% 27% • • •



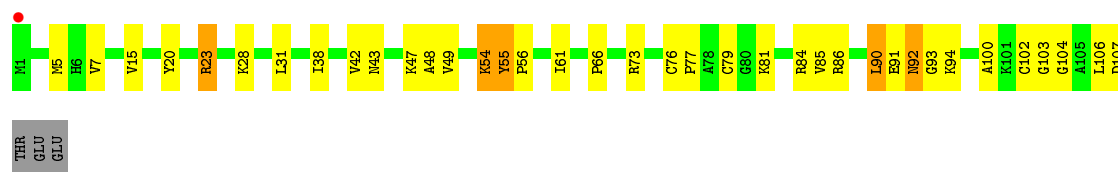
- Molecule 21: 50S ribosomal protein L23

Chain CX: 67% 28% • •



- Molecule 22: 50S ribosomal protein L24

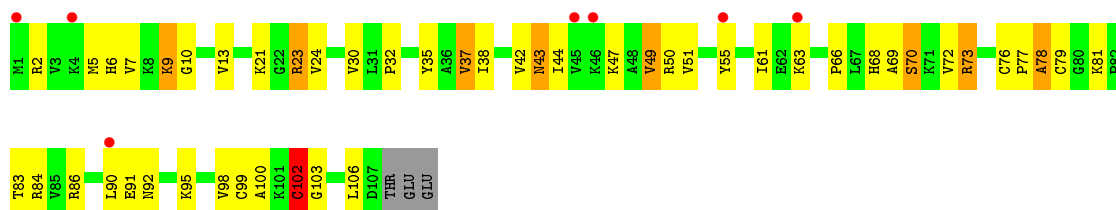
Chain AY: 64% 29% 5% •



- Molecule 22: 50S ribosomal protein L24

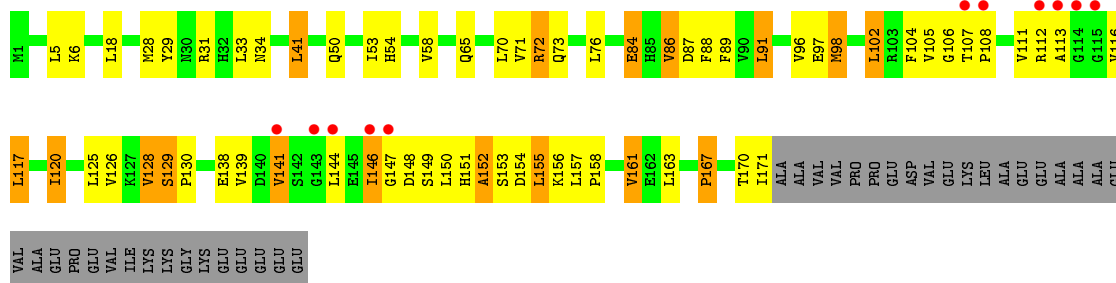


Chain CY: 



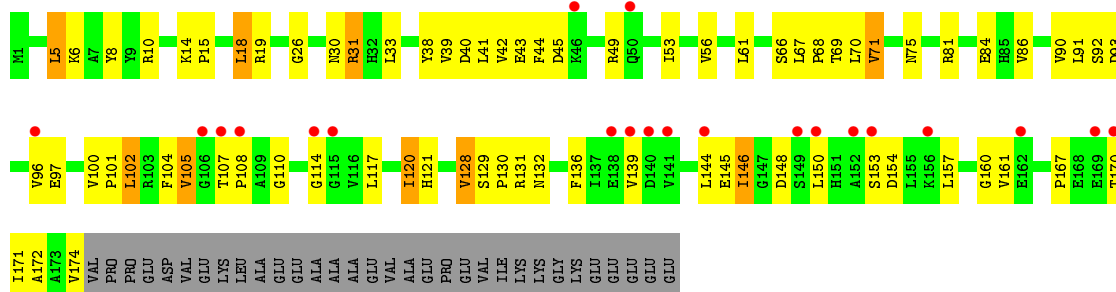
- Molecule 23: 50S ribosomal protein L25

Chain AZ: 




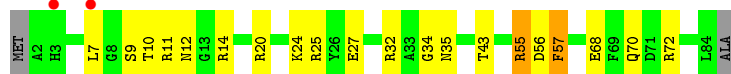
- Molecule 23: 50S ribosomal protein L25

Chain CZ: 



- Molecule 24: 50S ribosomal protein L27

Chain A0: 



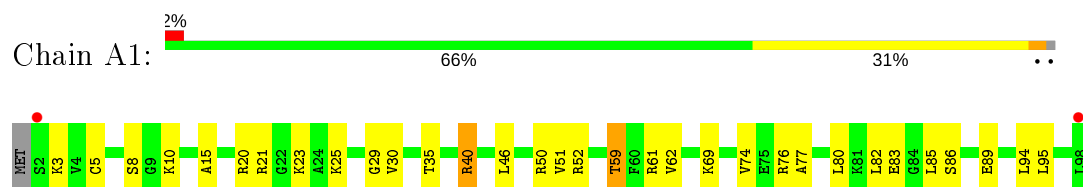
- Molecule 24: 50S ribosomal protein L27

Chain C0: 

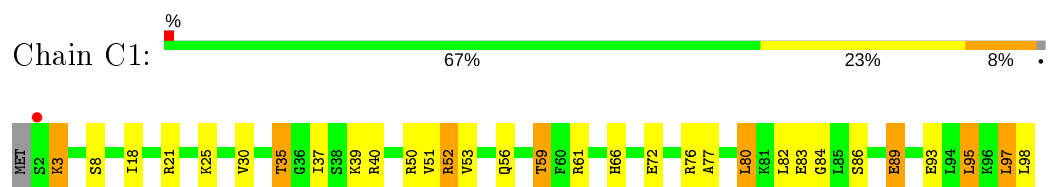




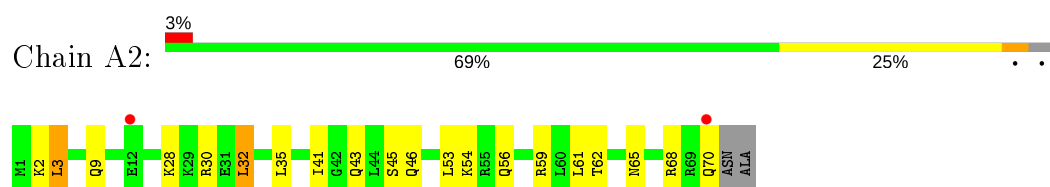
## • Molecule 25: 50S ribosomal protein L28



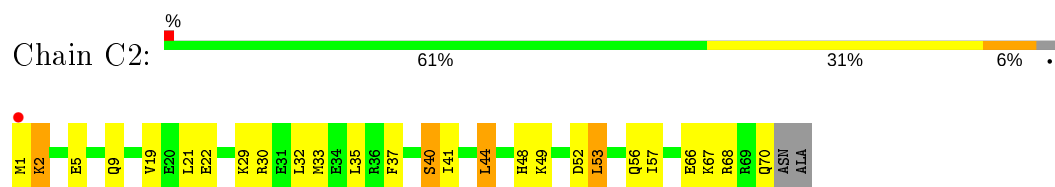
## • Molecule 25: 50S ribosomal protein L28



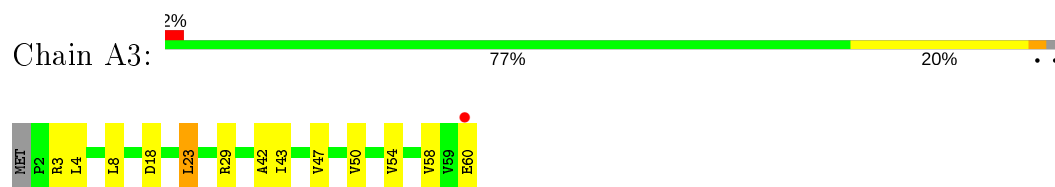
## • Molecule 26: 50S ribosomal protein L29



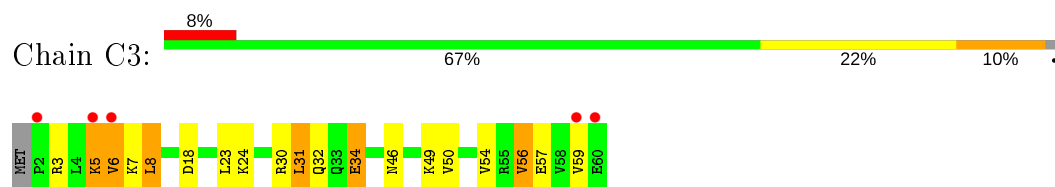
## • Molecule 26: 50S ribosomal protein L29



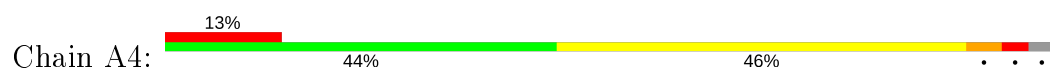
## • Molecule 27: 50S ribosomal protein L30



## • Molecule 27: 50S ribosomal protein L30



## • Molecule 28: 50S ribosomal protein L31







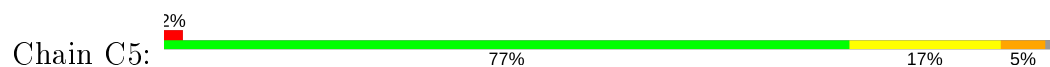
- Molecule 28: 50S ribosomal protein L31



- 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



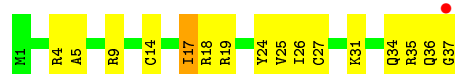
- Molecule 32: 50S ribosomal protein L35



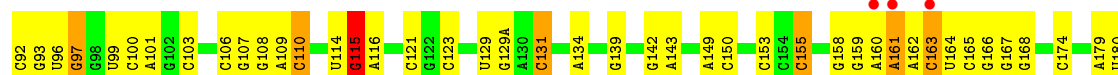
- Molecule 33: 50S ribosomal protein L36



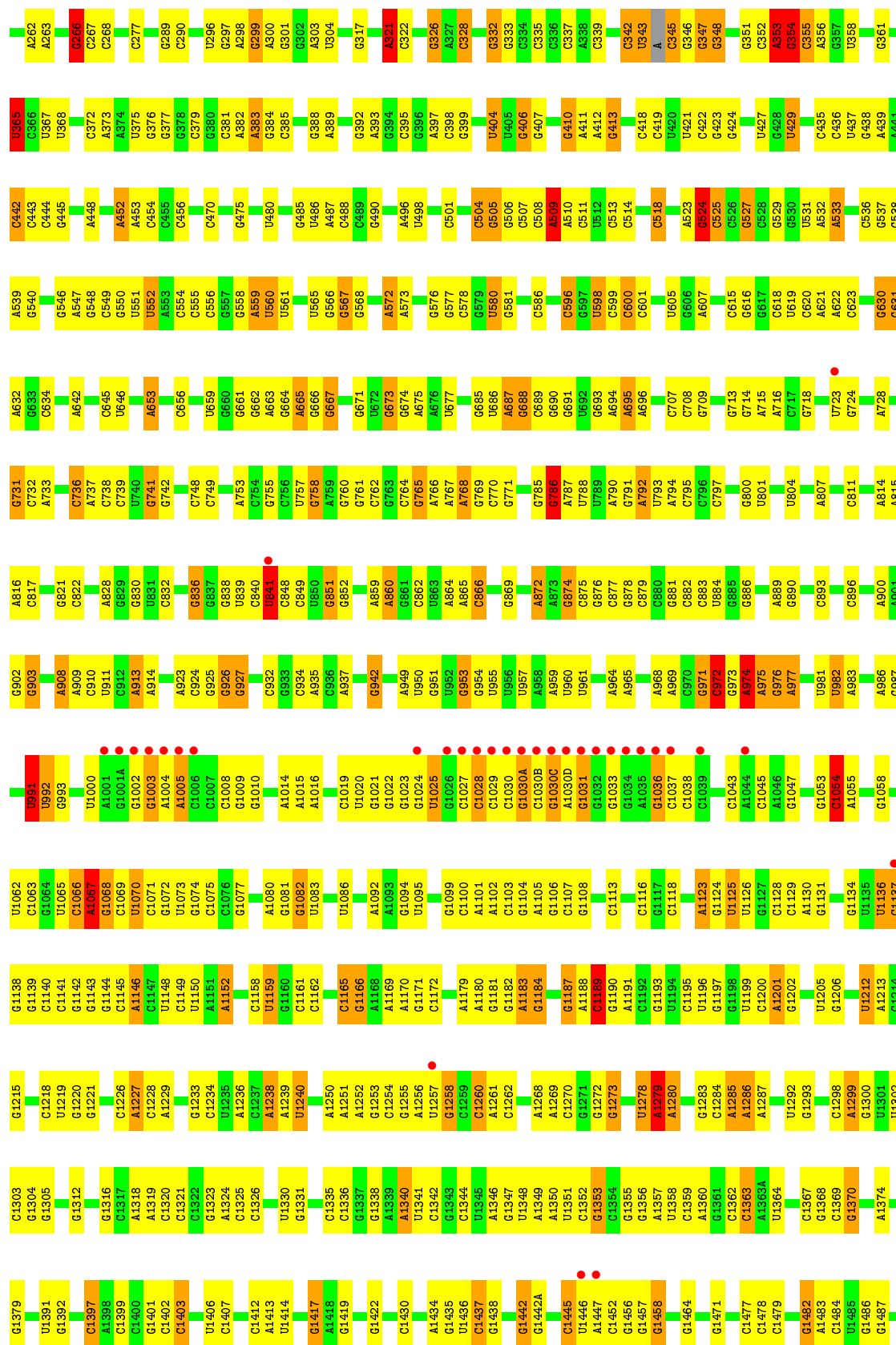
- Molecule 33: 50S ribosomal protein L36



- Molecule 34: 16S Ribosomal RNA



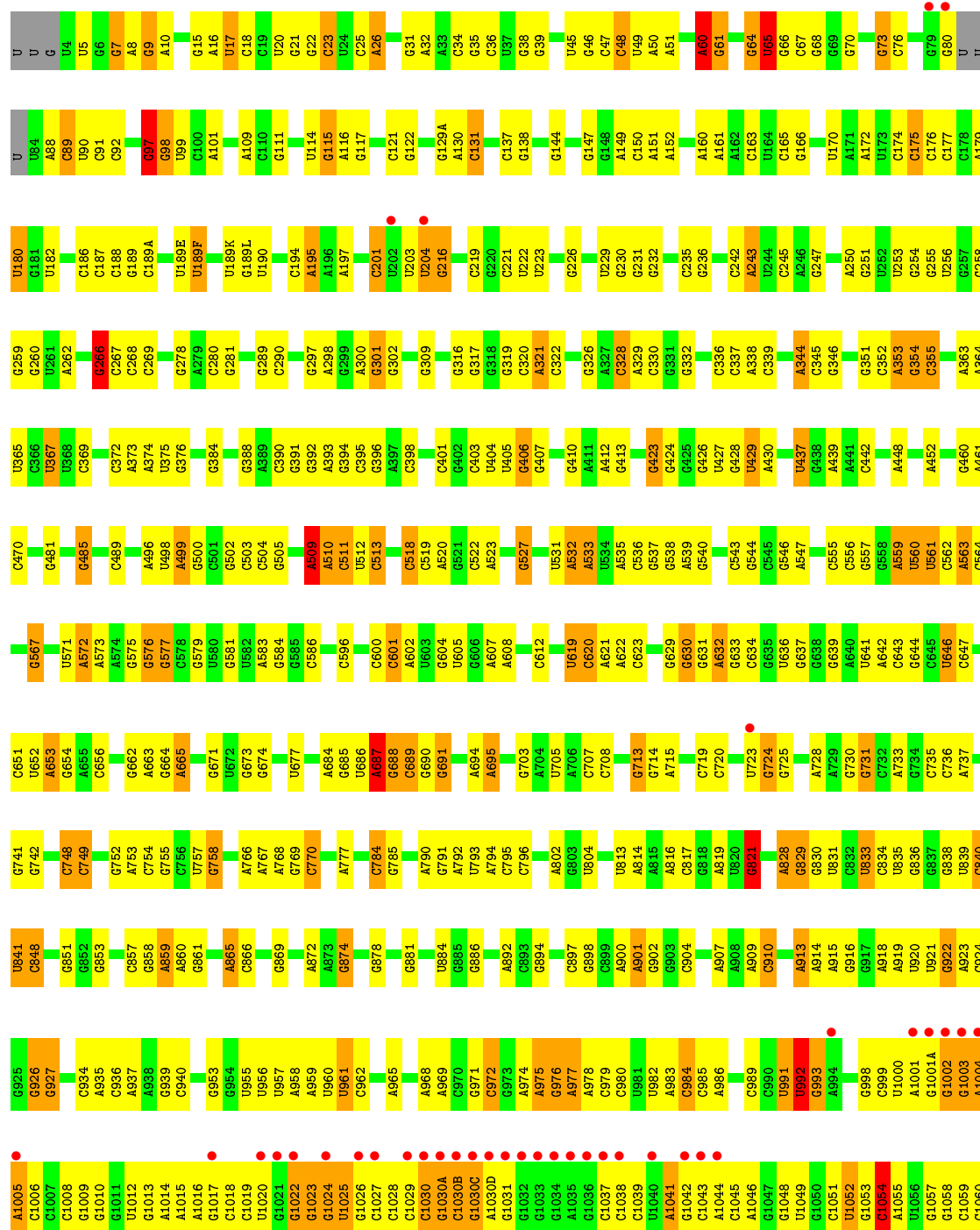




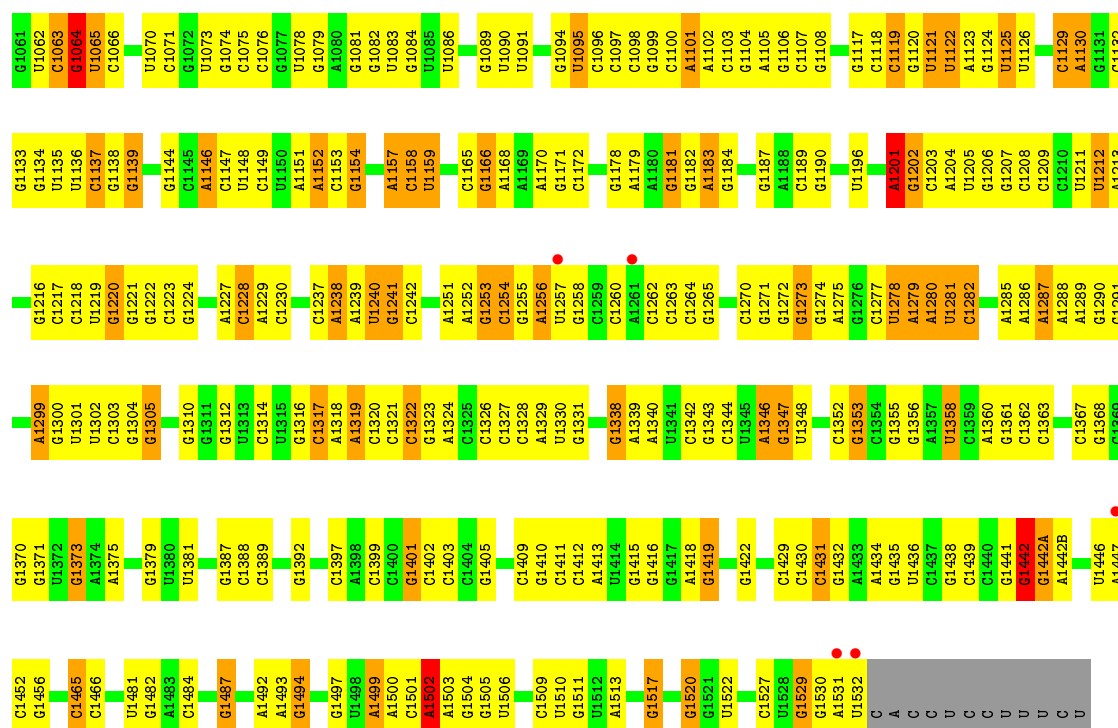




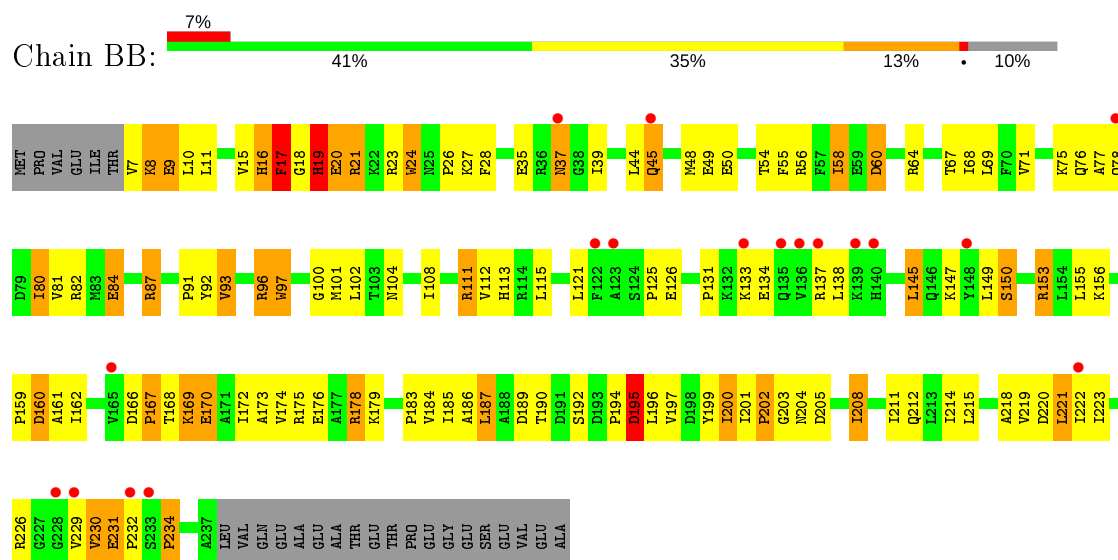
• Molecule 34: 16S Ribosomal RNA



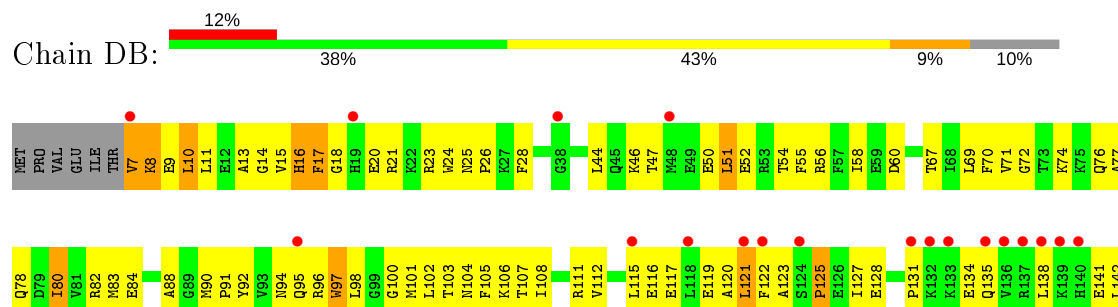




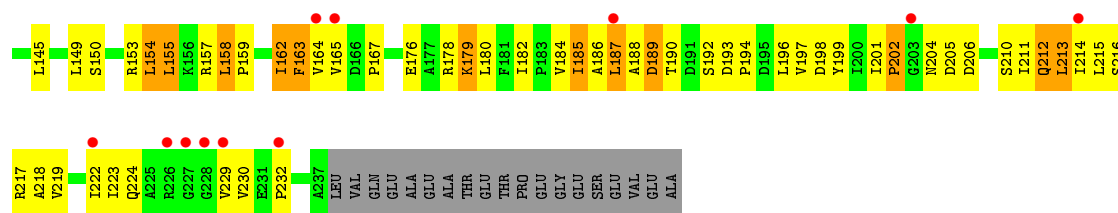
• Molecule 35: 30S ribosomal protein S2



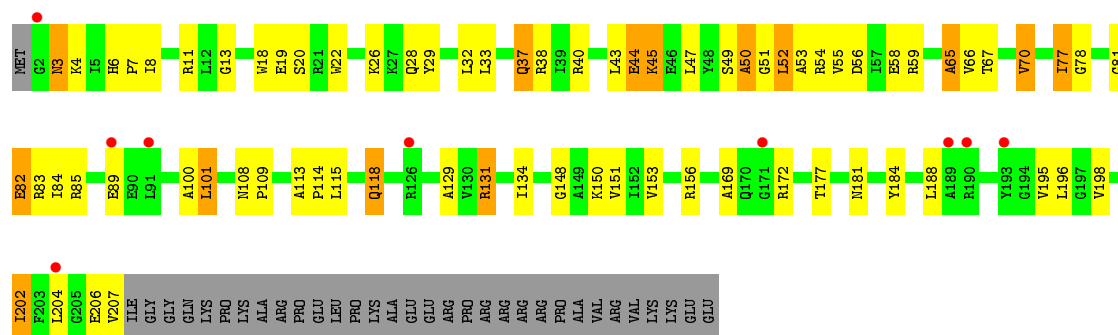
• Molecule 35: 30S ribosomal protein S2



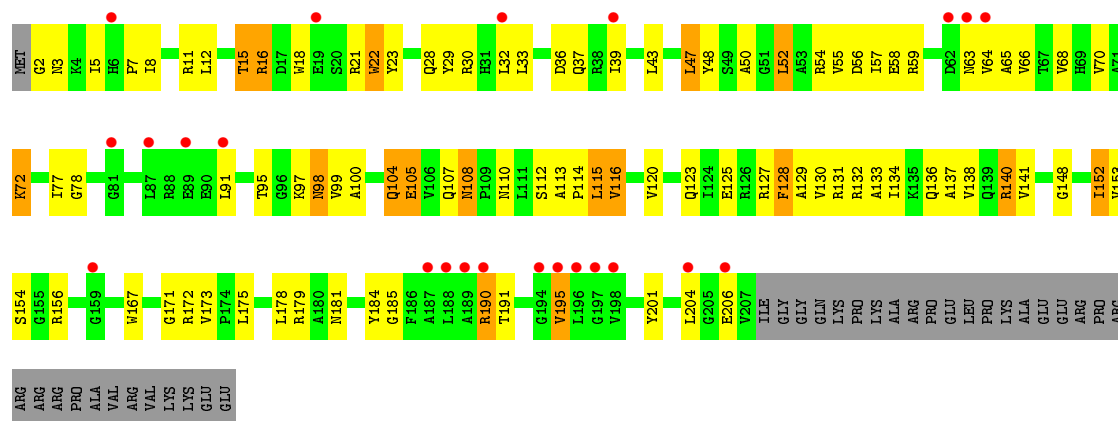




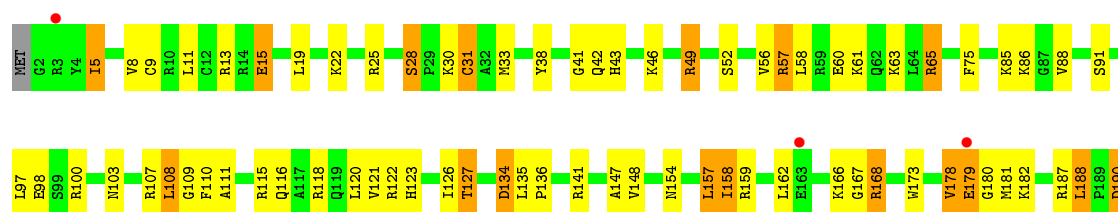
• Molecule 36: 30S ribosomal protein S3



• Molecule 36: 30S ribosomal protein S3



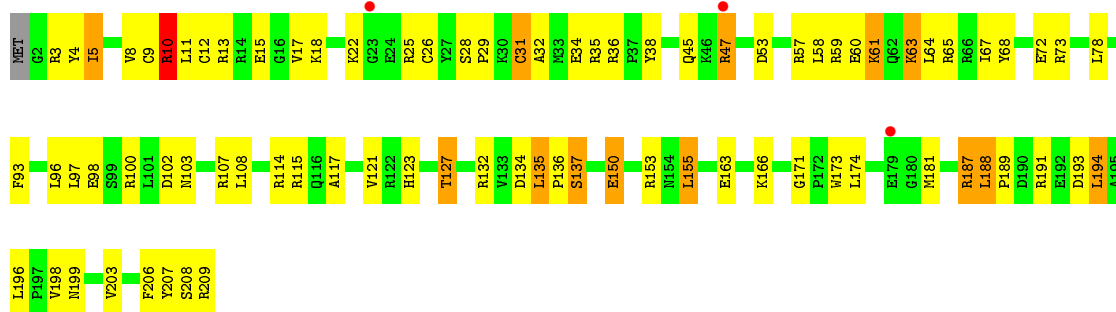
• Molecule 37: 30S ribosomal protein S4



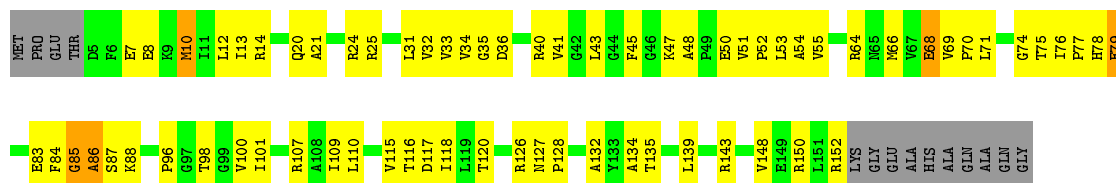




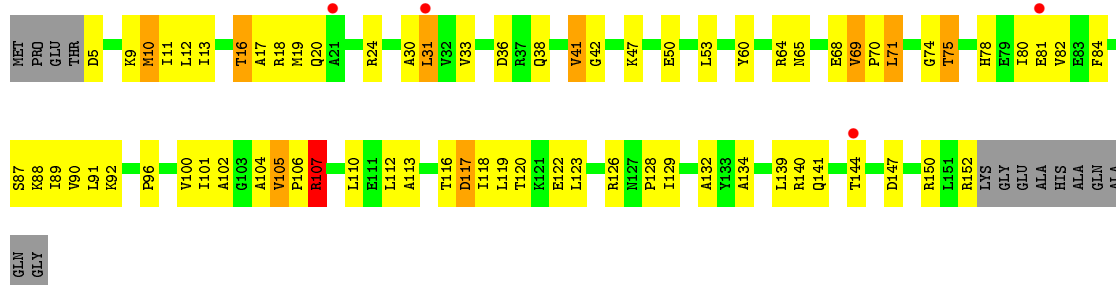
• Molecule 37: 30S ribosomal protein S4



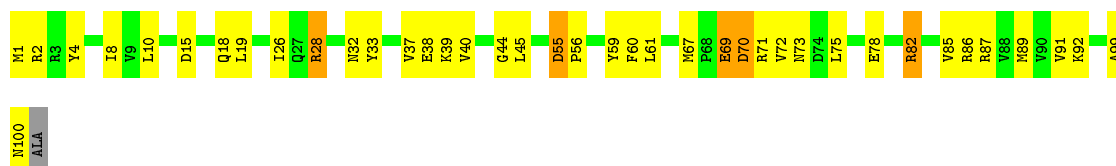
• Molecule 38: 30S ribosomal protein S5



• Molecule 38: 30S ribosomal protein S5



• Molecule 39: 30S ribosomal protein S6





- Molecule 39: 30S ribosomal protein S6

Chain DF:  69% 24% 5% ..



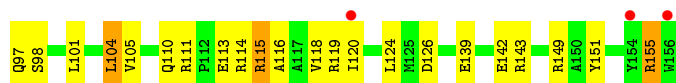
- Molecule 40: 30S ribosomal protein S7

Chain BG:  8% 72% 21% 5% ..



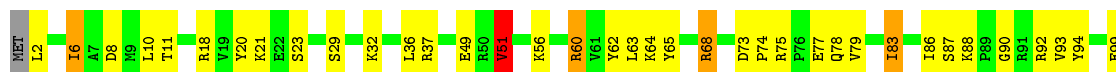
- Molecule 40: 30S ribosomal protein S7

Chain DG:  11% 69% 28% ..



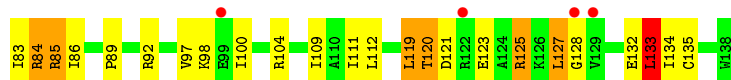
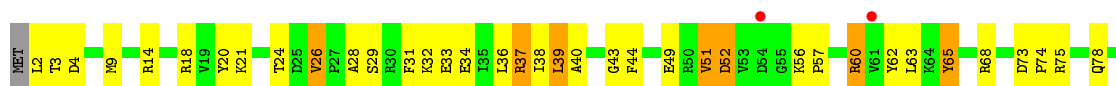
- Molecule 41: 30S ribosomal protein S8

Chain BH:  % 60% 34% ..



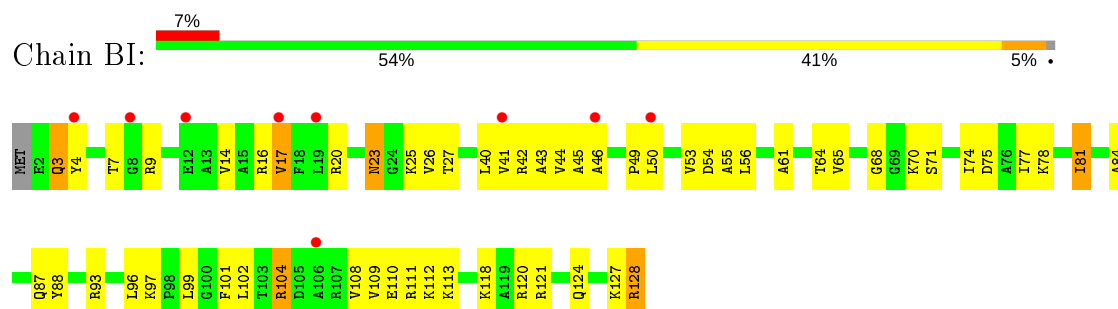
- Molecule 41: 30S ribosomal protein S8

Chain DH:  4% 55% 34% 9% ..

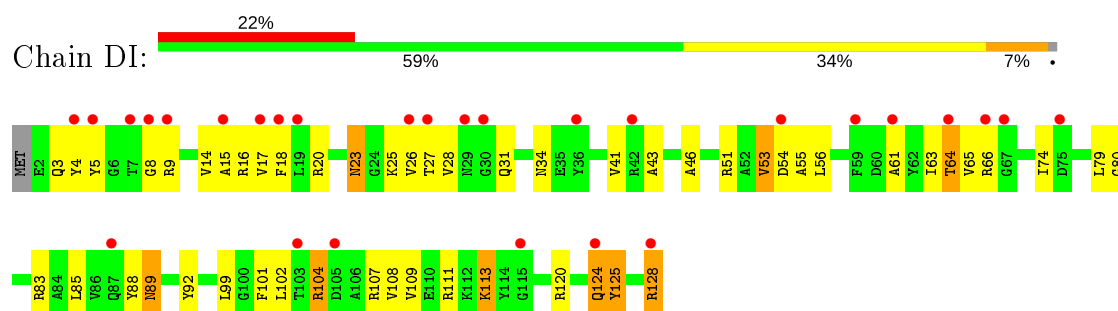




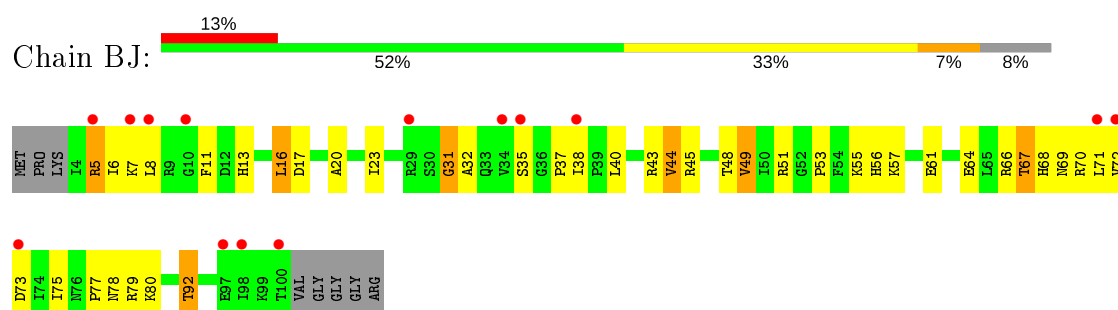
- Molecule 42: 30S ribosomal protein S9



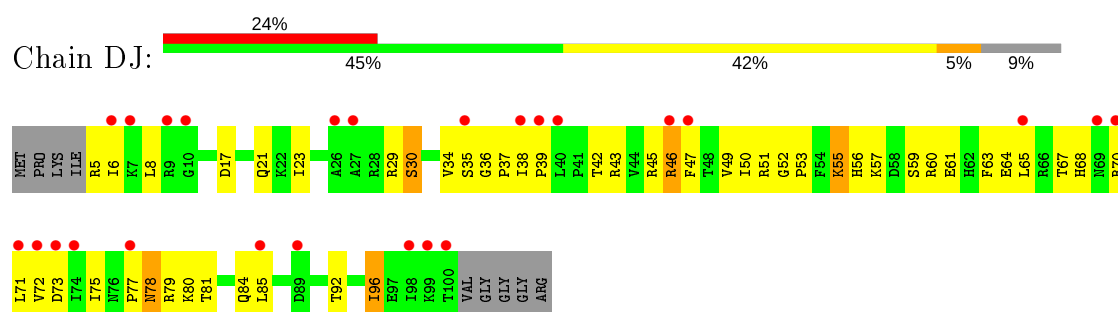
- Molecule 42: 30S ribosomal protein S9



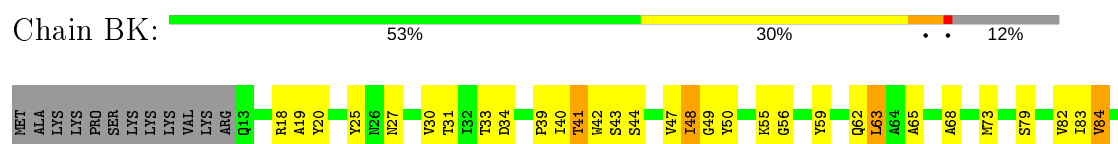
- Molecule 43: 30S ribosomal protein S10



- Molecule 43: 30S ribosomal protein S10



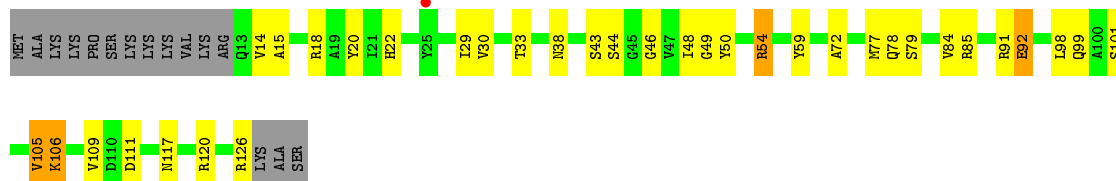
- Molecule 44: 30S ribosomal protein S11



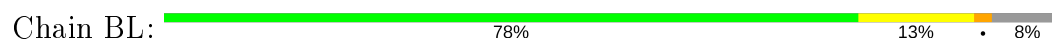




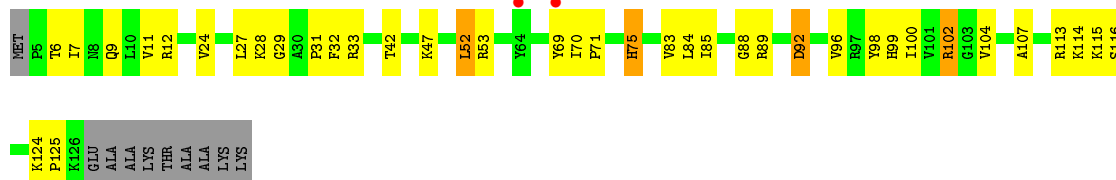
- Molecule 44: 30S ribosomal protein S11



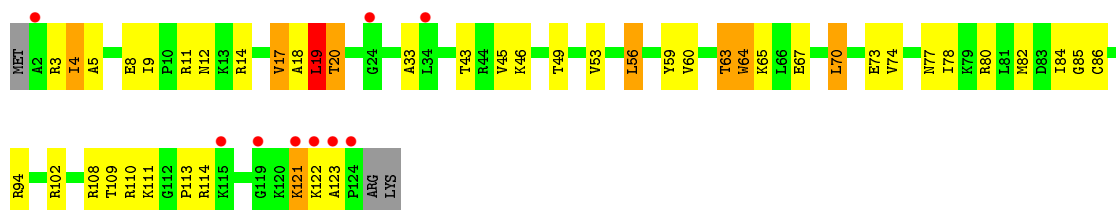
- Molecule 45: 30S ribosomal protein S12



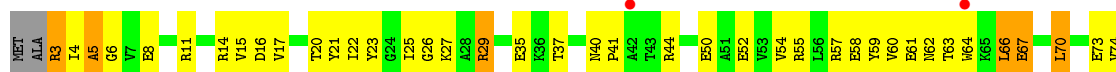
- Molecule 45: 30S ribosomal protein S12



- Molecule 46: 30S ribosomal protein S13



- Molecule 46: 30S ribosomal protein S13



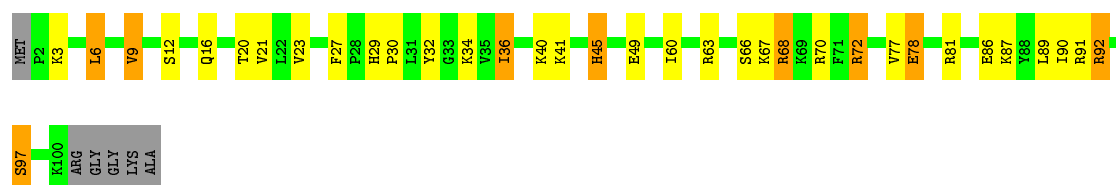






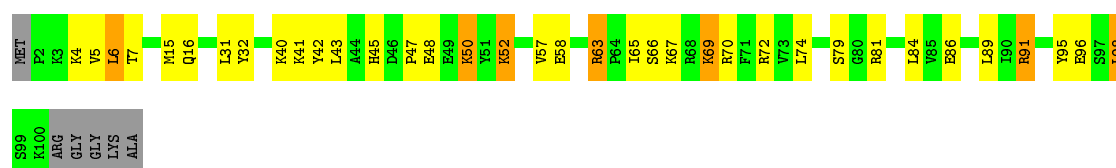
- Molecule 50: 30S ribosomal protein S17

Chain BQ: 




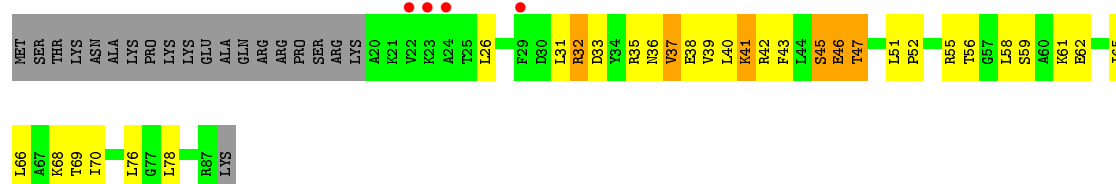
- Molecule 50: 30S ribosomal protein S17

Chain DQ: 



- Molecule 51: 30S ribosomal protein S18

Chain BR: 




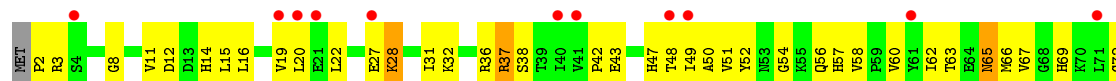
- Molecule 51: 30S ribosomal protein S18

Chain DR: 

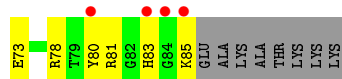


- Molecule 52: 30S ribosomal protein S19

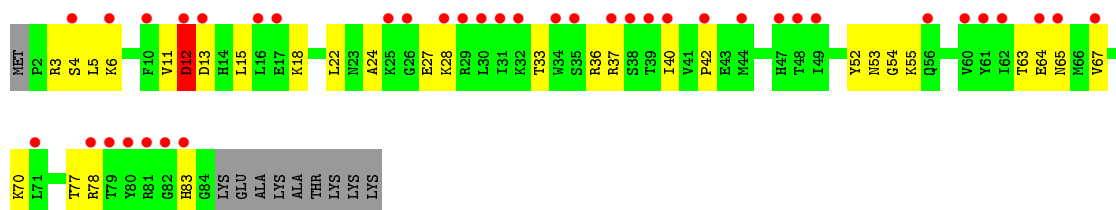
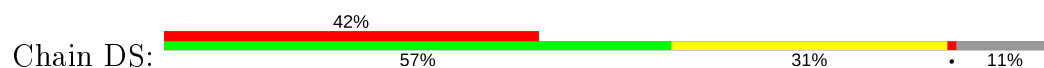
Chain BS: 



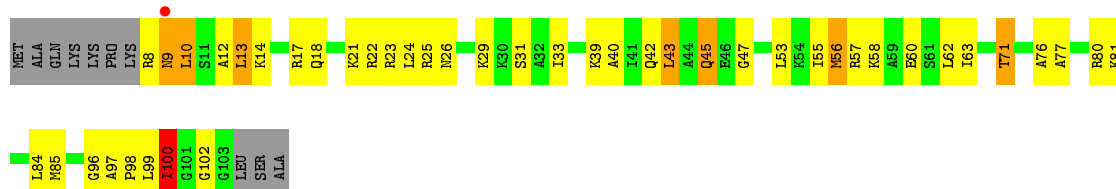




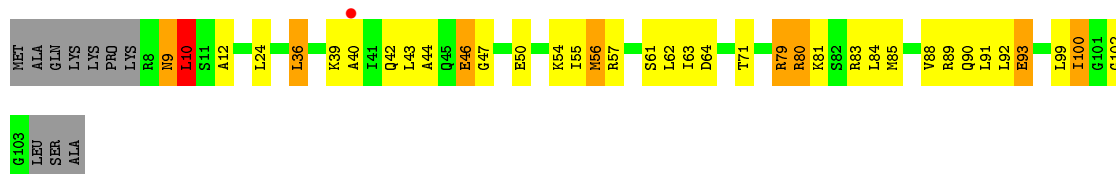
- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20



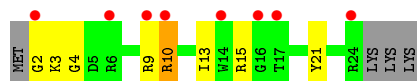
- Molecule 53: 30S ribosomal protein S20



- Molecule 54: 30S ribosomal protein Thx

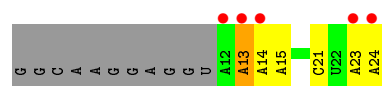
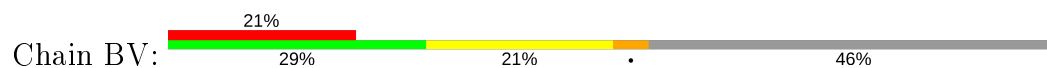


- Molecule 54: 30S ribosomal protein Thx

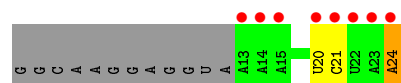
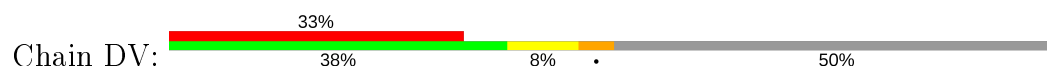




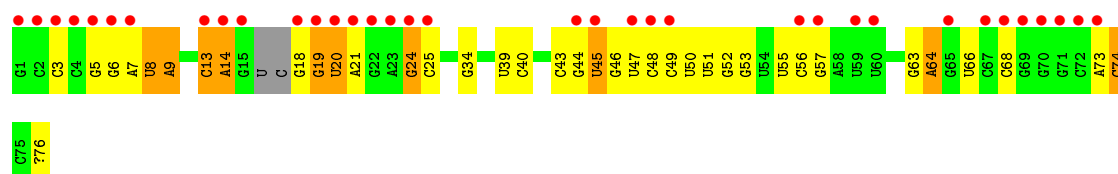
- Molecule 55: mRNA



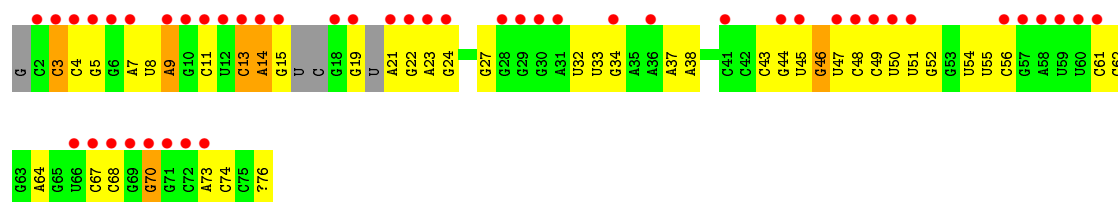
- Molecule 55: mRNA



- Molecule 56: A-site tRNA



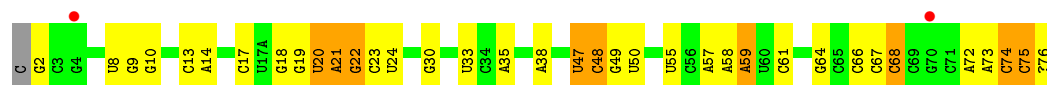
- Molecule 56: A-site tRNA



- Molecule 57: P-site tRNA

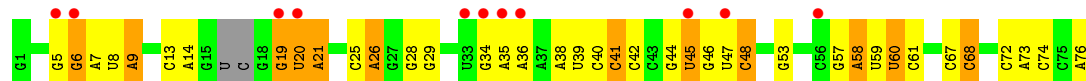


- Molecule 57: P-site tRNA

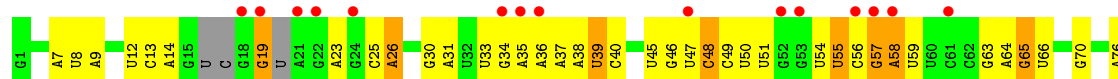


- Molecule 58: E-site tRNA

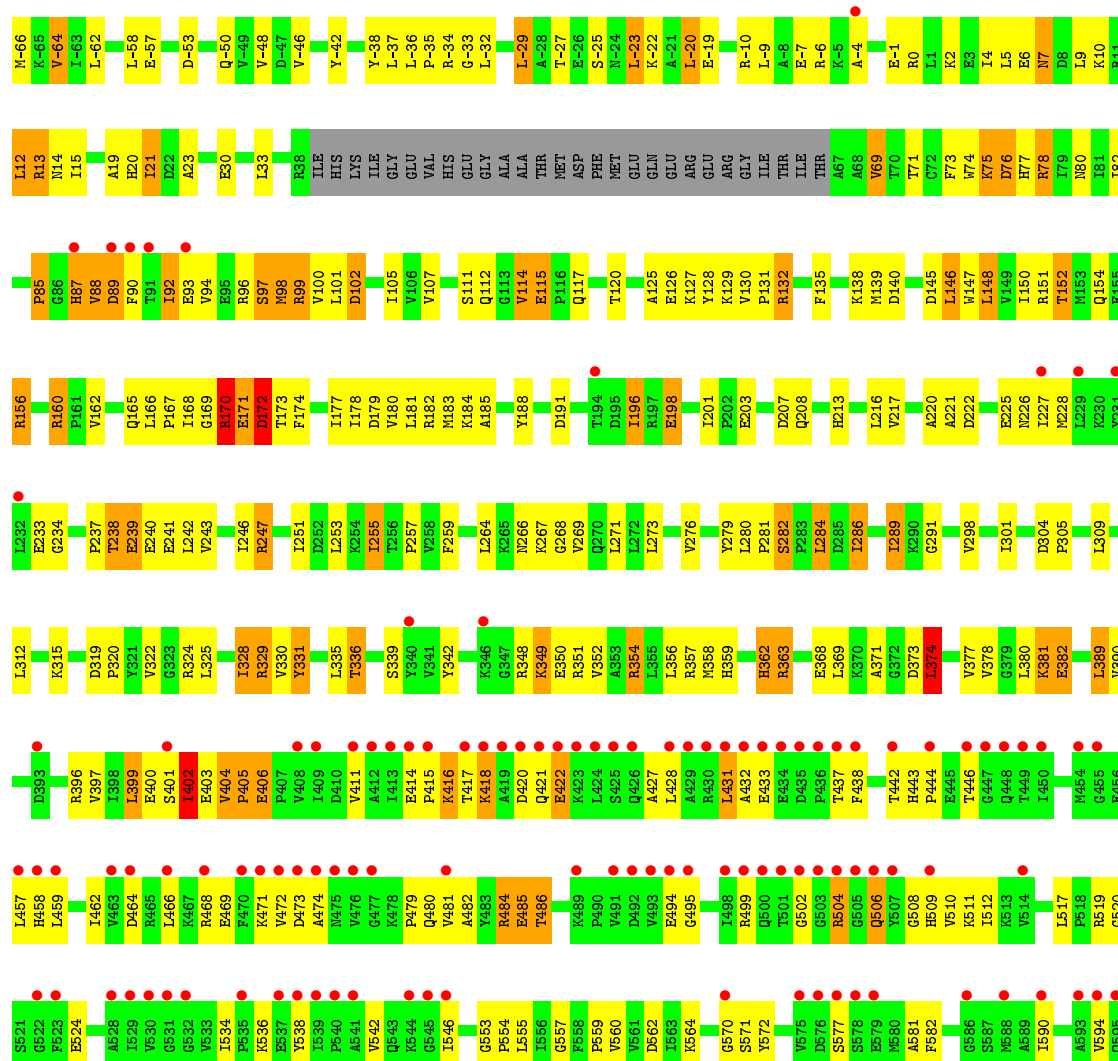




• Molecule 58: E-site tRNA



• Molecule 59: 50S ribosomal protein L9,Elongation factor G









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.89 Å   449.03 Å   622.90 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	49.63 – 2.80 49.63 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.63-2.80) 99.0 (49.63-2.80)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.81 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, $R_{free}$	0.202   ,   0.252 0.203   ,   0.252	Depositor DCC
$R_{free}$ test set	71166 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.8	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 67.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	313372	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, GDP, ZN, MIA, SF4, MG, F3N, 31H, 5MC, 4SU, 7MG, K, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	AA	1.20	165/69281 (0.2%)	1.78	2173/108144 (2.0%)
1	CA	0.89	30/69179 (0.0%)	1.46	878/107984 (0.8%)
2	AB	0.97	0/2878	1.65	57/4490 (1.3%)
2	CB	0.63	0/2878	1.24	15/4490 (0.3%)
3	AC	0.34	0/1083	0.65	0/1460
3	CC	0.34	0/1083	0.65	0/1460
4	AD	0.80	2/2186 (0.1%)	0.91	2/2944 (0.1%)
4	CD	0.65	0/2192	0.81	2/2951 (0.1%)
5	AE	0.81	0/1592	0.89	1/2149 (0.0%)
5	CE	0.63	0/1592	0.80	0/2149
6	AF	0.75	0/1619	0.91	2/2193 (0.1%)
6	CF	0.57	0/1615	0.74	0/2188
7	AG	0.51	0/1450	0.70	0/1959
7	CG	0.39	0/1449	0.59	0/1958
8	AH	0.67	0/1356	0.79	0/1834
8	CH	0.41	0/1356	0.62	0/1834
9	AK	0.33	0/640	0.63	0/889
9	CK	0.26	0/640	0.58	0/889
10	AL	0.31	0/503	0.53	0/673
10	CL	0.34	0/503	0.54	0/673
11	AN	0.81	0/1144	0.90	1/1543 (0.1%)
11	CN	0.57	0/1144	0.71	0/1543
12	AO	0.76	0/943	0.84	1/1269 (0.1%)
12	CO	0.68	0/943	0.75	0/1269
13	AP	0.70	0/1156	0.87	2/1537 (0.1%)
13	CP	0.51	0/1152	0.80	0/1533
14	AQ	0.77	0/1143	0.86	1/1527 (0.1%)
14	CQ	0.58	0/1143	0.69	0/1527
15	AR	0.73	0/982	0.87	0/1312
15	CR	0.58	0/982	0.77	0/1312
16	AS	0.58	0/887	0.76	1/1180 (0.1%)
16	CS	0.46	0/880	0.71	0/1172



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AT	0.74	0/1105	0.88	0/1477
17	CT	0.58	0/1097	0.74	0/1468
18	AU	0.89	1/977 (0.1%)	0.92	1/1301 (0.1%)
18	CU	0.62	0/977	0.71	2/1301 (0.2%)
19	AV	0.80	0/782	0.90	1/1049 (0.1%)
19	CV	0.52	0/782	0.74	0/1049
20	AW	0.91	0/897	0.93	3/1205 (0.2%)
20	CW	0.70	0/897	0.81	0/1205
21	AX	0.82	1/764 (0.1%)	0.80	1/1025 (0.1%)
21	CX	0.62	0/764	0.75	1/1025 (0.1%)
22	AY	0.74	0/819	0.85	0/1095
22	CY	0.54	0/819	0.69	0/1095
23	AZ	0.52	0/1379	0.70	1/1873 (0.1%)
23	CZ	0.39	0/1390	0.58	0/1890
24	A0	0.67	0/662	0.88	1/881 (0.1%)
24	C0	0.56	0/662	0.68	0/881
25	A1	0.70	0/762	0.81	0/1014
25	C1	0.61	0/762	0.77	0/1014
26	A2	0.78	0/590	0.78	0/781
26	C2	0.53	0/590	0.63	0/781
27	A3	0.82	0/474	0.91	0/635
27	C3	0.49	0/469	0.69	0/630
28	A4	0.43	0/571	0.70	0/768
28	C4	0.35	0/545	0.60	0/737
29	A5	0.89	1/469 (0.2%)	1.00	2/635 (0.3%)
29	C5	0.66	0/469	0.82	0/635
30	A6	0.86	1/460 (0.2%)	0.79	0/613
30	C6	0.62	0/456	0.74	0/608
31	A7	0.84	0/426	0.99	2/561 (0.4%)
31	C7	0.70	0/426	0.78	0/561
32	A8	0.82	0/525	0.90	0/691
32	C8	0.61	0/525	0.78	0/691
33	A9	0.80	0/310	0.94	0/407
33	C9	0.60	0/310	0.73	0/407
34	BA	0.70	4/36027 (0.0%)	1.28	246/56227 (0.4%)
34	DA	0.64	1/36170 (0.0%)	1.21	131/56452 (0.2%)
35	BB	0.40	0/1881	0.67	1/2542 (0.0%)
35	DB	0.36	0/1860	0.61	0/2518
36	BC	0.38	0/1576	0.59	0/2130
36	DC	0.35	0/1568	0.57	0/2122
37	BD	0.48	0/1689	0.67	0/2267
37	DD	0.48	0/1708	0.70	1/2289 (0.0%)
38	BE	0.51	0/1145	0.69	1/1543 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DE	0.44	0/1149	0.67	0/1548
39	BF	0.52	0/825	0.70	0/1118
39	DF	0.52	0/833	0.69	1/1128 (0.1%)
40	BG	0.43	0/1250	0.58	0/1679
40	DG	0.37	0/1254	0.56	0/1683
41	BH	0.48	0/1108	0.68	0/1494
41	DH	0.42	0/1108	0.64	0/1494
42	BI	0.42	0/1005	0.62	0/1350
42	DI	0.36	0/997	0.58	0/1343
43	BJ	0.38	0/722	0.58	0/982
43	DJ	0.34	0/727	0.59	0/988
44	BK	0.49	0/848	0.66	0/1149
44	DK	0.50	0/848	0.66	0/1149
45	BL	0.56	0/946	0.70	0/1274
45	DL	0.52	0/946	0.68	0/1274
46	BM	0.41	0/977	0.64	0/1310
46	DM	0.35	0/961	0.56	0/1291
47	BN	0.44	0/501	0.70	0/664
47	DN	0.37	0/501	0.59	1/664 (0.2%)
48	BO	0.50	0/739	0.71	0/985
48	DO	0.46	0/739	0.63	0/985
49	BP	0.53	0/697	0.69	0/939
49	DP	0.52	0/693	0.66	0/935
50	BQ	0.53	0/836	0.69	1/1117 (0.1%)
50	DQ	0.50	0/836	0.68	0/1117
51	BR	0.51	0/560	0.74	0/746
51	DR	0.52	0/560	0.66	0/746
52	BS	0.36	0/676	0.58	0/911
52	DS	0.32	0/661	0.64	0/893
53	BT	0.45	0/730	0.71	0/965
53	DT	0.46	0/733	0.69	0/969
54	BU	0.40	0/203	0.62	0/266
54	DU	0.35	0/203	0.62	0/266
55	BV	0.65	0/310	1.02	1/480 (0.2%)
55	DV	0.54	0/282	0.91	0/437
56	BW	0.43	0/1577	0.96	1/2454 (0.0%)
56	DW	0.36	0/1531	0.94	0/2379
57	BX	0.71	1/1700 (0.1%)	1.22	2/2650 (0.1%)
57	DX	0.63	1/1700 (0.1%)	1.12	4/2650 (0.2%)
58	BY	0.43	0/1602	0.98	1/2493 (0.0%)
58	DY	0.36	0/1579	0.86	0/2455
59	BZ	0.44	0/5763	0.68	2/7804 (0.0%)
59	DZ	0.41	0/5784	0.63	0/7835



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.82	208/333310 (0.1%)	1.32	3545/497173 (0.7%)

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
1	AA	0	1
28	A4	0	1
35	BB	0	1
53	BT	0	1
53	DT	0	1
59	DZ	0	1
All	All	0	6

The worst 5 of 208 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1188	A	N9-C4	-13.96	1.29	1.37
1	AA	354	A	N9-C4	-13.07	1.30	1.37
1	CA	528	A	N9-C4	-11.34	1.31	1.37
57	DX	74	C	O3'-P	-11.14	1.47	1.61
1	AA	2299	A	N9-C4	-10.50	1.31	1.37

The worst 5 of 3545 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	990	A	N1-C6-N6	23.54	132.72	118.60
1	AA	354	A	C2-N3-C4	-21.82	99.69	110.60
1	AA	990	A	C6-C5-N7	-21.49	117.25	132.30
1	AA	1188	A	C2-N3-C4	-21.02	100.09	110.60
1	AA	990	A	C5-N7-C8	-19.83	93.98	103.90

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	A4	59	PHE	Peptide
1	AA	537	G	Sidechain
35	BB	8	LYS	Peptide

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
53	BT	9	ASN	Peptide
53	DT	9	ASN	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	31186	660	2
1	CA	61771	0	31146	786	0
2	AB	2573	0	1306	15	0
2	CB	2573	0	1306	26	0
3	AC	1063	0	1091	140	5
3	CC	1063	0	1089	150	10
4	AD	2136	0	2218	55	0
4	CD	2142	0	2229	67	0
5	AE	1559	0	1618	48	0
5	CE	1559	0	1618	42	0
6	AF	1584	0	1625	39	0
6	CF	1580	0	1619	50	0
7	AG	1425	0	1443	47	0
7	CG	1424	0	1434	42	0
8	AH	1330	0	1407	24	0
8	CH	1330	0	1407	42	0
9	AK	641	0	309	11	0
9	CK	641	0	309	13	0
10	AL	498	0	521	17	0
10	CL	498	0	521	21	0
11	AN	1117	0	1184	26	0
11	CN	1117	0	1184	21	0
12	AO	933	0	996	29	0
12	CO	933	0	996	22	0
13	AP	1139	0	1223	34	0
13	CP	1135	0	1212	47	0
14	AQ	1122	0	1179	36	0
14	CQ	1122	0	1179	36	0
15	AR	968	0	1033	19	0
15	CR	968	0	1033	27	0
16	AS	877	0	938	20	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	35	0
17	AT	1091	0	1151	31	0
17	CT	1083	0	1136	28	0
18	AU	959	0	1019	25	0
18	CU	959	0	1019	30	0
19	AV	771	0	830	13	0
19	CV	771	0	830	19	0
20	AW	886	0	940	15	0
20	CW	886	0	940	18	0
21	AX	750	0	814	20	0
21	CX	750	0	814	19	0
22	AY	806	0	881	29	0
22	CY	806	0	882	37	0
23	AZ	1349	0	1355	38	0
23	CZ	1360	0	1363	41	0
24	A0	653	0	674	20	0
24	C0	653	0	674	20	0
25	A1	755	0	826	20	0
25	C1	755	0	826	20	0
26	A2	588	0	643	9	0
26	C2	588	0	643	14	0
27	A3	469	0	518	6	0
27	C3	464	0	514	8	0
28	A4	558	0	545	22	0
28	C4	532	0	506	20	0
29	A5	455	0	465	7	0
29	C5	455	0	465	11	0
30	A6	453	0	473	13	0
30	C6	449	0	469	13	0
31	A7	418	0	467	11	0
31	C7	418	0	467	9	0
32	A8	517	0	582	23	0
32	C8	517	0	582	19	0
33	A9	307	0	335	8	0
33	C9	307	0	335	11	0
34	BA	32185	0	16245	438	0
34	DA	32312	0	16308	510	1
35	BB	1846	0	1867	80	0
35	DB	1825	0	1828	101	0
36	BC	1552	0	1546	52	0
36	DC	1544	0	1524	65	0
37	BD	1659	0	1676	58	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	DD	1678	0	1718	53	0
38	BE	1129	0	1185	42	0
38	DE	1133	0	1191	41	0
39	BF	812	0	804	18	0
39	DF	820	0	814	23	0
40	BG	1231	0	1238	21	0
40	DG	1235	0	1249	31	0
41	BH	1088	0	1126	39	0
41	DH	1088	0	1126	37	0
42	BI	986	0	995	39	0
42	DI	978	0	966	42	0
43	BJ	709	0	650	34	0
43	DJ	714	0	672	33	0
44	BK	833	0	836	23	0
44	DK	833	0	836	16	0
45	BL	930	0	980	10	0
45	DL	930	0	980	30	0
46	BM	966	0	1024	33	0
46	DM	950	0	988	39	0
47	BN	492	0	529	22	0
47	DN	492	0	531	33	0
48	BO	728	0	760	17	0
48	DO	728	0	760	14	0
49	BP	681	0	697	27	0
49	DP	677	0	686	20	0
50	BQ	823	0	891	24	0
50	DQ	823	0	891	23	0
51	BR	555	0	618	16	0
51	DR	555	0	618	20	0
52	BS	661	0	675	39	0
52	DS	646	0	644	25	0
53	BT	728	0	798	29	0
53	DT	731	0	807	22	0
54	BU	199	0	208	7	0
54	DU	199	0	208	5	0
55	BV	277	0	140	3	0
55	DV	252	0	130	3	0
56	BW	1599	0	830	26	0
56	DW	1552	0	794	21	0
57	BX	1635	0	838	15	0
57	DX	1635	0	839	25	0
58	BY	1581	0	805	21	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	DY	1561	0	796	18	0
59	BZ	5663	0	5746	246	10
59	DZ	5682	0	5766	192	6
60	A0	5	0	0	0	0
60	A1	2	0	0	0	0
60	A2	1	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	A7	1	0	0	0	0
60	A8	2	0	0	0	0
60	A9	1	0	0	0	0
60	AA	834	0	0	0	0
60	AB	23	0	0	0	0
60	AD	10	0	0	0	0
60	AE	5	0	0	0	0
60	AF	5	0	0	0	0
60	AG	2	0	0	0	0
60	AH	1	0	0	0	0
60	AN	3	0	0	0	0
60	AO	1	0	0	0	0
60	AP	2	0	0	0	0
60	AQ	3	0	0	0	0
60	AR	1	0	0	0	0
60	AU	4	0	0	0	0
60	AV	1	0	0	0	0
60	AW	4	0	0	0	0
60	AX	2	0	0	0	0
60	AY	1	0	0	0	0
60	AZ	1	0	0	0	0
60	BA	213	0	0	0	0
60	BB	1	0	0	0	0
60	BD	1	0	0	0	0
60	BE	1	0	0	0	0
60	BF	1	0	0	0	0
60	BK	1	0	0	0	0
60	BL	2	0	0	0	0
60	BM	1	0	0	0	0
60	BN	2	0	0	0	0
60	BT	1	0	0	0	0
60	BV	1	0	0	0	0
60	BW	2	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	BX	15	0	0	0	0
60	BY	2	0	0	0	0
60	BZ	1	0	0	0	0
60	C0	2	0	0	0	0
60	C3	1	0	0	0	0
60	C5	1	0	0	0	0
60	C7	1	0	0	0	0
60	C8	1	0	0	0	0
60	CA	664	0	0	0	0
60	CB	13	0	0	0	0
60	CD	4	0	0	0	0
60	CE	6	0	0	0	0
60	CF	6	0	0	0	0
60	CG	1	0	0	0	0
60	CN	1	0	0	0	0
60	CO	2	0	0	0	0
60	CP	1	0	0	0	0
60	CQ	4	0	0	0	0
60	CR	2	0	0	0	0
60	CU	1	0	0	0	0
60	CV	2	0	0	0	0
60	CY	1	0	0	0	0
60	DA	168	0	0	0	0
60	DD	1	0	0	0	0
60	DE	2	0	0	0	0
60	DF	1	0	0	0	0
60	DJ	1	0	0	0	0
60	DK	2	0	0	0	0
60	DT	1	0	0	0	0
60	DW	1	0	0	0	0
60	DX	1	0	0	0	0
60	DZ	1	0	0	0	0
61	AA	1	0	0	0	0
62	A4	1	0	0	0	0
62	A5	1	0	0	0	0
62	A6	1	0	0	0	0
62	A9	1	0	0	0	0
62	AY	1	0	0	0	0
62	BN	1	0	0	0	0
62	C4	1	0	0	0	0
62	C5	1	0	0	0	0
62	C6	1	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	C9	1	0	0	0	0
62	CY	1	0	0	0	0
62	DN	1	0	0	0	0
63	BD	8	0	0	1	0
63	DD	8	0	0	1	0
64	BZ	28	0	12	6	0
64	DZ	28	0	12	7	0
65	A0	6	0	0	0	0
65	A1	1	0	0	0	0
65	A3	1	0	0	0	0
65	A5	3	0	0	0	0
65	A6	2	0	0	0	0
65	A7	4	0	0	1	0
65	A8	10	0	0	1	0
65	AA	1408	0	0	48	0
65	AB	36	0	0	1	0
65	AD	15	0	0	1	0
65	AE	19	0	0	1	0
65	AF	7	0	0	0	0
65	AG	3	0	0	0	0
65	AH	1	0	0	0	0
65	AN	2	0	0	0	0
65	AO	1	0	0	0	0
65	AP	15	0	0	2	0
65	AQ	4	0	0	2	0
65	AR	2	0	0	2	0
65	AS	1	0	0	0	0
65	AT	2	0	0	0	0
65	AU	5	0	0	0	0
65	AV	2	0	0	0	0
65	AW	2	0	0	0	0
65	AX	3	0	0	0	0
65	AZ	1	0	0	0	0
65	BA	212	0	0	13	0
65	BD	2	0	0	0	0
65	BE	2	0	0	0	0
65	BL	1	0	0	0	0
65	BM	1	0	0	0	0
65	BV	2	0	0	0	0
65	BW	3	0	0	0	0
65	BX	8	0	0	0	0
65	BY	1	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	BZ	2	0	0	0	0
65	C0	6	0	0	1	0
65	C1	2	0	0	0	0
65	C3	2	0	0	0	0
65	C6	1	0	0	1	0
65	C7	1	0	0	0	0
65	C8	3	0	0	0	0
65	CA	985	0	0	52	0
65	CB	9	0	0	1	0
65	CD	14	0	0	0	0
65	CE	13	0	0	1	0
65	CF	7	0	0	0	0
65	CN	2	0	0	0	0
65	CP	10	0	0	1	0
65	CQ	1	0	0	0	0
65	CR	1	0	0	0	0
65	CT	3	0	0	0	0
65	CU	2	0	0	0	0
65	CV	1	0	0	0	0
65	CY	1	0	0	0	0
65	DA	155	0	0	6	0
65	DE	4	0	0	0	0
65	DJ	1	0	0	0	0
65	DK	2	0	0	0	0
65	DL	1	0	0	0	0
65	DW	2	0	0	0	0
65	DX	1	0	0	0	0
All	All	313372	0	210866	5329	17

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 11.

The worst 5 of 5329 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:CA:1860:G:H5'	3:CC:206:LYS:CD	1.27	1.64
1:CA:1860:G:H5''	3:CC:206:LYS:CG	1.28	1.64
1:AA:1891:G:C5'	3:AC:206:LYS:HD2	1.35	1.54
1:CA:1860:G:C5'	3:CC:206:LYS:HD2	1.25	1.53
1:CA:1860:G:C5'	3:CC:206:LYS:CG	1.84	1.50



The worst 5 of 17 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)
3:AC:9:ARG:NH2	59:DZ:504:ARG:NH1[3_654]	0.73	1.47
59:BZ:504:ARG:NH2	3:CC:9:ARG:NE[2_655]	1.08	1.12
59:BZ:504:ARG:NH1	3:CC:9:ARG:NH1[2_655]	1.09	1.11
3:AC:6:LYS:O	59:DZ:501:THR:O[3_654]	1.74	0.46
59:BZ:504:ARG:NH1	3:CC:9:ARG:NE[2_655]	1.80	0.40

## 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%)	248 (91%)	22 (8%)	3 (1%)	14	41
4	CD	273/276 (99%)	245 (90%)	25 (9%)	3 (1%)	14	41
5	AE	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	29	61
5	CE	202/206 (98%)	189 (94%)	10 (5%)	3 (2%)	10	33
6	AF	201/210 (96%)	185 (92%)	16 (8%)	0	100	100
6	CF	201/210 (96%)	189 (94%)	8 (4%)	4 (2%)	7	24
7	AG	179/182 (98%)	159 (89%)	14 (8%)	6 (3%)	3	13
7	CG	179/182 (98%)	154 (86%)	19 (11%)	6 (3%)	3	13
8	AH	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	25	56
8	CH	172/180 (96%)	153 (89%)	13 (8%)	6 (4%)	3	12
9	AK	128/173 (74%)	74 (58%)	26 (20%)	28 (22%)	0	0
9	CK	128/173 (74%)	80 (62%)	28 (22%)	20 (16%)	0	0
10	AL	64/147 (44%)	47 (73%)	13 (20%)	4 (6%)	1	3
10	CL	64/147 (44%)	44 (69%)	17 (27%)	3 (5%)	2	7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AN	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
11	CN	138/140 (99%)	126 (91%)	10 (7%)	2 (1%)	11	34
12	AO	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	19	49
12	CO	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	19	49
13	AP	147/150 (98%)	133 (90%)	12 (8%)	2 (1%)	11	34
13	CP	147/150 (98%)	129 (88%)	15 (10%)	3 (2%)	7	24
14	AQ	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
14	CQ	139/141 (99%)	123 (88%)	13 (9%)	3 (2%)	6	22
15	AR	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	17	46
15	CR	116/118 (98%)	104 (90%)	11 (10%)	1 (1%)	17	46
16	AS	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	17	46
16	CS	108/112 (96%)	89 (82%)	17 (16%)	2 (2%)	8	26
17	AT	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
17	CT	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
18	AU	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
18	CU	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
19	AV	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	44
19	CV	99/101 (98%)	90 (91%)	7 (7%)	2 (2%)	7	24
20	AW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
20	CW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
21	AX	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14	41
21	CX	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	14	41
22	AY	105/110 (96%)	95 (90%)	9 (9%)	1 (1%)	15	44
22	CY	105/110 (96%)	90 (86%)	11 (10%)	4 (4%)	3	10
23	AZ	169/206 (82%)	136 (80%)	28 (17%)	5 (3%)	4	15
23	CZ	172/206 (84%)	144 (84%)	25 (14%)	3 (2%)	9	29
24	A0	81/85 (95%)	74 (91%)	6 (7%)	1 (1%)	13	39
24	C0	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
25	A1	95/98 (97%)	86 (90%)	9 (10%)	0	100	100
25	C1	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	14	41
26	A2	68/72 (94%)	66 (97%)	2 (3%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	C2	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
27	A3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	C3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	8	28
28	A4	67/71 (94%)	44 (66%)	16 (24%)	7 (10%)	0	1
28	C4	67/71 (94%)	49 (73%)	13 (19%)	5 (8%)	1	2
29	A5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	C5	57/60 (95%)	57 (100%)	0	0	100	100
30	A6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
30	C6	51/54 (94%)	45 (88%)	6 (12%)	0	100	100
31	A7	46/49 (94%)	46 (100%)	0	0	100	100
31	C7	46/49 (94%)	44 (96%)	0	2 (4%)	2	8
32	A8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
32	C8	62/65 (95%)	58 (94%)	2 (3%)	2 (3%)	4	13
33	A9	35/37 (95%)	35 (100%)	0	0	100	100
33	C9	35/37 (95%)	35 (100%)	0	0	100	100
35	BB	229/256 (90%)	187 (82%)	29 (13%)	13 (6%)	1	5
35	DB	229/256 (90%)	177 (77%)	37 (16%)	15 (7%)	1	3
36	BC	204/239 (85%)	171 (84%)	25 (12%)	8 (4%)	3	10
36	DC	204/239 (85%)	171 (84%)	30 (15%)	3 (2%)	10	33
37	BD	206/209 (99%)	186 (90%)	16 (8%)	4 (2%)	8	26
37	DD	206/209 (99%)	180 (87%)	20 (10%)	6 (3%)	4	15
38	BE	146/162 (90%)	128 (88%)	13 (9%)	5 (3%)	3	13
38	DE	146/162 (90%)	128 (88%)	12 (8%)	6 (4%)	3	9
39	BF	98/101 (97%)	89 (91%)	7 (7%)	2 (2%)	7	24
39	DF	98/101 (97%)	91 (93%)	6 (6%)	1 (1%)	15	44
40	BG	153/156 (98%)	142 (93%)	9 (6%)	2 (1%)	12	36
40	DG	153/156 (98%)	132 (86%)	19 (12%)	2 (1%)	12	36
41	BH	135/138 (98%)	120 (89%)	12 (9%)	3 (2%)	6	22
41	DH	135/138 (98%)	121 (90%)	12 (9%)	2 (2%)	10	33
42	BI	125/128 (98%)	111 (89%)	10 (8%)	4 (3%)	4	13
42	DI	125/128 (98%)	111 (89%)	12 (10%)	2 (2%)	9	31

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BJ	95/105 (90%)	81 (85%)	9 (10%)	5 (5%)	2	6
43	DJ	94/105 (90%)	77 (82%)	10 (11%)	7 (7%)	1	2
44	BK	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	8	28
44	DK	112/129 (87%)	98 (88%)	10 (9%)	4 (4%)	3	11
45	BL	120/132 (91%)	106 (88%)	13 (11%)	1 (1%)	19	49
45	DL	120/132 (91%)	109 (91%)	11 (9%)	0	100	100
46	BM	121/126 (96%)	101 (84%)	17 (14%)	3 (2%)	5	19
46	DM	120/126 (95%)	98 (82%)	13 (11%)	9 (8%)	1	2
47	BN	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	9	29
47	DN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9	29
48	BO	86/89 (97%)	77 (90%)	7 (8%)	2 (2%)	6	21
48	DO	86/89 (97%)	72 (84%)	12 (14%)	2 (2%)	6	21
49	BP	80/88 (91%)	66 (82%)	12 (15%)	2 (2%)	5	19
49	DP	80/88 (91%)	66 (82%)	13 (16%)	1 (1%)	12	36
50	BQ	97/105 (92%)	87 (90%)	9 (9%)	1 (1%)	15	44
50	DQ	97/105 (92%)	85 (88%)	12 (12%)	0	100	100
51	BR	66/88 (75%)	61 (92%)	4 (6%)	1 (2%)	10	33
51	DR	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
52	BS	82/93 (88%)	73 (89%)	9 (11%)	0	100	100
52	DS	81/93 (87%)	67 (83%)	12 (15%)	2 (2%)	5	19
53	BT	94/106 (89%)	78 (83%)	10 (11%)	6 (6%)	1	3
53	DT	94/106 (89%)	78 (83%)	12 (13%)	4 (4%)	2	8
54	BU	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
54	DU	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	7
59	BZ	722/758 (95%)	598 (83%)	92 (13%)	32 (4%)	2	8
59	DZ	726/758 (96%)	594 (82%)	97 (13%)	35 (5%)	2	7
All	All	13220/14444 (92%)	11544 (87%)	1298 (10%)	378 (3%)	4	15

5 of 378 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 ⓘ

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%)	14	38
3	CC	111/180 (62%)	103 (93%)	8 (7%)	14	38
4	AD	215/218 (99%)	189 (88%)	26 (12%)	5	15
4	CD	216/218 (99%)	181 (84%)	35 (16%)	2	7
5	AE	164/166 (99%)	140 (85%)	24 (15%)	3	9
5	CE	164/166 (99%)	139 (85%)	25 (15%)	3	8
6	AF	160/166 (96%)	134 (84%)	26 (16%)	2	7
6	CF	159/166 (96%)	135 (85%)	24 (15%)	3	9
7	AG	143/156 (92%)	119 (83%)	24 (17%)	2	6
7	CG	142/156 (91%)	108 (76%)	34 (24%)	0	2
8	AH	144/148 (97%)	128 (89%)	16 (11%)	6	19
8	CH	144/148 (97%)	125 (87%)	19 (13%)	4	12
10	AL	50/111 (45%)	45 (90%)	5 (10%)	7	22
10	CL	50/111 (45%)	45 (90%)	5 (10%)	7	22
11	AN	118/119 (99%)	94 (80%)	24 (20%)	1	4
11	CN	118/119 (99%)	98 (83%)	20 (17%)	2	6
12	AO	100/100 (100%)	83 (83%)	17 (17%)	2	6
12	CO	100/100 (100%)	83 (83%)	17 (17%)	2	6
13	AP	116/116 (100%)	97 (84%)	19 (16%)	2	7
13	CP	115/116 (99%)	99 (86%)	16 (14%)	3	11
14	AQ	111/111 (100%)	90 (81%)	21 (19%)	1	5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	CQ	111/111 (100%)	95 (86%)	16 (14%)	3	10
15	AR	101/101 (100%)	79 (78%)	22 (22%)	1	3
15	CR	101/101 (100%)	84 (83%)	17 (17%)	2	6
16	AS	87/88 (99%)	71 (82%)	16 (18%)	1	5
16	CS	85/88 (97%)	67 (79%)	18 (21%)	1	3
17	AT	115/127 (91%)	97 (84%)	18 (16%)	2	8
17	CT	113/127 (89%)	93 (82%)	20 (18%)	2	5
18	AU	93/94 (99%)	77 (83%)	16 (17%)	2	6
18	CU	93/94 (99%)	82 (88%)	11 (12%)	5	16
19	AV	80/82 (98%)	65 (81%)	15 (19%)	1	5
19	CV	80/82 (98%)	67 (84%)	13 (16%)	2	7
20	AW	90/92 (98%)	80 (89%)	10 (11%)	6	19
20	CW	90/92 (98%)	79 (88%)	11 (12%)	5	15
21	AX	77/78 (99%)	73 (95%)	4 (5%)	23	55
21	CX	77/78 (99%)	70 (91%)	7 (9%)	9	27
22	AY	85/91 (93%)	73 (86%)	12 (14%)	3	10
22	CY	85/91 (93%)	70 (82%)	15 (18%)	2	5
23	AZ	145/179 (81%)	117 (81%)	28 (19%)	1	4
23	CZ	145/179 (81%)	125 (86%)	20 (14%)	3	11
24	A0	65/67 (97%)	63 (97%)	2 (3%)	40	74
24	C0	65/67 (97%)	60 (92%)	5 (8%)	13	35
25	A1	80/83 (96%)	72 (90%)	8 (10%)	7	22
25	C1	80/83 (96%)	69 (86%)	11 (14%)	3	11
26	A2	65/67 (97%)	54 (83%)	11 (17%)	2	6
26	C2	65/67 (97%)	55 (85%)	10 (15%)	2	8
27	A3	51/52 (98%)	44 (86%)	7 (14%)	3	11
27	C3	50/52 (96%)	38 (76%)	12 (24%)	0	2
28	A4	60/63 (95%)	49 (82%)	11 (18%)	1	5
28	C4	53/63 (84%)	39 (74%)	14 (26%)	0	1
29	A5	50/52 (96%)	43 (86%)	7 (14%)	3	11
29	C5	50/52 (96%)	44 (88%)	6 (12%)	5	15

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	A6	51/52 (98%)	40 (78%)	11 (22%)	1	3
30	C6	50/52 (96%)	43 (86%)	7 (14%)	3	11
31	A7	41/42 (98%)	35 (85%)	6 (15%)	3	9
31	C7	41/42 (98%)	36 (88%)	5 (12%)	5	15
32	A8	54/55 (98%)	47 (87%)	7 (13%)	4	13
32	C8	54/55 (98%)	49 (91%)	5 (9%)	9	26
33	A9	34/34 (100%)	31 (91%)	3 (9%)	10	29
33	C9	34/34 (100%)	29 (85%)	5 (15%)	3	9
35	BB	192/220 (87%)	144 (75%)	48 (25%)	0	2
35	DB	187/220 (85%)	157 (84%)	30 (16%)	2	7
36	BC	143/188 (76%)	124 (87%)	19 (13%)	4	12
36	DC	141/188 (75%)	115 (82%)	26 (18%)	1	5
37	BD	170/181 (94%)	146 (86%)	24 (14%)	3	10
37	DD	174/181 (96%)	148 (85%)	26 (15%)	3	9
38	BE	113/123 (92%)	104 (92%)	9 (8%)	12	34
38	DE	114/123 (93%)	96 (84%)	18 (16%)	2	8
39	BF	84/90 (93%)	71 (84%)	13 (16%)	2	8
39	DF	86/90 (96%)	75 (87%)	11 (13%)	4	13
40	BG	119/127 (94%)	98 (82%)	21 (18%)	2	5
40	DG	120/127 (94%)	112 (93%)	8 (7%)	16	43
41	BH	114/119 (96%)	98 (86%)	16 (14%)	3	11
41	DH	114/119 (96%)	92 (81%)	22 (19%)	1	4
42	BI	91/99 (92%)	72 (79%)	19 (21%)	1	3
42	DI	89/99 (90%)	71 (80%)	18 (20%)	1	4
43	BJ	66/92 (72%)	58 (88%)	8 (12%)	5	15
43	DJ	69/92 (75%)	58 (84%)	11 (16%)	2	7
44	BK	83/99 (84%)	71 (86%)	12 (14%)	3	9
44	DK	83/99 (84%)	74 (89%)	9 (11%)	6	19
45	BL	97/109 (89%)	90 (93%)	7 (7%)	14	38
45	DL	97/109 (89%)	86 (89%)	11 (11%)	6	18
46	BM	95/101 (94%)	82 (86%)	13 (14%)	3	11

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	DM	92/101 (91%)	76 (83%)	16 (17%)	2	6
47	BN	49/50 (98%)	39 (80%)	10 (20%)	1	4
47	DN	49/50 (98%)	40 (82%)	9 (18%)	1	5
48	BO	78/80 (98%)	64 (82%)	14 (18%)	2	5
48	DO	78/80 (98%)	68 (87%)	10 (13%)	4	13
49	BP	69/74 (93%)	56 (81%)	13 (19%)	1	5
49	DP	68/74 (92%)	61 (90%)	7 (10%)	7	21
50	BQ	94/97 (97%)	81 (86%)	13 (14%)	3	11
50	DQ	94/97 (97%)	82 (87%)	12 (13%)	4	13
51	BR	59/77 (77%)	47 (80%)	12 (20%)	1	4
51	DR	59/77 (77%)	51 (86%)	8 (14%)	3	11
52	BS	70/80 (88%)	61 (87%)	9 (13%)	4	13
52	DS	67/80 (84%)	60 (90%)	7 (10%)	7	21
53	BT	70/82 (85%)	59 (84%)	11 (16%)	2	8
53	DT	71/82 (87%)	58 (82%)	13 (18%)	1	5
54	BU	18/22 (82%)	16 (89%)	2 (11%)	6	19
54	DU	18/22 (82%)	16 (89%)	2 (11%)	6	19
59	BZ	604/636 (95%)	489 (81%)	115 (19%)	1	4
59	DZ	607/636 (95%)	505 (83%)	102 (17%)	2	6
All	All	10652/11672 (91%)	9013 (85%)	1639 (15%)	2	8

5 of 1639 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
59	BZ	89	ASP
6	CF	140	LEU
51	DR	85	LEU
59	BZ	222	ASP
3	CC	28	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 154 such sidechains are listed below:

Mol	Chain	Res	Type
59	BZ	573	HIS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
10	CL	116	ASN
59	DZ	-50	GLN
59	BZ	675	HIS
4	CD	96	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2866/2915 (98%)	477 (16%)	41 (1%)
1	CA	2860/2915 (98%)	517 (18%)	37 (1%)
2	AB	119/121 (98%)	11 (9%)	0
2	CB	119/121 (98%)	19 (15%)	0
34	BA	1494/1521 (98%)	265 (17%)	21 (1%)
34	DA	1501/1521 (98%)	284 (18%)	23 (1%)
55	BV	12/24 (50%)	3 (25%)	0
55	DV	11/24 (45%)	1 (9%)	0
56	BW	70/76 (92%)	18 (25%)	1 (1%)
56	DW	67/76 (88%)	22 (32%)	2 (2%)
57	BX	74/77 (96%)	10 (13%)	0
57	DX	74/77 (96%)	13 (17%)	0
58	BY	71/76 (93%)	20 (28%)	2 (2%)
58	DY	69/76 (90%)	19 (27%)	0
All	All	9407/9620 (97%)	1679 (17%)	127 (1%)

5 of 1679 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	U
1	AA	13	A
1	AA	34	C
1	AA	45	C
1	AA	62	U

5 of 127 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	BA	1201	A
1	CA	310	A
34	DA	991	U
34	BA	1335	C
58	BY	58	A



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

40 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	PSU	BW	39	56	17,21,22	1.41	2 (11%)	20,30,33	3.19	5 (25%)
58	MIA	BY	37	58	18,24,32	1.18	2 (11%)	18,35,47	1.42	3 (16%)
56	4SU	BW	8	56	14,21,22	1.31	1 (7%)	15,30,33	1.41	2 (13%)
58	5MU	DY	54	58	15,22,23	1.09	1 (6%)	16,32,35	1.89	2 (12%)
56	PSU	BW	55	56	17,21,22	1.31	2 (11%)	20,30,33	3.22	7 (35%)
58	4SU	BY	8	58	14,21,22	1.32	1 (7%)	15,30,33	1.48	2 (13%)
58	PSU	DY	32	58	17,21,22	1.47	2 (11%)	20,30,33	3.17	6 (30%)
57	PSU	BX	55	57	17,21,22	1.60	2 (11%)	20,30,33	3.20	6 (30%)
58	PSU	BY	55	58	17,21,22	1.52	2 (11%)	20,30,33	3.17	6 (30%)
58	MIA	DY	37	58	18,24,32	1.07	2 (11%)	18,35,47	1.31	2 (11%)
57	5MU	DX	54	57	15,22,23	1.16	2 (13%)	16,32,35	1.77	2 (12%)
57	31H	BX	76	60,57	28,34,35	1.29	4 (14%)	23,47,50	1.60	3 (13%)
56	5MU	BW	54	56	15,22,23	1.31	1 (6%)	16,32,35	2.00	2 (12%)
58	PSU	DY	55	58	17,21,22	1.55	4 (23%)	20,30,33	3.12	6 (30%)
58	7MG	BY	46	58	22,26,27	1.79	3 (13%)	28,39,42	2.80	9 (32%)
57	5MC	BX	32	57	15,22,23	1.05	1 (6%)	19,32,35	1.88	5 (26%)
56	7MG	DW	46	56	22,26,27	1.76	4 (18%)	28,39,42	2.63	8 (28%)
56	PSU	BW	32	60,56	17,21,22	1.52	2 (11%)	20,30,33	3.15	6 (30%)
57	31H	DX	76	60,57	28,34,35	1.29	4 (14%)	23,47,50	1.59	3 (13%)
56	PSU	DW	32	56	17,21,22	1.39	2 (11%)	20,30,33	3.19	7 (35%)
56	PSU	DW	55	56	17,21,22	1.37	2 (11%)	20,30,33	3.34	7 (35%)
58	PSU	BY	32	58	17,21,22	1.34	2 (11%)	20,30,33	3.18	5 (25%)
56	5MU	DW	54	56	15,22,23	1.13	1 (6%)	16,32,35	1.92	2 (12%)
58	4SU	DY	8	58	14,21,22	1.31	1 (7%)	15,30,33	1.45	2 (13%)
56	MIA	DW	37	56	18,24,32	1.11	2 (11%)	18,35,47	1.24	2 (11%)
57	4SU	BX	8	57	14,21,22	1.29	2 (14%)	15,30,33	1.39	2 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	F3N	BW	76	1,56	30,36,37	1.37	6 (20%)	29,51,54	1.27	1 (3%)
58	7MG	DY	46	58	22,26,27	1.78	3 (13%)	28,39,42	2.98	11 (39%)
56	7MG	BW	46	56	22,26,27	1.78	4 (18%)	28,39,42	2.71	9 (32%)
56	4SU	DW	8	56	14,21,22	1.29	1 (7%)	15,30,33	1.46	2 (13%)
56	PSU	DW	39	56	17,21,22	1.61	2 (11%)	20,30,33	3.28	6 (30%)
57	5MU	BX	54	60,57	15,22,23	1.23	1 (6%)	16,32,35	1.87	1 (6%)
58	PSU	DY	39	58	17,21,22	1.53	4 (23%)	20,30,33	3.31	6 (30%)
57	4SU	DX	8	57	14,21,22	1.44	2 (14%)	15,30,33	1.25	2 (13%)
56	MIA	BW	37	56	24,31,32	2.33	3 (12%)	26,44,47	2.76	9 (34%)
56	F3N	DW	76	1,56	30,36,37	1.46	6 (20%)	29,51,54	1.36	2 (6%)
58	5MU	BY	54	58	15,22,23	1.07	1 (6%)	16,32,35	1.90	1 (6%)
57	5MC	DX	32	57	15,22,23	1.43	1 (6%)	19,32,35	1.51	5 (26%)
58	PSU	BY	39	58	17,21,22	1.54	2 (11%)	20,30,33	3.15	6 (30%)
57	PSU	DX	55	57	17,21,22	1.39	2 (11%)	20,30,33	3.16	5 (25%)

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	PSU	BW	39	56	-	0/7/25/26	0/2/2/2
58	MIA	BY	37	58	-	2/3/25/34	0/3/3/3
56	4SU	BW	8	56	-	0/5/25/26	0/2/2/2
58	5MU	DY	54	58	-	2/5/25/26	0/2/2/2
56	PSU	BW	55	56	-	0/7/25/26	0/2/2/2
58	4SU	BY	8	58	-	1/5/25/26	0/2/2/2
58	PSU	DY	32	58	-	0/7/25/26	0/2/2/2
57	PSU	BX	55	57	-	0/7/25/26	0/2/2/2
58	PSU	BY	55	58	-	0/7/25/26	0/2/2/2
58	MIA	DY	37	58	-	2/3/25/34	0/3/3/3
57	5MU	DX	54	57	-	0/5/25/26	0/2/2/2
57	31H	BX	76	60,57	-	9/18/40/41	0/3/3/3
56	5MU	BW	54	56	-	0/5/25/26	0/2/2/2
58	PSU	DY	55	58	-	5/7/25/26	0/2/2/2
58	7MG	BY	46	58	-	6/7/37/38	0/3/3/3
57	5MC	BX	32	57	-	0/5/25/26	0/2/2/2
56	7MG	DW	46	56	-	3/7/37/38	0/3/3/3

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PSU	BW	32	60,56	-	0/7/25/26	0/2/2/2
57	31H	DX	76	60,57	-	9/18/40/41	0/3/3/3
56	PSU	DW	32	56	-	0/7/25/26	0/2/2/2
56	PSU	DW	55	56	-	0/7/25/26	0/2/2/2
58	PSU	BY	32	58	-	0/7/25/26	0/2/2/2
56	5MU	DW	54	56	-	0/5/25/26	0/2/2/2
58	4SU	DY	8	58	-	1/5/25/26	0/2/2/2
56	MIA	DW	37	56	-	0/3/25/34	0/3/3/3
57	4SU	BX	8	57	-	0/5/25/26	0/2/2/2
56	F3N	BW	76	1,56	-	1/15/37/38	0/4/4/4
58	7MG	DY	46	58	-	3/7/37/38	0/3/3/3
56	7MG	BW	46	56	-	3/7/37/38	0/3/3/3
56	4SU	DW	8	56	-	0/5/25/26	0/2/2/2
56	PSU	DW	39	56	-	0/7/25/26	0/2/2/2
57	5MU	BX	54	60,57	-	0/5/25/26	0/2/2/2
58	PSU	DY	39	58	-	2/7/25/26	0/2/2/2
57	4SU	DX	8	57	-	0/5/25/26	0/2/2/2
56	MIA	BW	37	56	-	3/11/33/34	0/3/3/3
56	F3N	DW	76	1,56	-	0/15/37/38	0/4/4/4
58	5MU	BY	54	58	-	1/5/25/26	0/2/2/2
57	5MC	DX	32	57	-	0/5/25/26	0/2/2/2
58	PSU	BY	39	58	-	0/7/25/26	0/2/2/2
57	PSU	DX	55	57	-	0/7/25/26	0/2/2/2

The worst 5 of 92 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BW	37	MIA	C2-S10	-7.54	1.69	1.75
56	BW	37	MIA	C13-C14	7.36	1.53	1.32
58	BY	46	7MG	C6-C5	5.25	1.48	1.41
57	DX	32	5MC	C5-C4	5.25	1.49	1.41
56	DW	46	7MG	C6-C5	5.02	1.48	1.41

The worst 5 of 178 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	DY	46	7MG	N3-C4-N9	10.14	139.93	126.91
58	BY	46	7MG	N3-C4-N9	9.35	138.92	126.91
56	BW	39	PSU	N1-C2-N3	-9.32	121.02	128.43
58	BY	32	PSU	N1-C2-N3	-9.16	121.15	128.43
56	DW	39	PSU	N1-C2-N3	-9.04	121.24	128.43



There are no chirality outliers.

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	DY	54	5MU	O4'-C4'-C5'-O5'
58	BY	8	4SU	C2'-C1'-N1-C6
58	DY	37	MIA	C3'-C4'-C5'-O5'
57	BX	76	31H	C3'-C4'-C5'-O5'
57	BX	76	31H	C4'-C5'-O5'-P

There are no ring outliers.

21 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	BW	39	PSU	1	0
56	BW	8	4SU	1	0
56	BW	55	PSU	1	0
58	BY	8	4SU	1	0
57	BX	55	PSU	1	0
58	DY	37	MIA	2	0
58	DY	55	PSU	3	0
57	BX	32	5MC	2	0
56	DW	46	7MG	2	0
57	DX	76	31H	3	0
56	DW	32	PSU	1	0
56	DW	55	PSU	1	0
56	DW	54	5MU	1	0
58	DY	8	4SU	1	0
56	DW	37	MIA	1	0
56	BW	76	F3N	2	0
58	DY	39	PSU	1	0
57	DX	8	4SU	1	0
56	DW	76	F3N	4	0
58	BY	39	PSU	1	0
57	DX	55	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2073 ligands modelled in this entry, 2069 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
64	GDP	BZ	702	60	24,30,30	1.20	3 (12%)	31,47,47	1.87	6 (19%)
64	GDP	DZ	702	60	24,30,30	1.08	2 (8%)	31,47,47	1.98	9 (29%)
63	SF4	BD	501	37	0,12,12	0.00	-	-		
63	SF4	DD	501	37	0,12,12	0.00	-	-		

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
64	GDP	BZ	702	60	-	0/12/32/32	0/3/3/3
64	GDP	DZ	702	60	-	2/12/32/32	0/3/3/3
63	SF4	BD	501	37	-	-	0/6/5/5
63	SF4	DD	501	37	-	-	0/6/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	DZ	702	GDP	C6-C5	3.53	1.47	1.41
64	BZ	702	GDP	C6-C5	3.04	1.46	1.41
64	BZ	702	GDP	C5-C4	2.50	1.47	1.40
64	DZ	702	GDP	C5-C4	2.36	1.47	1.40
64	BZ	702	GDP	C2'-C1'	-2.21	1.50	1.53

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	BZ	702	GDP	C5-C6-N1	-4.94	116.67	123.43
64	DZ	702	GDP	C5-C6-N1	-4.28	117.57	123.43
64	BZ	702	GDP	C2-N3-C4	4.10	120.04	115.36
64	DZ	702	GDP	C6-N1-C2	4.10	122.44	115.93
64	BZ	702	GDP	C6-N1-C2	4.01	122.29	115.93



There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
64	DZ	702	GDP	PA-O3A-PB-O2B
64	DZ	702	GDP	C5'-O5'-PA-O1A

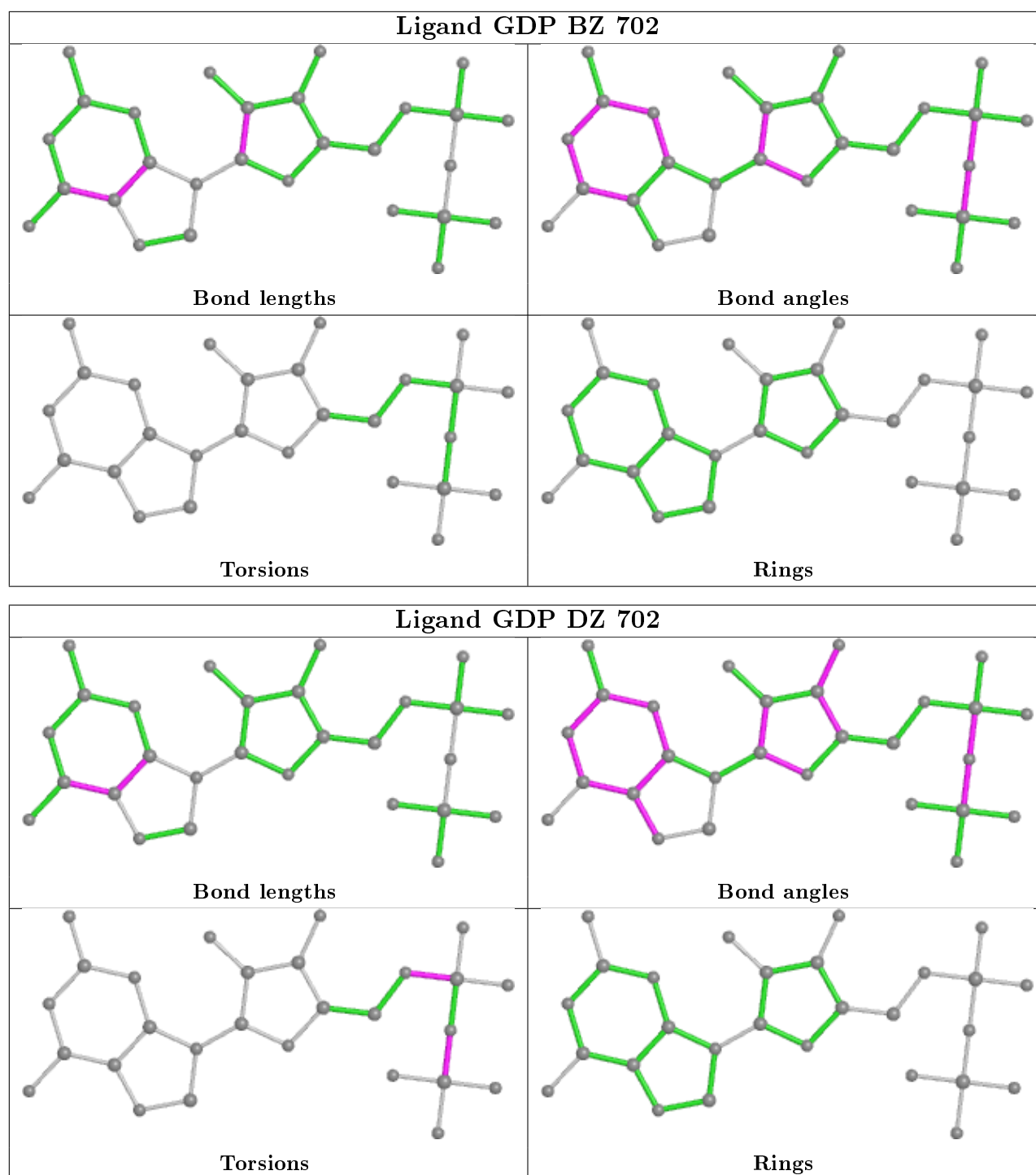
There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	BZ	702	GDP	6	0
64	DZ	702	GDP	7	0
63	BD	501	SF4	1	0
63	DD	501	SF4	1	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	2872/2915 (98%)	-0.17	64 (2%) 62 52	16, 36, 153, 292	0
1	CA	2868/2915 (98%)	-0.05	119 (4%) 37 27	25, 54, 187, 320	0
2	AB	120/121 (99%)	-0.44	0 100 100	26, 52, 72, 110	0
2	CB	120/121 (99%)	-0.13	0 100 100	55, 87, 110, 177	0
3	AC	137/228 (60%)	4.00	113 (82%) 0 0	95, 162, 210, 232	0
3	CC	137/228 (60%)	5.74	125 (91%) 0 0	115, 183, 225, 239	0
4	AD	275/276 (99%)	-0.47	2 (0%) 87 84	16, 35, 59, 113	0
4	CD	275/276 (99%)	-0.34	1 (0%) 92 91	19, 46, 73, 142	0
5	AE	204/206 (99%)	-0.47	0 100 100	8, 36, 67, 101	0
5	CE	204/206 (99%)	-0.28	0 100 100	25, 53, 88, 136	0
6	AF	203/210 (96%)	-0.41	1 (0%) 91 88	12, 37, 91, 175	0
6	CF	203/210 (96%)	-0.29	0 100 100	23, 63, 114, 164	0
7	AG	181/182 (99%)	-0.23	3 (1%) 70 63	41, 71, 110, 179	0
7	CG	181/182 (99%)	0.30	8 (4%) 34 24	74, 106, 143, 190	0
8	AH	174/180 (96%)	-0.35	2 (1%) 80 75	30, 51, 81, 174	0
8	CH	174/180 (96%)	0.62	12 (6%) 16 10	45, 94, 139, 208	0
9	AK	130/173 (75%)	1.28	27 (20%) 1 0	62, 125, 191, 235	0
9	CK	130/173 (75%)	2.90	71 (54%) 0 0	104, 173, 211, 231	0
10	AL	66/147 (44%)	4.16	50 (75%) 0 0	134, 182, 226, 242	0
10	CL	66/147 (44%)	5.90	53 (80%) 0 0	115, 198, 249, 257	0
11	AN	140/140 (100%)	-0.53	0 100 100	17, 34, 76, 106	0
11	CN	140/140 (100%)	-0.10	1 (0%) 87 84	33, 59, 97, 139	0
12	AO	122/122 (100%)	-0.33	0 100 100	20, 40, 67, 95	0
12	CO	122/122 (100%)	-0.30	0 100 100	33, 52, 83, 102	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AP	149/150 (99%)	-0.30	0 100 100	14, 44, 83, 127	0
13	CP	149/150 (99%)	0.21	4 (2%) 54 44	29, 66, 112, 154	0
14	AQ	141/141 (100%)	-0.37	0 100 100	17, 39, 66, 97	0
14	CQ	141/141 (100%)	-0.33	0 100 100	33, 62, 91, 156	0
15	AR	118/118 (100%)	-0.48	0 100 100	17, 32, 57, 96	0
15	CR	118/118 (100%)	-0.27	0 100 100	29, 52, 78, 97	0
16	AS	110/112 (98%)	-0.16	0 100 100	32, 54, 81, 102	0
16	CS	110/112 (98%)	0.27	4 (3%) 42 32	53, 82, 112, 143	0
17	AT	131/146 (89%)	-0.30	2 (1%) 73 68	23, 44, 94, 160	0
17	CT	131/146 (89%)	-0.31	0 100 100	37, 58, 99, 155	0
18	AU	116/118 (98%)	-0.57	0 100 100	15, 28, 48, 110	0
18	CU	116/118 (98%)	-0.28	1 (0%) 84 80	36, 52, 82, 123	0
19	AV	101/101 (100%)	-0.56	1 (0%) 82 77	19, 34, 63, 119	0
19	CV	101/101 (100%)	-0.03	1 (0%) 82 77	33, 72, 108, 138	0
20	AW	112/113 (99%)	-0.45	0 100 100	15, 29, 56, 134	0
20	CW	112/113 (99%)	-0.23	1 (0%) 84 80	27, 48, 86, 149	0
21	AX	95/96 (98%)	-0.44	1 (1%) 80 75	22, 38, 69, 125	0
21	CX	95/96 (98%)	0.03	4 (4%) 36 26	40, 61, 93, 134	0
22	AY	107/110 (97%)	-0.29	1 (0%) 84 80	25, 48, 92, 129	0
22	CY	107/110 (97%)	0.67	7 (6%) 18 11	43, 78, 114, 172	0
23	AZ	171/206 (83%)	0.07	11 (6%) 19 12	33, 73, 144, 235	0
23	CZ	174/206 (84%)	0.83	21 (12%) 4 2	60, 107, 174, 243	0
24	A0	83/85 (97%)	-0.31	2 (2%) 59 49	18, 38, 68, 147	0
24	C0	83/85 (97%)	0.31	6 (7%) 15 8	37, 62, 96, 135	0
25	A1	97/98 (98%)	-0.22	2 (2%) 63 54	23, 44, 85, 108	0
25	C1	97/98 (98%)	-0.10	1 (1%) 82 77	33, 54, 107, 119	0
26	A2	70/72 (97%)	-0.28	2 (2%) 51 41	22, 47, 74, 149	0
26	C2	70/72 (97%)	0.02	1 (1%) 75 70	51, 78, 99, 121	0
27	A3	59/60 (98%)	-0.28	1 (1%) 70 63	18, 34, 63, 112	0
27	C3	59/60 (98%)	0.60	5 (8%) 10 5	43, 62, 108, 167	0
28	A4	69/71 (97%)	0.48	9 (13%) 3 2	60, 100, 186, 194	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	C4	69/71 (97%)	0.96	11 (15%) 1 1	89, 138, 197, 212	0
29	A5	59/60 (98%)	-0.56	0 100 100	15, 30, 55, 84	0
29	C5	59/60 (98%)	-0.24	1 (1%) 70 63	29, 46, 77, 112	0
30	A6	53/54 (98%)	-0.39	0 100 100	24, 42, 67, 91	0
30	C6	53/54 (98%)	-0.09	1 (1%) 66 59	43, 63, 88, 103	0
31	A7	48/49 (97%)	-0.27	2 (4%) 36 26	14, 26, 63, 126	0
31	C7	48/49 (97%)	-0.10	1 (2%) 63 54	26, 38, 83, 105	0
32	A8	64/65 (98%)	-0.44	0 100 100	17, 32, 46, 72	0
32	C8	64/65 (98%)	-0.24	0 100 100	36, 51, 70, 101	0
33	A9	37/37 (100%)	-0.12	0 100 100	23, 39, 60, 80	0
33	C9	37/37 (100%)	0.24	1 (2%) 54 44	42, 66, 96, 108	0
34	BA	1497/1521 (98%)	0.01	40 (2%) 54 44	32, 76, 169, 302	0
34	DA	1503/1521 (98%)	0.10	42 (2%) 53 43	40, 83, 174, 317	0
35	BB	231/256 (90%)	0.48	18 (7%) 13 7	61, 108, 167, 197	0
35	DB	231/256 (90%)	0.82	30 (12%) 3 2	77, 129, 184, 232	0
36	BC	206/239 (86%)	0.32	9 (4%) 34 24	60, 103, 138, 194	0
36	DC	206/239 (86%)	0.90	23 (11%) 5 3	77, 127, 170, 196	0
37	BD	208/209 (99%)	0.06	3 (1%) 75 70	51, 82, 121, 168	0
37	DD	208/209 (99%)	-0.02	3 (1%) 75 70	47, 80, 112, 165	0
38	BE	148/162 (91%)	-0.08	0 100 100	48, 73, 111, 140	0
38	DE	148/162 (91%)	0.19	4 (2%) 54 44	46, 89, 128, 151	0
39	BF	100/101 (99%)	-0.22	0 100 100	45, 80, 116, 137	0
39	DF	100/101 (99%)	-0.18	0 100 100	49, 80, 104, 121	0
40	BG	155/156 (99%)	0.27	13 (8%) 11 5	59, 88, 132, 174	0
40	DG	155/156 (99%)	0.67	17 (10%) 5 3	67, 103, 142, 192	0
41	BH	137/138 (99%)	0.08	1 (0%) 87 84	45, 76, 106, 135	0
41	DH	137/138 (99%)	0.37	6 (4%) 34 24	55, 88, 127, 170	0
42	BI	127/128 (99%)	0.59	9 (7%) 16 9	50, 101, 140, 166	0
42	DI	127/128 (99%)	1.30	28 (22%) 0 0	66, 118, 159, 201	0
43	BJ	97/105 (92%)	0.80	14 (14%) 2 1	53, 113, 158, 199	0
43	DJ	96/105 (91%)	1.45	25 (26%) 0 0	70, 134, 181, 195	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BK	114/129 (88%)	-0.26	0 100 100	45, 72, 112, 129	0
44	DK	114/129 (88%)	-0.02	1 (0%) 84 80	44, 80, 118, 139	0
45	BL	122/132 (92%)	-0.22	0 100 100	38, 63, 88, 113	0
45	DL	122/132 (92%)	-0.02	2 (1%) 72 66	37, 72, 94, 141	0
46	BM	123/126 (97%)	0.53	9 (7%) 15 8	55, 95, 129, 222	0
46	DM	122/126 (96%)	0.88	16 (13%) 3 2	71, 125, 153, 188	0
47	BN	60/61 (98%)	0.56	5 (8%) 11 6	65, 95, 123, 138	0
47	DN	60/61 (98%)	1.69	20 (33%) 0 0	84, 123, 166, 208	0
48	BO	88/89 (98%)	-0.05	2 (2%) 60 51	39, 68, 110, 142	0
48	DO	88/89 (98%)	0.25	0 100 100	43, 78, 112, 127	0
49	BP	82/88 (93%)	0.34	1 (1%) 79 73	54, 76, 109, 134	0
49	DP	82/88 (93%)	0.18	2 (2%) 59 49	53, 70, 96, 131	0
50	BQ	99/105 (94%)	-0.08	0 100 100	43, 69, 97, 110	0
50	DQ	99/105 (94%)	0.09	0 100 100	51, 74, 103, 123	0
51	BR	68/88 (77%)	0.47	4 (5%) 22 14	48, 73, 112, 135	0
51	DR	68/88 (77%)	0.47	4 (5%) 22 14	46, 78, 116, 135	0
52	BS	84/93 (90%)	1.05	15 (17%) 1 1	67, 110, 163, 180	0
52	DS	83/93 (89%)	1.86	39 (46%) 0 0	92, 141, 187, 229	0
53	BT	96/106 (90%)	0.24	1 (1%) 82 77	53, 77, 115, 169	0
53	DT	96/106 (90%)	0.28	1 (1%) 82 77	52, 77, 117, 132	0
54	BU	23/27 (85%)	0.77	3 (13%) 3 2	56, 89, 104, 114	0
54	DU	23/27 (85%)	1.72	8 (34%) 0 0	79, 109, 130, 142	0
55	BV	13/24 (54%)	1.80	5 (38%) 0 0	49, 87, 172, 178	0
55	DV	12/24 (50%)	2.83	8 (66%) 0 0	63, 120, 171, 199	0
56	BW	66/76 (86%)	2.57	35 (53%) 0 0	64, 169, 230, 256	0
56	DW	64/76 (84%)	3.63	47 (73%) 0 0	92, 197, 239, 263	0
57	BX	71/77 (92%)	-0.05	1 (1%) 75 70	34, 78, 124, 188	0
57	DX	71/77 (92%)	0.18	2 (2%) 53 43	34, 100, 148, 162	0
58	BY	67/76 (88%)	0.92	11 (16%) 1 1	39, 159, 224, 266	0
58	DY	66/76 (86%)	1.34	15 (22%) 0 0	57, 178, 229, 251	0
59	BZ	728/758 (96%)	1.08	151 (20%) 1 0	41, 107, 195, 257	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
59	DZ	730/758 (96%)	1.54	227 (31%) 0 0	38, 116, 213, 248	0
All	All	22848/24064 (94%)	0.24	1677 (7%) 15 8	8, 68, 177, 320	0

The worst 5 of 1677 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
59	BZ	503	GLY	25.5
10	CL	137	GLU	19.3
3	CC	174	ALA	18.6
10	CL	138	VAL	16.1
59	BZ	502	GLY	15.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	5MU	BY	54	21/22	0.30	0.33	217,217,217,217	0
58	PSU	DY	55	20/21	0.51	0.54	222,222,222,222	0
56	PSU	DW	55	20/21	0.52	0.44	190,190,190,190	0
56	4SU	DW	8	20/21	0.58	0.49	225,225,225,225	0
58	4SU	DY	8	20/21	0.62	0.21	193,193,193,193	0
58	7MG	DY	46	24/25	0.64	0.24	206,206,206,206	0
58	PSU	BY	55	20/21	0.64	0.24	205,205,205,205	0
56	4SU	BW	8	20/21	0.64	0.28	200,200,200,200	0
56	7MG	DW	46	24/25	0.65	0.34	244,244,244,244	0
58	MIA	DY	37	22/30	0.68	0.29	156,156,156,156	0
58	4SU	BY	8	20/21	0.71	0.21	191,191,191,191	0
58	7MG	BY	46	24/25	0.71	0.21	200,200,200,200	0
56	7MG	BW	46	24/25	0.72	0.27	203,203,203,203	0
56	PSU	BW	55	20/21	0.72	0.31	113,113,113,113	0
58	5MU	DY	54	21/22	0.72	0.36	200,200,200,200	0
58	PSU	DY	32	20/21	0.82	0.20	154,154,154,154	0
58	PSU	DY	39	20/21	0.84	0.21	138,138,138,138	0
58	PSU	BY	32	20/21	0.84	0.20	126,126,126,126	0
58	MIA	BY	37	22/30	0.85	0.18	118,118,118,118	0
57	31H	DX	76	32/33	0.87	0.31	58,58,58,58	4
56	5MU	DW	54	21/22	0.87	0.22	118,118,118,118	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	PSU	DW	39	20/21	0.89	0.24	118,118,118,118	0
56	PSU	DW	32	20/21	0.89	0.36	139,139,139,139	0
56	5MU	BW	54	21/22	0.89	0.25	89,89,89,89	0
56	PSU	BW	39	20/21	0.90	0.23	96,96,96,96	0
57	4SU	DX	8	20/21	0.90	0.14	96,96,96,96	0
56	MIA	BW	37	29/30	0.90	0.30	95,95,95,95	1
56	MIA	DW	37	22/30	0.90	0.27	116,116,116,116	0
56	F3N	DW	76	33/34	0.91	0.35	75,75,75,75	1
58	PSU	BY	39	20/21	0.91	0.17	106,106,106,106	0
57	PSU	DX	55	20/21	0.91	0.13	95,95,95,95	0
56	PSU	BW	32	20/21	0.92	0.21	110,110,110,110	0
57	5MC	DX	32	21/22	0.93	0.20	86,86,86,86	0
57	5MU	BX	54	21/22	0.93	0.17	85,85,85,85	0
57	4SU	BX	8	20/21	0.93	0.14	70,70,70,70	1
57	31H	BX	76	32/33	0.94	0.26	58,58,58,58	4
57	PSU	BX	55	20/21	0.94	0.13	74,74,74,74	0
57	5MU	DX	54	21/22	0.94	0.18	108,108,108,108	0
57	5MC	BX	32	21/22	0.95	0.17	65,65,65,65	0
56	F3N	BW	76	33/34	0.96	0.25	54,54,54,54	1

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	1800	1/1	0.10	0.56	116,116,116,116	0
60	MG	CA	3543	1/1	0.17	0.55	114,114,114,114	0
60	MG	DA	1686	1/1	0.22	0.36	102,102,102,102	0
60	MG	CA	3491	1/1	0.26	0.61	99,99,99,99	0
60	MG	AA	3108	1/1	0.31	0.41	88,88,88,88	0
60	MG	CA	3527	1/1	0.34	0.38	83,83,83,83	0
60	MG	AA	3203	1/1	0.35	1.03	125,125,125,125	0
60	MG	CA	3206	1/1	0.37	0.65	109,109,109,109	0
60	MG	CA	3073	1/1	0.38	0.73	94,94,94,94	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3550	1/1	0.39	0.36	88,88,88,88	0
60	MG	AA	3805	1/1	0.39	1.54	117,117,117,117	0
60	MG	CA	3478	1/1	0.41	0.29	91,91,91,91	0
60	MG	CA	3653	1/1	0.41	0.51	102,102,102,102	0
60	MG	AA	3136	1/1	0.42	0.46	74,74,74,74	0
60	MG	AA	3490	1/1	0.43	0.52	87,87,87,87	0
60	MG	DA	1715	1/1	0.43	0.46	87,87,87,87	0
60	MG	AA	3770	1/1	0.44	0.80	57,57,57,57	1
60	MG	CA	3098	1/1	0.45	1.04	90,90,90,90	0
60	MG	CA	3514	1/1	0.46	0.16	68,68,68,68	0
60	MG	AA	3040	1/1	0.47	0.13	93,93,93,93	0
60	MG	CB	3008	1/1	0.47	0.26	87,87,87,87	0
60	MG	CA	3031	1/1	0.48	0.73	102,102,102,102	0
60	MG	CA	3177	1/1	0.49	0.65	98,98,98,98	0
60	MG	CA	3597	1/1	0.50	0.48	108,108,108,108	0
60	MG	CA	3139	1/1	0.50	0.53	83,83,83,83	0
60	MG	BK	3101	1/1	0.51	0.57	95,95,95,95	0
60	MG	CA	3481	1/1	0.51	0.24	86,86,86,86	0
60	MG	DA	1615	1/1	0.51	0.52	87,87,87,87	0
60	MG	CA	3042	1/1	0.52	0.89	84,84,84,84	0
60	MG	CA	3079	1/1	0.52	0.57	82,82,82,82	0
60	MG	BA	1740	1/1	0.52	0.12	89,89,89,89	0
60	MG	AA	3736	1/1	0.53	0.37	74,74,74,74	0
60	MG	AA	3246	1/1	0.54	0.60	86,86,86,86	0
60	MG	CA	3581	1/1	0.54	0.22	100,100,100,100	0
60	MG	AA	3327	1/1	0.55	0.23	36,36,36,36	0
60	MG	BA	1779	1/1	0.55	0.33	82,82,82,82	0
60	MG	CA	3502	1/1	0.56	0.14	66,66,66,66	0
60	MG	AA	3225	1/1	0.56	0.89	91,91,91,91	0
60	MG	CA	3588	1/1	0.57	0.19	78,78,78,78	0
60	MG	CA	3070	1/1	0.57	0.57	78,78,78,78	0
60	MG	CA	3578	1/1	0.57	0.12	96,96,96,96	0
60	MG	AA	3271	1/1	0.58	0.29	81,81,81,81	0
60	MG	BA	1803	1/1	0.58	0.22	79,79,79,79	0
60	MG	CQ	201	1/1	0.58	0.76	85,85,85,85	0
60	MG	DA	1764	1/1	0.58	0.41	94,94,94,94	0
60	MG	BA	1709	1/1	0.59	0.27	96,96,96,96	0
60	MG	AA	3051	1/1	0.59	0.69	84,84,84,84	0
60	MG	CA	3090	1/1	0.59	0.46	98,98,98,98	0
60	MG	BA	1624	1/1	0.59	0.21	75,75,75,75	0
60	MG	DX	3001	1/1	0.59	0.41	75,75,75,75	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	DA	1671	1/1	0.60	0.65	77,77,77,77	0
60	MG	CA	3376	1/1	0.60	0.17	94,94,94,94	0
60	MG	AA	3694	1/1	0.60	0.17	49,49,49,49	0
60	MG	AA	3242	1/1	0.61	0.20	69,69,69,69	0
60	MG	DA	1753	1/1	0.61	0.26	85,85,85,85	0
60	MG	AA	3739	1/1	0.61	0.42	90,90,90,90	0
60	MG	CA	3049	1/1	0.62	0.29	63,63,63,63	0
60	MG	CA	3085	1/1	0.62	0.53	82,82,82,82	0
60	MG	AA	3725	1/1	0.62	0.27	42,42,42,42	0
60	MG	CA	3575	1/1	0.62	0.47	77,77,77,77	0
60	MG	AA	3026	1/1	0.64	0.38	69,69,69,69	0
60	MG	BW	101	1/1	0.64	0.47	82,82,82,82	0
60	MG	CA	3622	1/1	0.64	0.17	106,106,106,106	0
60	MG	CA	3101	1/1	0.64	0.11	86,86,86,86	0
60	MG	CA	3111	1/1	0.64	0.20	82,82,82,82	0
60	MG	CA	3613	1/1	0.64	0.31	42,42,42,42	0
60	MG	AA	3579	1/1	0.65	0.14	66,66,66,66	0
60	MG	DA	1623	1/1	0.65	0.38	70,70,70,70	0
60	MG	CA	3239	1/1	0.65	0.32	76,76,76,76	0
60	MG	DA	1651	1/1	0.65	0.26	86,86,86,86	0
60	MG	BA	1706	1/1	0.65	0.25	82,82,82,82	0
60	MG	AA	3150	1/1	0.65	0.32	63,63,63,63	0
60	MG	AA	3664	1/1	0.66	0.21	94,94,94,94	0
60	MG	CA	3016	1/1	0.66	0.48	69,69,69,69	0
60	MG	AA	3070	1/1	0.66	0.35	68,68,68,68	0
60	MG	AA	3625	1/1	0.66	0.30	88,88,88,88	0
60	MG	CA	3506	1/1	0.66	0.25	120,120,120,120	0
60	MG	CA	3092	1/1	0.66	0.49	74,74,74,74	0
60	MG	DA	1610	1/1	0.66	0.29	59,59,59,59	0
60	MG	CA	3212	1/1	0.66	0.10	78,78,78,78	0
60	MG	CA	3063	1/1	0.66	0.71	74,74,74,74	0
60	MG	CA	3592	1/1	0.66	0.23	87,87,87,87	0
60	MG	CA	3526	1/1	0.67	0.13	69,69,69,69	0
60	MG	CA	3482	1/1	0.67	0.29	89,89,89,89	0
60	MG	BA	1691	1/1	0.67	0.34	98,98,98,98	0
60	MG	BA	1703	1/1	0.67	0.22	65,65,65,65	0
60	MG	AA	3324	1/1	0.67	0.10	69,69,69,69	0
60	MG	AA	3692	1/1	0.67	0.48	86,86,86,86	0
60	MG	CA	3199	1/1	0.67	0.58	92,92,92,92	0
60	MG	CB	3006	1/1	0.67	0.19	82,82,82,82	0
60	MG	DA	1739	1/1	0.67	0.43	85,85,85,85	0
60	MG	AA	3599	1/1	0.67	0.43	113,113,113,113	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3348	1/1	0.68	0.14	78,78,78,78	0
60	MG	BA	1674	1/1	0.68	0.08	78,78,78,78	0
60	MG	DA	1676	1/1	0.68	0.29	69,69,69,69	0
60	MG	BA	1722	1/1	0.68	0.29	86,86,86,86	0
60	MG	BX	112	1/1	0.68	0.21	78,78,78,78	0
60	MG	AA	3263	1/1	0.68	0.44	75,75,75,75	0
60	MG	CA	3244	1/1	0.69	0.32	70,70,70,70	0
60	MG	DA	1734	1/1	0.69	0.28	75,75,75,75	0
60	MG	DA	1762	1/1	0.69	0.16	86,86,86,86	0
60	MG	AA	3192	1/1	0.69	0.42	69,69,69,69	0
60	MG	DA	1704	1/1	0.69	0.31	83,83,83,83	0
60	MG	CA	3089	1/1	0.69	0.71	78,78,78,78	0
60	MG	CA	3590	1/1	0.70	0.53	78,78,78,78	0
60	MG	CA	3664	1/1	0.70	0.31	69,69,69,69	0
60	MG	BA	1763	1/1	0.70	0.08	75,75,75,75	0
60	MG	CA	3152	1/1	0.70	0.17	67,67,67,67	0
60	MG	CA	3234	1/1	0.70	0.35	96,96,96,96	0
60	MG	AA	3648	1/1	0.70	0.17	80,80,80,80	0
60	MG	DA	1608	1/1	0.70	0.50	79,79,79,79	0
60	MG	AA	3537	1/1	0.70	0.12	90,90,90,90	0
60	MG	AA	3015	1/1	0.71	0.46	74,74,74,74	0
60	MG	AA	3249	1/1	0.71	0.45	64,64,64,64	0
60	MG	AA	3632	1/1	0.71	0.26	97,97,97,97	0
60	MG	AA	3773	1/1	0.71	0.20	77,77,77,77	0
60	MG	AA	3766	1/1	0.71	0.22	69,69,69,69	0
60	MG	BY	3002	1/1	0.71	0.17	83,83,83,83	0
60	MG	AA	3828	1/1	0.71	0.55	68,68,68,68	0
60	MG	AA	3783	1/1	0.71	0.38	68,68,68,68	0
60	MG	CA	3245	1/1	0.71	0.30	53,53,53,53	0
60	MG	CA	3311	1/1	0.72	0.29	54,54,54,54	0
60	MG	AA	3689	1/1	0.72	0.16	84,84,84,84	0
60	MG	BA	1770	1/1	0.72	0.12	62,62,62,62	0
60	MG	BA	1767	1/1	0.72	0.27	73,73,73,73	0
60	MG	BA	1737	1/1	0.72	0.27	87,87,87,87	0
60	MG	DA	1765	1/1	0.72	0.26	66,66,66,66	0
60	MG	CA	3303	1/1	0.72	0.28	52,52,52,52	0
60	MG	AA	3183	1/1	0.72	0.97	89,89,89,89	0
60	MG	AA	3571	1/1	0.72	0.11	53,53,53,53	0
60	MG	CA	3374	1/1	0.72	0.15	74,74,74,74	0
60	MG	AQ	3002	1/1	0.72	0.31	79,79,79,79	0
60	MG	AA	3059	1/1	0.73	0.52	62,62,62,62	0
60	MG	BA	1790	1/1	0.73	0.32	87,87,87,87	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	1699	1/1	0.73	0.19	70,70,70,70	0
60	MG	CA	3059	1/1	0.73	0.38	66,66,66,66	0
60	MG	CA	3535	1/1	0.73	0.19	74,74,74,74	0
60	MG	CA	3282	1/1	0.73	0.38	75,75,75,75	0
60	MG	CE	303	1/1	0.73	0.39	55,55,55,55	0
60	MG	CA	3411	1/1	0.73	0.24	49,49,49,49	0
60	MG	CA	3616	1/1	0.73	0.34	62,62,62,62	0
60	MG	CA	3529	1/1	0.73	0.31	69,69,69,69	0
60	MG	CA	3475	1/1	0.73	0.17	55,55,55,55	0
60	MG	AB	3014	1/1	0.73	0.23	70,70,70,70	0
60	MG	A0	104	1/1	0.73	0.80	81,81,81,81	0
60	MG	DA	1743	1/1	0.73	0.13	83,83,83,83	0
60	MG	AA	3347	1/1	0.74	0.32	63,63,63,63	0
60	MG	AA	3088	1/1	0.74	0.53	42,42,42,42	0
60	MG	AA	3221	1/1	0.74	0.16	72,72,72,72	0
60	MG	CA	3241	1/1	0.74	0.19	69,69,69,69	0
60	MG	AA	3578	1/1	0.74	0.37	71,71,71,71	0
60	MG	CA	3195	1/1	0.74	0.18	36,36,36,36	0
60	MG	AA	3755	1/1	0.74	0.23	77,77,77,77	0
60	MG	CF	306	1/1	0.74	0.94	85,85,85,85	0
60	MG	CA	3542	1/1	0.74	0.20	82,82,82,82	0
60	MG	DA	1611	1/1	0.74	0.23	80,80,80,80	0
60	MG	CA	3194	1/1	0.74	0.55	87,87,87,87	0
60	MG	CA	3642	1/1	0.74	0.11	75,75,75,75	0
60	MG	AD	307	1/1	0.74	0.20	54,54,54,54	0
60	MG	CA	3619	1/1	0.75	0.36	78,78,78,78	0
60	MG	CA	3652	1/1	0.75	0.23	79,79,79,79	0
60	MG	CA	3183	1/1	0.75	0.43	83,83,83,83	0
60	MG	DW	3001	1/1	0.75	0.80	90,90,90,90	0
60	MG	AA	3234	1/1	0.75	0.42	58,58,58,58	0
60	MG	AA	3751	1/1	0.75	0.20	76,76,76,76	0
60	MG	AA	3713	1/1	0.75	0.52	48,48,48,48	0
60	MG	CA	3247	1/1	0.75	0.16	45,45,45,45	0
60	MG	CA	3067	1/1	0.75	0.60	82,82,82,82	0
60	MG	AA	3245	1/1	0.75	0.22	79,79,79,79	0
60	MG	AA	3582	1/1	0.75	0.36	78,78,78,78	0
60	MG	CA	3524	1/1	0.75	0.29	87,87,87,87	0
60	MG	AA	3763	1/1	0.75	0.25	66,66,66,66	0
60	MG	BA	1804	1/1	0.75	0.47	94,94,94,94	0
60	MG	AA	3487	1/1	0.76	0.10	66,66,66,66	0
60	MG	BA	1670	1/1	0.76	0.30	76,76,76,76	0
60	MG	CA	3083	1/1	0.76	0.22	80,80,80,80	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	1646	1/1	0.76	0.52	71,71,71,71	0
60	MG	CA	3298	1/1	0.76	0.21	68,68,68,68	0
60	MG	CA	3113	1/1	0.76	0.47	75,75,75,75	0
60	MG	AA	3638	1/1	0.76	0.36	72,72,72,72	0
60	MG	CA	3094	1/1	0.76	0.35	92,92,92,92	0
60	MG	CA	3511	1/1	0.76	0.34	66,66,66,66	0
60	MG	AA	3480	1/1	0.76	0.13	78,78,78,78	0
60	MG	AA	3700	1/1	0.76	0.21	48,48,48,48	0
60	MG	CA	3505	1/1	0.76	0.26	66,66,66,66	0
60	MG	AF	304	1/1	0.76	0.43	69,69,69,69	0
60	MG	CA	3631	1/1	0.76	0.29	88,88,88,88	0
60	MG	CA	3091	1/1	0.77	0.40	60,60,60,60	0
60	MG	AB	3019	1/1	0.77	0.18	61,61,61,61	0
60	MG	BA	1657	1/1	0.77	0.47	72,72,72,72	0
60	MG	DA	1631	1/1	0.77	0.22	55,55,55,55	0
60	MG	AA	3002	1/1	0.77	0.24	53,53,53,53	0
60	MG	AX	102	1/1	0.77	0.37	78,78,78,78	0
60	MG	CA	3103	1/1	0.77	0.19	80,80,80,80	0
60	MG	DA	1620	1/1	0.77	0.23	68,68,68,68	0
60	MG	CA	3096	1/1	0.77	0.28	75,75,75,75	0
60	MG	BA	1627	1/1	0.77	0.21	63,63,63,63	0
60	MG	CA	3032	1/1	0.77	0.43	67,67,67,67	0
60	MG	CA	3273	1/1	0.77	0.21	42,42,42,42	0
60	MG	AA	3548	1/1	0.77	0.13	69,69,69,69	0
60	MG	DE	201	1/1	0.78	0.31	93,93,93,93	0
60	MG	BN	503	1/1	0.78	0.23	61,61,61,61	0
60	MG	CA	3509	1/1	0.78	0.19	52,52,52,52	0
60	MG	CB	3012	1/1	0.78	0.16	74,74,74,74	0
60	MG	BA	1752	1/1	0.78	0.07	48,48,48,48	0
60	MG	CA	3467	1/1	0.78	0.44	99,99,99,99	0
60	MG	CA	3431	1/1	0.78	0.17	80,80,80,80	0
60	MG	A2	3001	1/1	0.78	0.25	62,62,62,62	0
60	MG	BA	1786	1/1	0.78	0.33	79,79,79,79	0
60	MG	CA	3187	1/1	0.78	0.32	70,70,70,70	0
60	MG	BA	1621	1/1	0.78	0.66	78,78,78,78	0
60	MG	CA	3018	1/1	0.78	0.18	59,59,59,59	0
60	MG	CA	3645	1/1	0.78	0.13	78,78,78,78	0
60	MG	AA	3541	1/1	0.78	0.20	61,61,61,61	0
60	MG	DA	1634	1/1	0.78	0.34	66,66,66,66	0
60	MG	DA	1702	1/1	0.78	0.27	58,58,58,58	0
60	MG	DA	1735	1/1	0.78	0.10	75,75,75,75	0
60	MG	AA	3732	1/1	0.78	0.18	63,63,63,63	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3152	1/1	0.78	0.41	80,80,80,80	0
60	MG	AA	3164	1/1	0.78	0.21	106,106,106,106	0
60	MG	BA	1629	1/1	0.78	0.25	71,71,71,71	0
60	MG	CA	3057	1/1	0.78	0.71	77,77,77,77	0
60	MG	CA	3202	1/1	0.79	0.32	67,67,67,67	0
60	MG	AZ	5001	1/1	0.79	0.11	67,67,67,67	0
60	MG	CA	3122	1/1	0.79	0.33	95,95,95,95	0
60	MG	CA	3291	1/1	0.79	0.17	74,74,74,74	0
60	MG	BW	102	1/1	0.79	0.20	75,75,75,75	0
60	MG	AA	3146	1/1	0.79	0.20	53,53,53,53	0
60	MG	AA	3161	1/1	0.79	0.57	89,89,89,89	0
60	MG	CA	3080	1/1	0.79	0.58	78,78,78,78	0
60	MG	AA	3210	1/1	0.79	0.55	106,106,106,106	0
60	MG	CA	3633	1/1	0.79	0.19	85,85,85,85	0
60	MG	AA	3640	1/1	0.79	0.49	74,74,74,74	0
60	MG	CA	3015	1/1	0.79	0.48	66,66,66,66	0
60	MG	CA	3155	1/1	0.79	0.48	69,69,69,69	0
60	MG	CA	3483	1/1	0.79	0.17	67,67,67,67	0
60	MG	AA	3793	1/1	0.79	0.35	76,76,76,76	0
60	MG	AA	3093	1/1	0.79	0.86	81,81,81,81	0
60	MG	AA	3744	1/1	0.79	0.15	79,79,79,79	0
60	MG	CA	3087	1/1	0.79	0.41	107,107,107,107	0
60	MG	A0	101	1/1	0.79	0.23	88,88,88,88	0
60	MG	CA	3474	1/1	0.79	0.14	72,72,72,72	0
60	MG	BA	1671	1/1	0.80	0.36	71,71,71,71	0
60	MG	CA	3599	1/1	0.80	0.09	75,75,75,75	0
60	MG	CA	3659	1/1	0.80	0.35	72,72,72,72	0
60	MG	AA	3444	1/1	0.80	0.10	52,52,52,52	0
60	MG	AA	3649	1/1	0.80	0.07	78,78,78,78	0
60	MG	BA	1630	1/1	0.80	0.19	61,61,61,61	0
60	MG	CA	3249	1/1	0.80	0.18	67,67,67,67	0
60	MG	DA	1602	1/1	0.80	0.22	65,65,65,65	0
60	MG	BA	1757	1/1	0.80	0.35	63,63,63,63	0
60	MG	AA	3061	1/1	0.80	0.77	64,64,64,64	0
60	MG	AD	309	1/1	0.80	0.34	58,58,58,58	0
60	MG	CA	3521	1/1	0.80	0.34	59,59,59,59	0
60	MG	CA	3235	1/1	0.80	0.37	78,78,78,78	0
60	MG	CB	3010	1/1	0.80	0.16	67,67,67,67	0
60	MG	BA	1808	1/1	0.80	0.16	80,80,80,80	0
60	MG	AA	3486	1/1	0.80	0.21	34,34,34,34	0
60	MG	AA	3605	1/1	0.80	0.11	66,66,66,66	0
60	MG	AD	306	1/1	0.80	0.22	108,108,108,108	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3407	1/1	0.80	0.28	41,41,41,41	0
60	MG	BX	106	1/1	0.80	0.17	85,85,85,85	0
60	MG	BA	1689	1/1	0.80	0.29	65,65,65,65	0
60	MG	AA	3182	1/1	0.80	0.27	73,73,73,73	0
60	MG	AA	3165	1/1	0.80	0.41	64,64,64,64	0
60	MG	AA	3702	1/1	0.80	0.44	45,45,45,45	1
60	MG	CA	3222	1/1	0.80	0.70	81,81,81,81	0
60	MG	AA	3159	1/1	0.80	0.41	66,66,66,66	0
60	MG	CA	3445	1/1	0.80	0.36	70,70,70,70	0
60	MG	AA	3110	1/1	0.80	0.48	57,57,57,57	0
60	MG	AB	3005	1/1	0.81	0.17	70,70,70,70	0
60	MG	CA	3156	1/1	0.81	1.42	92,92,92,92	0
60	MG	BA	1788	1/1	0.81	0.17	79,79,79,79	0
60	MG	AA	3753	1/1	0.81	0.15	59,59,59,59	0
60	MG	CA	3555	1/1	0.81	0.08	59,59,59,59	0
60	MG	CA	3296	1/1	0.81	0.14	61,61,61,61	0
60	MG	CA	3043	1/1	0.81	0.19	75,75,75,75	0
60	MG	CA	3371	1/1	0.81	0.61	70,70,70,70	0
60	MG	AA	3585	1/1	0.81	0.15	60,60,60,60	0
60	MG	CA	3576	1/1	0.81	0.35	91,91,91,91	0
60	MG	CA	3387	1/1	0.81	0.40	73,73,73,73	0
60	MG	CE	305	1/1	0.81	0.26	37,37,37,37	0
60	MG	AA	3351	1/1	0.81	0.10	80,80,80,80	0
60	MG	CA	3329	1/1	0.81	0.22	59,59,59,59	0
60	MG	AA	3204	1/1	0.81	0.45	83,83,83,83	0
60	MG	CA	3628	1/1	0.81	0.12	76,76,76,76	0
60	MG	AA	3321	1/1	0.81	0.08	45,45,45,45	0
60	MG	CA	3462	1/1	0.81	0.34	63,63,63,63	0
60	MG	BV	101	1/1	0.81	0.16	78,78,78,78	0
60	MG	AA	3018	1/1	0.81	0.66	55,55,55,55	0
60	MG	AA	3758	1/1	0.81	0.35	70,70,70,70	0
60	MG	CA	3151	1/1	0.81	0.21	66,66,66,66	0
60	MG	BA	1622	1/1	0.81	0.63	64,64,64,64	0
60	MG	DA	1638	1/1	0.81	0.28	60,60,60,60	0
60	MG	AA	3657	1/1	0.81	0.11	73,73,73,73	0
60	MG	AA	3089	1/1	0.81	0.39	58,58,58,58	0
60	MG	AA	3098	1/1	0.81	0.29	65,65,65,65	0
60	MG	DD	502	1/1	0.82	0.50	64,64,64,64	0
60	MG	BA	1787	1/1	0.82	0.13	64,64,64,64	0
60	MG	CA	3459	1/1	0.82	0.12	46,46,46,46	0
60	MG	CA	3051	1/1	0.82	0.18	52,52,52,52	0
60	MG	CA	3226	1/1	0.82	0.37	56,56,56,56	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3279	1/1	0.82	0.55	62,62,62,62	0
60	MG	AA	3299	1/1	0.82	0.18	64,64,64,64	0
60	MG	DA	1661	1/1	0.82	0.14	74,74,74,74	0
60	MG	DA	1677	1/1	0.82	0.38	67,67,67,67	0
60	MG	AA	3300	1/1	0.82	0.30	43,43,43,43	0
60	MG	AA	3440	1/1	0.82	0.18	63,63,63,63	0
60	MG	AA	3639	1/1	0.82	0.23	74,74,74,74	0
60	MG	CA	3077	1/1	0.82	0.28	62,62,62,62	0
60	MG	AA	3829	1/1	0.82	0.40	89,89,89,89	0
60	MG	CA	3487	1/1	0.82	0.29	64,64,64,64	0
60	MG	BA	1601	1/1	0.82	0.19	66,66,66,66	0
60	MG	DA	1737	1/1	0.82	0.40	73,73,73,73	0
60	MG	DA	1614	1/1	0.82	0.15	71,71,71,71	0
60	MG	BA	1755	1/1	0.82	0.18	92,92,92,92	0
60	MG	AA	3127	1/1	0.82	0.45	83,83,83,83	0
60	MG	DA	1757	1/1	0.82	0.12	77,77,77,77	0
60	MG	AA	3027	1/1	0.82	0.55	85,85,85,85	0
60	MG	CA	3167	1/1	0.82	0.32	68,68,68,68	0
60	MG	CA	3240	1/1	0.82	0.14	49,49,49,49	0
60	MG	DA	1700	1/1	0.82	0.21	66,66,66,66	0
60	MG	CA	3281	1/1	0.82	0.20	74,74,74,74	0
60	MG	CA	3030	1/1	0.82	0.43	52,52,52,52	0
60	MG	CA	3532	1/1	0.82	0.16	59,59,59,59	0
60	MG	CA	3169	1/1	0.82	0.28	65,65,65,65	0
60	MG	AA	3408	1/1	0.82	0.26	41,41,41,41	0
60	MG	BX	103	1/1	0.82	0.08	88,88,88,88	0
60	MG	CA	3112	1/1	0.82	0.47	76,76,76,76	0
60	MG	CA	3496	1/1	0.82	0.55	58,58,58,58	0
60	MG	CA	3071	1/1	0.82	0.31	53,53,53,53	0
60	MG	AA	3243	1/1	0.82	0.29	79,79,79,79	0
60	MG	AA	3716	1/1	0.82	0.20	63,63,63,63	0
60	MG	AA	3005	1/1	0.82	0.20	63,63,63,63	0
60	MG	AA	3048	1/1	0.82	0.16	39,39,39,39	0
60	MG	CA	3280	1/1	0.82	0.17	43,43,43,43	0
60	MG	AA	3056	1/1	0.82	0.49	72,72,72,72	0
60	MG	CA	3538	1/1	0.82	0.31	58,58,58,58	0
60	MG	BA	1776	1/1	0.83	0.10	64,64,64,64	0
60	MG	CA	3533	1/1	0.83	0.14	63,63,63,63	0
60	MG	AA	3538	1/1	0.83	0.20	62,62,62,62	0
60	MG	C3	101	1/1	0.83	0.46	91,91,91,91	0
60	MG	CA	3132	1/1	0.83	0.19	67,67,67,67	0
60	MG	AA	3346	1/1	0.83	0.23	32,32,32,32	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	DA	1749	1/1	0.83	0.23	72,72,72,72	0
60	MG	BA	1766	1/1	0.83	0.16	81,81,81,81	0
60	MG	AA	3036	1/1	0.83	0.21	63,63,63,63	0
60	MG	CF	301	1/1	0.83	0.45	61,61,61,61	0
60	MG	CA	3213	1/1	0.83	0.34	62,62,62,62	0
60	MG	CA	3646	1/1	0.83	0.10	90,90,90,90	0
60	MG	BA	1758	1/1	0.83	0.18	56,56,56,56	0
60	MG	CA	3583	1/1	0.83	0.28	114,114,114,114	0
60	MG	DT	3001	1/1	0.83	0.25	59,59,59,59	0
60	MG	CA	3250	1/1	0.83	0.17	69,69,69,69	0
60	MG	CA	3660	1/1	0.83	0.14	65,65,65,65	0
60	MG	AA	3489	1/1	0.83	0.32	39,39,39,39	0
60	MG	AA	3105	1/1	0.83	0.18	77,77,77,77	0
60	MG	AH	201	1/1	0.83	1.23	83,83,83,83	0
60	MG	CA	3129	1/1	0.83	0.30	76,76,76,76	0
60	MG	AA	3688	1/1	0.83	0.16	76,76,76,76	0
60	MG	BA	1712	1/1	0.83	0.60	68,68,68,68	0
60	MG	AA	3612	1/1	0.83	0.20	60,60,60,60	0
60	MG	AA	3650	1/1	0.83	0.29	62,62,62,62	0
60	MG	DA	1718	1/1	0.83	0.11	66,66,66,66	0
60	MG	AA	3181	1/1	0.83	0.40	55,55,55,55	0
60	MG	BA	1672	1/1	0.83	0.22	61,61,61,61	0
60	MG	CA	3377	1/1	0.83	0.14	53,53,53,53	0
60	MG	AA	3413	1/1	0.83	0.15	34,34,34,34	0
60	MG	DE	202	1/1	0.83	0.17	92,92,92,92	0
60	MG	AA	3208	1/1	0.83	0.27	55,55,55,55	0
60	MG	AA	3230	1/1	0.83	0.34	55,55,55,55	0
60	MG	DA	1673	1/1	0.83	0.40	68,68,68,68	0
60	MG	AA	3265	1/1	0.83	0.36	64,64,64,64	0
60	MG	AA	3767	1/1	0.83	0.29	75,75,75,75	0
60	MG	CA	3218	1/1	0.83	0.88	63,63,63,63	0
60	MG	AA	3443	1/1	0.83	0.21	58,58,58,58	0
60	MG	CA	3146	1/1	0.83	0.31	79,79,79,79	0
60	MG	AA	3252	1/1	0.83	0.37	76,76,76,76	0
60	MG	AA	3479	1/1	0.83	0.14	66,66,66,66	0
60	MG	CA	3560	1/1	0.83	0.16	103,103,103,103	0
60	MG	BA	1638	1/1	0.84	0.64	83,83,83,83	0
60	MG	AA	3266	1/1	0.84	0.28	55,55,55,55	0
60	MG	AA	3163	1/1	0.84	0.27	73,73,73,73	0
60	MG	AA	3654	1/1	0.84	0.25	81,81,81,81	0
60	MG	DA	1621	1/1	0.84	0.08	69,69,69,69	0
60	MG	AA	3109	1/1	0.84	0.35	75,75,75,75	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3764	1/1	0.84	0.38	48,48,48,48	0
60	MG	BA	1602	1/1	0.84	0.20	75,75,75,75	0
60	MG	AA	3543	1/1	0.84	0.17	84,84,84,84	0
60	MG	AA	3369	1/1	0.84	0.19	59,59,59,59	0
60	MG	CA	3341	1/1	0.84	0.19	35,35,35,35	0
60	MG	CA	3498	1/1	0.84	0.34	68,68,68,68	0
60	MG	BA	1715	1/1	0.84	0.21	90,90,90,90	0
60	MG	CA	3069	1/1	0.84	0.28	66,66,66,66	0
60	MG	BX	105	1/1	0.84	0.09	87,87,87,87	0
60	MG	AA	3202	1/1	0.84	0.12	46,46,46,46	0
60	MG	CA	3068	1/1	0.84	0.19	73,73,73,73	0
60	MG	AA	3442	1/1	0.84	0.13	73,73,73,73	0
60	MG	CA	3545	1/1	0.84	0.11	93,93,93,93	0
60	MG	BX	102	1/1	0.84	0.10	78,78,78,78	0
60	MG	DA	1655	1/1	0.84	0.22	72,72,72,72	0
60	MG	CA	3261	1/1	0.84	0.12	50,50,50,50	0
60	MG	AA	3175	1/1	0.84	0.33	50,50,50,50	1
60	MG	AA	3768	1/1	0.84	0.35	67,67,67,67	0
60	MG	CA	3584	1/1	0.84	0.27	91,91,91,91	0
60	MG	AA	3151	1/1	0.84	0.32	63,63,63,63	0
60	MG	DA	1767	1/1	0.84	0.56	88,88,88,88	0
60	MG	AA	3337	1/1	0.84	0.22	52,52,52,52	0
60	MG	AA	3615	1/1	0.84	0.39	65,65,65,65	0
60	MG	DA	1648	1/1	0.84	0.46	66,66,66,66	0
60	MG	CA	3011	1/1	0.84	0.25	75,75,75,75	0
60	MG	AA	3624	1/1	0.84	0.27	56,56,56,56	0
60	MG	CA	3383	1/1	0.84	0.34	66,66,66,66	0
60	MG	AA	3747	1/1	0.84	0.33	65,65,65,65	0
60	MG	CA	3355	1/1	0.84	0.13	71,71,71,71	0
60	MG	CA	3115	1/1	0.84	0.54	71,71,71,71	0
60	MG	BA	1696	1/1	0.84	0.14	84,84,84,84	0
60	MG	AA	3806	1/1	0.85	0.55	56,56,56,56	0
60	MG	AF	301	1/1	0.85	0.20	49,49,49,49	0
60	MG	AB	3010	1/1	0.85	0.09	56,56,56,56	1
60	MG	CA	3589	1/1	0.85	0.16	67,67,67,67	0
60	MG	AA	3412	1/1	0.85	0.16	58,58,58,58	0
60	MG	AA	3655	1/1	0.85	0.20	55,55,55,55	0
60	MG	AA	3441	1/1	0.85	0.18	62,62,62,62	0
60	MG	AA	3028	1/1	0.85	0.30	40,40,40,40	1
60	MG	CA	3503	1/1	0.85	0.09	67,67,67,67	0
60	MG	AA	3795	1/1	0.85	0.28	26,26,26,26	1
60	MG	CA	3573	1/1	0.85	0.12	82,82,82,82	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3366	1/1	0.85	0.24	60,60,60,60	0
60	MG	CA	3397	1/1	0.85	0.10	80,80,80,80	0
60	MG	AA	3160	1/1	0.85	0.48	96,96,96,96	0
60	MG	CA	3388	1/1	0.85	0.18	97,97,97,97	0
60	MG	CA	3236	1/1	0.85	0.30	80,80,80,80	0
60	MG	CA	3142	1/1	0.85	0.25	73,73,73,73	0
60	MG	DA	1719	1/1	0.85	0.22	87,87,87,87	0
60	MG	AA	3745	1/1	0.85	0.28	42,42,42,42	0
60	MG	DA	1758	1/1	0.85	0.35	80,80,80,80	0
60	MG	CA	3490	1/1	0.85	0.41	81,81,81,81	0
60	MG	BA	1656	1/1	0.85	0.19	83,83,83,83	0
60	MG	DA	1642	1/1	0.85	0.17	67,67,67,67	0
60	MG	AA	3524	1/1	0.85	0.30	41,41,41,41	0
60	MG	CA	3293	1/1	0.85	0.31	82,82,82,82	0
60	MG	AE	301	1/1	0.85	0.40	65,65,65,65	0
60	MG	CA	3548	1/1	0.85	0.12	53,53,53,53	0
60	MG	CA	3081	1/1	0.85	0.41	69,69,69,69	0
60	MG	AA	3544	1/1	0.85	0.17	16,16,16,16	0
60	MG	DA	1748	1/1	0.85	0.18	78,78,78,78	0
60	MG	BA	1609	1/1	0.85	0.20	77,77,77,77	0
60	MG	CA	3275	1/1	0.85	0.13	73,73,73,73	0
60	MG	AA	3106	1/1	0.85	0.19	43,43,43,43	0
60	MG	BA	1618	1/1	0.85	0.52	54,54,54,54	0
60	MG	AA	3121	1/1	0.85	0.30	63,63,63,63	0
60	MG	AB	3021	1/1	0.85	0.14	75,75,75,75	0
60	MG	BA	1603	1/1	0.85	0.20	65,65,65,65	0
60	MG	CA	3634	1/1	0.85	0.21	82,82,82,82	0
60	MG	CA	3219	1/1	0.85	0.32	57,57,57,57	0
60	MG	DA	1738	1/1	0.85	0.25	100,100,100,100	0
60	MG	AA	3789	1/1	0.85	0.21	71,71,71,71	0
60	MG	BA	1759	1/1	0.85	0.14	60,60,60,60	0
60	MG	CA	3357	1/1	0.85	0.17	34,34,34,34	0
60	MG	BA	1733	1/1	0.85	0.09	57,57,57,57	0
60	MG	CA	3607	1/1	0.85	0.18	76,76,76,76	0
60	MG	AA	3316	1/1	0.85	0.20	64,64,64,64	0
60	MG	CA	3412	1/1	0.85	0.21	52,52,52,52	0
60	MG	AA	3580	1/1	0.85	0.14	26,26,26,26	0
60	MG	AA	3237	1/1	0.85	0.08	51,51,51,51	0
60	MG	CA	3058	1/1	0.85	0.44	74,74,74,74	0
60	MG	CA	3086	1/1	0.85	0.15	65,65,65,65	0
60	MG	CA	3055	1/1	0.85	0.29	77,77,77,77	0
60	MG	CA	3410	1/1	0.85	0.19	72,72,72,72	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3661	1/1	0.85	0.17	78,78,78,78	0
60	MG	CA	3637	1/1	0.86	0.24	78,78,78,78	0
60	MG	AA	3756	1/1	0.86	0.24	57,57,57,57	0
60	MG	AA	3646	1/1	0.86	0.28	82,82,82,82	0
60	MG	CA	3382	1/1	0.86	0.18	70,70,70,70	0
60	MG	CA	3075	1/1	0.86	0.15	51,51,51,51	0
60	MG	AB	3006	1/1	0.86	0.22	84,84,84,84	0
60	MG	AA	3595	1/1	0.86	0.18	60,60,60,60	0
60	MG	AA	3177	1/1	0.86	0.21	43,43,43,43	0
60	MG	CQ	203	1/1	0.86	0.28	62,62,62,62	0
60	MG	BA	1784	1/1	0.86	0.18	59,59,59,59	0
60	MG	DA	1624	1/1	0.86	0.07	83,83,83,83	0
60	MG	AQ	3001	1/1	0.86	0.26	56,56,56,56	0
60	MG	DA	1662	1/1	0.86	0.10	51,51,51,51	0
60	MG	CA	3486	1/1	0.86	0.14	48,48,48,48	0
60	MG	AA	3250	1/1	0.86	0.45	46,46,46,46	1
60	MG	AA	3652	1/1	0.86	0.44	87,87,87,87	0
60	MG	DA	1722	1/1	0.86	0.19	69,69,69,69	0
60	MG	CA	3114	1/1	0.86	0.20	59,59,59,59	0
60	MG	CA	3191	1/1	0.86	0.28	61,61,61,61	0
60	MG	AA	3708	1/1	0.86	0.30	71,71,71,71	0
60	MG	AN	3001	1/1	0.86	0.47	64,64,64,64	0
60	MG	AA	3434	1/1	0.86	0.27	58,58,58,58	0
60	MG	CA	3021	1/1	0.86	0.33	91,91,91,91	0
60	MG	AA	3171	1/1	0.86	0.51	71,71,71,71	0
60	MG	CA	3540	1/1	0.86	0.24	71,71,71,71	0
60	MG	AA	3025	1/1	0.86	0.44	60,60,60,60	0
60	MG	BA	1669	1/1	0.86	0.17	70,70,70,70	0
60	MG	CA	3401	1/1	0.86	0.07	75,75,75,75	0
60	MG	A0	105	1/1	0.86	0.08	52,52,52,52	0
60	MG	BA	1642	1/1	0.86	0.18	59,59,59,59	0
60	MG	BX	111	1/1	0.86	0.14	67,67,67,67	0
60	MG	CA	3497	1/1	0.86	0.18	85,85,85,85	0
60	MG	CA	3394	1/1	0.86	0.26	54,54,54,54	0
60	MG	AA	3180	1/1	0.86	0.25	53,53,53,53	0
60	MG	AA	3195	1/1	0.86	0.20	55,55,55,55	0
60	MG	CA	3640	1/1	0.86	0.24	47,47,47,47	0
60	MG	CA	3005	1/1	0.86	0.18	69,69,69,69	0
60	MG	AA	3438	1/1	0.86	0.21	75,75,75,75	0
60	MG	AA	3140	1/1	0.86	0.90	66,66,66,66	0
60	MG	DA	1729	1/1	0.86	0.10	82,82,82,82	0
60	MG	CA	3617	1/1	0.86	0.38	41,41,41,41	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3429	1/1	0.86	0.22	58,58,58,58	0
60	MG	CA	3338	1/1	0.86	0.14	58,58,58,58	0
60	MG	AA	3238	1/1	0.86	0.13	68,68,68,68	0
60	MG	AA	3727	1/1	0.86	0.16	64,64,64,64	0
60	MG	CA	3386	1/1	0.86	0.14	79,79,79,79	0
60	MG	AA	3631	1/1	0.86	0.39	74,74,74,74	0
60	MG	AE	304	1/1	0.86	0.53	70,70,70,70	0
60	MG	AA	3378	1/1	0.86	0.21	24,24,24,24	0
60	MG	AA	3029	1/1	0.86	0.20	50,50,50,50	0
60	MG	AA	3621	1/1	0.86	0.12	34,34,34,34	0
60	MG	CE	304	1/1	0.86	0.74	74,74,74,74	0
60	MG	DA	1763	1/1	0.86	0.15	61,61,61,61	0
60	MG	CA	3001	1/1	0.86	0.17	81,81,81,81	0
60	MG	CA	3629	1/1	0.86	0.14	74,74,74,74	0
60	MG	AB	3018	1/1	0.86	0.13	76,76,76,76	0
60	MG	AA	3024	1/1	0.86	0.13	60,60,60,60	0
60	MG	A4	502	1/1	0.86	0.18	81,81,81,81	0
60	MG	CA	3517	1/1	0.86	0.21	75,75,75,75	0
60	MG	DA	1761	1/1	0.86	0.08	68,68,68,68	0
60	MG	CA	3265	1/1	0.86	0.19	66,66,66,66	0
60	MG	AA	3425	1/1	0.86	0.17	40,40,40,40	0
60	MG	BA	1617	1/1	0.86	0.16	64,64,64,64	0
60	MG	BA	1688	1/1	0.86	0.30	71,71,71,71	0
60	MG	AG	202	1/1	0.86	0.08	69,69,69,69	0
60	MG	DA	1658	1/1	0.86	0.13	89,89,89,89	0
60	MG	CA	3201	1/1	0.86	0.32	70,70,70,70	0
60	MG	AA	3132	1/1	0.86	0.45	43,43,43,43	0
60	MG	C0	102	1/1	0.86	0.08	56,56,56,56	0
60	MG	CE	301	1/1	0.86	0.61	54,54,54,54	0
60	MG	AA	3671	1/1	0.86	0.58	31,31,31,31	1
60	MG	DA	1609	1/1	0.86	0.18	49,49,49,49	0
60	MG	BA	1607	1/1	0.86	0.11	64,64,64,64	0
60	MG	CA	3663	1/1	0.87	0.26	74,74,74,74	0
60	MG	DA	1746	1/1	0.87	0.28	67,67,67,67	0
60	MG	DA	1628	1/1	0.87	0.20	69,69,69,69	0
60	MG	DA	1657	1/1	0.87	0.14	75,75,75,75	0
60	MG	BA	1694	1/1	0.87	0.23	78,78,78,78	0
60	MG	AA	3158	1/1	0.87	0.37	50,50,50,50	0
60	MG	CA	3361	1/1	0.87	0.14	70,70,70,70	0
60	MG	BA	1681	1/1	0.87	0.66	69,69,69,69	0
60	MG	AA	3542	1/1	0.87	0.10	47,47,47,47	0
60	MG	AB	3015	1/1	0.87	0.12	51,51,51,51	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AB	3016	1/1	0.87	0.14	47,47,47,47	0
60	MG	AA	3738	1/1	0.87	0.14	73,73,73,73	0
60	MG	AA	3130	1/1	0.87	0.33	59,59,59,59	0
60	MG	CA	3035	1/1	0.87	0.36	47,47,47,47	0
60	MG	AA	3678	1/1	0.87	0.13	62,62,62,62	0
60	MG	CA	3536	1/1	0.87	0.13	95,95,95,95	0
60	MG	AA	3575	1/1	0.87	0.16	63,63,63,63	0
60	MG	BD	502	1/1	0.87	0.42	56,56,56,56	0
60	MG	AA	3062	1/1	0.87	0.36	60,60,60,60	0
60	MG	BA	1774	1/1	0.87	0.09	79,79,79,79	0
60	MG	AA	3291	1/1	0.87	0.13	84,84,84,84	0
60	MG	AA	3270	1/1	0.87	0.20	92,92,92,92	0
60	MG	AA	3644	1/1	0.87	0.21	74,74,74,74	0
60	MG	AA	3258	1/1	0.87	0.26	32,32,32,32	0
60	MG	DA	1668	1/1	0.87	0.27	68,68,68,68	0
60	MG	AA	3017	1/1	0.87	0.11	71,71,71,71	0
60	MG	AA	3509	1/1	0.87	0.26	51,51,51,51	0
60	MG	DA	1664	1/1	0.87	0.24	49,49,49,49	0
60	MG	AA	3111	1/1	0.87	0.31	47,47,47,47	0
60	MG	AA	3268	1/1	0.87	0.23	80,80,80,80	0
60	MG	AA	3200	1/1	0.87	0.28	73,73,73,73	0
60	MG	CA	3528	1/1	0.87	0.07	51,51,51,51	1
60	MG	CO	201	1/1	0.87	0.16	72,72,72,72	0
60	MG	AA	3656	1/1	0.87	0.24	62,62,62,62	1
60	MG	DA	1630	1/1	0.87	0.27	51,51,51,51	0
60	MG	CA	3464	1/1	0.87	0.61	78,78,78,78	0
60	MG	CA	3485	1/1	0.87	0.24	76,76,76,76	0
60	MG	BA	1632	1/1	0.87	0.23	60,60,60,60	0
60	MG	DA	1670	1/1	0.87	0.25	74,74,74,74	0
60	MG	BX	107	1/1	0.87	0.11	69,69,69,69	0
60	MG	CA	3045	1/1	0.87	0.23	68,68,68,68	0
60	MG	CA	3384	1/1	0.87	0.20	52,52,52,52	0
60	MG	CA	3184	1/1	0.87	0.26	43,43,43,43	0
60	MG	CA	3390	1/1	0.87	0.21	42,42,42,42	0
60	MG	AA	3362	1/1	0.87	0.21	69,69,69,69	0
60	MG	AA	3780	1/1	0.87	0.35	51,51,51,51	1
60	MG	CA	3552	1/1	0.87	0.09	60,60,60,60	0
60	MG	DA	1695	1/1	0.87	0.18	79,79,79,79	0
60	MG	AA	3297	1/1	0.87	0.08	56,56,56,56	0
60	MG	AF	303	1/1	0.87	0.56	54,54,54,54	0
60	MG	AA	3447	1/1	0.87	0.19	44,44,44,44	0
60	MG	CA	3562	1/1	0.87	0.17	69,69,69,69	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3016	1/1	0.87	0.31	44,44,44,44	0
60	MG	DA	1720	1/1	0.87	0.12	61,61,61,61	0
60	MG	BA	1666	1/1	0.87	0.34	70,70,70,70	0
60	MG	CA	3276	1/1	0.87	0.17	32,32,32,32	0
60	MG	CA	3494	1/1	0.87	0.17	58,58,58,58	0
60	MG	CA	3013	1/1	0.87	0.32	52,52,52,52	0
60	MG	BA	1782	1/1	0.87	0.29	72,72,72,72	0
60	MG	BA	1661	1/1	0.87	0.45	59,59,59,59	0
60	MG	AA	3010	1/1	0.87	0.29	68,68,68,68	0
60	MG	AA	3247	1/1	0.87	0.43	75,75,75,75	0
60	MG	AA	3589	1/1	0.87	0.33	31,31,31,31	1
60	MG	CA	3305	1/1	0.88	0.31	64,64,64,64	0
60	MG	CA	3648	1/1	0.88	0.60	78,78,78,78	0
60	MG	CA	3442	1/1	0.88	0.13	70,70,70,70	0
60	MG	CA	3230	1/1	0.88	0.11	64,64,64,64	0
60	MG	AA	3388	1/1	0.88	0.16	55,55,55,55	0
60	MG	AA	3033	1/1	0.88	0.41	48,48,48,48	0
60	MG	DA	1618	1/1	0.88	0.09	51,51,51,51	0
60	MG	CA	3135	1/1	0.88	0.11	73,73,73,73	0
60	MG	BY	3001	1/1	0.88	0.07	78,78,78,78	0
60	MG	DA	1617	1/1	0.88	0.18	47,47,47,47	0
60	MG	AA	3248	1/1	0.88	0.49	79,79,79,79	0
60	MG	CA	3630	1/1	0.88	0.21	91,91,91,91	0
60	MG	AA	3156	1/1	0.88	0.23	46,46,46,46	0
60	MG	CA	3242	1/1	0.88	0.33	48,48,48,48	0
60	MG	CA	3138	1/1	0.88	0.28	67,67,67,67	0
60	MG	CB	3011	1/1	0.88	0.27	51,51,51,51	0
60	MG	CA	3643	1/1	0.88	0.33	83,83,83,83	0
60	MG	DA	1712	1/1	0.88	0.17	67,67,67,67	0
60	MG	CR	202	1/1	0.88	0.39	61,61,61,61	0
60	MG	CA	3039	1/1	0.88	0.39	76,76,76,76	0
60	MG	CA	3210	1/1	0.88	0.23	44,44,44,44	0
60	MG	BA	1645	1/1	0.88	0.77	58,58,58,58	0
60	MG	AA	3078	1/1	0.88	0.26	54,54,54,54	0
60	MG	AA	3637	1/1	0.88	0.19	54,54,54,54	0
60	MG	DA	1747	1/1	0.88	0.11	67,67,67,67	0
60	MG	AA	3329	1/1	0.88	0.23	82,82,82,82	0
60	MG	CA	3587	1/1	0.88	0.13	72,72,72,72	0
60	MG	CA	3510	1/1	0.88	0.17	71,71,71,71	0
60	MG	CA	3007	1/1	0.88	0.24	75,75,75,75	0
60	MG	DA	1742	1/1	0.88	0.25	52,52,52,52	0
60	MG	BA	1732	1/1	0.88	0.25	65,65,65,65	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	DA	1751	1/1	0.88	0.25	84,84,84,84	0
60	MG	BA	1633	1/1	0.88	0.36	65,65,65,65	0
60	MG	CA	3064	1/1	0.88	0.20	72,72,72,72	0
60	MG	AA	3107	1/1	0.88	0.17	51,51,51,51	0
60	MG	AA	3199	1/1	0.88	0.22	61,61,61,61	0
60	MG	AA	3598	1/1	0.88	0.20	57,57,57,57	0
60	MG	BA	1739	1/1	0.88	0.18	52,52,52,52	0
60	MG	AA	3087	1/1	0.88	0.32	62,62,62,62	0
60	MG	AE	305	1/1	0.88	0.43	44,44,44,44	0
60	MG	CA	3598	1/1	0.88	0.21	66,66,66,66	0
60	MG	AA	3364	1/1	0.88	0.24	57,57,57,57	0
60	MG	CA	3309	1/1	0.88	0.11	50,50,50,50	0
60	MG	AA	3285	1/1	0.88	0.22	72,72,72,72	0
60	MG	AA	3802	1/1	0.88	0.27	55,55,55,55	0
60	MG	AA	3769	1/1	0.88	0.46	48,48,48,48	1
60	MG	BA	1813	1/1	0.88	0.17	66,66,66,66	0
60	MG	BA	1649	1/1	0.88	0.34	56,56,56,56	0
60	MG	AA	3287	1/1	0.88	0.20	25,25,25,25	0
60	MG	CA	3409	1/1	0.88	0.32	63,63,63,63	0
60	MG	DJ	5001	1/1	0.88	0.17	94,94,94,94	0
60	MG	AA	3824	1/1	0.88	0.33	53,53,53,53	0
60	MG	BA	1793	1/1	0.88	0.10	68,68,68,68	0
60	MG	DA	1688	1/1	0.88	0.20	46,46,46,46	0
60	MG	AA	3228	1/1	0.88	0.32	63,63,63,63	0
60	MG	BA	1724	1/1	0.88	0.31	60,60,60,60	0
60	MG	AA	3236	1/1	0.88	0.10	61,61,61,61	0
60	MG	CA	3569	1/1	0.88	0.17	71,71,71,71	0
60	MG	AB	3001	1/1	0.88	0.18	80,80,80,80	0
60	MG	CA	3136	1/1	0.88	0.21	112,112,112,112	0
60	MG	CA	3658	1/1	0.88	0.19	62,62,62,62	0
60	MG	BX	113	1/1	0.88	0.21	78,78,78,78	0
60	MG	AA	3455	1/1	0.88	0.23	80,80,80,80	0
60	MG	CA	3457	1/1	0.88	0.22	60,60,60,60	0
60	MG	CA	3181	1/1	0.88	0.31	68,68,68,68	0
60	MG	A8	5001	1/1	0.88	0.31	66,66,66,66	0
60	MG	AA	3439	1/1	0.88	0.18	43,43,43,43	0
60	MG	BA	1613	1/1	0.88	0.07	92,92,92,92	0
60	MG	CA	3500	1/1	0.88	0.47	56,56,56,56	0
60	MG	CA	3041	1/1	0.88	0.47	67,67,67,67	0
60	MG	BA	1789	1/1	0.88	0.11	68,68,68,68	0
60	MG	BA	1799	1/1	0.88	0.07	69,69,69,69	0
60	MG	CA	3097	1/1	0.88	0.17	79,79,79,79	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AB	3011	1/1	0.88	0.18	47,47,47,47	0
60	MG	AA	3353	1/1	0.88	0.11	68,68,68,68	0
60	MG	DA	1667	1/1	0.89	0.43	70,70,70,70	0
60	MG	AA	3303	1/1	0.89	0.21	30,30,30,30	0
60	MG	CD	302	1/1	0.89	0.43	51,51,51,51	0
60	MG	AA	3604	1/1	0.89	0.23	44,44,44,44	1
60	MG	CA	3170	1/1	0.89	0.36	68,68,68,68	0
60	MG	AA	3119	1/1	0.89	0.23	41,41,41,41	0
60	MG	AA	3491	1/1	0.89	0.30	40,40,40,40	0
60	MG	CA	3287	1/1	0.89	0.35	43,43,43,43	0
60	MG	AA	3800	1/1	0.89	0.28	59,59,59,59	0
60	MG	AW	3002	1/1	0.89	0.18	59,59,59,59	0
60	MG	CA	3123	1/1	0.89	0.27	63,63,63,63	0
60	MG	AA	3563	1/1	0.89	0.07	37,37,37,37	1
60	MG	CA	3200	1/1	0.89	0.15	65,65,65,65	0
60	MG	AN	3003	1/1	0.89	0.07	52,52,52,52	0
60	MG	CA	3054	1/1	0.89	0.13	50,50,50,50	0
60	MG	AA	3608	1/1	0.89	0.15	66,66,66,66	0
60	MG	CA	3608	1/1	0.89	0.11	69,69,69,69	0
60	MG	AA	3419	1/1	0.89	0.05	88,88,88,88	0
60	MG	CA	3379	1/1	0.89	0.22	62,62,62,62	0
60	MG	AB	3004	1/1	0.89	0.29	69,69,69,69	0
60	MG	AA	3559	1/1	0.89	0.21	37,37,37,37	0
60	MG	AA	3360	1/1	0.89	0.45	72,72,72,72	0
60	MG	AA	3482	1/1	0.89	0.26	46,46,46,46	0
60	MG	AA	3822	1/1	0.89	0.60	67,67,67,67	0
60	MG	CA	3557	1/1	0.89	0.26	76,76,76,76	0
60	MG	AA	3342	1/1	0.89	0.11	77,77,77,77	0
60	MG	CA	3133	1/1	0.89	0.20	72,72,72,72	0
60	MG	CA	3523	1/1	0.89	0.09	77,77,77,77	0
60	MG	CA	3317	1/1	0.89	0.16	61,61,61,61	0
60	MG	CR	201	1/1	0.89	0.36	63,63,63,63	0
60	MG	BX	110	1/1	0.89	0.14	67,67,67,67	0
60	MG	CA	3611	1/1	0.89	0.29	64,64,64,64	0
60	MG	BA	1612	1/1	0.89	0.14	79,79,79,79	0
60	MG	BL	201	1/1	0.89	0.19	104,104,104,104	0
60	MG	AA	3476	1/1	0.89	0.10	50,50,50,50	0
60	MG	BA	1785	1/1	0.89	0.19	69,69,69,69	0
60	MG	CA	3033	1/1	0.89	0.13	47,47,47,47	0
60	MG	AA	3592	1/1	0.89	0.27	67,67,67,67	0
60	MG	CA	3144	1/1	0.89	0.29	84,84,84,84	0
60	MG	CE	306	1/1	0.89	0.09	69,69,69,69	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3477	1/1	0.89	0.15	47,47,47,47	0
60	MG	AA	3473	1/1	0.89	0.15	57,57,57,57	0
60	MG	AA	3743	1/1	0.89	0.20	66,66,66,66	0
60	MG	CA	3418	1/1	0.89	0.31	53,53,53,53	0
60	MG	CA	3480	1/1	0.89	0.14	61,61,61,61	0
60	MG	CA	3204	1/1	0.89	0.25	88,88,88,88	0
60	MG	CA	3539	1/1	0.89	0.31	72,72,72,72	0
60	MG	BA	1807	1/1	0.89	0.20	72,72,72,72	0
60	MG	AA	3191	1/1	0.89	0.29	57,57,57,57	0
60	MG	CA	3036	1/1	0.89	0.26	65,65,65,65	0
60	MG	AA	3187	1/1	0.89	0.17	29,29,29,29	0
60	MG	AA	3500	1/1	0.89	0.14	27,27,27,27	0
60	MG	CA	3175	1/1	0.89	0.14	59,59,59,59	0
60	MG	CA	3312	1/1	0.89	0.38	52,52,52,52	0
60	MG	AY	502	1/1	0.89	0.24	54,54,54,54	0
60	MG	DA	1721	1/1	0.89	0.32	60,60,60,60	0
60	MG	CA	3596	1/1	0.89	0.10	75,75,75,75	0
60	MG	CA	3302	1/1	0.89	0.11	67,67,67,67	0
60	MG	CA	3254	1/1	0.89	0.15	35,35,35,35	0
60	MG	AA	3381	1/1	0.89	0.12	34,34,34,34	0
60	MG	AA	3194	1/1	0.89	0.35	58,58,58,58	0
60	MG	DK	202	1/1	0.89	0.23	80,80,80,80	0
60	MG	CA	3153	1/1	0.89	0.31	54,54,54,54	0
60	MG	CA	3477	1/1	0.89	0.24	65,65,65,65	0
60	MG	DA	1750	1/1	0.89	0.18	86,86,86,86	0
60	MG	AA	3198	1/1	0.89	0.09	47,47,47,47	0
60	MG	CA	3606	1/1	0.89	0.27	58,58,58,58	0
60	MG	AA	3154	1/1	0.89	0.16	64,64,64,64	0
60	MG	AA	3120	1/1	0.89	0.26	54,54,54,54	0
60	MG	CA	3614	1/1	0.89	0.28	79,79,79,79	0
60	MG	AU	201	1/1	0.89	0.53	72,72,72,72	0
60	MG	AA	3101	1/1	0.89	0.48	68,68,68,68	0
60	MG	BA	1702	1/1	0.89	0.46	56,56,56,56	0
60	MG	AA	3080	1/1	0.89	0.36	54,54,54,54	0
60	MG	CA	3549	1/1	0.89	0.18	29,29,29,29	0
60	MG	AA	3095	1/1	0.89	0.16	58,58,58,58	0
60	MG	AA	3063	1/1	0.89	0.17	46,46,46,46	0
60	MG	AA	3778	1/1	0.89	0.10	68,68,68,68	0
60	MG	AU	203	1/1	0.89	0.24	55,55,55,55	0
60	MG	AA	3379	1/1	0.89	0.14	40,40,40,40	1
60	MG	AA	3568	1/1	0.89	0.22	23,23,23,23	0
60	MG	DA	1666	1/1	0.89	0.19	45,45,45,45	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3093	1/1	0.89	0.34	77,77,77,77	0
60	MG	AA	3157	1/1	0.89	0.33	93,93,93,93	0
60	MG	CA	3530	1/1	0.89	0.15	68,68,68,68	0
60	MG	AA	3740	1/1	0.89	0.25	54,54,54,54	0
60	MG	CA	3323	1/1	0.90	0.16	32,32,32,32	0
60	MG	AA	3460	1/1	0.90	0.30	81,81,81,81	0
60	MG	BA	1619	1/1	0.90	0.13	54,54,54,54	0
60	MG	CA	3437	1/1	0.90	0.25	41,41,41,41	0
60	MG	CA	3108	1/1	0.90	0.18	84,84,84,84	0
60	MG	AA	3307	1/1	0.90	0.12	35,35,35,35	0
60	MG	BA	1623	1/1	0.90	0.25	67,67,67,67	0
60	MG	BA	1625	1/1	0.90	0.24	53,53,53,53	0
60	MG	DA	1672	1/1	0.90	0.16	61,61,61,61	0
60	MG	AA	3079	1/1	0.90	0.10	27,27,27,27	0
60	MG	AA	3622	1/1	0.90	0.13	52,52,52,52	0
60	MG	DA	1636	1/1	0.90	0.32	77,77,77,77	0
60	MG	DA	1714	1/1	0.90	0.39	82,82,82,82	0
60	MG	BM	201	1/1	0.90	0.06	60,60,60,60	0
60	MG	CA	3295	1/1	0.90	0.30	55,55,55,55	0
60	MG	AA	3784	1/1	0.90	0.15	69,69,69,69	0
60	MG	CA	3458	1/1	0.90	0.14	28,28,28,28	0
60	MG	BA	1698	1/1	0.90	0.31	57,57,57,57	0
60	MG	CA	3333	1/1	0.90	0.20	64,64,64,64	0
60	MG	CA	3065	1/1	0.90	0.15	56,56,56,56	0
60	MG	AA	3698	1/1	0.90	0.31	51,51,51,51	1
60	MG	CA	3544	1/1	0.90	0.18	74,74,74,74	0
60	MG	AA	3516	1/1	0.90	0.27	38,38,38,38	0
60	MG	DA	1613	1/1	0.90	0.25	50,50,50,50	0
60	MG	CA	3220	1/1	0.90	0.50	89,89,89,89	0
60	MG	BA	1604	1/1	0.90	0.16	85,85,85,85	0
60	MG	CA	3662	1/1	0.90	0.37	60,60,60,60	0
60	MG	AA	3445	1/1	0.90	0.06	59,59,59,59	0
60	MG	CF	303	1/1	0.90	0.28	63,63,63,63	0
60	MG	AA	3724	1/1	0.90	0.31	37,37,37,37	0
60	MG	AA	3081	1/1	0.90	0.20	38,38,38,38	0
60	MG	AA	3494	1/1	0.90	0.14	66,66,66,66	0
60	MG	AA	3055	1/1	0.90	0.17	61,61,61,61	0
60	MG	BA	1662	1/1	0.90	0.17	45,45,45,45	0
60	MG	AA	3483	1/1	0.90	0.18	21,21,21,21	0
60	MG	AA	3572	1/1	0.90	0.16	51,51,51,51	0
60	MG	BA	1762	1/1	0.90	0.07	57,57,57,57	0
60	MG	CA	3603	1/1	0.90	0.28	93,93,93,93	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3226	1/1	0.90	0.27	51,51,51,51	0
60	MG	BA	1708	1/1	0.90	0.27	55,55,55,55	0
60	MG	CA	3534	1/1	0.90	0.12	58,58,58,58	0
60	MG	DA	1768	1/1	0.90	0.10	57,57,57,57	0
60	MG	AA	3142	1/1	0.90	0.27	50,50,50,50	0
60	MG	AA	3377	1/1	0.90	0.15	19,19,19,19	0
60	MG	C5	101	1/1	0.90	0.43	64,64,64,64	0
60	MG	DA	1626	1/1	0.90	0.41	63,63,63,63	0
60	MG	BA	1673	1/1	0.90	0.72	63,63,63,63	0
60	MG	CA	3127	1/1	0.90	0.15	68,68,68,68	0
60	MG	AA	3096	1/1	0.90	0.22	54,54,54,54	0
60	MG	CA	3519	1/1	0.90	0.20	68,68,68,68	0
60	MG	AA	3530	1/1	0.90	0.10	60,60,60,60	0
60	MG	CB	3013	1/1	0.90	0.12	90,90,90,90	0
60	MG	CA	3314	1/1	0.90	0.15	41,41,41,41	0
60	MG	CA	3271	1/1	0.90	0.11	59,59,59,59	0
60	MG	CA	3460	1/1	0.90	0.28	57,57,57,57	0
60	MG	CA	3267	1/1	0.90	0.24	110,110,110,110	0
60	MG	CA	3228	1/1	0.90	0.71	68,68,68,68	0
60	MG	AA	3019	1/1	0.90	0.26	53,53,53,53	0
60	MG	AD	303	1/1	0.90	0.13	46,46,46,46	0
60	MG	CA	3257	1/1	0.90	0.14	45,45,45,45	0
60	MG	AA	3721	1/1	0.90	0.20	21,21,21,21	0
60	MG	AA	3235	1/1	0.90	0.28	42,42,42,42	0
60	MG	CA	3074	1/1	0.90	0.31	64,64,64,64	0
60	MG	BA	1640	1/1	0.90	0.19	56,56,56,56	0
60	MG	AA	3498	1/1	0.90	0.17	56,56,56,56	0
60	MG	AA	3092	1/1	0.90	0.23	41,41,41,41	0
60	MG	DA	1724	1/1	0.90	0.19	74,74,74,74	0
60	MG	CA	3088	1/1	0.90	0.43	85,85,85,85	0
60	MG	AA	3728	1/1	0.90	0.27	75,75,75,75	0
60	MG	CA	3655	1/1	0.90	0.47	69,69,69,69	0
60	MG	AA	3504	1/1	0.90	0.14	44,44,44,44	0
60	MG	CB	3007	1/1	0.90	0.14	57,57,57,57	0
60	MG	CA	3288	1/1	0.90	0.34	39,39,39,39	0
60	MG	AA	3046	1/1	0.90	0.36	47,47,47,47	0
60	MG	AA	3402	1/1	0.90	0.33	53,53,53,53	0
60	MG	CA	3286	1/1	0.90	0.21	62,62,62,62	0
60	MG	AA	3288	1/1	0.90	0.13	39,39,39,39	0
60	MG	AA	3812	1/1	0.90	0.20	78,78,78,78	0
60	MG	CA	3283	1/1	0.90	0.23	57,57,57,57	0
60	MG	CA	3404	1/1	0.90	0.11	46,46,46,46	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	DA	1725	1/1	0.90	0.13	78,78,78,78	0
60	MG	CA	3215	1/1	0.90	0.43	50,50,50,50	0
60	MG	AA	3630	1/1	0.90	0.15	66,66,66,66	0
60	MG	BA	1719	1/1	0.90	0.27	75,75,75,75	0
60	MG	AA	3752	1/1	0.90	0.63	75,75,75,75	0
60	MG	AA	3550	1/1	0.90	0.21	47,47,47,47	0
60	MG	AA	3021	1/1	0.90	0.20	49,49,49,49	0
60	MG	DA	1707	1/1	0.90	0.09	79,79,79,79	0
60	MG	AN	3002	1/1	0.90	0.20	76,76,76,76	0
60	MG	DA	1629	1/1	0.90	0.80	79,79,79,79	0
60	MG	CA	3322	1/1	0.90	0.28	41,41,41,41	0
60	MG	CA	3626	1/1	0.90	0.09	52,52,52,52	0
60	MG	AA	3273	1/1	0.90	0.27	57,57,57,57	0
60	MG	CA	3062	1/1	0.90	0.09	41,41,41,41	0
60	MG	CD	303	1/1	0.90	0.14	70,70,70,70	0
60	MG	CA	3143	1/1	0.90	0.23	62,62,62,62	0
60	MG	AA	3488	1/1	0.90	0.09	56,56,56,56	0
60	MG	A6	101	1/1	0.90	0.21	69,69,69,69	0
60	MG	AA	3294	1/1	0.90	0.19	56,56,56,56	0
60	MG	DA	1640	1/1	0.91	0.35	73,73,73,73	0
60	MG	AA	3167	1/1	0.91	0.29	69,69,69,69	0
60	MG	CF	302	1/1	0.91	0.32	64,64,64,64	0
60	MG	AA	3269	1/1	0.91	0.54	78,78,78,78	0
60	MG	CA	3076	1/1	0.91	0.32	48,48,48,48	0
60	MG	BF	3001	1/1	0.91	0.15	49,49,49,49	0
60	MG	CA	3238	1/1	0.91	0.34	73,73,73,73	0
60	MG	BA	1801	1/1	0.91	0.12	55,55,55,55	0
60	MG	AA	3618	1/1	0.91	0.13	39,39,39,39	0
60	MG	BA	1628	1/1	0.91	0.30	59,59,59,59	0
60	MG	AA	3811	1/1	0.91	0.59	65,65,65,65	0
60	MG	BA	1667	1/1	0.91	0.15	69,69,69,69	0
60	MG	BA	1684	1/1	0.91	0.21	64,64,64,64	0
60	MG	AA	3614	1/1	0.91	0.13	66,66,66,66	0
60	MG	AA	3788	1/1	0.91	0.17	64,64,64,64	0
60	MG	AA	3289	1/1	0.91	0.19	47,47,47,47	0
60	MG	BA	1605	1/1	0.91	0.11	76,76,76,76	0
60	MG	AA	3679	1/1	0.91	0.18	64,64,64,64	0
60	MG	AA	3690	1/1	0.91	0.11	58,58,58,58	0
60	MG	CA	3315	1/1	0.91	0.21	44,44,44,44	0
60	MG	AA	3797	1/1	0.91	0.30	60,60,60,60	0
60	MG	DA	1635	1/1	0.91	0.44	61,61,61,61	0
60	MG	BA	1643	1/1	0.91	0.09	56,56,56,56	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3715	1/1	0.91	0.09	62,62,62,62	0
60	MG	CA	3495	1/1	0.91	0.18	64,64,64,64	0
60	MG	AA	3170	1/1	0.91	0.57	44,44,44,44	1
60	MG	AD	305	1/1	0.91	0.55	75,75,75,75	0
60	MG	CA	3268	1/1	0.91	0.21	46,46,46,46	0
60	MG	AA	3499	1/1	0.91	0.11	46,46,46,46	0
60	MG	AA	3827	1/1	0.91	0.29	39,39,39,39	0
60	MG	AA	3014	1/1	0.91	0.17	45,45,45,45	0
60	MG	CA	3363	1/1	0.91	0.18	55,55,55,55	0
60	MG	DA	1689	1/1	0.91	0.24	68,68,68,68	0
60	MG	DA	1639	1/1	0.91	0.10	59,59,59,59	0
60	MG	AA	3785	1/1	0.91	0.21	54,54,54,54	0
60	MG	BX	104	1/1	0.91	0.20	67,67,67,67	0
60	MG	DA	1675	1/1	0.91	0.13	61,61,61,61	0
60	MG	CA	3349	1/1	0.91	0.15	36,36,36,36	0
60	MG	DA	1691	1/1	0.91	0.18	66,66,66,66	0
60	MG	AU	202	1/1	0.91	0.28	65,65,65,65	0
60	MG	AA	3004	1/1	0.91	0.14	30,30,30,30	0
60	MG	AA	3058	1/1	0.91	0.12	38,38,38,38	0
60	MG	CA	3335	1/1	0.91	0.16	38,38,38,38	0
60	MG	CA	3551	1/1	0.91	0.15	76,76,76,76	0
60	MG	AA	3257	1/1	0.91	0.22	18,18,18,18	0
60	MG	BA	1809	1/1	0.91	0.18	74,74,74,74	0
60	MG	CB	3001	1/1	0.91	0.21	68,68,68,68	0
60	MG	C7	101	1/1	0.91	0.43	47,47,47,47	0
60	MG	AA	3466	1/1	0.91	0.17	48,48,48,48	0
60	MG	AA	3765	1/1	0.91	0.20	62,62,62,62	0
60	MG	AA	3794	1/1	0.91	0.20	47,47,47,47	0
60	MG	BA	1683	1/1	0.91	0.24	50,50,50,50	0
60	MG	AA	3179	1/1	0.91	0.23	62,62,62,62	0
60	MG	CA	3372	1/1	0.91	0.29	63,63,63,63	0
60	MG	BA	1668	1/1	0.91	0.18	72,72,72,72	0
60	MG	AA	3420	1/1	0.91	0.13	26,26,26,26	0
60	MG	AA	3209	1/1	0.91	0.26	64,64,64,64	0
60	MG	AA	3394	1/1	0.91	0.13	22,22,22,22	0
60	MG	AA	3481	1/1	0.91	0.06	53,53,53,53	0
60	MG	AA	3683	1/1	0.91	0.10	40,40,40,40	0
60	MG	AA	3380	1/1	0.91	0.18	75,75,75,75	0
60	MG	BA	1720	1/1	0.91	0.14	51,51,51,51	0
60	MG	AA	3495	1/1	0.91	0.20	58,58,58,58	0
60	MG	CA	3402	1/1	0.91	0.16	46,46,46,46	0
60	MG	DA	1716	1/1	0.91	0.27	56,56,56,56	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	1738	1/1	0.91	0.23	55,55,55,55	0
60	MG	AA	3437	1/1	0.91	0.20	25,25,25,25	0
60	MG	AA	3587	1/1	0.91	0.17	44,44,44,44	0
60	MG	BA	1644	1/1	0.91	0.27	72,72,72,72	0
60	MG	DA	1605	1/1	0.91	0.29	59,59,59,59	0
60	MG	CA	3095	1/1	0.91	0.09	92,92,92,92	0
60	MG	BA	1723	1/1	0.91	0.27	61,61,61,61	0
60	MG	AA	3507	1/1	0.91	0.25	53,53,53,53	0
60	MG	CA	3484	1/1	0.91	0.26	56,56,56,56	0
60	MG	BA	1658	1/1	0.91	0.55	68,68,68,68	0
60	MG	AA	3435	1/1	0.91	0.27	54,54,54,54	0
60	MG	AA	3667	1/1	0.91	0.14	45,45,45,45	0
60	MG	AA	3240	1/1	0.91	0.51	39,39,39,39	0
60	MG	AA	3254	1/1	0.91	0.29	47,47,47,47	0
60	MG	CA	3037	1/1	0.91	0.19	65,65,65,65	0
60	MG	AA	3277	1/1	0.91	0.19	48,48,48,48	0
60	MG	CA	3050	1/1	0.91	0.65	55,55,55,55	0
60	MG	AA	3613	1/1	0.91	0.12	96,96,96,96	0
60	MG	AA	3813	1/1	0.91	0.21	68,68,68,68	0
60	MG	CA	3214	1/1	0.91	0.28	50,50,50,50	0
60	MG	DA	1705	1/1	0.91	0.17	61,61,61,61	0
60	MG	AA	3804	1/1	0.91	0.38	70,70,70,70	0
60	MG	AA	3562	1/1	0.91	0.06	45,45,45,45	0
60	MG	DA	1694	1/1	0.91	0.27	60,60,60,60	0
60	MG	CA	3650	1/1	0.91	0.17	42,42,42,42	0
60	MG	AA	3777	1/1	0.91	0.32	58,58,58,58	0
60	MG	AA	3561	1/1	0.91	0.17	64,64,64,64	0
60	MG	AA	3687	1/1	0.91	0.11	48,48,48,48	0
60	MG	DA	1622	1/1	0.91	0.15	43,43,43,43	0
60	MG	CA	3515	1/1	0.91	0.11	72,72,72,72	0
60	MG	CA	3168	1/1	0.91	0.23	65,65,65,65	0
60	MG	CA	3470	1/1	0.91	0.10	55,55,55,55	0
60	MG	AA	3782	1/1	0.91	0.17	70,70,70,70	0
60	MG	CA	3396	1/1	0.91	0.14	59,59,59,59	0
60	MG	BA	1634	1/1	0.91	0.21	71,71,71,71	0
60	MG	AA	3201	1/1	0.91	0.32	71,71,71,71	0
60	MG	CA	3263	1/1	0.91	0.12	50,50,50,50	0
60	MG	CA	3260	1/1	0.91	0.14	59,59,59,59	0
60	MG	AA	3069	1/1	0.91	0.08	32,32,32,32	0
60	MG	CA	3162	1/1	0.91	0.27	57,57,57,57	0
60	MG	AA	3421	1/1	0.91	0.12	73,73,73,73	0
60	MG	AA	3104	1/1	0.91	0.25	55,55,55,55	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3246	1/1	0.91	0.28	79,79,79,79	0
60	MG	AA	3309	1/1	0.91	0.18	72,72,72,72	0
60	MG	AA	3512	1/1	0.91	0.13	32,32,32,32	0
60	MG	AA	3280	1/1	0.91	0.20	63,63,63,63	0
61	K	AA	3814	1/1	0.91	0.27	87,87,87,87	0
60	MG	AA	3705	1/1	0.91	0.44	29,29,29,29	1
60	MG	AA	3125	1/1	0.91	0.35	74,74,74,74	0
60	MG	CA	3389	1/1	0.91	0.09	55,55,55,55	0
60	MG	AA	3141	1/1	0.91	0.20	46,46,46,46	0
60	MG	BA	1647	1/1	0.91	0.09	57,57,57,57	0
60	MG	AA	3066	1/1	0.91	0.20	63,63,63,63	0
60	MG	AA	3525	1/1	0.92	0.21	45,45,45,45	0
60	MG	CA	3126	1/1	0.92	0.54	71,71,71,71	0
60	MG	DA	1752	1/1	0.92	0.32	73,73,73,73	0
60	MG	BA	1717	1/1	0.92	0.15	77,77,77,77	0
60	MG	CA	3620	1/1	0.92	0.22	41,41,41,41	0
60	MG	AA	3137	1/1	0.92	0.36	55,55,55,55	0
60	MG	AA	3674	1/1	0.92	0.09	56,56,56,56	0
60	MG	AA	3552	1/1	0.92	0.14	73,73,73,73	0
60	MG	AA	3609	1/1	0.92	0.21	57,57,57,57	0
60	MG	AA	3452	1/1	0.92	0.07	53,53,53,53	0
60	MG	CA	3188	1/1	0.92	0.27	55,55,55,55	0
60	MG	AA	3810	1/1	0.92	0.34	49,49,49,49	0
60	MG	AA	3072	1/1	0.92	0.08	20,20,20,20	0
60	MG	CA	3330	1/1	0.92	0.27	37,37,37,37	0
60	MG	AA	3139	1/1	0.92	0.25	64,64,64,64	0
60	MG	CA	3205	1/1	0.92	0.31	66,66,66,66	0
60	MG	BA	1679	1/1	0.92	0.20	51,51,51,51	0
60	MG	DA	1710	1/1	0.92	0.23	56,56,56,56	0
60	MG	AA	3693	1/1	0.92	0.19	47,47,47,47	0
60	MG	AA	3735	1/1	0.92	0.27	30,30,30,30	0
60	MG	AA	3729	1/1	0.92	0.07	40,40,40,40	0
60	MG	AA	3619	1/1	0.92	0.12	39,39,39,39	0
60	MG	AA	3261	1/1	0.92	0.27	53,53,53,53	0
60	MG	CA	3499	1/1	0.92	0.21	68,68,68,68	0
60	MG	AA	3370	1/1	0.92	0.16	43,43,43,43	0
60	MG	C0	101	1/1	0.92	0.07	50,50,50,50	0
60	MG	A5	102	1/1	0.92	0.25	46,46,46,46	0
60	MG	DA	1607	1/1	0.92	0.83	63,63,63,63	0
60	MG	BA	1620	1/1	0.92	0.09	60,60,60,60	0
60	MG	CA	3102	1/1	0.92	0.34	50,50,50,50	0
60	MG	CA	3351	1/1	0.92	0.13	50,50,50,50	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3295	1/1	0.92	0.16	24,24,24,24	0
60	MG	CA	3334	1/1	0.92	0.09	56,56,56,56	0
60	MG	AA	3215	1/1	0.92	0.18	48,48,48,48	0
60	MG	CA	3656	1/1	0.92	0.55	75,75,75,75	0
60	MG	BA	1626	1/1	0.92	0.25	72,72,72,72	0
60	MG	CB	3009	1/1	0.92	0.16	66,66,66,66	0
60	MG	BA	1731	1/1	0.92	0.06	65,65,65,65	0
60	MG	BA	1636	1/1	0.92	0.27	66,66,66,66	0
60	MG	AA	3712	1/1	0.92	0.20	50,50,50,50	0
60	MG	CA	3595	1/1	0.92	0.26	67,67,67,67	0
60	MG	AA	3043	1/1	0.92	0.29	39,39,39,39	0
60	MG	BA	1773	1/1	0.92	0.24	69,69,69,69	0
60	MG	DA	1654	1/1	0.92	0.40	48,48,48,48	0
60	MG	AB	3023	1/1	0.92	0.26	63,63,63,63	0
60	MG	AA	3217	1/1	0.92	0.16	50,50,50,50	0
60	MG	CA	3221	1/1	0.92	0.56	60,60,60,60	0
60	MG	BA	1608	1/1	0.92	0.35	52,52,52,52	0
60	MG	CA	3154	1/1	0.92	0.22	68,68,68,68	0
60	MG	AA	3581	1/1	0.92	0.26	48,48,48,48	0
60	MG	DA	1733	1/1	0.92	0.09	73,73,73,73	0
60	MG	CA	3601	1/1	0.92	0.36	61,61,61,61	0
60	MG	AA	3450	1/1	0.92	0.27	71,71,71,71	0
60	MG	AA	3659	1/1	0.92	0.10	56,56,56,56	0
60	MG	AA	3099	1/1	0.92	0.08	48,48,48,48	0
60	MG	CA	3105	1/1	0.92	0.12	47,47,47,47	0
60	MG	CA	3350	1/1	0.92	0.07	74,74,74,74	0
60	MG	AA	3401	1/1	0.92	0.22	26,26,26,26	0
60	MG	DA	1698	1/1	0.92	0.15	75,75,75,75	0
60	MG	CA	3566	1/1	0.92	0.24	47,47,47,47	0
60	MG	CA	3346	1/1	0.92	0.30	48,48,48,48	0
60	MG	CA	3022	1/1	0.92	0.62	76,76,76,76	0
60	MG	CA	3572	1/1	0.92	0.22	82,82,82,82	0
60	MG	CD	301	1/1	0.92	0.35	61,61,61,61	0
60	MG	AA	3746	1/1	0.92	0.43	62,62,62,62	0
60	MG	CA	3342	1/1	0.92	0.17	84,84,84,84	0
60	MG	AA	3798	1/1	0.92	0.10	34,34,34,34	0
60	MG	AA	3222	1/1	0.92	0.26	58,58,58,58	0
60	MG	CA	3150	1/1	0.92	0.12	52,52,52,52	0
60	MG	CA	3023	1/1	0.92	0.19	56,56,56,56	0
60	MG	BA	1631	1/1	0.92	0.09	44,44,44,44	0
60	MG	AA	3147	1/1	0.92	0.51	52,52,52,52	0
60	MG	AA	3352	1/1	0.92	0.18	64,64,64,64	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3190	1/1	0.92	0.30	77,77,77,77	0
60	MG	CA	3644	1/1	0.92	0.17	60,60,60,60	0
60	MG	AA	3313	1/1	0.92	0.17	31,31,31,31	0
60	MG	BA	1650	1/1	0.92	0.22	49,49,49,49	0
60	MG	AA	3458	1/1	0.92	0.20	79,79,79,79	0
60	MG	AA	3567	1/1	0.92	0.14	69,69,69,69	0
60	MG	CA	3525	1/1	0.92	0.07	30,30,30,30	0
60	MG	CA	3610	1/1	0.92	0.45	94,94,94,94	0
60	MG	BA	1798	1/1	0.92	0.38	62,62,62,62	0
60	MG	CA	3393	1/1	0.92	0.35	47,47,47,47	0
60	MG	DA	1754	1/1	0.92	0.23	77,77,77,77	0
60	MG	CQ	202	1/1	0.92	0.25	56,56,56,56	0
60	MG	BT	3001	1/1	0.92	0.27	47,47,47,47	0
60	MG	CA	3209	1/1	0.92	0.27	101,101,101,101	0
60	MG	AA	3274	1/1	0.92	0.49	48,48,48,48	1
60	MG	BA	1652	1/1	0.92	0.10	65,65,65,65	0
60	MG	DA	1741	1/1	0.92	0.32	81,81,81,81	0
60	MG	CA	3278	1/1	0.92	0.24	38,38,38,38	0
60	MG	BA	1659	1/1	0.92	0.33	68,68,68,68	0
60	MG	BA	1660	1/1	0.92	0.32	55,55,55,55	0
60	MG	AA	3310	1/1	0.92	0.17	37,37,37,37	0
60	MG	CA	3165	1/1	0.92	0.52	58,58,58,58	0
60	MG	BA	1791	1/1	0.92	0.18	58,58,58,58	0
60	MG	AA	3492	1/1	0.92	0.12	41,41,41,41	0
60	MG	AD	310	1/1	0.92	0.49	63,63,63,63	0
60	MG	AA	3332	1/1	0.92	0.18	55,55,55,55	0
60	MG	AA	3145	1/1	0.92	0.32	41,41,41,41	1
60	MG	CA	3048	1/1	0.92	0.30	48,48,48,48	0
60	MG	AA	3540	1/1	0.92	0.20	28,28,28,28	0
60	MG	BA	1710	1/1	0.92	0.10	83,83,83,83	0
60	MG	AA	3231	1/1	0.92	0.49	87,87,87,87	0
60	MG	BA	1761	1/1	0.92	0.18	74,74,74,74	0
60	MG	AA	3262	1/1	0.92	0.59	70,70,70,70	0
60	MG	CA	3125	1/1	0.92	0.48	58,58,58,58	0
60	MG	CA	3243	1/1	0.92	0.35	55,55,55,55	0
60	MG	CA	3507	1/1	0.92	0.14	99,99,99,99	0
60	MG	DA	1650	1/1	0.92	0.31	48,48,48,48	0
60	MG	CA	3419	1/1	0.92	0.18	55,55,55,55	0
60	MG	BA	1792	1/1	0.92	0.07	61,61,61,61	0
60	MG	AA	3497	1/1	0.92	0.10	36,36,36,36	0
60	MG	AA	3305	1/1	0.92	0.16	38,38,38,38	0
60	MG	AA	3501	1/1	0.92	0.16	45,45,45,45	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3278	1/1	0.92	0.35	58,58,58,58	0
60	MG	CA	3636	1/1	0.92	0.32	60,60,60,60	0
60	MG	AA	3113	1/1	0.92	0.23	41,41,41,41	0
60	MG	AA	3260	1/1	0.92	0.43	67,67,67,67	0
60	MG	AA	3484	1/1	0.92	0.23	48,48,48,48	0
60	MG	BA	1806	1/1	0.92	0.17	63,63,63,63	0
60	MG	BA	1687	1/1	0.92	0.59	73,73,73,73	0
60	MG	CA	3119	1/1	0.92	0.69	63,63,63,63	0
60	MG	CA	3066	1/1	0.92	0.42	69,69,69,69	0
60	MG	CA	3149	1/1	0.92	0.22	58,58,58,58	0
60	MG	AA	3233	1/1	0.92	0.28	85,85,85,85	0
60	MG	CB	3002	1/1	0.92	0.13	78,78,78,78	0
60	MG	BX	101	1/1	0.92	0.30	63,63,63,63	0
60	MG	BA	1614	1/1	0.92	0.18	70,70,70,70	0
60	MG	CA	3072	1/1	0.92	0.43	54,54,54,54	0
60	MG	DA	1678	1/1	0.92	0.40	66,66,66,66	0
60	MG	AA	3049	1/1	0.92	0.14	35,35,35,35	0
60	MG	AA	3325	1/1	0.92	0.11	78,78,78,78	0
60	MG	CA	3232	1/1	0.92	0.24	69,69,69,69	0
60	MG	BA	1736	1/1	0.92	0.09	66,66,66,66	0
60	MG	CA	3425	1/1	0.93	0.15	45,45,45,45	0
60	MG	CG	3001	1/1	0.93	0.19	66,66,66,66	0
60	MG	CA	3571	1/1	0.93	0.14	52,52,52,52	0
60	MG	DF	3001	1/1	0.93	0.12	53,53,53,53	0
60	MG	CA	3604	1/1	0.93	0.20	54,54,54,54	0
60	MG	BA	1676	1/1	0.93	0.24	39,39,39,39	0
60	MG	CA	3489	1/1	0.93	0.18	64,64,64,64	0
60	MG	BA	1794	1/1	0.93	0.15	63,63,63,63	0
60	MG	CA	3531	1/1	0.93	0.13	67,67,67,67	0
60	MG	CA	3044	1/1	0.93	0.14	64,64,64,64	0
60	MG	A9	502	1/1	0.93	0.28	52,52,52,52	0
60	MG	CA	3582	1/1	0.93	0.15	60,60,60,60	0
60	MG	BA	1735	1/1	0.93	0.14	58,58,58,58	0
60	MG	BA	1685	1/1	0.93	0.11	41,41,41,41	0
60	MG	CA	3148	1/1	0.93	0.15	41,41,41,41	0
60	MG	CA	3435	1/1	0.93	0.16	55,55,55,55	0
60	MG	AA	3591	1/1	0.93	0.23	61,61,61,61	0
60	MG	AA	3446	1/1	0.93	0.11	25,25,25,25	0
60	MG	DK	201	1/1	0.93	0.23	55,55,55,55	0
60	MG	CA	3434	1/1	0.93	0.17	67,67,67,67	0
60	MG	AA	3354	1/1	0.93	0.29	56,56,56,56	0
60	MG	CA	3284	1/1	0.93	0.22	49,49,49,49	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3041	1/1	0.93	0.33	41,41,41,41	0
60	MG	AA	3834	1/1	0.93	0.29	49,49,49,49	0
60	MG	BA	1653	1/1	0.93	0.23	62,62,62,62	0
60	MG	AA	3341	1/1	0.93	0.14	74,74,74,74	0
60	MG	AA	3600	1/1	0.93	0.39	70,70,70,70	0
60	MG	DA	1726	1/1	0.93	0.16	58,58,58,58	0
60	MG	AA	3681	1/1	0.93	0.21	52,52,52,52	0
60	MG	AA	3448	1/1	0.93	0.27	74,74,74,74	0
60	MG	BA	1680	1/1	0.93	0.08	50,50,50,50	0
60	MG	AA	3513	1/1	0.93	0.22	37,37,37,37	0
60	MG	CA	3040	1/1	0.93	0.18	63,63,63,63	0
60	MG	AA	3168	1/1	0.93	0.20	60,60,60,60	0
60	MG	AW	3001	1/1	0.93	0.19	46,46,46,46	0
60	MG	AA	3006	1/1	0.93	0.29	56,56,56,56	0
60	MG	CA	3428	1/1	0.93	0.36	50,50,50,50	0
60	MG	CA	3453	1/1	0.93	0.08	43,43,43,43	0
60	MG	AA	3068	1/1	0.93	0.34	52,52,52,52	0
60	MG	BX	114	1/1	0.93	0.27	57,57,57,57	0
60	MG	CA	3593	1/1	0.93	0.11	62,62,62,62	0
60	MG	BA	1675	1/1	0.93	0.19	50,50,50,50	0
60	MG	AA	3627	1/1	0.93	0.14	53,53,53,53	0
60	MG	AA	3577	1/1	0.93	0.13	65,65,65,65	0
60	MG	CQ	204	1/1	0.93	0.28	74,74,74,74	0
60	MG	CA	3124	1/1	0.93	0.38	68,68,68,68	0
60	MG	AA	3176	1/1	0.93	0.21	70,70,70,70	0
60	MG	CA	3084	1/1	0.93	0.39	73,73,73,73	0
60	MG	DA	1674	1/1	0.93	0.28	60,60,60,60	0
60	MG	AA	3123	1/1	0.93	0.49	55,55,55,55	0
60	MG	CA	3326	1/1	0.93	0.21	54,54,54,54	0
60	MG	AA	3211	1/1	0.93	0.59	53,53,53,53	0
60	MG	CA	3473	1/1	0.93	0.24	48,48,48,48	0
60	MG	CA	3492	1/1	0.93	0.26	60,60,60,60	0
60	MG	CA	3104	1/1	0.93	0.15	64,64,64,64	0
60	MG	AA	3757	1/1	0.93	0.29	67,67,67,67	0
60	MG	AA	3417	1/1	0.93	0.19	16,16,16,16	0
60	MG	CA	3512	1/1	0.93	0.12	58,58,58,58	0
60	MG	CA	3053	1/1	0.93	0.19	71,71,71,71	0
60	MG	AA	3821	1/1	0.93	0.13	59,59,59,59	0
60	MG	CA	3029	1/1	0.93	0.11	68,68,68,68	0
60	MG	CA	3417	1/1	0.93	0.18	58,58,58,58	0
60	MG	DA	1699	1/1	0.93	0.20	79,79,79,79	0
60	MG	BA	1682	1/1	0.93	0.11	71,71,71,71	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3441	1/1	0.93	0.16	37,37,37,37	0
60	MG	CA	3520	1/1	0.93	0.10	27,27,27,27	0
60	MG	CA	3420	1/1	0.93	0.26	50,50,50,50	0
60	MG	BA	1635	1/1	0.93	0.29	62,62,62,62	0
60	MG	CA	3056	1/1	0.93	0.34	83,83,83,83	0
60	MG	CA	3621	1/1	0.93	0.22	55,55,55,55	0
60	MG	AA	3601	1/1	0.93	0.28	44,44,44,44	0
60	MG	CA	3635	1/1	0.93	0.30	77,77,77,77	0
60	MG	CA	3012	1/1	0.93	0.09	41,41,41,41	0
60	MG	AA	3393	1/1	0.93	0.17	18,18,18,18	0
60	MG	AA	3392	1/1	0.93	0.17	31,31,31,31	0
60	MG	BA	1718	1/1	0.93	0.16	48,48,48,48	0
60	MG	CA	3339	1/1	0.93	0.33	75,75,75,75	0
60	MG	BA	1730	1/1	0.93	0.21	68,68,68,68	0
60	MG	DA	1665	1/1	0.93	0.15	57,57,57,57	0
60	MG	AA	3365	1/1	0.93	0.40	55,55,55,55	0
60	MG	CA	3197	1/1	0.93	0.28	48,48,48,48	0
60	MG	BA	1707	1/1	0.93	0.24	57,57,57,57	0
60	MG	AA	3283	1/1	0.93	0.31	48,48,48,48	0
60	MG	AA	3545	1/1	0.93	0.06	64,64,64,64	0
60	MG	CA	3623	1/1	0.93	0.58	71,71,71,71	0
60	MG	AA	3073	1/1	0.93	0.22	61,61,61,61	0
60	MG	AA	3772	1/1	0.93	0.53	37,37,37,37	0
60	MG	AA	3547	1/1	0.93	0.06	50,50,50,50	0
60	MG	CA	3106	1/1	0.93	0.27	45,45,45,45	0
60	MG	AP	202	1/1	0.93	0.26	70,70,70,70	0
60	MG	CA	3391	1/1	0.93	0.10	67,67,67,67	0
60	MG	CA	3292	1/1	0.93	0.15	56,56,56,56	0
60	MG	CA	3654	1/1	0.93	0.63	76,76,76,76	0
60	MG	AA	3808	1/1	0.93	0.16	47,47,47,47	0
60	MG	CA	3237	1/1	0.93	0.34	70,70,70,70	0
60	MG	A1	101	1/1	0.93	0.10	58,58,58,58	0
60	MG	AA	3511	1/1	0.93	0.26	84,84,84,84	0
60	MG	AA	3032	1/1	0.93	0.54	62,62,62,62	0
60	MG	BA	1812	1/1	0.93	0.16	47,47,47,47	0
60	MG	AA	3219	1/1	0.93	0.22	38,38,38,38	0
60	MG	BA	1745	1/1	0.93	0.09	46,46,46,46	0
60	MG	AA	3596	1/1	0.93	0.21	39,39,39,39	0
60	MG	BA	1664	1/1	0.93	0.57	64,64,64,64	0
60	MG	BA	1760	1/1	0.93	0.18	68,68,68,68	0
60	MG	CA	3661	1/1	0.93	0.18	78,78,78,78	0
60	MG	AA	3672	1/1	0.93	0.07	71,71,71,71	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	DA	1687	1/1	0.93	0.25	60,60,60,60	0
60	MG	CA	3353	1/1	0.93	0.13	48,48,48,48	0
60	MG	AA	3590	1/1	0.93	0.19	71,71,71,71	0
60	MG	DA	1684	1/1	0.93	0.29	54,54,54,54	0
60	MG	CA	3414	1/1	0.93	0.18	50,50,50,50	0
60	MG	AA	3213	1/1	0.93	0.60	49,49,49,49	0
60	MG	AA	3153	1/1	0.93	0.27	47,47,47,47	0
60	MG	AA	3114	1/1	0.93	0.34	55,55,55,55	0
60	MG	CA	3118	1/1	0.93	0.11	67,67,67,67	0
60	MG	AA	3461	1/1	0.93	0.22	57,57,57,57	0
60	MG	AA	3333	1/1	0.93	0.15	33,33,33,33	0
60	MG	AA	3251	1/1	0.93	0.26	50,50,50,50	0
60	MG	AA	3223	1/1	0.93	0.17	21,21,21,21	0
60	MG	AB	3003	1/1	0.93	0.12	40,40,40,40	0
60	MG	CA	3429	1/1	0.93	0.23	80,80,80,80	0
60	MG	CA	3563	1/1	0.93	0.29	30,30,30,30	0
60	MG	CA	3185	1/1	0.93	0.32	47,47,47,47	0
60	MG	BA	1781	1/1	0.93	0.14	63,63,63,63	0
60	MG	AA	3083	1/1	0.93	0.67	48,48,48,48	1
60	MG	AA	3570	1/1	0.93	0.14	22,22,22,22	0
60	MG	CA	3406	1/1	0.93	0.08	54,54,54,54	0
60	MG	AA	3428	1/1	0.93	0.14	36,36,36,36	0
60	MG	AA	3684	1/1	0.93	0.17	47,47,47,47	0
60	MG	AA	3623	1/1	0.93	0.10	58,58,58,58	0
60	MG	AA	3272	1/1	0.93	0.40	74,74,74,74	0
60	MG	DA	1632	1/1	0.93	0.21	77,77,77,77	0
60	MG	DA	1619	1/1	0.93	0.36	50,50,50,50	0
60	MG	AA	3382	1/1	0.93	0.13	29,29,29,29	0
60	MG	CA	3229	1/1	0.93	0.21	48,48,48,48	0
60	MG	AA	3054	1/1	0.93	0.28	26,26,26,26	0
60	MG	DA	1697	1/1	0.93	0.21	67,67,67,67	0
60	MG	CA	3140	1/1	0.93	0.55	54,54,54,54	0
60	MG	DA	1601	1/1	0.93	0.17	59,59,59,59	0
60	MG	AA	3138	1/1	0.93	0.14	58,58,58,58	0
60	MG	DA	1730	1/1	0.93	0.39	65,65,65,65	0
60	MG	AA	3406	1/1	0.93	0.14	52,52,52,52	0
60	MG	BX	115	1/1	0.93	0.20	44,44,44,44	0
60	MG	DA	1633	1/1	0.93	0.58	67,67,67,67	0
60	MG	CA	3602	1/1	0.93	0.07	49,49,49,49	0
60	MG	BA	1690	1/1	0.93	0.19	59,59,59,59	0
60	MG	AA	3680	1/1	0.94	0.12	70,70,70,70	0
60	MG	CA	3398	1/1	0.94	0.20	57,57,57,57	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3714	1/1	0.94	0.24	44,44,44,44	0
60	MG	AA	3090	1/1	0.94	0.27	52,52,52,52	0
60	MG	AA	3339	1/1	0.94	0.29	18,18,18,18	0
60	MG	CA	3452	1/1	0.94	0.17	37,37,37,37	0
60	MG	AA	3197	1/1	0.94	0.32	42,42,42,42	0
60	MG	AA	3343	1/1	0.94	0.07	60,60,60,60	0
60	MG	CA	3300	1/1	0.94	0.15	56,56,56,56	0
60	MG	CA	3508	1/1	0.94	0.14	74,74,74,74	0
60	MG	CA	3624	1/1	0.94	0.22	76,76,76,76	0
60	MG	AA	3256	1/1	0.94	0.18	24,24,24,24	0
60	MG	CA	3163	1/1	0.94	0.31	41,41,41,41	0
60	MG	AA	3549	1/1	0.94	0.12	53,53,53,53	0
60	MG	BA	1811	1/1	0.94	0.14	52,52,52,52	0
60	MG	CA	3586	1/1	0.94	0.25	75,75,75,75	0
60	MG	AA	3710	1/1	0.94	0.17	55,55,55,55	0
60	MG	BA	1726	1/1	0.94	0.17	59,59,59,59	0
60	MG	AA	3067	1/1	0.94	0.62	82,82,82,82	0
60	MG	AA	3771	1/1	0.94	0.18	40,40,40,40	0
60	MG	CA	3430	1/1	0.94	0.22	38,38,38,38	0
60	MG	AB	3013	1/1	0.94	0.13	55,55,55,55	0
60	MG	AB	3020	1/1	0.94	0.09	66,66,66,66	0
60	MG	BA	1754	1/1	0.94	0.05	75,75,75,75	0
60	MG	AA	3064	1/1	0.94	0.22	31,31,31,31	0
60	MG	AA	3707	1/1	0.94	0.43	59,59,59,59	0
60	MG	AA	3071	1/1	0.94	0.73	55,55,55,55	0
60	MG	AA	3047	1/1	0.94	0.30	40,40,40,40	0
60	MG	CA	3010	1/1	0.94	0.13	49,49,49,49	0
60	MG	CA	3141	1/1	0.94	0.32	51,51,51,51	0
60	MG	CA	3647	1/1	0.94	0.38	61,61,61,61	0
60	MG	CA	3145	1/1	0.94	0.33	65,65,65,65	0
60	MG	AA	3675	1/1	0.94	0.16	67,67,67,67	0
60	MG	BA	1783	1/1	0.94	0.15	61,61,61,61	0
60	MG	CA	3325	1/1	0.94	0.25	42,42,42,42	0
60	MG	AA	3791	1/1	0.94	0.23	48,48,48,48	0
60	MG	AA	3515	1/1	0.94	0.14	27,27,27,27	0
60	MG	CA	3308	1/1	0.94	0.19	35,35,35,35	0
60	MG	CA	3034	1/1	0.94	0.15	51,51,51,51	0
60	MG	CA	3638	1/1	0.94	0.48	68,68,68,68	0
60	MG	CA	3488	1/1	0.94	0.17	58,58,58,58	0
60	MG	BA	1751	1/1	0.94	0.30	49,49,49,49	0
60	MG	AA	3475	1/1	0.94	0.15	73,73,73,73	0
60	MG	AA	3207	1/1	0.94	0.34	67,67,67,67	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3670	1/1	0.94	0.17	66,66,66,66	0
60	MG	AA	3134	1/1	0.94	0.52	49,49,49,49	0
60	MG	CA	3269	1/1	0.94	0.40	64,64,64,64	0
60	MG	AA	3553	1/1	0.94	0.17	47,47,47,47	0
60	MG	BA	1728	1/1	0.94	0.18	53,53,53,53	0
60	MG	DA	1637	1/1	0.94	0.38	61,61,61,61	0
60	MG	AB	3022	1/1	0.94	0.06	79,79,79,79	0
60	MG	AA	3835	1/1	0.94	0.23	34,34,34,34	1
60	MG	AA	3642	1/1	0.94	0.23	60,60,60,60	0
60	MG	AB	3009	1/1	0.94	0.10	62,62,62,62	0
60	MG	CA	3537	1/1	0.94	0.10	64,64,64,64	0
60	MG	AA	3518	1/1	0.94	0.18	28,28,28,28	0
60	MG	DA	1756	1/1	0.94	0.24	60,60,60,60	0
60	MG	AA	3558	1/1	0.94	0.14	72,72,72,72	0
60	MG	CA	3019	1/1	0.94	0.14	23,23,23,23	0
60	MG	CA	3327	1/1	0.94	0.22	37,37,37,37	0
60	MG	CA	3078	1/1	0.94	0.14	49,49,49,49	0
60	MG	AA	3349	1/1	0.94	0.13	34,34,34,34	0
60	MG	DA	1649	1/1	0.94	0.30	53,53,53,53	0
60	MG	AA	3529	1/1	0.94	0.19	12,12,12,12	1
60	MG	A0	103	1/1	0.94	0.12	67,67,67,67	0
60	MG	CA	3290	1/1	0.94	0.15	61,61,61,61	0
60	MG	AA	3034	1/1	0.94	0.35	84,84,84,84	0
60	MG	CA	3469	1/1	0.94	0.58	76,76,76,76	0
60	MG	CA	3343	1/1	0.94	0.15	37,37,37,37	0
60	MG	CA	3354	1/1	0.94	0.18	40,40,40,40	0
60	MG	CA	3231	1/1	0.94	0.26	56,56,56,56	0
60	MG	CA	3413	1/1	0.94	0.25	38,38,38,38	0
60	MG	AA	3038	1/1	0.94	0.40	42,42,42,42	0
60	MG	CD	304	1/1	0.94	0.23	32,32,32,32	0
60	MG	CA	3465	1/1	0.94	0.08	64,64,64,64	0
60	MG	BN	502	1/1	0.94	0.29	64,64,64,64	0
60	MG	CE	302	1/1	0.94	0.13	31,31,31,31	0
60	MG	AA	3474	1/1	0.94	0.14	74,74,74,74	0
60	MG	AD	302	1/1	0.94	0.39	31,31,31,31	0
60	MG	CA	3173	1/1	0.94	0.53	72,72,72,72	0
60	MG	AA	3426	1/1	0.94	0.20	47,47,47,47	0
60	MG	AA	3593	1/1	0.94	0.14	49,49,49,49	0
60	MG	CA	3272	1/1	0.94	0.05	56,56,56,56	0
60	MG	AA	3050	1/1	0.94	0.25	29,29,29,29	0
60	MG	CB	3004	1/1	0.94	0.13	70,70,70,70	0
60	MG	CA	3574	1/1	0.94	0.11	31,31,31,31	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3366	1/1	0.94	0.18	35,35,35,35	0
60	MG	CA	3217	1/1	0.94	0.13	52,52,52,52	0
60	MG	CA	3052	1/1	0.94	0.34	46,46,46,46	0
60	MG	BA	1665	1/1	0.94	0.41	68,68,68,68	0
60	MG	AA	3174	1/1	0.94	0.27	39,39,39,39	0
60	MG	C8	5001	1/1	0.94	0.29	43,43,43,43	0
60	MG	AA	3720	1/1	0.94	0.35	78,78,78,78	0
60	MG	AA	3658	1/1	0.94	0.21	25,25,25,25	0
60	MG	AA	3214	1/1	0.94	0.08	47,47,47,47	0
60	MG	AA	3077	1/1	0.94	0.26	44,44,44,44	0
60	MG	AA	3383	1/1	0.94	0.21	31,31,31,31	0
60	MG	BA	1637	1/1	0.94	0.19	64,64,64,64	0
60	MG	AA	3759	1/1	0.94	0.13	29,29,29,29	0
60	MG	CA	3403	1/1	0.94	0.19	70,70,70,70	0
60	MG	AA	3322	1/1	0.94	0.19	37,37,37,37	0
60	MG	CA	3116	1/1	0.94	0.45	57,57,57,57	0
60	MG	BA	1697	1/1	0.94	0.47	80,80,80,80	0
60	MG	DA	1641	1/1	0.94	0.13	55,55,55,55	0
60	MG	BA	1651	1/1	0.94	0.12	69,69,69,69	0
60	MG	DA	1659	1/1	0.94	0.35	79,79,79,79	0
60	MG	AA	3535	1/1	0.94	0.18	37,37,37,37	0
60	MG	CA	3564	1/1	0.94	0.28	33,33,33,33	0
60	MG	CA	3301	1/1	0.94	0.43	56,56,56,56	0
60	MG	AA	3317	1/1	0.94	0.19	56,56,56,56	0
60	MG	DA	1701	1/1	0.94	0.14	61,61,61,61	0
60	MG	AA	3122	1/1	0.94	0.29	39,39,39,39	0
60	MG	AA	3787	1/1	0.94	0.27	55,55,55,55	0
60	MG	DA	1692	1/1	0.94	0.26	49,49,49,49	0
60	MG	CB	3005	1/1	0.94	0.22	65,65,65,65	0
60	MG	AA	3526	1/1	0.94	0.15	26,26,26,26	0
60	MG	AA	3636	1/1	0.94	0.21	71,71,71,71	0
60	MG	CA	3365	1/1	0.94	0.18	69,69,69,69	0
60	MG	CA	3554	1/1	0.94	0.16	60,60,60,60	0
60	MG	CA	3208	1/1	0.94	0.12	24,24,24,24	0
60	MG	BA	1713	1/1	0.94	0.24	61,61,61,61	0
60	MG	CA	3207	1/1	0.94	0.48	62,62,62,62	0
60	MG	AA	3799	1/1	0.94	0.12	45,45,45,45	0
60	MG	CA	3657	1/1	0.94	0.24	34,34,34,34	0
60	MG	CA	3568	1/1	0.94	0.24	71,71,71,71	0
60	MG	AA	3320	1/1	0.94	0.24	65,65,65,65	0
60	MG	AA	3749	1/1	0.94	0.14	30,30,30,30	0
60	MG	CA	3513	1/1	0.94	0.24	109,109,109,109	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3203	1/1	0.94	0.32	45,45,45,45	0
60	MG	BA	1693	1/1	0.94	0.14	69,69,69,69	0
60	MG	AA	3503	1/1	0.94	0.14	41,41,41,41	0
60	MG	AA	3001	1/1	0.94	0.21	39,39,39,39	0
60	MG	CA	3360	1/1	0.94	0.17	52,52,52,52	0
60	MG	CA	3134	1/1	0.94	0.18	64,64,64,64	0
60	MG	BA	1772	1/1	0.94	0.33	51,51,51,51	0
60	MG	BA	1802	1/1	0.94	0.13	58,58,58,58	0
60	MG	AA	3345	1/1	0.94	0.10	34,34,34,34	0
60	MG	AA	3573	1/1	0.94	0.09	47,47,47,47	0
60	MG	CA	3060	1/1	0.94	0.28	50,50,50,50	0
60	MG	AA	3533	1/1	0.94	0.12	20,20,20,20	0
60	MG	AA	3012	1/1	0.94	0.17	38,38,38,38	0
60	MG	AA	3493	1/1	0.94	0.22	56,56,56,56	0
60	MG	AA	3060	1/1	0.94	0.34	23,23,23,23	0
60	MG	AA	3531	1/1	0.94	0.15	61,61,61,61	0
60	MG	DA	1723	1/1	0.94	0.28	53,53,53,53	0
60	MG	AA	3173	1/1	0.94	0.26	74,74,74,74	0
60	MG	AA	3356	1/1	0.94	0.12	51,51,51,51	0
60	MG	CA	3408	1/1	0.94	0.27	35,35,35,35	0
60	MG	AA	3820	1/1	0.94	0.21	31,31,31,31	0
60	MG	AA	3830	1/1	0.94	0.30	75,75,75,75	0
60	MG	CA	3364	1/1	0.94	0.19	64,64,64,64	0
60	MG	AA	3823	1/1	0.94	0.33	51,51,51,51	0
60	MG	BA	1700	1/1	0.94	0.11	62,62,62,62	0
60	MG	CA	3570	1/1	0.94	0.09	61,61,61,61	0
60	MG	CA	3493	1/1	0.94	0.22	66,66,66,66	0
60	MG	CA	3046	1/1	0.94	0.07	72,72,72,72	0
60	MG	CA	3380	1/1	0.94	0.16	37,37,37,37	0
60	MG	AA	3586	1/1	0.94	0.19	75,75,75,75	0
60	MG	DA	1682	1/1	0.94	0.30	60,60,60,60	0
60	MG	CA	3002	1/1	0.94	0.24	32,32,32,32	0
60	MG	DA	1606	1/1	0.94	0.16	66,66,66,66	0
60	MG	CA	3440	1/1	0.94	0.41	69,69,69,69	0
60	MG	BA	1796	1/1	0.94	0.18	75,75,75,75	0
60	MG	DA	1693	1/1	0.94	0.15	50,50,50,50	0
60	MG	BA	1701	1/1	0.94	0.21	47,47,47,47	0
60	MG	AA	3556	1/1	0.94	0.17	54,54,54,54	0
60	MG	AA	3635	1/1	0.94	0.15	33,33,33,33	0
60	MG	BA	1615	1/1	0.94	0.30	65,65,65,65	0
60	MG	CA	3255	1/1	0.94	0.35	61,61,61,61	0
60	MG	AA	3298	1/1	0.94	0.15	28,28,28,28	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	DA	1717	1/1	0.94	0.17	70,70,70,70	0
60	MG	AA	3464	1/1	0.95	0.09	69,69,69,69	0
60	MG	AA	3634	1/1	0.95	0.25	63,63,63,63	0
60	MG	AA	3682	1/1	0.95	0.20	58,58,58,58	0
60	MG	AA	3433	1/1	0.95	0.28	50,50,50,50	0
60	MG	AA	3190	1/1	0.95	0.18	51,51,51,51	0
60	MG	AA	3372	1/1	0.95	0.27	59,59,59,59	0
60	MG	CA	3641	1/1	0.95	0.54	59,59,59,59	0
60	MG	CV	201	1/1	0.95	0.36	84,84,84,84	0
60	MG	AA	3610	1/1	0.95	0.10	66,66,66,66	0
60	MG	AA	3719	1/1	0.95	0.09	62,62,62,62	0
60	MG	AA	3602	1/1	0.95	0.21	39,39,39,39	0
60	MG	DA	1604	1/1	0.95	0.12	90,90,90,90	0
60	MG	DA	1663	1/1	0.95	0.10	53,53,53,53	0
60	MG	AU	204	1/1	0.95	0.45	55,55,55,55	0
60	MG	AA	3302	1/1	0.95	0.34	58,58,58,58	0
60	MG	AA	3129	1/1	0.95	0.27	52,52,52,52	0
60	MG	BA	1648	1/1	0.95	0.18	28,28,28,28	0
60	MG	AA	3338	1/1	0.95	0.13	49,49,49,49	0
60	MG	AA	3292	1/1	0.95	0.18	31,31,31,31	0
60	MG	AA	3468	1/1	0.95	0.12	34,34,34,34	0
60	MG	AA	3398	1/1	0.95	0.19	29,29,29,29	0
60	MG	AA	3084	1/1	0.95	0.10	27,27,27,27	0
60	MG	DA	1679	1/1	0.95	0.38	70,70,70,70	0
60	MG	AA	3424	1/1	0.95	0.11	48,48,48,48	0
60	MG	CA	3424	1/1	0.95	0.25	40,40,40,40	0
60	MG	AA	3133	1/1	0.95	0.47	92,92,92,92	1
60	MG	BA	1654	1/1	0.95	0.12	45,45,45,45	0
60	MG	CA	3358	1/1	0.95	0.13	41,41,41,41	0
60	MG	DA	1713	1/1	0.95	0.15	59,59,59,59	0
60	MG	CA	3319	1/1	0.95	0.07	32,32,32,32	0
60	MG	AA	3102	1/1	0.95	0.24	38,38,38,38	0
60	MG	CA	3176	1/1	0.95	0.35	60,60,60,60	0
60	MG	CA	3472	1/1	0.95	0.29	49,49,49,49	0
60	MG	CA	3471	1/1	0.95	0.21	59,59,59,59	0
60	MG	AA	3220	1/1	0.95	0.19	65,65,65,65	0
60	MG	CA	3518	1/1	0.95	0.18	72,72,72,72	0
60	MG	AA	3449	1/1	0.95	0.20	46,46,46,46	0
60	MG	CA	3433	1/1	0.95	0.15	45,45,45,45	0
60	MG	AA	3801	1/1	0.95	0.16	39,39,39,39	0
60	MG	CA	3426	1/1	0.95	0.16	46,46,46,46	0
60	MG	CA	3128	1/1	0.95	0.22	31,31,31,31	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3118	1/1	0.95	0.30	59,59,59,59	0
60	MG	AA	3255	1/1	0.95	0.28	64,64,64,64	0
60	MG	AA	3803	1/1	0.95	0.33	37,37,37,37	0
60	MG	AA	3376	1/1	0.95	0.21	39,39,39,39	0
60	MG	AA	3431	1/1	0.95	0.15	25,25,25,25	0
60	MG	A1	102	1/1	0.95	0.16	46,46,46,46	0
60	MG	AA	3454	1/1	0.95	0.16	27,27,27,27	0
60	MG	CA	3321	1/1	0.95	0.13	65,65,65,65	0
60	MG	CA	3615	1/1	0.95	0.15	33,33,33,33	0
60	MG	BA	1705	1/1	0.95	0.31	61,61,61,61	0
60	MG	AW	3003	1/1	0.95	0.33	38,38,38,38	0
60	MG	CA	3061	1/1	0.95	0.15	36,36,36,36	0
60	MG	AA	3695	1/1	0.95	0.29	50,50,50,50	0
60	MG	A8	5002	1/1	0.95	0.25	45,45,45,45	0
60	MG	BA	1610	1/1	0.95	0.14	112,112,112,112	0
60	MG	AA	3414	1/1	0.95	0.17	43,43,43,43	0
60	MG	AA	3344	1/1	0.95	0.18	65,65,65,65	0
60	MG	AA	3781	1/1	0.95	0.17	49,49,49,49	0
60	MG	BA	1678	1/1	0.95	0.22	52,52,52,52	0
60	MG	DA	1696	1/1	0.95	0.26	65,65,65,65	0
60	MG	CA	3627	1/1	0.95	0.07	59,59,59,59	0
60	MG	AA	3779	1/1	0.95	0.28	41,41,41,41	0
60	MG	CA	3310	1/1	0.95	0.21	45,45,45,45	0
60	MG	AA	3696	1/1	0.95	0.20	62,62,62,62	0
60	MG	AA	3314	1/1	0.95	0.20	43,43,43,43	0
60	MG	AA	3815	1/1	0.95	0.46	72,72,72,72	0
60	MG	AA	3184	1/1	0.95	0.20	39,39,39,39	0
60	MG	CA	3227	1/1	0.95	0.25	30,30,30,30	0
60	MG	CA	3328	1/1	0.95	0.17	40,40,40,40	0
60	MG	AA	3469	1/1	0.95	0.20	37,37,37,37	0
60	MG	DA	1706	1/1	0.95	0.19	70,70,70,70	0
60	MG	CA	3362	1/1	0.95	0.11	20,20,20,20	0
60	MG	CA	3266	1/1	0.95	0.15	67,67,67,67	0
60	MG	CA	3299	1/1	0.95	0.23	42,42,42,42	0
60	MG	CA	3565	1/1	0.95	0.14	36,36,36,36	0
60	MG	BA	1692	1/1	0.95	0.31	69,69,69,69	0
60	MG	AA	3792	1/1	0.95	0.26	35,35,35,35	0
60	MG	AA	3186	1/1	0.95	0.24	53,53,53,53	0
60	MG	AA	3539	1/1	0.95	0.23	42,42,42,42	0
60	MG	CV	202	1/1	0.95	0.36	82,82,82,82	0
60	MG	AA	3091	1/1	0.95	0.48	62,62,62,62	0
60	MG	AA	3135	1/1	0.95	0.16	53,53,53,53	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CU	201	1/1	0.95	0.51	62,62,62,62	0
60	MG	AA	3478	1/1	0.95	0.07	70,70,70,70	0
60	MG	CA	3463	1/1	0.95	0.43	75,75,75,75	0
60	MG	AA	3760	1/1	0.95	0.34	50,50,50,50	0
60	MG	BA	1805	1/1	0.95	0.10	55,55,55,55	0
60	MG	CA	3109	1/1	0.95	0.18	65,65,65,65	0
60	MG	AA	3666	1/1	0.95	0.29	28,28,28,28	0
60	MG	AB	3017	1/1	0.95	0.07	76,76,76,76	0
60	MG	AA	3472	1/1	0.95	0.24	37,37,37,37	0
60	MG	AA	3831	1/1	0.95	0.39	41,41,41,41	0
60	MG	AA	3761	1/1	0.95	0.19	72,72,72,72	0
60	MG	CA	3395	1/1	0.95	0.12	60,60,60,60	0
60	MG	AA	3117	1/1	0.95	0.17	64,64,64,64	0
60	MG	CA	3196	1/1	0.95	0.28	57,57,57,57	0
60	MG	BA	1711	1/1	0.95	0.37	63,63,63,63	0
60	MG	AA	3704	1/1	0.95	0.17	57,57,57,57	0
60	MG	AA	3312	1/1	0.95	0.14	25,25,25,25	0
60	MG	CA	3180	1/1	0.95	0.17	46,46,46,46	0
60	MG	AA	3463	1/1	0.95	0.19	41,41,41,41	0
60	MG	AA	3348	1/1	0.95	0.30	39,39,39,39	0
60	MG	CA	3131	1/1	0.95	0.28	61,61,61,61	0
60	MG	AA	3293	1/1	0.95	0.14	68,68,68,68	0
60	MG	DA	1690	1/1	0.95	0.20	74,74,74,74	0
60	MG	AA	3162	1/1	0.95	0.32	35,35,35,35	0
60	MG	AA	3662	1/1	0.95	0.33	60,60,60,60	0
60	MG	DA	1660	1/1	0.95	0.29	81,81,81,81	0
60	MG	AA	3418	1/1	0.95	0.17	22,22,22,22	0
60	MG	AA	3384	1/1	0.95	0.16	26,26,26,26	0
60	MG	BA	1748	1/1	0.95	0.33	75,75,75,75	0
60	MG	BA	1616	1/1	0.95	0.11	69,69,69,69	0
60	MG	BA	1777	1/1	0.95	0.12	76,76,76,76	0
60	MG	AA	3741	1/1	0.95	0.27	47,47,47,47	0
60	MG	CA	3556	1/1	0.95	0.05	77,77,77,77	0
60	MG	AA	3459	1/1	0.95	0.47	65,65,65,65	0
60	MG	CA	3591	1/1	0.95	0.14	69,69,69,69	0
60	MG	AA	3554	1/1	0.95	0.07	48,48,48,48	0
60	MG	AA	3462	1/1	0.95	0.06	73,73,73,73	0
60	MG	BA	1677	1/1	0.95	0.32	57,57,57,57	0
60	MG	DA	1656	1/1	0.95	0.07	67,67,67,67	0
60	MG	CA	3516	1/1	0.95	0.20	58,58,58,58	0
60	MG	AA	3331	1/1	0.95	0.20	61,61,61,61	0
60	MG	DA	1680	1/1	0.95	0.17	40,40,40,40	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3609	1/1	0.95	0.21	62,62,62,62	0
60	MG	BA	1655	1/1	0.95	0.27	65,65,65,65	0
60	MG	CA	3421	1/1	0.95	0.19	39,39,39,39	0
60	MG	AA	3676	1/1	0.95	0.17	46,46,46,46	0
60	MG	AA	3711	1/1	0.95	0.37	41,41,41,41	0
62	ZN	A4	501	1/1	0.95	0.08	120,120,120,120	0
60	MG	CA	3479	1/1	0.95	0.16	67,67,67,67	0
60	MG	BA	1756	1/1	0.95	0.25	43,43,43,43	0
60	MG	CA	3618	1/1	0.95	0.21	79,79,79,79	0
60	MG	AA	3373	1/1	0.95	0.22	23,23,23,23	0
60	MG	CA	3225	1/1	0.95	0.24	73,73,73,73	0
60	MG	AA	3701	1/1	0.95	0.56	62,62,62,62	0
62	ZN	C4	501	1/1	0.95	0.07	163,163,163,163	0
60	MG	AA	3044	1/1	0.95	0.35	62,62,62,62	0
60	MG	AA	3807	1/1	0.95	0.20	62,62,62,62	0
60	MG	CA	3160	1/1	0.95	0.27	33,33,33,33	0
60	MG	AA	3253	1/1	0.95	0.19	42,42,42,42	0
60	MG	CA	3107	1/1	0.95	0.11	64,64,64,64	0
60	MG	AA	3651	1/1	0.95	0.23	66,66,66,66	0
60	MG	DA	1727	1/1	0.95	0.17	65,65,65,65	0
60	MG	CA	3274	1/1	0.95	0.18	64,64,64,64	0
60	MG	CA	3009	1/1	0.95	0.05	24,24,24,24	0
60	MG	AA	3722	1/1	0.95	0.17	31,31,31,31	0
60	MG	AA	3607	1/1	0.95	0.15	39,39,39,39	0
60	MG	CA	3304	1/1	0.95	0.15	48,48,48,48	0
60	MG	BA	1641	1/1	0.95	0.29	56,56,56,56	0
60	MG	AB	3008	1/1	0.95	0.39	46,46,46,46	0
60	MG	CA	3546	1/1	0.95	0.17	59,59,59,59	0
60	MG	CA	3025	1/1	0.95	0.50	32,32,32,32	1
60	MG	AA	3551	1/1	0.95	0.17	58,58,58,58	0
60	MG	AA	3742	1/1	0.95	0.20	68,68,68,68	0
60	MG	CA	3038	1/1	0.95	0.21	26,26,26,26	0
60	MG	AA	3267	1/1	0.95	0.31	43,43,43,43	0
60	MG	AA	3389	1/1	0.95	0.18	46,46,46,46	0
60	MG	CA	3121	1/1	0.95	0.32	78,78,78,78	0
60	MG	CA	3378	1/1	0.95	0.15	63,63,63,63	0
60	MG	AF	302	1/1	0.95	0.09	42,42,42,42	0
60	MG	CA	3164	1/1	0.95	0.13	38,38,38,38	0
60	MG	CA	3179	1/1	0.95	0.27	27,27,27,27	0
60	MG	DA	1627	1/1	0.95	0.36	48,48,48,48	0
60	MG	CA	3612	1/1	0.95	0.13	59,59,59,59	0
60	MG	CA	3427	1/1	0.95	0.29	69,69,69,69	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3276	1/1	0.95	0.18	64,64,64,64	0
60	MG	BA	1704	1/1	0.95	0.26	68,68,68,68	0
60	MG	AA	3308	1/1	0.95	0.11	45,45,45,45	0
60	MG	AA	3546	1/1	0.95	0.17	36,36,36,36	0
60	MG	AA	3315	1/1	0.95	0.21	56,56,56,56	0
60	MG	CA	3605	1/1	0.95	0.19	72,72,72,72	0
60	MG	AA	3775	1/1	0.95	0.18	52,52,52,52	0
60	MG	AA	3416	1/1	0.95	0.19	31,31,31,31	0
60	MG	CA	3117	1/1	0.96	0.13	46,46,46,46	0
60	MG	AA	3686	1/1	0.96	0.24	62,62,62,62	0
60	MG	AA	3451	1/1	0.96	0.18	43,43,43,43	0
60	MG	AA	3013	1/1	0.96	0.14	38,38,38,38	0
60	MG	CA	3369	1/1	0.96	0.17	65,65,65,65	0
60	MG	AA	3052	1/1	0.96	0.20	15,15,15,15	0
60	MG	DA	1685	1/1	0.96	0.20	49,49,49,49	0
60	MG	AA	3534	1/1	0.96	0.20	34,34,34,34	0
60	MG	CA	3110	1/1	0.96	0.33	35,35,35,35	0
60	MG	AA	3510	1/1	0.96	0.22	13,13,13,13	0
60	MG	AA	3358	1/1	0.96	0.06	72,72,72,72	0
60	MG	CA	3233	1/1	0.96	0.30	52,52,52,52	0
60	MG	AA	3606	1/1	0.96	0.18	62,62,62,62	0
60	MG	DA	1759	1/1	0.96	0.42	64,64,64,64	0
60	MG	AA	3467	1/1	0.96	0.13	54,54,54,54	0
60	MG	CA	3444	1/1	0.96	0.24	70,70,70,70	0
60	MG	AA	3172	1/1	0.96	0.18	50,50,50,50	0
62	ZN	DN	501	1/1	0.96	0.07	120,120,120,120	0
60	MG	DA	1744	1/1	0.96	0.14	57,57,57,57	0
60	MG	AA	3626	1/1	0.96	0.23	59,59,59,59	0
60	MG	AA	3566	1/1	0.96	0.19	26,26,26,26	0
60	MG	CA	3561	1/1	0.96	0.12	62,62,62,62	0
60	MG	AA	3457	1/1	0.96	0.17	18,18,18,18	0
60	MG	CA	3443	1/1	0.96	0.31	40,40,40,40	0
60	MG	CA	3252	1/1	0.96	0.25	30,30,30,30	0
60	MG	AA	3528	1/1	0.96	0.19	26,26,26,26	0
60	MG	BX	108	1/1	0.96	0.10	78,78,78,78	0
60	MG	CA	3504	1/1	0.96	0.11	77,77,77,77	0
60	MG	AA	3387	1/1	0.96	0.21	34,34,34,34	0
60	MG	CA	3423	1/1	0.96	0.18	57,57,57,57	0
60	MG	CA	3082	1/1	0.96	0.21	31,31,31,31	0
60	MG	CA	3594	1/1	0.96	0.16	62,62,62,62	0
60	MG	AA	3748	1/1	0.96	0.18	62,62,62,62	0
60	MG	AA	3039	1/1	0.96	0.25	34,34,34,34	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	1742	1/1	0.96	0.09	45,45,45,45	0
60	MG	CA	3130	1/1	0.96	0.17	57,57,57,57	0
64	GDP	DZ	702	28/28	0.96	0.13	69,69,69,69	0
60	MG	AA	3334	1/1	0.96	0.21	62,62,62,62	0
60	MG	AA	3832	1/1	0.96	0.21	52,52,52,52	0
60	MG	AA	3629	1/1	0.96	0.11	51,51,51,51	0
60	MG	CA	3468	1/1	0.96	0.17	37,37,37,37	0
60	MG	CA	3331	1/1	0.96	0.47	62,62,62,62	0
60	MG	AA	3275	1/1	0.96	0.39	56,56,56,56	0
60	MG	AA	3825	1/1	0.96	0.29	45,45,45,45	0
60	MG	AA	3730	1/1	0.96	0.27	34,34,34,34	0
60	MG	AA	3326	1/1	0.96	0.14	22,22,22,22	0
60	MG	AA	3653	1/1	0.96	0.12	47,47,47,47	0
60	MG	AA	3645	1/1	0.96	0.10	57,57,57,57	0
60	MG	AA	3536	1/1	0.96	0.09	36,36,36,36	0
60	MG	AA	3100	1/1	0.96	0.21	34,34,34,34	0
60	MG	AA	3085	1/1	0.96	0.24	80,80,80,80	0
60	MG	DA	1745	1/1	0.96	0.23	54,54,54,54	0
60	MG	AA	3517	1/1	0.96	0.31	44,44,44,44	0
60	MG	AA	3502	1/1	0.96	0.09	41,41,41,41	0
60	MG	DA	1709	1/1	0.96	0.22	57,57,57,57	0
60	MG	AA	3391	1/1	0.96	0.13	27,27,27,27	0
60	MG	A7	101	1/1	0.96	0.10	57,57,57,57	0
60	MG	AA	3020	1/1	0.96	0.18	25,25,25,25	0
60	MG	BA	1695	1/1	0.96	0.06	64,64,64,64	0
60	MG	CA	3100	1/1	0.96	0.17	75,75,75,75	0
60	MG	CA	3392	1/1	0.96	0.09	66,66,66,66	0
60	MG	AA	3281	1/1	0.96	0.43	38,38,38,38	0
60	MG	CA	3345	1/1	0.96	0.19	41,41,41,41	0
60	MG	AA	3022	1/1	0.96	0.09	19,19,19,19	0
60	MG	AA	3436	1/1	0.96	0.13	31,31,31,31	0
60	MG	AA	3229	1/1	0.96	0.13	33,33,33,33	0
60	MG	AA	3697	1/1	0.96	0.15	71,71,71,71	0
60	MG	CA	3367	1/1	0.96	0.13	39,39,39,39	0
60	MG	CA	3436	1/1	0.96	0.15	34,34,34,34	0
60	MG	CA	3198	1/1	0.96	0.25	49,49,49,49	0
60	MG	AA	3143	1/1	0.96	0.05	37,37,37,37	0
60	MG	AW	3004	1/1	0.96	0.14	45,45,45,45	0
60	MG	AA	3647	1/1	0.96	0.14	35,35,35,35	0
60	MG	CA	3147	1/1	0.96	0.12	51,51,51,51	0
60	MG	AA	3311	1/1	0.96	0.21	46,46,46,46	0
60	MG	BA	1746	1/1	0.96	0.16	70,70,70,70	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3075	1/1	0.96	0.28	47,47,47,47	0
60	MG	AA	3665	1/1	0.96	0.06	63,63,63,63	0
60	MG	CA	3579	1/1	0.96	0.07	58,58,58,58	0
60	MG	AA	3774	1/1	0.96	0.10	44,44,44,44	0
60	MG	BA	1797	1/1	0.96	0.15	75,75,75,75	0
60	MG	AA	3633	1/1	0.96	0.25	51,51,51,51	0
60	MG	CA	3216	1/1	0.96	0.25	32,32,32,32	0
60	MG	AA	3620	1/1	0.96	0.14	49,49,49,49	0
60	MG	AA	3009	1/1	0.96	0.09	26,26,26,26	0
60	MG	DA	1711	1/1	0.96	0.10	64,64,64,64	0
60	MG	AE	302	1/1	0.96	0.18	62,62,62,62	0
60	MG	CA	3447	1/1	0.96	0.12	44,44,44,44	0
60	MG	CA	3297	1/1	0.96	0.16	55,55,55,55	0
60	MG	AA	3206	1/1	0.96	0.19	55,55,55,55	0
60	MG	BA	1741	1/1	0.96	0.15	49,49,49,49	0
60	MG	CA	3456	1/1	0.96	0.15	37,37,37,37	0
60	MG	CA	3248	1/1	0.96	0.08	58,58,58,58	0
60	MG	AA	3422	1/1	0.96	0.19	22,22,22,22	0
60	MG	BA	1663	1/1	0.96	0.13	66,66,66,66	0
60	MG	DA	1732	1/1	0.96	0.11	54,54,54,54	0
60	MG	CA	3344	1/1	0.96	0.18	27,27,27,27	0
60	MG	CA	3580	1/1	0.96	0.12	37,37,37,37	0
60	MG	AA	3569	1/1	0.96	0.19	17,17,17,17	0
60	MG	AA	3368	1/1	0.96	0.31	54,54,54,54	0
60	MG	AA	3762	1/1	0.96	0.26	63,63,63,63	0
60	MG	AA	3522	1/1	0.96	0.16	31,31,31,31	0
60	MG	DA	1755	1/1	0.96	0.14	69,69,69,69	0
60	MG	CA	3047	1/1	0.96	0.06	54,54,54,54	0
60	MG	AA	3594	1/1	0.96	0.26	48,48,48,48	0
60	MG	AA	3375	1/1	0.96	0.13	16,16,16,16	0
60	MG	AA	3094	1/1	0.96	0.31	82,82,82,82	0
60	MG	AA	3726	1/1	0.96	0.13	74,74,74,74	0
60	MG	CA	3270	1/1	0.96	0.33	69,69,69,69	0
60	MG	DA	1728	1/1	0.96	0.09	53,53,53,53	0
60	MG	CA	3356	1/1	0.96	0.24	28,28,28,28	0
60	MG	AA	3205	1/1	0.96	0.31	45,45,45,45	0
60	MG	AA	3155	1/1	0.96	0.24	31,31,31,31	0
60	MG	CA	3375	1/1	0.96	0.09	65,65,65,65	0
60	MG	AA	3734	1/1	0.96	0.12	23,23,23,23	0
60	MG	AA	3367	1/1	0.96	0.11	52,52,52,52	0
60	MG	DA	1646	1/1	0.96	0.30	51,51,51,51	0
60	MG	AA	3074	1/1	0.96	0.37	26,26,26,26	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3385	1/1	0.96	0.20	24,24,24,24	0
60	MG	AA	3086	1/1	0.96	0.35	43,43,43,43	1
60	MG	BA	1744	1/1	0.96	0.13	48,48,48,48	0
60	MG	AA	3816	1/1	0.96	0.25	64,64,64,64	0
60	MG	BA	1716	1/1	0.96	0.27	71,71,71,71	0
60	MG	AA	3390	1/1	0.96	0.14	23,23,23,23	0
60	MG	DA	1760	1/1	0.96	0.27	53,53,53,53	0
60	MG	CA	3405	1/1	0.96	0.15	50,50,50,50	0
60	MG	CA	3585	1/1	0.96	0.11	44,44,44,44	0
60	MG	AA	3035	1/1	0.96	0.22	69,69,69,69	0
60	MG	CA	3020	1/1	0.96	0.18	38,38,38,38	0
60	MG	CA	3289	1/1	0.96	0.13	23,23,23,23	0
60	MG	DA	1644	1/1	0.96	0.18	49,49,49,49	0
60	MG	CA	3501	1/1	0.96	0.17	78,78,78,78	0
60	MG	AA	3336	1/1	0.96	0.27	52,52,52,52	0
60	MG	CA	3172	1/1	0.96	0.17	41,41,41,41	0
60	MG	AA	3685	1/1	0.96	0.15	58,58,58,58	0
60	MG	BX	109	1/1	0.96	0.22	55,55,55,55	0
60	MG	CA	3264	1/1	0.96	0.20	54,54,54,54	0
60	MG	AA	3611	1/1	0.96	0.26	57,57,57,57	0
60	MG	AA	3754	1/1	0.96	0.09	25,25,25,25	0
60	MG	DA	1736	1/1	0.96	0.17	63,63,63,63	0
60	MG	CA	3558	1/1	0.96	0.20	49,49,49,49	1
60	MG	CF	305	1/1	0.96	0.20	45,45,45,45	0
60	MG	AA	3264	1/1	0.96	0.09	54,54,54,54	0
60	MG	CA	3014	1/1	0.96	0.14	58,58,58,58	0
60	MG	CA	3189	1/1	0.96	0.07	40,40,40,40	0
60	MG	AA	3817	1/1	0.96	0.46	40,40,40,40	0
60	MG	AA	3809	1/1	0.96	0.25	46,46,46,46	0
60	MG	AA	3357	1/1	0.96	0.18	52,52,52,52	0
60	MG	CP	201	1/1	0.96	0.13	57,57,57,57	0
60	MG	AA	3691	1/1	0.96	0.09	51,51,51,51	0
60	MG	AA	3131	1/1	0.96	0.29	39,39,39,39	0
60	MG	CA	3253	1/1	0.96	0.38	61,61,61,61	0
60	MG	BA	1725	1/1	0.96	0.31	52,52,52,52	0
60	MG	BA	1753	1/1	0.96	0.14	48,48,48,48	0
60	MG	DA	1683	1/1	0.96	0.42	60,60,60,60	0
60	MG	DA	1681	1/1	0.96	0.14	44,44,44,44	0
60	MG	AA	3407	1/1	0.96	0.19	22,22,22,22	0
60	MG	CA	3026	1/1	0.96	0.47	55,55,55,55	0
60	MG	AA	3282	1/1	0.96	0.39	65,65,65,65	0
60	MG	BB	3001	1/1	0.96	0.23	67,67,67,67	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	1771	1/1	0.96	0.13	48,48,48,48	0
60	MG	AA	3003	1/1	0.96	0.07	14,14,14,14	0
60	MG	CA	3256	1/1	0.96	0.29	73,73,73,73	0
60	MG	AA	3241	1/1	0.96	0.26	29,29,29,29	0
60	MG	AA	3259	1/1	0.96	0.37	27,27,27,27	0
60	MG	CA	3024	1/1	0.96	0.62	67,67,67,67	0
60	MG	AA	3188	1/1	0.96	0.16	15,15,15,15	0
60	MG	CA	3448	1/1	0.96	0.08	64,64,64,64	0
60	MG	AA	3776	1/1	0.96	0.12	21,21,21,21	0
60	MG	AA	3699	1/1	0.96	0.22	61,61,61,61	0
60	MG	AA	3239	1/1	0.96	0.21	63,63,63,63	0
60	MG	CA	3373	1/1	0.96	0.38	71,71,71,71	0
60	MG	CA	3577	1/1	0.96	0.12	52,52,52,52	0
60	MG	AA	3057	1/1	0.96	0.29	56,56,56,56	0
60	MG	AA	3564	1/1	0.97	0.23	17,17,17,17	0
60	MG	CA	3332	1/1	0.97	0.24	47,47,47,47	0
60	MG	CA	3318	1/1	0.97	0.16	31,31,31,31	0
60	MG	AA	3557	1/1	0.97	0.17	21,21,21,21	0
60	MG	AA	3521	1/1	0.97	0.19	30,30,30,30	0
60	MG	CA	3262	1/1	0.97	0.28	59,59,59,59	0
60	MG	AR	5001	1/1	0.97	0.14	34,34,34,34	0
60	MG	AA	3588	1/1	0.97	0.15	33,33,33,33	0
60	MG	AA	3355	1/1	0.97	0.14	19,19,19,19	0
60	MG	CA	3359	1/1	0.97	0.22	44,44,44,44	0
60	MG	AV	201	1/1	0.97	0.28	46,46,46,46	0
60	MG	BA	1768	1/1	0.97	0.18	64,64,64,64	0
60	MG	AA	3193	1/1	0.97	0.20	63,63,63,63	0
60	MG	CA	3316	1/1	0.97	0.19	34,34,34,34	0
60	MG	BZ	701	1/1	0.97	0.20	58,58,58,58	0
60	MG	AA	3284	1/1	0.97	0.39	45,45,45,45	0
60	MG	CA	3251	1/1	0.97	0.15	62,62,62,62	0
60	MG	AA	3216	1/1	0.97	0.17	68,68,68,68	0
60	MG	AA	3663	1/1	0.97	0.20	61,61,61,61	0
60	MG	BE	3001	1/1	0.97	0.08	83,83,83,83	0
60	MG	AA	3323	1/1	0.97	0.18	42,42,42,42	0
60	MG	AA	3030	1/1	0.97	0.33	44,44,44,44	1
60	MG	CA	3416	1/1	0.97	0.28	33,33,33,33	0
60	MG	BA	1750	1/1	0.97	0.10	54,54,54,54	0
60	MG	CA	3649	1/1	0.97	0.19	15,15,15,15	0
60	MG	AA	3519	1/1	0.97	0.13	39,39,39,39	0
60	MG	CA	3553	1/1	0.97	0.14	77,77,77,77	0
60	MG	DA	1603	1/1	0.97	0.07	52,52,52,52	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3446	1/1	0.97	0.24	37,37,37,37	0
60	MG	BA	1606	1/1	0.97	0.28	74,74,74,74	0
60	MG	CA	3008	1/1	0.97	0.39	52,52,52,52	0
60	MG	AA	3403	1/1	0.97	0.14	55,55,55,55	0
60	MG	AA	3318	1/1	0.97	0.16	64,64,64,64	0
60	MG	CA	3455	1/1	0.97	0.27	37,37,37,37	0
60	MG	AA	3506	1/1	0.97	0.20	19,19,19,19	0
60	MG	CA	3003	1/1	0.97	0.31	49,49,49,49	0
60	MG	BL	202	1/1	0.97	0.14	56,56,56,56	0
60	MG	CY	502	1/1	0.97	0.14	53,53,53,53	0
60	MG	BA	1734	1/1	0.97	0.13	35,35,35,35	0
60	MG	CA	3192	1/1	0.97	0.26	47,47,47,47	0
60	MG	AA	3399	1/1	0.97	0.24	51,51,51,51	0
60	MG	CA	3439	1/1	0.97	0.23	47,47,47,47	0
60	MG	AA	3643	1/1	0.97	0.14	56,56,56,56	0
60	MG	AA	3505	1/1	0.97	0.23	29,29,29,29	0
60	MG	CA	3157	1/1	0.97	0.23	56,56,56,56	0
60	MG	AA	3668	1/1	0.97	0.10	25,25,25,25	0
60	MG	CA	3324	1/1	0.97	0.22	31,31,31,31	0
60	MG	CA	3028	1/1	0.97	0.64	60,60,60,60	0
60	MG	AA	3555	1/1	0.97	0.16	57,57,57,57	0
60	MG	AA	3411	1/1	0.97	0.15	21,21,21,21	0
60	MG	CO	202	1/1	0.97	0.13	53,53,53,53	0
60	MG	AX	101	1/1	0.97	0.11	37,37,37,37	0
60	MG	DA	1708	1/1	0.97	0.10	67,67,67,67	0
60	MG	BA	1686	1/1	0.97	0.25	58,58,58,58	0
60	MG	AA	3733	1/1	0.97	0.13	40,40,40,40	0
60	MG	AA	3496	1/1	0.97	0.05	43,43,43,43	0
60	MG	BA	1743	1/1	0.97	0.08	60,60,60,60	0
60	MG	BA	1727	1/1	0.97	0.28	53,53,53,53	0
60	MG	AB	3012	1/1	0.97	0.14	24,24,24,24	1
60	MG	CA	3120	1/1	0.97	0.12	47,47,47,47	0
60	MG	AA	3560	1/1	0.97	0.20	49,49,49,49	0
60	MG	CA	3449	1/1	0.97	0.21	52,52,52,52	0
60	MG	AA	3423	1/1	0.97	0.22	53,53,53,53	0
60	MG	AA	3359	1/1	0.97	0.18	31,31,31,31	0
60	MG	CA	3381	1/1	0.97	0.22	37,37,37,37	0
60	MG	AF	305	1/1	0.97	0.09	48,48,48,48	0
60	MG	AA	3584	1/1	0.97	0.12	63,63,63,63	0
60	MG	CA	3258	1/1	0.97	0.17	54,54,54,54	0
64	GDP	BZ	702	28/28	0.97	0.14	57,57,57,57	1
60	MG	CA	3651	1/1	0.97	0.17	41,41,41,41	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3576	1/1	0.97	0.29	49,49,49,49	0
60	MG	DZ	701	1/1	0.97	0.24	47,47,47,47	0
60	MG	AA	3185	1/1	0.97	0.20	35,35,35,35	0
60	MG	AA	3669	1/1	0.97	0.21	36,36,36,36	0
60	MG	AA	3350	1/1	0.97	0.16	54,54,54,54	0
60	MG	CA	3368	1/1	0.97	0.12	45,45,45,45	0
60	MG	AE	303	1/1	0.97	0.19	23,23,23,23	0
60	MG	AA	3045	1/1	0.97	0.33	58,58,58,58	0
60	MG	CA	3415	1/1	0.97	0.18	43,43,43,43	0
60	MG	AA	3833	1/1	0.97	0.25	39,39,39,39	0
60	MG	AA	3405	1/1	0.97	0.15	27,27,27,27	0
60	MG	BA	1810	1/1	0.97	0.13	39,39,39,39	0
60	MG	AA	3790	1/1	0.97	0.23	11,11,11,11	0
60	MG	AA	3011	1/1	0.97	0.10	27,27,27,27	0
60	MG	CA	3522	1/1	0.97	0.24	25,25,25,25	0
60	MG	CA	3399	1/1	0.97	0.18	45,45,45,45	0
60	MG	DA	1625	1/1	0.97	0.12	38,38,38,38	0
60	MG	AD	304	1/1	0.97	0.34	49,49,49,49	0
60	MG	DA	1731	1/1	0.97	0.20	51,51,51,51	0
60	MG	AA	3400	1/1	0.97	0.07	19,19,19,19	0
60	MG	BA	1611	1/1	0.97	0.09	31,31,31,31	0
60	MG	AA	3717	1/1	0.97	0.23	47,47,47,47	0
60	MG	DA	1653	1/1	0.97	0.08	29,29,29,29	0
60	MG	AA	3703	1/1	0.97	0.07	76,76,76,76	0
60	MG	AA	3527	1/1	0.97	0.16	20,20,20,20	0
60	MG	AD	301	1/1	0.97	0.34	46,46,46,46	0
60	MG	BA	1729	1/1	0.97	0.13	38,38,38,38	0
60	MG	AA	3128	1/1	0.97	0.46	53,53,53,53	1
60	MG	AA	3514	1/1	0.97	0.21	32,32,32,32	0
60	MG	AA	3115	1/1	0.97	0.47	44,44,44,44	0
60	MG	AA	3189	1/1	0.97	0.26	31,31,31,31	0
60	MG	BA	1747	1/1	0.97	0.14	53,53,53,53	0
60	MG	AD	308	1/1	0.97	0.36	49,49,49,49	0
60	MG	CF	304	1/1	0.97	0.15	46,46,46,46	0
60	MG	AA	3673	1/1	0.97	0.24	58,58,58,58	0
60	MG	AA	3116	1/1	0.97	0.32	36,36,36,36	0
60	MG	CA	3547	1/1	0.97	0.06	57,57,57,57	1
60	MG	AA	3597	1/1	0.97	0.12	58,58,58,58	0
60	MG	AA	3628	1/1	0.97	0.18	62,62,62,62	0
60	MG	AA	3532	1/1	0.97	0.18	20,20,20,20	0
60	MG	AA	3290	1/1	0.97	0.16	78,78,78,78	0
60	MG	CA	3279	1/1	0.97	0.26	46,46,46,46	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3169	1/1	0.97	0.26	36,36,36,36	0
60	MG	CA	3224	1/1	0.97	0.18	32,32,32,32	0
60	MG	AA	3386	1/1	0.97	0.21	19,19,19,19	0
60	MG	AA	3126	1/1	0.97	0.24	68,68,68,68	0
60	MG	AA	3042	1/1	0.97	0.20	43,43,43,43	0
60	MG	AA	3397	1/1	0.97	0.36	41,41,41,41	0
60	MG	CA	3099	1/1	0.97	0.46	55,55,55,55	0
60	MG	CA	3541	1/1	0.97	0.34	58,58,58,58	0
60	MG	AA	3617	1/1	0.97	0.12	32,32,32,32	0
60	MG	CA	3004	1/1	0.97	0.18	43,43,43,43	0
60	MG	AA	3409	1/1	0.97	0.19	51,51,51,51	0
60	MG	AA	3453	1/1	0.97	0.11	51,51,51,51	0
60	MG	CA	3451	1/1	0.97	0.12	78,78,78,78	0
60	MG	CA	3137	1/1	0.97	0.18	64,64,64,64	0
60	MG	AA	3374	1/1	0.97	0.15	22,22,22,22	0
60	MG	CA	3161	1/1	0.97	0.44	45,45,45,45	0
60	MG	AA	3076	1/1	0.97	0.13	6,6,6,6	0
60	MG	CA	3559	1/1	0.97	0.14	30,30,30,30	0
60	MG	CA	3438	1/1	0.97	0.29	45,45,45,45	0
60	MG	AA	3335	1/1	0.97	0.19	14,14,14,14	0
60	MG	AA	3603	1/1	0.97	0.10	68,68,68,68	0
60	MG	CA	3639	1/1	0.97	0.31	54,54,54,54	0
60	MG	AA	3404	1/1	0.97	0.10	50,50,50,50	0
60	MG	CA	3182	1/1	0.97	0.58	45,45,45,45	0
60	MG	AA	3103	1/1	0.97	0.12	11,11,11,11	0
60	MG	A0	102	1/1	0.97	0.06	41,41,41,41	0
60	MG	CA	3171	1/1	0.97	0.43	48,48,48,48	0
60	MG	CA	3006	1/1	0.97	0.09	24,24,24,24	0
60	MG	AP	201	1/1	0.97	0.31	35,35,35,35	0
60	MG	BA	1780	1/1	0.97	0.07	44,44,44,44	0
60	MG	AA	3065	1/1	0.97	0.41	51,51,51,51	0
60	MG	AA	3144	1/1	0.97	0.49	48,48,48,48	0
60	MG	CA	3285	1/1	0.97	0.07	41,41,41,41	0
60	MG	DA	1647	1/1	0.97	0.14	39,39,39,39	0
60	MG	AA	3232	1/1	0.97	0.22	58,58,58,58	0
60	MG	AA	3786	1/1	0.97	0.19	57,57,57,57	0
60	MG	AA	3565	1/1	0.97	0.21	26,26,26,26	0
60	MG	AA	3718	1/1	0.97	0.14	40,40,40,40	0
60	MG	AA	3196	1/1	0.97	0.34	48,48,48,48	0
60	MG	BA	1764	1/1	0.97	0.16	55,55,55,55	0
60	MG	CA	3320	1/1	0.97	0.25	47,47,47,47	0
60	MG	AA	3430	1/1	0.97	0.24	23,23,23,23	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3330	1/1	0.97	0.21	33,33,33,33	0
60	MG	DA	1703	1/1	0.98	0.06	59,59,59,59	0
60	MG	AA	3819	1/1	0.98	0.37	46,46,46,46	0
60	MG	AB	3002	1/1	0.98	0.22	55,55,55,55	0
60	MG	CA	3432	1/1	0.98	0.13	29,29,29,29	0
60	MG	AA	3082	1/1	0.98	0.58	57,57,57,57	1
60	MG	CA	3277	1/1	0.98	0.18	43,43,43,43	0
60	MG	AA	3037	1/1	0.98	0.12	12,12,12,12	0
60	MG	AA	3007	1/1	0.98	0.10	18,18,18,18	0
60	MG	AA	3723	1/1	0.98	0.16	30,30,30,30	0
60	MG	AA	3818	1/1	0.98	0.36	46,46,46,46	0
60	MG	CA	3422	1/1	0.98	0.18	43,43,43,43	0
60	MG	CA	3600	1/1	0.98	0.12	60,60,60,60	0
60	MG	BA	1795	1/1	0.98	0.15	64,64,64,64	0
60	MG	AA	3053	1/1	0.98	0.15	21,21,21,21	0
60	MG	CA	3174	1/1	0.98	0.12	31,31,31,31	0
60	MG	AA	3319	1/1	0.98	0.17	28,28,28,28	0
60	MG	AA	3371	1/1	0.98	0.07	21,21,21,21	0
60	MG	CA	3307	1/1	0.98	0.21	31,31,31,31	0
60	MG	CA	3400	1/1	0.98	0.10	48,48,48,48	0
60	MG	BA	1765	1/1	0.98	0.29	67,67,67,67	0
60	MG	AA	3306	1/1	0.98	0.14	3,3,3,3	0
60	MG	AA	3574	1/1	0.98	0.15	26,26,26,26	0
60	MG	AA	3023	1/1	0.98	0.46	40,40,40,40	1
60	MG	AA	3826	1/1	0.98	0.22	56,56,56,56	0
60	MG	AA	3124	1/1	0.98	0.24	39,39,39,39	1
60	MG	DA	1669	1/1	0.98	0.20	63,63,63,63	0
60	MG	CA	3476	1/1	0.98	0.22	60,60,60,60	0
60	MG	AA	3301	1/1	0.98	0.17	59,59,59,59	0
60	MG	AA	3731	1/1	0.98	0.14	34,34,34,34	0
60	MG	CA	3461	1/1	0.98	0.10	46,46,46,46	0
60	MG	BA	1769	1/1	0.98	0.26	80,80,80,80	0
60	MG	AA	3008	1/1	0.98	0.17	28,28,28,28	0
60	MG	AA	3224	1/1	0.98	0.19	26,26,26,26	0
62	ZN	CY	501	1/1	0.98	0.05	92,92,92,92	0
60	MG	CA	3294	1/1	0.98	0.31	40,40,40,40	0
60	MG	CA	3466	1/1	0.98	0.14	56,56,56,56	0
60	MG	AA	3363	1/1	0.98	0.24	47,47,47,47	0
60	MG	CA	3017	1/1	0.98	0.15	28,28,28,28	0
60	MG	CA	3352	1/1	0.98	0.23	40,40,40,40	0
60	MG	DA	1616	1/1	0.98	0.41	44,44,44,44	0
60	MG	AA	3328	1/1	0.98	0.22	21,21,21,21	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	DA	1652	1/1	0.98	0.09	68,68,68,68	0
60	MG	AQ	3003	1/1	0.98	0.34	37,37,37,37	0
60	MG	CA	3340	1/1	0.98	0.13	38,38,38,38	0
60	MG	DA	1612	1/1	0.98	0.13	46,46,46,46	0
60	MG	CA	3166	1/1	0.98	0.20	31,31,31,31	0
60	MG	AA	3583	1/1	0.98	0.12	18,18,18,18	0
60	MG	AA	3149	1/1	0.98	0.25	15,15,15,15	0
60	MG	AA	3523	1/1	0.98	0.17	35,35,35,35	0
60	MG	AA	3641	1/1	0.98	0.14	45,45,45,45	0
60	MG	CA	3567	1/1	0.98	0.12	42,42,42,42	0
60	MG	CA	3259	1/1	0.98	0.17	19,19,19,19	0
60	MG	AA	3470	1/1	0.98	0.13	24,24,24,24	0
60	MG	AA	3031	1/1	0.98	0.25	29,29,29,29	1
60	MG	CA	3193	1/1	0.98	0.36	47,47,47,47	0
60	MG	BA	1639	1/1	0.98	0.37	42,42,42,42	0
60	MG	CA	3450	1/1	0.98	0.24	38,38,38,38	0
60	MG	AA	3286	1/1	0.98	0.25	48,48,48,48	0
60	MG	BA	1778	1/1	0.98	0.26	52,52,52,52	0
60	MG	AA	3427	1/1	0.98	0.12	34,34,34,34	0
60	MG	AA	3616	1/1	0.98	0.10	33,33,33,33	0
63	SF4	DD	501	8/8	0.98	0.11	71,71,71,71	0
60	MG	CA	3347	1/1	0.98	0.14	37,37,37,37	0
60	MG	CN	5001	1/1	0.98	0.10	64,64,64,64	0
60	MG	CA	3223	1/1	0.98	0.18	46,46,46,46	0
60	MG	AA	3485	1/1	0.98	0.17	34,34,34,34	0
60	MG	AA	3410	1/1	0.98	0.13	19,19,19,19	0
60	MG	BA	1721	1/1	0.98	0.26	60,60,60,60	0
60	MG	AA	3166	1/1	0.98	0.12	52,52,52,52	0
60	MG	CA	3027	1/1	0.98	0.05	29,29,29,29	0
60	MG	AG	201	1/1	0.98	0.05	41,41,41,41	0
60	MG	CA	3178	1/1	0.98	0.21	54,54,54,54	0
60	MG	AA	3395	1/1	0.98	0.14	21,21,21,21	0
60	MG	AA	3508	1/1	0.98	0.13	42,42,42,42	0
60	MG	CA	3313	1/1	0.98	0.14	54,54,54,54	0
60	MG	CA	3186	1/1	0.98	0.07	49,49,49,49	0
60	MG	AA	3218	1/1	0.98	0.20	10,10,10,10	0
60	MG	AA	3112	1/1	0.98	0.36	44,44,44,44	0
60	MG	CA	3159	1/1	0.98	0.42	42,42,42,42	0
62	ZN	BN	501	1/1	0.98	0.09	83,83,83,83	0
62	ZN	C6	501	1/1	0.98	0.09	66,66,66,66	0
60	MG	DA	1766	1/1	0.98	0.07	41,41,41,41	0
60	MG	CA	3211	1/1	0.98	0.14	19,19,19,19	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3296	1/1	0.98	0.27	40,40,40,40	0
60	MG	CA	3454	1/1	0.98	0.23	43,43,43,43	0
60	MG	DA	1740	1/1	0.98	0.17	56,56,56,56	0
60	MG	AA	3244	1/1	0.98	0.40	42,42,42,42	0
60	MG	AA	3737	1/1	0.98	0.15	25,25,25,25	0
60	MG	AA	3660	1/1	0.98	0.34	58,58,58,58	0
60	MG	CA	3632	1/1	0.98	0.15	55,55,55,55	0
60	MG	CB	3003	1/1	0.98	0.13	61,61,61,61	0
60	MG	AB	3007	1/1	0.98	0.07	37,37,37,37	0
60	MG	DA	1645	1/1	0.98	0.34	58,58,58,58	0
60	MG	CA	3625	1/1	0.98	0.22	46,46,46,46	0
60	MG	DA	1643	1/1	0.98	0.14	51,51,51,51	0
62	ZN	C9	501	1/1	0.99	0.07	70,70,70,70	0
60	MG	AA	3796	1/1	0.99	0.24	45,45,45,45	0
60	MG	AA	3396	1/1	0.99	0.14	22,22,22,22	0
60	MG	AO	5001	1/1	0.99	0.10	43,43,43,43	0
60	MG	BA	1714	1/1	0.99	0.17	44,44,44,44	0
60	MG	AA	3706	1/1	0.99	0.35	26,26,26,26	1
60	MG	AA	3212	1/1	0.99	0.40	43,43,43,43	0
60	MG	CA	3336	1/1	0.99	0.12	64,64,64,64	0
60	MG	AA	3361	1/1	0.99	0.17	33,33,33,33	0
60	MG	AA	3520	1/1	0.99	0.15	34,34,34,34	0
60	MG	AA	3677	1/1	0.99	0.20	26,26,26,26	0
62	ZN	A6	102	1/1	0.99	0.10	47,47,47,47	0
60	MG	AA	3465	1/1	0.99	0.05	49,49,49,49	0
60	MG	AA	3304	1/1	0.99	0.17	44,44,44,44	0
60	MG	AA	3750	1/1	0.99	0.10	26,26,26,26	0
60	MG	AA	3178	1/1	0.99	0.43	50,50,50,50	0
60	MG	AA	3227	1/1	0.99	0.25	75,75,75,75	0
60	MG	CA	3158	1/1	0.99	0.33	54,54,54,54	0
60	MG	CA	3385	1/1	0.99	0.26	48,48,48,48	0
60	MG	BA	1749	1/1	0.99	0.27	52,52,52,52	0
60	MG	AA	3456	1/1	0.99	0.13	64,64,64,64	0
60	MG	AA	3709	1/1	0.99	0.47	39,39,39,39	0
60	MG	AA	3415	1/1	0.99	0.20	29,29,29,29	0
62	ZN	A9	501	1/1	0.99	0.11	45,45,45,45	0
60	MG	CA	3306	1/1	0.99	0.11	39,39,39,39	0
60	MG	BA	1775	1/1	0.99	0.22	47,47,47,47	0
60	MG	CA	3370	1/1	0.99	0.13	31,31,31,31	0
60	MG	AA	3148	1/1	0.99	0.24	48,48,48,48	0
62	ZN	AY	501	1/1	0.99	0.06	68,68,68,68	0
63	SF4	BD	501	8/8	0.99	0.11	67,67,67,67	0

*Continued on next page...*



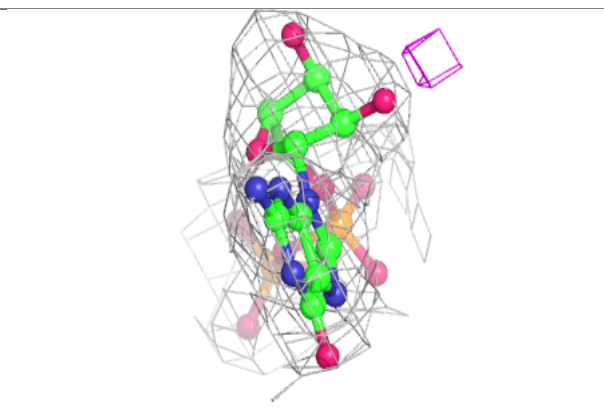
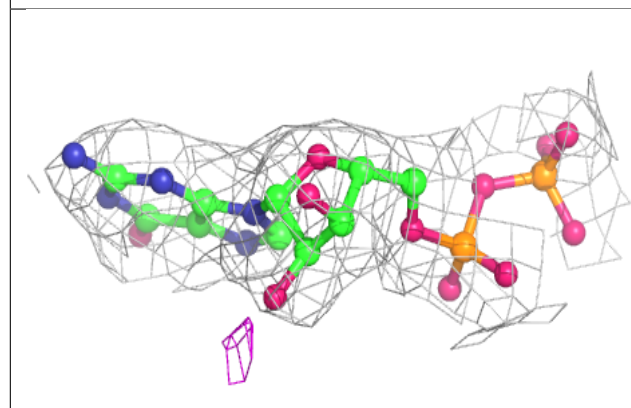
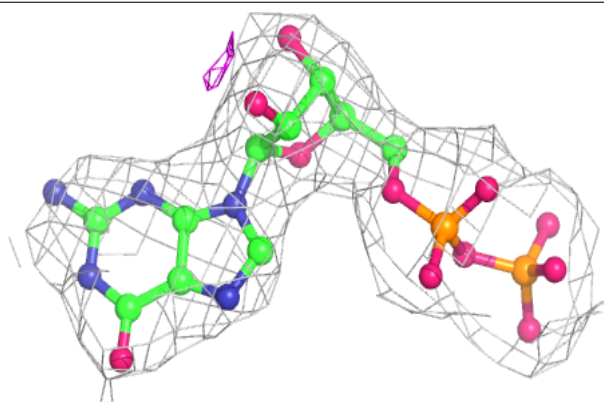
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3097	1/1	0.99	0.25	29,29,29,29	0
60	MG	AA	3340	1/1	0.99	0.10	3,3,3,3	0
62	ZN	C5	102	1/1	0.99	0.07	66,66,66,66	0
60	MG	CA	3337	1/1	0.99	0.13	27,27,27,27	0
60	MG	AA	3471	1/1	0.99	0.18	24,24,24,24	0
60	MG	AA	3432	1/1	0.99	0.16	24,24,24,24	0
62	ZN	A5	101	1/1	1.00	0.12	40,40,40,40	0

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

**Electron density around GDP DZ 702:**

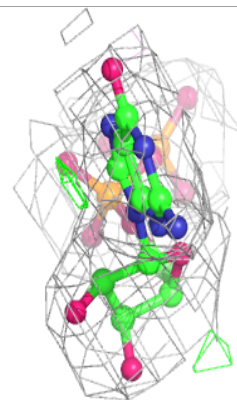
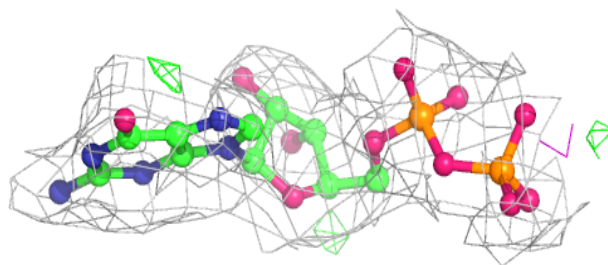
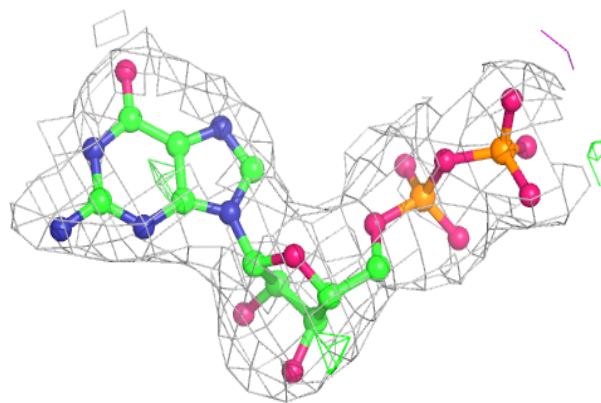
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around GDP BZ 702:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.