wwPDB X-ray Structure Validation Summary Report (i)

Aug 3, 2026 – 04:42 PM EDT

PDB ID	:	4WQU / pdb_00004wqu
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with elongation factor G trapped by the antibiotic dityromycin
Authors	:	Lin, J.; Gagnon, M.G.; Steitz, T.A.
Deposited on	:	2014-10-22
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

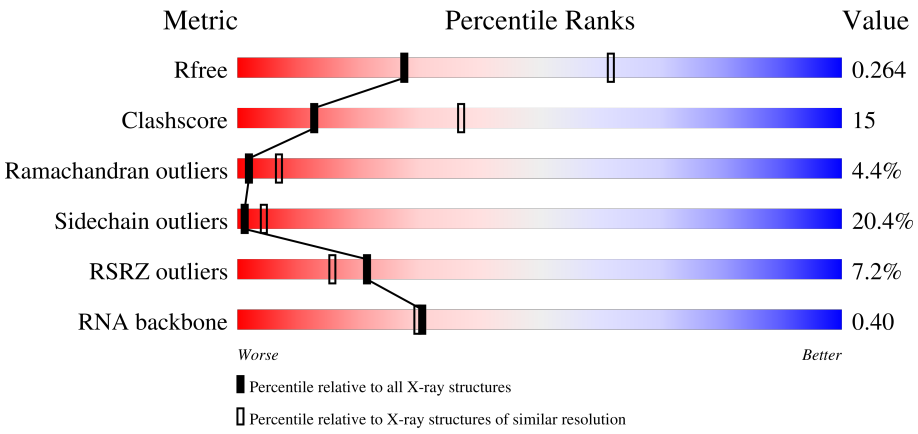
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	%, 56%, 34%, 9%
1	CA	2915	2%, 47%, 42%, 10%
2	AB	121	%, 66%, 31%
2	CB	121	4%, 39%, 50%, 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AC	228	41% 21% 28% 10% • 40%
3	CC	228	43% 19% 29% 10% • 40%
4	AD	276	% 55% 33% 10% •
4	CD	276	% 53% 33% 13% •
5	AE	206	53% 33% 13% •
5	CE	206	% 45% 40% 13% ••
6	AF	210	50% 36% 9% • •
6	CF	210	% 41% 44% 10% •
7	AG	182	% 49% 36% 12% • •
7	CG	182	15% 41% 48% 11% •
8	AH	180	% 43% 41% 12% • •
8	CH	180	8% 41% 45% 11% •
9	AK	173	20% 44% 25% 6% 25%
9	CK	173	31% 53% 17% 5% 25%
10	AL	147	15% 18% 22% • • 55%
10	CL	147	26% 18% 17% 10% 55%
11	AN	140	% 61% 27% 11% •
11	CN	140	% 45% 40% 14% •
12	AO	122	57% 33% 10%
12	CO	122	58% 36% 6%
13	AP	150	56% 31% 12% ••
13	CP	150	4% 55% 33% 11% ••
14	AQ	141	57% 35% 8%
14	CQ	141	2% 50% 37% 11% •
15	AR	118	54% 32% 13% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	CR	118	56% 32% 12%
16	AS	112	% 46% 39% 13% •
16	CS	112	18% 22% 62% 13% •
17	AT	146	3% 42% 35% 12% 10%
17	CT	146	2% 47% 34% 9% 10%
18	AU	118	57% 32% 9% •
18	CU	118	55% 33% 10% •
19	AV	101	64% 30% 6%
19	CV	101	% 58% 33% 8% •
20	AW	113	58% 30% 9% • •
20	CW	113	55% 35% 9% • •
21	AX	96	% 63% 26% 9% • •
21	CX	96	6% 48% 41% 9% • •
22	AY	110	2% 48% 35% 11% • •
22	CY	110	6% 34% 52% 10% • •
23	AZ	206	% 42% 33% 13% • 10%
23	CZ	206	4% 35% 39% 13% • 10%
24	A0	85	% 64% 16% 11% 9%
24	C0	85	8% 45% 34% 9% • 9%
25	A1	98	% 51% 37% 8% • •
25	C1	98	3% 53% 35% 11% •
26	A2	72	3% 58% 32% 7% •
26	C2	72	4% 35% 50% 12% •
27	A3	60	2% 53% 33% 12% •
27	C3	60	3% 45% 37% 17% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	A4	71	11% 34% 48% 15%
28	C4	71	15% 35% 46% 15%
29	A5	60	62% 28% 8%
29	C5	60	52% 40% 7%
30	A6	54	39% 52% 7%
30	C6	54	44% 39% 15%
31	A7	49	4% 51% 37% 8%
31	C7	49	8% 51% 39% 8%
32	A8	65	46% 40% 11%
32	C8	65	2% 46% 49%
33	A9	37	3% 46% 43% 11%
33	C9	37	3% 46% 49% 5%
34	BA	1521	2% 38% 49% 11%
34	DA	1521	4% 38% 48% 13%
35	BB	256	9% 42% 35% 12% 10%
35	DB	256	18% 39% 37% 13% 10%
36	BC	239	12% 47% 32% 6% 14%
36	DC	239	22% 42% 38% 7% 14%
37	BD	209	18% 52% 35% 11%
37	DD	209	14% 44% 42% 12%
38	BE	162	% 44% 35% 11% 9%
38	DE	162	8% 33% 41% 16% 9%
39	BF	101	% 48% 37% 15%
39	DF	101	3% 50% 42% 7%
40	BG	156	11% 51% 35% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	DG	156	14% 51% 41% 8% •
41	BH	138	5% 42% 43% 13% ••
41	DH	138	9% 38% 43% 14% • •
42	BI	128	30% 50% 41% 8% •
42	DI	128	46% 49% 37% 12% ••
43	BJ	105	30% 44% 43% 5% • 8%
43	DJ	105	43% 50% 35% 6% 9%
44	BK	129	% 49% 32% 6% • 12%
44	DK	129	7% 49% 32% 7% • 12%
45	BL	132	4% 54% 32% 7% 8%
45	DL	132	4% 48% 33% 11% 8%
46	BM	126	10% 52% 31% 10% 7%
46	DM	126	27% 44% 36% 13% 8%
47	BN	61	25% 36% 52% 10% •
47	DN	61	57% 33% 57% 8% •
48	BO	89	6% 45% 46% 8% •
48	DO	89	3% 47% 42% 10% •
49	BP	88	11% 33% 36% 23% • 7%
49	DP	88	5% 36% 40% 16% • 7%
50	BQ	105	5% 48% 34% 11% • 6%
50	DQ	105	11% 45% 41% 9% 6%
51	BR	88	% 31% 39% 8% 23%
51	DR	88	% 39% 32% 6% • 23%
52	BS	93	29% 43% 32% 15% 10%
52	DS	93	40% 47% 33% 9% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	BT	106	9% 37% 43% 8% 9%
53	DT	106	8% 51% 30% 9% 9%
54	BU	27	41% 52% 33% 15%
54	DU	27	41% 37% 41% 7% 15%
55	BV	18	17% 22% 11% 6% 61%
55	DV	18	17% 22% 11% 67%
56	BW	76	4% 42% 42% 16%
56	BY	76	16% 39% 36% 22%
56	DW	76	39% 43% 12% 5%
56	DY	76	18% 33% 47% 13%
57	BZ	758	9% 42% 39% 14%
57	DZ	758	12% 45% 38% 12%
58	BX	10	20% 70% 10%
58	DX	10	10% 10% 10% 80%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	2QY	DX	10	-	-	X	-
59	MG	AA	3056	-	-	-	X
59	MG	AA	3093	-	-	-	X
59	MG	AA	3108	-	-	-	X
59	MG	AA	3717	-	-	-	X
59	MG	AA	3773	-	-	-	X
59	MG	DA	1611	-	-	-	X
61	SF4	DD	501	-	-	X	-

2 Entry composition (i)

There are 63 unique types of molecules in this entry. The entry contains 310038 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AA	2872	61861	27532	11574	19884	2871	0	0	0
1	CA	2868	61771	27492	11554	19858	2867	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 55 is a RNA chain called mRNA.

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

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

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

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

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

- Molecule 58 is a protein called Dityromycin.

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

- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

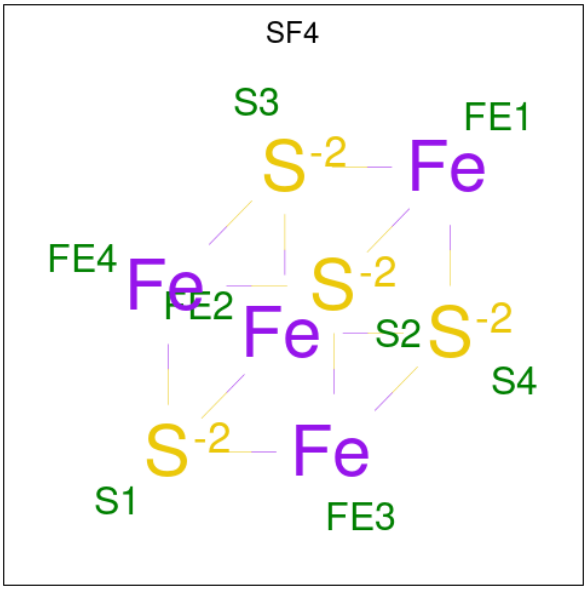
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
60	AY	1	1	1	0	0
			Total	Zn		
60	A4	1	1	1	0	0
			Total	Zn		
60	A5	1	1	1	0	0
			Total	Zn		
60	A6	1	1	1	0	0
			Total	Zn		
60	A9	1	1	1	0	0
			Total	Zn		
60	BN	1	1	1	0	0
			Total	Zn		
60	CY	1	1	1	0	0
			Total	Zn		
60	C4	1	1	1	0	0
			Total	Zn		
60	C5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

Continued on next page...

Continued from previous page...

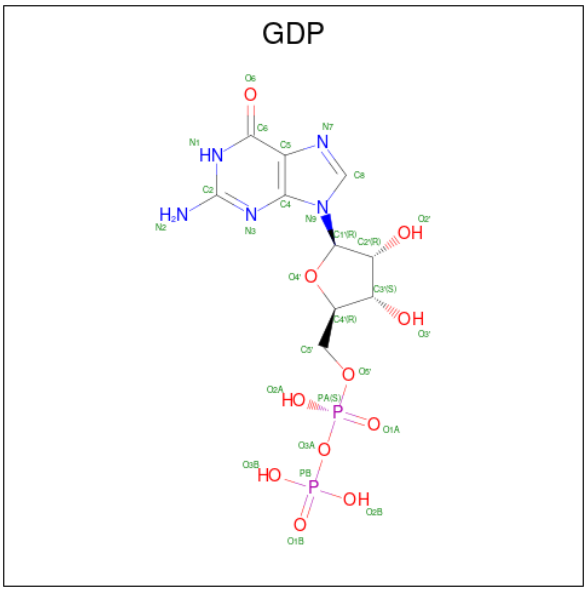
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
60	DN	1	1	1	0	0

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



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

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 63 is water.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

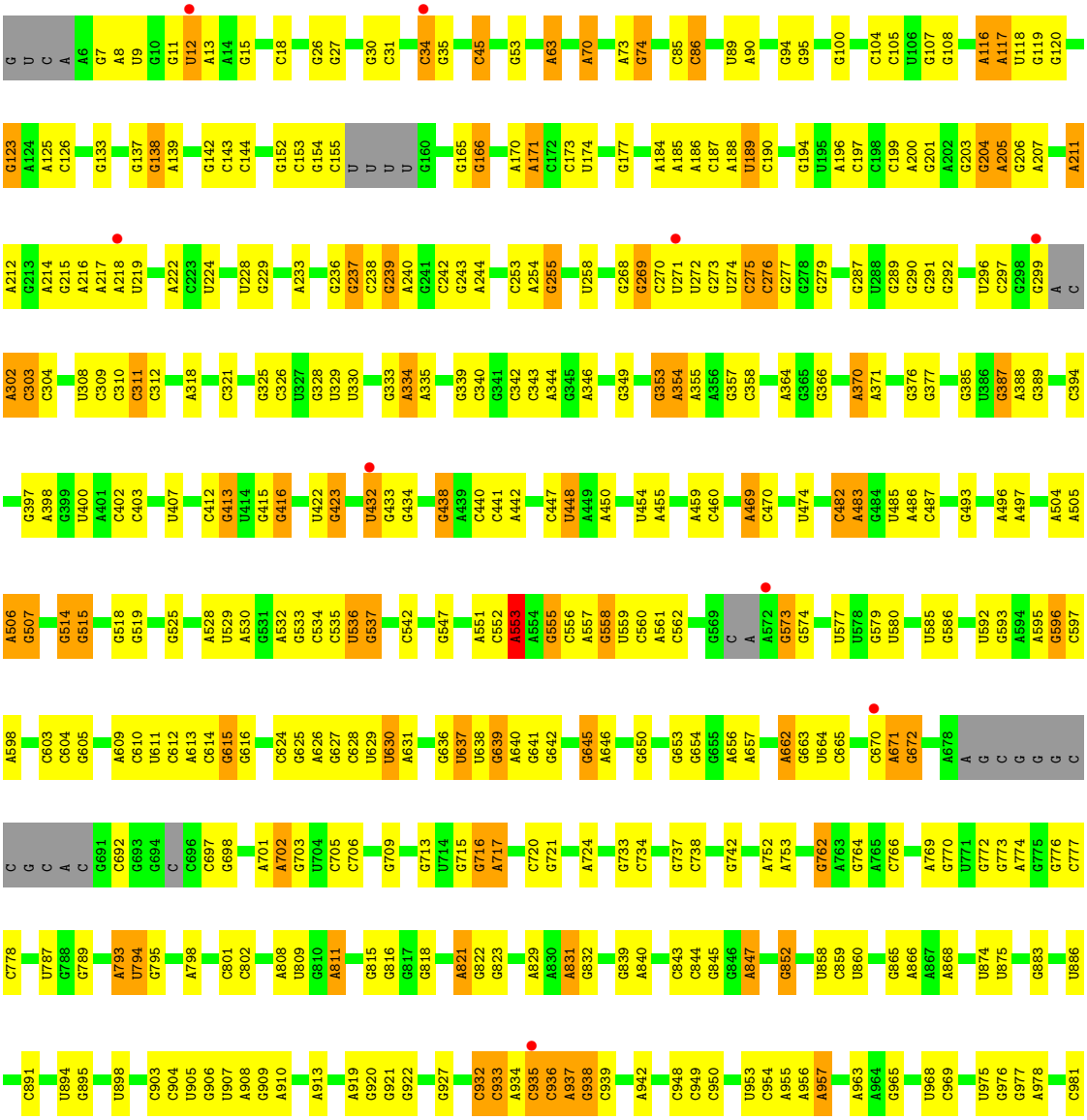
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	C5	1	Total O 1 1	0	0
63	C7	2	Total O 2 2	0	0
63	C8	4	Total O 4 4	0	0
63	DA	157	Total O 157 157	0	0
63	DD	1	Total O 1 1	0	0
63	DE	2	Total O 2 2	0	0
63	DH	1	Total O 1 1	0	0
63	DJ	1	Total O 1 1	0	0
63	DK	2	Total O 2 2	0	0
63	DL	1	Total O 1 1	0	0
63	DT	1	Total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

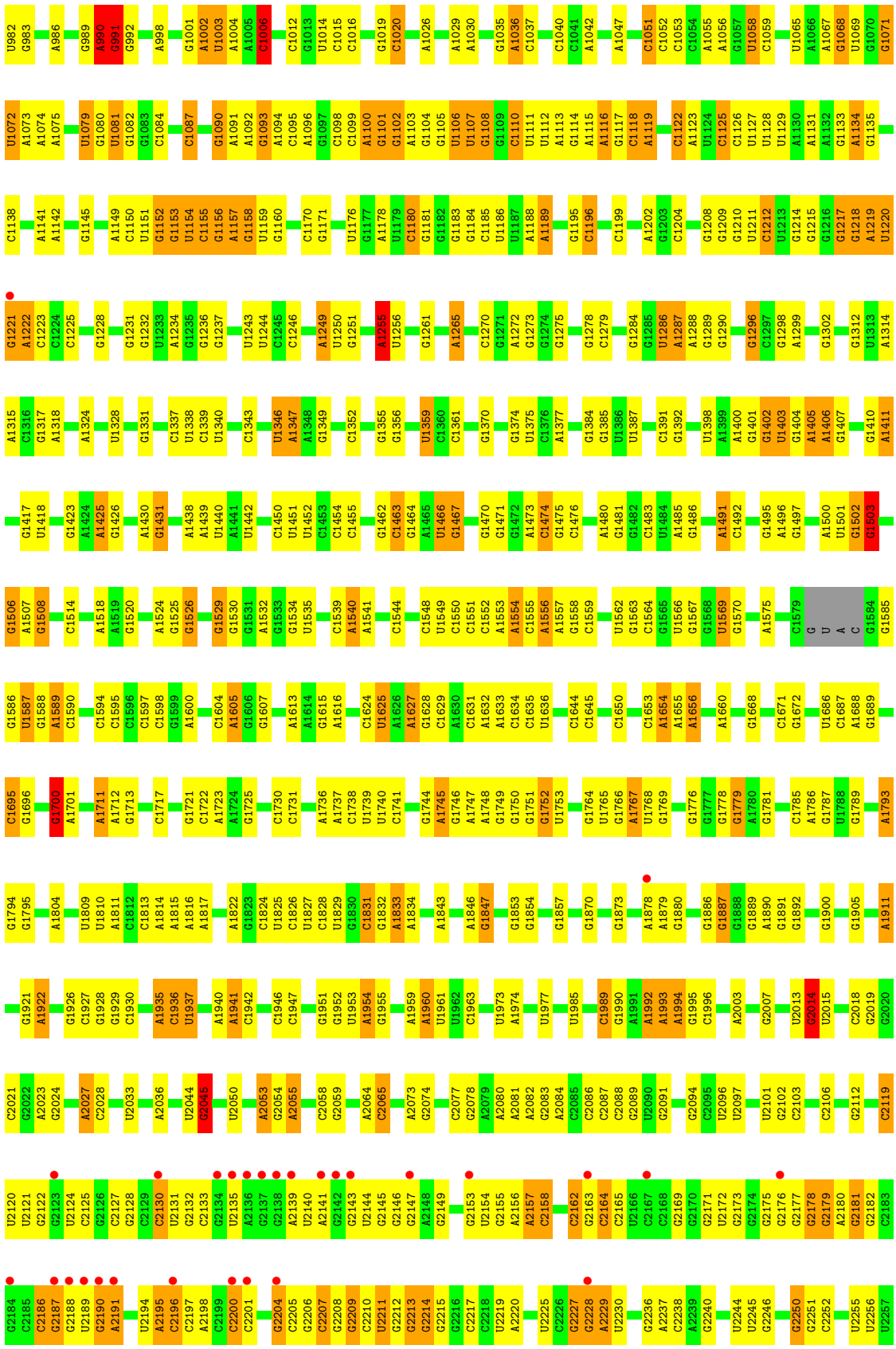
3 Residue-property plots (i)

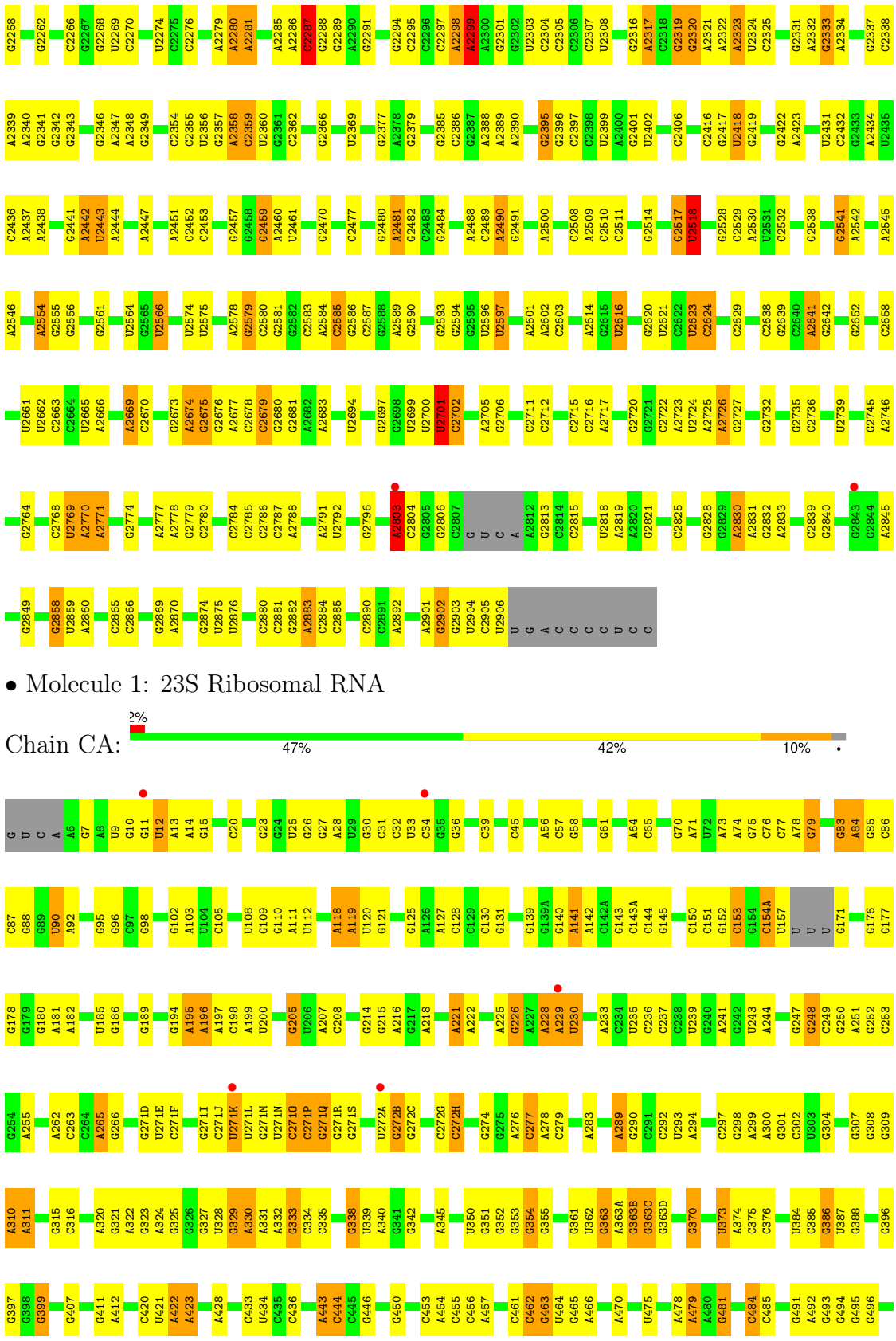
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23S Ribosomal RNA

Chain AA:

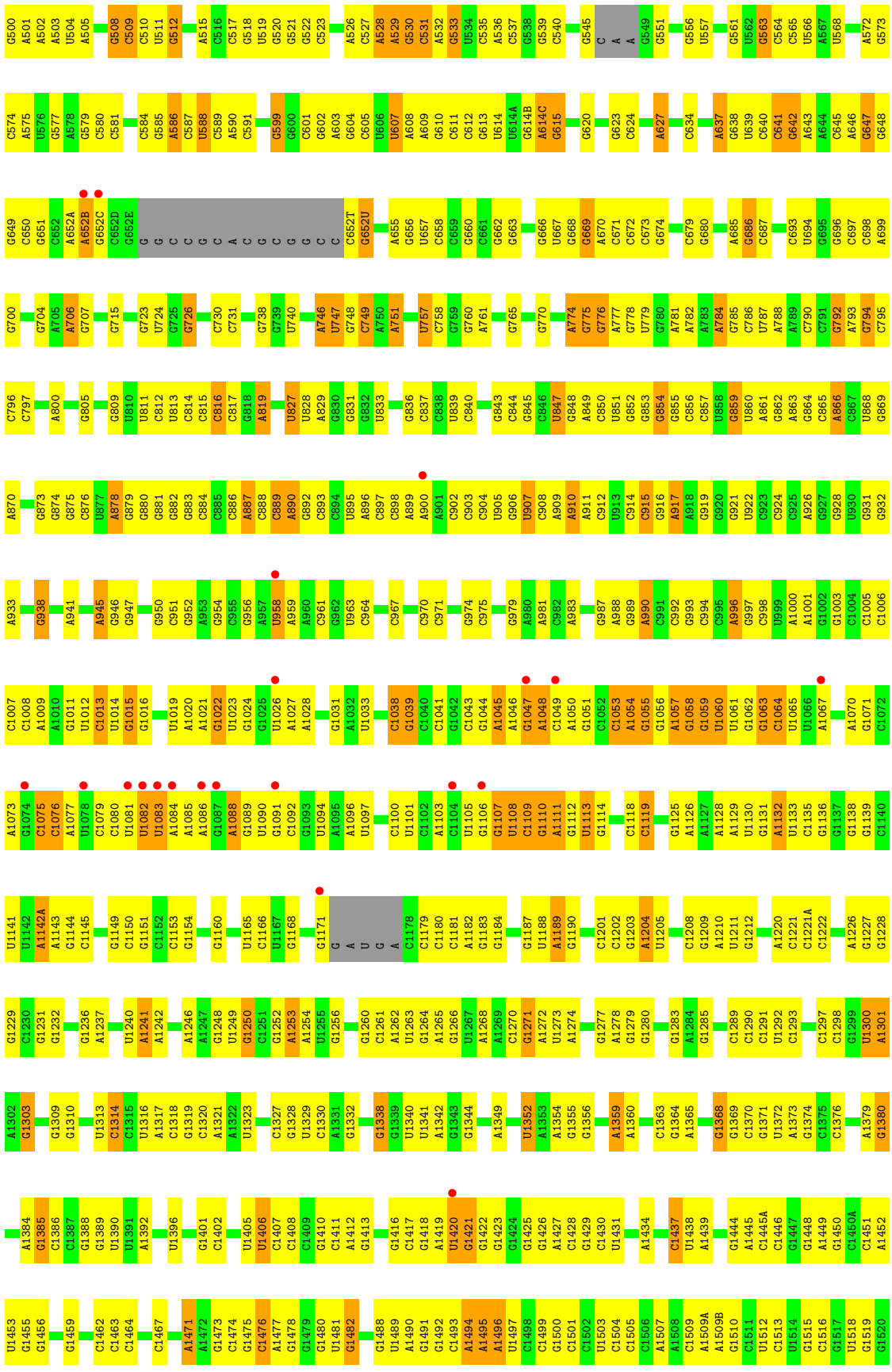


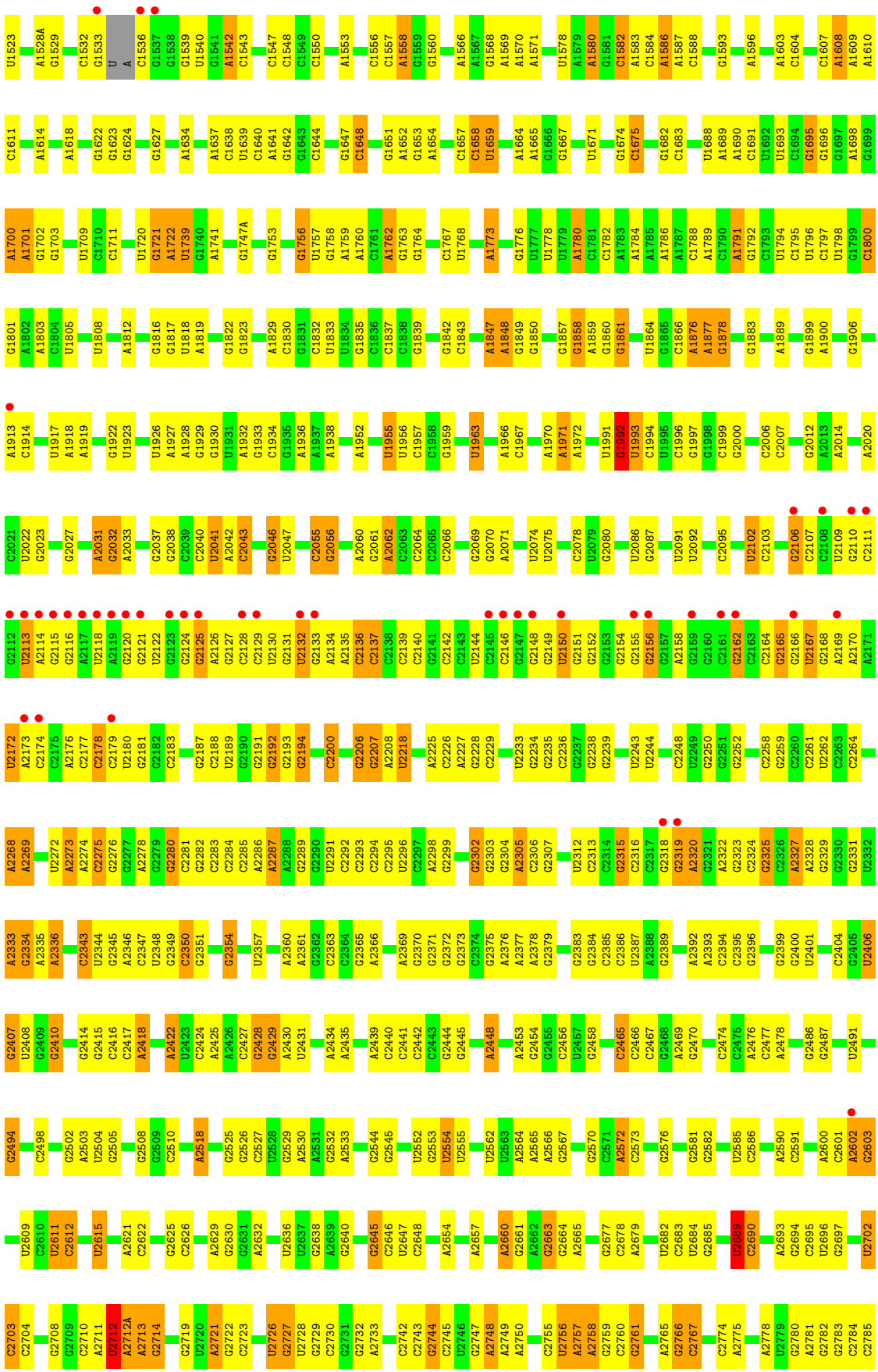

U982 G983 A986 G989 A990 G991 G992 A998 G1001 A1002 U1003 A1004 A1005 G1006 C1012 G1013 U1014 C1015 C1016 G1019 C1020 A1026 A1029 A1030 G1035 A1036 C1037 C1040 C1041 A1042 A1047 C1051 C1052 C1053 C1054 A1055 A1056 G1057 U1058 C1059 U1065 A1066 A1067 G1068 U1069 G1070 G1071
U1072 A1073 A1074 A1075 U1079 G1080 U1081 G1082 G1083 C1084 C1087 G1090 A1091 A1092 G1093 A1094 C1095 A1096 G1097 C1098 C1099 A1100 G1101 G1102 A1103 G1104 G1105 U1106 U1107 G1108 G1109 C1110 U1111 U1112 A1113 G1114 A1115 A1116 G1117 C1118 A1119 C1122 A1123 U1124 C1125 C1126 U1127 U1128 U1129 A1130 A1131 A1132 G1133 A1134 G1135
C1138 A1141 A1142 G1145 A1149 C1150 U1151 G1152 G1153 U1154 C1155 G1156 A1157 G1158 U1159 G1160 C1170 G1171 U1176 G1177 A1178 U1179 C1180 G1181 G1182 G1183 G1184 C1185 U1186 U1187 A1188 A1189 G1195 C1196 C1199 A1202 G1203 C1204 G1208 G1209 G1210 U1211 C1212 U1213 G1214 G1215 G1216 G1217 G1218 A1219 U1220
G1221 A1222 C1223 C1224 C1225 G1228 G1231 G1232 U1233 A1234 G1235 G1236 G1237 U1243 U1244 C1245 C1246 A1249 U1250 G1251 A1255 U1256 G1261 A1265 C1270 G1271 A1272 G1273 G1274 G1275 G1278 C1279 G1284 G1285 U1286 A1287 A1288 G1289 G1290 G1296 C1297 G1298 A1299 G1302 G1312 U1313 A1314
A1315 C1316 G1317 A1318 A1324 U1328 G1331 C1337 U1338 C1339 U1340 C1343 U1346 A1347 A1348 G1349 C1352 G1355 G1356 U1359 C1360 C1361 G1370 G1374 U1375 C1376 A1377 G1384 G1385 U1386 U1387 C1391 G1392 U1398 A1399 A1400 G1401 G1402 U1403 G1404 A1405 A1406 G1407 G1410 A1411
G1417 U1418 G1423 A1424 A1425 G1426 A1430 G1431 A1438 A1439 U1440 A1441 U1442 C1450 U1451 U1452 C1453 C1454 C1455 G1462 C1463 G1464 A1465 U1466 G1467 G1470 G1471 G1472 A1473 C1474 G1475 C1476 A1480 G1481 G1482 C1483 U1484 A1485 G1486 A1491 C1492 G1495 A1496 G1497 A1500 U1501 G1502 G1503
G1506 A1507 G1508 C1514 A1518 A1519 G1520 A1524 G1525 G1526 G1529 G1530 G1531 A1532 G1533 G1534 U1535 C1539 A1540 A1541 C1544 C1548 U1549 C1550 C1551 C1552 A1553 A1554 C1555 A1556 A1557 G1558 C1559 U1562 G1563 C1564 G1565 U1566 G1567 G1568 U1569 G1570 A1575 C1579 G U A C G1584 G1585
G1586 U1587 G1588 A1589 C1590 C1594 C1595 C1596 C1597 C1598 G1599 A1600 C1604 A1605 G1606 G1607 A1613 A1614 G1615 A1616 C1624 U1625 A1626 A1627 G1628 C1629 A1630 C1631 A1632 A1633 C1634 C1635 U1636 C1644 C1645 C1650 C1653 A1654 A1655 A1656 A1660 G1668 C1671 G1672 U1686 C1687 A1688 G1689
C1695 G1696 G1700 A1701 A1711 A1712 G1713 C1717 G1721 C1722 A1723 A1724 G1725 C1730 C1731 A1736 A1737 C1738 U1739 U1740 C1741 G1744 A1745 G1746 A1747 A1748 G1749 G1750 G1751 G1752 U1753 G1764 U1765 G1766 A1767 U1768 G1769 G1776 G1777 G1778 G1779 A1780 G1781 C1785 A1786 G1787 U1788 G1789 A1793
G1794 G1795 A1804 U1809 U1810 A1811 C1812 C1813 A1814 A1815 A1816 A1817 A1822 G1823 C1824 U1825 C1826 U1827 C1828 U1829 G1830 C1831 G1832 A1833 A1834 A1843 A1846 G1847 G1853 G1854 G1857 G1870 G1873 A1878 A1879 G1880 G1886 G1887 G1888 G1889 A1890 G1891 G1892 G1900 G1905 A1911
G1921 A1922 G1926 C1927 G1928 G1929 C1930 A1935 C1936 U1937 A1940 A1941 C1942 C1946 C1947 G1951 G1952 U1953 A1954 G1955 A1959 A1960 U1961 U1962 C1963 U1973 A1974 U1977 U1985 C1989 G1990 A1991 A1992 A1993 A1994 G1995 C1996 A2003 G2007 U2013 G2014 U2015 C2018 G2019 G2020
C2021 G2022 A2023 G2024 A2027 C2028 U2033 A2036 U2044 G2045 U2050 A2053 G2054 A2055 C2058 G2059 A2064 C2065 A2073 G2074 C2077 G2078 A2079 A2080 A2081 A2082 G2083 A2084 C2085 C2086 C2087 C2088 G2089 U2090 G2091 G2094 C2095 U2096 U2097 U2101 G2102 C2103 C2106 G2112 C2119
U2120 U2121 G2122 G2123 U2124 C2125 G2126 C2127 G2128 C2129 C2130 U2131 G2132 C2133 G2134 U2135 A2136 G2137 G2138 A2139 U2140 A2141 G2142 G2143 U2144 G2145 G2146 G2147 A2148 G2149 G2153 U2154 G2155 A2156 A2157 C2158 C2162 G2163 C2164 C2165 U2166 C2167 C2168 G2169 G2170 G2171 U2172 G2173 G2174 G2175 G2176 G2177 G2178 G2179 A2180 G2181 C2182 C2183
G2184 C2185 C2186 G2187 G2188 U2189 G2190 A2191 U2194 A2195 C2196 C2197 A2198 C2199 C2200 C2201 G2204 C2205 C2206 C2207 G2208 G2209 C2210 U2211 G2212 G2213 G2214 G2215 G2216 C2217 C2218 U2219 A2220 U2225 C2226 G2227 G2228 A2229 U2230 G2236 A2237 C2238 A2239 G2240 U2244 U2245 G2246 G2250 G2251 C2252 U2255 U2256 U2257

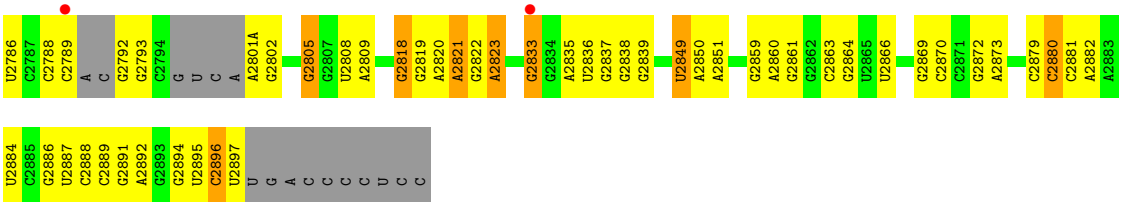


• Molecule 1: 23S Ribosomal RNA

Chain CA:

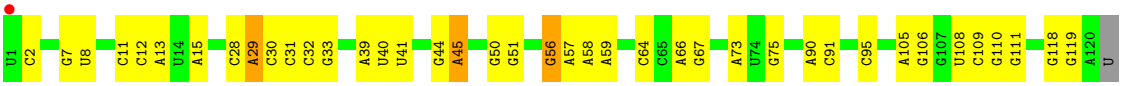

G500 A501 A502 A503 U504 A505 G508 C509 C510 U511 G512 A515 C516 C517 G518 U519 G520 G521 G522 C523 A526 C527 A528 A529 G530 C531 A532 G533 U534 C535 A536 C537 G538 G539 C540 G545 C A A G549 G551 G556 U557 G561 U562 G563 C564 C565 U566 A567 U568 A572 G573
C574 A575 U576 G577 A578 G579 C580 C581 C584 G585 A586 C587 U588 C589 A590 C591 G599 G600 C601 G602 A603 G604 C605 U606 U607 A608 A609 C610 C611 C612 G613 U614 U614A G614B A614C G615 G620 G623 C624 A627 C634 A637 G638 U639 C640 C641 G642 A643 A644 C645 A646 G647 G648
G649 C650 G651 C652 A652A A652B G652C C652D G652E G G C C G C A C G C G G C C C652T G652U A655 G656 U657 C658 C659 G660 C661 G662 G663 G666 U667 G668 G669 A670 C671 C672 C673 G674 C679 G680 A685 G686 C687 C693 U694 G695 G696 C697 C698 A699
G700 G704 A705 A706 G707 G715 G723 U724 G725 G726 C730 C731 G738 G739 U740 A746 U747 G748 C749 A750 A751 U757 C758 G759 G760 A761 G765 G770 A774 G775 G776 A777 G778 U779 G780 A781 A782 A783 A784 G785 C786 U787 A788 A789 C790 C791 G792 A793 G794 C795
C796 C797 A800 G805 G809 U810 U811 C812 U813 C814 C815 C816 C817 G818 A819 U827 U828 A829 G830 G831 G832 U833 G836 C837 C838 U839 C840 G843 C844 G845 C846 U847 G848 A849 C850 U851 G852 G853 G854 G855 C856 C857 U858 G859 U860 A861 G862 A863 G864 C865 A866 C867 U868 G869
A870 G873 G874 G875 C876 U877 A878 G879 G880 G881 G882 G883 C884 C885 C886 A887 C888 C889 A890 G892 C893 C894 U895 A896 C897 C898 A899 A900 A901 C902 C903 C904 U905 G906 U907 C908 A909 A910 A911 C912 U913 C914 C915 G916 A917 A918 G919 G920 G921 U922 C923 C924 C925 A926 G927 G928 U930 G931 G932
A933 G938 A941 A945 G946 G947 G950 C951 G952 A953 G954 C955 G956 A957 U958 A959 A960 C961 G962 U963 C964 C967 C970 C971 G974 C975 G979 A980 A981 C982 A983 G987 A988 G989 A990 C991 C992 G993 C994 C995 A996 G997 C998 U999 A1000 A1001 G1002 G1003 C1004 C1005 C1006
C1007 C1008 A1009 A1010 G1011 U1012 C1013 U1014 G1015 G1016 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 G1031 A1032 U1033 C1038 G1039 C1040 C1041 G1042 C1043 G1044 A1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 C1053 A1054 G1055 G1056 A1057 G1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 A1070 G1071 C1072
A1073 G1074 C1075 C1076 A1077 U1078 C1079 C1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 G1110 A1111 G1112 U1113 G1114 C1118 C1119 G1125 A1126 A1127 A1128 A1129 U1130 G1131 A1132 U1133 C1135 G1136 G1137 G1138 G1139 C1140
U1141 U1142 A1142A A1143 G1144 C1145 G1149 C1150 G1151 C1152 C1153 G1154 G1160 U1165 C1166 U1167 G1168 G1171 G A U G A C1178 C1179 C1180 C1181 A1182 G1183 G1184 G1187 U1188 A1189 G1190 C1201 C1202 G1203 A1204 U1205 C1208 G1209 A1210 U1211 G1212 A1220 C1221 C1221A C1222 A1226 G1227 G1228
G1229 C1230 G1231 G1232 G1236 A1237 U1240 A1241 A1242 A1246 A1247 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 G1260 C1261 A1262 U1263 G1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 G1277 A1278 G1279 G1280 G1283 A1284 G1285 C1289 C1290 C1291 U1292 C1293 C1297 C1298 G1299 U1300 A1301
A1302 G1303 G1309 G1310 U1313 C1314 C1315 U1316 A1317 C1318 G1319 C1320 A1321 A1322 U1323 C1327 G1328 U1329 C1330 A1331 G1332 G1338 G1339 U1340 U1341 A1342 G1343 G1344 A1349 U1352 A1353 A1354 G1355 G1356 A1359 A1360 C1363 G1364 A1365 G1368 G1369 C1370 G1371 U1372 A1373 G1374 C1375 C1376 A1379 G1380
A1384 G1385 C1386 C1387 G1388 G1389 U1390 U1391 A1392 U1396 G1401 C1402 U1405 U1406 C1407 C1408 C1409 G1410 C1411 A1412 G1413 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1423 G1424 G1425 G1426 A1427 C1428 G1429 C1430 U1431 A1434 C1437 U1438 A1439 G1444 A1445 C1445A C1446 G1447 G1448 A1449 G1450 C1450A C1451 A1452
U1453 G1455 G1456 G1459 C1462 C1463 C1464 C1467 A1471 A1472 G1473 C1474 G1475 C1476 A1477 G1478 G1479 G1480 U1481 G1482 G1488 U1489 A1490 G1491 G1492 G1493 A1494 A1495 A1496 U1497 C1498 C1499 G1500 C1501 C1502 U1503 C1504 C1505 C1506 A1507 A1508 C1509 A1509A A1509B G1510 C1511 U1512 C1513 U1514 G1515 C1516 G1517 U1518 G1519 G1520


U1523 A1528A G1529 C1532 G1533 U A C1536 G1537 G1538 G1539 U1540 G1541 A1542 C1543 C1547 C1548 C1549 C1550 A1553 C1556 C1557 A1558 G1559 G1560 A1566 A1567 G1568 A1569 A1570 A1571 U1578 A1579 A1580 G1581 C1582 A1583 C1584 A1586 A1587 C1588 G1593 A1596 A1603 C1604 C1607 A1608 A1609 A1610
C1611 A1614 A1618 G1622 G1623 G1624 G1627 A1634 A1637 C1638 U1639 C1640 A1641 G1642 G1643 C1644 G1647 C1648 G1651 A1652 G1653 A1654 C1657 C1658 U1659 A1664 A1665 G1666 G1667 U1671 G1674 C1675 G1682 C1683 U1688 A1689 A1690 C1691 U1692 U1693 C1694 G1695 G1696 G1697 A1698 G1699
A1700 A1701 G1702 G1703 U1709 C1710 C1711 U1720 G1721 A1722 U1739 G1740 A1741 G1747A G1753 G1756 U1757 G1758 A1759 A1760 C1761 A1762 G1763 G1764 C1767 U1768 A1773 G1776 U1777 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 G1792 C1793 U1794 C1795 U1796 C1797 U1798 G1799 C1800
G1801 A1802 A1803 C1804 U1805 U1808 A1812 G1816 G1817 U1818 A1819 G1822 G1823 A1829 C1830 G1831 C1832 U1833 U1834 G1835 C1836 C1837 C1838 G1839 G1842 C1843 A1847 A1848 G1849 G1850 G1857 G1858 A1859 G1860 G1861 U1864 G1865 C1866 A1876 A1877 G1878 G1883 A1889 G1899 A1900 G1906
A1913 C1914 U1917 A1918 A1919 G1922 U1923 U1926 A1927 A1928 G1929 G1930 U1931 A1932 G1933 C1934 G1935 A1936 A1937 A1938 A1952 U1955 U1956 C1957 C1958 G1959 U1963 A1966 C1967 A1970 A1971 A1972 U1991 G1992 U1993 C1994 U1995 C1996 G1997 G1998 C1999 G2000 C2006 C2007 G2012 A2013 A2014 A2020
C2021 U2022 G2023 G2027 A2031 G2032 A2033 G2037 G2038 C2039 C2040 U2041 A2042 C2043 G2046 U2047 C2055 G2056 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2069 G2070 A2071 U2074 U2075 C2078 U2079 G2080 U2086 G2087 U2091 U2092 C2095 U2102 C2103 G2106 C2107 C2108 U2109 G2110 C2111
G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 G2147 G2148 G2149 U2150 G2151 G2152 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171
U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 G2181 G2182 C2183 G2187 C2188 U2189 G2190 G2191 G2192 G2193 G2194 C2200 G2206 G2207 A2208 U2218 A2225 C2226 A2227 G2228 C2229 U2233 G2234 G2235 C2236 G2237 G2238 G2239 U2243 U2244 C2248 U2249 G2250 G2251 G2252 C2258 G2259 C2260 C2261 U2262 C2263 C2264
A2268 A2269 U2272 A2273 A2274 C2275 G2276 G2277 A2278 G2279 G2280 C2281 G2282 C2283 C2284 C2285 A2286 A2287 A2288 G2289 G2290 U2291 C2292 C2293 C2294 C2295 U2296 C2297 A2298 G2299 G2302 G2303 G2304 A2305 C2306 G2307 U2312 C2313 C2314 G2315 C2316 C2317 G2318 G2319 A2320 G2321 A2322 G2323 C2324 G2325 C2326 A2327 A2328 G2329 G2330 G2331 U2332
A2333 G2334 A2335 A2336 C2343 U2344 G2345 A2346 C2347 U2348 G2349 C2350 G2351 G2354 U2357 A2360 A2361 G2362 C2363 C2364 G2365 A2366 A2369 G2370 C2371 G2372 G2373 C2374 G2375 A2376 A2377 A2378 G2379 G2383 G2384 C2385 C2386 U2387 A2388 G2389 A2392 A2393 C2394 C2395 G2396 G2399 G2400 U2401 C2404 G2405 U2406
G2407 U2408 G2409 G2410 G2414 G2415 C2416 C2417 A2418 A2422 U2423 C2424 A2425 A2426 C2427 G2428 G2429 A2430 U2431 A2434 A2435 A2439 C2440 C2441 C2442 C2443 G2444 G2445 A2448 A2453 G2454 G2455 C2456 U2457 G2458 C2465 C2466 C2467 G2468 A2469 G2470 C2474 C2475 A2476 C2477 A2478 G2486 G2487 U2491
G2494 C2498 G2502 A2503 U2504 G2505 G2508 G2509 C2510 A2518 G2525 G2526 C2527 U2528 G2529 A2530 A2531 G2532 A2533 G2544 G2545 U2552 G2553 U2554 U2555 U2562 U2563 A2564 A2565 A2566 G2567 G2570 C2571 A2572 C2573 G2576 G2581 G2582 U2585 C2586 A2590 C2591 A2600 C2601 A2602 G2603
U2609 C2610 U2611 C2612 U2615 A2621 C2622 G2625 C2626 A2629 G2630 G2631 A2632 U2636 U2637 G2638 A2639 G2640 G2645 C2646 U2647 C2648 A2654 A2657 A2660 G2661 A2662 G2663 G2664 A2665 G2677 C2678 A2679 U2682 C2683 U2684 G2685 U2689 C2690 A2693 G2694 C2695 U2696 G2697 U2702
C2703 C2704 G2708 G2709 C2710 A2711 U2712 A2712A A2713 G2714 G2719 U2720 A2721 G2722 C2723 U2726 G2727 U2728 G2729 C2730 G2731 G2732 A2733 C2742 C2743 G2744 C2745 U2746 G2747 A2748 A2749 A2750 C2755 U2756 A2757 A2758 G2759 C2760 G2761 A2765 G2766 C2767 C2774 A2775 A2778 U2779 G2780 A2781 G2782 G2783 C2784 C2785



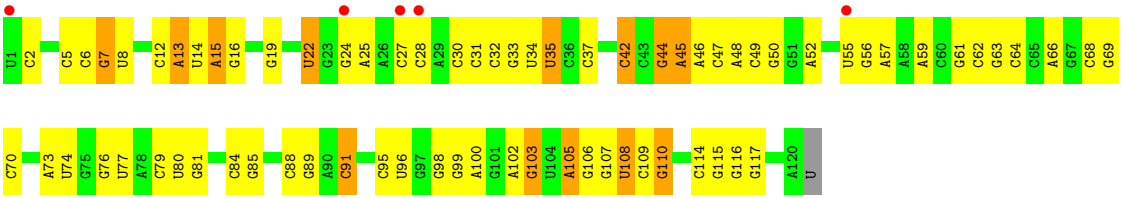
• Molecule 2: 5S Ribosomal RNA

Chain AB:



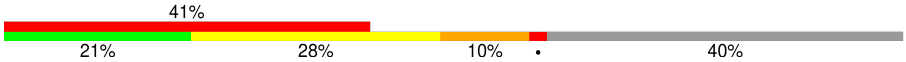
• Molecule 2: 5S Ribosomal RNA

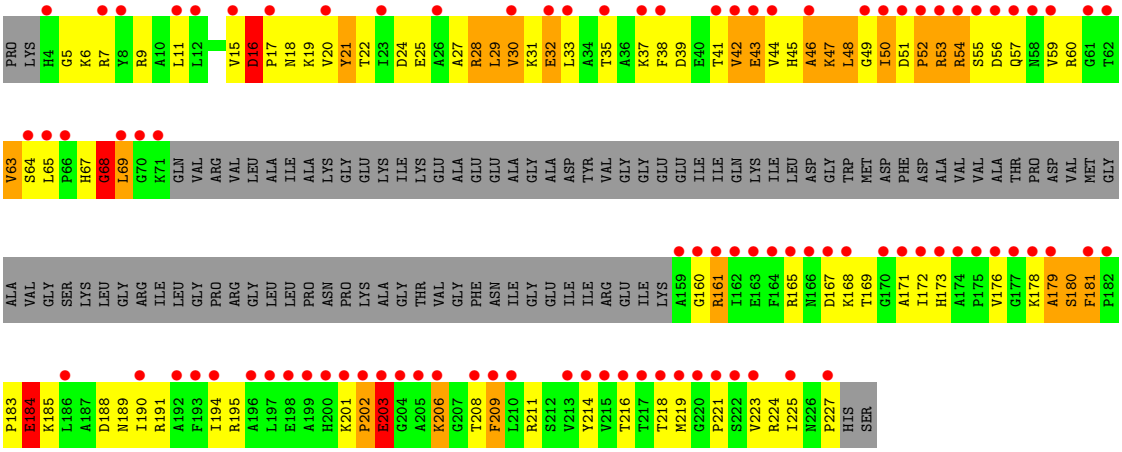
Chain CB:



• Molecule 3: 50S ribosomal protein L1

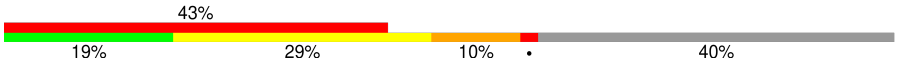
Chain AC:

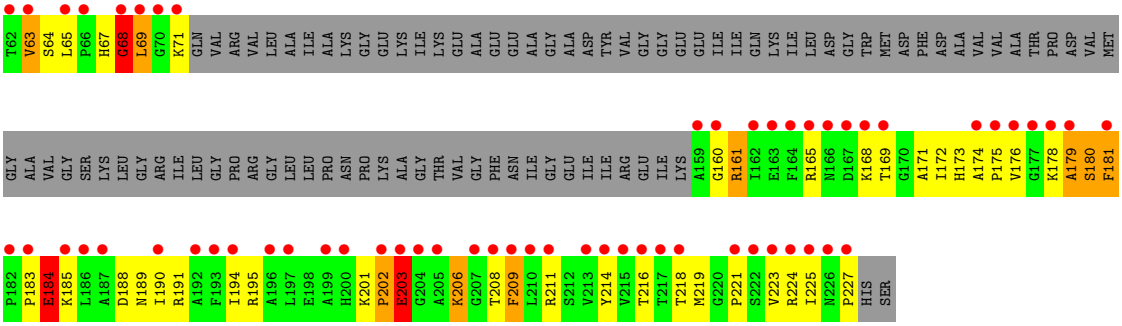




• Molecule 3: 50S ribosomal protein L1

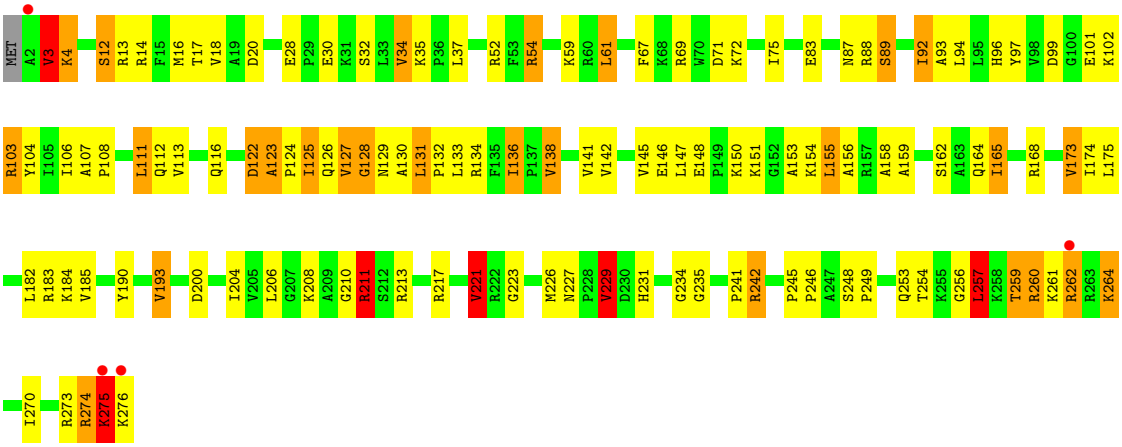
Chain CC:





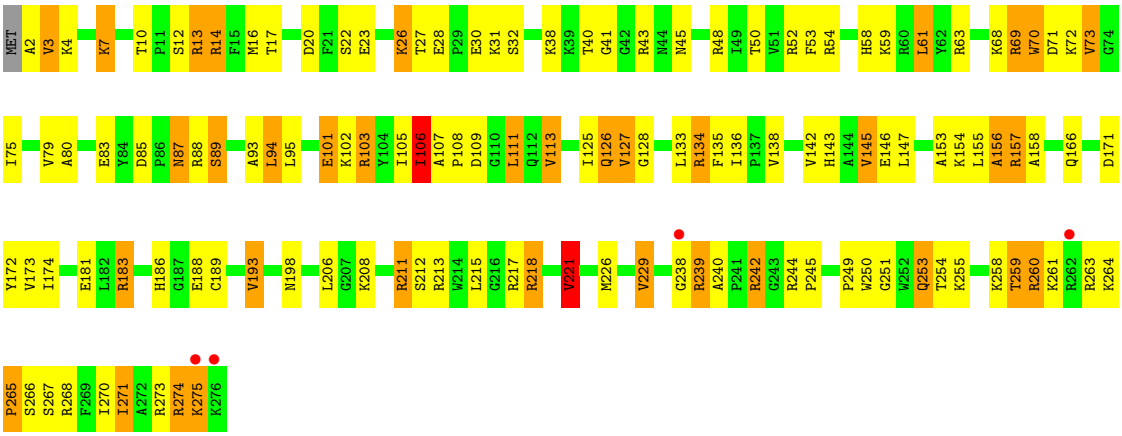
- Molecule 4: 50S ribosomal protein L2

Chain AD:



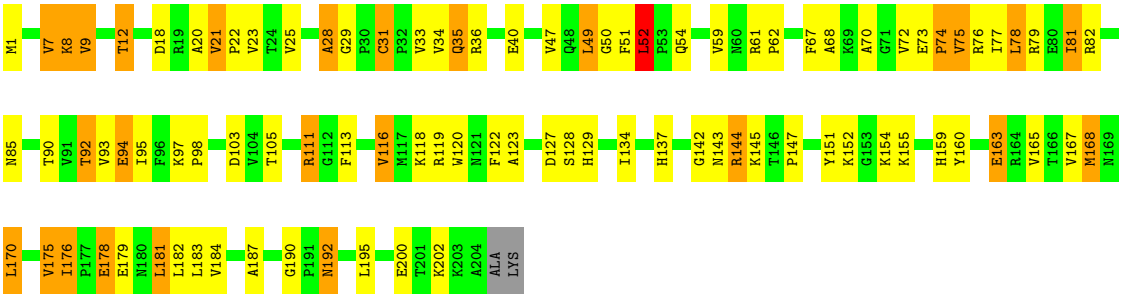
- Molecule 4: 50S ribosomal protein L2

Chain CD:



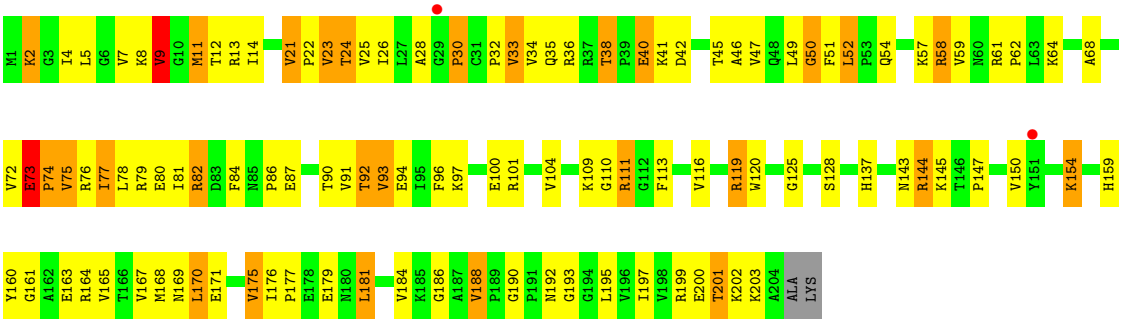
- Molecule 5: 50S ribosomal protein L3

Chain AE:



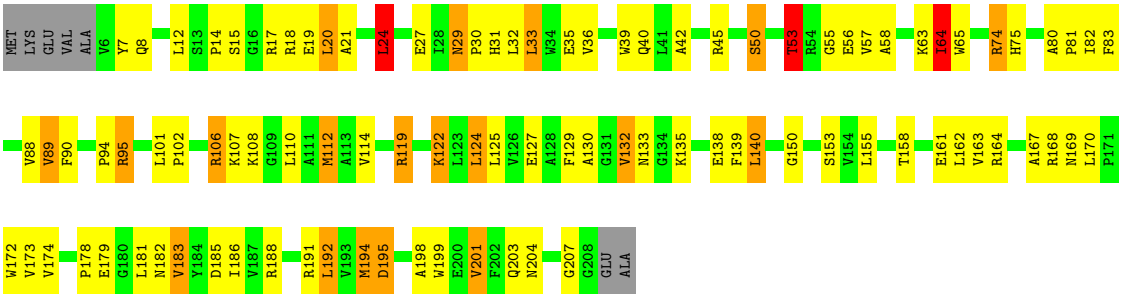
- Molecule 5: 50S ribosomal protein L3

Chain CE:



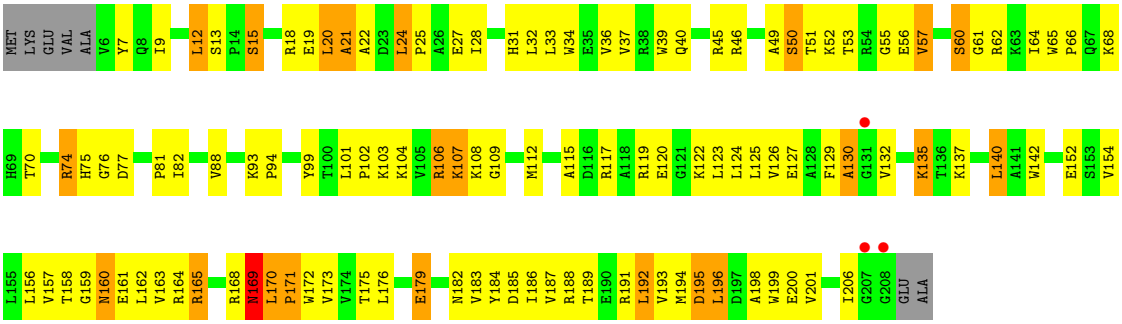
- Molecule 6: 50S ribosomal protein L4

Chain AF:



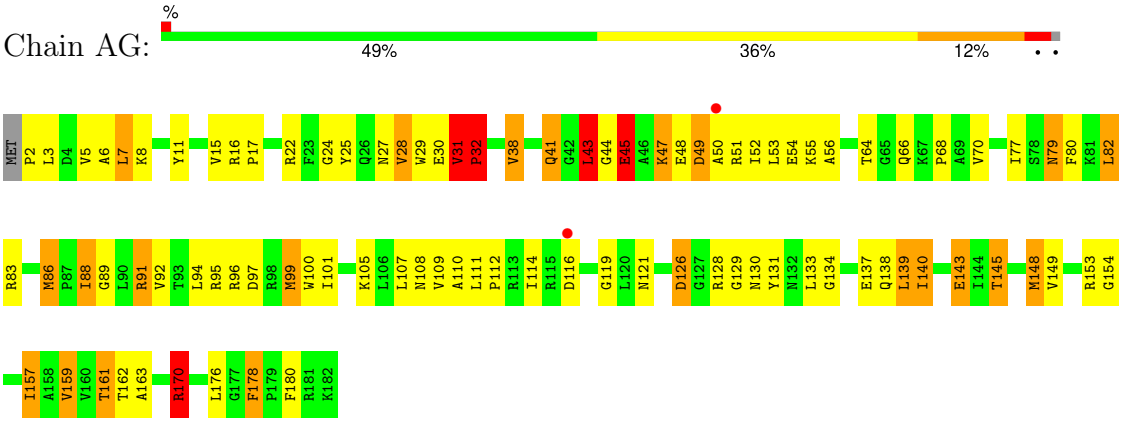
- Molecule 6: 50S ribosomal protein L4

Chain CF:



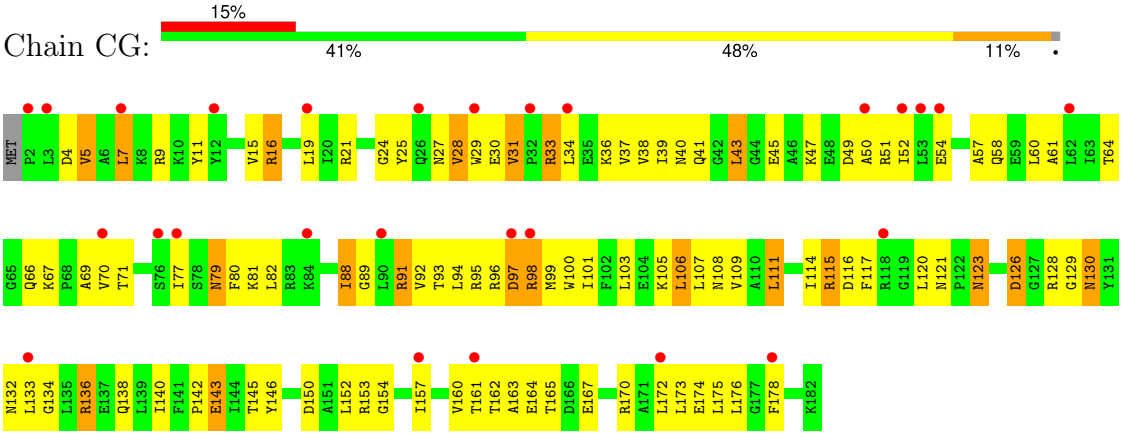
• Molecule 7: 50S ribosomal protein L5

Chain AG:



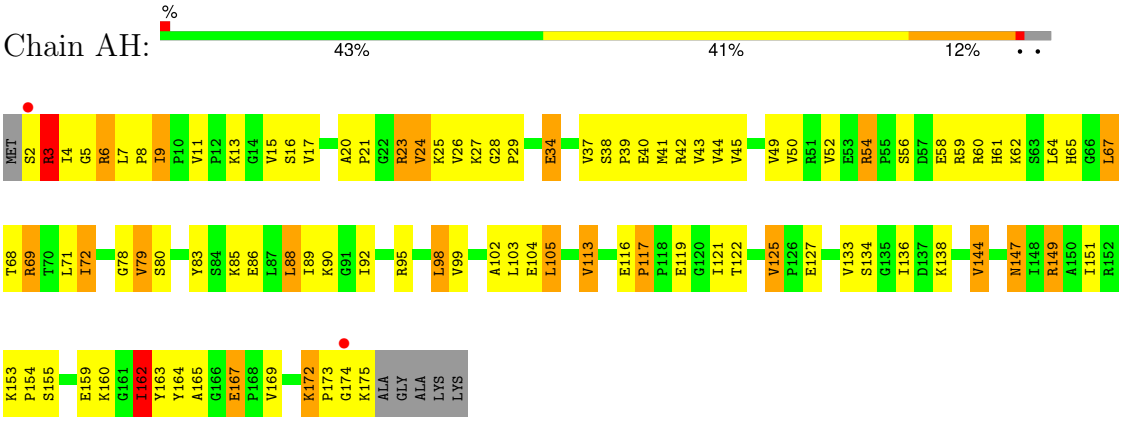
• Molecule 7: 50S ribosomal protein L5

Chain CG:



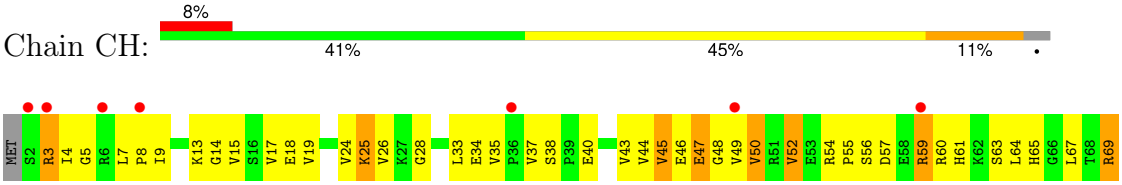
• Molecule 8: 50S ribosomal protein L6

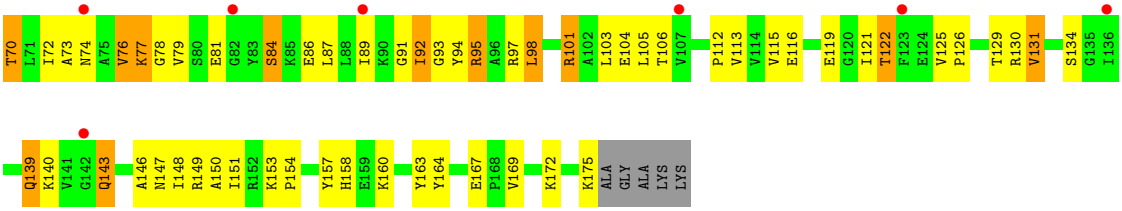
Chain AH:



• Molecule 8: 50S ribosomal protein L6

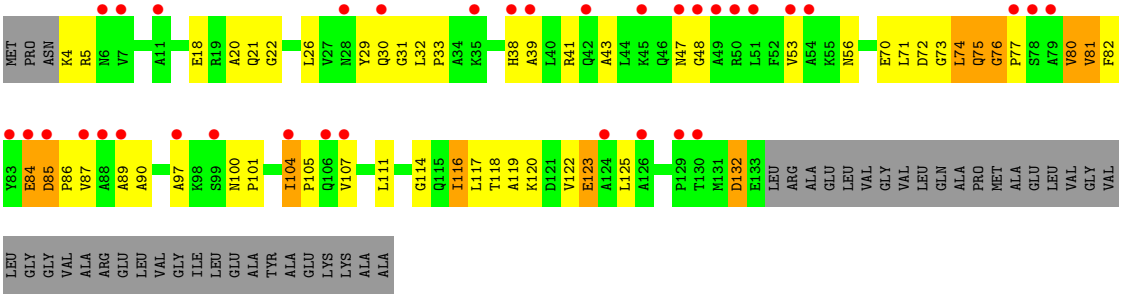
Chain CH:





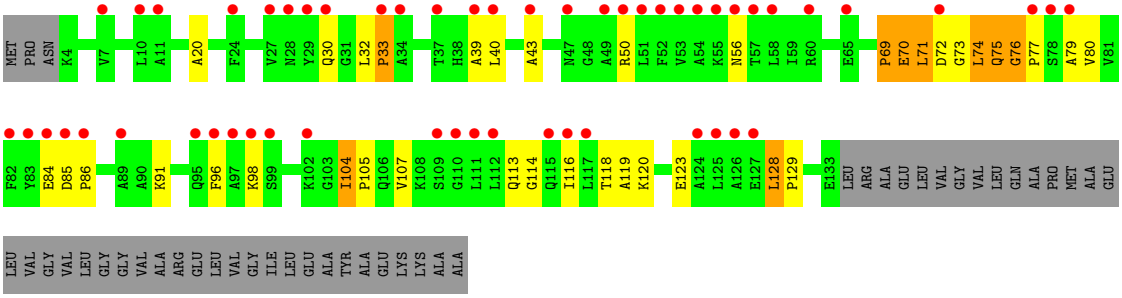
- Molecule 9: 50S ribosomal protein L10

Chain AK:



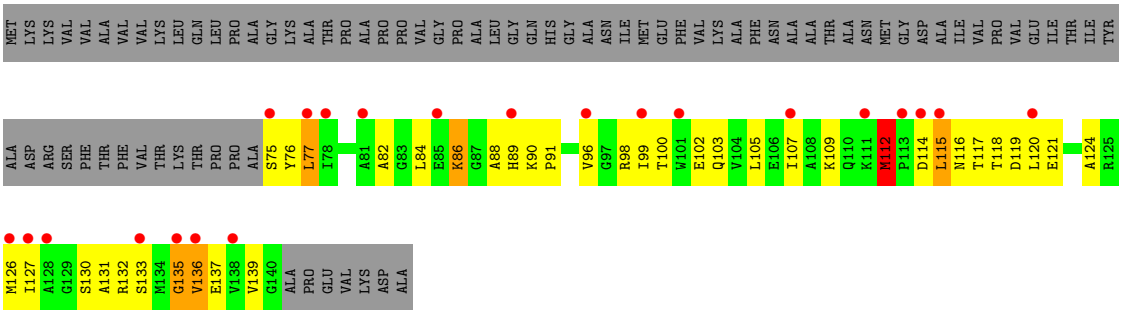
- Molecule 9: 50S ribosomal protein L10

Chain CK:



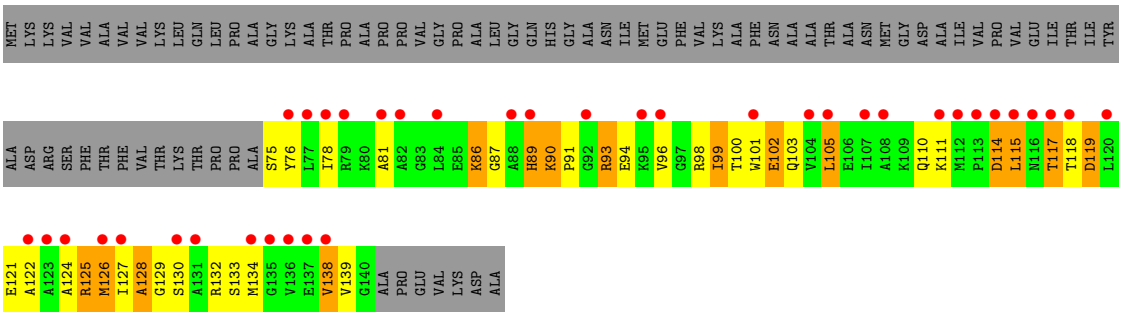
- Molecule 10: 50S ribosomal protein L11

Chain AL:



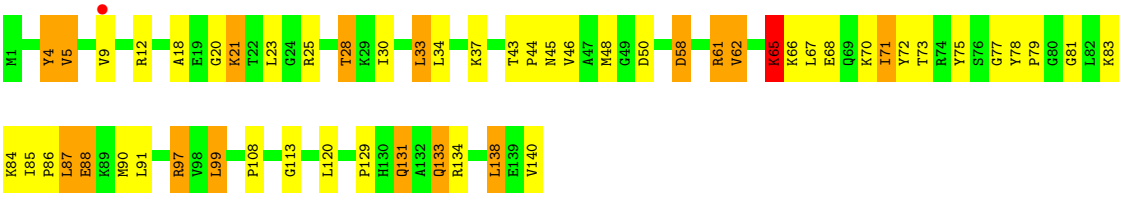
- Molecule 10: 50S ribosomal protein L11

Chain CL:



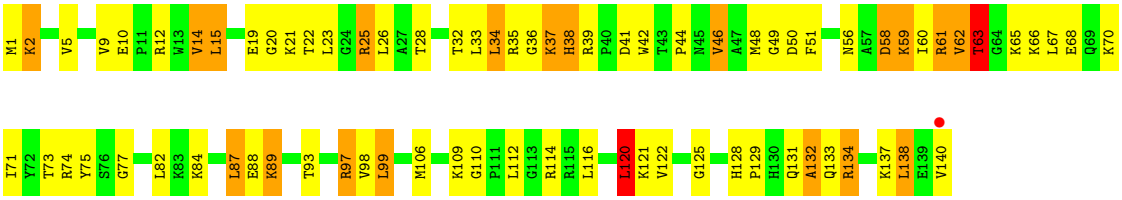
- Molecule 11: 50S ribosomal protein L13

Chain AN:



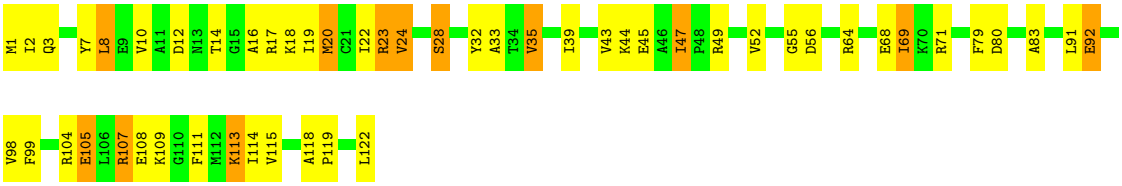
- Molecule 11: 50S ribosomal protein L13

Chain CN:



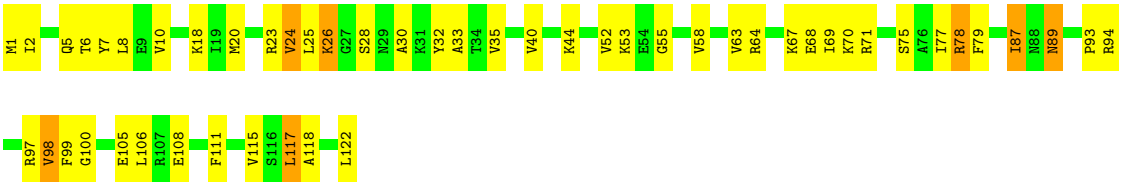
- Molecule 12: 50S ribosomal protein L14

Chain AO:



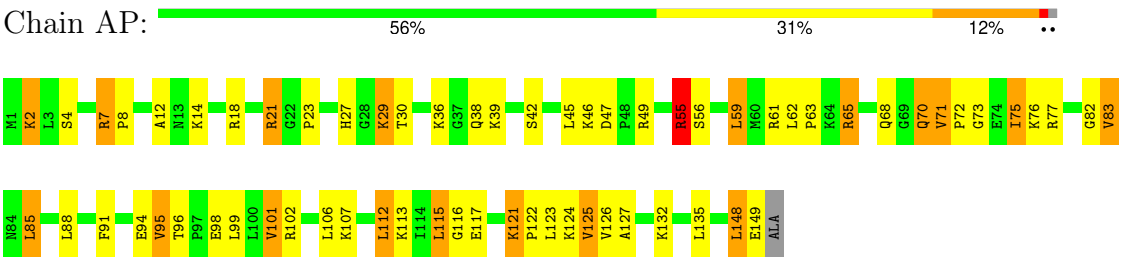
- Molecule 12: 50S ribosomal protein L14

Chain CO:



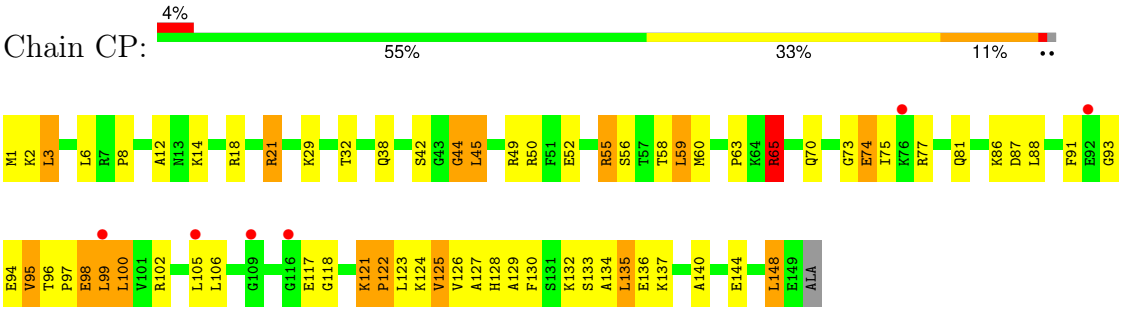
- Molecule 13: 50S ribosomal protein L15

Chain AP:



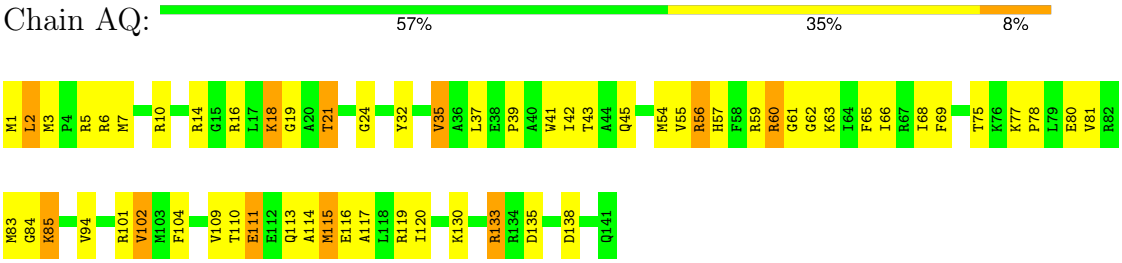
- Molecule 13: 50S ribosomal protein L15

Chain CP:



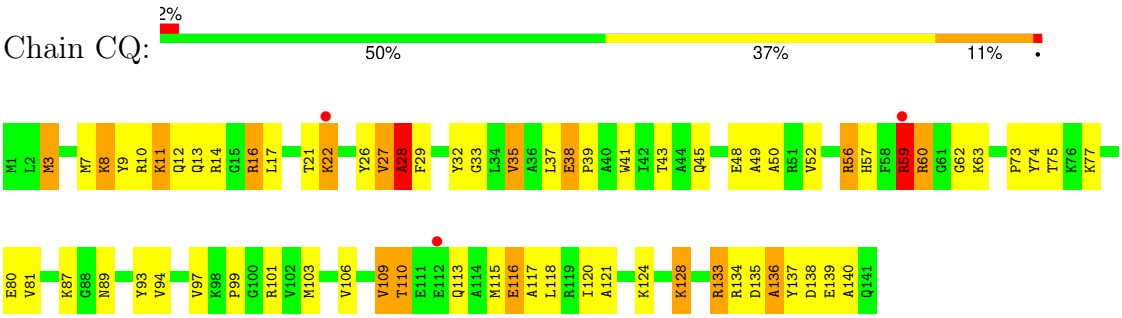
- Molecule 14: 50S ribosomal protein L16

Chain AQ:



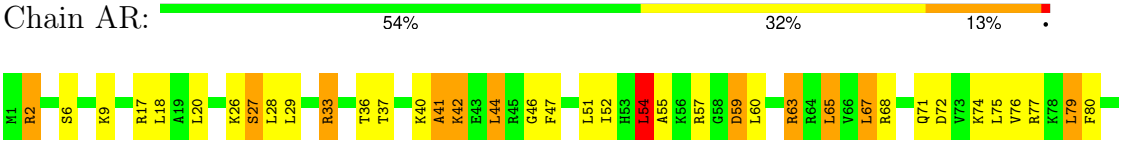
- Molecule 14: 50S ribosomal protein L16

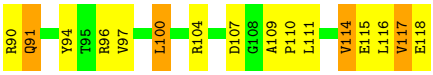
Chain CQ:



- Molecule 15: 50S ribosomal protein L17

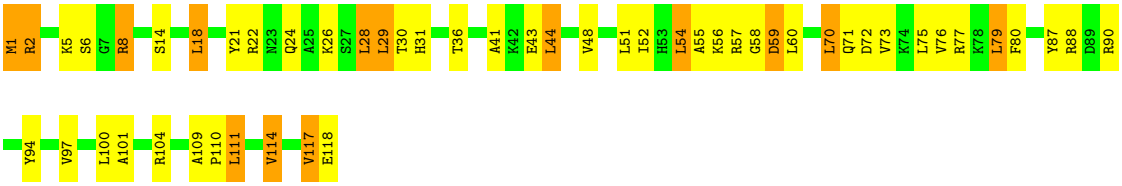
Chain AR:





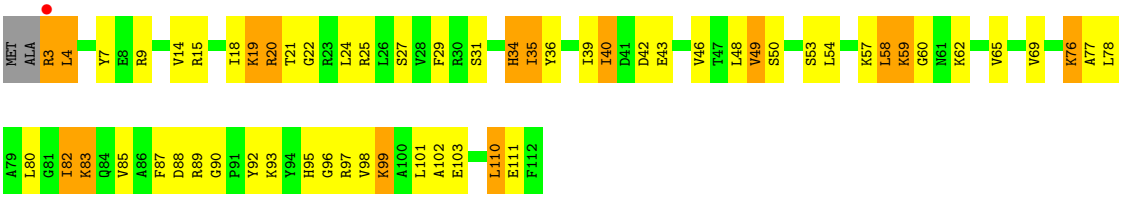
• Molecule 15: 50S ribosomal protein L17

Chain CR:



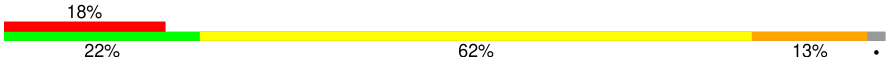
• Molecule 16: 50S ribosomal protein L18

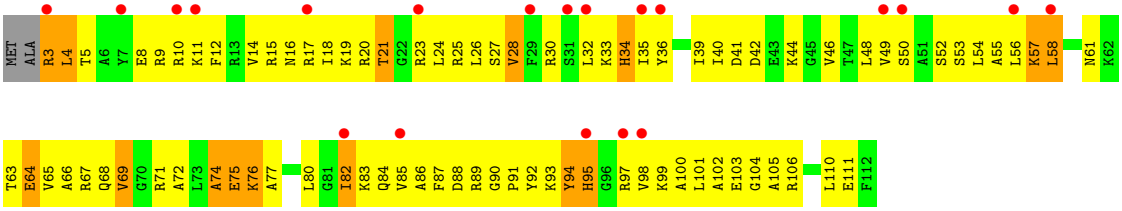
Chain AS:



• Molecule 16: 50S ribosomal protein L18

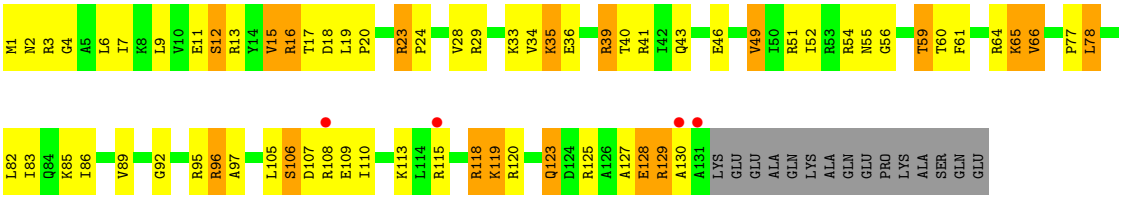
Chain CS:





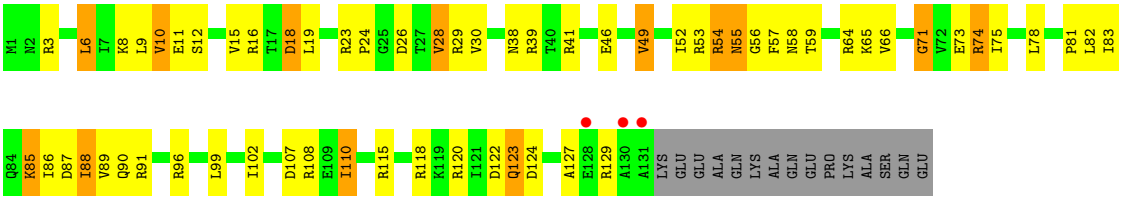
• Molecule 17: 50S ribosomal protein L19

Chain AT:



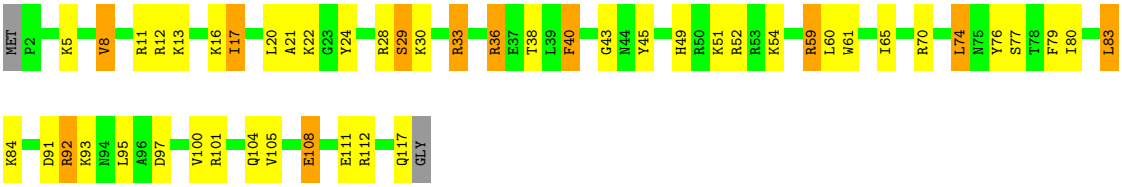
• Molecule 17: 50S ribosomal protein L19

Chain CT:



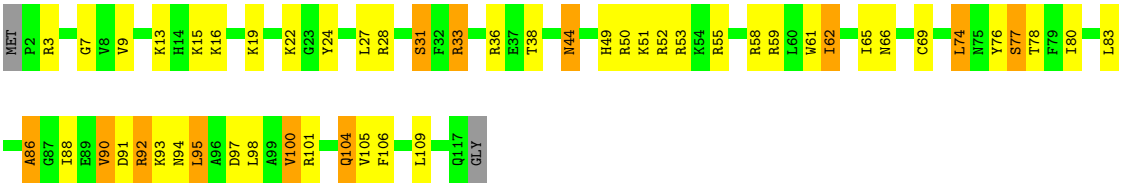
- Molecule 18: 50S ribosomal protein L20

Chain AU:



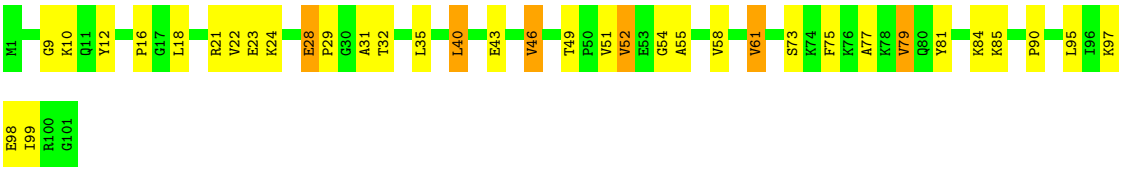
- Molecule 18: 50S ribosomal protein L20

Chain CU:



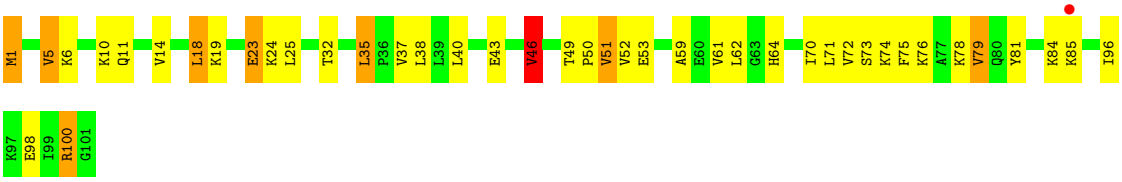
- Molecule 19: 50S ribosomal protein L21

Chain AV:



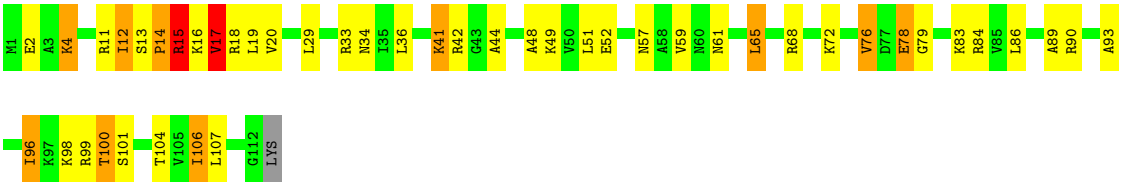
- Molecule 19: 50S ribosomal protein L21

Chain CV:



- Molecule 20: 50S ribosomal protein L22

Chain AW:

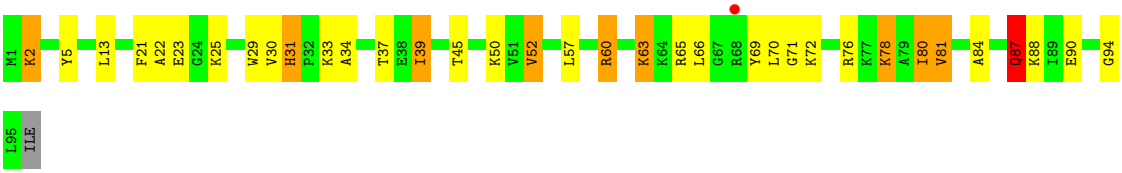


- Molecule 20: 50S ribosomal protein L22

Chain CW:

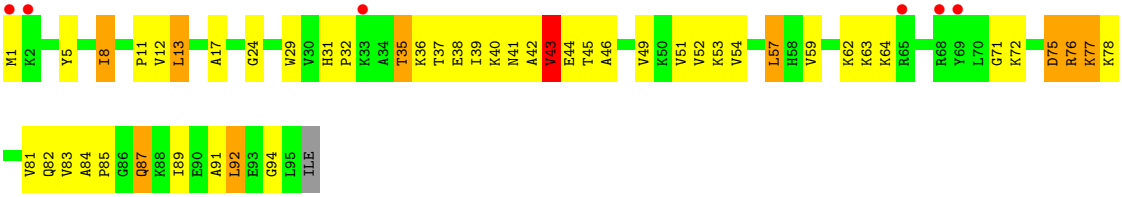
- Molecule 21: 50S ribosomal protein L23

Chain AX:



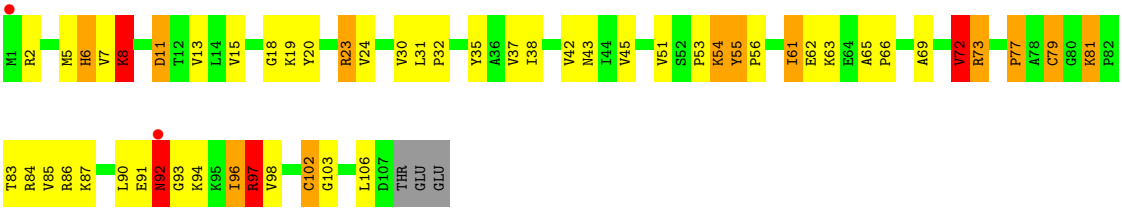
- Molecule 21: 50S ribosomal protein L23

Chain CX:



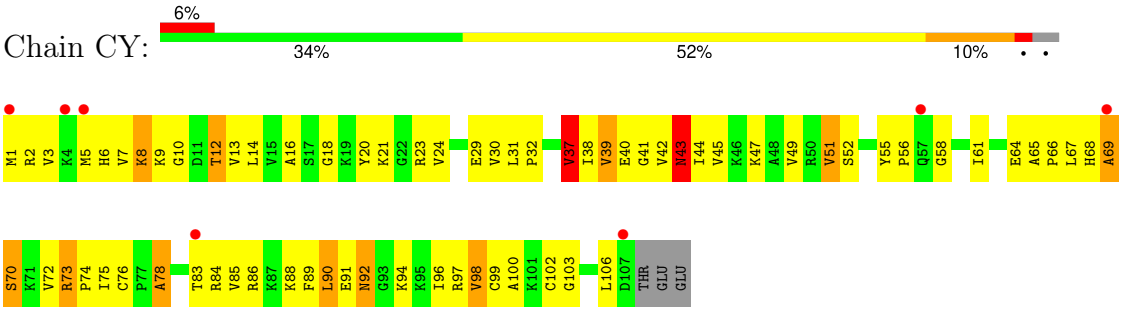
- Molecule 22: 50S ribosomal protein L24

Chain AY:



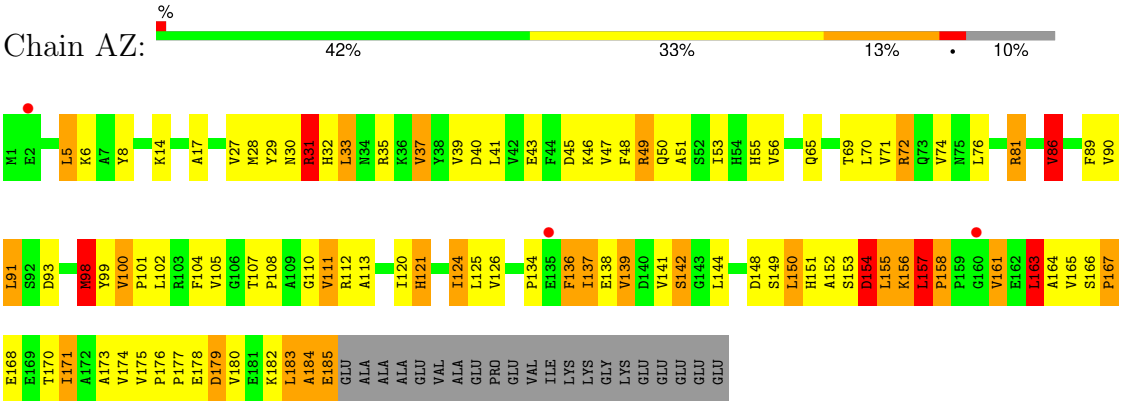
- Molecule 22: 50S ribosomal protein L24

Chain CY:



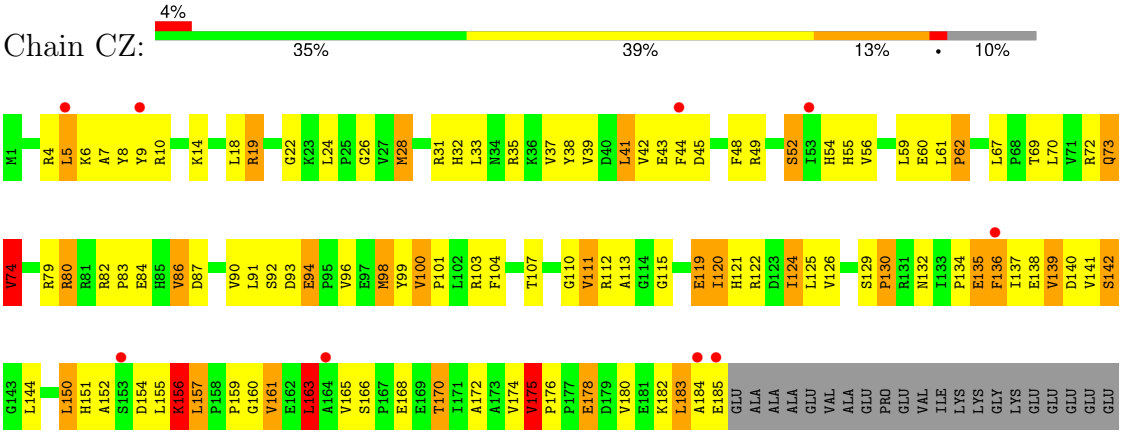
- Molecule 23: 50S ribosomal protein L25

Chain AZ:



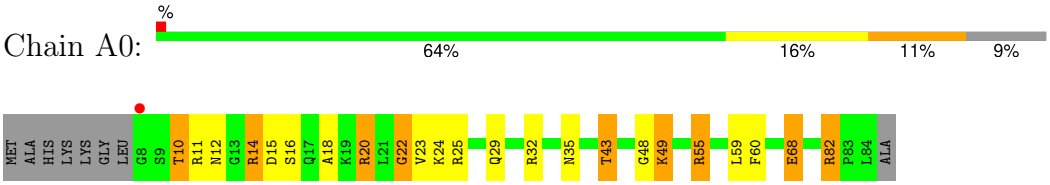
- Molecule 23: 50S ribosomal protein L25

Chain CZ:



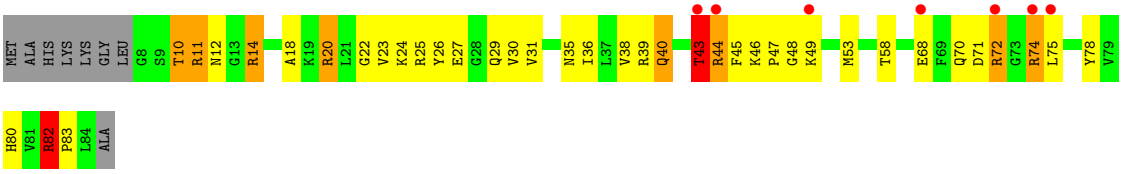
- Molecule 24: 50S ribosomal protein L27

Chain A0:



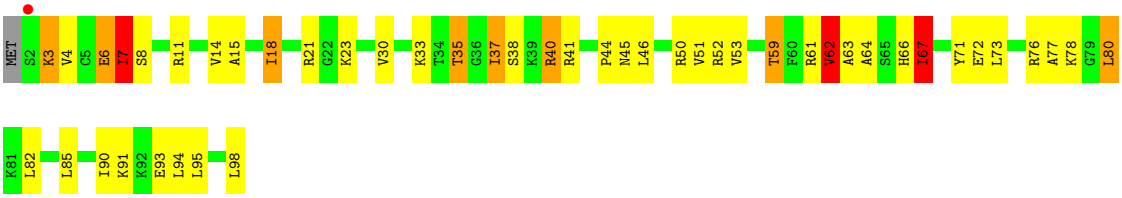
- Molecule 24: 50S ribosomal protein L27

Chain C0:



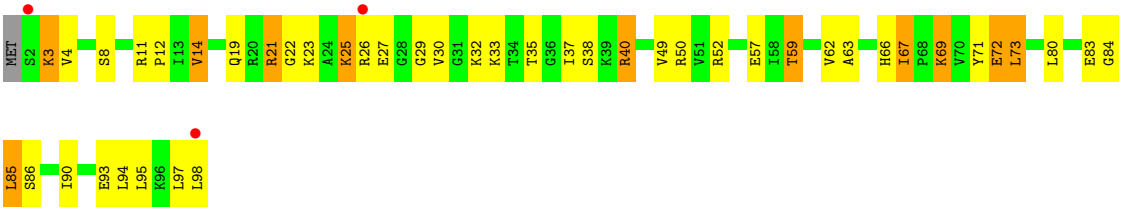
• Molecule 25: 50S ribosomal protein L28

Chain A1:



• Molecule 25: 50S ribosomal protein L28

Chain C1:

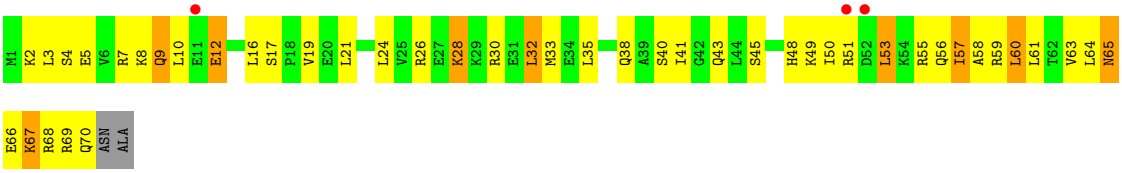


• Molecule 26: 50S ribosomal protein L29

Chain A2:

• Molecule 26: 50S ribosomal protein L29

Chain C2:



• Molecule 27: 50S ribosomal protein L30

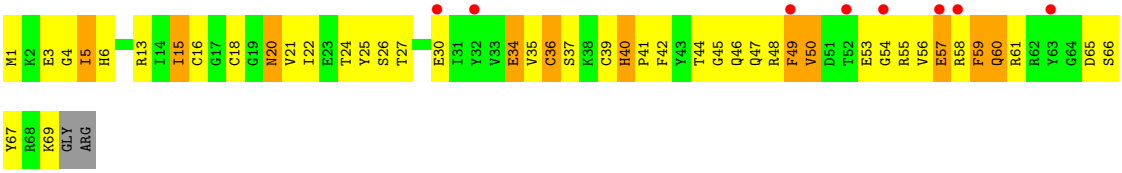
Chain A3:

• Molecule 27: 50S ribosomal protein L30

Chain C3:

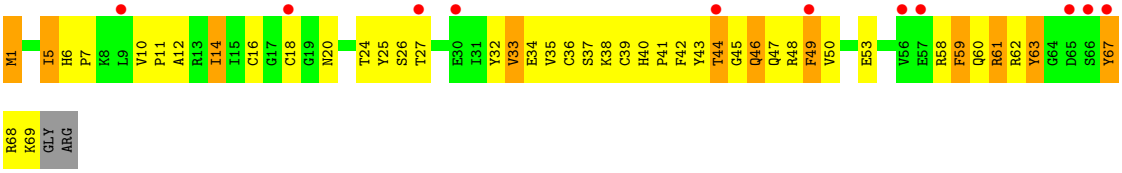
• Molecule 28: 50S ribosomal protein L31

Chain A4:



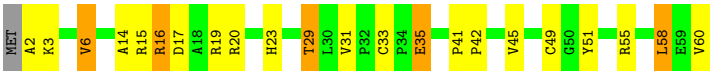
• Molecule 28: 50S ribosomal protein L31

Chain C4:



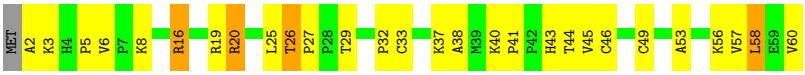
• Molecule 29: 50S ribosomal protein L32

Chain A5:



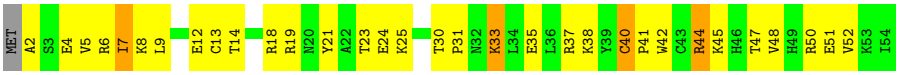
• Molecule 29: 50S ribosomal protein L32

Chain C5:



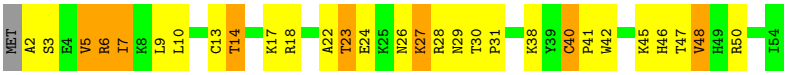
• Molecule 30: 50S ribosomal protein L33

Chain A6:



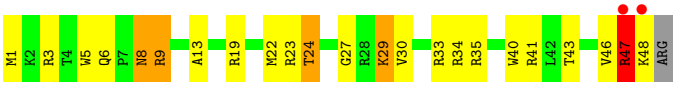
• Molecule 30: 50S ribosomal protein L33

Chain C6:



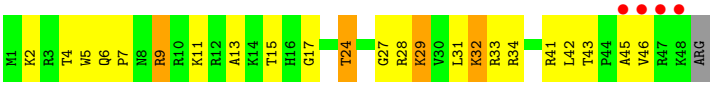
• Molecule 31: 50S ribosomal protein L34

Chain A7:



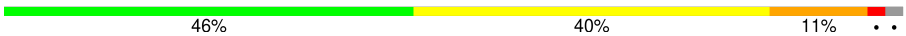
• Molecule 31: 50S ribosomal protein L34

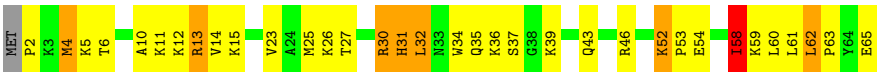
Chain C7:



• Molecule 32: 50S ribosomal protein L35

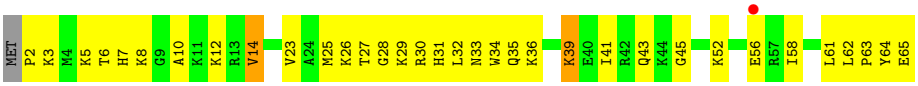
Chain A8:





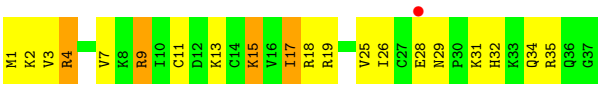
• Molecule 32: 50S ribosomal protein L35

Chain C8:



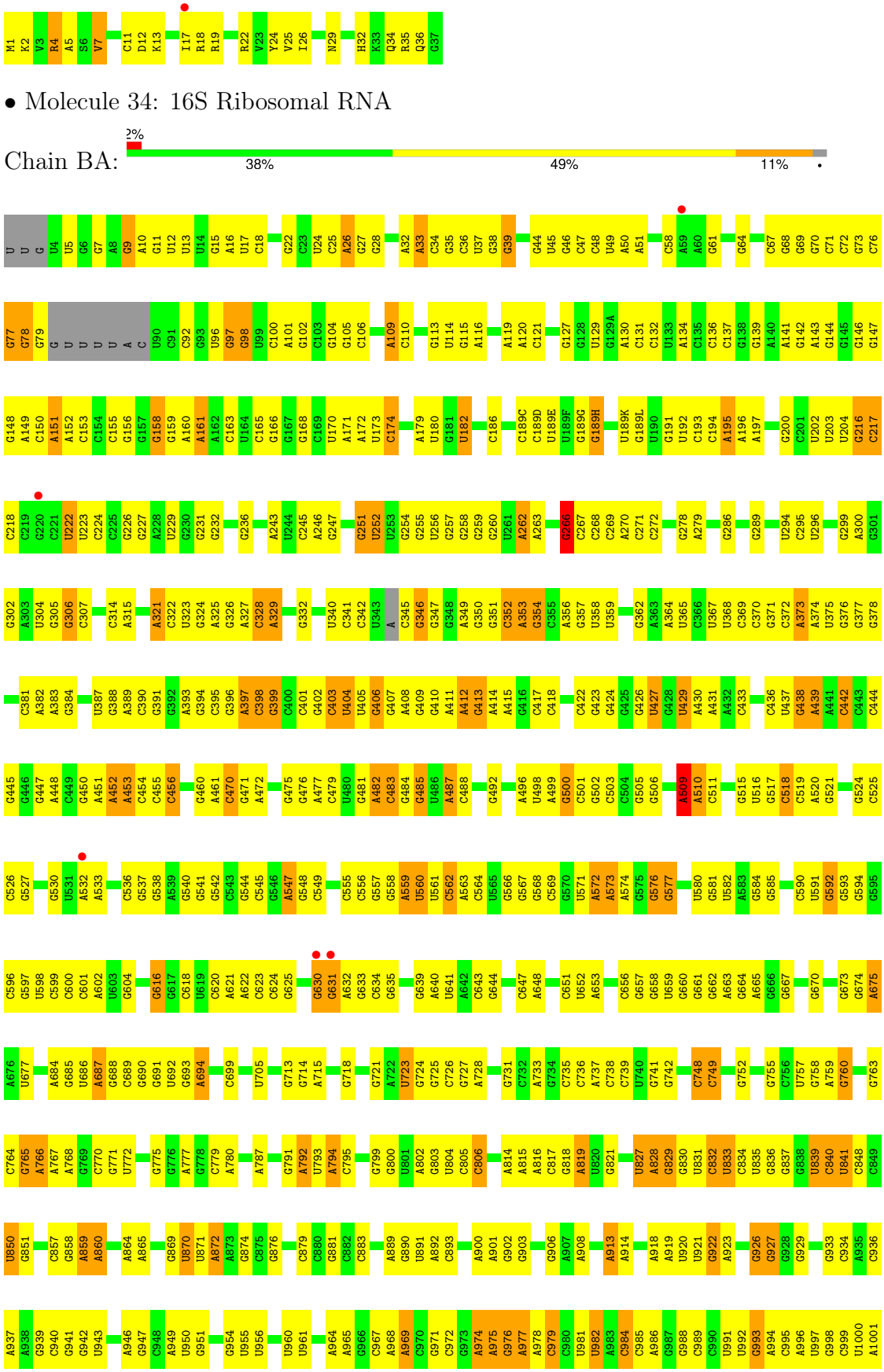
• Molecule 33: 50S ribosomal protein L36

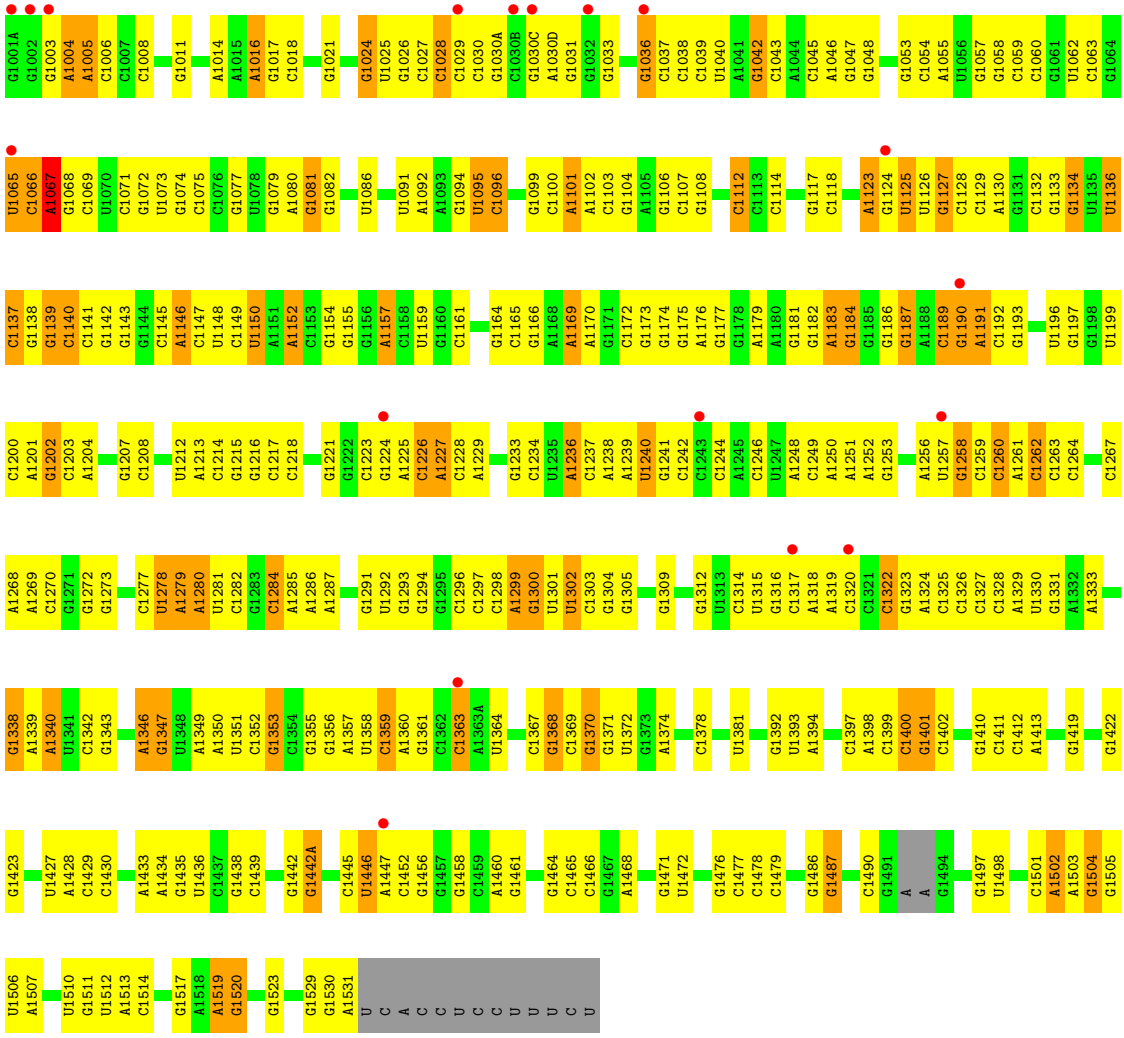
Chain A9:



• Molecule 33: 50S ribosomal protein L36

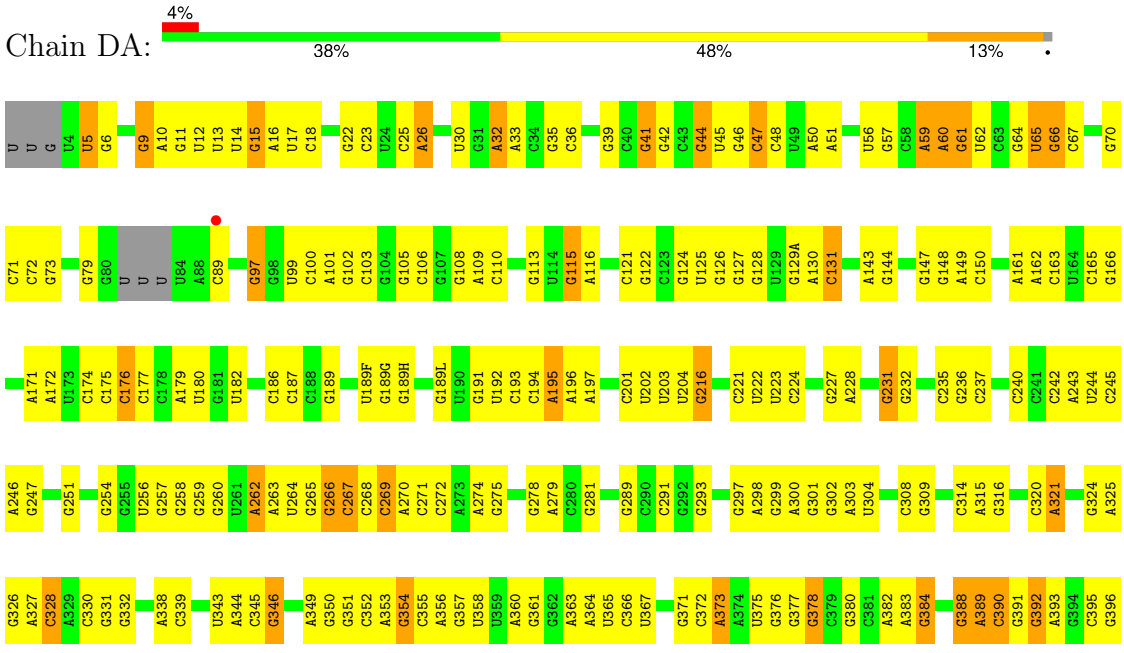
Chain C9:

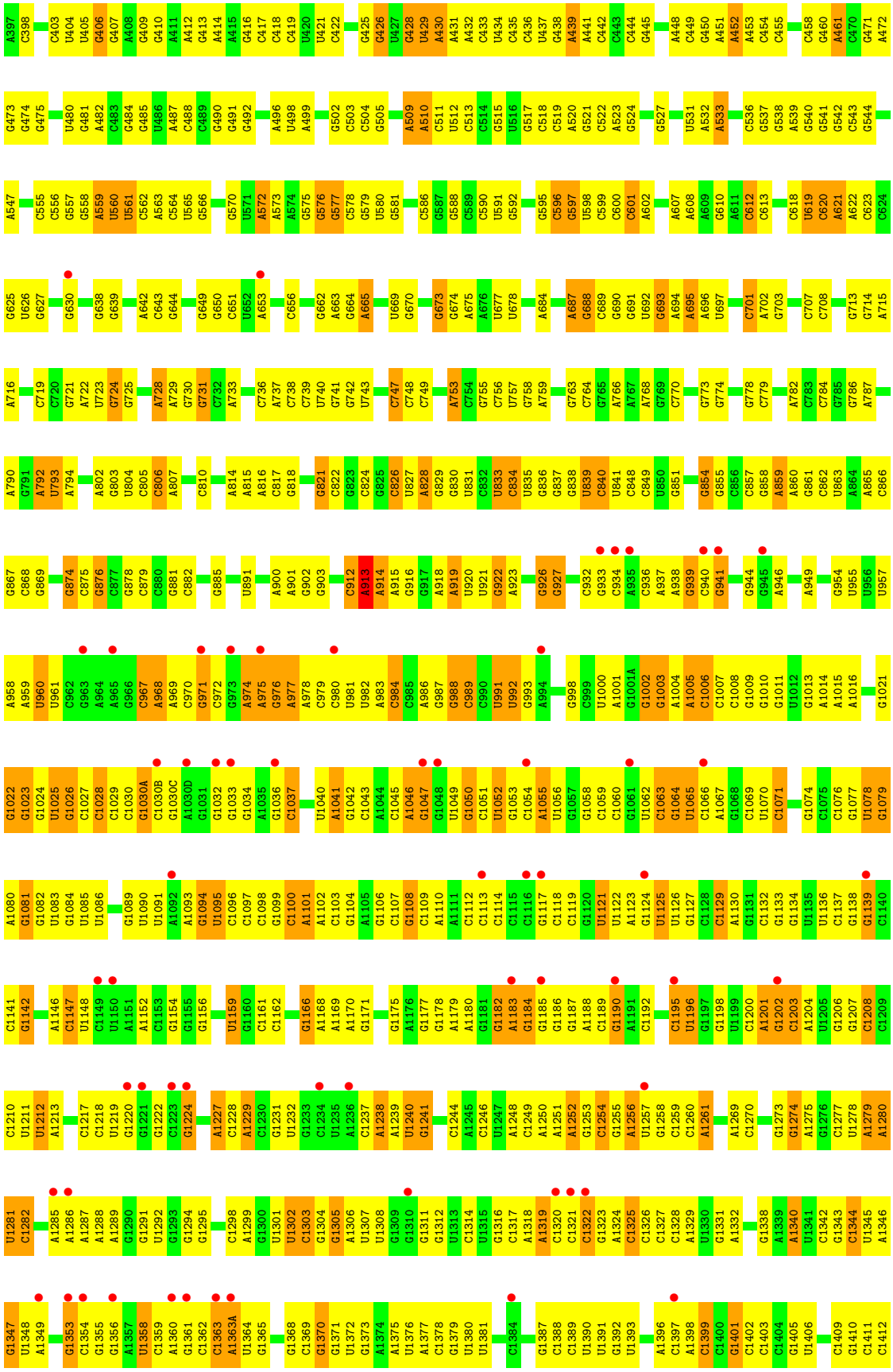

M1 K2 V3 R4 A5 S6 V7 C11 D12 K13 I17 R18 R19 R22 V23 Y24 V25 I26 N29 H32 K33 Q34 R35 Q36 G37
• Molecule 34: 16S Ribosomal RNA
Chain BA:
2%
38%
49%
11%

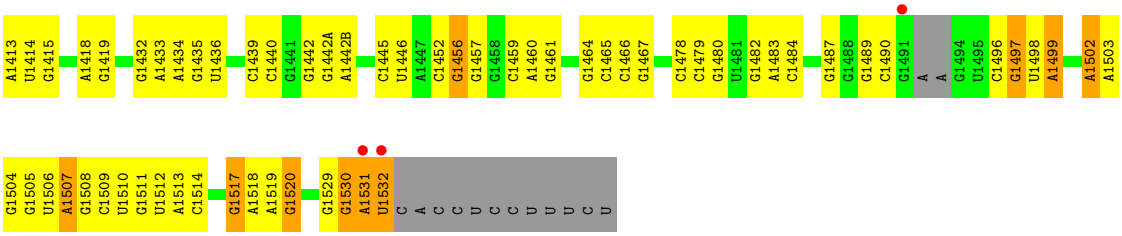


• Molecule 34: 16S Ribosomal RNA

Chain DA:

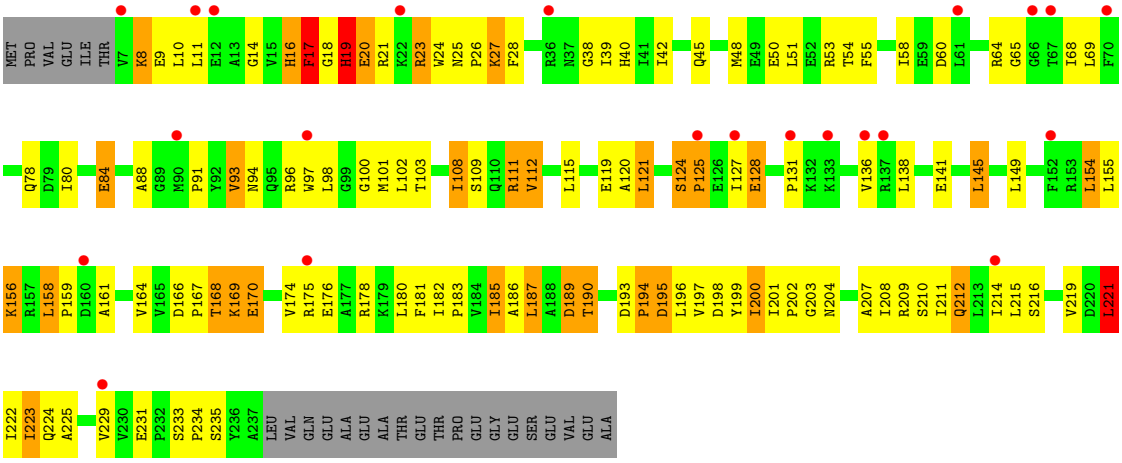



A397 C398 C403 U404 U405 G406 G407 A408 G409 G410 A411 A412 G413 A414 A415 G416 C417 C418 C419 U420 U421 C422 G425 G426 U427 G428 U429 A430 A431 A432 C433 U434 C435 C436 U437 G438 A439 A441 C442 C443 C444 G445 A448 C449 G450 A451 A452 A453 C454 C455 C458 G460 A461 C470 G471 A472
G473 G474 G475 U480 G481 A482 C483 G484 G485 U486 A487 C488 C489 G490 G491 G492 A496 U498 A499 G502 C503 C504 G505 A509 A510 C511 U512 C513 C514 G515 U516 G517 C518 C519 A520 G521 C522 A523 G524 G527 U531 A532 A533 C536 G537 G538 A539 G540 G541 G542 C543 G544
A547 C555 C556 G557 G558 A559 U560 U561 C562 A563 C564 U565 G566 G570 U571 A572 A573 A574 G575 G576 G577 C578 G579 U580 G581 C586 G587 G588 C589 C590 U591 G592 G595 C596 G597 U598 C599 C600 C601 A602 A607 A608 A609 G610 A611 C612 C613 C618 U619 C620 A621 A622 C623 C624
G625 U626 G627 G630 G638 G639 A642 C643 G644 G649 G650 C651 U652 A653 C656 G662 A663 G664 A665 U669 G670 G673 G674 A675 A676 U677 U678 A684 A687 G688 C689 G690 G691 U692 G693 A694 A695 A696 U697 C701 A702 G703 C707 C708 G713 G714 A715
A716 C719 C720 G721 A722 U723 G724 G725 A728 A729 G730 G731 C732 A733 C736 A737 C738 C739 U740 G741 G742 U743 C747 C748 C749 A753 C754 G755 C756 U757 G758 A759 G763 C764 G765 A766 A767 A768 G769 C770 G773 G774 G778 C779 A782 C783 C784 G785 G786 A787
A790 G791 A792 U793 A794 A802 G803 U804 C805 C806 A807 C810 A814 A815 A816 C817 G818 G821 C822 G823 C824 G825 C826 U827 A828 G829 G830 U831 C832 U833 C834 U835 G836 G837 G838 U839 C840 U841 C848 C849 U850 G851 G854 G855 C856 C857 G858 A859 A860 G861 C862 U863 A864 A865 C866
G867 C868 G869 G874 C875 G876 C877 C878 C879 C880 G881 C882 G885 U891 A900 A901 G902 G903 G912 A913 A914 A915 G916 G917 A918 A919 U920 U921 G922 A923 G926 G927 C932 G933 C934 A935 C936 A937 A938 G939 C940 G941 G944 G945 A946 A949 G954 U955 U956 U957
A958 A959 U960 U961 C962 G963 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 A986 G987 G988 C989 C990 U991 U992 G993 A994 G998 C999 U1000 A1001 G1001A G1002 G1003 A1004 A1005 C1006 C1007 C1008 G1009 G1010 G1011 U1012 G1013 A1014 A1015 A1016 G1021
G1022 G1023 G1024 U1025 G1026 C1027 C1028 C1029 C1030 G1030A C1030B C1030C A1030D G1031 G1032 G1033 G1034 A1035 G1036 C1037 U1040 A1041 G1042 C1043 A1044 C1045 A1046 G1047 G1048 U1049 G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 G1058 C1059 C1060 G1061 U1062 C1063 G1064 U1065 C1066 A1067 G1068 C1069 U1070 C1071 G1074 C1075 C1076 G1077 U1078 G1079
A1080 G1081 G1082 U1083 G1084 U1085 U1086 G1089 U1090 U1091 A1092 A1093 G1094 U1095 C1096 C1097 C1098 G1099 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1109 A1110 A1111 C1112 C1113 C1114 C1115 C1116 G1117 C1118 C1119 G1120 U1121 U1122 A1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 C1132 G1133 G1134 U1135 U1136 C1137 G1138 G1139 C1140
C1141 G1142 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154 G1155 G1156 U1159 G1160 C1161 C1162 G1166 A1168 A1169 A1170 G1171 G1175 A1176 U1177 G1178 A1179 A1180 G1181 G1182 A1183 G1184 G1185 G1186 G1187 A1188 C1189 G1190 A1191 C1192 C1195 U1196 G1197 G1198 U1199 C1200 A1201 G1202 C1203 A1204 U1205 G1206 G1207 C1208 C1209
C1210 U1211 U1212 A1213 C1217 C1218 U1219 G1220 G1221 G1222 C1223 G1224 A1227 C1228 A1229 C1230 G1231 U1232 G1233 C1234 U1235 A1236 C1237 A1238 A1239 U1240 G1241 C1244 A1245 C1246 U1247 A1248 C1249 A1250 A1251 A1252 C1253 C1254 G1255 A1256 U1257 G1258 C1259 C1260 A1261 A1269 C1270 G1273 G1274 A1275 G1276 C1277 U1278 A1279 A1280
U1281 C1282 A1285 A1286 A1287 A1288 A1289 G1290 G1291 U1292 G1293 G1294 G1295 C1298 A1299 G1300 U1301 U1302 C1303 G1304 G1305 A1306 U1307 U1308 G1309 G1310 G1311 G1312 U1313 C1314 U1315 G1316 C1317 A1318 A1319 C1320 C1321 C1322 G1323 A1324 C1325 C1326 C1327 C1328 A1329 U1330 G1331 A1332 G1338 A1339 A1340 U1341 C1342 G1343 C1344 U1345 A1346
G1347 U1348 A1349 G1353 C1354 G1355 G1356 A1357 U1358 C1359 A1360 G1361 C1362 C1363 A1363A U1364 G1365 G1368 C1369 G1370 G1371 U1372 G1373 A1374 A1375 U1376 A1377 C1378 G1379 U1380 U1381 C1384 G1387 C1388 C1389 U1390 U1391 G1392 U1393 A1396 C1397 A1398 C1399 C1400 G1401 C1402 C1403 C1404 G1405 U1406 C1409 G1410 C1411 C1412



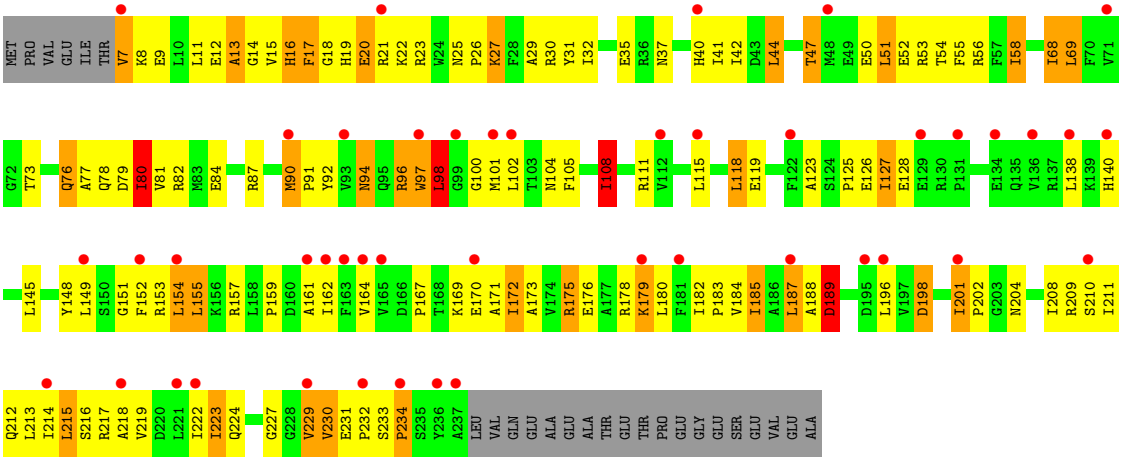
- Molecule 35: 30S ribosomal protein S2

Chain BB:



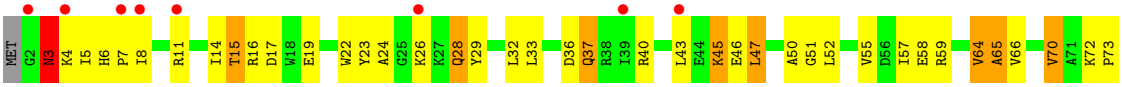
- Molecule 35: 30S ribosomal protein S2

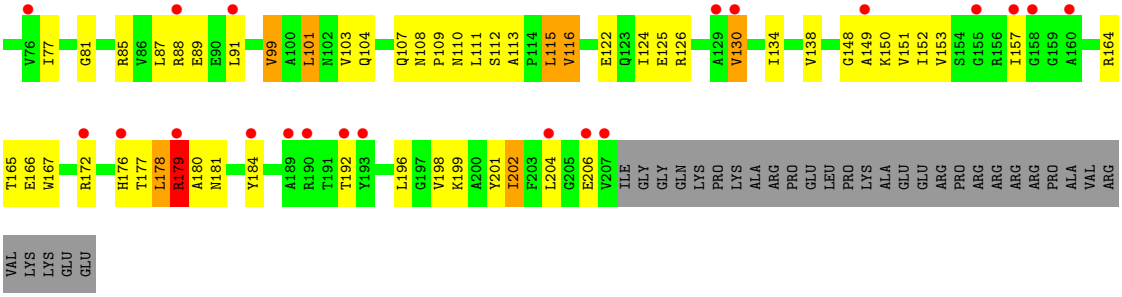
Chain DB:



- Molecule 36: 30S ribosomal protein S3

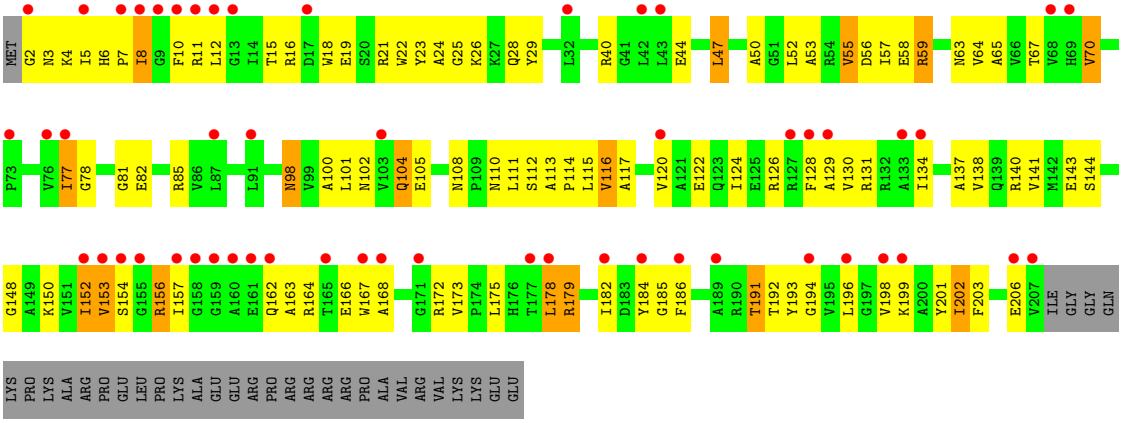
Chain BC:





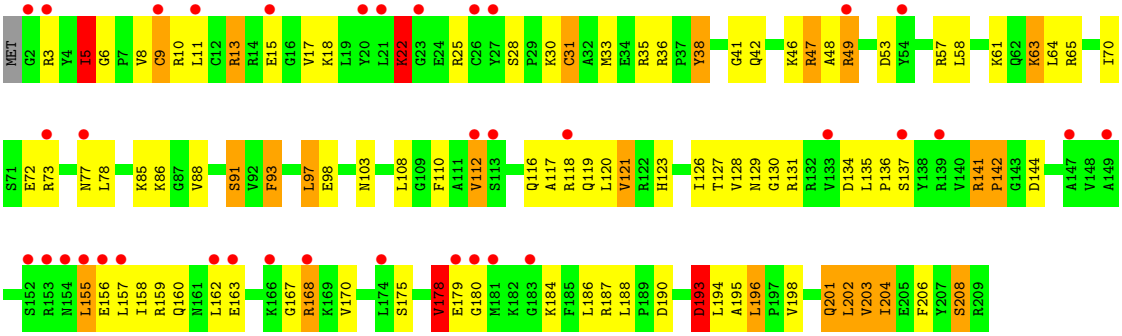
- Molecule 36: 30S ribosomal protein S3

Chain DC:



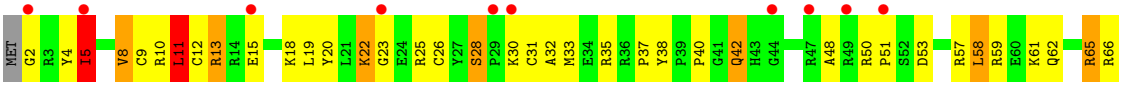
- Molecule 37: 30S ribosomal protein S4

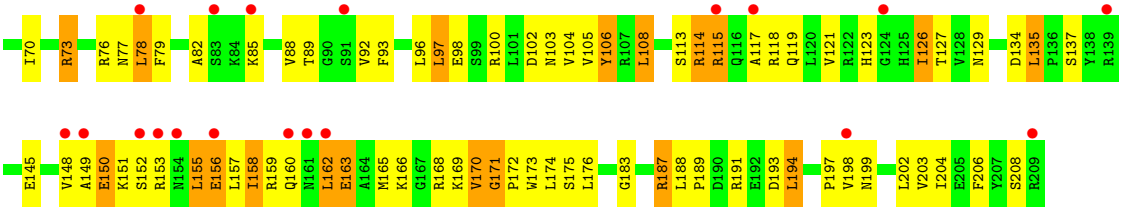
Chain BD:



- Molecule 37: 30S ribosomal protein S4

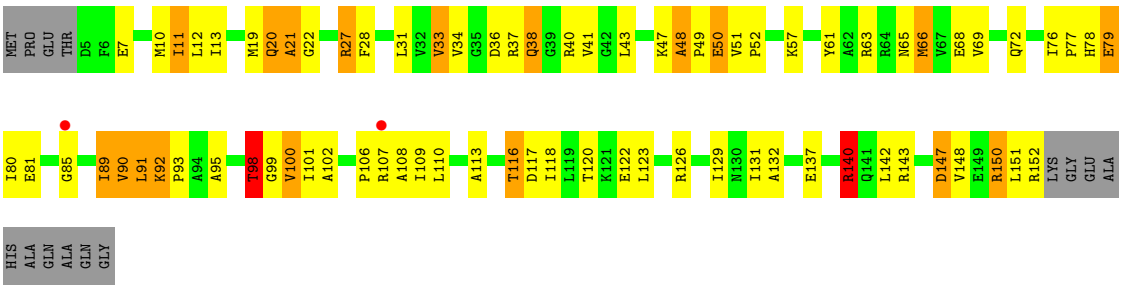
Chain DD:





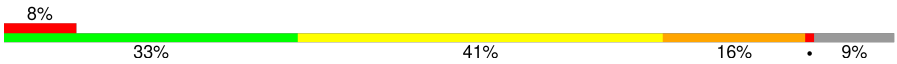
- Molecule 38: 30S ribosomal protein S5

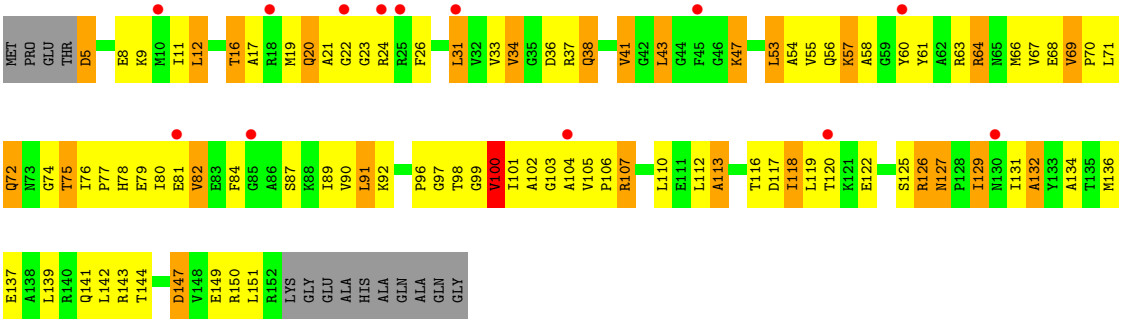
Chain BE:



- Molecule 38: 30S ribosomal protein S5

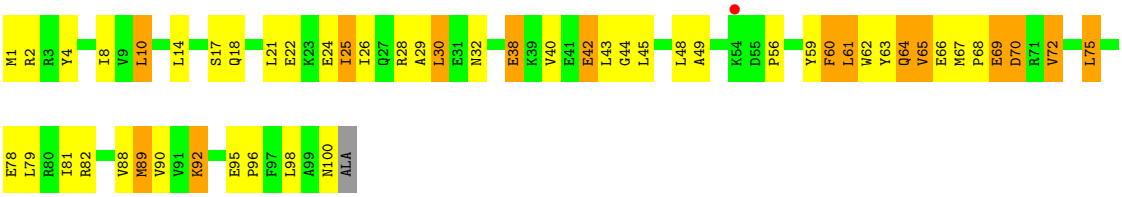
Chain DE:





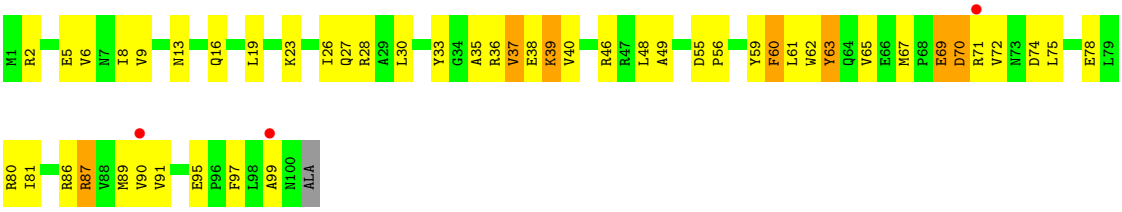
- Molecule 39: 30S ribosomal protein S6

Chain BF:



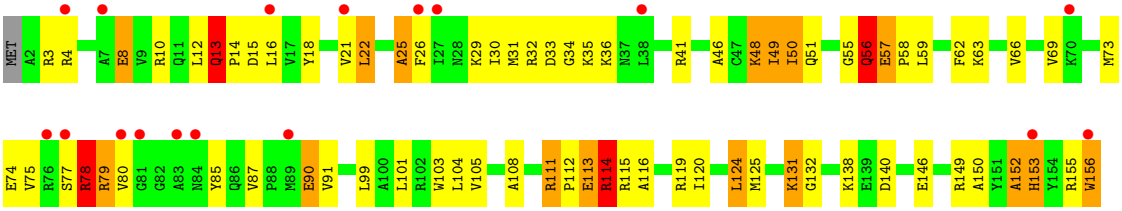
- Molecule 39: 30S ribosomal protein S6

Chain DF:



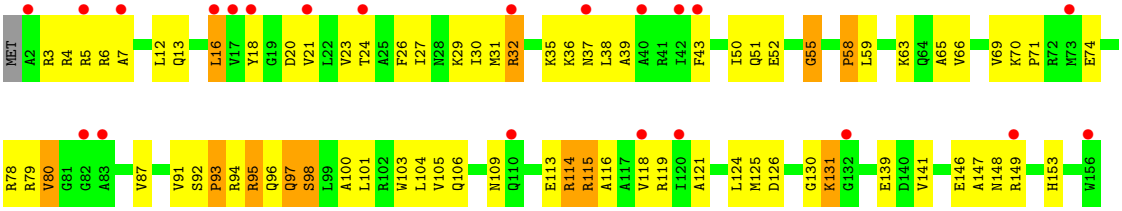
- Molecule 40: 30S ribosomal protein S7

Chain BG:



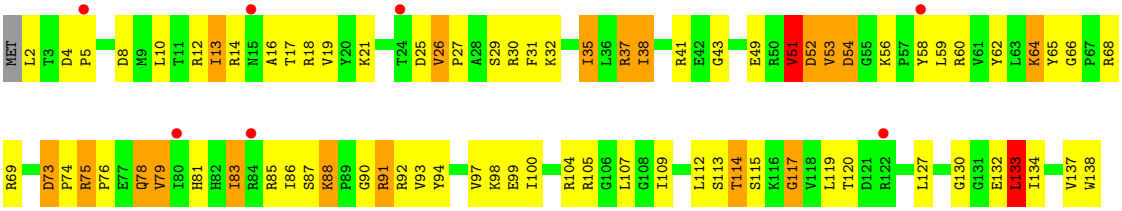
- Molecule 40: 30S ribosomal protein S7

Chain DG:



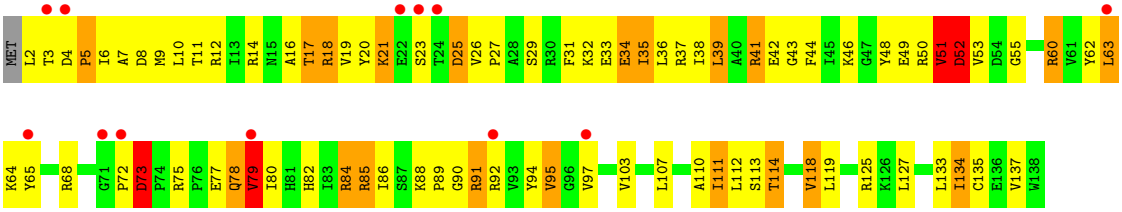
- Molecule 41: 30S ribosomal protein S8

Chain BH:



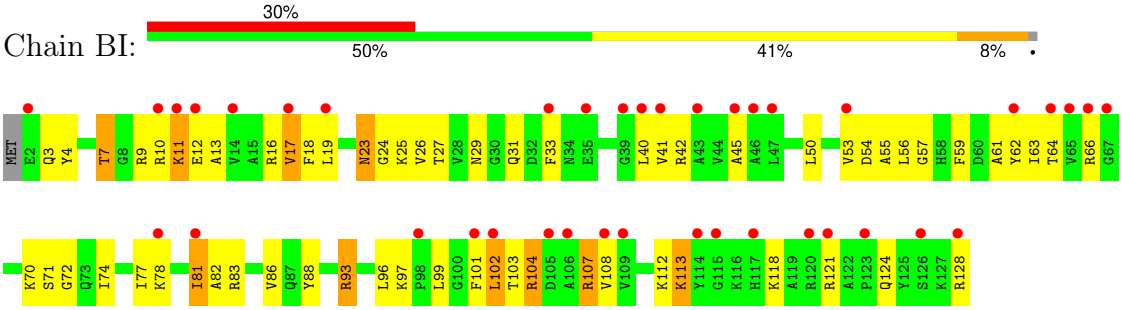
- Molecule 41: 30S ribosomal protein S8

Chain DH:



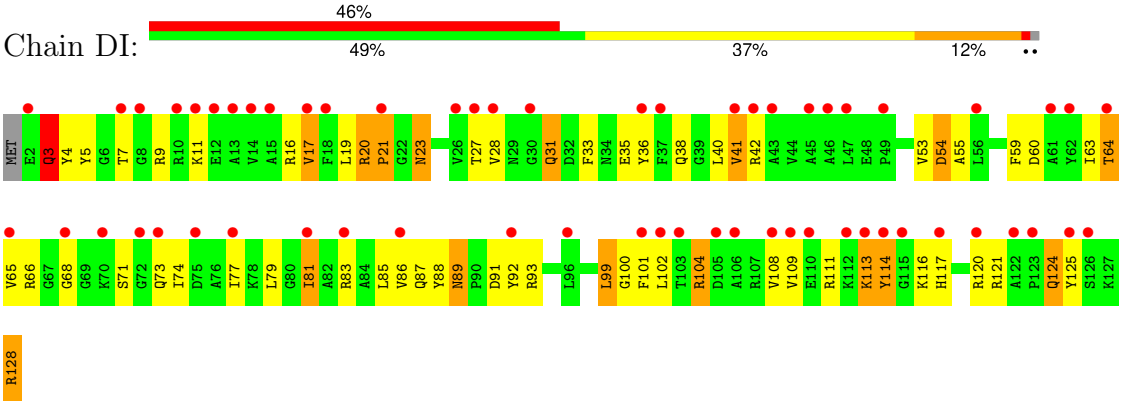
- Molecule 42: 30S ribosomal protein S9

Chain BI:



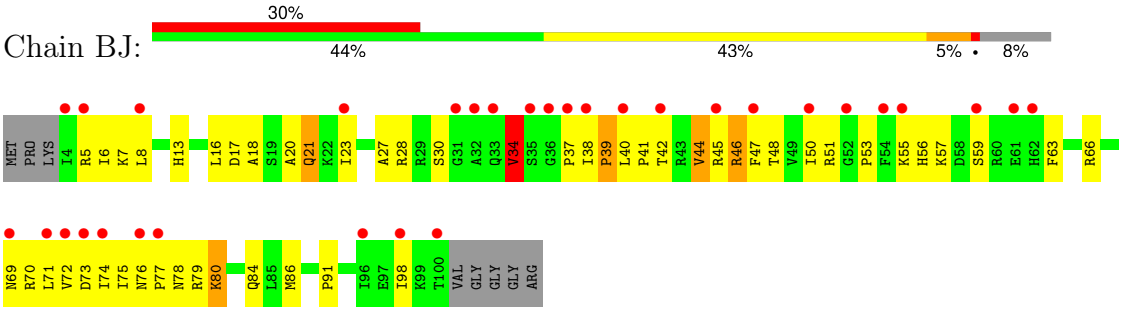
- Molecule 42: 30S ribosomal protein S9

Chain DI:



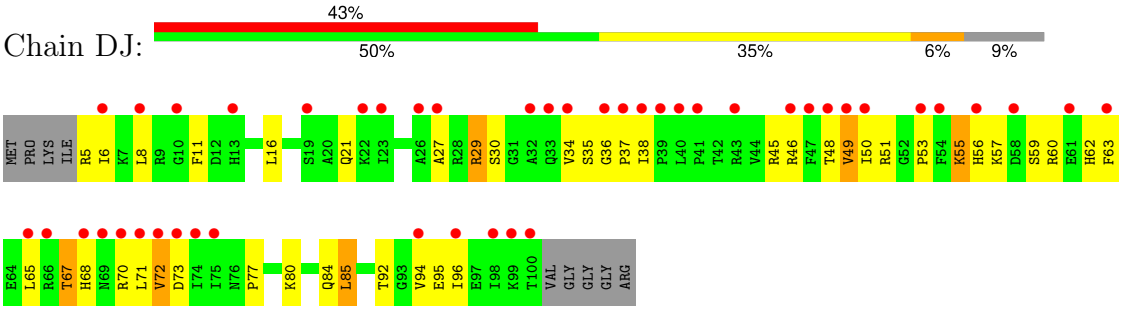
- Molecule 43: 30S ribosomal protein S10

Chain BJ:



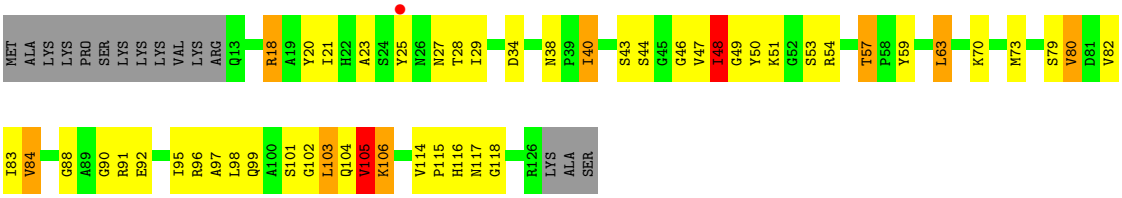
- Molecule 43: 30S ribosomal protein S10

Chain DJ:



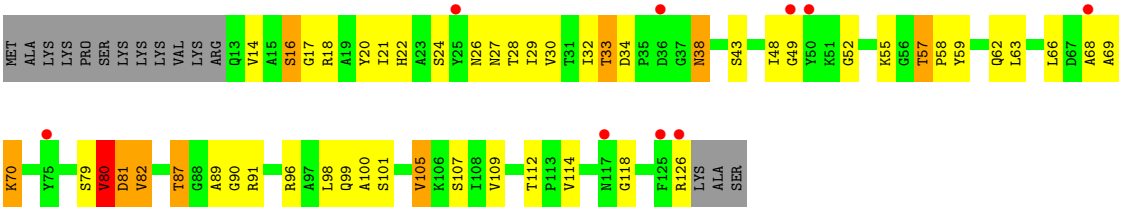
- Molecule 44: 30S ribosomal protein S11

Chain BK:



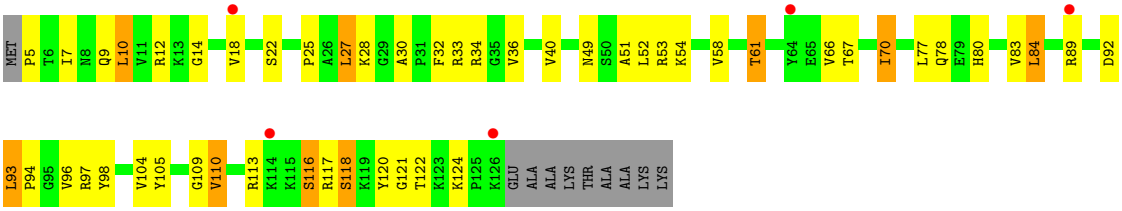
• Molecule 44: 30S ribosomal protein S11

Chain DK:



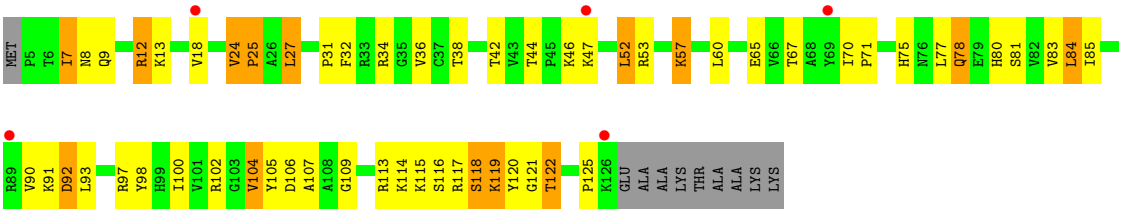
• Molecule 45: 30S ribosomal protein S12

Chain BL:



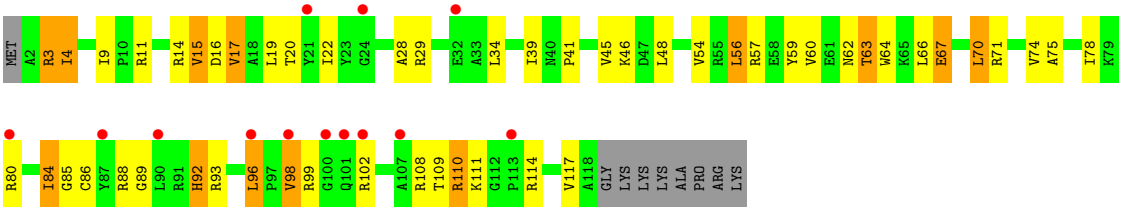
• Molecule 45: 30S ribosomal protein S12

Chain DL:



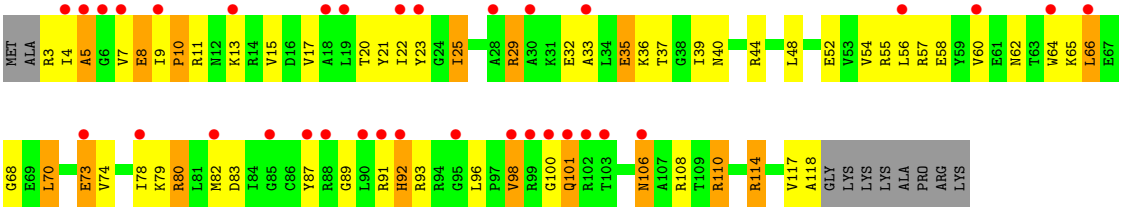
• Molecule 46: 30S ribosomal protein S13

Chain BM:



- Molecule 46: 30S ribosomal protein S13

Chain DM:

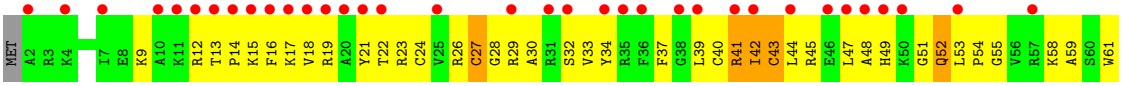


- Molecule 47: 30S ribosomal protein S14 type Z

Chain BN:

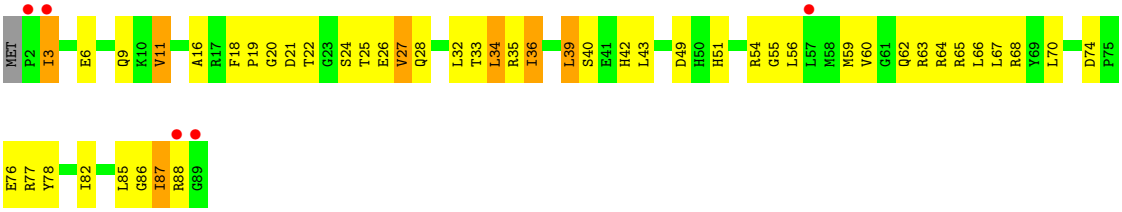
- Molecule 47: 30S ribosomal protein S14 type Z

Chain DN:



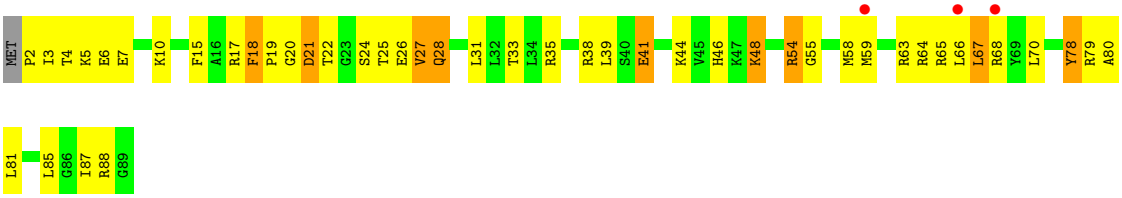
- Molecule 48: 30S ribosomal protein S15

Chain BO:



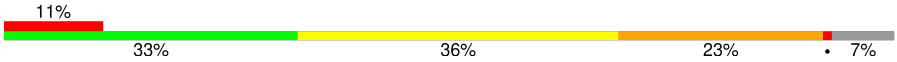
- Molecule 48: 30S ribosomal protein S15

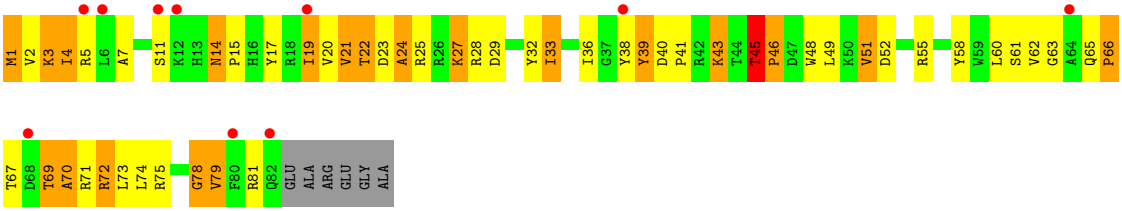
Chain DO:



- Molecule 49: 30S ribosomal protein S16

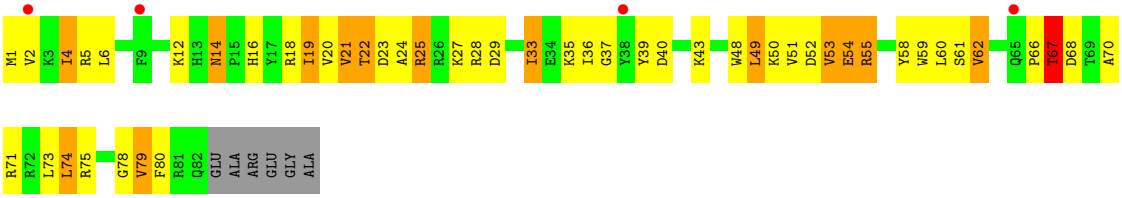
Chain BP:





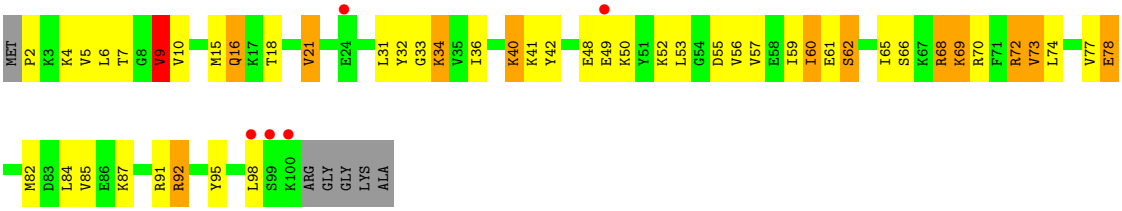
- Molecule 49: 30S ribosomal protein S16

Chain DP:



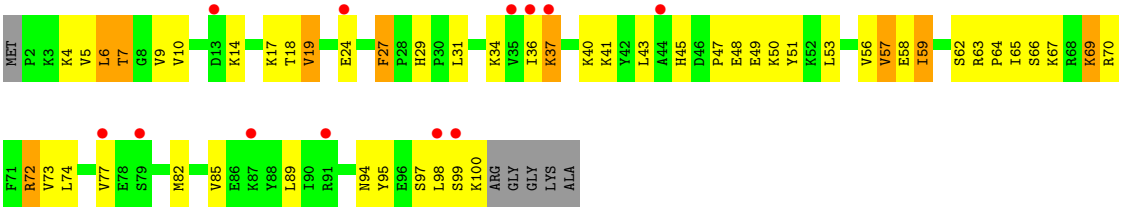
- Molecule 50: 30S ribosomal protein S17

Chain BQ:



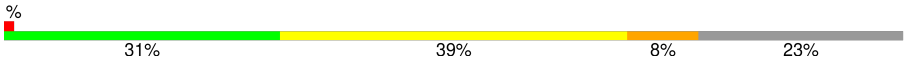
- Molecule 50: 30S ribosomal protein S17

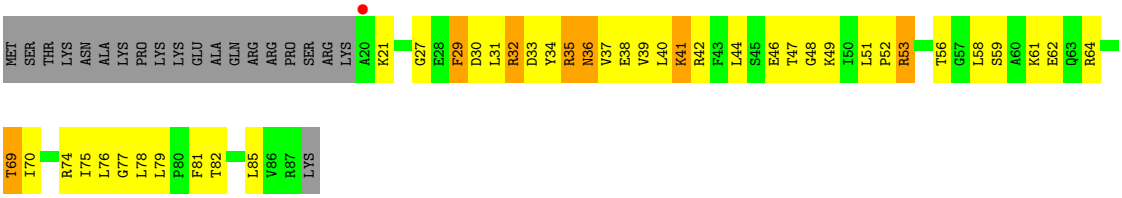
Chain DQ:



- Molecule 51: 30S ribosomal protein S18

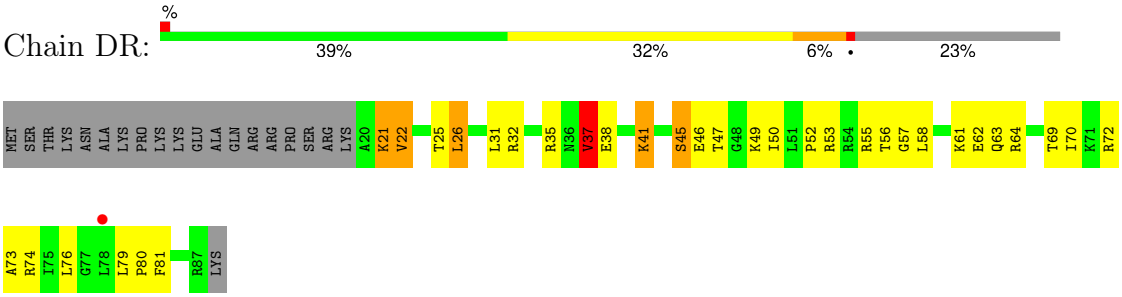
Chain BR:





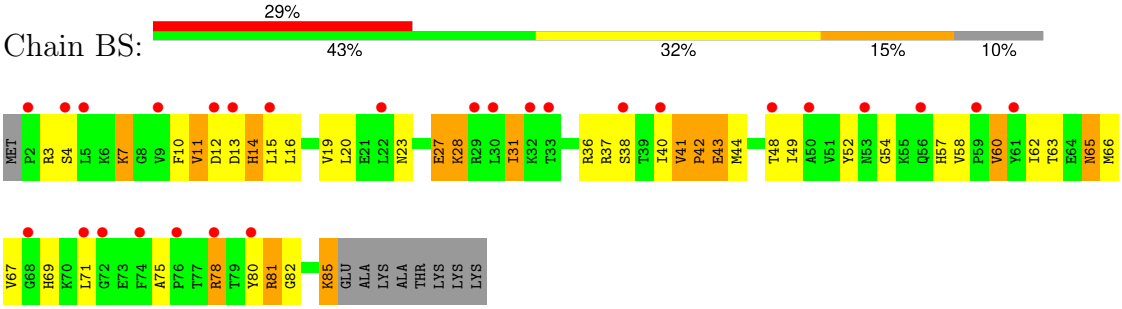
- Molecule 51: 30S ribosomal protein S18

Chain DR:



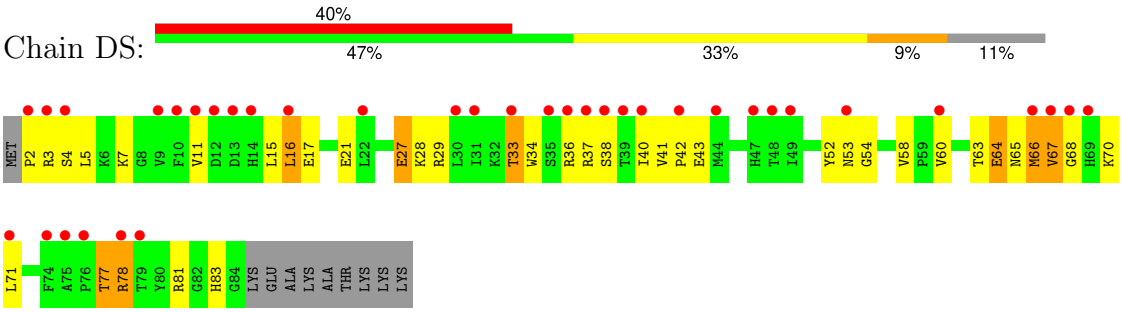
- Molecule 52: 30S ribosomal protein S19

Chain BS:



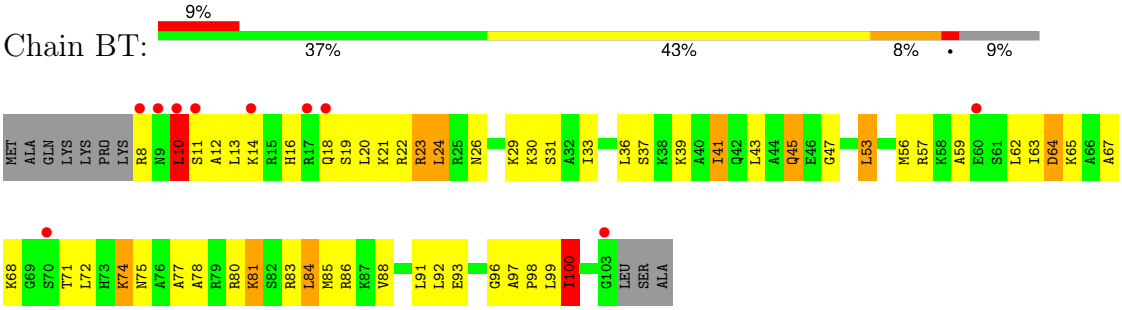
- Molecule 52: 30S ribosomal protein S19

Chain DS:



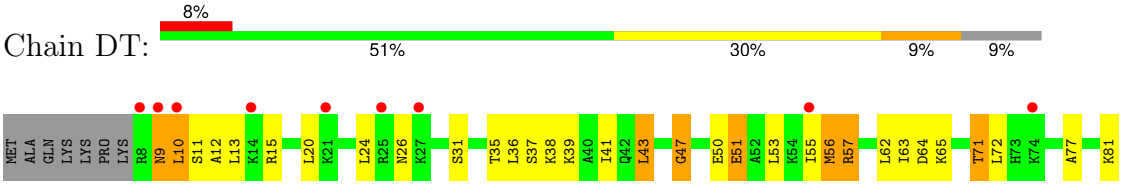
- Molecule 53: 30S ribosomal protein S20

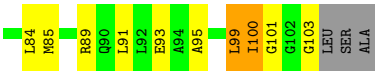
Chain BT:



- Molecule 53: 30S ribosomal protein S20

Chain DT:





• Molecule 54: 30S ribosomal protein Thx

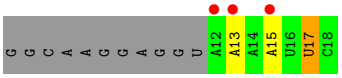
Chain BU:

• Molecule 54: 30S ribosomal protein Thx

Chain DU:

• Molecule 55: mRNA

Chain BV:

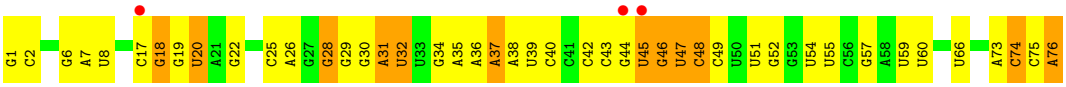


• Molecule 55: mRNA

Chain DV:

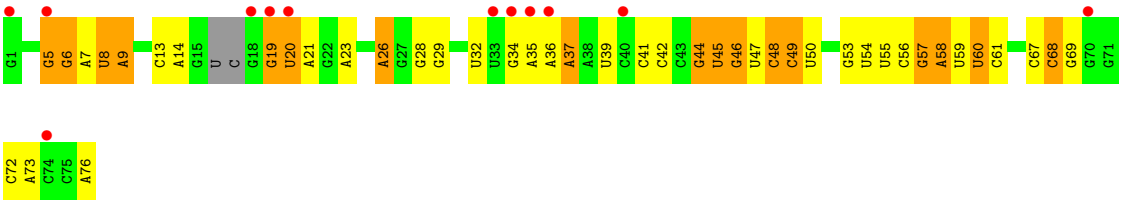
• Molecule 56: P-site tRNA

Chain BW:



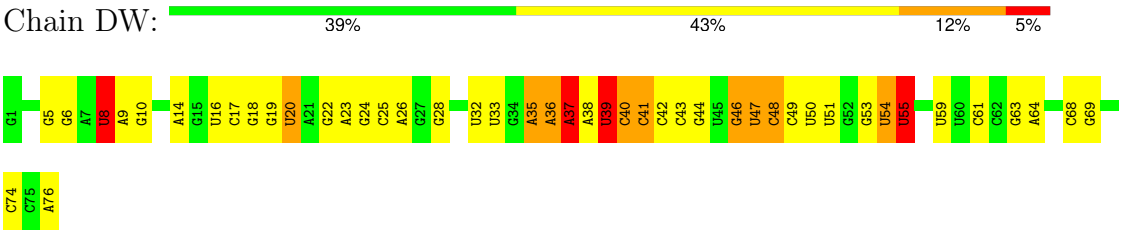
• Molecule 56: P-site tRNA

Chain BY:



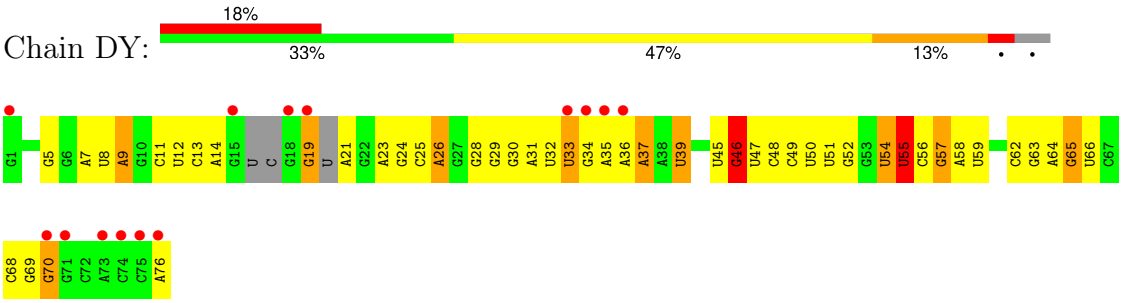
- Molecule 56: P-site tRNA

Chain DW:



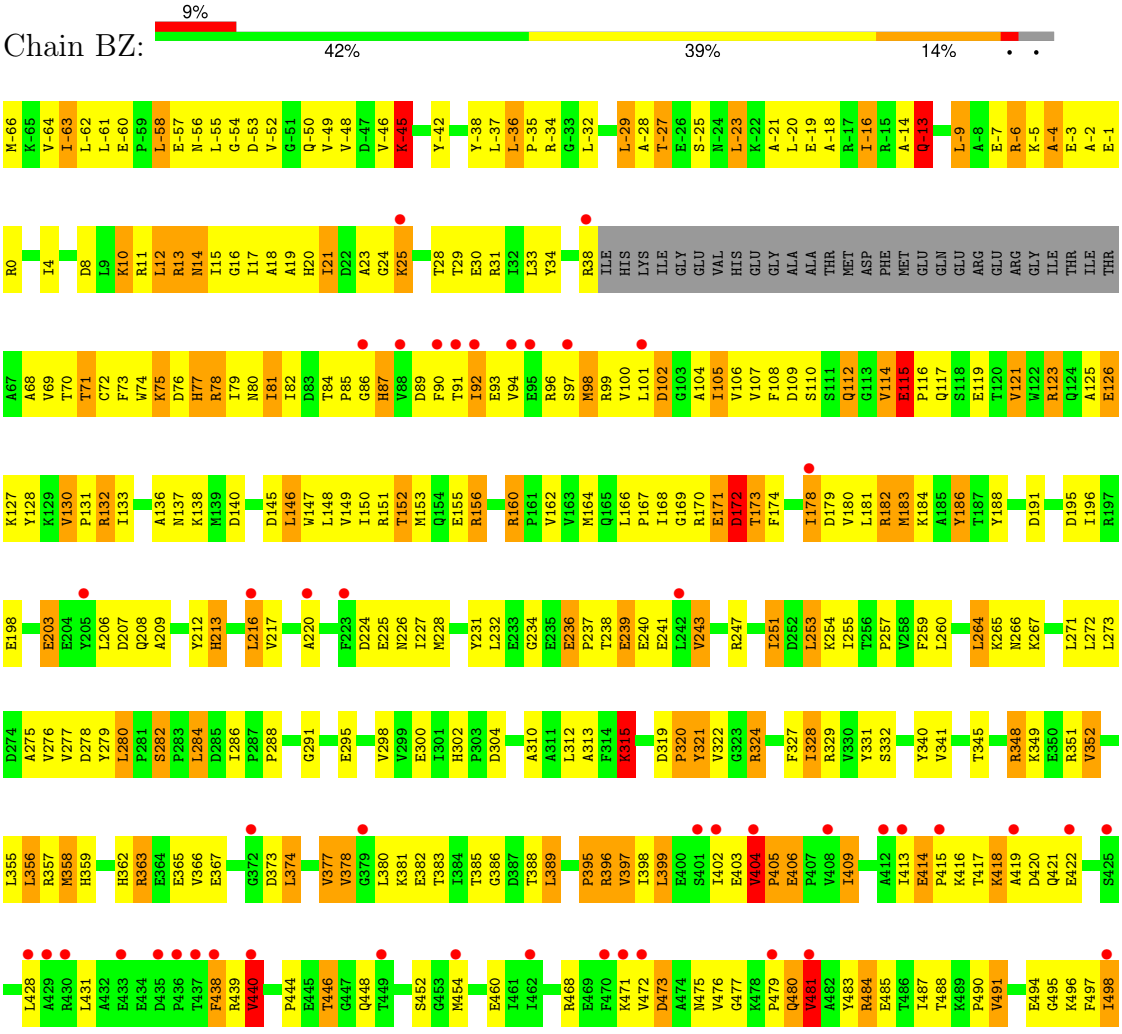
- Molecule 56: P-site tRNA

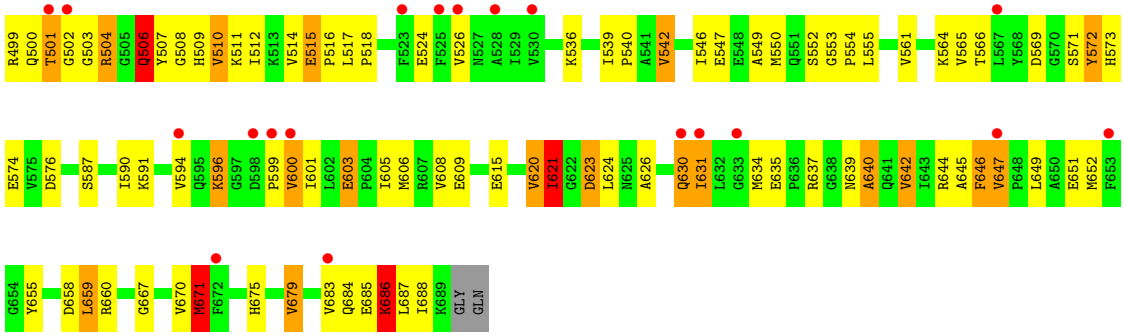
Chain DY:



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

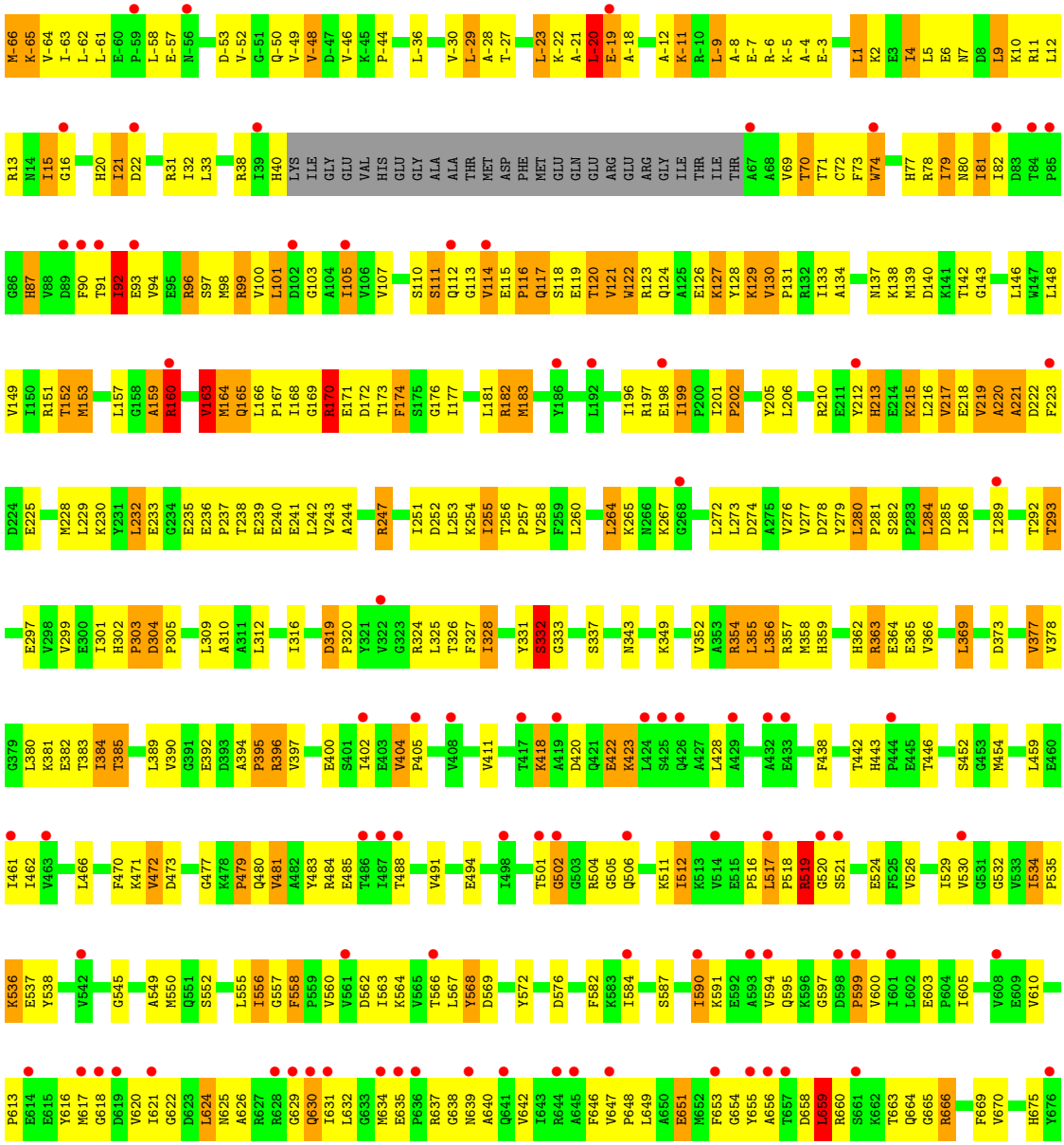
Chain BZ:

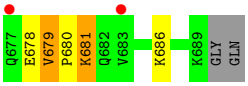




• Molecule 57: 50S ribosomal protein L9,Elongation factor G

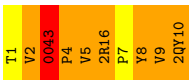
Chain DZ:





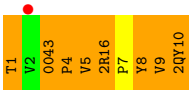
- Molecule 58: Dityromycin

Chain BX:



- Molecule 58: Dityromycin

Chain DX:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.84Å 450.58Å 623.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 2.80 49.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.5 (49.81-2.80) 94.5 (49.81-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.209 , 0.264 0.210 , 0.264	Depositor DCC
R_{free} test set	67916 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 73.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	310038	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MVA, PSU, 4SU, 5MU, SF4, GDP, 2R3, 7MG, MIA, 2QY, 004, 2R1, MG, 2QZ, ZN

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	0.75	0/69281	0.92	47/108144 (0.0%)
1	CA	0.54	0/69179	0.76	7/107984 (0.0%)
2	AB	0.63	0/2878	0.88	0/4490
2	CB	0.37	0/2878	0.62	0/4490
3	AC	0.42	0/1083	0.97	6/1460 (0.4%)
3	CC	0.42	0/1083	0.97	5/1460 (0.3%)
4	AD	1.14	5/2186 (0.2%)	1.39	19/2944 (0.6%)
4	CD	0.95	2/2192 (0.1%)	1.30	12/2951 (0.4%)
5	AE	1.17	1/1592 (0.1%)	1.54	28/2149 (1.3%)
5	CE	0.91	1/1592 (0.1%)	1.34	20/2149 (0.9%)
6	AF	1.14	1/1619 (0.1%)	1.42	14/2193 (0.6%)
6	CF	0.77	0/1615	1.17	7/2188 (0.3%)
7	AG	0.75	0/1450	1.24	16/1959 (0.8%)
7	CG	0.49	0/1449	1.03	3/1958 (0.2%)
8	AH	1.06	3/1356 (0.2%)	1.40	16/1834 (0.9%)
8	CH	0.64	0/1356	1.05	8/1834 (0.4%)
9	AK	0.59	0/640	1.53	12/889 (1.3%)
9	CK	0.48	0/640	1.62	10/889 (1.1%)
10	AL	0.48	0/503	0.96	3/673 (0.4%)
10	CL	0.53	0/503	1.13	4/673 (0.6%)
11	AN	1.14	1/1144 (0.1%)	1.33	6/1543 (0.4%)
11	CN	0.78	0/1144	1.20	6/1543 (0.4%)
12	AO	1.14	2/943 (0.2%)	1.39	8/1269 (0.6%)
12	CO	0.94	0/943	1.27	5/1269 (0.4%)
13	AP	1.02	0/1156	1.37	10/1537 (0.7%)
13	CP	0.71	0/1152	1.25	12/1533 (0.8%)
14	AQ	1.14	0/1143	1.32	9/1527 (0.6%)
14	CQ	0.79	0/1143	1.23	8/1527 (0.5%)
15	AR	1.18	2/982 (0.2%)	1.35	7/1312 (0.5%)
15	CR	0.84	0/982	1.16	1/1312 (0.1%)
16	AS	0.90	0/887	1.22	9/1180 (0.8%)
16	CS	0.59	0/880	1.07	1/1172 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AT	1.08	1/1105 (0.1%)	1.30	6/1477 (0.4%)
17	CT	0.83	0/1097	1.15	5/1468 (0.3%)
18	AU	1.31	0/977	1.39	9/1301 (0.7%)
18	CU	0.85	0/977	1.09	3/1301 (0.2%)
19	AV	1.21	2/782 (0.3%)	1.54	9/1049 (0.9%)
19	CV	0.76	0/782	1.12	2/1049 (0.2%)
20	AW	1.30	3/897 (0.3%)	1.34	7/1205 (0.6%)
20	CW	0.99	0/897	1.29	6/1205 (0.5%)
21	AX	1.17	2/764 (0.3%)	1.34	7/1025 (0.7%)
21	CX	0.82	0/764	1.19	6/1025 (0.6%)
22	AY	1.06	1/819 (0.1%)	1.46	9/1095 (0.8%)
22	CY	0.66	0/819	1.10	5/1095 (0.5%)
23	AZ	0.87	0/1483	1.31	13/2017 (0.6%)
23	CZ	0.61	1/1483 (0.1%)	1.16	11/2017 (0.5%)
24	A0	1.12	1/616 (0.2%)	1.35	3/821 (0.4%)
24	C0	0.73	0/616	1.16	6/821 (0.7%)
25	A1	1.08	1/762 (0.1%)	1.32	6/1014 (0.6%)
25	C1	0.82	0/762	1.22	6/1014 (0.6%)
26	A2	0.97	0/590	1.21	1/781 (0.1%)
26	C2	0.72	0/590	1.10	2/781 (0.3%)
27	A3	1.28	3/474 (0.6%)	1.51	6/635 (0.9%)
27	C3	0.75	0/469	1.20	3/630 (0.5%)
28	A4	0.58	0/571	1.21	7/768 (0.9%)
28	C4	0.50	0/545	1.08	4/737 (0.5%)
29	A5	1.29	2/469 (0.4%)	1.48	6/635 (0.9%)
29	C5	0.96	0/469	1.30	5/635 (0.8%)
30	A6	1.13	2/460 (0.4%)	1.32	1/613 (0.2%)
30	C6	0.79	0/456	1.04	0/608
31	A7	1.22	1/426 (0.2%)	1.27	3/561 (0.5%)
31	C7	0.96	1/426 (0.2%)	1.32	4/561 (0.7%)
32	A8	1.15	0/525	1.35	6/691 (0.9%)
32	C8	0.78	0/525	1.19	1/691 (0.1%)
33	A9	1.18	1/310 (0.3%)	1.43	4/407 (1.0%)
33	C9	0.78	0/310	1.17	1/407 (0.2%)
34	BA	0.43	0/35976	0.67	5/56145 (0.0%)
34	DA	0.38	0/36119	0.60	2/56370 (0.0%)
35	BB	0.55	0/1881	1.13	15/2542 (0.6%)
35	DB	0.51	0/1860	1.04	8/2518 (0.3%)
36	BC	0.54	0/1576	0.94	2/2130 (0.1%)
36	DC	0.51	0/1568	0.93	4/2122 (0.2%)
37	BD	0.64	1/1689 (0.1%)	1.09	9/2267 (0.4%)
37	DD	0.61	0/1708	1.12	9/2289 (0.4%)
38	BE	0.75	0/1145	1.11	4/1543 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	DE	0.66	0/1149	1.19	9/1548 (0.6%)
39	BF	0.65	0/825	1.12	5/1118 (0.4%)
39	DF	0.63	0/833	1.05	3/1128 (0.3%)
40	BG	0.54	0/1250	0.99	9/1679 (0.5%)
40	DG	0.45	0/1254	0.98	3/1683 (0.2%)
41	BH	0.69	0/1108	1.19	9/1494 (0.6%)
41	DH	0.58	0/1108	1.10	5/1494 (0.3%)
42	BI	0.58	0/1005	0.99	1/1350 (0.1%)
42	DI	0.49	0/997	0.95	4/1343 (0.3%)
43	BJ	0.53	0/722	1.08	7/982 (0.7%)
43	DJ	0.49	0/727	0.96	1/988 (0.1%)
44	BK	0.73	0/848	1.18	7/1149 (0.6%)
44	DK	0.59	0/848	1.08	4/1149 (0.3%)
45	BL	0.78	0/946	1.16	6/1274 (0.5%)
45	DL	0.76	0/946	1.14	2/1274 (0.2%)
46	BM	0.52	0/933	1.03	1/1253 (0.1%)
46	DM	0.41	0/917	0.86	2/1234 (0.2%)
47	BN	0.55	0/501	1.05	2/664 (0.3%)
47	DN	0.43	0/501	0.91	0/664
48	BO	0.76	0/739	1.14	4/985 (0.4%)
48	DO	0.61	0/739	1.02	3/985 (0.3%)
49	BP	0.70	0/697	1.15	6/939 (0.6%)
49	DP	0.66	0/693	1.10	6/935 (0.6%)
50	BQ	0.69	0/836	1.12	5/1117 (0.4%)
50	DQ	0.61	0/836	1.05	3/1117 (0.3%)
51	BR	0.70	0/560	1.17	4/746 (0.5%)
51	DR	0.62	0/560	1.03	2/746 (0.3%)
52	BS	0.48	0/676	1.03	4/911 (0.4%)
52	DS	0.46	0/661	1.02	1/893 (0.1%)
53	BT	0.66	0/730	1.19	2/965 (0.2%)
53	DT	0.61	0/733	1.07	1/969 (0.1%)
54	BU	0.48	0/203	0.93	0/266
54	DU	0.48	0/203	0.95	1/266 (0.4%)
55	BV	0.36	0/165	0.61	0/254
55	DV	0.32	0/137	0.64	0/211
56	BW	0.48	0/1650	0.74	0/2569
56	BY	0.27	1/1602 (0.1%)	0.43	0/2493
56	DW	0.38	0/1650	0.59	0/2569
56	DY	0.23	0/1579	0.34	0/2455
57	BZ	0.64	0/5763	1.10	29/7804 (0.4%)
57	DZ	0.61	0/5784	1.11	41/7835 (0.5%)
58	BX	0.65	0/20	0.73	0/23
58	DX	0.72	0/20	1.46	0/23

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.65	42/329767 (0.0%)	0.91	742/491645 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	AE	0	1
6	AF	0	1
19	AV	0	1
35	BB	0	1
57	DZ	0	1
58	BX	0	1
All	All	0	6

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	AO	24	VAL	CA-CB	12.14	1.68	1.54
8	AH	11	VAL	CA-CB	-7.32	1.47	1.54
15	AR	52	ILE	CA-CB	-7.18	1.46	1.54
29	A5	35	GLU	CA-C	-7.03	1.46	1.53
5	AE	12	THR	CA-C	-6.95	1.47	1.53

The worst 5 of 742 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	CK	76	GLY	CA-C-N	15.68	139.44	119.84
9	CK	76	GLY	C-N-CA	15.68	139.44	119.84
9	AK	76	GLY	CA-C-N	13.99	137.33	119.84
9	AK	76	GLY	C-N-CA	13.99	137.33	119.84
9	CK	128	LEU	CA-C-N	11.91	134.73	119.84

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
35	BB	93	VAL	Peptide
58	BX	3	004	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	61861	0	31172	862	0
1	CA	61771	0	31146	1176	0
2	AB	2573	0	1306	27	0
2	CB	2573	0	1306	57	0
3	AC	1063	0	1091	157	4
3	CC	1063	0	1090	183	17
4	AD	2136	0	2218	88	0
4	CD	2142	0	2229	89	0
5	AE	1559	0	1618	64	0
5	CE	1559	0	1618	78	0
6	AF	1584	0	1625	67	0
6	CF	1580	0	1619	79	0
7	AG	1425	0	1443	68	0
7	CG	1424	0	1434	85	0
8	AH	1330	0	1407	56	0
8	CH	1330	0	1407	54	0
9	AK	641	0	309	16	0
9	CK	641	0	309	10	0
10	AL	498	0	521	23	0
10	CL	498	0	521	29	0
11	AN	1117	0	1184	35	0
11	CN	1117	0	1184	40	0
12	AO	933	0	996	32	0
12	CO	933	0	996	28	0
13	AP	1139	0	1223	44	0
13	CP	1135	0	1212	58	0
14	AQ	1122	0	1179	39	0
14	CQ	1122	0	1179	56	0
15	AR	968	0	1033	34	0
15	CR	968	0	1033	40	0
16	AS	877	0	938	43	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	68	0
17	AT	1091	0	1151	51	0
17	CT	1083	0	1136	43	0
18	AU	959	0	1019	30	0
18	CU	959	0	1018	41	0
19	AV	771	0	830	12	0
19	CV	771	0	830	25	0
20	AW	886	0	940	24	0
20	CW	886	0	940	41	0
21	AX	750	0	814	24	0
21	CX	750	0	814	28	0
22	AY	806	0	881	37	0
22	CY	806	0	882	45	0
23	AZ	1451	0	1457	64	0
23	CZ	1451	0	1457	74	0
24	A0	608	0	622	20	0
24	C0	608	0	622	27	0
25	A1	755	0	826	30	0
25	C1	755	0	826	24	0
26	A2	588	0	643	18	0
26	C2	588	0	643	31	0
27	A3	469	0	518	12	0
27	C3	464	0	514	25	0
28	A4	558	0	545	31	0
28	C4	532	0	507	30	0
29	A5	455	0	465	15	0
29	C5	455	0	465	17	0
30	A6	453	0	473	17	0
30	C6	449	0	469	21	0
31	A7	418	0	467	17	0
31	C7	418	0	467	12	0
32	A8	517	0	582	28	0
32	C8	517	0	582	25	0
33	A9	307	0	335	11	0
33	C9	307	0	335	14	0
34	BA	32141	0	16224	691	0
34	DA	32268	0	16287	744	0
35	BB	1846	0	1867	83	0
35	DB	1825	0	1828	102	0
36	BC	1552	0	1546	66	0
36	DC	1544	0	1524	65	0
37	BD	1659	0	1679	68	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	DD	1678	0	1719	86	0
38	BE	1129	0	1185	54	0
38	DE	1133	0	1191	69	0
39	BF	812	0	804	32	0
39	DF	820	0	814	38	0
40	BG	1231	0	1238	49	0
40	DG	1235	0	1249	54	0
41	BH	1088	0	1126	54	0
41	DH	1088	0	1126	77	0
42	BI	986	0	995	54	0
42	DI	978	0	966	55	0
43	BJ	709	0	650	32	0
43	DJ	714	0	672	32	0
44	BK	833	0	836	35	0
44	DK	833	0	836	27	0
45	BL	930	0	980	39	0
45	DL	930	0	980	47	0
46	BM	923	0	970	39	0
46	DM	907	0	934	42	0
47	BN	492	0	529	31	0
47	DN	492	0	531	46	0
48	BO	728	0	760	33	0
48	DO	728	0	760	31	0
49	BP	681	0	697	52	0
49	DP	677	0	686	37	0
50	BQ	823	0	891	35	0
50	DQ	823	0	891	35	0
51	BR	555	0	618	27	0
51	DR	555	0	618	30	0
52	BS	661	0	675	38	0
52	DS	646	0	644	34	0
53	BT	728	0	798	39	0
53	DT	731	0	807	28	0
54	BU	199	0	208	7	0
54	DU	199	0	208	9	0
55	BV	148	0	76	3	0
55	DV	123	0	66	1	0
56	BW	1631	0	839	25	0
56	BY	1581	0	805	25	0
56	DW	1631	0	839	33	0
56	DY	1561	0	796	33	0
57	BZ	5663	0	5747	286	17

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DZ	5682	0	5766	243	4
58	BX	93	0	85	14	0
58	DX	93	0	85	15	0
59	A0	5	0	0	0	0
59	A2	1	0	0	0	0
59	A5	1	0	0	0	0
59	A6	2	0	0	0	0
59	A7	4	0	0	0	0
59	A8	1	0	0	0	0
59	A9	1	0	0	0	0
59	AA	821	0	0	0	0
59	AB	23	0	0	0	0
59	AD	12	0	0	0	0
59	AE	5	0	0	0	0
59	AF	8	0	0	0	0
59	AG	2	0	0	0	0
59	AH	1	0	0	0	0
59	AN	3	0	0	0	0
59	AO	1	0	0	0	0
59	AP	4	0	0	0	0
59	AQ	3	0	0	0	0
59	AR	2	0	0	0	0
59	AU	3	0	0	0	0
59	AV	6	0	0	0	0
59	AW	3	0	0	0	0
59	AX	1	0	0	0	0
59	AY	1	0	0	0	0
59	AZ	2	0	0	0	0
59	BA	215	0	0	0	0
59	BB	1	0	0	0	0
59	BD	1	0	0	0	0
59	BE	1	0	0	0	0
59	BF	1	0	0	0	0
59	BK	1	0	0	0	0
59	BL	2	0	0	0	0
59	BM	1	0	0	0	0
59	BN	2	0	0	0	0
59	BS	1	0	0	0	0
59	BT	1	0	0	0	0
59	BW	3	0	0	0	0
59	BZ	1	0	0	0	0
59	C0	1	0	0	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	C8	4	0	0	0	0
63	CA	983	0	0	79	0
63	CB	9	0	0	1	0
63	CD	15	0	0	1	0
63	CE	9	0	0	1	0
63	CF	6	0	0	0	0
63	CN	1	0	0	0	0
63	CO	1	0	0	0	0
63	CP	11	0	0	2	0
63	CQ	2	0	0	1	0
63	CT	3	0	0	0	0
63	CU	2	0	0	0	0
63	CV	1	0	0	1	0
63	CW	1	0	0	0	0
63	CX	1	0	0	0	0
63	CY	2	0	0	1	0
63	DA	157	0	0	13	0
63	DD	1	0	0	0	0
63	DE	2	0	0	2	0
63	DH	1	0	0	0	0
63	DJ	1	0	0	0	0
63	DK	2	0	0	0	0
63	DL	1	0	0	0	0
63	DT	1	0	0	0	0
All	All	310038	0	209219	7561	21

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 7561 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1891:G:H5”	3:AC:206:LYS:CG	1.32	1.59
1:AA:1891:G:C5’	3:AC:206:LYS:HD2	1.36	1.52
1:CA:2128:C:H5”	3:CC:219:MET:CE	1.36	1.51
1:CA:2132:U:C4	3:CC:6:LYS:HE3	1.51	1.41
1:CA:2128:C:C5’	3:CC:219:MET:HE1	1.50	1.38

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

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	0
3	CC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	0
4	AD	273/276 (99%)	249 (91%)	19 (7%)	5 (2%)	6	23
4	CD	273/276 (99%)	234 (86%)	26 (10%)	13 (5%)	2	6
5	AE	202/206 (98%)	186 (92%)	14 (7%)	2 (1%)	12	38
5	CE	202/206 (98%)	179 (89%)	20 (10%)	3 (2%)	8	28
6	AF	201/210 (96%)	182 (90%)	18 (9%)	1 (0%)	24	55
6	CF	201/210 (96%)	177 (88%)	17 (8%)	7 (4%)	3	10
7	AG	179/182 (98%)	154 (86%)	19 (11%)	6 (3%)	3	11
7	CG	179/182 (98%)	141 (79%)	31 (17%)	7 (4%)	2	8
8	AH	172/180 (96%)	154 (90%)	15 (9%)	3 (2%)	7	25
8	CH	172/180 (96%)	144 (84%)	17 (10%)	11 (6%)	1	3
9	AK	128/173 (74%)	66 (52%)	36 (28%)	26 (20%)	0	0
9	CK	128/173 (74%)	76 (59%)	27 (21%)	25 (20%)	0	0
10	AL	64/147 (44%)	43 (67%)	17 (27%)	4 (6%)	1	3
10	CL	64/147 (44%)	42 (66%)	19 (30%)	3 (5%)	2	6
11	AN	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	18	47
11	CN	138/140 (99%)	120 (87%)	15 (11%)	3 (2%)	5	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
12	CO	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	4	16
13	AP	147/150 (98%)	130 (88%)	15 (10%)	2 (1%)	9	30
13	CP	147/150 (98%)	119 (81%)	25 (17%)	3 (2%)	6	21
14	AQ	139/141 (99%)	126 (91%)	12 (9%)	1 (1%)	18	47
14	CQ	139/141 (99%)	123 (88%)	14 (10%)	2 (1%)	9	30
15	AR	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
15	CR	116/118 (98%)	102 (88%)	11 (10%)	3 (3%)	4	15
16	AS	108/112 (96%)	88 (82%)	16 (15%)	4 (4%)	2	9
16	CS	108/112 (96%)	83 (77%)	20 (18%)	5 (5%)	2	6
17	AT	129/146 (88%)	114 (88%)	13 (10%)	2 (2%)	7	27
17	CT	129/146 (88%)	116 (90%)	11 (8%)	2 (2%)	7	27
18	AU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
18	CU	114/118 (97%)	100 (88%)	11 (10%)	3 (3%)	4	15
19	AV	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	12	38
19	CV	99/101 (98%)	86 (87%)	10 (10%)	3 (3%)	3	12
20	AW	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
20	CW	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
21	AX	93/96 (97%)	85 (91%)	6 (6%)	2 (2%)	5	19
21	CX	93/96 (97%)	77 (83%)	11 (12%)	5 (5%)	1	4
22	AY	105/110 (96%)	93 (89%)	9 (9%)	3 (3%)	3	13
22	CY	105/110 (96%)	86 (82%)	14 (13%)	5 (5%)	2	6
23	AZ	183/206 (89%)	147 (80%)	24 (13%)	12 (7%)	1	3
23	CZ	183/206 (89%)	134 (73%)	33 (18%)	16 (9%)	0	1
24	A0	75/85 (88%)	70 (93%)	5 (7%)	0	100	100
24	C0	75/85 (88%)	67 (89%)	7 (9%)	1 (1%)	9	31
25	A1	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
25	C1	95/98 (97%)	85 (90%)	7 (7%)	3 (3%)	3	11
26	A2	68/72 (94%)	62 (91%)	6 (9%)	0	100	100
26	C2	68/72 (94%)	60 (88%)	7 (10%)	1 (2%)	8	28
27	A3	57/60 (95%)	51 (90%)	6 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	C3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	3	10
28	A4	67/71 (94%)	46 (69%)	12 (18%)	9 (13%)	0	0
28	C4	67/71 (94%)	43 (64%)	15 (22%)	9 (13%)	0	0
29	A5	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
29	C5	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	6	23
30	A6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
30	C6	51/54 (94%)	42 (82%)	8 (16%)	1 (2%)	6	21
31	A7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
31	C7	46/49 (94%)	41 (89%)	4 (9%)	1 (2%)	5	19
32	A8	62/65 (95%)	60 (97%)	1 (2%)	1 (2%)	7	27
32	C8	62/65 (95%)	54 (87%)	7 (11%)	1 (2%)	7	27
33	A9	35/37 (95%)	35 (100%)	0	0	100	100
33	C9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
35	BB	229/256 (90%)	182 (80%)	33 (14%)	14 (6%)	1	3
35	DB	229/256 (90%)	170 (74%)	41 (18%)	18 (8%)	1	1
36	BC	204/239 (85%)	155 (76%)	38 (19%)	11 (5%)	1	4
36	DC	204/239 (85%)	169 (83%)	29 (14%)	6 (3%)	3	13
37	BD	206/209 (99%)	166 (81%)	28 (14%)	12 (6%)	1	4
37	DD	206/209 (99%)	171 (83%)	27 (13%)	8 (4%)	2	8
38	BE	146/162 (90%)	114 (78%)	24 (16%)	8 (6%)	1	4
38	DE	146/162 (90%)	117 (80%)	22 (15%)	7 (5%)	2	6
39	BF	98/101 (97%)	84 (86%)	11 (11%)	3 (3%)	3	12
39	DF	98/101 (97%)	90 (92%)	5 (5%)	3 (3%)	3	12
40	BG	153/156 (98%)	128 (84%)	13 (8%)	12 (8%)	1	2
40	DG	153/156 (98%)	126 (82%)	22 (14%)	5 (3%)	3	11
41	BH	135/138 (98%)	110 (82%)	22 (16%)	3 (2%)	5	19
41	DH	135/138 (98%)	114 (84%)	14 (10%)	7 (5%)	1	5
42	BI	125/128 (98%)	103 (82%)	15 (12%)	7 (6%)	1	4
42	DI	125/128 (98%)	100 (80%)	21 (17%)	4 (3%)	3	11
43	BJ	95/105 (90%)	76 (80%)	12 (13%)	7 (7%)	1	2
43	DJ	94/105 (90%)	75 (80%)	16 (17%)	3 (3%)	3	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	BK	112/129 (87%)	96 (86%)	14 (12%)	2 (2%)	6	23
44	DK	112/129 (87%)	92 (82%)	16 (14%)	4 (4%)	2	10
45	BL	120/132 (91%)	108 (90%)	11 (9%)	1 (1%)	16	44
45	DL	120/132 (91%)	100 (83%)	16 (13%)	4 (3%)	3	11
46	BM	115/126 (91%)	93 (81%)	18 (16%)	4 (4%)	3	10
46	DM	114/126 (90%)	88 (77%)	17 (15%)	9 (8%)	1	1
47	BN	58/61 (95%)	46 (79%)	9 (16%)	3 (5%)	1	5
47	DN	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	11
48	BO	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	3	10
48	DO	86/89 (97%)	72 (84%)	10 (12%)	4 (5%)	2	6
49	BP	80/88 (91%)	54 (68%)	17 (21%)	9 (11%)	0	1
49	DP	80/88 (91%)	58 (72%)	18 (22%)	4 (5%)	1	5
50	BQ	97/105 (92%)	87 (90%)	7 (7%)	3 (3%)	3	12
50	DQ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
51	BR	66/88 (75%)	57 (86%)	7 (11%)	2 (3%)	3	12
51	DR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
52	BS	82/93 (88%)	64 (78%)	14 (17%)	4 (5%)	1	6
52	DS	81/93 (87%)	63 (78%)	15 (18%)	3 (4%)	2	9
53	BT	94/106 (89%)	78 (83%)	12 (13%)	4 (4%)	2	7
53	DT	94/106 (89%)	75 (80%)	13 (14%)	6 (6%)	1	3
54	BU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
54	DU	21/27 (78%)	17 (81%)	2 (10%)	2 (10%)	0	1
57	BZ	722/758 (95%)	563 (78%)	107 (15%)	52 (7%)	1	2
57	DZ	726/758 (96%)	537 (74%)	132 (18%)	57 (8%)	1	1
58	BX	3/10 (30%)	1 (33%)	0	2 (67%)	0	0
58	DX	3/10 (30%)	0	2 (67%)	1 (33%)	0	0
All	All	13227/14464 (91%)	10975 (83%)	1666 (13%)	586 (4%)	2	7

5 of 586 Ramachandran outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	AC	111/180 (62%)	100 (90%)	11 (10%)	7 24
3	CC	111/180 (62%)	100 (90%)	11 (10%)	7 24
4	AD	215/218 (99%)	169 (79%)	46 (21%)	1 4
4	CD	216/218 (99%)	173 (80%)	43 (20%)	1 5
5	AE	164/166 (99%)	133 (81%)	31 (19%)	1 5
5	CE	164/166 (99%)	127 (77%)	37 (23%)	1 3
6	AF	160/166 (96%)	126 (79%)	34 (21%)	1 4
6	CF	159/166 (96%)	120 (76%)	39 (24%)	1 2
7	AG	143/156 (92%)	112 (78%)	31 (22%)	1 3
7	CG	142/156 (91%)	108 (76%)	34 (24%)	1 3
8	AH	144/148 (97%)	107 (74%)	37 (26%)	0 2
8	CH	144/148 (97%)	113 (78%)	31 (22%)	1 4
10	AL	50/111 (45%)	39 (78%)	11 (22%)	1 3
10	CL	50/111 (45%)	32 (64%)	18 (36%)	0 0
11	AN	118/119 (99%)	92 (78%)	26 (22%)	1 3
11	CN	118/119 (99%)	82 (70%)	36 (30%)	0 1
12	AO	100/100 (100%)	83 (83%)	17 (17%)	2 7
12	CO	100/100 (100%)	84 (84%)	16 (16%)	2 9
13	AP	116/116 (100%)	94 (81%)	22 (19%)	1 5
13	CP	115/116 (99%)	92 (80%)	23 (20%)	1 4
14	AQ	111/111 (100%)	91 (82%)	20 (18%)	2 6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	CQ	111/111 (100%)	84 (76%)	27 (24%)	1	2
15	AR	101/101 (100%)	78 (77%)	23 (23%)	1	3
15	CR	101/101 (100%)	86 (85%)	15 (15%)	3	10
16	AS	87/88 (99%)	66 (76%)	21 (24%)	1	2
16	CS	85/88 (97%)	64 (75%)	21 (25%)	1	2
17	AT	115/127 (91%)	94 (82%)	21 (18%)	2	6
17	CT	113/127 (89%)	96 (85%)	17 (15%)	3	10
18	AU	93/94 (99%)	74 (80%)	19 (20%)	1	4
18	CU	93/94 (99%)	79 (85%)	14 (15%)	3	10
19	AV	80/82 (98%)	65 (81%)	15 (19%)	1	5
19	CV	80/82 (98%)	62 (78%)	18 (22%)	1	3
20	AW	90/92 (98%)	74 (82%)	16 (18%)	2	6
20	CW	90/92 (98%)	72 (80%)	18 (20%)	1	4
21	AX	77/78 (99%)	63 (82%)	14 (18%)	2	6
21	CX	77/78 (99%)	62 (80%)	15 (20%)	1	5
22	AY	85/91 (93%)	65 (76%)	20 (24%)	1	3
22	CY	85/91 (93%)	62 (73%)	23 (27%)	0	1
23	AZ	156/179 (87%)	114 (73%)	42 (27%)	0	1
23	CZ	156/179 (87%)	123 (79%)	33 (21%)	1	4
24	A0	61/67 (91%)	55 (90%)	6 (10%)	7	25
24	C0	61/67 (91%)	48 (79%)	13 (21%)	1	4
25	A1	80/83 (96%)	62 (78%)	18 (22%)	1	3
25	C1	80/83 (96%)	63 (79%)	17 (21%)	1	4
26	A2	65/67 (97%)	55 (85%)	10 (15%)	2	10
26	C2	65/67 (97%)	50 (77%)	15 (23%)	1	3
27	A3	51/52 (98%)	42 (82%)	9 (18%)	2	7
27	C3	50/52 (96%)	38 (76%)	12 (24%)	1	2
28	A4	60/63 (95%)	52 (87%)	8 (13%)	4	14
28	C4	53/63 (84%)	41 (77%)	12 (23%)	1	3
29	A5	50/52 (96%)	43 (86%)	7 (14%)	3	12
29	C5	50/52 (96%)	41 (82%)	9 (18%)	2	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	A6	51/52 (98%)	37 (72%)	14 (28%)	0	1
30	C6	50/52 (96%)	40 (80%)	10 (20%)	1	4
31	A7	41/42 (98%)	31 (76%)	10 (24%)	1	2
31	C7	41/42 (98%)	33 (80%)	8 (20%)	1	5
32	A8	54/55 (98%)	43 (80%)	11 (20%)	1	4
32	C8	54/55 (98%)	47 (87%)	7 (13%)	4	14
33	A9	34/34 (100%)	29 (85%)	5 (15%)	3	10
33	C9	34/34 (100%)	31 (91%)	3 (9%)	9	29
35	BB	192/220 (87%)	150 (78%)	42 (22%)	1	3
35	DB	187/220 (85%)	145 (78%)	42 (22%)	1	3
36	BC	143/188 (76%)	122 (85%)	21 (15%)	3	10
36	DC	141/188 (75%)	104 (74%)	37 (26%)	0	2
37	BD	170/181 (94%)	135 (79%)	35 (21%)	1	4
37	DD	174/181 (96%)	136 (78%)	38 (22%)	1	3
38	BE	113/123 (92%)	85 (75%)	28 (25%)	1	2
38	DE	114/123 (93%)	80 (70%)	34 (30%)	0	1
39	BF	84/90 (93%)	68 (81%)	16 (19%)	1	5
39	DF	86/90 (96%)	73 (85%)	13 (15%)	3	10
40	BG	119/127 (94%)	93 (78%)	26 (22%)	1	3
40	DG	120/127 (94%)	103 (86%)	17 (14%)	3	12
41	BH	114/119 (96%)	87 (76%)	27 (24%)	1	3
41	DH	114/119 (96%)	84 (74%)	30 (26%)	0	2
42	BI	91/99 (92%)	76 (84%)	15 (16%)	2	8
42	DI	89/99 (90%)	66 (74%)	23 (26%)	0	2
43	BJ	66/92 (72%)	56 (85%)	10 (15%)	3	10
43	DJ	69/92 (75%)	58 (84%)	11 (16%)	2	9
44	BK	83/99 (84%)	65 (78%)	18 (22%)	1	3
44	DK	83/99 (84%)	63 (76%)	20 (24%)	1	2
45	BL	97/109 (89%)	79 (81%)	18 (19%)	1	5
45	DL	97/109 (89%)	73 (75%)	24 (25%)	1	2
46	BM	91/101 (90%)	76 (84%)	15 (16%)	2	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	DM	88/101 (87%)	73 (83%)	15 (17%)	2	7
47	BN	49/50 (98%)	38 (78%)	11 (22%)	1	3
47	DN	49/50 (98%)	42 (86%)	7 (14%)	3	11
48	BO	78/80 (98%)	69 (88%)	9 (12%)	5	18
48	DO	78/80 (98%)	61 (78%)	17 (22%)	1	3
49	BP	69/74 (93%)	53 (77%)	16 (23%)	1	3
49	DP	68/74 (92%)	52 (76%)	16 (24%)	1	3
50	BQ	94/97 (97%)	75 (80%)	19 (20%)	1	4
50	DQ	94/97 (97%)	80 (85%)	14 (15%)	3	10
51	BR	59/77 (77%)	48 (81%)	11 (19%)	1	5
51	DR	59/77 (77%)	53 (90%)	6 (10%)	7	23
52	BS	70/80 (88%)	58 (83%)	12 (17%)	2	7
52	DS	67/80 (84%)	54 (81%)	13 (19%)	1	5
53	BT	70/82 (85%)	51 (73%)	19 (27%)	0	1
53	DT	71/82 (87%)	59 (83%)	12 (17%)	2	7
54	BU	18/22 (82%)	17 (94%)	1 (6%)	19	50
54	DU	18/22 (82%)	17 (94%)	1 (6%)	19	50
57	BZ	604/636 (95%)	470 (78%)	134 (22%)	1	3
57	DZ	607/636 (95%)	491 (81%)	116 (19%)	1	5
58	BX	3/3 (100%)	3 (100%)	0	100	100
58	DX	3/3 (100%)	3 (100%)	0	100	100
All	All	10664/11678 (91%)	8485 (80%)	2179 (20%)	1	4

5 of 2179 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	DG	146	GLU
43	DJ	29	ARG
40	DG	131	LYS
57	DZ	33	LEU
42	BI	66	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 211 such sidechains are listed below:

Mol	Chain	Res	Type
8	CH	147	ASN
23	CZ	65	GLN
57	DZ	-50	GLN
12	CO	89	ASN
17	CT	58	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2865/2915 (98%)	536 (18%)	51 (1%)
1	CA	2860/2915 (98%)	615 (21%)	39 (1%)
2	AB	119/121 (98%)	15 (12%)	0
2	CB	119/121 (98%)	27 (22%)	0
34	BA	1491/1521 (98%)	331 (22%)	20 (1%)
34	DA	1498/1521 (98%)	352 (23%)	22 (1%)
55	BV	6/18 (33%)	2 (33%)	0
55	DV	5/18 (27%)	1 (20%)	0
56	BW	75/76 (98%)	16 (21%)	1 (1%)
56	BY	72/76 (94%)	24 (33%)	2 (2%)
56	DW	75/76 (98%)	24 (32%)	2 (2%)
56	DY	71/76 (93%)	23 (32%)	1 (1%)
All	All	9256/9454 (97%)	1966 (21%)	138 (1%)

5 of 1966 RNA backbone outliers are listed below:

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

5 of 138 RNA pucker outliers are listed below:

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	MIA	BY	37	56	21,24,32	1.68	3 (14%)	30,35,47	2.03	8 (26%)
56	PSU	DW	55	56	18,21,22	1.40	2 (11%)	21,30,33	2.01	5 (23%)
56	PSU	BW	32	56	18,21,22	1.34	3 (16%)	21,30,33	1.83	5 (23%)
58	2QZ	BX	1	58	7,8,9	0.67	0	7,10,12	4.73	4 (57%)
58	MVA	DX	9	58	6,7,8	1.14	1 (16%)	6,8,10	1.58	1 (16%)
56	MIA	DY	37	56	21,24,32	1.60	4 (19%)	30,35,47	2.07	7 (23%)
58	2R1	DX	6	58	10,10,11	1.65	2 (20%)	8,13,15	2.10	3 (37%)
56	PSU	BW	55	56	18,21,22	1.37	1 (5%)	21,30,33	1.95	3 (14%)
56	7MG	BY	46	56	23,26,27	1.30	3 (13%)	27,39,42	2.71	7 (25%)
56	4SU	BY	8	56	18,21,22	1.75	4 (22%)	25,30,33	2.14	6 (24%)
56	4SU	DW	8	56	18,21,22	1.83	5 (27%)	25,30,33	2.31	4 (16%)
58	MVA	DX	5	58	6,7,8	1.06	0	6,8,10	1.57	1 (16%)
56	PSU	BY	55	56	18,21,22	1.39	2 (11%)	21,30,33	1.98	3 (14%)
56	7MG	BW	46	56	23,26,27	1.29	4 (17%)	27,39,42	2.77	7 (25%)
56	PSU	DY	39	56	18,21,22	1.43	2 (11%)	21,30,33	1.97	3 (14%)
56	PSU	DY	55	56	18,21,22	1.42	2 (11%)	21,30,33	2.01	3 (14%)
58	2QY	DX	10	58	12,13,14	1.66	1 (8%)	14,16,18	3.67	6 (42%)
56	MIA	DW	37	56	28,31,32	2.31	6 (21%)	38,44,47	2.62	13 (34%)
58	2R3	BX	8	58	12,14,15	0.70	0	16,18,20	2.13	9 (56%)
56	PSU	BY	39	56	18,21,22	1.39	2 (11%)	21,30,33	1.93	3 (14%)
58	2R1	BX	6	58	10,10,11	2.35	3 (30%)	8,13,15	3.80	3 (37%)
56	7MG	DY	46	56	23,26,27	1.24	3 (13%)	27,39,42	2.76	7 (25%)
56	PSU	DW	32	56	18,21,22	1.43	3 (16%)	21,30,33	2.14	4 (19%)
56	5MU	BW	54	56	19,22,23	1.44	4 (21%)	27,32,35	1.98	7 (25%)
56	4SU	BW	8	56	18,21,22	1.49	3 (16%)	25,30,33	2.18	5 (20%)
56	PSU	BY	32	56	18,21,22	1.40	2 (11%)	21,30,33	1.94	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	PSU	BW	39	56	18,21,22	1.37	2 (11%)	21,30,33	2.02	5 (23%)
58	2QZ	DX	1	58	7,8,9	0.55	0	7,10,12	4.52	3 (42%)
58	2R3	DX	8	58	12,14,15	0.60	0	16,18,20	1.77	5 (31%)
56	4SU	DY	8	56	18,21,22	1.84	4 (22%)	25,30,33	2.35	6 (24%)
56	PSU	DY	32	56	18,21,22	1.36	2 (11%)	21,30,33	1.95	4 (19%)
58	MVA	BX	5	58	6,7,8	0.52	0	6,8,10	1.39	1 (16%)
56	5MU	DY	54	56	19,22,23	1.44	6 (31%)	27,32,35	2.07	5 (18%)
58	004	BX	3	58	9,10,11	1.39	1 (11%)	9,12,14	1.32	1 (11%)
58	2QY	BX	10	58	12,13,14	1.73	2 (16%)	14,16,18	4.12	6 (42%)
56	PSU	DW	39	56	18,21,22	1.35	2 (11%)	21,30,33	2.08	4 (19%)
56	MIA	BW	37	56	28,31,32	2.41	8 (28%)	38,44,47	2.62	14 (36%)
56	5MU	BY	54	56	19,22,23	1.53	5 (26%)	27,32,35	2.21	8 (29%)
56	5MU	DW	54	56	19,22,23	1.49	4 (21%)	27,32,35	2.07	7 (25%)
58	004	DX	3	58	9,10,11	1.53	1 (11%)	9,12,14	1.28	1 (11%)
58	MVA	BX	9	58	6,7,8	0.77	0	6,8,10	1.50	1 (16%)
56	7MG	DW	46	56	23,26,27	1.30	3 (13%)	27,39,42	2.71	7 (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	MIA	BY	37	56	-	2/7/25/34	0/3/3/3
56	PSU	DW	55	56	-	2/7/25/26	0/2/2/2
56	PSU	BW	32	56	-	4/7/25/26	0/2/2/2
58	2QZ	BX	1	58	-	1/8/10/12	-
58	MVA	DX	9	58	-	4/6/8/10	-
56	MIA	DY	37	56	-	3/7/25/34	0/3/3/3
58	2R1	DX	6	58	-	2/2/14/16	0/1/1/1
56	PSU	BW	55	56	-	2/7/25/26	0/2/2/2
56	7MG	BY	46	56	-	4/7/37/38	0/3/3/3
56	4SU	BY	8	56	-	1/7/25/26	0/2/2/2
56	4SU	DW	8	56	-	0/7/25/26	0/2/2/2
58	MVA	DX	5	58	-	4/6/8/10	-
56	PSU	BY	55	56	-	2/7/25/26	0/2/2/2
56	7MG	BW	46	56	-	1/7/37/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PSU	DY	39	56	-	2/7/25/26	0/2/2/2
56	PSU	DY	55	56	-	3/7/25/26	0/2/2/2
58	2QY	DX	10	58	-	3/5/8/10	0/1/1/1
56	MIA	DW	37	56	-	7/15/33/34	0/3/3/3
58	2R3	BX	8	58	-	6/11/12/14	0/1/1/1
56	PSU	BY	39	56	-	0/7/25/26	0/2/2/2
58	2R1	BX	6	58	-	0/2/14/16	0/1/1/1
56	7MG	DY	46	56	-	3/7/37/38	0/3/3/3
56	PSU	DW	32	56	-	2/7/25/26	0/2/2/2
56	5MU	BW	54	56	-	1/7/25/26	0/2/2/2
56	4SU	BW	8	56	-	0/7/25/26	0/2/2/2
56	PSU	BY	32	56	-	0/7/25/26	0/2/2/2
56	PSU	BW	39	56	-	0/7/25/26	0/2/2/2
58	2QZ	DX	1	58	-	1/8/10/12	-
58	2R3	DX	8	58	-	6/11/12/14	0/1/1/1
56	4SU	DY	8	56	-	1/7/25/26	0/2/2/2
56	PSU	DY	32	56	-	0/7/25/26	0/2/2/2
58	MVA	BX	5	58	-	4/6/8/10	-
56	5MU	DY	54	56	-	2/7/25/26	0/2/2/2
58	004	BX	3	58	-	0/4/6/8	0/1/1/1
58	2QY	BX	10	58	-	3/5/8/10	0/1/1/1
56	PSU	DW	39	56	-	1/7/25/26	0/2/2/2
56	MIA	BW	37	56	-	5/15/33/34	0/3/3/3
56	5MU	BY	54	56	-	2/7/25/26	0/2/2/2
56	5MU	DW	54	56	-	0/7/25/26	0/2/2/2
58	004	DX	3	58	-	0/4/6/8	0/1/1/1
58	MVA	BX	9	58	-	2/6/8/10	-
56	7MG	DW	46	56	-	4/7/37/38	0/3/3/3

The worst 5 of 105 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BW	37	MIA	C13-C14	7.51	1.54	1.32
56	DW	37	MIA	C13-C14	7.11	1.53	1.32
56	BW	37	MIA	C2-S10	-7.10	1.69	1.75
56	DW	37	MIA	C2-S10	-5.65	1.71	1.75
56	BY	37	MIA	C5-C4	5.34	1.48	1.39

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

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

There are no chirality outliers.

5 of 90 torsion outliers are listed below:

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

There are no ring outliers.

23 monomers are involved in 47 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
62	GDP	DZ	703	59	29,30,30	1.25	3 (10%)	45,47,47	1.68	6 (13%)
62	GDP	BZ	702	59	29,30,30	1.18	2 (6%)	45,47,47	1.66	8 (17%)
61	SF4	DD	501	37	0,12,12	-	-	-		
61	SF4	BD	501	-	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	SF4	BD	501	-	-	-	0/6/5/5
62	GDP	BZ	702	59	-	3/16/32/32	0/3/3/3
61	SF4	DD	501	37	-	-	0/6/5/5
62	GDP	DZ	703	59	-	1/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	BZ	702	GDP	C5-C4	3.41	1.48	1.38
62	DZ	703	GDP	C5-C4	3.29	1.47	1.38
62	BZ	702	GDP	C5-N7	-2.38	1.34	1.39
62	DZ	703	GDP	C4-N9	-2.25	1.32	1.38
62	DZ	703	GDP	C6-N1	-2.13	1.34	1.38

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	DZ	703	GDP	C5-C4-N3	-5.05	120.35	128.39
62	BZ	702	GDP	C5-C4-N3	-5.03	120.38	128.39
62	DZ	703	GDP	C2-N3-C4	4.36	119.80	112.30
62	BZ	702	GDP	N9-C4-N3	4.16	134.27	125.95
62	DZ	703	GDP	N9-C4-N3	4.09	134.13	125.95

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

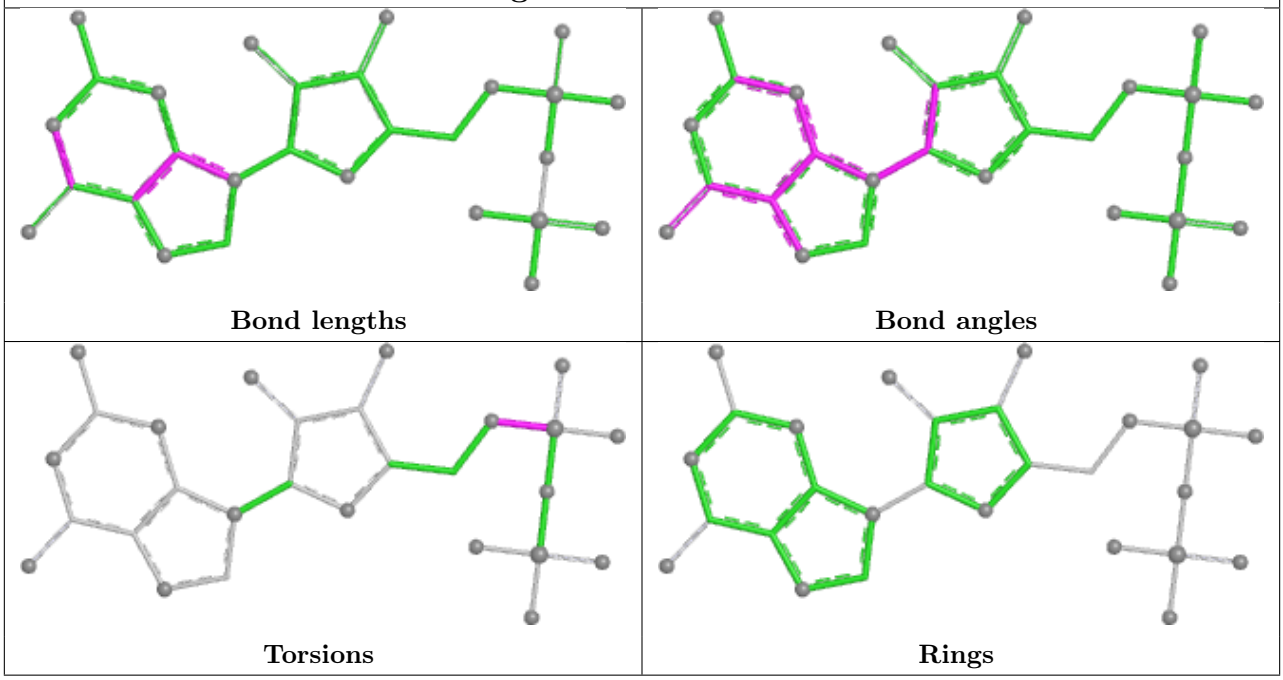
There are no ring outliers.

4 monomers are involved in 15 short contacts:

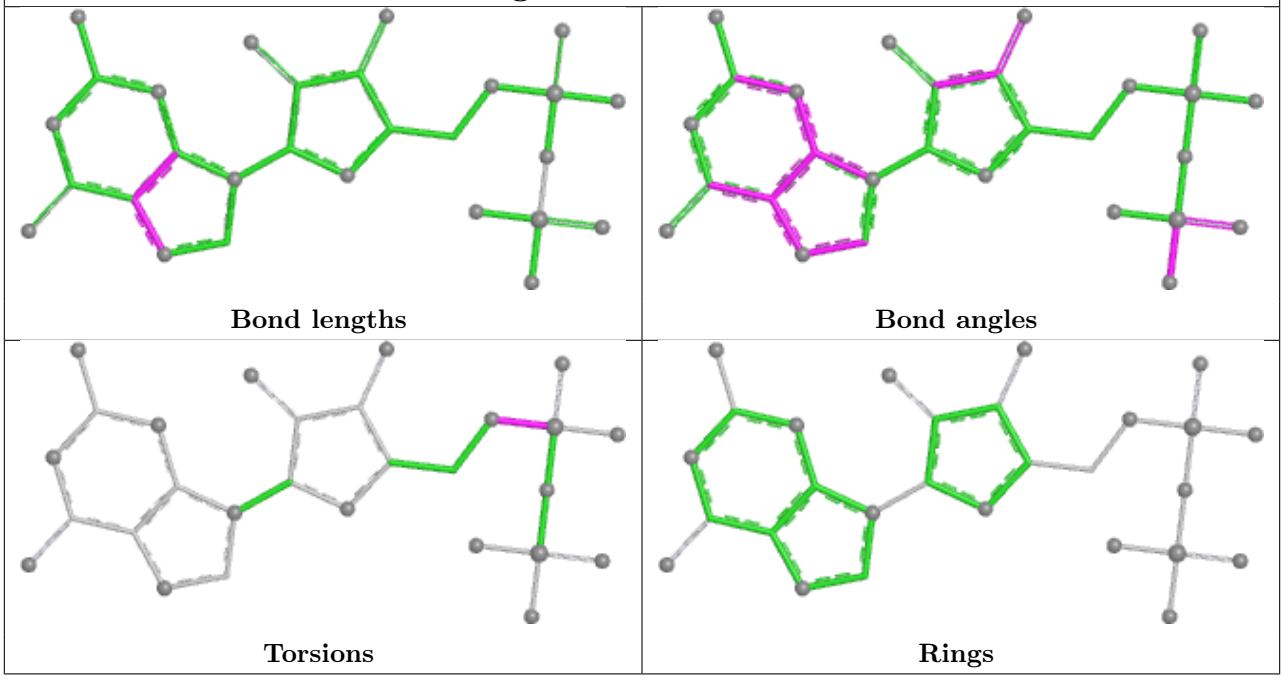
Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	DZ	703	GDP	7	0
62	BZ	702	GDP	5	0
61	DD	501	SF4	2	0
61	BD	501	SF4	1	0

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 then 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.

Ligand GDP DZ 703



Ligand GDP BZ 702



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AA	2872/2915 (98%)	-0.84	40 (1%)	73	64	13, 31, 166, 310	0
1	CA	2868/2915 (98%)	-0.32	71 (2%)	58	48	23, 54, 175, 327	0
2	AB	120/121 (99%)	-0.71	1 (0%)	82	75	23, 46, 65, 111	0
2	CB	120/121 (99%)	0.58	5 (4%)	40	32	54, 103, 145, 177	0
3	AC	137/228 (60%)	2.68	94 (68%)	0	0	89, 187, 231, 259	0
3	CC	137/228 (60%)	2.84	98 (71%)	0	0	142, 205, 249, 270	0
4	AD	275/276 (99%)	-0.59	4 (1%)	72	63	8, 30, 56, 122	0
4	CD	275/276 (99%)	-0.25	4 (1%)	72	63	13, 43, 76, 133	0
5	AE	204/206 (99%)	-0.65	0	100	100	7, 30, 60, 99	0
5	CE	204/206 (99%)	-0.23	2 (0%)	79	72	15, 51, 85, 143	0
6	AF	203/210 (96%)	-0.60	0	100	100	5, 31, 75, 140	0
6	CF	203/210 (96%)	0.13	3 (1%)	72	63	20, 66, 122, 158	0
7	AG	181/182 (99%)	0.14	2 (1%)	78	70	33, 66, 114, 178	0
7	CG	181/182 (99%)	1.20	27 (14%)	5	4	73, 124, 181, 208	0
8	AH	174/180 (96%)	-0.31	2 (1%)	78	70	21, 45, 72, 198	0
8	CH	174/180 (96%)	0.72	14 (8%)	18	13	51, 90, 139, 171	0
9	AK	130/173 (75%)	1.59	35 (26%)	1	1	65, 130, 195, 217	0
9	CK	130/173 (75%)	1.99	54 (41%)	0	0	84, 161, 205, 230	0
10	AL	66/147 (44%)	1.91	22 (33%)	1	1	109, 180, 227, 243	0
10	CL	66/147 (44%)	2.51	38 (57%)	0	0	104, 180, 226, 260	0
11	AN	140/140 (100%)	-0.68	1 (0%)	84	77	11, 27, 54, 96	0
11	CN	140/140 (100%)	0.03	1 (0%)	84	77	35, 58, 92, 142	0
12	AO	122/122 (100%)	-0.66	0	100	100	16, 35, 64, 91	0
12	CO	122/122 (100%)	-0.28	0	100	100	28, 48, 80, 94	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AP	149/150 (99%)	-0.49	0 100 100	8, 37, 77, 126	0
13	CP	149/150 (99%)	0.37	6 (4%) 42 33	26, 73, 123, 155	0
14	AQ	141/141 (100%)	-0.59	0 100 100	9, 31, 53, 97	0
14	CQ	141/141 (100%)	0.23	3 (2%) 63 54	18, 62, 94, 145	0
15	AR	118/118 (100%)	-0.77	0 100 100	13, 27, 51, 75	0
15	CR	118/118 (100%)	-0.23	0 100 100	25, 49, 73, 106	0
16	AS	110/112 (98%)	-0.25	1 (0%) 81 74	24, 46, 74, 86	0
16	CS	110/112 (98%)	1.38	20 (18%) 3 2	59, 95, 139, 166	0
17	AT	131/146 (89%)	-0.25	4 (3%) 51 41	20, 39, 93, 218	0
17	CT	131/146 (89%)	0.06	3 (2%) 61 51	35, 56, 103, 151	0
18	AU	116/118 (98%)	-0.88	0 100 100	7, 22, 38, 87	0
18	CU	116/118 (98%)	0.09	0 100 100	31, 55, 88, 107	0
19	AV	101/101 (100%)	-0.88	0 100 100	10, 27, 56, 76	0
19	CV	101/101 (100%)	0.05	1 (0%) 79 72	28, 68, 101, 162	0
20	AW	112/113 (99%)	-0.77	0 100 100	10, 23, 47, 145	0
20	CW	112/113 (99%)	-0.19	0 100 100	26, 44, 74, 159	0
21	AX	95/96 (98%)	-0.45	1 (1%) 78 70	12, 33, 63, 107	0
21	CX	95/96 (98%)	0.37	6 (6%) 26 19	36, 62, 97, 173	0
22	AY	107/110 (97%)	-0.29	2 (1%) 66 57	18, 42, 88, 117	0
22	CY	107/110 (97%)	0.63	7 (6%) 25 18	48, 80, 124, 170	0
23	AZ	185/206 (89%)	-0.06	3 (1%) 70 61	27, 55, 94, 136	0
23	CZ	185/206 (89%)	0.81	9 (4%) 35 27	52, 97, 144, 173	0
24	A0	77/85 (90%)	-0.58	1 (1%) 75 66	9, 31, 53, 82	0
24	C0	77/85 (90%)	0.65	7 (9%) 15 11	27, 67, 104, 127	0
25	A1	97/98 (98%)	-0.40	1 (1%) 79 72	15, 38, 79, 97	0
25	C1	97/98 (98%)	0.17	3 (3%) 51 41	30, 55, 94, 139	0
26	A2	70/72 (97%)	-0.16	2 (2%) 53 43	14, 43, 63, 135	0
26	C2	70/72 (97%)	0.64	3 (4%) 40 31	47, 78, 109, 151	0
27	A3	59/60 (98%)	-0.62	1 (1%) 69 60	10, 26, 50, 110	0
27	C3	59/60 (98%)	0.30	2 (3%) 48 39	31, 62, 102, 162	0
28	A4	69/71 (97%)	0.77	8 (11%) 9 7	47, 101, 187, 216	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	C4	69/71 (97%)	1.26	11 (15%)	5	4	86, 158, 194, 226	0
29	A5	59/60 (98%)	-0.79	0	100	100	11, 22, 48, 66	0
29	C5	59/60 (98%)	-0.29	0	100	100	16, 46, 81, 120	0
30	A6	53/54 (98%)	-0.48	0	100	100	17, 35, 61, 75	0
30	C6	53/54 (98%)	0.21	0	100	100	40, 62, 85, 101	0
31	A7	48/49 (97%)	-0.53	2 (4%)	40	32	11, 20, 52, 99	0
31	C7	48/49 (97%)	-0.03	4 (8%)	17	12	23, 35, 95, 120	0
32	A8	64/65 (98%)	-0.72	0	100	100	13, 26, 39, 61	0
32	C8	64/65 (98%)	0.05	1 (1%)	70	61	26, 53, 71, 93	0
33	A9	37/37 (100%)	-0.42	1 (2%)	56	46	19, 32, 61, 65	0
33	C9	37/37 (100%)	0.39	1 (2%)	56	46	43, 61, 90, 101	0
34	BA	1495/1521 (98%)	0.22	23 (1%)	72	63	23, 81, 179, 326	0
34	DA	1501/1521 (98%)	0.46	65 (4%)	40	31	39, 93, 206, 304	0
35	BB	231/256 (90%)	0.89	22 (9%)	14	10	52, 103, 165, 193	0
35	DB	231/256 (90%)	1.34	45 (19%)	3	2	66, 134, 196, 226	0
36	BC	206/239 (86%)	1.03	29 (14%)	6	5	72, 113, 168, 187	0
36	DC	206/239 (86%)	1.48	53 (25%)	1	1	88, 150, 194, 221	0
37	BD	208/209 (99%)	1.13	37 (17%)	4	3	53, 90, 140, 180	0
37	DD	208/209 (99%)	0.95	29 (13%)	6	5	52, 87, 132, 197	0
38	BE	148/162 (91%)	0.33	2 (1%)	73	64	36, 71, 108, 150	0
38	DE	148/162 (91%)	0.80	13 (8%)	15	11	42, 88, 131, 177	0
39	BF	100/101 (99%)	0.44	1 (1%)	79	72	42, 80, 123, 144	0
39	DF	100/101 (99%)	0.56	3 (3%)	52	42	48, 90, 133, 146	0
40	BG	155/156 (99%)	0.80	17 (10%)	10	8	65, 100, 155, 193	0
40	DG	155/156 (99%)	1.10	22 (14%)	6	5	79, 130, 177, 212	0
41	BH	137/138 (99%)	0.57	7 (5%)	33	25	44, 72, 105, 119	0
41	DH	137/138 (99%)	0.84	12 (8%)	15	11	51, 90, 124, 159	0
42	BI	127/128 (99%)	1.58	39 (30%)	1	1	58, 114, 168, 190	0
42	DI	127/128 (99%)	2.03	59 (46%)	0	0	78, 153, 189, 243	0
43	BJ	97/105 (92%)	1.67	32 (32%)	1	1	74, 121, 172, 194	0
43	DJ	96/105 (91%)	1.96	45 (46%)	0	0	75, 158, 198, 215	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	BK	114/129 (88%)	0.25	1 (0%)	81	74	29, 73, 115, 125	0
44	DK	114/129 (88%)	0.66	9 (7%)	18	13	59, 92, 138, 168	0
45	BL	122/132 (92%)	0.24	5 (4%)	41	33	26, 60, 88, 110	0
45	DL	122/132 (92%)	0.55	5 (4%)	41	33	40, 70, 99, 142	0
46	BM	117/126 (92%)	0.92	13 (11%)	10	7	62, 107, 151, 187	0
46	DM	116/126 (92%)	1.63	34 (29%)	1	1	64, 154, 201, 235	0
47	BN	60/61 (98%)	1.55	15 (25%)	2	1	59, 109, 151, 171	0
47	DN	60/61 (98%)	2.27	35 (58%)	0	0	94, 141, 190, 208	0
48	BO	88/89 (98%)	0.35	5 (5%)	29	22	34, 68, 106, 139	0
48	DO	88/89 (98%)	0.58	3 (3%)	48	39	49, 81, 115, 139	0
49	BP	82/88 (93%)	0.94	10 (12%)	8	6	45, 80, 125, 150	0
49	DP	82/88 (93%)	0.74	4 (4%)	35	27	48, 76, 108, 120	0
50	BQ	99/105 (94%)	0.34	5 (5%)	33	25	43, 71, 103, 118	0
50	DQ	99/105 (94%)	0.79	12 (12%)	8	6	46, 79, 116, 148	0
51	BR	68/88 (77%)	0.27	1 (1%)	72	63	44, 71, 115, 135	0
51	DR	68/88 (77%)	0.54	1 (1%)	72	63	57, 89, 127, 146	0
52	BS	84/93 (90%)	1.63	27 (32%)	1	1	64, 126, 168, 222	0
52	DS	83/93 (89%)	2.01	37 (44%)	0	0	98, 162, 210, 220	0
53	BT	96/106 (90%)	0.82	10 (10%)	11	8	49, 84, 117, 159	0
53	DT	96/106 (90%)	0.76	9 (9%)	14	10	47, 81, 126, 145	0
54	BU	23/27 (85%)	1.93	11 (47%)	0	0	59, 99, 112, 154	0
54	DU	23/27 (85%)	2.42	11 (47%)	0	0	78, 132, 157, 179	0
55	BV	7/18 (38%)	1.50	3 (42%)	0	0	60, 68, 174, 188	0
55	DV	6/18 (33%)	1.98	3 (50%)	0	0	87, 94, 180, 202	0
56	BW	69/76 (90%)	-0.15	3 (4%)	40	31	37, 69, 117, 208	0
56	BY	67/76 (88%)	1.14	12 (17%)	3	3	74, 230, 278, 300	0
56	DW	69/76 (90%)	0.29	0	100	100	46, 106, 150, 254	0
56	DY	66/76 (86%)	1.36	14 (21%)	2	2	141, 280, 312, 332	0
57	BZ	728/758 (96%)	0.70	66 (9%)	15	11	37, 96, 187, 244	0
57	DZ	730/758 (96%)	0.89	90 (12%)	8	6	27, 112, 210, 259	0
58	BX	3/10 (30%)	0.69	0	100	100	81, 81, 81, 82	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
58	DX	3/10 (30%)	1.10	1 (33%) 1 1	78, 78, 80, 81	0
All	All	22705/23918 (94%)	0.20	1642 (7%) 21 16	5, 69, 187, 332	0

The worst 5 of 1642 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
42	DI	106	ALA	11.1
25	C1	2	SER	10.3
3	CC	213	VAL	7.5
36	BC	2	GLY	7.4
10	CL	127	ILE	7.3

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

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

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

Continued on next page...

Continued from previous page...

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	1718	1/1	0.23	0.19	101,101,101,101	0
59	MG	BA	1776	1/1	0.27	0.18	97,97,97,97	0
59	MG	CB	3013	1/1	0.33	0.16	100,100,100,100	0
59	MG	BA	1790	1/1	0.39	0.17	96,96,96,96	0
59	MG	DA	1757	1/1	0.43	0.27	111,111,111,111	0
59	MG	CA	3624	1/1	0.51	0.22	118,118,118,118	0
59	MG	BA	1691	1/1	0.55	0.22	86,86,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3773	1/1	0.55	0.63	35,35,35,35	1
59	MG	BA	1616	1/1	0.55	0.22	122,122,122,122	0
59	MG	DA	1754	1/1	0.55	0.28	120,120,120,120	0
59	MG	BB	3001	1/1	0.55	0.27	91,91,91,91	0
59	MG	CA	3363	1/1	0.58	0.13	88,88,88,88	0
59	MG	AA	3056	1/1	0.58	0.45	96,96,96,96	0
59	MG	DA	1609	1/1	0.59	0.13	89,89,89,89	0
59	MG	AA	3277	1/1	0.59	0.24	99,99,99,99	0
59	MG	CA	3488	1/1	0.60	0.25	88,88,88,88	0
59	MG	CA	3620	1/1	0.60	0.24	96,96,96,96	0
59	MG	BA	1660	1/1	0.61	0.24	82,82,82,82	0
59	MG	CA	3289	1/1	0.62	0.14	65,65,65,65	0
59	MG	AA	3418	1/1	0.62	0.12	74,74,74,74	0
59	MG	CA	3566	1/1	0.64	0.17	30,30,30,30	1
59	MG	DA	1710	1/1	0.65	0.10	104,104,104,104	0
59	MG	BL	201	1/1	0.65	0.12	84,84,84,84	0
59	MG	CA	3579	1/1	0.65	0.14	65,65,65,65	0
59	MG	AA	3643	1/1	0.65	0.23	84,84,84,84	0
59	MG	CA	3545	1/1	0.66	0.20	86,86,86,86	0
59	MG	DA	1738	1/1	0.66	0.14	95,95,95,95	0
59	MG	CA	3304	1/1	0.67	0.14	67,67,67,67	0
59	MG	CA	3546	1/1	0.67	0.14	88,88,88,88	0
59	MG	AA	3717	1/1	0.67	0.50	68,68,68,68	0
59	MG	CQ	202	1/1	0.67	0.27	74,74,74,74	0
59	MG	BA	1673	1/1	0.67	0.14	80,80,80,80	0
59	MG	AA	3747	1/1	0.68	0.16	85,85,85,85	0
59	MG	AA	3347	1/1	0.68	0.13	88,88,88,88	0
59	MG	DA	1611	1/1	0.68	0.41	89,89,89,89	0
59	MG	AA	3296	1/1	0.68	0.18	67,67,67,67	0
59	MG	AA	3617	1/1	0.69	0.10	77,77,77,77	0
59	MG	AA	3780	1/1	0.69	0.11	72,72,72,72	0
59	MG	DA	1749	1/1	0.69	0.12	77,77,77,77	0
59	MG	CA	3089	1/1	0.69	0.25	87,87,87,87	0
59	MG	CA	3444	1/1	0.69	0.09	67,67,67,67	0
59	MG	DA	1631	1/1	0.70	0.10	74,74,74,74	0
59	MG	BA	1741	1/1	0.70	0.10	88,88,88,88	0
59	MG	AA	3242	1/1	0.70	0.21	85,85,85,85	0
59	MG	CA	3557	1/1	0.70	0.21	76,76,76,76	0
59	MG	CA	3560	1/1	0.70	0.23	79,79,79,79	0
59	MG	CA	3485	1/1	0.70	0.10	85,85,85,85	0
59	MG	BA	1786	1/1	0.70	0.15	82,82,82,82	0
59	MG	AA	3629	1/1	0.71	0.18	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3096	1/1	0.71	0.37	125,125,125,125	0
59	MG	BA	1707	1/1	0.71	0.13	72,72,72,72	0
59	MG	AA	3464	1/1	0.72	0.17	66,66,66,66	0
59	MG	AA	3040	1/1	0.72	0.24	113,113,113,113	0
59	MG	AA	3678	1/1	0.72	0.17	77,77,77,77	0
59	MG	AA	3619	1/1	0.72	0.12	47,47,47,47	0
59	MG	CA	3125	1/1	0.72	0.38	78,78,78,78	0
59	MG	BA	1812	1/1	0.72	0.19	79,79,79,79	0
59	MG	CA	3535	1/1	0.73	0.22	77,77,77,77	0
59	MG	CA	3172	1/1	0.73	0.25	81,81,81,81	0
59	MG	CA	3055	1/1	0.73	0.16	77,77,77,77	0
59	MG	BA	1675	1/1	0.73	0.20	100,100,100,100	0
59	MG	CA	3350	1/1	0.73	0.13	82,82,82,82	0
59	MG	AA	3781	1/1	0.73	0.17	72,72,72,72	0
59	MG	BA	1775	1/1	0.73	0.17	90,90,90,90	0
59	MG	CA	3460	1/1	0.73	0.33	104,104,104,104	0
59	MG	CA	3127	1/1	0.73	0.22	94,94,94,94	0
59	MG	DA	1756	1/1	0.73	0.23	86,86,86,86	0
59	MG	CA	3139	1/1	0.73	0.22	126,126,126,126	0
59	MG	DA	1769	1/1	0.73	0.21	74,74,74,74	0
59	MG	BA	1657	1/1	0.74	0.26	78,78,78,78	0
59	MG	AA	3232	1/1	0.74	0.18	58,58,58,58	0
59	MG	BA	1719	1/1	0.74	0.14	62,62,62,62	0
59	MG	A0	101	1/1	0.74	0.12	69,69,69,69	0
59	MG	AA	3122	1/1	0.74	0.33	99,99,99,99	0
59	MG	BA	1679	1/1	0.74	0.21	59,59,59,59	0
59	MG	CA	3587	1/1	0.75	0.10	70,70,70,70	0
59	MG	AA	3625	1/1	0.75	0.18	51,51,51,51	0
59	MG	BA	1694	1/1	0.75	0.28	83,83,83,83	0
59	MG	AA	3480	1/1	0.75	0.23	88,88,88,88	0
59	MG	CA	3149	1/1	0.75	0.24	100,100,100,100	0
59	MG	CA	3100	1/1	0.75	0.29	81,81,81,81	0
59	MG	CA	3583	1/1	0.75	0.13	80,80,80,80	0
59	MG	CA	3586	1/1	0.75	0.31	93,93,93,93	0
59	MG	DT	3001	1/1	0.75	0.23	60,60,60,60	0
59	MG	DA	1727	1/1	0.76	0.08	61,61,61,61	0
59	MG	CQ	204	1/1	0.76	0.15	74,74,74,74	0
59	MG	CA	3376	1/1	0.76	0.12	78,78,78,78	0
59	MG	AA	3275	1/1	0.76	0.39	89,89,89,89	0
59	MG	CA	3646	1/1	0.76	0.14	91,91,91,91	0
59	MG	DA	1663	1/1	0.76	0.22	91,91,91,91	0
59	MG	AA	3269	1/1	0.76	0.23	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3467	1/1	0.76	0.32	77,77,77,77	0
59	MG	BA	1758	1/1	0.77	0.26	76,76,76,76	0
59	MG	DA	1715	1/1	0.77	0.18	79,79,79,79	0
59	MG	CA	3235	1/1	0.77	0.16	78,78,78,78	0
59	MG	CQ	201	1/1	0.77	0.18	72,72,72,72	0
59	MG	DA	1732	1/1	0.77	0.11	85,85,85,85	0
59	MG	AA	3016	1/1	0.77	0.20	64,64,64,64	0
59	MG	DA	1740	1/1	0.77	0.17	68,68,68,68	0
59	MG	CA	3108	1/1	0.77	0.22	78,78,78,78	0
59	MG	AA	3219	1/1	0.77	0.18	61,61,61,61	0
59	MG	AA	3481	1/1	0.77	0.19	78,78,78,78	0
59	MG	CA	3066	1/1	0.77	0.15	69,69,69,69	0
59	MG	DA	1762	1/1	0.77	0.18	61,61,61,61	0
59	MG	BA	1670	1/1	0.77	0.13	69,69,69,69	0
59	MG	DA	1668	1/1	0.77	0.31	65,65,65,65	0
59	MG	DW	503	1/1	0.77	0.19	85,85,85,85	0
59	MG	CA	3619	1/1	0.78	0.14	40,40,40,40	0
59	MG	CA	3240	1/1	0.78	0.24	71,71,71,71	0
59	MG	CA	3244	1/1	0.78	0.25	89,89,89,89	0
59	MG	CA	3246	1/1	0.78	0.26	57,57,57,57	0
59	MG	AA	3708	1/1	0.78	0.26	61,61,61,61	0
59	MG	AA	3093	1/1	0.78	0.68	92,92,92,92	0
59	MG	CA	3093	1/1	0.78	0.39	75,75,75,75	0
59	MG	CA	3357	1/1	0.78	0.13	66,66,66,66	0
59	MG	AA	3622	1/1	0.78	0.17	60,60,60,60	0
59	MG	CA	3007	1/1	0.78	0.25	92,92,92,92	0
59	MG	AA	3700	1/1	0.78	0.12	70,70,70,70	0
59	MG	DA	1635	1/1	0.78	0.21	75,75,75,75	0
59	MG	DA	1655	1/1	0.78	0.24	83,83,83,83	0
59	MG	CA	3236	1/1	0.78	0.36	81,81,81,81	0
59	MG	CA	3237	1/1	0.78	0.15	94,94,94,94	0
59	MG	AA	3583	1/1	0.79	0.13	63,63,63,63	0
59	MG	BA	1628	1/1	0.79	0.20	87,87,87,87	0
59	MG	DA	1724	1/1	0.79	0.15	70,70,70,70	0
59	MG	CA	3032	1/1	0.79	0.28	100,100,100,100	0
59	MG	CA	3050	1/1	0.79	0.21	75,75,75,75	0
59	MG	CA	3395	1/1	0.79	0.25	50,50,50,50	0
59	MG	CA	3408	1/1	0.79	0.11	58,58,58,58	0
59	MG	DA	1746	1/1	0.79	0.12	81,81,81,81	0
59	MG	BA	1671	1/1	0.79	0.36	101,101,101,101	0
59	MG	BA	1748	1/1	0.79	0.10	63,63,63,63	0
59	MG	CA	3465	1/1	0.79	0.25	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	1755	1/1	0.79	0.10	86,86,86,86	0
59	MG	CA	3295	1/1	0.79	0.17	66,66,66,66	0
59	MG	AA	3108	1/1	0.79	0.45	101,101,101,101	0
59	MG	DA	1708	1/1	0.79	0.20	77,77,77,77	0
59	MG	CA	3516	1/1	0.79	0.16	79,79,79,79	0
59	MG	AA	3571	1/1	0.80	0.19	94,94,94,94	0
59	MG	CA	3323	1/1	0.80	0.21	87,87,87,87	0
59	MG	AA	3642	1/1	0.80	0.17	71,71,71,71	0
59	MG	BA	1733	1/1	0.80	0.20	78,78,78,78	0
59	MG	AA	3776	1/1	0.80	0.10	69,69,69,69	0
59	MG	CA	3146	1/1	0.80	0.33	82,82,82,82	0
59	MG	AA	3246	1/1	0.80	0.10	52,52,52,52	0
59	MG	AA	3202	1/1	0.80	0.17	61,61,61,61	0
59	MG	CA	3186	1/1	0.80	0.20	77,77,77,77	0
59	MG	AA	3323	1/1	0.80	0.09	64,64,64,64	0
59	MG	CA	3065	1/1	0.80	0.23	56,56,56,56	0
59	MG	DA	1733	1/1	0.80	0.20	92,92,92,92	0
59	MG	DA	1737	1/1	0.80	0.15	69,69,69,69	0
59	MG	CA	3644	1/1	0.80	0.20	66,66,66,66	0
59	MG	BA	1612	1/1	0.80	0.17	92,92,92,92	0
59	MG	CB	3001	1/1	0.80	0.16	72,72,72,72	0
59	MG	CA	3078	1/1	0.80	0.21	57,57,57,57	0
59	MG	AA	3198	1/1	0.80	0.19	63,63,63,63	0
59	MG	CA	3492	1/1	0.80	0.15	59,59,59,59	0
59	MG	CA	3507	1/1	0.80	0.18	83,83,83,83	0
59	MG	DA	1604	1/1	0.80	0.18	80,80,80,80	0
59	MG	AA	3536	1/1	0.80	0.17	66,66,66,66	0
59	MG	BA	1697	1/1	0.80	0.32	99,99,99,99	0
59	MG	BA	1800	1/1	0.80	0.18	77,77,77,77	0
59	MG	AA	3660	1/1	0.81	0.16	61,61,61,61	0
59	MG	CA	3539	1/1	0.81	0.15	90,90,90,90	0
59	MG	BA	1603	1/1	0.81	0.17	61,61,61,61	0
59	MG	AA	3266	1/1	0.81	0.50	90,90,90,90	0
59	MG	CF	301	1/1	0.81	0.17	61,61,61,61	0
59	MG	BA	1721	1/1	0.81	0.09	66,66,66,66	0
59	MG	AA	3274	1/1	0.81	0.15	75,75,75,75	0
59	MG	BA	1625	1/1	0.81	0.20	86,86,86,86	0
59	MG	AA	3267	1/1	0.81	0.11	53,53,53,53	0
59	MG	CA	3223	1/1	0.81	0.09	59,59,59,59	0
59	MG	BA	1648	1/1	0.81	0.08	74,74,74,74	0
59	MG	DA	1748	1/1	0.81	0.11	70,70,70,70	0
59	MG	DA	1623	1/1	0.81	0.13	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	1753	1/1	0.81	0.30	79,79,79,79	0
59	MG	CA	3494	1/1	0.81	0.14	97,97,97,97	0
59	MG	CA	3594	1/1	0.81	0.08	73,73,73,73	0
59	MG	CA	3506	1/1	0.81	0.12	63,63,63,63	0
59	MG	AA	3644	1/1	0.81	0.21	56,56,56,56	0
59	MG	BA	1767	1/1	0.81	0.11	96,96,96,96	0
59	MG	DA	1674	1/1	0.81	0.20	77,77,77,77	0
59	MG	CA	3638	1/1	0.81	0.24	76,76,76,76	0
59	MG	CA	3428	1/1	0.82	0.14	58,58,58,58	0
59	MG	CA	3069	1/1	0.82	0.43	81,81,81,81	0
59	MG	AA	3542	1/1	0.82	0.13	58,58,58,58	0
59	MG	DA	1704	1/1	0.82	0.11	49,49,49,49	0
59	MG	BA	1792	1/1	0.82	0.17	80,80,80,80	0
59	MG	CA	3605	1/1	0.82	0.19	70,70,70,70	0
59	MG	AA	3719	1/1	0.82	0.15	59,59,59,59	0
59	MG	BA	1619	1/1	0.82	0.11	59,59,59,59	0
59	MG	AA	3737	1/1	0.82	0.10	54,54,54,54	0
59	MG	AB	3017	1/1	0.82	0.10	59,59,59,59	0
59	MG	CA	3111	1/1	0.82	0.23	79,79,79,79	0
59	MG	BA	1634	1/1	0.82	0.26	64,64,64,64	0
59	MG	AD	301	1/1	0.82	0.18	57,57,57,57	0
59	MG	CA	3035	1/1	0.82	0.38	69,69,69,69	0
59	MG	CA	3530	1/1	0.82	0.23	71,71,71,71	0
59	MG	AA	3063	1/1	0.82	0.15	54,54,54,54	0
59	MG	BA	1659	1/1	0.82	0.21	67,67,67,67	0
59	MG	CA	3542	1/1	0.82	0.14	87,87,87,87	0
59	MG	CA	3155	1/1	0.82	0.29	112,112,112,112	0
59	MG	BA	1782	1/1	0.82	0.11	47,47,47,47	0
59	MG	DA	1755	1/1	0.82	0.32	88,88,88,88	0
59	MG	AA	3441	1/1	0.82	0.18	58,58,58,58	0
59	MG	CA	3202	1/1	0.82	0.23	73,73,73,73	0
59	MG	CA	3411	1/1	0.82	0.13	57,57,57,57	0
59	MG	CA	3420	1/1	0.82	0.19	69,69,69,69	0
59	MG	DA	1638	1/1	0.82	0.15	80,80,80,80	0
59	MG	CA	3581	1/1	0.82	0.12	38,38,38,38	0
59	MG	BA	1601	1/1	0.83	0.13	95,95,95,95	0
59	MG	CA	3591	1/1	0.83	0.10	60,60,60,60	0
59	MG	BA	1693	1/1	0.83	0.17	76,76,76,76	0
59	MG	BA	1764	1/1	0.83	0.10	71,71,71,71	0
59	MG	DA	1676	1/1	0.83	0.16	74,74,74,74	0
59	MG	DA	1677	1/1	0.83	0.15	78,78,78,78	0
59	MG	DA	1678	1/1	0.83	0.20	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3706	1/1	0.83	0.24	41,41,41,41	1
59	MG	CA	3117	1/1	0.83	0.20	67,67,67,67	0
59	MG	CA	3622	1/1	0.83	0.13	50,50,50,50	0
59	MG	CA	3502	1/1	0.83	0.27	90,90,90,90	0
59	MG	CA	3124	1/1	0.83	0.23	65,65,65,65	0
59	MG	BA	1610	1/1	0.83	0.15	78,78,78,78	0
59	MG	CA	3126	1/1	0.83	0.15	62,62,62,62	0
59	MG	AA	3235	1/1	0.83	0.25	93,93,93,93	0
59	MG	CA	3044	1/1	0.83	0.19	89,89,89,89	0
59	MG	BA	1778	1/1	0.83	0.10	54,54,54,54	0
59	MG	AA	3018	1/1	0.83	0.60	67,67,67,67	0
59	MG	AA	3582	1/1	0.83	0.23	76,76,76,76	0
59	MG	CA	3164	1/1	0.83	0.23	64,64,64,64	0
59	MG	AA	3495	1/1	0.83	0.15	35,35,35,35	0
59	MG	CA	3184	1/1	0.83	0.26	77,77,77,77	0
59	MG	AA	3133	1/1	0.83	0.21	50,50,50,50	0
59	MG	DA	1618	1/1	0.83	0.29	91,91,91,91	0
59	MG	BA	1797	1/1	0.83	0.14	59,59,59,59	0
59	MG	DA	1629	1/1	0.83	0.17	59,59,59,59	0
59	MG	CA	3203	1/1	0.83	0.10	73,73,73,73	0
59	MG	AA	3756	1/1	0.83	0.09	49,49,49,49	0
59	MG	BA	1811	1/1	0.83	0.13	77,77,77,77	0
59	MG	DA	1639	1/1	0.83	0.14	69,69,69,69	0
59	MG	DA	1643	1/1	0.83	0.17	79,79,79,79	0
59	MG	DA	1634	1/1	0.84	0.23	66,66,66,66	0
59	MG	BA	1704	1/1	0.84	0.20	71,71,71,71	0
59	MG	CA	3565	1/1	0.84	0.11	95,95,95,95	0
59	MG	CA	3398	1/1	0.84	0.14	67,67,67,67	0
59	MG	CA	3070	1/1	0.84	0.13	60,60,60,60	0
59	MG	AA	3212	1/1	0.84	0.24	81,81,81,81	0
59	MG	AA	3758	1/1	0.84	0.23	43,43,43,43	1
59	MG	AA	3425	1/1	0.84	0.16	77,77,77,77	0
59	MG	CA	3204	1/1	0.84	0.10	54,54,54,54	0
59	MG	DA	1675	1/1	0.84	0.48	70,70,70,70	0
59	MG	CA	3216	1/1	0.84	0.21	79,79,79,79	0
59	MG	BA	1662	1/1	0.84	0.24	70,70,70,70	0
59	MG	BA	1669	1/1	0.84	0.20	66,66,66,66	0
59	MG	CA	3470	1/1	0.84	0.17	74,74,74,74	0
59	MG	BA	1744	1/1	0.84	0.12	57,57,57,57	0
59	MG	AA	3141	1/1	0.84	0.09	68,68,68,68	0
59	MG	BA	1614	1/1	0.84	0.17	72,72,72,72	0
59	MG	CA	3634	1/1	0.84	0.12	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BS	101	1/1	0.84	0.09	79,79,79,79	0
59	MG	CA	3643	1/1	0.84	0.09	79,79,79,79	0
59	MG	DA	1730	1/1	0.84	0.17	71,71,71,71	0
59	MG	CA	3501	1/1	0.84	0.17	74,74,74,74	0
59	MG	AA	3653	1/1	0.84	0.10	60,60,60,60	0
59	MG	CA	3649	1/1	0.84	0.18	51,51,51,51	0
59	MG	AA	3157	1/1	0.84	0.22	91,91,91,91	0
59	MG	AA	3677	1/1	0.84	0.20	69,69,69,69	0
59	MG	DA	1742	1/1	0.84	0.11	72,72,72,72	0
59	MG	CE	301	1/1	0.84	0.16	53,53,53,53	0
59	MG	CA	3508	1/1	0.84	0.09	52,52,52,52	0
59	MG	CA	3129	1/1	0.84	0.14	64,64,64,64	0
59	MG	DA	1750	1/1	0.84	0.14	67,67,67,67	0
59	MG	CA	3518	1/1	0.84	0.11	65,65,65,65	0
59	MG	CA	3314	1/1	0.84	0.12	57,57,57,57	0
59	MG	AA	3607	1/1	0.84	0.14	60,60,60,60	1
59	MG	CA	3538	1/1	0.84	0.14	72,72,72,72	0
59	MG	AD	308	1/1	0.84	0.14	65,65,65,65	0
59	MG	BA	1644	1/1	0.84	0.15	74,74,74,74	0
59	MG	BA	1780	1/1	0.84	0.12	60,60,60,60	0
59	MG	CA	3367	1/1	0.84	0.14	63,63,63,63	0
59	MG	AA	3754	1/1	0.84	0.16	64,64,64,64	0
59	MG	CA	3294	1/1	0.85	0.06	72,72,72,72	0
59	MG	BA	1646	1/1	0.85	0.24	66,66,66,66	0
59	MG	AA	3651	1/1	0.85	0.17	77,77,77,77	0
59	MG	AA	3206	1/1	0.85	0.25	106,106,106,106	0
59	MG	AA	3068	1/1	0.85	0.32	73,73,73,73	0
59	MG	CA	3333	1/1	0.85	0.17	68,68,68,68	0
59	MG	CA	3340	1/1	0.85	0.16	66,66,66,66	0
59	MG	CA	3341	1/1	0.85	0.12	73,73,73,73	0
59	MG	CA	3555	1/1	0.85	0.07	71,71,71,71	0
59	MG	AE	305	1/1	0.85	0.18	48,48,48,48	0
59	MG	AA	3675	1/1	0.85	0.12	64,64,64,64	0
59	MG	CA	3134	1/1	0.85	0.17	71,71,71,71	0
59	MG	CA	3135	1/1	0.85	0.23	59,59,59,59	0
59	MG	A7	104	1/1	0.85	0.09	55,55,55,55	0
59	MG	CA	3379	1/1	0.85	0.10	83,83,83,83	0
59	MG	CA	3389	1/1	0.85	0.17	59,59,59,59	0
59	MG	CA	3392	1/1	0.85	0.11	43,43,43,43	0
59	MG	DA	1692	1/1	0.85	0.12	53,53,53,53	0
59	MG	DA	1694	1/1	0.85	0.12	106,106,106,106	0
59	MG	AA	3676	1/1	0.85	0.10	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3148	1/1	0.85	0.26	62,62,62,62	0
59	MG	DA	1709	1/1	0.85	0.13	70,70,70,70	0
59	MG	CA	3038	1/1	0.85	0.31	97,97,97,97	0
59	MG	DA	1713	1/1	0.85	0.08	49,49,49,49	0
59	MG	CA	3042	1/1	0.85	0.27	65,65,65,65	0
59	MG	CA	3612	1/1	0.85	0.28	83,83,83,83	0
59	MG	DA	1722	1/1	0.85	0.10	77,77,77,77	0
59	MG	AA	3755	1/1	0.85	0.29	78,78,78,78	0
59	MG	AA	3453	1/1	0.85	0.14	39,39,39,39	0
59	MG	CA	3432	1/1	0.85	0.16	32,32,32,32	0
59	MG	AA	3213	1/1	0.85	0.33	76,76,76,76	0
59	MG	BA	1676	1/1	0.85	0.24	61,61,61,61	0
59	MG	DA	1736	1/1	0.85	0.10	78,78,78,78	0
59	MG	AA	3769	1/1	0.85	0.15	63,63,63,63	0
59	MG	AA	3680	1/1	0.85	0.20	79,79,79,79	0
59	MG	BA	1781	1/1	0.85	0.09	63,63,63,63	0
59	MG	CA	3076	1/1	0.85	0.24	64,64,64,64	0
59	MG	AA	3189	1/1	0.85	0.20	62,62,62,62	0
59	MG	CA	3226	1/1	0.85	0.24	52,52,52,52	0
59	MG	AA	3138	1/1	0.85	0.09	38,38,38,38	0
59	MG	BA	1788	1/1	0.85	0.35	79,79,79,79	0
59	MG	AA	3096	1/1	0.85	0.17	59,59,59,59	0
59	MG	BA	1699	1/1	0.85	0.07	72,72,72,72	0
59	MG	CA	3107	1/1	0.85	0.20	77,77,77,77	0
59	MG	AA	3787	1/1	0.85	0.13	82,82,82,82	0
59	MG	CA	3510	1/1	0.85	0.17	95,95,95,95	0
59	MG	DA	1605	1/1	0.85	0.14	105,105,105,105	0
59	MG	CA	3511	1/1	0.85	0.10	81,81,81,81	0
59	MG	AA	3796	1/1	0.85	0.19	78,78,78,78	0
59	MG	DA	1614	1/1	0.85	0.09	65,65,65,65	0
59	MG	DA	1610	1/1	0.86	0.21	71,71,71,71	0
59	MG	CA	3524	1/1	0.86	0.10	52,52,52,52	0
59	MG	BA	1783	1/1	0.86	0.15	57,57,57,57	0
59	MG	AA	3715	1/1	0.86	0.23	33,33,33,33	1
59	MG	AA	3344	1/1	0.86	0.11	22,22,22,22	0
59	MG	A2	3001	1/1	0.86	0.11	53,53,53,53	0
59	MG	AA	3775	1/1	0.86	0.27	25,25,25,25	1
59	MG	DA	1632	1/1	0.86	0.21	57,57,57,57	0
59	MG	CA	3194	1/1	0.86	0.10	52,52,52,52	0
59	MG	CA	3378	1/1	0.86	0.16	97,97,97,97	0
59	MG	BA	1795	1/1	0.86	0.07	59,59,59,59	0
59	MG	AA	3614	1/1	0.86	0.14	50,50,50,50	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	1641	1/1	0.86	0.10	74,74,74,74	0
59	MG	AA	3273	1/1	0.86	0.09	90,90,90,90	0
59	MG	DA	1652	1/1	0.86	0.14	80,80,80,80	0
59	MG	CA	3205	1/1	0.86	0.11	81,81,81,81	0
59	MG	DA	1659	1/1	0.86	0.26	78,78,78,78	0
59	MG	DA	1662	1/1	0.86	0.23	75,75,75,75	0
59	MG	BA	1664	1/1	0.86	0.10	56,56,56,56	0
59	MG	CA	3573	1/1	0.86	0.11	65,65,65,65	0
59	MG	CA	3222	1/1	0.86	0.15	57,57,57,57	0
59	MG	CA	3104	1/1	0.86	0.17	80,80,80,80	0
59	MG	CA	3414	1/1	0.86	0.14	34,34,34,34	1
59	MG	BA	1668	1/1	0.86	0.09	69,69,69,69	0
59	MG	CA	3230	1/1	0.86	0.24	49,49,49,49	0
59	MG	DA	1690	1/1	0.86	0.19	73,73,73,73	0
59	MG	CA	3233	1/1	0.86	0.12	59,59,59,59	0
59	MG	CA	3433	1/1	0.86	0.10	82,82,82,82	0
59	MG	DA	1698	1/1	0.86	0.20	97,97,97,97	0
59	MG	CA	3603	1/1	0.86	0.16	49,49,49,49	0
59	MG	AA	3740	1/1	0.86	0.17	61,61,61,61	0
59	MG	CA	3606	1/1	0.86	0.29	73,73,73,73	0
59	MG	CA	3610	1/1	0.86	0.11	69,69,69,69	0
59	MG	CA	3456	1/1	0.86	0.11	54,54,54,54	0
59	MG	CA	3614	1/1	0.86	0.11	62,62,62,62	0
59	MG	DA	1717	1/1	0.86	0.19	95,95,95,95	0
59	MG	CA	3615	1/1	0.86	0.12	28,28,28,28	0
59	MG	AA	3098	1/1	0.86	0.26	51,51,51,51	0
59	MG	AA	3792	1/1	0.86	0.08	48,48,48,48	0
59	MG	CA	3238	1/1	0.86	0.18	69,69,69,69	0
59	MG	AA	3315	1/1	0.86	0.23	65,65,65,65	0
59	MG	CA	3626	1/1	0.86	0.16	61,61,61,61	0
59	MG	CA	3474	1/1	0.86	0.14	59,59,59,59	0
59	MG	AA	3814	1/1	0.86	0.26	72,72,72,72	0
59	MG	AA	3181	1/1	0.86	0.23	79,79,79,79	0
59	MG	CA	3249	1/1	0.86	0.10	61,61,61,61	0
59	MG	DA	1739	1/1	0.86	0.14	73,73,73,73	0
59	MG	CA	3256	1/1	0.86	0.19	65,65,65,65	0
59	MG	CA	3647	1/1	0.86	0.10	85,85,85,85	0
59	MG	DA	1743	1/1	0.86	0.11	59,59,59,59	0
59	MG	AB	3021	1/1	0.86	0.21	65,65,65,65	0
59	MG	CA	3041	1/1	0.86	0.24	61,61,61,61	0
59	MG	CA	3504	1/1	0.86	0.12	79,79,79,79	0
59	MG	BA	1687	1/1	0.86	0.23	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CE	305	1/1	0.86	0.06	58,58,58,58	0
59	MG	AA	3586	1/1	0.86	0.20	74,74,74,74	0
59	MG	CP	201	1/1	0.86	0.08	62,62,62,62	1
59	MG	CA	3307	1/1	0.86	0.11	60,60,60,60	0
59	MG	CA	3509	1/1	0.86	0.08	83,83,83,83	0
59	MG	CA	3047	1/1	0.86	0.19	84,84,84,84	0
59	MG	BA	1638	1/1	0.86	0.17	66,66,66,66	0
59	MG	DE	201	1/1	0.86	0.15	84,84,84,84	0
59	MG	AA	3711	1/1	0.86	0.29	43,43,43,43	1
59	MG	BA	1695	1/1	0.86	0.10	83,83,83,83	0
59	MG	BA	1724	1/1	0.87	0.11	67,67,67,67	0
59	MG	AA	3786	1/1	0.87	0.09	53,53,53,53	0
59	MG	CA	3057	1/1	0.87	0.19	60,60,60,60	0
59	MG	AA	3186	1/1	0.87	0.12	48,48,48,48	0
59	MG	BA	1645	1/1	0.87	0.12	74,74,74,74	0
59	MG	CA	3067	1/1	0.87	0.13	63,63,63,63	0
59	MG	AA	3705	1/1	0.87	0.23	53,53,53,53	1
59	MG	AA	3150	1/1	0.87	0.14	45,45,45,45	0
59	MG	DA	1622	1/1	0.87	0.14	60,60,60,60	0
59	MG	AA	3194	1/1	0.87	0.21	82,82,82,82	0
59	MG	BA	1658	1/1	0.87	0.31	66,66,66,66	0
59	MG	CA	3254	1/1	0.87	0.15	85,85,85,85	0
59	MG	AA	3337	1/1	0.87	0.12	75,75,75,75	0
59	MG	CA	3273	1/1	0.87	0.11	58,58,58,58	0
59	MG	CA	3532	1/1	0.87	0.13	49,49,49,49	0
59	MG	CA	3288	1/1	0.87	0.14	49,49,49,49	0
59	MG	CA	3537	1/1	0.87	0.16	59,59,59,59	0
59	MG	DA	1640	1/1	0.87	0.27	77,77,77,77	0
59	MG	BA	1772	1/1	0.87	0.10	66,66,66,66	0
59	MG	BA	1774	1/1	0.87	0.13	50,50,50,50	0
59	MG	DA	1644	1/1	0.87	0.15	94,94,94,94	0
59	MG	DA	1649	1/1	0.87	0.27	69,69,69,69	0
59	MG	AB	3020	1/1	0.87	0.15	62,62,62,62	0
59	MG	DA	1654	1/1	0.87	0.26	63,63,63,63	0
59	MG	AA	3712	1/1	0.87	0.29	70,70,70,70	0
59	MG	AA	3486	1/1	0.87	0.13	67,67,67,67	0
59	MG	BA	1779	1/1	0.87	0.13	85,85,85,85	0
59	MG	BA	1665	1/1	0.87	0.20	73,73,73,73	0
59	MG	CA	3112	1/1	0.87	0.21	69,69,69,69	0
59	MG	CA	3563	1/1	0.87	0.11	75,75,75,75	0
59	MG	CA	3116	1/1	0.87	0.21	52,52,52,52	0
59	MG	AA	3626	1/1	0.87	0.12	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3493	1/1	0.87	0.09	77,77,77,77	0
59	MG	AG	202	1/1	0.87	0.08	54,54,54,54	0
59	MG	AA	3195	1/1	0.87	0.26	69,69,69,69	0
59	MG	AA	3516	1/1	0.87	0.15	65,65,65,65	0
59	MG	AA	3128	1/1	0.87	0.31	89,89,89,89	0
59	MG	DA	1695	1/1	0.87	0.14	63,63,63,63	0
59	MG	AA	3367	1/1	0.87	0.13	60,60,60,60	0
59	MG	BA	1602	1/1	0.87	0.19	79,79,79,79	0
59	MG	BA	1682	1/1	0.87	0.29	70,70,70,70	0
59	MG	CA	3596	1/1	0.87	0.10	51,51,51,51	0
59	MG	CA	3598	1/1	0.87	0.07	65,65,65,65	0
59	MG	BA	1683	1/1	0.87	0.22	71,71,71,71	0
59	MG	BA	1810	1/1	0.87	0.09	82,82,82,82	0
59	MG	AA	3409	1/1	0.87	0.14	60,60,60,60	0
59	MG	AA	3169	1/1	0.87	0.19	35,35,35,35	0
59	MG	CA	3157	1/1	0.87	0.19	81,81,81,81	0
59	MG	AA	3664	1/1	0.87	0.14	62,62,62,62	0
59	MG	CA	3165	1/1	0.87	0.19	57,57,57,57	0
59	MG	BE	3001	1/1	0.87	0.08	78,78,78,78	0
59	MG	AA	3055	1/1	0.87	0.26	65,65,65,65	0
59	MG	CA	3621	1/1	0.87	0.11	61,61,61,61	0
59	MG	AA	3435	1/1	0.87	0.11	52,52,52,52	0
59	MG	CA	3442	1/1	0.87	0.30	74,74,74,74	0
59	MG	AA	3288	1/1	0.87	0.13	39,39,39,39	0
59	MG	CA	3633	1/1	0.87	0.12	68,68,68,68	0
59	MG	BA	1623	1/1	0.87	0.15	67,67,67,67	0
59	MG	CA	3034	1/1	0.87	0.24	77,77,77,77	0
59	MG	AA	3608	1/1	0.87	0.13	60,60,60,60	0
59	MG	AA	3611	1/1	0.87	0.14	47,47,47,47	0
59	MG	CA	3212	1/1	0.87	0.28	84,84,84,84	0
59	MG	BA	1714	1/1	0.87	0.21	74,74,74,74	0
59	MG	CA	3478	1/1	0.87	0.12	65,65,65,65	0
59	MG	CA	3656	1/1	0.87	0.23	63,63,63,63	0
59	MG	CA	3480	1/1	0.87	0.11	50,50,50,50	0
59	MG	CB	3005	1/1	0.87	0.18	63,63,63,63	0
59	MG	CA	3481	1/1	0.87	0.11	64,64,64,64	0
59	MG	CA	3217	1/1	0.87	0.17	62,62,62,62	0
59	MG	BA	1716	1/1	0.87	0.14	86,86,86,86	0
59	MG	CA	3490	1/1	0.87	0.09	50,50,50,50	0
59	MG	BA	1631	1/1	0.87	0.11	71,71,71,71	0
59	MG	DJ	5001	1/1	0.87	0.09	82,82,82,82	0
59	MG	DK	5001	1/1	0.87	0.10	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3698	1/1	0.87	0.07	41,41,41,41	0
59	MG	CA	3499	1/1	0.87	0.19	62,62,62,62	0
59	MG	DZ	701	1/1	0.87	0.10	72,72,72,72	0
59	MG	CA	3072	1/1	0.88	0.12	66,66,66,66	0
59	MG	CA	3075	1/1	0.88	0.16	90,90,90,90	0
59	MG	BA	1713	1/1	0.88	0.23	68,68,68,68	0
59	MG	AA	3771	1/1	0.88	0.16	60,60,60,60	0
59	MG	CA	3577	1/1	0.88	0.10	51,51,51,51	1
59	MG	CA	3080	1/1	0.88	0.15	75,75,75,75	0
59	MG	CA	3081	1/1	0.88	0.15	63,63,63,63	0
59	MG	AA	3051	1/1	0.88	0.30	48,48,48,48	0
59	MG	DA	1646	1/1	0.88	0.08	57,57,57,57	0
59	MG	CA	3221	1/1	0.88	0.19	65,65,65,65	0
59	MG	AA	3066	1/1	0.88	0.14	51,51,51,51	0
59	MG	BA	1803	1/1	0.88	0.12	64,64,64,64	0
59	MG	CA	3224	1/1	0.88	0.22	59,59,59,59	0
59	MG	CA	3098	1/1	0.88	0.10	70,70,70,70	0
59	MG	BA	1805	1/1	0.88	0.12	71,71,71,71	0
59	MG	AA	3415	1/1	0.88	0.18	62,62,62,62	0
59	MG	DA	1665	1/1	0.88	0.11	63,63,63,63	0
59	MG	BA	1609	1/1	0.88	0.08	62,62,62,62	0
59	MG	DA	1669	1/1	0.88	0.12	65,65,65,65	0
59	MG	BA	1727	1/1	0.88	0.11	77,77,77,77	0
59	MG	CA	3608	1/1	0.88	0.21	50,50,50,50	1
59	MG	AA	3027	1/1	0.88	0.37	75,75,75,75	0
59	MG	CA	3477	1/1	0.88	0.14	69,69,69,69	0
59	MG	AA	3627	1/1	0.88	0.10	76,76,76,76	0
59	MG	DA	1679	1/1	0.88	0.12	70,70,70,70	0
59	MG	DA	1683	1/1	0.88	0.13	58,58,58,58	0
59	MG	CA	3239	1/1	0.88	0.10	69,69,69,69	0
59	MG	CA	3114	1/1	0.88	0.24	66,66,66,66	0
59	MG	CA	3241	1/1	0.88	0.18	72,72,72,72	0
59	MG	CA	3486	1/1	0.88	0.13	81,81,81,81	0
59	MG	AA	3314	1/1	0.88	0.13	57,57,57,57	0
59	MG	AA	3630	1/1	0.88	0.34	72,72,72,72	0
59	MG	CA	3001	1/1	0.88	0.16	64,64,64,64	0
59	MG	CA	3628	1/1	0.88	0.10	54,54,54,54	0
59	MG	CA	3003	1/1	0.88	0.21	62,62,62,62	0
59	MG	AA	3640	1/1	0.88	0.10	68,68,68,68	0
59	MG	AA	3551	1/1	0.88	0.08	39,39,39,39	0
59	MG	CA	3284	1/1	0.88	0.18	75,75,75,75	0
59	MG	AA	3427	1/1	0.88	0.06	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3215	1/1	0.88	0.19	59,59,59,59	0
59	MG	AA	3124	1/1	0.88	0.30	62,62,62,62	0
59	MG	BA	1633	1/1	0.88	0.25	63,63,63,63	0
59	MG	DA	1728	1/1	0.88	0.09	71,71,71,71	0
59	MG	CA	3296	1/1	0.88	0.09	79,79,79,79	0
59	MG	CA	3298	1/1	0.88	0.21	57,57,57,57	0
59	MG	CA	3140	1/1	0.88	0.25	63,63,63,63	0
59	MG	CB	3011	1/1	0.88	0.20	56,56,56,56	0
59	MG	CB	3012	1/1	0.88	0.14	62,62,62,62	0
59	MG	CA	3514	1/1	0.88	0.22	64,64,64,64	0
59	MG	CA	3515	1/1	0.88	0.07	54,54,54,54	0
59	MG	AA	3450	1/1	0.88	0.08	58,58,58,58	0
59	MG	AA	3601	1/1	0.88	0.10	61,61,61,61	0
59	MG	AA	3010	1/1	0.88	0.18	46,46,46,46	0
59	MG	AA	3061	1/1	0.88	0.17	59,59,59,59	0
59	MG	AF	307	1/1	0.88	0.18	76,76,76,76	0
59	MG	CA	3534	1/1	0.88	0.07	73,73,73,73	0
59	MG	AA	3241	1/1	0.88	0.17	65,65,65,65	0
59	MG	CA	3536	1/1	0.88	0.13	84,84,84,84	0
59	MG	BA	1698	1/1	0.88	0.18	63,63,63,63	0
59	MG	CA	3171	1/1	0.88	0.16	56,56,56,56	0
59	MG	BA	1654	1/1	0.88	0.14	76,76,76,76	0
59	MG	CA	3180	1/1	0.88	0.19	62,62,62,62	0
59	MG	DA	1761	1/1	0.88	0.12	72,72,72,72	0
59	MG	AA	3357	1/1	0.88	0.13	55,55,55,55	0
59	MG	AA	3365	1/1	0.88	0.20	77,77,77,77	0
59	MG	DA	1770	1/1	0.88	0.09	63,63,63,63	0
59	MG	CA	3553	1/1	0.88	0.12	90,90,90,90	0
59	MG	DA	1624	1/1	0.88	0.07	82,82,82,82	0
59	MG	DA	1626	1/1	0.88	0.14	71,71,71,71	0
59	MG	CA	3190	1/1	0.88	0.16	66,66,66,66	0
59	MG	CA	3193	1/1	0.88	0.15	89,89,89,89	0
59	MG	BA	1711	1/1	0.88	0.10	61,61,61,61	0
59	MG	CA	3219	1/1	0.89	0.14	42,42,42,42	0
59	MG	BA	1808	1/1	0.89	0.10	54,54,54,54	0
59	MG	CA	3576	1/1	0.89	0.08	71,71,71,71	0
59	MG	AA	3603	1/1	0.89	0.24	76,76,76,76	0
59	MG	BA	1717	1/1	0.89	0.13	78,78,78,78	0
59	MG	BA	1718	1/1	0.89	0.06	63,63,63,63	0
59	MG	CA	3441	1/1	0.89	0.16	56,56,56,56	0
59	MG	BA	1663	1/1	0.89	0.13	43,43,43,43	0
59	MG	CA	3229	1/1	0.89	0.12	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3589	1/1	0.89	0.14	71,71,71,71	0
59	MG	CA	3454	1/1	0.89	0.08	81,81,81,81	0
59	MG	CA	3593	1/1	0.89	0.18	61,61,61,61	0
59	MG	AA	3604	1/1	0.89	0.17	81,81,81,81	0
59	MG	CA	3113	1/1	0.89	0.15	38,38,38,38	0
59	MG	AA	3180	1/1	0.89	0.22	69,69,69,69	0
59	MG	BA	1666	1/1	0.89	0.18	61,61,61,61	0
59	MG	CA	3604	1/1	0.89	0.07	62,62,62,62	0
59	MG	BA	1667	1/1	0.89	0.16	74,74,74,74	0
59	MG	CA	3120	1/1	0.89	0.17	42,42,42,42	0
59	MG	DA	1672	1/1	0.89	0.09	77,77,77,77	0
59	MG	AA	3251	1/1	0.89	0.21	56,56,56,56	0
59	MG	AA	3530	1/1	0.89	0.14	20,20,20,20	1
59	MG	AA	3240	1/1	0.89	0.15	69,69,69,69	0
59	MG	BA	1754	1/1	0.89	0.12	49,49,49,49	0
59	MG	AA	3615	1/1	0.89	0.17	43,43,43,43	0
59	MG	BA	1672	1/1	0.89	0.24	65,65,65,65	0
59	MG	CA	3040	1/1	0.89	0.29	79,79,79,79	0
59	MG	AA	3736	1/1	0.89	0.11	59,59,59,59	0
59	MG	CA	3264	1/1	0.89	0.16	60,60,60,60	0
59	MG	CA	3268	1/1	0.89	0.20	52,52,52,52	0
59	MG	CA	3495	1/1	0.89	0.13	70,70,70,70	0
59	MG	AA	3800	1/1	0.89	0.10	35,35,35,35	0
59	MG	CA	3043	1/1	0.89	0.17	61,61,61,61	0
59	MG	AA	3375	1/1	0.89	0.14	48,48,48,48	0
59	MG	CA	3636	1/1	0.89	0.10	64,64,64,64	0
59	MG	CA	3046	1/1	0.89	0.14	68,68,68,68	0
59	MG	CA	3639	1/1	0.89	0.22	61,61,61,61	0
59	MG	CA	3291	1/1	0.89	0.17	48,48,48,48	0
59	MG	AA	3739	1/1	0.89	0.09	38,38,38,38	0
59	MG	CA	3645	1/1	0.89	0.10	69,69,69,69	0
59	MG	BA	1630	1/1	0.89	0.17	61,61,61,61	0
59	MG	AA	3140	1/1	0.89	0.23	62,62,62,62	0
59	MG	AA	3565	1/1	0.89	0.13	44,44,44,44	0
59	MG	BA	1689	1/1	0.89	0.36	71,71,71,71	0
59	MG	AA	3466	1/1	0.89	0.19	76,76,76,76	0
59	MG	CB	3003	1/1	0.89	0.09	65,65,65,65	0
59	MG	AD	307	1/1	0.89	0.21	86,86,86,86	0
59	MG	AA	3278	1/1	0.89	0.17	60,60,60,60	0
59	MG	CA	3517	1/1	0.89	0.11	62,62,62,62	0
59	MG	AA	3339	1/1	0.89	0.12	49,49,49,49	0
59	MG	CA	3521	1/1	0.89	0.17	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3335	1/1	0.89	0.17	66,66,66,66	0
59	MG	CA	3529	1/1	0.89	0.09	68,68,68,68	0
59	MG	CA	3189	1/1	0.89	0.14	50,50,50,50	0
59	MG	AA	3692	1/1	0.89	0.10	36,36,36,36	1
59	MG	CA	3343	1/1	0.89	0.09	32,32,32,32	0
59	MG	CQ	203	1/1	0.89	0.15	54,54,54,54	0
59	MG	AA	3761	1/1	0.89	0.40	92,92,92,92	0
59	MG	DA	1752	1/1	0.89	0.20	52,52,52,52	0
59	MG	BA	1789	1/1	0.89	0.14	72,72,72,72	0
59	MG	CA	3199	1/1	0.89	0.17	55,55,55,55	0
59	MG	CA	3200	1/1	0.89	0.12	51,51,51,51	0
59	MG	BA	1652	1/1	0.89	0.09	59,59,59,59	0
59	MG	CA	3540	1/1	0.89	0.08	54,54,54,54	0
59	MG	AZ	302	1/1	0.89	0.10	55,55,55,55	0
59	MG	BA	1706	1/1	0.89	0.10	63,63,63,63	0
59	MG	AA	3767	1/1	0.89	0.19	67,67,67,67	0
59	MG	CA	3207	1/1	0.89	0.19	75,75,75,75	0
59	MG	DA	1771	1/1	0.89	0.09	60,60,60,60	0
59	MG	CA	3210	1/1	0.89	0.18	62,62,62,62	0
59	MG	AA	3628	1/1	0.89	0.12	70,70,70,70	0
59	MG	CA	3406	1/1	0.89	0.09	77,77,77,77	0
59	MG	AA	3281	1/1	0.89	0.24	75,75,75,75	0
59	MG	AA	3203	1/1	0.89	0.07	59,59,59,59	0
59	MG	DA	1633	1/1	0.89	0.21	55,55,55,55	0
59	MG	CA	3368	1/1	0.90	0.10	44,44,44,44	0
59	MG	AE	302	1/1	0.90	0.11	57,57,57,57	0
59	MG	BA	1739	1/1	0.90	0.11	62,62,62,62	0
59	MG	AA	3057	1/1	0.90	0.11	46,46,46,46	0
59	MG	BA	1661	1/1	0.90	0.24	63,63,63,63	0
59	MG	CA	3571	1/1	0.90	0.07	45,45,45,45	0
59	MG	DA	1637	1/1	0.90	0.17	68,68,68,68	0
59	MG	CA	3572	1/1	0.90	0.17	70,70,70,70	0
59	MG	AA	3541	1/1	0.90	0.10	74,74,74,74	0
59	MG	BA	1749	1/1	0.90	0.11	61,61,61,61	0
59	MG	AA	3170	1/1	0.90	0.14	54,54,54,54	0
59	MG	AR	202	1/1	0.90	0.08	28,28,28,28	0
59	MG	BA	1756	1/1	0.90	0.07	85,85,85,85	0
59	MG	AA	3101	1/1	0.90	0.39	68,68,68,68	0
59	MG	CA	3585	1/1	0.90	0.12	36,36,36,36	1
59	MG	CA	3412	1/1	0.90	0.13	59,59,59,59	0
59	MG	BA	1763	1/1	0.90	0.12	76,76,76,76	0
59	MG	AA	3556	1/1	0.90	0.13	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	A0	105	1/1	0.90	0.05	30,30,30,30	0
59	MG	DA	1660	1/1	0.90	0.07	80,80,80,80	0
59	MG	DA	1661	1/1	0.90	0.13	66,66,66,66	0
59	MG	AA	3106	1/1	0.90	0.09	33,33,33,33	0
59	MG	A6	101	1/1	0.90	0.16	60,60,60,60	0
59	MG	A6	103	1/1	0.90	0.26	72,72,72,72	0
59	MG	A7	103	1/1	0.90	0.17	55,55,55,55	0
59	MG	AA	3683	1/1	0.90	0.12	62,62,62,62	0
59	MG	AA	3688	1/1	0.90	0.09	25,25,25,25	0
59	MG	CA	3455	1/1	0.90	0.22	49,49,49,49	0
59	MG	AA	3772	1/1	0.90	0.26	61,61,61,61	1
59	MG	AA	3184	1/1	0.90	0.16	75,75,75,75	0
59	MG	BA	1605	1/1	0.90	0.13	73,73,73,73	0
59	MG	CA	3092	1/1	0.90	0.36	79,79,79,79	0
59	MG	AA	3139	1/1	0.90	0.16	60,60,60,60	0
59	MG	CA	3228	1/1	0.90	0.27	59,59,59,59	0
59	MG	AA	3699	1/1	0.90	0.15	71,71,71,71	0
59	MG	AA	3070	1/1	0.90	0.36	81,81,81,81	0
59	MG	AA	3467	1/1	0.90	0.14	49,49,49,49	0
59	MG	CA	3101	1/1	0.90	0.20	84,84,84,84	0
59	MG	AA	3782	1/1	0.90	0.09	44,44,44,44	0
59	MG	AA	3783	1/1	0.90	0.25	53,53,53,53	1
59	MG	BA	1620	1/1	0.90	0.09	52,52,52,52	0
59	MG	AA	3633	1/1	0.90	0.12	48,48,48,48	0
59	MG	BA	1696	1/1	0.90	0.10	98,98,98,98	0
59	MG	CA	3635	1/1	0.90	0.10	48,48,48,48	0
59	MG	AA	3635	1/1	0.90	0.07	49,49,49,49	0
59	MG	CA	3242	1/1	0.90	0.22	82,82,82,82	0
59	MG	AA	3109	1/1	0.90	0.12	56,56,56,56	0
59	MG	DA	1721	1/1	0.90	0.07	80,80,80,80	0
59	MG	CA	3500	1/1	0.90	0.13	75,75,75,75	0
59	MG	CA	3115	1/1	0.90	0.28	67,67,67,67	0
59	MG	AA	3065	1/1	0.90	0.21	62,62,62,62	0
59	MG	AA	3153	1/1	0.90	0.16	59,59,59,59	0
59	MG	CA	3118	1/1	0.90	0.14	65,65,65,65	0
59	MG	AA	3414	1/1	0.90	0.06	37,37,37,37	0
59	MG	CA	3654	1/1	0.90	0.20	90,90,90,90	0
59	MG	AA	3816	1/1	0.90	0.25	66,66,66,66	0
59	MG	CA	3270	1/1	0.90	0.18	76,76,76,76	0
59	MG	AA	3817	1/1	0.90	0.09	75,75,75,75	0
59	MG	CA	3278	1/1	0.90	0.08	58,58,58,58	0
59	MG	BD	502	1/1	0.90	0.23	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	1640	1/1	0.90	0.17	52,52,52,52	0
59	MG	CA	3128	1/1	0.90	0.17	50,50,50,50	0
59	MG	AA	3819	1/1	0.90	0.14	35,35,35,35	1
59	MG	CA	3133	1/1	0.90	0.13	85,85,85,85	0
59	MG	BN	503	1/1	0.90	0.07	62,62,62,62	0
59	MG	AB	3004	1/1	0.90	0.25	69,69,69,69	0
59	MG	DA	1751	1/1	0.90	0.12	64,64,64,64	0
59	MG	AA	3041	1/1	0.90	0.12	37,37,37,37	0
59	MG	AA	3652	1/1	0.90	0.10	53,53,53,53	0
59	MG	CA	3141	1/1	0.90	0.22	68,68,68,68	0
59	MG	AA	3158	1/1	0.90	0.22	68,68,68,68	0
59	MG	DA	1601	1/1	0.90	0.15	74,74,74,74	0
59	MG	CA	3020	1/1	0.90	0.10	47,47,47,47	0
59	MG	DA	1758	1/1	0.90	0.15	75,75,75,75	0
59	MG	CA	3022	1/1	0.90	0.28	69,69,69,69	0
59	MG	DA	1608	1/1	0.90	0.09	57,57,57,57	0
59	MG	DA	1767	1/1	0.90	0.08	74,74,74,74	0
59	MG	CA	3154	1/1	0.90	0.19	64,64,64,64	0
59	MG	CA	3023	1/1	0.90	0.13	68,68,68,68	0
59	MG	CA	3030	1/1	0.90	0.20	59,59,59,59	0
59	MG	CA	3159	1/1	0.90	0.15	69,69,69,69	0
59	MG	AA	3657	1/1	0.90	0.09	63,63,63,63	0
59	MG	CA	3354	1/1	0.90	0.12	49,49,49,49	0
59	MG	AA	3659	1/1	0.90	0.15	73,73,73,73	0
59	MG	BA	1726	1/1	0.90	0.10	46,46,46,46	0
59	MG	AA	3253	1/1	0.90	0.12	64,64,64,64	0
60	ZN	C4	501	1/1	0.90	0.07	194,194,194,194	0
59	MG	AA	3165	1/1	0.91	0.14	52,52,52,52	0
59	MG	CA	3348	1/1	0.91	0.14	44,44,44,44	0
59	MG	BA	1752	1/1	0.91	0.15	59,59,59,59	0
59	MG	CA	3352	1/1	0.91	0.09	79,79,79,79	0
59	MG	AA	3035	1/1	0.91	0.09	48,48,48,48	0
59	MG	DA	1619	1/1	0.91	0.17	59,59,59,59	0
59	MG	AA	3086	1/1	0.91	0.12	55,55,55,55	0
59	MG	CA	3548	1/1	0.91	0.08	90,90,90,90	0
59	MG	CA	3551	1/1	0.91	0.09	63,63,63,63	0
59	MG	AA	3174	1/1	0.91	0.21	59,59,59,59	0
59	MG	CA	3366	1/1	0.91	0.14	49,49,49,49	0
59	MG	AA	3356	1/1	0.91	0.13	80,80,80,80	0
59	MG	CA	3558	1/1	0.91	0.08	64,64,64,64	0
59	MG	CA	3559	1/1	0.91	0.09	75,75,75,75	0
59	MG	BA	1759	1/1	0.91	0.17	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3373	1/1	0.91	0.17	58,58,58,58	0
59	MG	AA	3649	1/1	0.91	0.13	62,62,62,62	0
59	MG	AA	3143	1/1	0.91	0.09	48,48,48,48	0
59	MG	CA	3059	1/1	0.91	0.13	58,58,58,58	0
59	MG	BA	1604	1/1	0.91	0.15	63,63,63,63	0
59	MG	AA	3718	1/1	0.91	0.14	42,42,42,42	0
59	MG	CA	3575	1/1	0.91	0.09	71,71,71,71	0
59	MG	BA	1606	1/1	0.91	0.22	126,126,126,126	0
59	MG	AA	3468	1/1	0.91	0.07	55,55,55,55	0
59	MG	AA	3722	1/1	0.91	0.12	37,37,37,37	0
59	MG	BA	1611	1/1	0.91	0.07	31,31,31,31	0
59	MG	BA	1678	1/1	0.91	0.13	54,54,54,54	0
59	MG	CA	3208	1/1	0.91	0.17	74,74,74,74	0
59	MG	DA	1656	1/1	0.91	0.13	63,63,63,63	0
59	MG	DA	1658	1/1	0.91	0.23	51,51,51,51	0
59	MG	AA	3724	1/1	0.91	0.11	47,47,47,47	0
59	MG	CA	3077	1/1	0.91	0.11	42,42,42,42	0
59	MG	AA	3474	1/1	0.91	0.06	18,18,18,18	1
59	MG	BA	1615	1/1	0.91	0.07	62,62,62,62	0
59	MG	AA	3363	1/1	0.91	0.10	82,82,82,82	0
59	MG	CA	3435	1/1	0.91	0.07	55,55,55,55	0
59	MG	CA	3595	1/1	0.91	0.12	70,70,70,70	0
59	MG	AB	3003	1/1	0.91	0.15	60,60,60,60	0
59	MG	DA	1670	1/1	0.91	0.10	49,49,49,49	0
59	MG	AA	3012	1/1	0.91	0.14	49,49,49,49	0
59	MG	CA	3600	1/1	0.91	0.13	86,86,86,86	0
59	MG	AB	3006	1/1	0.91	0.11	57,57,57,57	0
59	MG	CA	3094	1/1	0.91	0.13	59,59,59,59	0
59	MG	BA	1624	1/1	0.91	0.10	58,58,58,58	0
59	MG	AA	3209	1/1	0.91	0.13	62,62,62,62	0
59	MG	AA	3285	1/1	0.91	0.19	51,51,51,51	0
59	MG	AA	3378	1/1	0.91	0.19	56,56,56,56	0
59	MG	AA	3135	1/1	0.91	0.14	55,55,55,55	0
59	MG	CA	3106	1/1	0.91	0.18	66,66,66,66	0
59	MG	BA	1801	1/1	0.91	0.07	65,65,65,65	0
59	MG	CA	3616	1/1	0.91	0.22	74,74,74,74	0
59	MG	BA	1802	1/1	0.91	0.17	76,76,76,76	0
59	MG	DA	1700	1/1	0.91	0.13	61,61,61,61	0
59	MG	DA	1703	1/1	0.91	0.10	89,89,89,89	0
59	MG	AD	302	1/1	0.91	0.27	85,85,85,85	0
59	MG	BA	1700	1/1	0.91	0.22	52,52,52,52	0
59	MG	BA	1703	1/1	0.91	0.18	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3483	1/1	0.91	0.13	64,64,64,64	0
59	MG	CA	3484	1/1	0.91	0.10	78,78,78,78	0
59	MG	AA	3290	1/1	0.91	0.09	64,64,64,64	0
59	MG	CA	3630	1/1	0.91	0.10	65,65,65,65	0
59	MG	CA	3631	1/1	0.91	0.10	65,65,65,65	0
59	MG	BA	1635	1/1	0.91	0.31	65,65,65,65	0
59	MG	AA	3293	1/1	0.91	0.07	27,27,27,27	0
59	MG	BA	1814	1/1	0.91	0.09	69,69,69,69	0
59	MG	DA	1725	1/1	0.91	0.11	58,58,58,58	0
59	MG	CA	3247	1/1	0.91	0.16	39,39,39,39	0
59	MG	BA	1708	1/1	0.91	0.07	64,64,64,64	0
59	MG	AA	3252	1/1	0.91	0.08	44,44,44,44	0
59	MG	BA	1643	1/1	0.91	0.17	66,66,66,66	0
59	MG	CA	3257	1/1	0.91	0.10	35,35,35,35	0
59	MG	AA	3765	1/1	0.91	0.15	60,60,60,60	0
59	MG	BL	202	1/1	0.91	0.10	54,54,54,54	0
59	MG	AA	3118	1/1	0.91	0.22	76,76,76,76	0
59	MG	AF	308	1/1	0.91	0.12	57,57,57,57	0
59	MG	BW	502	1/1	0.91	0.12	59,59,59,59	0
59	MG	CA	3130	1/1	0.91	0.07	55,55,55,55	0
59	MG	CA	3660	1/1	0.91	0.20	60,60,60,60	0
59	MG	BW	503	1/1	0.91	0.20	60,60,60,60	0
59	MG	CB	3002	1/1	0.91	0.07	63,63,63,63	0
59	MG	BA	1647	1/1	0.91	0.25	57,57,57,57	0
59	MG	AA	3550	1/1	0.91	0.09	38,38,38,38	0
59	MG	CB	3007	1/1	0.91	0.16	52,52,52,52	0
59	MG	CB	3008	1/1	0.91	0.14	66,66,66,66	0
59	MG	CA	3293	1/1	0.91	0.12	60,60,60,60	0
59	MG	AN	3001	1/1	0.91	0.12	58,58,58,58	0
59	MG	AP	204	1/1	0.91	0.08	59,59,59,59	0
59	MG	CD	302	1/1	0.91	0.21	56,56,56,56	0
59	MG	BA	1655	1/1	0.91	0.06	59,59,59,59	0
59	MG	AQ	203	1/1	0.91	0.10	32,32,32,32	0
59	MG	DA	1759	1/1	0.91	0.08	53,53,53,53	0
59	MG	BA	1729	1/1	0.91	0.12	53,53,53,53	0
59	MG	CG	3001	1/1	0.91	0.08	65,65,65,65	0
59	MG	DA	1763	1/1	0.91	0.10	76,76,76,76	0
59	MG	CN	5001	1/1	0.91	0.08	65,65,65,65	0
59	MG	CA	3031	1/1	0.91	0.20	68,68,68,68	0
59	MG	CA	3526	1/1	0.91	0.14	58,58,58,58	0
59	MG	CA	3150	1/1	0.91	0.15	57,57,57,57	0
59	MG	AA	3102	1/1	0.91	0.23	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DE	202	1/1	0.91	0.08	100,100,100,100	0
59	MG	CA	3325	1/1	0.91	0.08	38,38,38,38	0
59	MG	AA	3694	1/1	0.91	0.07	53,53,53,53	0
59	MG	AA	3218	1/1	0.91	0.17	67,67,67,67	0
59	MG	DW	502	1/1	0.91	0.08	58,58,58,58	0
59	MG	AA	3632	1/1	0.91	0.12	54,54,54,54	0
59	MG	DA	1606	1/1	0.91	0.06	85,85,85,85	0
59	MG	AA	3440	1/1	0.91	0.09	63,63,63,63	0
59	MG	AA	3229	1/1	0.92	0.27	67,67,67,67	0
59	MG	BA	1771	1/1	0.92	0.11	65,65,65,65	0
59	MG	AF	302	1/1	0.92	0.14	47,47,47,47	0
59	MG	CV	201	1/1	0.92	0.17	117,117,117,117	0
59	MG	CX	5001	1/1	0.92	0.11	65,65,65,65	0
59	MG	AA	3646	1/1	0.92	0.12	53,53,53,53	0
59	MG	CA	3087	1/1	0.92	0.33	68,68,68,68	0
59	MG	CA	3243	1/1	0.92	0.12	58,58,58,58	0
59	MG	CA	3088	1/1	0.92	0.18	67,67,67,67	0
59	MG	AA	3558	1/1	0.92	0.07	48,48,48,48	0
59	MG	AA	3448	1/1	0.92	0.07	62,62,62,62	0
59	MG	AA	3752	1/1	0.92	0.10	42,42,42,42	0
59	MG	AA	3134	1/1	0.92	0.12	62,62,62,62	0
59	MG	CA	3520	1/1	0.92	0.10	73,73,73,73	0
59	MG	AA	3451	1/1	0.92	0.12	57,57,57,57	0
59	MG	AR	201	1/1	0.92	0.12	63,63,63,63	0
59	MG	AA	3655	1/1	0.92	0.11	55,55,55,55	0
59	MG	AX	3001	1/1	0.92	0.10	52,52,52,52	0
59	MG	AA	3160	1/1	0.92	0.07	30,30,30,30	0
59	MG	AA	3455	1/1	0.92	0.13	32,32,32,32	1
59	MG	DA	1627	1/1	0.92	0.05	77,77,77,77	0
59	MG	CA	3274	1/1	0.92	0.13	52,52,52,52	0
59	MG	A0	102	1/1	0.92	0.07	56,56,56,56	0
59	MG	CA	3280	1/1	0.92	0.07	48,48,48,48	0
59	MG	AA	3763	1/1	0.92	0.10	47,47,47,47	0
59	MG	CA	3285	1/1	0.92	0.09	63,63,63,63	0
59	MG	CA	3287	1/1	0.92	0.13	45,45,45,45	0
59	MG	DA	1636	1/1	0.92	0.24	62,62,62,62	0
59	MG	BA	1791	1/1	0.92	0.11	72,72,72,72	0
59	MG	AA	3596	1/1	0.92	0.12	65,65,65,65	0
59	MG	AA	3346	1/1	0.92	0.19	59,59,59,59	0
59	MG	BA	1796	1/1	0.92	0.16	57,57,57,57	0
59	MG	CA	3547	1/1	0.92	0.12	69,69,69,69	0
59	MG	DA	1642	1/1	0.92	0.10	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3768	1/1	0.92	0.07	58,58,58,58	0
59	MG	BA	1798	1/1	0.92	0.11	73,73,73,73	0
59	MG	DA	1645	1/1	0.92	0.07	58,58,58,58	0
59	MG	AA	3670	1/1	0.92	0.07	54,54,54,54	0
59	MG	AA	3238	1/1	0.92	0.16	76,76,76,76	0
59	MG	CA	3119	1/1	0.92	0.32	55,55,55,55	0
59	MG	AA	3019	1/1	0.92	0.16	70,70,70,70	0
59	MG	AA	3606	1/1	0.92	0.09	34,34,34,34	0
59	MG	CA	3319	1/1	0.92	0.08	65,65,65,65	0
59	MG	AA	3208	1/1	0.92	0.27	54,54,54,54	0
59	MG	AA	3280	1/1	0.92	0.12	53,53,53,53	0
59	MG	AA	3682	1/1	0.92	0.09	31,31,31,31	0
59	MG	AA	3166	1/1	0.92	0.17	40,40,40,40	0
59	MG	BA	1608	1/1	0.92	0.22	57,57,57,57	0
59	MG	AA	3687	1/1	0.92	0.20	52,52,52,52	0
59	MG	AA	3283	1/1	0.92	0.24	43,43,43,43	0
59	MG	AA	3127	1/1	0.92	0.16	57,57,57,57	0
59	MG	AA	3693	1/1	0.92	0.16	69,69,69,69	0
59	MG	CA	3137	1/1	0.92	0.14	69,69,69,69	0
59	MG	AA	3490	1/1	0.92	0.12	27,27,27,27	0
59	MG	AA	3794	1/1	0.92	0.18	60,60,60,60	0
59	MG	AA	3695	1/1	0.92	0.10	67,67,67,67	0
59	MG	BA	1617	1/1	0.92	0.11	118,118,118,118	0
59	MG	CA	3147	1/1	0.92	0.13	55,55,55,55	0
59	MG	BA	1618	1/1	0.92	0.14	52,52,52,52	0
59	MG	CA	3590	1/1	0.92	0.11	59,59,59,59	0
59	MG	AA	3286	1/1	0.92	0.29	40,40,40,40	0
59	MG	DA	1684	1/1	0.92	0.12	69,69,69,69	0
59	MG	AA	3802	1/1	0.92	0.13	86,86,86,86	0
59	MG	AA	3803	1/1	0.92	0.14	45,45,45,45	0
59	MG	CA	3005	1/1	0.92	0.11	48,48,48,48	0
59	MG	CA	3380	1/1	0.92	0.16	59,59,59,59	0
59	MG	CA	3388	1/1	0.92	0.10	90,90,90,90	0
59	MG	AA	3249	1/1	0.92	0.16	59,59,59,59	0
59	MG	CA	3015	1/1	0.92	0.14	51,51,51,51	0
59	MG	AA	3496	1/1	0.92	0.19	31,31,31,31	0
59	MG	DA	1705	1/1	0.92	0.09	68,68,68,68	0
59	MG	DA	1706	1/1	0.92	0.13	66,66,66,66	0
59	MG	BA	1627	1/1	0.92	0.07	51,51,51,51	0
59	MG	AA	3499	1/1	0.92	0.06	48,48,48,48	0
59	MG	CA	3024	1/1	0.92	0.18	100,100,100,100	0
59	MG	CA	3409	1/1	0.92	0.13	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3176	1/1	0.92	0.23	60,60,60,60	0
59	MG	AA	3818	1/1	0.92	0.12	61,61,61,61	0
59	MG	CA	3413	1/1	0.92	0.09	39,39,39,39	0
59	MG	CA	3182	1/1	0.92	0.16	38,38,38,38	0
59	MG	CA	3419	1/1	0.92	0.08	59,59,59,59	0
59	MG	BA	1720	1/1	0.92	0.09	61,61,61,61	0
59	MG	AA	3508	1/1	0.92	0.15	43,43,43,43	0
59	MG	CA	3431	1/1	0.92	0.13	75,75,75,75	0
59	MG	CA	3033	1/1	0.92	0.20	55,55,55,55	0
59	MG	AB	3002	1/1	0.92	0.13	52,52,52,52	0
59	MG	AA	3193	1/1	0.92	0.21	40,40,40,40	0
59	MG	CA	3436	1/1	0.92	0.13	64,64,64,64	0
59	MG	CA	3037	1/1	0.92	0.31	57,57,57,57	0
59	MG	AA	3710	1/1	0.92	0.20	29,29,29,29	1
59	MG	AA	3099	1/1	0.92	0.15	53,53,53,53	0
59	MG	CA	3447	1/1	0.92	0.12	73,73,73,73	0
59	MG	CA	3451	1/1	0.92	0.14	62,62,62,62	0
59	MG	DA	1741	1/1	0.92	0.20	67,67,67,67	0
59	MG	CA	3637	1/1	0.92	0.34	61,61,61,61	0
59	MG	BA	1732	1/1	0.92	0.07	70,70,70,70	0
59	MG	BA	1639	1/1	0.92	0.23	61,61,61,61	0
59	MG	BA	1737	1/1	0.92	0.23	79,79,79,79	0
59	MG	AB	3009	1/1	0.92	0.07	50,50,50,50	0
59	MG	AA	3028	1/1	0.92	0.10	39,39,39,39	0
59	MG	BA	1742	1/1	0.92	0.09	48,48,48,48	0
59	MG	CA	3209	1/1	0.92	0.13	73,73,73,73	0
59	MG	CA	3048	1/1	0.92	0.05	47,47,47,47	0
59	MG	AB	3018	1/1	0.92	0.09	69,69,69,69	0
59	MG	CA	3213	1/1	0.92	0.18	51,51,51,51	0
59	MG	CA	3051	1/1	0.92	0.22	57,57,57,57	0
59	MG	CA	3662	1/1	0.92	0.14	33,33,33,33	0
59	MG	CA	3663	1/1	0.92	0.11	64,64,64,64	0
59	MG	CA	3054	1/1	0.92	0.14	36,36,36,36	0
59	MG	AA	3300	1/1	0.92	0.09	22,22,22,22	0
59	MG	AA	3264	1/1	0.92	0.22	51,51,51,51	0
59	MG	AA	3544	1/1	0.92	0.09	26,26,26,26	0
59	MG	CA	3061	1/1	0.92	0.14	68,68,68,68	0
59	MG	AA	3177	1/1	0.92	0.12	59,59,59,59	0
59	MG	CA	3225	1/1	0.92	0.15	64,64,64,64	0
59	MG	AD	303	1/1	0.92	0.24	58,58,58,58	0
59	MG	CA	3493	1/1	0.92	0.15	65,65,65,65	0
59	MG	AA	3641	1/1	0.92	0.09	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3224	1/1	0.92	0.19	56,56,56,56	0
59	MG	BA	1656	1/1	0.92	0.20	75,75,75,75	0
59	MG	BA	1762	1/1	0.92	0.08	74,74,74,74	0
59	MG	CA	3073	1/1	0.92	0.09	49,49,49,49	0
59	MG	AE	301	1/1	0.92	0.11	69,69,69,69	0
59	MG	CA	3503	1/1	0.92	0.18	52,52,52,52	0
59	MG	DZ	702	1/1	0.92	0.13	57,57,57,57	0
59	MG	AA	3555	1/1	0.92	0.07	45,45,45,45	0
59	MG	DA	1603	1/1	0.93	0.08	72,72,72,72	0
59	MG	AA	3237	1/1	0.93	0.17	76,76,76,76	0
59	MG	AA	3080	1/1	0.93	0.29	61,61,61,61	0
59	MG	BA	1681	1/1	0.93	0.06	53,53,53,53	0
59	MG	DA	1607	1/1	0.93	0.07	86,86,86,86	0
59	MG	AA	3187	1/1	0.93	0.28	56,56,56,56	0
59	MG	A7	102	1/1	0.93	0.11	37,37,37,37	0
59	MG	BA	1807	1/1	0.93	0.11	61,61,61,61	0
59	MG	BA	1684	1/1	0.93	0.17	61,61,61,61	0
59	MG	CA	3122	1/1	0.93	0.13	58,58,58,58	0
59	MG	DA	1616	1/1	0.93	0.19	51,51,51,51	0
59	MG	AA	3210	1/1	0.93	0.17	59,59,59,59	1
59	MG	AA	3684	1/1	0.93	0.11	51,51,51,51	0
59	MG	DA	1620	1/1	0.93	0.16	57,57,57,57	0
59	MG	AA	3017	1/1	0.93	0.09	61,61,61,61	0
59	MG	AA	3471	1/1	0.93	0.08	56,56,56,56	0
59	MG	AA	3610	1/1	0.93	0.15	59,59,59,59	0
59	MG	DA	1625	1/1	0.93	0.08	50,50,50,50	0
59	MG	CA	3313	1/1	0.93	0.16	38,38,38,38	0
59	MG	AA	3473	1/1	0.93	0.07	53,53,53,53	0
59	MG	CA	3543	1/1	0.93	0.09	71,71,71,71	0
59	MG	AA	3791	1/1	0.93	0.14	51,51,51,51	0
59	MG	BK	201	1/1	0.93	0.09	44,44,44,44	0
59	MG	AA	3244	1/1	0.93	0.19	52,52,52,52	0
59	MG	BA	1607	1/1	0.93	0.08	64,64,64,64	0
59	MG	AA	3025	1/1	0.93	0.12	68,68,68,68	0
59	MG	CA	3336	1/1	0.93	0.10	64,64,64,64	0
59	MG	AA	3361	1/1	0.93	0.16	53,53,53,53	0
59	MG	CA	3556	1/1	0.93	0.12	62,62,62,62	0
59	MG	AA	3798	1/1	0.93	0.09	25,25,25,25	0
59	MG	AA	3618	1/1	0.93	0.10	72,72,72,72	0
59	MG	CA	3344	1/1	0.93	0.05	68,68,68,68	0
59	MG	CA	3145	1/1	0.93	0.08	76,76,76,76	0
59	MG	BZ	701	1/1	0.93	0.11	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	1705	1/1	0.93	0.14	53,53,53,53	0
59	MG	AA	3282	1/1	0.93	0.13	33,33,33,33	0
59	MG	AA	3703	1/1	0.93	0.15	56,56,56,56	0
59	MG	AA	3804	1/1	0.93	0.06	50,50,50,50	0
59	MG	DA	1650	1/1	0.93	0.15	50,50,50,50	0
59	MG	CA	3365	1/1	0.93	0.07	55,55,55,55	0
59	MG	CA	3011	1/1	0.93	0.15	63,63,63,63	0
59	MG	AA	3805	1/1	0.93	0.12	58,58,58,58	0
59	MG	CA	3016	1/1	0.93	0.16	52,52,52,52	0
59	MG	BA	1712	1/1	0.93	0.33	57,57,57,57	0
59	MG	AA	3810	1/1	0.93	0.20	67,67,67,67	0
59	MG	AA	3026	1/1	0.93	0.06	47,47,47,47	0
59	MG	AA	3492	1/1	0.93	0.08	26,26,26,26	0
59	MG	CA	3026	1/1	0.93	0.12	32,32,32,32	1
59	MG	CA	3384	1/1	0.93	0.10	55,55,55,55	0
59	MG	CA	3028	1/1	0.93	0.21	51,51,51,51	0
59	MG	DA	1666	1/1	0.93	0.19	53,53,53,53	0
59	MG	DA	1667	1/1	0.93	0.07	66,66,66,66	0
59	MG	CA	3177	1/1	0.93	0.12	29,29,29,29	0
59	MG	CA	3390	1/1	0.93	0.05	80,80,80,80	0
59	MG	CA	3178	1/1	0.93	0.09	54,54,54,54	0
59	MG	CA	3394	1/1	0.93	0.15	69,69,69,69	0
59	MG	AA	3179	1/1	0.93	0.14	45,45,45,45	1
59	MG	BA	1622	1/1	0.93	0.16	65,65,65,65	0
59	MG	CA	3402	1/1	0.93	0.10	66,66,66,66	0
59	MG	AA	3371	1/1	0.93	0.09	53,53,53,53	0
59	MG	AA	3374	1/1	0.93	0.14	49,49,49,49	0
59	MG	CA	3188	1/1	0.93	0.14	94,94,94,94	0
59	MG	AB	3001	1/1	0.93	0.15	74,74,74,74	0
59	MG	AA	3001	1/1	0.93	0.08	25,25,25,25	0
59	MG	DA	1685	1/1	0.93	0.07	46,46,46,46	0
59	MG	DA	1689	1/1	0.93	0.08	56,56,56,56	0
59	MG	AA	3714	1/1	0.93	0.14	70,70,70,70	0
59	MG	BA	1629	1/1	0.93	0.12	61,61,61,61	0
59	MG	AA	3501	1/1	0.93	0.07	49,49,49,49	0
59	MG	BA	1730	1/1	0.93	0.11	53,53,53,53	0
59	MG	CA	3421	1/1	0.93	0.15	57,57,57,57	0
59	MG	CA	3201	1/1	0.93	0.21	45,45,45,45	0
59	MG	DA	1701	1/1	0.93	0.13	68,68,68,68	0
59	MG	AA	3716	1/1	0.93	0.15	66,66,66,66	0
59	MG	BA	1632	1/1	0.93	0.09	48,48,48,48	0
59	MG	AB	3008	1/1	0.93	0.17	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3287	1/1	0.93	0.21	43,43,43,43	0
59	MG	AA	3142	1/1	0.93	0.14	64,64,64,64	0
59	MG	CA	3625	1/1	0.93	0.11	64,64,64,64	0
59	MG	BA	1637	1/1	0.93	0.22	72,72,72,72	0
59	MG	AA	3520	1/1	0.93	0.07	17,17,17,17	0
59	MG	DA	1714	1/1	0.93	0.08	68,68,68,68	0
59	MG	BA	1747	1/1	0.93	0.09	65,65,65,65	0
59	MG	AA	3636	1/1	0.93	0.12	86,86,86,86	0
59	MG	AA	3289	1/1	0.93	0.10	53,53,53,53	0
59	MG	BA	1641	1/1	0.93	0.11	54,54,54,54	0
59	MG	BA	1642	1/1	0.93	0.11	60,60,60,60	0
59	MG	AA	3732	1/1	0.93	0.15	70,70,70,70	0
59	MG	AA	3258	1/1	0.93	0.15	68,68,68,68	0
59	MG	DA	1726	1/1	0.93	0.13	60,60,60,60	0
59	MG	AA	3263	1/1	0.93	0.16	24,24,24,24	1
59	MG	AA	3420	1/1	0.93	0.07	25,25,25,25	1
59	MG	AA	3050	1/1	0.93	0.13	28,28,28,28	0
59	MG	CA	3472	1/1	0.93	0.22	62,62,62,62	0
59	MG	AD	309	1/1	0.93	0.09	56,56,56,56	0
59	MG	DA	1734	1/1	0.93	0.05	65,65,65,65	0
59	MG	DA	1735	1/1	0.93	0.07	73,73,73,73	0
59	MG	AA	3742	1/1	0.93	0.14	68,68,68,68	0
59	MG	AA	3746	1/1	0.93	0.13	73,73,73,73	0
59	MG	AA	3298	1/1	0.93	0.09	58,58,58,58	0
59	MG	CA	3652	1/1	0.93	0.07	23,23,23,23	0
59	MG	AA	3751	1/1	0.93	0.23	61,61,61,61	0
59	MG	AA	3231	1/1	0.93	0.13	64,64,64,64	0
59	MG	CA	3658	1/1	0.93	0.17	64,64,64,64	0
59	MG	CA	3659	1/1	0.93	0.07	55,55,55,55	0
59	MG	AA	3313	1/1	0.93	0.13	39,39,39,39	0
59	MG	AA	3204	1/1	0.93	0.13	54,54,54,54	0
59	MG	AA	3446	1/1	0.93	0.17	59,59,59,59	0
59	MG	CA	3083	1/1	0.93	0.16	61,61,61,61	0
59	MG	CA	3086	1/1	0.93	0.36	85,85,85,85	0
59	MG	AN	3003	1/1	0.93	0.07	55,55,55,55	0
59	MG	CB	3004	1/1	0.93	0.09	55,55,55,55	0
59	MG	AP	203	1/1	0.93	0.08	44,44,44,44	0
59	MG	AA	3563	1/1	0.93	0.12	34,34,34,34	0
59	MG	AA	3447	1/1	0.93	0.10	56,56,56,56	0
59	MG	AA	3185	1/1	0.93	0.14	76,76,76,76	0
59	MG	CA	3245	1/1	0.93	0.24	62,62,62,62	0
59	MG	AA	3575	1/1	0.93	0.09	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CD	301	1/1	0.93	0.12	43,43,43,43	0
59	MG	CA	3095	1/1	0.93	0.12	58,58,58,58	0
59	MG	AV	201	1/1	0.93	0.11	38,38,38,38	0
59	MG	DA	1765	1/1	0.93	0.07	64,64,64,64	0
59	MG	DA	1766	1/1	0.93	0.07	74,74,74,74	0
59	MG	CA	3253	1/1	0.93	0.10	70,70,70,70	0
59	MG	AW	3002	1/1	0.93	0.11	47,47,47,47	0
59	MG	AA	3449	1/1	0.93	0.10	50,50,50,50	0
59	MG	AY	502	1/1	0.93	0.17	60,60,60,60	0
59	MG	AZ	301	1/1	0.93	0.13	86,86,86,86	0
59	MG	BA	1793	1/1	0.93	0.07	65,65,65,65	0
59	MG	CA	3269	1/1	0.93	0.18	81,81,81,81	0
59	MG	BA	1794	1/1	0.93	0.06	38,38,38,38	0
59	MG	AA	3322	1/1	0.93	0.13	61,61,61,61	0
59	MG	CU	201	1/1	0.93	0.15	74,74,74,74	0
59	MG	AA	3270	1/1	0.93	0.22	55,55,55,55	0
59	MG	AA	3593	1/1	0.93	0.19	15,15,15,15	1
59	MG	C5	101	1/1	0.93	0.20	66,66,66,66	0
59	MG	AA	3329	1/1	0.93	0.07	40,40,40,40	1
62	GDP	DZ	703	28/28	0.93	0.08	66,66,66,66	1
59	MG	AA	3325	1/1	0.94	0.11	70,70,70,70	0
59	MG	AA	3808	1/1	0.94	0.13	72,72,72,72	0
59	MG	CB	3010	1/1	0.94	0.08	51,51,51,51	0
59	MG	AA	3148	1/1	0.94	0.22	29,29,29,29	1
59	MG	BA	1731	1/1	0.94	0.10	45,45,45,45	0
59	MG	CA	3464	1/1	0.94	0.08	36,36,36,36	0
59	MG	AA	3813	1/1	0.94	0.07	29,29,29,29	1
59	MG	AA	3599	1/1	0.94	0.07	59,59,59,59	0
59	MG	CA	3469	1/1	0.94	0.14	61,61,61,61	0
59	MG	CE	302	1/1	0.94	0.06	64,64,64,64	0
59	MG	CE	304	1/1	0.94	0.15	75,75,75,75	0
59	MG	BA	1734	1/1	0.94	0.09	61,61,61,61	0
59	MG	AA	3014	1/1	0.94	0.11	31,31,31,31	0
59	MG	BA	1738	1/1	0.94	0.05	66,66,66,66	0
59	MG	AA	3602	1/1	0.94	0.10	51,51,51,51	0
59	MG	AA	3454	1/1	0.94	0.11	61,61,61,61	0
59	MG	AA	3182	1/1	0.94	0.15	46,46,46,46	0
59	MG	CA	3056	1/1	0.94	0.07	63,63,63,63	0
59	MG	AA	3701	1/1	0.94	0.12	81,81,81,81	0
59	MG	AA	3456	1/1	0.94	0.08	56,56,56,56	0
59	MG	CA	3060	1/1	0.94	0.28	72,72,72,72	0
59	MG	AA	3704	1/1	0.94	0.09	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3073	1/1	0.94	0.05	31,31,31,31	0
59	MG	C3	3001	1/1	0.94	0.09	72,72,72,72	0
59	MG	CA	3489	1/1	0.94	0.08	39,39,39,39	0
59	MG	AA	3220	1/1	0.94	0.08	62,62,62,62	0
59	MG	DA	1602	1/1	0.94	0.06	45,45,45,45	0
59	MG	AA	3609	1/1	0.94	0.07	58,58,58,58	0
59	MG	CA	3231	1/1	0.94	0.23	60,60,60,60	0
59	MG	CA	3232	1/1	0.94	0.21	54,54,54,54	0
59	MG	CA	3068	1/1	0.94	0.31	66,66,66,66	0
59	MG	CA	3498	1/1	0.94	0.06	49,49,49,49	0
59	MG	AA	3709	1/1	0.94	0.21	23,23,23,23	1
59	MG	AB	3014	1/1	0.94	0.09	56,56,56,56	0
59	MG	AB	3015	1/1	0.94	0.06	28,28,28,28	0
59	MG	AA	3002	1/1	0.94	0.12	57,57,57,57	0
59	MG	AA	3349	1/1	0.94	0.08	47,47,47,47	0
59	MG	DA	1615	1/1	0.94	0.06	58,58,58,58	0
59	MG	AA	3355	1/1	0.94	0.12	57,57,57,57	0
59	MG	AA	3226	1/1	0.94	0.10	46,46,46,46	0
59	MG	BA	1766	1/1	0.94	0.07	62,62,62,62	0
59	MG	CA	3079	1/1	0.94	0.07	41,41,41,41	0
59	MG	AB	3023	1/1	0.94	0.19	54,54,54,54	0
59	MG	BA	1770	1/1	0.94	0.06	54,54,54,54	0
59	MG	AA	3616	1/1	0.94	0.09	57,57,57,57	0
59	MG	CA	3513	1/1	0.94	0.10	70,70,70,70	0
59	MG	CA	3084	1/1	0.94	0.10	56,56,56,56	0
59	MG	AA	3228	1/1	0.94	0.07	32,32,32,32	0
59	MG	CA	3251	1/1	0.94	0.13	82,82,82,82	0
59	MG	DA	1630	1/1	0.94	0.27	62,62,62,62	0
59	MG	AA	3479	1/1	0.94	0.07	55,55,55,55	0
59	MG	BA	1651	1/1	0.94	0.16	55,55,55,55	0
59	MG	CA	3519	1/1	0.94	0.13	48,48,48,48	0
59	MG	AD	305	1/1	0.94	0.09	50,50,50,50	0
59	MG	AA	3046	1/1	0.94	0.12	35,35,35,35	0
59	MG	CA	3259	1/1	0.94	0.11	80,80,80,80	0
59	MG	AA	3362	1/1	0.94	0.07	46,46,46,46	0
59	MG	CA	3527	1/1	0.94	0.15	76,76,76,76	0
59	MG	CA	3528	1/1	0.94	0.08	38,38,38,38	0
59	MG	AA	3485	1/1	0.94	0.06	48,48,48,48	0
59	MG	AD	311	1/1	0.94	0.13	37,37,37,37	0
59	MG	AA	3088	1/1	0.94	0.15	39,39,39,39	0
59	MG	AA	3730	1/1	0.94	0.09	75,75,75,75	0
59	MG	CA	3099	1/1	0.94	0.20	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	1784	1/1	0.94	0.08	68,68,68,68	0
59	MG	AA	3731	1/1	0.94	0.10	51,51,51,51	0
59	MG	CA	3281	1/1	0.94	0.07	21,21,21,21	0
59	MG	BA	1787	1/1	0.94	0.12	55,55,55,55	0
59	MG	DA	1651	1/1	0.94	0.10	63,63,63,63	0
59	MG	AA	3161	1/1	0.94	0.06	43,43,43,43	0
59	MG	AA	3733	1/1	0.94	0.08	49,49,49,49	0
59	MG	AA	3162	1/1	0.94	0.22	67,67,67,67	0
59	MG	CA	3544	1/1	0.94	0.10	60,60,60,60	0
59	MG	CA	3109	1/1	0.94	0.06	35,35,35,35	0
59	MG	CA	3110	1/1	0.94	0.11	56,56,56,56	0
59	MG	AA	3370	1/1	0.94	0.08	47,47,47,47	0
59	MG	AA	3164	1/1	0.94	0.21	71,71,71,71	0
59	MG	CA	3549	1/1	0.94	0.11	70,70,70,70	0
59	MG	CA	3550	1/1	0.94	0.07	62,62,62,62	1
59	MG	DA	1664	1/1	0.94	0.05	66,66,66,66	0
59	MG	AA	3090	1/1	0.94	0.12	53,53,53,53	0
59	MG	AA	3497	1/1	0.94	0.08	44,44,44,44	0
59	MG	CA	3554	1/1	0.94	0.08	66,66,66,66	0
59	MG	AA	3743	1/1	0.94	0.15	67,67,67,67	0
59	MG	CA	3299	1/1	0.94	0.07	64,64,64,64	0
59	MG	AQ	201	1/1	0.94	0.11	48,48,48,48	0
59	MG	DA	1671	1/1	0.94	0.21	56,56,56,56	0
59	MG	AQ	202	1/1	0.94	0.14	35,35,35,35	0
59	MG	CA	3310	1/1	0.94	0.08	47,47,47,47	0
59	MG	AA	3196	1/1	0.94	0.16	55,55,55,55	0
59	MG	CA	3561	1/1	0.94	0.08	41,41,41,41	1
59	MG	AA	3114	1/1	0.94	0.09	26,26,26,26	0
59	MG	AA	3381	1/1	0.94	0.07	16,16,16,16	0
59	MG	CA	3121	1/1	0.94	0.06	49,49,49,49	0
59	MG	CA	3569	1/1	0.94	0.08	41,41,41,41	0
59	MG	AA	3385	1/1	0.94	0.10	49,49,49,49	0
59	MG	CA	3331	1/1	0.94	0.12	52,52,52,52	0
59	MG	DA	1688	1/1	0.94	0.12	51,51,51,51	0
59	MG	AV	206	1/1	0.94	0.09	33,33,33,33	0
59	MG	CA	3334	1/1	0.94	0.12	47,47,47,47	0
59	MG	AA	3753	1/1	0.94	0.08	30,30,30,30	0
59	MG	AA	3400	1/1	0.94	0.07	13,13,13,13	0
59	MG	AA	3521	1/1	0.94	0.08	19,19,19,19	0
59	MG	AA	3529	1/1	0.94	0.12	30,30,30,30	0
59	MG	DA	1699	1/1	0.94	0.10	74,74,74,74	0
59	MG	CA	3582	1/1	0.94	0.08	99,99,99,99	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3645	1/1	0.94	0.11	58,58,58,58	0
59	MG	AA	3403	1/1	0.94	0.08	42,42,42,42	0
59	MG	CA	3347	1/1	0.94	0.07	45,45,45,45	0
59	MG	BA	1813	1/1	0.94	0.10	55,55,55,55	0
59	MG	BA	1685	1/1	0.94	0.09	50,50,50,50	0
59	MG	DA	1707	1/1	0.94	0.12	61,61,61,61	0
59	MG	BA	1815	1/1	0.94	0.18	53,53,53,53	0
59	MG	AA	3199	1/1	0.94	0.14	41,41,41,41	0
59	MG	A0	103	1/1	0.94	0.07	70,70,70,70	0
59	MG	CA	3360	1/1	0.94	0.09	38,38,38,38	0
59	MG	AA	3650	1/1	0.94	0.08	49,49,49,49	0
59	MG	BA	1692	1/1	0.94	0.18	55,55,55,55	0
59	MG	DA	1716	1/1	0.94	0.05	57,57,57,57	0
59	MG	CA	3142	1/1	0.94	0.17	61,61,61,61	0
59	MG	CA	3599	1/1	0.94	0.07	70,70,70,70	0
59	MG	DA	1719	1/1	0.94	0.17	61,61,61,61	0
59	MG	AA	3039	1/1	0.94	0.20	34,34,34,34	1
59	MG	CA	3602	1/1	0.94	0.09	84,84,84,84	0
59	MG	A5	502	1/1	0.94	0.11	51,51,51,51	0
59	MG	CA	3371	1/1	0.94	0.11	52,52,52,52	0
59	MG	BN	502	1/1	0.94	0.09	87,87,87,87	0
59	MG	CA	3375	1/1	0.94	0.16	68,68,68,68	0
59	MG	AA	3120	1/1	0.94	0.10	33,33,33,33	0
59	MG	DA	1729	1/1	0.94	0.14	49,49,49,49	0
59	MG	CA	3609	1/1	0.94	0.09	52,52,52,52	0
59	MG	AA	3172	1/1	0.94	0.13	47,47,47,47	0
59	MG	CA	3611	1/1	0.94	0.10	59,59,59,59	0
59	MG	AA	3250	1/1	0.94	0.13	123,123,123,123	0
59	MG	CA	3153	1/1	0.94	0.18	73,73,73,73	0
59	MG	CA	3381	1/1	0.94	0.07	50,50,50,50	0
59	MG	AA	3067	1/1	0.94	0.21	61,61,61,61	0
59	MG	AA	3175	1/1	0.94	0.25	63,63,63,63	0
59	MG	AA	3307	1/1	0.94	0.17	61,61,61,61	0
59	MG	AA	3176	1/1	0.94	0.16	70,70,70,70	0
59	MG	CA	3391	1/1	0.94	0.11	51,51,51,51	0
59	MG	CA	3623	1/1	0.94	0.08	64,64,64,64	0
59	MG	CA	3161	1/1	0.94	0.16	57,57,57,57	0
59	MG	AA	3667	1/1	0.94	0.12	41,41,41,41	0
59	MG	AA	3669	1/1	0.94	0.09	81,81,81,81	0
59	MG	CA	3396	1/1	0.94	0.06	39,39,39,39	0
59	MG	CA	3166	1/1	0.94	0.14	27,27,27,27	0
59	MG	CA	3399	1/1	0.94	0.06	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3559	1/1	0.94	0.09	46,46,46,46	0
59	MG	CA	3012	1/1	0.94	0.10	65,65,65,65	0
59	MG	AA	3562	1/1	0.94	0.06	56,56,56,56	0
59	MG	AA	3785	1/1	0.94	0.10	61,61,61,61	0
59	MG	AA	3256	1/1	0.94	0.09	49,49,49,49	0
59	MG	AA	3444	1/1	0.94	0.12	66,66,66,66	0
59	MG	AA	3445	1/1	0.94	0.07	23,23,23,23	0
59	MG	CA	3642	1/1	0.94	0.20	52,52,52,52	0
59	MG	CA	3183	1/1	0.94	0.08	49,49,49,49	0
59	MG	CA	3417	1/1	0.94	0.10	56,56,56,56	0
59	MG	AA	3059	1/1	0.94	0.19	40,40,40,40	0
59	MG	AA	3321	1/1	0.94	0.11	61,61,61,61	0
59	MG	BA	1613	1/1	0.94	0.06	76,76,76,76	0
59	MG	CA	3426	1/1	0.94	0.14	38,38,38,38	0
59	MG	AA	3211	1/1	0.94	0.11	56,56,56,56	0
59	MG	CA	3430	1/1	0.94	0.17	41,41,41,41	0
59	MG	CA	3655	1/1	0.94	0.22	52,52,52,52	0
59	MG	AA	3584	1/1	0.94	0.07	17,17,17,17	0
59	MG	AA	3686	1/1	0.94	0.12	61,61,61,61	0
59	MG	AA	3145	1/1	0.94	0.11	44,44,44,44	0
59	MG	CA	3434	1/1	0.94	0.09	32,32,32,32	0
59	MG	CA	3196	1/1	0.94	0.32	68,68,68,68	0
59	MG	CA	3198	1/1	0.94	0.11	34,34,34,34	0
59	MG	BA	1722	1/1	0.94	0.14	51,51,51,51	0
59	MG	AA	3590	1/1	0.94	0.08	60,60,60,60	0
59	MG	CA	3036	1/1	0.94	0.16	32,32,32,32	0
59	MG	BA	1725	1/1	0.94	0.07	54,54,54,54	0
59	MG	AA	3690	1/1	0.94	0.10	50,50,50,50	0
59	MG	AA	3078	1/1	0.95	0.24	70,70,70,70	0
59	MG	AA	3060	1/1	0.95	0.12	20,20,20,20	0
59	MG	BW	501	1/1	0.95	0.21	47,47,47,47	0
59	MG	AA	3230	1/1	0.95	0.16	69,69,69,69	0
59	MG	AA	3405	1/1	0.95	0.15	44,44,44,44	0
59	MG	AA	3131	1/1	0.95	0.10	63,63,63,63	0
59	MG	CA	3531	1/1	0.95	0.06	47,47,47,47	0
59	MG	BA	1710	1/1	0.95	0.08	81,81,81,81	0
59	MG	DA	1612	1/1	0.95	0.10	57,57,57,57	0
59	MG	CA	3138	1/1	0.95	0.08	86,86,86,86	0
59	MG	CA	3002	1/1	0.95	0.14	28,28,28,28	0
59	MG	CA	3322	1/1	0.95	0.15	40,40,40,40	0
59	MG	AA	3613	1/1	0.95	0.07	48,48,48,48	0
59	MG	AA	3807	1/1	0.95	0.15	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3319	1/1	0.95	0.11	58,58,58,58	0
59	MG	CA	3008	1/1	0.95	0.11	46,46,46,46	0
59	MG	CA	3541	1/1	0.95	0.12	63,63,63,63	0
59	MG	CA	3010	1/1	0.95	0.07	43,43,43,43	0
59	MG	AA	3809	1/1	0.95	0.17	57,57,57,57	0
59	MG	AA	3500	1/1	0.95	0.11	59,59,59,59	0
59	MG	CA	3338	1/1	0.95	0.09	64,64,64,64	0
59	MG	CA	3013	1/1	0.95	0.09	42,42,42,42	0
59	MG	AA	3271	1/1	0.95	0.14	34,34,34,34	0
59	MG	CA	3152	1/1	0.95	0.13	64,64,64,64	0
59	MG	AA	3081	1/1	0.95	0.12	56,56,56,56	0
59	MG	CA	3018	1/1	0.95	0.06	41,41,41,41	0
59	MG	AA	3234	1/1	0.95	0.18	36,36,36,36	0
59	MG	AA	3112	1/1	0.95	0.17	61,61,61,61	0
59	MG	CA	3351	1/1	0.95	0.08	46,46,46,46	0
59	MG	CA	3158	1/1	0.95	0.16	54,54,54,54	0
59	MG	AA	3178	1/1	0.95	0.17	48,48,48,48	0
59	MG	CA	3160	1/1	0.95	0.17	57,57,57,57	0
59	MG	CA	3358	1/1	0.95	0.14	36,36,36,36	0
59	MG	AA	3623	1/1	0.95	0.05	28,28,28,28	0
59	MG	CA	3362	1/1	0.95	0.08	43,43,43,43	0
59	MG	CA	3162	1/1	0.95	0.23	31,31,31,31	0
59	MG	AA	3431	1/1	0.95	0.10	25,25,25,25	0
59	MG	BA	1621	1/1	0.95	0.05	51,51,51,51	0
59	MG	AA	3331	1/1	0.95	0.07	15,15,15,15	0
59	MG	AA	3532	1/1	0.95	0.11	20,20,20,20	0
59	MG	AA	3535	1/1	0.95	0.06	48,48,48,48	0
59	MG	AB	3005	1/1	0.95	0.16	44,44,44,44	0
59	MG	CA	3374	1/1	0.95	0.08	60,60,60,60	0
59	MG	AA	3044	1/1	0.95	0.18	52,52,52,52	0
59	MG	AA	3136	1/1	0.95	0.15	63,63,63,63	0
59	MG	CA	3179	1/1	0.95	0.14	60,60,60,60	0
59	MG	AA	3443	1/1	0.95	0.09	33,33,33,33	0
59	MG	AA	3342	1/1	0.95	0.13	51,51,51,51	0
59	MG	BA	1736	1/1	0.95	0.10	67,67,67,67	0
59	MG	AA	3546	1/1	0.95	0.07	60,60,60,60	0
59	MG	AA	3723	1/1	0.95	0.07	49,49,49,49	0
59	MG	CA	3187	1/1	0.95	0.11	37,37,37,37	0
59	MG	AA	3547	1/1	0.95	0.13	60,60,60,60	0
59	MG	AA	3637	1/1	0.95	0.18	17,17,17,17	1
59	MG	AA	3638	1/1	0.95	0.11	71,71,71,71	0
59	MG	BA	1636	1/1	0.95	0.20	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AB	3022	1/1	0.95	0.11	61,61,61,61	0
59	MG	AA	3549	1/1	0.95	0.05	66,66,66,66	0
59	MG	CA	3197	1/1	0.95	0.12	45,45,45,45	0
59	MG	CA	3049	1/1	0.95	0.18	46,46,46,46	0
59	MG	CA	3597	1/1	0.95	0.10	58,58,58,58	0
59	MG	CA	3400	1/1	0.95	0.10	57,57,57,57	0
59	MG	AA	3116	1/1	0.95	0.24	35,35,35,35	0
59	MG	AA	3049	1/1	0.95	0.10	35,35,35,35	0
59	MG	AA	3183	1/1	0.95	0.10	58,58,58,58	0
59	MG	AA	3284	1/1	0.95	0.20	60,60,60,60	0
59	MG	AD	306	1/1	0.95	0.21	41,41,41,41	0
59	MG	DA	1681	1/1	0.95	0.20	70,70,70,70	0
59	MG	AA	3350	1/1	0.95	0.06	36,36,36,36	0
59	MG	CA	3058	1/1	0.95	0.17	67,67,67,67	0
59	MG	CA	3607	1/1	0.95	0.07	64,64,64,64	0
59	MG	DA	1687	1/1	0.95	0.25	56,56,56,56	0
59	MG	AA	3352	1/1	0.95	0.16	47,47,47,47	0
59	MG	AA	3119	1/1	0.95	0.09	47,47,47,47	0
59	MG	CA	3418	1/1	0.95	0.12	34,34,34,34	0
59	MG	AA	3744	1/1	0.95	0.07	34,34,34,34	0
59	MG	CA	3062	1/1	0.95	0.12	38,38,38,38	0
59	MG	CA	3063	1/1	0.95	0.08	34,34,34,34	0
59	MG	AA	3077	1/1	0.95	0.19	43,43,43,43	0
59	MG	CA	3215	1/1	0.95	0.12	54,54,54,54	0
59	MG	CA	3429	1/1	0.95	0.07	59,59,59,59	0
59	MG	AA	3104	1/1	0.95	0.11	54,54,54,54	0
59	MG	AE	304	1/1	0.95	0.07	52,52,52,52	0
59	MG	BA	1653	1/1	0.95	0.13	56,56,56,56	0
59	MG	AA	3748	1/1	0.95	0.07	45,45,45,45	0
59	MG	AA	3570	1/1	0.95	0.06	14,14,14,14	0
59	MG	CA	3071	1/1	0.95	0.07	45,45,45,45	0
59	MG	AF	303	1/1	0.95	0.15	39,39,39,39	0
59	MG	CA	3440	1/1	0.95	0.16	49,49,49,49	0
59	MG	AF	304	1/1	0.95	0.18	41,41,41,41	0
59	MG	AA	3217	1/1	0.95	0.17	29,29,29,29	1
59	MG	CA	3632	1/1	0.95	0.09	74,74,74,74	0
59	MG	AA	3167	1/1	0.95	0.07	45,45,45,45	0
59	MG	CA	3446	1/1	0.95	0.05	33,33,33,33	0
59	MG	AG	201	1/1	0.95	0.07	38,38,38,38	0
59	MG	AA	3656	1/1	0.95	0.18	80,80,80,80	0
59	MG	AA	3576	1/1	0.95	0.08	52,52,52,52	0
59	MG	AA	3658	1/1	0.95	0.08	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AO	5001	1/1	0.95	0.06	34,34,34,34	0
59	MG	CA	3234	1/1	0.95	0.17	50,50,50,50	0
59	MG	CA	3461	1/1	0.95	0.09	34,34,34,34	0
59	MG	CA	3462	1/1	0.95	0.10	63,63,63,63	0
59	MG	AA	3577	1/1	0.95	0.06	42,42,42,42	0
59	MG	BA	1785	1/1	0.95	0.07	62,62,62,62	0
59	MG	AA	3579	1/1	0.95	0.11	54,54,54,54	0
59	MG	CA	3648	1/1	0.95	0.16	52,52,52,52	0
59	MG	CA	3468	1/1	0.95	0.05	53,53,53,53	0
59	MG	AA	3762	1/1	0.95	0.07	23,23,23,23	0
59	MG	AA	3580	1/1	0.95	0.15	54,54,54,54	0
59	MG	AA	3168	1/1	0.95	0.07	47,47,47,47	0
59	MG	CA	3090	1/1	0.95	0.16	77,77,77,77	0
59	MG	AA	3291	1/1	0.95	0.07	45,45,45,45	0
59	MG	AA	3366	1/1	0.95	0.06	35,35,35,35	1
59	MG	AU	201	1/1	0.95	0.10	46,46,46,46	0
59	MG	AA	3673	1/1	0.95	0.07	38,38,38,38	0
59	MG	BA	1674	1/1	0.95	0.19	48,48,48,48	0
59	MG	AV	203	1/1	0.95	0.08	47,47,47,47	0
59	MG	AA	3674	1/1	0.95	0.10	30,30,30,30	0
59	MG	DA	1745	1/1	0.95	0.20	50,50,50,50	0
59	MG	AW	3001	1/1	0.95	0.21	54,54,54,54	0
59	MG	CA	3487	1/1	0.95	0.16	60,60,60,60	0
59	MG	CA	3252	1/1	0.95	0.16	62,62,62,62	0
59	MG	CB	3006	1/1	0.95	0.08	71,71,71,71	0
59	MG	AA	3105	1/1	0.95	0.14	52,52,52,52	0
59	MG	BA	1799	1/1	0.95	0.10	64,64,64,64	0
59	MG	AA	3588	1/1	0.95	0.09	47,47,47,47	0
59	MG	AA	3368	1/1	0.95	0.14	49,49,49,49	0
59	MG	CA	3258	1/1	0.95	0.24	51,51,51,51	0
59	MG	AA	3294	1/1	0.95	0.10	37,37,37,37	0
59	MG	AA	3594	1/1	0.95	0.09	56,56,56,56	0
59	MG	CA	3265	1/1	0.95	0.14	61,61,61,61	0
59	MG	AA	3144	1/1	0.95	0.14	50,50,50,50	0
59	MG	BA	1806	1/1	0.95	0.11	55,55,55,55	0
59	MG	AA	3373	1/1	0.95	0.10	48,48,48,48	0
59	MG	BA	1688	1/1	0.95	0.19	61,61,61,61	0
59	MG	AA	3225	1/1	0.95	0.16	73,73,73,73	0
59	MG	CA	3277	1/1	0.95	0.15	55,55,55,55	0
59	MG	AA	3685	1/1	0.95	0.07	72,72,72,72	0
59	MG	DA	1768	1/1	0.95	0.06	59,59,59,59	0
59	MG	CA	3279	1/1	0.95	0.07	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3171	1/1	0.95	0.14	54,54,54,54	0
59	MG	AA	3377	1/1	0.95	0.06	20,20,20,20	0
59	MG	AA	3788	1/1	0.95	0.14	61,61,61,61	0
59	MG	AA	3789	1/1	0.95	0.10	44,44,44,44	0
59	MG	CR	201	1/1	0.95	0.06	34,34,34,34	0
59	MG	AA	3790	1/1	0.95	0.23	57,57,57,57	0
59	MG	AA	3302	1/1	0.95	0.09	51,51,51,51	0
59	MG	AA	3689	1/1	0.95	0.05	35,35,35,35	0
59	MG	CA	3290	1/1	0.95	0.15	34,34,34,34	0
59	MG	AA	3605	1/1	0.95	0.17	45,45,45,45	0
59	MG	AA	3306	1/1	0.95	0.12	52,52,52,52	0
59	MG	BA	1701	1/1	0.95	0.07	54,54,54,54	0
62	GDP	BZ	702	28/28	0.95	0.07	57,57,57,57	0
59	MG	AA	3797	1/1	0.95	0.08	52,52,52,52	0
59	MG	CA	3286	1/1	0.96	0.09	58,58,58,58	0
59	MG	BM	201	1/1	0.96	0.04	62,62,62,62	0
59	MG	BA	1702	1/1	0.96	0.15	46,46,46,46	0
59	MG	CA	3505	1/1	0.96	0.05	67,67,67,67	0
59	MG	AA	3197	1/1	0.96	0.08	45,45,45,45	0
59	MG	AA	3472	1/1	0.96	0.08	42,42,42,42	0
59	MG	AA	3799	1/1	0.96	0.10	42,42,42,42	0
59	MG	CW	201	1/1	0.96	0.13	46,46,46,46	0
59	MG	CA	3131	1/1	0.96	0.09	26,26,26,26	0
59	MG	C1	101	1/1	0.96	0.10	57,57,57,57	0
59	MG	AA	3600	1/1	0.96	0.07	25,25,25,25	0
59	MG	AA	3033	1/1	0.96	0.11	55,55,55,55	0
59	MG	C7	101	1/1	0.96	0.10	56,56,56,56	0
59	MG	C8	5001	1/1	0.96	0.11	37,37,37,37	0
59	MG	AA	3079	1/1	0.96	0.07	27,27,27,27	0
59	MG	AA	3201	1/1	0.96	0.11	53,53,53,53	0
59	MG	AA	3047	1/1	0.96	0.04	29,29,29,29	0
59	MG	AA	3034	1/1	0.96	0.12	49,49,49,49	0
59	MG	CA	3004	1/1	0.96	0.15	49,49,49,49	0
59	MG	AA	3483	1/1	0.96	0.07	46,46,46,46	0
59	MG	CA	3312	1/1	0.96	0.09	38,38,38,38	0
59	MG	AA	3696	1/1	0.96	0.08	66,66,66,66	0
59	MG	CA	3144	1/1	0.96	0.13	40,40,40,40	0
59	MG	CA	3522	1/1	0.96	0.10	54,54,54,54	0
59	MG	CA	3315	1/1	0.96	0.09	47,47,47,47	0
59	MG	CA	3316	1/1	0.96	0.09	43,43,43,43	0
59	MG	BA	1715	1/1	0.96	0.07	60,60,60,60	0
59	MG	AA	3372	1/1	0.96	0.12	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3082	1/1	0.96	0.15	60,60,60,60	0
59	MG	DA	1617	1/1	0.96	0.13	64,64,64,64	0
59	MG	AA	3488	1/1	0.96	0.07	36,36,36,36	0
59	MG	CA	3326	1/1	0.96	0.08	28,28,28,28	0
59	MG	AA	3205	1/1	0.96	0.09	42,42,42,42	0
59	MG	CA	3332	1/1	0.96	0.09	29,29,29,29	0
59	MG	AA	3083	1/1	0.96	0.14	61,61,61,61	0
59	MG	AA	3299	1/1	0.96	0.19	47,47,47,47	0
59	MG	CA	3017	1/1	0.96	0.05	30,30,30,30	0
59	MG	AA	3207	1/1	0.96	0.11	60,60,60,60	0
59	MG	BA	1723	1/1	0.96	0.06	70,70,70,70	0
59	MG	CA	3156	1/1	0.96	0.14	52,52,52,52	0
59	MG	AA	3064	1/1	0.96	0.05	32,32,32,32	0
59	MG	AA	3113	1/1	0.96	0.11	45,45,45,45	0
59	MG	AA	3386	1/1	0.96	0.08	45,45,45,45	0
59	MG	CA	3025	1/1	0.96	0.16	59,59,59,59	0
59	MG	AA	3389	1/1	0.96	0.07	25,25,25,25	0
59	MG	AA	3390	1/1	0.96	0.06	23,23,23,23	0
59	MG	AA	3620	1/1	0.96	0.05	22,22,22,22	0
59	MG	AA	3621	1/1	0.96	0.04	17,17,17,17	0
59	MG	AA	3503	1/1	0.96	0.05	54,54,54,54	0
59	MG	CA	3167	1/1	0.96	0.07	50,50,50,50	0
59	MG	CA	3168	1/1	0.96	0.20	58,58,58,58	0
59	MG	AB	3012	1/1	0.96	0.06	23,23,23,23	1
59	MG	AB	3013	1/1	0.96	0.07	53,53,53,53	0
59	MG	CA	3173	1/1	0.96	0.19	61,61,61,61	0
59	MG	AA	3395	1/1	0.96	0.07	54,54,54,54	0
59	MG	AA	3624	1/1	0.96	0.07	42,42,42,42	0
59	MG	AA	3398	1/1	0.96	0.13	31,31,31,31	0
59	MG	DA	1647	1/1	0.96	0.14	51,51,51,51	0
59	MG	AA	3254	1/1	0.96	0.13	52,52,52,52	0
59	MG	AB	3019	1/1	0.96	0.11	70,70,70,70	0
59	MG	AA	3309	1/1	0.96	0.14	46,46,46,46	0
59	MG	BA	1743	1/1	0.96	0.04	41,41,41,41	0
59	MG	CA	3564	1/1	0.96	0.14	80,80,80,80	0
59	MG	AA	3255	1/1	0.96	0.08	38,38,38,38	0
59	MG	AA	3015	1/1	0.96	0.26	57,57,57,57	0
59	MG	CA	3567	1/1	0.96	0.05	26,26,26,26	0
59	MG	CA	3377	1/1	0.96	0.07	52,52,52,52	0
59	MG	CA	3045	1/1	0.96	0.21	60,60,60,60	0
59	MG	AA	3729	1/1	0.96	0.10	41,41,41,41	0
59	MG	AA	3257	1/1	0.96	0.18	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3533	1/1	0.96	0.09	22,22,22,22	0
59	MG	AA	3036	1/1	0.96	0.08	25,25,25,25	0
59	MG	CA	3385	1/1	0.96	0.27	61,61,61,61	0
59	MG	CA	3387	1/1	0.96	0.06	50,50,50,50	0
59	MG	AA	3634	1/1	0.96	0.17	76,76,76,76	0
59	MG	AA	3417	1/1	0.96	0.06	25,25,25,25	0
59	MG	CA	3053	1/1	0.96	0.13	32,32,32,32	0
59	MG	BA	1757	1/1	0.96	0.11	43,43,43,43	0
59	MG	AA	3261	1/1	0.96	0.10	25,25,25,25	0
59	MG	AA	3091	1/1	0.96	0.32	47,47,47,47	1
59	MG	DA	1673	1/1	0.96	0.06	82,82,82,82	0
59	MG	BA	1761	1/1	0.96	0.09	62,62,62,62	0
59	MG	AA	3092	1/1	0.96	0.18	39,39,39,39	0
59	MG	AA	3149	1/1	0.96	0.08	51,51,51,51	0
59	MG	CA	3592	1/1	0.96	0.08	64,64,64,64	0
59	MG	BA	1649	1/1	0.96	0.11	35,35,35,35	0
59	MG	BA	1765	1/1	0.96	0.13	54,54,54,54	0
59	MG	CA	3206	1/1	0.96	0.16	44,44,44,44	0
59	MG	DA	1682	1/1	0.96	0.16	52,52,52,52	0
59	MG	CA	3403	1/1	0.96	0.06	70,70,70,70	0
59	MG	CA	3404	1/1	0.96	0.08	65,65,65,65	0
59	MG	CA	3405	1/1	0.96	0.08	55,55,55,55	0
59	MG	DA	1686	1/1	0.96	0.16	56,56,56,56	0
59	MG	BA	1650	1/1	0.96	0.10	55,55,55,55	0
59	MG	AD	312	1/1	0.96	0.18	78,78,78,78	0
59	MG	CA	3601	1/1	0.96	0.05	57,57,57,57	0
59	MG	BA	1768	1/1	0.96	0.08	64,64,64,64	0
59	MG	CA	3410	1/1	0.96	0.08	25,25,25,25	0
59	MG	AA	3023	1/1	0.96	0.17	53,53,53,53	0
59	MG	AA	3094	1/1	0.96	0.26	80,80,80,80	0
59	MG	DA	1696	1/1	0.96	0.12	53,53,53,53	0
59	MG	AA	3334	1/1	0.96	0.08	63,63,63,63	0
59	MG	BA	1773	1/1	0.96	0.07	40,40,40,40	0
59	MG	CA	3416	1/1	0.96	0.07	44,44,44,44	0
59	MG	AA	3154	1/1	0.96	0.08	57,57,57,57	0
59	MG	AA	3442	1/1	0.96	0.09	23,23,23,23	0
59	MG	AA	3750	1/1	0.96	0.15	51,51,51,51	0
59	MG	AA	3338	1/1	0.96	0.06	28,28,28,28	0
59	MG	CA	3613	1/1	0.96	0.10	57,57,57,57	0
59	MG	AA	3648	1/1	0.96	0.07	41,41,41,41	0
59	MG	CA	3422	1/1	0.96	0.10	43,43,43,43	0
59	MG	AA	3155	1/1	0.96	0.18	93,93,93,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3221	1/1	0.96	0.05	30,30,30,30	0
59	MG	DA	1711	1/1	0.96	0.12	60,60,60,60	0
59	MG	AA	3156	1/1	0.96	0.17	49,49,49,49	0
59	MG	AA	3123	1/1	0.96	0.12	54,54,54,54	0
59	MG	CA	3227	1/1	0.96	0.15	41,41,41,41	0
59	MG	AA	3564	1/1	0.96	0.06	44,44,44,44	0
59	MG	AA	3760	1/1	0.96	0.14	55,55,55,55	0
59	MG	CA	3082	1/1	0.96	0.15	76,76,76,76	0
59	MG	AP	201	1/1	0.96	0.20	72,72,72,72	0
59	MG	DA	1720	1/1	0.96	0.09	60,60,60,60	0
59	MG	AA	3654	1/1	0.96	0.05	67,67,67,67	0
59	MG	CA	3437	1/1	0.96	0.08	64,64,64,64	0
59	MG	DA	1723	1/1	0.96	0.06	53,53,53,53	0
59	MG	AA	3276	1/1	0.96	0.10	67,67,67,67	0
59	MG	AA	3566	1/1	0.96	0.06	56,56,56,56	0
59	MG	AA	3764	1/1	0.96	0.07	73,73,73,73	0
59	MG	AA	3567	1/1	0.96	0.07	26,26,26,26	0
59	MG	CA	3445	1/1	0.96	0.07	22,22,22,22	0
59	MG	AA	3348	1/1	0.96	0.05	53,53,53,53	0
59	MG	AA	3095	1/1	0.96	0.12	75,75,75,75	0
59	MG	CA	3448	1/1	0.96	0.09	37,37,37,37	0
59	MG	AA	3573	1/1	0.96	0.07	12,12,12,12	0
59	MG	CA	3640	1/1	0.96	0.10	43,43,43,43	0
59	MG	AA	3662	1/1	0.96	0.05	60,60,60,60	0
59	MG	AA	3006	1/1	0.96	0.08	52,52,52,52	0
59	MG	BA	1677	1/1	0.96	0.08	28,28,28,28	0
59	MG	CA	3097	1/1	0.96	0.16	66,66,66,66	0
59	MG	AA	3452	1/1	0.96	0.04	14,14,14,14	0
59	MG	AA	3668	1/1	0.96	0.10	54,54,54,54	0
59	MG	CA	3463	1/1	0.96	0.10	56,56,56,56	0
59	MG	AA	3188	1/1	0.96	0.14	31,31,31,31	0
59	MG	CA	3651	1/1	0.96	0.27	76,76,76,76	0
59	MG	AA	3777	1/1	0.96	0.06	41,41,41,41	0
59	MG	CA	3102	1/1	0.96	0.13	62,62,62,62	0
59	MG	DA	1747	1/1	0.96	0.07	48,48,48,48	0
59	MG	CA	3250	1/1	0.96	0.06	38,38,38,38	0
59	MG	CA	3103	1/1	0.96	0.16	53,53,53,53	0
59	MG	CA	3657	1/1	0.96	0.15	41,41,41,41	0
59	MG	AA	3779	1/1	0.96	0.05	22,22,22,22	0
59	MG	CA	3105	1/1	0.96	0.06	39,39,39,39	0
59	MG	CA	3473	1/1	0.96	0.08	51,51,51,51	0
59	MG	AA	3578	1/1	0.96	0.06	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3671	1/1	0.96	0.11	19,19,19,19	0
59	MG	CA	3664	1/1	0.96	0.10	48,48,48,48	0
59	MG	AA	3672	1/1	0.96	0.06	48,48,48,48	0
59	MG	CA	3479	1/1	0.96	0.08	50,50,50,50	0
59	MG	AA	3030	1/1	0.96	0.20	24,24,24,24	1
59	MG	DA	1760	1/1	0.96	0.07	61,61,61,61	0
59	MG	AA	3129	1/1	0.96	0.07	34,34,34,34	1
59	MG	CA	3260	1/1	0.96	0.07	35,35,35,35	0
59	MG	BA	1809	1/1	0.96	0.08	61,61,61,61	0
59	MG	BA	1690	1/1	0.96	0.16	71,71,71,71	0
59	MG	A0	104	1/1	0.96	0.13	51,51,51,51	0
59	MG	AA	3163	1/1	0.96	0.14	72,72,72,72	0
59	MG	AA	3458	1/1	0.96	0.08	40,40,40,40	0
59	MG	AA	3460	1/1	0.96	0.07	27,27,27,27	0
59	MG	AA	3461	1/1	0.96	0.10	62,62,62,62	0
59	MG	CA	3491	1/1	0.96	0.04	44,44,44,44	0
59	MG	DD	502	1/1	0.96	0.18	50,50,50,50	0
59	MG	CA	3275	1/1	0.96	0.07	61,61,61,61	0
59	MG	CD	303	1/1	0.96	0.08	70,70,70,70	0
59	MG	DF	3001	1/1	0.96	0.10	54,54,54,54	0
59	MG	AA	3359	1/1	0.96	0.06	31,31,31,31	0
59	MG	AA	3233	1/1	0.96	0.14	46,46,46,46	0
59	MG	AA	3058	1/1	0.96	0.03	22,22,22,22	0
59	MG	CA	3496	1/1	0.96	0.10	56,56,56,56	0
59	MG	BF	3001	1/1	0.96	0.06	49,49,49,49	0
59	MG	CF	302	1/1	0.96	0.20	69,69,69,69	0
59	MG	CF	304	1/1	0.96	0.07	65,65,65,65	0
60	ZN	A4	501	1/1	0.96	0.04	117,117,117,117	0
59	MG	AA	3031	1/1	0.96	0.14	63,63,63,63	0
59	MG	A8	5001	1/1	0.96	0.06	30,30,30,30	0
59	MG	AA	3595	1/1	0.96	0.07	42,42,42,42	0
59	MG	AA	3612	1/1	0.97	0.05	68,68,68,68	0
59	MG	CO	5001	1/1	0.97	0.08	50,50,50,50	0
59	MG	CA	3497	1/1	0.97	0.07	45,45,45,45	0
59	MG	AA	3806	1/1	0.97	0.12	42,42,42,42	0
59	MG	CA	3297	1/1	0.97	0.10	36,36,36,36	0
59	MG	CA	3143	1/1	0.97	0.19	41,41,41,41	0
59	MG	AA	3413	1/1	0.97	0.07	25,25,25,25	0
59	MG	CA	3300	1/1	0.97	0.05	47,47,47,47	0
59	MG	CA	3301	1/1	0.97	0.07	60,60,60,60	0
59	MG	CA	3014	1/1	0.97	0.08	50,50,50,50	0
59	MG	CA	3305	1/1	0.97	0.11	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3115	1/1	0.97	0.09	44,44,44,44	0
59	MG	C0	101	1/1	0.97	0.11	59,59,59,59	0
59	MG	CA	3308	1/1	0.97	0.04	39,39,39,39	0
59	MG	AA	3507	1/1	0.97	0.06	50,50,50,50	0
59	MG	AA	3005	1/1	0.97	0.11	64,64,64,64	0
59	MG	AA	3811	1/1	0.97	0.08	56,56,56,56	0
59	MG	AA	3812	1/1	0.97	0.06	41,41,41,41	0
59	MG	CA	3021	1/1	0.97	0.13	69,69,69,69	0
59	MG	AA	3509	1/1	0.97	0.07	40,40,40,40	0
59	MG	CA	3317	1/1	0.97	0.06	49,49,49,49	0
59	MG	CA	3318	1/1	0.97	0.05	24,24,24,24	0
59	MG	AA	3511	1/1	0.97	0.06	14,14,14,14	0
59	MG	BA	1728	1/1	0.97	0.12	47,47,47,47	0
59	MG	AA	3815	1/1	0.97	0.08	30,30,30,30	0
59	MG	AA	3514	1/1	0.97	0.06	42,42,42,42	0
59	MG	CA	3027	1/1	0.97	0.04	31,31,31,31	0
59	MG	CA	3328	1/1	0.97	0.06	35,35,35,35	0
59	MG	CA	3523	1/1	0.97	0.10	37,37,37,37	0
59	MG	CA	3330	1/1	0.97	0.08	36,36,36,36	0
59	MG	DA	1613	1/1	0.97	0.21	48,48,48,48	0
59	MG	CA	3525	1/1	0.97	0.10	23,23,23,23	0
59	MG	AA	3245	1/1	0.97	0.06	11,11,11,11	0
59	MG	CA	3029	1/1	0.97	0.10	56,56,56,56	0
59	MG	AA	3341	1/1	0.97	0.06	25,25,25,25	0
59	MG	AA	3008	1/1	0.97	0.06	26,26,26,26	0
59	MG	AA	3820	1/1	0.97	0.05	25,25,25,25	0
59	MG	BA	1735	1/1	0.97	0.13	41,41,41,41	0
59	MG	DA	1621	1/1	0.97	0.06	42,42,42,42	0
59	MG	CA	3337	1/1	0.97	0.05	20,20,20,20	0
59	MG	CA	3533	1/1	0.97	0.07	45,45,45,45	0
59	MG	AA	3524	1/1	0.97	0.07	41,41,41,41	0
59	MG	AA	3713	1/1	0.97	0.18	27,27,27,27	0
59	MG	BA	1626	1/1	0.97	0.11	41,41,41,41	0
59	MG	AA	3424	1/1	0.97	0.08	14,14,14,14	0
59	MG	DA	1628	1/1	0.97	0.04	39,39,39,39	0
59	MG	AA	3247	1/1	0.97	0.19	55,55,55,55	0
59	MG	CA	3345	1/1	0.97	0.06	46,46,46,46	0
59	MG	CA	3039	1/1	0.97	0.21	37,37,37,37	0
59	MG	CA	3174	1/1	0.97	0.26	50,50,50,50	0
59	MG	CA	3175	1/1	0.97	0.10	31,31,31,31	0
59	MG	AA	3216	1/1	0.97	0.27	38,38,38,38	0
59	MG	AA	3429	1/1	0.97	0.08	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3353	1/1	0.97	0.06	45,45,45,45	0
59	MG	AB	3007	1/1	0.97	0.04	39,39,39,39	0
59	MG	CA	3355	1/1	0.97	0.08	35,35,35,35	0
59	MG	BA	1745	1/1	0.97	0.04	46,46,46,46	0
59	MG	AA	3430	1/1	0.97	0.05	39,39,39,39	0
59	MG	CA	3359	1/1	0.97	0.04	33,33,33,33	0
59	MG	CA	3181	1/1	0.97	0.13	40,40,40,40	0
59	MG	CA	3552	1/1	0.97	0.09	30,30,30,30	0
59	MG	CA	3361	1/1	0.97	0.14	43,43,43,43	0
59	MG	AA	3100	1/1	0.97	0.10	29,29,29,29	0
59	MG	AB	3010	1/1	0.97	0.04	62,62,62,62	0
59	MG	CA	3364	1/1	0.97	0.04	22,22,22,22	0
59	MG	BA	1751	1/1	0.97	0.06	48,48,48,48	0
59	MG	CA	3185	1/1	0.97	0.09	48,48,48,48	0
59	MG	AA	3720	1/1	0.97	0.08	55,55,55,55	0
59	MG	AA	3721	1/1	0.97	0.12	40,40,40,40	0
59	MG	CA	3370	1/1	0.97	0.06	41,41,41,41	0
59	MG	AA	3432	1/1	0.97	0.13	42,42,42,42	0
59	MG	AA	3631	1/1	0.97	0.13	46,46,46,46	0
59	MG	AB	3016	1/1	0.97	0.06	34,34,34,34	0
59	MG	CA	3191	1/1	0.97	0.16	46,46,46,46	0
59	MG	CA	3192	1/1	0.97	0.03	45,45,45,45	0
59	MG	AA	3433	1/1	0.97	0.10	37,37,37,37	0
59	MG	CA	3570	1/1	0.97	0.04	36,36,36,36	0
59	MG	AA	3725	1/1	0.97	0.05	13,13,13,13	0
59	MG	CA	3195	1/1	0.97	0.18	47,47,47,47	0
59	MG	AA	3728	1/1	0.97	0.11	29,29,29,29	0
59	MG	AA	3434	1/1	0.97	0.06	17,17,17,17	0
59	MG	AA	3545	1/1	0.97	0.09	43,43,43,43	0
59	MG	AA	3191	1/1	0.97	0.03	16,16,16,16	0
59	MG	CA	3386	1/1	0.97	0.09	50,50,50,50	0
59	MG	CA	3580	1/1	0.97	0.09	76,76,76,76	0
59	MG	AA	3069	1/1	0.97	0.03	28,28,28,28	0
59	MG	AA	3121	1/1	0.97	0.08	53,53,53,53	0
59	MG	AA	3735	1/1	0.97	0.04	25,25,25,25	0
59	MG	CA	3584	1/1	0.97	0.05	32,32,32,32	0
59	MG	AA	3351	1/1	0.97	0.08	29,29,29,29	0
59	MG	CA	3064	1/1	0.97	0.07	48,48,48,48	0
59	MG	AA	3087	1/1	0.97	0.17	55,55,55,55	0
59	MG	AA	3552	1/1	0.97	0.09	63,63,63,63	0
59	MG	AA	3222	1/1	0.97	0.06	4,4,4,4	0
59	MG	DA	1680	1/1	0.97	0.09	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3741	1/1	0.97	0.05	21,21,21,21	0
59	MG	AA	3146	1/1	0.97	0.05	29,29,29,29	0
59	MG	AA	3557	1/1	0.97	0.08	37,37,37,37	0
59	MG	AA	3021	1/1	0.97	0.07	33,33,33,33	0
59	MG	AA	3745	1/1	0.97	0.09	68,68,68,68	0
59	MG	AA	3358	1/1	0.97	0.04	45,45,45,45	0
59	MG	CA	3074	1/1	0.97	0.05	49,49,49,49	0
59	MG	AA	3009	1/1	0.97	0.04	22,22,22,22	0
59	MG	CA	3218	1/1	0.97	0.27	40,40,40,40	0
59	MG	AA	3360	1/1	0.97	0.09	22,22,22,22	0
59	MG	CA	3220	1/1	0.97	0.05	59,59,59,59	0
59	MG	DA	1693	1/1	0.97	0.06	67,67,67,67	0
59	MG	AF	301	1/1	0.97	0.10	38,38,38,38	0
59	MG	AA	3749	1/1	0.97	0.08	73,73,73,73	0
59	MG	AA	3297	1/1	0.97	0.09	27,27,27,27	0
59	MG	DA	1697	1/1	0.97	0.03	48,48,48,48	0
59	MG	AA	3259	1/1	0.97	0.12	41,41,41,41	1
59	MG	AA	3227	1/1	0.97	0.04	22,22,22,22	0
59	MG	CA	3415	1/1	0.97	0.09	34,34,34,34	0
59	MG	AA	3126	1/1	0.97	0.14	79,79,79,79	0
59	MG	DA	1702	1/1	0.97	0.08	63,63,63,63	0
59	MG	AA	3152	1/1	0.97	0.12	10,10,10,10	0
59	MG	AA	3305	1/1	0.97	0.06	25,25,25,25	0
59	MG	AH	201	1/1	0.97	0.19	64,64,64,64	0
59	MG	AA	3572	1/1	0.97	0.10	17,17,17,17	0
59	MG	AN	3002	1/1	0.97	0.08	69,69,69,69	0
59	MG	AA	3265	1/1	0.97	0.12	43,43,43,43	0
59	MG	CA	3424	1/1	0.97	0.09	66,66,66,66	0
59	MG	CA	3425	1/1	0.97	0.06	50,50,50,50	0
59	MG	AA	3075	1/1	0.97	0.10	49,49,49,49	0
59	MG	DA	1712	1/1	0.97	0.12	53,53,53,53	0
59	MG	CA	3427	1/1	0.97	0.11	37,37,37,37	0
59	MG	CA	3091	1/1	0.97	0.14	69,69,69,69	0
59	MG	AA	3459	1/1	0.97	0.11	53,53,53,53	0
59	MG	AA	3107	1/1	0.97	0.06	49,49,49,49	0
59	MG	AA	3661	1/1	0.97	0.09	41,41,41,41	1
59	MG	AA	3310	1/1	0.97	0.08	56,56,56,56	0
59	MG	AA	3462	1/1	0.97	0.04	54,54,54,54	0
59	MG	CA	3627	1/1	0.97	0.09	60,60,60,60	0
59	MG	AA	3766	1/1	0.97	0.10	54,54,54,54	0
59	MG	CA	3629	1/1	0.97	0.05	55,55,55,55	0
59	MG	AA	3665	1/1	0.97	0.15	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3666	1/1	0.97	0.14	41,41,41,41	0
59	MG	AA	3268	1/1	0.97	0.10	66,66,66,66	0
59	MG	BA	1804	1/1	0.97	0.06	45,45,45,45	0
59	MG	AA	3062	1/1	0.97	0.10	47,47,47,47	0
59	MG	AA	3042	1/1	0.97	0.09	32,32,32,32	0
59	MG	BA	1686	1/1	0.97	0.12	36,36,36,36	0
59	MG	CA	3248	1/1	0.97	0.10	53,53,53,53	0
59	MG	DA	1731	1/1	0.97	0.07	49,49,49,49	0
59	MG	AV	204	1/1	0.97	0.09	45,45,45,45	0
59	MG	AA	3376	1/1	0.97	0.11	35,35,35,35	0
59	MG	AA	3774	1/1	0.97	0.21	25,25,25,25	1
59	MG	CA	3641	1/1	0.97	0.04	46,46,46,46	0
59	MG	CA	3449	1/1	0.97	0.04	55,55,55,55	0
59	MG	CA	3450	1/1	0.97	0.05	54,54,54,54	0
59	MG	AA	3585	1/1	0.97	0.07	35,35,35,35	0
59	MG	CA	3453	1/1	0.97	0.06	35,35,35,35	0
59	MG	AW	3003	1/1	0.97	0.06	28,28,28,28	0
59	MG	AA	3470	1/1	0.97	0.05	39,39,39,39	0
59	MG	AA	3587	1/1	0.97	0.12	28,28,28,28	0
59	MG	CA	3457	1/1	0.97	0.09	43,43,43,43	0
59	MG	DA	1744	1/1	0.97	0.07	66,66,66,66	0
59	MG	CA	3458	1/1	0.97	0.05	54,54,54,54	0
59	MG	AA	3316	1/1	0.97	0.10	36,36,36,36	0
59	MG	CA	3653	1/1	0.97	0.05	32,32,32,32	0
59	MG	AA	3318	1/1	0.97	0.09	23,23,23,23	0
59	MG	AA	3592	1/1	0.97	0.05	26,26,26,26	0
59	MG	AA	3110	1/1	0.97	0.15	52,52,52,52	0
59	MG	CA	3261	1/1	0.97	0.07	47,47,47,47	0
59	MG	CA	3263	1/1	0.97	0.07	64,64,64,64	0
59	MG	CA	3466	1/1	0.97	0.20	56,56,56,56	0
59	MG	AA	3384	1/1	0.97	0.06	22,22,22,22	0
59	MG	CA	3661	1/1	0.97	0.09	27,27,27,27	0
59	MG	AA	3272	1/1	0.97	0.05	55,55,55,55	0
59	MG	AA	3111	1/1	0.97	0.06	24,24,24,24	0
59	MG	AA	3598	1/1	0.97	0.12	51,51,51,51	0
59	MG	AA	3387	1/1	0.97	0.05	29,29,29,29	0
59	MG	CA	3272	1/1	0.97	0.14	49,49,49,49	0
59	MG	AA	3236	1/1	0.97	0.10	57,57,57,57	0
59	MG	CA	3475	1/1	0.97	0.17	50,50,50,50	0
59	MG	CA	3476	1/1	0.97	0.04	38,38,38,38	0
59	MG	DA	1764	1/1	0.97	0.05	71,71,71,71	0
59	MG	AA	3159	1/1	0.97	0.15	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3391	1/1	0.97	0.07	19,19,19,19	0
59	MG	CA	3276	1/1	0.97	0.07	44,44,44,44	0
59	MG	CB	3009	1/1	0.97	0.12	67,67,67,67	0
59	MG	BT	3001	1/1	0.97	0.05	46,46,46,46	0
59	MG	AA	3394	1/1	0.97	0.07	39,39,39,39	0
59	MG	AA	3326	1/1	0.97	0.05	36,36,36,36	1
59	MG	AA	3327	1/1	0.97	0.04	31,31,31,31	0
59	MG	BA	1709	1/1	0.97	0.15	50,50,50,50	0
59	MG	A9	502	1/1	0.97	0.12	41,41,41,41	0
59	MG	AA	3043	1/1	0.97	0.15	45,45,45,45	0
59	MG	CD	304	1/1	0.97	0.10	28,28,28,28	0
59	MG	CA	3132	1/1	0.97	0.06	48,48,48,48	0
59	MG	AA	3029	1/1	0.97	0.10	28,28,28,28	0
59	MG	DW	501	1/1	0.97	0.14	44,44,44,44	0
59	MG	CE	303	1/1	0.97	0.17	51,51,51,51	0
59	MG	AA	3045	1/1	0.97	0.11	55,55,55,55	0
59	MG	AA	3408	1/1	0.97	0.11	41,41,41,41	0
59	MG	AA	3336	1/1	0.97	0.08	51,51,51,51	0
59	MG	AA	3697	1/1	0.97	0.07	40,40,40,40	0
60	ZN	BN	501	1/1	0.97	0.04	132,132,132,132	0
59	MG	CF	303	1/1	0.97	0.10	51,51,51,51	0
61	SF4	DD	501	8/8	0.97	0.05	82,82,82,82	1
59	MG	CA	3009	1/1	0.97	0.05	27,27,27,27	0
59	MG	AA	3411	1/1	0.97	0.04	12,12,12,12	0
59	MG	CA	3019	1/1	0.98	0.03	22,22,22,22	0
59	MG	AA	3054	1/1	0.98	0.06	21,21,21,21	0
59	MG	AA	3301	1/1	0.98	0.05	39,39,39,39	0
59	MG	AA	3498	1/1	0.98	0.12	47,47,47,47	0
59	MG	CA	3439	1/1	0.98	0.08	32,32,32,32	0
59	MG	CA	3283	1/1	0.98	0.03	31,31,31,31	0
59	MG	AA	3097	1/1	0.98	0.09	22,22,22,22	0
59	MG	AA	3353	1/1	0.98	0.07	39,39,39,39	0
59	MG	AA	3354	1/1	0.98	0.04	27,27,27,27	0
59	MG	AA	3502	1/1	0.98	0.04	29,29,29,29	1
59	MG	AA	3421	1/1	0.98	0.07	28,28,28,28	0
59	MG	AA	3504	1/1	0.98	0.03	29,29,29,29	0
59	MG	AA	3422	1/1	0.98	0.09	23,23,23,23	0
59	MG	AA	3423	1/1	0.98	0.10	16,16,16,16	0
59	MG	CA	3292	1/1	0.98	0.03	12,12,12,12	0
59	MG	DA	1648	1/1	0.98	0.10	40,40,40,40	0
59	MG	BA	1740	1/1	0.98	0.10	50,50,50,50	0
59	MG	CA	3452	1/1	0.98	0.05	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3303	1/1	0.98	0.06	24,24,24,24	0
59	MG	AA	3510	1/1	0.98	0.05	17,17,17,17	0
59	MG	DA	1653	1/1	0.98	0.18	55,55,55,55	0
59	MG	AA	3304	1/1	0.98	0.06	47,47,47,47	0
59	MG	AA	3512	1/1	0.98	0.05	38,38,38,38	0
59	MG	AA	3426	1/1	0.98	0.07	20,20,20,20	0
59	MG	DA	1657	1/1	0.98	0.04	23,23,23,23	0
59	MG	AB	3011	1/1	0.98	0.05	29,29,29,29	0
59	MG	CA	3459	1/1	0.98	0.04	28,28,28,28	0
59	MG	AA	3515	1/1	0.98	0.07	12,12,12,12	0
59	MG	AA	3137	1/1	0.98	0.25	53,53,53,53	0
59	MG	CA	3302	1/1	0.98	0.06	37,37,37,37	0
59	MG	CA	3303	1/1	0.98	0.09	43,43,43,43	0
59	MG	CA	3617	1/1	0.98	0.07	41,41,41,41	0
59	MG	CA	3618	1/1	0.98	0.14	40,40,40,40	0
59	MG	BA	1750	1/1	0.98	0.05	55,55,55,55	0
59	MG	AA	3428	1/1	0.98	0.04	18,18,18,18	0
59	MG	CA	3306	1/1	0.98	0.04	24,24,24,24	0
59	MG	AA	3013	1/1	0.98	0.05	28,28,28,28	0
59	MG	CA	3169	1/1	0.98	0.10	34,34,34,34	0
59	MG	CA	3309	1/1	0.98	0.10	22,22,22,22	0
59	MG	CA	3170	1/1	0.98	0.04	32,32,32,32	0
59	MG	CA	3471	1/1	0.98	0.10	33,33,33,33	0
59	MG	BA	1753	1/1	0.98	0.06	48,48,48,48	0
59	MG	AA	3522	1/1	0.98	0.06	30,30,30,30	0
59	MG	AA	3523	1/1	0.98	0.03	13,13,13,13	0
59	MG	AA	3117	1/1	0.98	0.20	25,25,25,25	1
59	MG	AA	3525	1/1	0.98	0.07	35,35,35,35	0
59	MG	AA	3527	1/1	0.98	0.06	27,27,27,27	0
59	MG	AA	3528	1/1	0.98	0.06	19,19,19,19	0
59	MG	BA	1760	1/1	0.98	0.07	53,53,53,53	0
59	MG	CA	3320	1/1	0.98	0.06	36,36,36,36	0
59	MG	AA	3308	1/1	0.98	0.09	18,18,18,18	0
59	MG	CA	3482	1/1	0.98	0.09	61,61,61,61	0
59	MG	CA	3052	1/1	0.98	0.09	44,44,44,44	0
59	MG	CA	3324	1/1	0.98	0.05	26,26,26,26	0
59	MG	AA	3037	1/1	0.98	0.04	4,4,4,4	0
59	MG	AA	3734	1/1	0.98	0.09	26,26,26,26	0
59	MG	CA	3327	1/1	0.98	0.05	38,38,38,38	0
59	MG	AA	3531	1/1	0.98	0.06	24,24,24,24	0
59	MG	AA	3020	1/1	0.98	0.04	11,11,11,11	0
59	MG	AD	304	1/1	0.98	0.05	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3311	1/1	0.98	0.06	2,2,2,2	0
59	MG	AA	3534	1/1	0.98	0.10	14,14,14,14	0
59	MG	AA	3364	1/1	0.98	0.08	23,23,23,23	0
59	MG	AA	3437	1/1	0.98	0.05	17,17,17,17	0
59	MG	AA	3537	1/1	0.98	0.10	20,20,20,20	0
59	MG	AD	310	1/1	0.98	0.08	46,46,46,46	0
59	MG	AA	3539	1/1	0.98	0.10	34,34,34,34	0
59	MG	AA	3439	1/1	0.98	0.08	37,37,37,37	0
59	MG	AA	3243	1/1	0.98	0.10	43,43,43,43	0
59	MG	BA	1777	1/1	0.98	0.12	71,71,71,71	0
59	MG	AA	3639	1/1	0.98	0.07	18,18,18,18	0
59	MG	AA	3543	1/1	0.98	0.06	32,32,32,32	0
59	MG	AA	3084	1/1	0.98	0.07	23,23,23,23	0
59	MG	AA	3085	1/1	0.98	0.11	46,46,46,46	0
59	MG	CA	3349	1/1	0.98	0.07	23,23,23,23	0
59	MG	AA	3190	1/1	0.98	0.03	24,24,24,24	0
59	MG	AA	3369	1/1	0.98	0.04	47,47,47,47	0
59	MG	AA	3548	1/1	0.98	0.04	7,7,7,7	0
59	MG	AA	3317	1/1	0.98	0.07	24,24,24,24	0
59	MG	AA	3647	1/1	0.98	0.04	43,43,43,43	0
59	MG	AA	3032	1/1	0.98	0.11	59,59,59,59	0
59	MG	CA	3512	1/1	0.98	0.07	53,53,53,53	0
59	MG	AA	3279	1/1	0.98	0.09	34,34,34,34	0
59	MG	AA	3757	1/1	0.98	0.03	14,14,14,14	0
59	MG	AA	3192	1/1	0.98	0.05	30,30,30,30	0
59	MG	AA	3759	1/1	0.98	0.05	57,57,57,57	0
59	MG	AA	3553	1/1	0.98	0.04	43,43,43,43	0
59	MG	AA	3554	1/1	0.98	0.08	40,40,40,40	0
59	MG	AA	3048	1/1	0.98	0.04	28,28,28,28	0
59	MG	CA	3085	1/1	0.98	0.07	25,25,25,25	0
59	MG	AP	202	1/1	0.98	0.21	21,21,21,21	1
59	MG	AA	3071	1/1	0.98	0.13	40,40,40,40	0
59	MG	AA	3147	1/1	0.98	0.21	40,40,40,40	1
59	MG	AA	3223	1/1	0.98	0.04	15,15,15,15	0
59	MG	CA	3369	1/1	0.98	0.07	48,48,48,48	0
59	MG	AA	3089	1/1	0.98	0.10	49,49,49,49	0
59	MG	BA	1680	1/1	0.98	0.09	40,40,40,40	0
59	MG	AA	3560	1/1	0.98	0.05	29,29,29,29	0
59	MG	AA	3561	1/1	0.98	0.06	21,21,21,21	0
59	MG	AA	3379	1/1	0.98	0.11	23,23,23,23	0
59	MG	AA	3770	1/1	0.98	0.07	43,43,43,43	0
59	MG	AU	202	1/1	0.98	0.06	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AU	203	1/1	0.98	0.12	25,25,25,25	0
59	MG	AA	3380	1/1	0.98	0.04	18,18,18,18	0
59	MG	AV	202	1/1	0.98	0.07	38,38,38,38	0
59	MG	AA	3072	1/1	0.98	0.03	19,19,19,19	0
59	MG	AA	3382	1/1	0.98	0.05	37,37,37,37	0
59	MG	AA	3383	1/1	0.98	0.05	20,20,20,20	0
59	MG	AA	3330	1/1	0.98	0.05	66,66,66,66	0
59	MG	AA	3568	1/1	0.98	0.04	15,15,15,15	0
59	MG	AA	3173	1/1	0.98	0.08	46,46,46,46	0
59	MG	AA	3333	1/1	0.98	0.06	11,11,11,11	0
59	MG	AA	3004	1/1	0.98	0.09	21,21,21,21	0
59	MG	AA	3200	1/1	0.98	0.14	30,30,30,30	0
59	MG	AA	3574	1/1	0.98	0.05	12,12,12,12	0
59	MG	CV	202	1/1	0.98	0.08	38,38,38,38	0
59	MG	AA	3007	1/1	0.98	0.03	12,12,12,12	0
59	MG	AA	3260	1/1	0.98	0.07	21,21,21,21	0
59	MG	AA	3469	1/1	0.98	0.03	32,32,32,32	0
59	MG	CA	3397	1/1	0.98	0.08	57,57,57,57	0
59	MG	AA	3392	1/1	0.98	0.07	17,17,17,17	0
59	MG	AA	3292	1/1	0.98	0.07	24,24,24,24	0
59	MG	AA	3340	1/1	0.98	0.04	3,3,3,3	0
59	MG	AA	3581	1/1	0.98	0.07	52,52,52,52	0
59	MG	AA	3681	1/1	0.98	0.04	42,42,42,42	0
59	MG	AA	3130	1/1	0.98	0.07	34,34,34,34	0
59	MG	A7	101	1/1	0.98	0.08	47,47,47,47	0
59	MG	AA	3399	1/1	0.98	0.03	16,16,16,16	0
59	MG	CA	3407	1/1	0.98	0.07	36,36,36,36	0
59	MG	AA	3795	1/1	0.98	0.12	22,22,22,22	0
59	MG	AA	3262	1/1	0.98	0.03	15,15,15,15	0
59	MG	CA	3123	1/1	0.98	0.04	29,29,29,29	0
59	MG	AA	3295	1/1	0.98	0.07	57,57,57,57	0
59	MG	CA	3255	1/1	0.98	0.08	28,28,28,28	0
59	MG	AA	3345	1/1	0.98	0.06	6,6,6,6	0
59	MG	AA	3406	1/1	0.98	0.04	20,20,20,20	0
59	MG	AA	3484	1/1	0.98	0.07	53,53,53,53	0
59	MG	CA	3568	1/1	0.98	0.04	39,39,39,39	0
59	MG	AA	3589	1/1	0.98	0.04	55,55,55,55	0
59	MG	CA	3006	1/1	0.98	0.03	22,22,22,22	0
59	MG	AA	3407	1/1	0.98	0.05	10,10,10,10	0
59	MG	AA	3691	1/1	0.98	0.05	62,62,62,62	0
59	MG	AA	3591	1/1	0.98	0.11	52,52,52,52	0
59	MG	AA	3024	1/1	0.98	0.13	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3267	1/1	0.98	0.04	38,38,38,38	0
59	MG	AA	3132	1/1	0.98	0.07	41,41,41,41	0
59	MG	AA	3410	1/1	0.98	0.10	57,57,57,57	0
59	MG	CA	3136	1/1	0.98	0.03	63,63,63,63	0
59	MG	CA	3271	1/1	0.98	0.07	48,48,48,48	0
59	MG	AA	3491	1/1	0.98	0.04	46,46,46,46	0
59	MG	AA	3052	1/1	0.98	0.07	11,11,11,11	0
59	MG	AA	3597	1/1	0.98	0.04	33,33,33,33	0
59	MG	AA	3412	1/1	0.98	0.10	39,39,39,39	0
60	ZN	DN	501	1/1	0.98	0.04	117,117,117,117	0
61	SF4	BD	501	8/8	0.98	0.04	78,78,78,78	0
59	MG	AA	3494	1/1	0.98	0.06	34,34,34,34	0
59	MG	AA	3053	1/1	0.98	0.11	19,19,19,19	0
59	MG	CA	3588	1/1	0.98	0.04	32,32,32,32	0
59	MG	CA	3321	1/1	0.99	0.06	28,28,28,28	0
59	MG	CA	3562	1/1	0.99	0.03	29,29,29,29	0
59	MG	AA	3519	1/1	0.99	0.12	27,27,27,27	0
59	MG	CA	3401	1/1	0.99	0.04	28,28,28,28	0
59	MG	AA	3343	1/1	0.99	0.06	46,46,46,46	0
59	MG	CA	3650	1/1	0.99	0.07	14,14,14,14	0
59	MG	AA	3312	1/1	0.99	0.02	23,23,23,23	0
59	MG	AA	3074	1/1	0.99	0.06	14,14,14,14	0
59	MG	AA	3702	1/1	0.99	0.10	14,14,14,14	0
59	MG	AA	3482	1/1	0.99	0.03	41,41,41,41	0
59	MG	AF	305	1/1	0.99	0.07	19,19,19,19	0
59	MG	CA	3329	1/1	0.99	0.04	21,21,21,21	0
59	MG	AF	306	1/1	0.99	0.06	36,36,36,36	0
59	MG	AA	3401	1/1	0.99	0.04	21,21,21,21	0
59	MG	CA	3574	1/1	0.99	0.04	37,37,37,37	0
59	MG	CA	3262	1/1	0.99	0.03	11,11,11,11	0
59	MG	AA	3402	1/1	0.99	0.04	27,27,27,27	0
59	MG	AA	3526	1/1	0.99	0.11	19,19,19,19	0
59	MG	CA	3578	1/1	0.99	0.05	38,38,38,38	0
59	MG	AA	3707	1/1	0.99	0.03	59,59,59,59	0
59	MG	CA	3266	1/1	0.99	0.07	36,36,36,36	0
59	MG	AA	3328	1/1	0.99	0.05	42,42,42,42	0
59	MG	AA	3404	1/1	0.99	0.08	27,27,27,27	0
59	MG	AA	3487	1/1	0.99	0.03	49,49,49,49	0
59	MG	AA	3663	1/1	0.99	0.05	11,11,11,11	0
59	MG	CA	3342	1/1	0.99	0.03	33,33,33,33	0
59	MG	AA	3125	1/1	0.99	0.06	22,22,22,22	1
59	MG	AA	3489	1/1	0.99	0.04	15,15,15,15	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	3423	1/1	0.99	0.10	46,46,46,46	0
59	MG	AA	3248	1/1	0.99	0.07	22,22,22,22	0
59	MG	CA	3346	1/1	0.99	0.06	30,30,30,30	0
59	MG	AA	3821	1/1	0.99	0.09	82,82,82,82	0
59	MG	AA	3038	1/1	0.99	0.15	29,29,29,29	1
59	MG	AA	3457	1/1	0.99	0.04	30,30,30,30	0
59	MG	CA	3211	1/1	0.99	0.04	29,29,29,29	0
59	MG	AA	3332	1/1	0.99	0.04	17,17,17,17	0
59	MG	AA	3239	1/1	0.99	0.13	25,25,25,25	1
59	MG	CA	3214	1/1	0.99	0.07	22,22,22,22	0
59	MG	CA	3151	1/1	0.99	0.03	38,38,38,38	0
59	MG	CA	3282	1/1	0.99	0.05	36,36,36,36	0
59	MG	CA	3356	1/1	0.99	0.07	44,44,44,44	0
59	MG	AA	3003	1/1	0.99	0.02	8,8,8,8	0
59	MG	AA	3538	1/1	0.99	0.05	15,15,15,15	0
59	MG	CA	3438	1/1	0.99	0.04	24,24,24,24	0
59	MG	AA	3103	1/1	0.99	0.02	5,5,5,5	0
59	MG	AA	3540	1/1	0.99	0.03	36,36,36,36	0
59	MG	BA	1746	1/1	0.99	0.04	33,33,33,33	0
59	MG	AA	3436	1/1	0.99	0.03	12,12,12,12	0
59	MG	CA	3443	1/1	0.99	0.04	28,28,28,28	0
59	MG	AA	3463	1/1	0.99	0.03	15,15,15,15	0
59	MG	AA	3388	1/1	0.99	0.02	28,28,28,28	0
59	MG	AA	3726	1/1	0.99	0.06	12,12,12,12	0
59	MG	AA	3778	1/1	0.99	0.04	43,43,43,43	0
59	MG	AV	205	1/1	0.99	0.04	42,42,42,42	0
59	MG	CA	3163	1/1	0.99	0.13	30,30,30,30	0
59	MG	AA	3727	1/1	0.99	0.03	23,23,23,23	0
59	MG	AA	3465	1/1	0.99	0.06	42,42,42,42	0
59	MG	AA	3679	1/1	0.99	0.04	36,36,36,36	0
59	MG	CA	3372	1/1	0.99	0.08	35,35,35,35	0
59	MG	AA	3438	1/1	0.99	0.06	17,17,17,17	0
59	MG	AA	3320	1/1	0.99	0.08	37,37,37,37	0
59	MG	AA	3784	1/1	0.99	0.07	59,59,59,59	0
59	MG	AA	3214	1/1	0.99	0.22	58,58,58,58	1
59	MG	AA	3011	1/1	0.99	0.04	16,16,16,16	0
59	MG	AA	3505	1/1	0.99	0.04	30,30,30,30	0
59	MG	AA	3506	1/1	0.99	0.03	48,48,48,48	0
59	MG	AA	3151	1/1	0.99	0.07	62,62,62,62	0
59	MG	AA	3393	1/1	0.99	0.07	23,23,23,23	0
59	MG	CA	3382	1/1	0.99	0.07	38,38,38,38	0
59	MG	CA	3383	1/1	0.99	0.05	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	3738	1/1	0.99	0.07	24,24,24,24	0
59	MG	DA	1691	1/1	0.99	0.06	63,63,63,63	0
59	MG	AA	3419	1/1	0.99	0.06	20,20,20,20	0
59	MG	AA	3793	1/1	0.99	0.07	7,7,7,7	0
59	MG	AA	3324	1/1	0.99	0.02	15,15,15,15	0
59	MG	CA	3311	1/1	0.99	0.05	50,50,50,50	0
59	MG	BA	1769	1/1	0.99	0.05	58,58,58,58	0
59	MG	AA	3022	1/1	0.99	0.02	5,5,5,5	0
59	MG	AA	3475	1/1	0.99	0.08	45,45,45,45	0
59	MG	AA	3513	1/1	0.99	0.03	41,41,41,41	0
60	ZN	CY	501	1/1	0.99	0.03	101,101,101,101	0
59	MG	CA	3393	1/1	0.99	0.05	68,68,68,68	0
60	ZN	C5	102	1/1	0.99	0.04	66,66,66,66	0
60	ZN	C6	501	1/1	0.99	0.03	66,66,66,66	0
60	ZN	C9	501	1/1	0.99	0.03	75,75,75,75	0
59	MG	AA	3476	1/1	0.99	0.03	28,28,28,28	0
59	MG	AA	3477	1/1	0.99	0.03	14,14,14,14	0
59	MG	AA	3478	1/1	0.99	0.04	33,33,33,33	0
59	MG	AA	3517	1/1	0.99	0.03	23,23,23,23	0
59	MG	AA	3518	1/1	0.99	0.04	14,14,14,14	0
60	ZN	A6	102	1/1	1.00	0.03	40,40,40,40	0
60	ZN	A9	501	1/1	1.00	0.02	42,42,42,42	0
59	MG	AA	3397	1/1	1.00	0.05	13,13,13,13	0
59	MG	AA	3569	1/1	1.00	0.04	17,17,17,17	0
59	MG	CA	3339	1/1	1.00	0.03	24,24,24,24	0
59	MG	AA	3076	1/1	1.00	0.03	0,0,0,0	0
59	MG	AA	3335	1/1	1.00	0.08	15,15,15,15	0
59	MG	AA	3416	1/1	1.00	0.03	14,14,14,14	0
59	MG	AA	3801	1/1	1.00	0.05	27,27,27,27	0
59	MG	AA	3396	1/1	1.00	0.06	16,16,16,16	0
60	ZN	AY	501	1/1	1.00	0.01	61,61,61,61	0
59	MG	AE	303	1/1	1.00	0.09	19,19,19,19	0
60	ZN	A5	501	1/1	1.00	0.01	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.