wwPDB X-ray Structure Validation Summary Report (i)

Sep 15, 2026 – 11:09 PM EDT

PDB ID	:	5DFE / pdb_00005dfe
Title	:	70S termination complex containing E. coli RF2
Authors	:	Hoffer, E.D.; Dunham, C.M.
Deposited on	:	2015-08-26
Resolution	:	3.10 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:

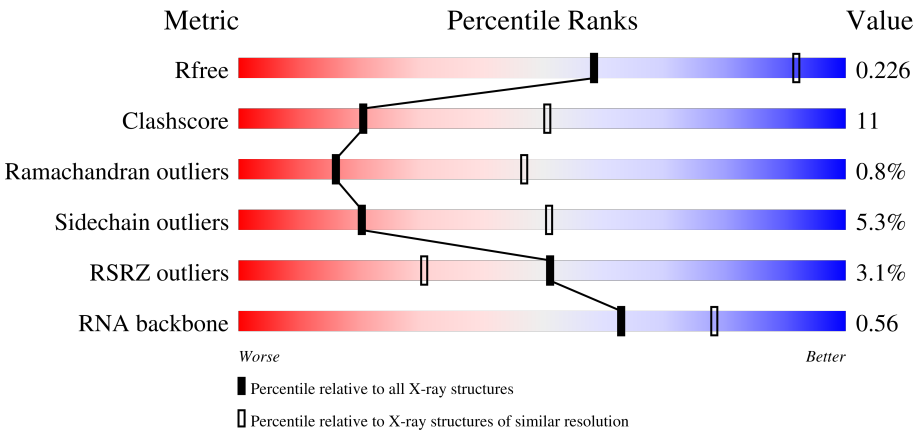
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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	QV	77	3%, 58%, 34%, 6% •
1	XV	77	3%, 65%, 26%, 9%
2	QX	25	12%, 24%, 12% •, 60%
2	XX	25	12%, 20%, 12%, 8%, 60%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	QY	380	10% 52% 37% 6%
3	XY	380	11% 49% 38% 6% 6%
4	RA	2915	% 59% 33% 7%
4	YA	2915	2% 58% 33% 7%
5	RB	122	2% 75% 23%
5	YB	122	2% 70% 23% 5%
6	RD	276	% 78% 19%
6	YD	276	75% 20%
7	RE	206	% 74% 21%
7	YE	206	73% 21% 5%
8	RF	210	% 68% 23% 6%
8	YF	210	64% 27% 5%
9	RG	182	3% 63% 32%
9	YG	182	3% 56% 39%
10	RH	180	5% 74% 20%
10	YH	180	2% 64% 28%
11	RI	148	9% 72% 24%
11	YI	148	6% 70% 26%
12	RN	140	% 73% 24%
12	YN	140	% 76% 21%
13	RO	122	2% 77% 20%
13	YO	122	% 75% 22%
14	RP	150	% 77% 20%
14	YP	150	% 73% 22%
15	RQ	141	% 72% 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	YQ	141	%, 74%, 20%, 6%
16	RR	118	65%, 31%, •
16	YR	118	%, 71%, 26%, •
17	RS	112	4%, 66%, 29%, • • •
17	YS	112	2%, 62%, 31%, • • •
18	RT	146	2%, 57%, 29%, • •, 10%
18	YT	146	%, 58%, 27%, • •, 10%
19	RU	118	%, 72%, 19%, 6%, • •
19	YU	118	74%, 19%, 5%, •
20	RV	101	73%, 19%, 7%, •
20	YV	101	2%, 73%, 24%, • •
21	RW	113	3%, 78%, 19%, • ••
21	YW	113	78%, 17%, • ••
22	RX	96	%, 82%, 15%, • •
22	YX	96	%, 82%, 17%, •
23	RY	110	12%, 65%, 28%, • •
23	YY	110	3%, 67%, 26%, • • •
24	RZ	206	7%, 74%, 20%, • •
24	YZ	206	6%, 69%, 26%, • •
25	R0	85	2%, 71%, 15%, • •, 9%
25	Y0	85	4%, 68%, 18%, • •, 9%
26	R1	98	3%, 76%, 19%, • •
26	Y1	98	64%, 29%, 5%, ••
27	R2	72	3%, 69%, 26%, • •
27	Y2	72	4%, 68%, 25%, • • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	R3	60	2% 80% 18%
28	Y3	60	3% 82% 15%
29	R4	71	% 52% 34% 10%
29	Y4	71	7% 44% 44% 6%
30	R5	60	73% 23%
30	Y5	60	2% 78% 15% 5%
31	R6	54	6% 67% 28%
31	Y6	54	2% 81% 15%
32	R7	49	6% 63% 33%
32	Y7	49	4% 73% 20%
33	R8	65	2% 63% 32%
33	Y8	65	2% 60% 37%
34	R9	37	70% 24%
34	Y9	37	5% 78% 19%
35	QA	1521	2% 52% 39% 7%
35	XA	1521	% 53% 39% 6%
36	QB	256	7% 50% 34% 10%
36	XB	256	6% 47% 35% 6% 10%
37	QC	239	3% 63% 22% 14%
37	XC	239	4% 60% 23% 14%
38	QD	209	6% 59% 36%
38	XD	209	7% 64% 30% 5%
39	QE	162	2% 62% 27% 9%
39	XE	162	% 54% 33% 9%
40	QF	101	3% 61% 29% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	XF	101	66% 23% 10%
41	QG	156	4% 82% 16%
41	XG	156	3% 68% 27%
42	QH	138	2% 68% 28%
42	XH	138	% 70% 28%
43	QI	128	12% 64% 30%
43	XI	128	11% 50% 45%
44	QJ	105	7% 54% 35% 8%
44	XJ	105	10% 57% 31% 9%
45	QK	129	5% 72% 15% 12%
45	XK	129	4% 69% 17% 12%
46	QL	132	3% 65% 24% 8%
46	XL	132	5% 68% 21% 8%
47	QM	126	9% 63% 29% 8%
47	XM	126	6% 59% 31% 10%
48	QN	61	11% 66% 25% 8%
48	XN	61	10% 75% 20%
49	QO	89	69% 28%
49	XO	89	3% 72% 25%
50	QP	88	5% 55% 36% 7%
50	XP	88	5% 61% 26% 7%
51	QQ	105	5% 70% 21% 6%
51	XQ	105	2% 72% 17% 5% 6%
52	QR	88	53% 17% 6% 23%
52	XR	88	51% 20% 6% 23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	QS	93	8% 66% 20% • 11%
53	XS	93	8% 60% 28% • 11%
54	QT	106	4% 74% 15% • 9%
54	XT	106	8% 66% 24% • 8%
55	QU	27	33% 56% 26% • 15%
55	XU	27	33% 59% 22% • 15%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	QA	1601	-	-	-	X
56	MG	QA	1611	-	-	-	X
56	MG	QA	1624	-	-	-	X
56	MG	QA	1657	-	-	-	X
56	MG	QA	1661	-	-	-	X
56	MG	QA	1718	-	-	-	X
56	MG	QA	1720	-	-	-	X
56	MG	QA	1725	-	-	-	X
56	MG	QA	1736	-	-	-	X
56	MG	QA	1737	-	-	-	X
56	MG	QA	1761	-	-	-	X
56	MG	QA	1762	-	-	-	X
56	MG	QA	1793	-	-	-	X
56	MG	QA	1812	-	-	-	X
56	MG	QA	1816	-	-	-	X
56	MG	QA	1831	-	-	-	X
56	MG	QA	1847	-	-	-	X
56	MG	QA	1849	-	-	-	X
56	MG	QA	1858	-	-	-	X
56	MG	QA	1866	-	-	-	X
56	MG	QN	103	-	-	-	X
56	MG	QY	403	-	-	-	X
56	MG	R0	103	-	-	-	X
56	MG	R1	102	-	-	-	X
56	MG	R3	101	-	-	-	X
56	MG	RA	3017	-	-	-	X
56	MG	RA	3058	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3076	-	-	-	X
56	MG	RA	3187	-	-	-	X
56	MG	RA	3193	-	-	-	X
56	MG	RA	3203	-	-	-	X
56	MG	RA	3212	-	-	-	X
56	MG	RA	3237	-	-	-	X
56	MG	RA	3239	-	-	-	X
56	MG	RA	3249	-	-	-	X
56	MG	RA	3252	-	-	-	X
56	MG	RA	3256	-	-	-	X
56	MG	RA	3299	-	-	-	X
56	MG	RA	3331	-	-	-	X
56	MG	RA	3367	-	-	-	X
56	MG	RA	3368	-	-	-	X
56	MG	RA	3370	-	-	-	X
56	MG	RA	3374	-	-	-	X
56	MG	RA	3444	-	-	-	X
56	MG	RA	3457	-	-	-	X
56	MG	RA	3459	-	-	-	X
56	MG	RA	3486	-	-	-	X
56	MG	RA	3511	-	-	-	X
56	MG	RA	3512	-	-	-	X
56	MG	RA	3517	-	-	-	X
56	MG	RA	3527	-	-	-	X
56	MG	RA	3564	-	-	-	X
56	MG	RA	3572	-	-	-	X
56	MG	RA	3573	-	-	-	X
56	MG	RA	3598	-	-	-	X
56	MG	RA	3625	-	-	-	X
56	MG	RA	3630	-	-	-	X
56	MG	RA	3631	-	-	-	X
56	MG	RA	3636	-	-	-	X
56	MG	RA	3639	-	-	-	X
56	MG	RA	3647	-	-	-	X
56	MG	RA	3694	-	-	-	X
56	MG	RA	3710	-	-	-	X
56	MG	RA	3727	-	-	-	X
56	MG	RA	3728	-	-	-	X
56	MG	RA	3733	-	-	-	X
56	MG	RA	3752	-	-	-	X
56	MG	RA	3777	-	-	-	X
56	MG	RA	3780	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3782	-	-	-	X
56	MG	RA	3872	-	-	-	X
56	MG	RA	3890	-	-	-	X
56	MG	RA	3951	-	-	-	X
56	MG	RA	3960	-	-	-	X
56	MG	RA	4002	-	-	-	X
56	MG	RA	4004	-	-	-	X
56	MG	RA	4015	-	-	-	X
56	MG	RA	4019	-	-	-	X
56	MG	RA	4035	-	-	-	X
56	MG	RA	4046	-	-	-	X
56	MG	RA	4058	-	-	-	X
56	MG	RB	223	-	-	-	X
56	MG	RF	301	-	-	-	X
56	MG	XA	1609	-	-	-	X
56	MG	XA	1682	-	-	-	X
56	MG	XA	1708	-	-	-	X
56	MG	XA	1719	-	-	-	X
56	MG	XA	1725	-	-	-	X
56	MG	XA	1753	-	-	-	X
56	MG	XA	1754	-	-	-	X
56	MG	XA	1773	-	-	-	X
56	MG	XA	1777	-	-	-	X
56	MG	XA	1781	-	-	-	X
56	MG	XA	1783	-	-	-	X
56	MG	XA	1787	-	-	-	X
56	MG	YA	3108	-	-	-	X
56	MG	YA	3150	-	-	-	X
56	MG	YA	3160	-	-	-	X
56	MG	YA	3164	-	-	-	X
56	MG	YA	3171	-	-	-	X
56	MG	YA	3185	-	-	-	X
56	MG	YA	3236	-	-	-	X
56	MG	YA	3239	-	-	-	X
56	MG	YA	3242	-	-	-	X
56	MG	YA	3246	-	-	-	X
56	MG	YA	3281	-	-	-	X
56	MG	YA	3311	-	-	-	X
56	MG	YA	3414	-	-	-	X
56	MG	YA	3417	-	-	-	X
56	MG	YA	3432	-	-	-	X
56	MG	YA	3455	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3465	-	-	-	X
56	MG	YA	3467	-	-	-	X
56	MG	YA	3468	-	-	-	X
56	MG	YA	3469	-	-	-	X
56	MG	YA	3490	-	-	-	X
56	MG	YA	3501	-	-	-	X
56	MG	YA	3528	-	-	-	X
56	MG	YA	3534	-	-	-	X
56	MG	YA	3582	-	-	-	X
56	MG	YA	3603	-	-	-	X
56	MG	YA	3637	-	-	-	X
56	MG	YA	3655	-	-	-	X
56	MG	YA	3662	-	-	-	X
56	MG	YA	3695	-	-	-	X
56	MG	YA	3707	-	-	-	X
56	MG	YA	3737	-	-	-	X
56	MG	YA	3747	-	-	-	X
56	MG	YB	209	-	-	-	X
56	MG	YE	303	-	-	-	X
56	MG	YF	302	-	-	-	X

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 296662 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 P-site tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	QV	77	1644	732	297	538	77	0	0	0
1	XV	77	1644	732	297	538	77	0	0	0

- Molecule 2 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	QX	10	215	97	42	66	10	0	0	0
2	XX	10	215	97	42	66	10	0	0	0

- Molecule 3 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	QY	357	2833	1742	498	583	10	0	0	0
3	XY	357	2833	1742	498	583	10	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QY	-14	MET	-	initiating methionine	UNP P07012
QY	-13	GLY	-	expression tag	UNP P07012
QY	-12	SER	-	expression tag	UNP P07012
QY	-11	SER	-	expression tag	UNP P07012
QY	-10	HIS	-	expression tag	UNP P07012
QY	-9	HIS	-	expression tag	UNP P07012
QY	-8	HIS	-	expression tag	UNP P07012
QY	-7	HIS	-	expression tag	UNP P07012

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
QY	-6	HIS	-	expression tag	UNP P07012
QY	-5	HIS	-	expression tag	UNP P07012
QY	-4	SER	-	expression tag	UNP P07012
QY	-3	GLU	-	expression tag	UNP P07012
QY	-2	ASP	-	expression tag	UNP P07012
QY	-1	PRO	-	expression tag	UNP P07012
QY	0	ALA	-	expression tag	UNP P07012
XY	-14	MET	-	initiating methionine	UNP P07012
XY	-13	GLY	-	expression tag	UNP P07012
XY	-12	SER	-	expression tag	UNP P07012
XY	-11	SER	-	expression tag	UNP P07012
XY	-10	HIS	-	expression tag	UNP P07012
XY	-9	HIS	-	expression tag	UNP P07012
XY	-8	HIS	-	expression tag	UNP P07012
XY	-7	HIS	-	expression tag	UNP P07012
XY	-6	HIS	-	expression tag	UNP P07012
XY	-5	HIS	-	expression tag	UNP P07012
XY	-4	SER	-	expression tag	UNP P07012
XY	-3	GLU	-	expression tag	UNP P07012
XY	-2	ASP	-	expression tag	UNP P07012
XY	-1	PRO	-	expression tag	UNP P07012
XY	0	ALA	-	expression tag	UNP P07012

- Molecule 4 is a RNA chain called T23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	YA	2867	61758	27491	11552	19850	2865	0	0	0
4	RA	2867	61758	27491	11552	19850	2865	0	0	0

- Molecule 5 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	YB	120	2573	1146	476	832	119	0	0	0
5	RB	120	2572	1145	476	832	119	0	0	0

- Molecule 6 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	YD	275	2136	1349	423	361	3	0	0	0
6	RD	275	2131	1346	422	360	3	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	YE	204	1559	985	298	270	6	0	0	0
7	RE	204	1559	985	298	270	6	0	0	0

- Molecule 8 is a protein called 50S ribosomal protein L4.

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

- Molecule 9 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	YG	181	1424	912	259	249	4	0	0	0
9	RG	181	1426	916	253	253	4	0	0	0

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	YH	173	1324	842	247	234	1	0	0	0
10	RH	174	1330	845	248	236	1	0	0	0

- Molecule 11 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	YI	146	1076	687	186	202	1	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	RI	147	1094	699	191	203	1	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	YN	140	1117	719	207	187	4	0	0	0
12	RN	140	1121	722	208	187	4	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	YO	122	933	588	171	170	4	0	0	0
13	RO	122	933	588	171	170	4	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	YP	149	1135	706	230	196	3	0	0	0
14	RP	149	1135	706	230	196	3	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	YQ	141	1122	715	212	188	7	0	0	0
15	RQ	141	1122	715	212	188	7	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	YR	118	968	604	203	160	1	0	0	0
16	RR	118	968	604	203	160	1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
17	YS	110	870	549	173	148	0	0	0
17	RS	110	877	553	175	149	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	YT	131	1083	675	224	183	1	0	0	0
18	RT	131	1091	680	225	185	1	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	YU	116	959	608	201	149	1	0	0	0
19	RU	116	959	608	201	149	1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	YV	101	771	495	140	135	1	0	0	0
20	RV	101	775	498	141	135	1	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	YW	112	886	557	174	153	2	0	0	0
21	RW	112	886	557	174	153	2	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	YX	95	750	488	135	126	1	0	0	0
22	RX	95	750	488	135	126	1	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	YY	107	810	519	153	132	6	0	0	0
23	RY	107	810	520	153	131	6	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	YZ	201	1557	995	274	286	2	0	0	0
24	RZ	203	1587	1011	282	292	2	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	Y0	77	608	375	129	103	1	0	0	0
25	R0	77	608	375	129	103	1	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	Y1	97	759	478	149	131	1	0	0	0
26	R1	97	754	475	148	130	1	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	Y2	70	592	368	119	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			
27	R2	70	588	365	118	103	2	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
28	Y3	59	464	296	90	78	0	0	0
28	R3	59	469	298	90	81	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	Y4	69	536	342	98	91	5	0	0	0
29	R4	69	546	346	96	99	5	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	Y5	59	455	285	89	76	5	0	0	0
30	R5	59	459	288	90	76	5	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	Y6	53	449	279	91	75	4	0	0	0
31	R6	53	453	281	91	77	4	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	Y7	48	418	257	104	55	2	0	0	0
32	R7	48	418	257	104	55	2	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	Y8	64	517	331	102	82	2	0	0	0
33	R8	64	517	331	102	82	2	0	0	0

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	Y9	37	307	188	68	47	4	0	0	0
34	R9	37	307	188	68	47	4	0	0	0

- Molecule 35 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
35	XA	1504	32331	14396	5990	10441	1504	0	0	0
35	QA	1500	32246	14358	5975	10413	1500	0	0	0

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	XB	231	1825	1167	326	327	5	0	0	0
36	QB	231	1842	1175	330	332	5	0	0	0

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	XC	206	1542	968	300	273	1	0	0	0
37	QC	206	1558	979	305	273	1	0	0	0

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	XD	208	1668	1047	330	284	7	0	0	0
38	QD	208	1665	1043	329	286	7	0	0	0

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	XE	148	1133	716	214	199	4	0	0	0
39	QE	148	1133	716	214	199	4	0	0	0

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	XF	100	816	516	146	151	3	0	0	0
40	QF	100	814	516	144	151	3	0	0	0

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	XG	155	1229	766	241	216	6	0	0	0
41	QG	155	1235	769	244	216	6	0	0	0

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	XH	137	1088	689	206	191	2	0	0	0
42	QH	137	1098	694	210	192	2	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
43	XI	126	966	613	186	167	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
43	QI	127	986	625	193	168	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
44	XJ	96	710	442	137	131	0	0	0
44	QJ	97	719	446	142	131	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	XK	114	833	519	156	155	3	0	0	0
45	QK	114	834	520	156	155	3	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	XL	122	932	586	185	159	2	0	0	0
46	QL	122	932	586	185	159	2	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	XM	114	895	550	186	157	2	0	0	0
47	QM	116	914	564	189	159	2	0	0	0

- Molecule 48 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	XN	60	492	312	104	72	4	0	0	0
48	QN	60	492	312	104	72	4	0	0	0

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	XO	88	728	456	144	126	2	0	0	0
49	QO	88	728	456	144	126	2	0	0	0

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	XP	82	677	430	133	113	1	0	0	0
50	QP	82	681	433	134	113	1	0	0	0

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	XQ	99	823	528	151	142	2	0	0	0
51	QQ	99	823	528	151	142	2	0	0	0

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
52	XR	68	555	355	108	92	0	0	0
52	QR	68	555	355	108	92	0	0	0

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	XS	83	645	410	118	115	2	0	0	0
53	QS	83	648	415	120	111	2	0	0	0

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	XT	98	733	451	154	126	2	0	0	0
54	QT	96	732	449	157	124	2	0	0	0

- Molecule 55 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
55	XU	23	199	122	48	29	0	0	0
55	QU	23	199	122	48	29	0	0	0

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	QV	2	2	2	0	0
56	QY	3	3	3	0	0
56	XX	1	1	1	0	0
56	YA	760	760	760	0	0
56	YB	19	19	19	0	0
56	YD	10	10	10	0	0
56	YE	7	7	7	0	0
56	YF	3	3	3	0	0
56	YG	3	3	3	0	0
56	YI	1	1	1	0	0
56	YN	1	1	1	0	0
56	YO	1	1	1	0	0
56	YP	1	1	1	0	0
56	YQ	2	2	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	YR	1	1	1	0	0
56	YT	3	3	3	0	0
56	YV	1	1	1	0	0
56	YW	2	2	2	0	0
56	YX	1	1	1	0	0
56	Y0	1	1	1	0	0
56	Y1	1	1	1	0	0
56	Y5	1	1	1	0	0
56	Y7	1	1	1	0	0
56	Y8	2	2	2	0	0
56	XA	190	190	190	0	0
56	XE	2	2	2	0	0
56	XF	4	4	4	0	0
56	XH	1	1	1	0	0
56	XJ	1	1	1	0	0
56	XK	1	1	1	0	0
56	XL	1	1	1	0	0
56	XR	1	1	1	0	0
56	XT	1	1	1	0	0
56	QA	279	279	279	0	0
56	QB	1	1	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	QD	3	3	3	0	0
56	QE	2	2	2	0	0
56	QF	1	1	1	0	0
56	QG	3	3	3	0	0
56	QH	2	2	2	0	0
56	QI	1	1	1	0	0
56	QL	3	3	3	0	0
56	QM	1	1	1	0	0
56	QN	2	2	2	0	0
56	QO	1	1	1	0	0
56	QQ	2	2	2	0	0
56	QR	1	1	1	0	0
56	QT	1	1	1	0	0
56	QU	1	1	1	0	0
56	RA	1066	1066	1066	0	0
56	RB	29	29	29	0	0
56	RD	13	13	13	0	0
56	RE	6	6	6	0	0
56	RF	12	12	12	0	0
56	RG	4	4	4	0	0
56	RH	2	2	2	0	0

Continued on next page...

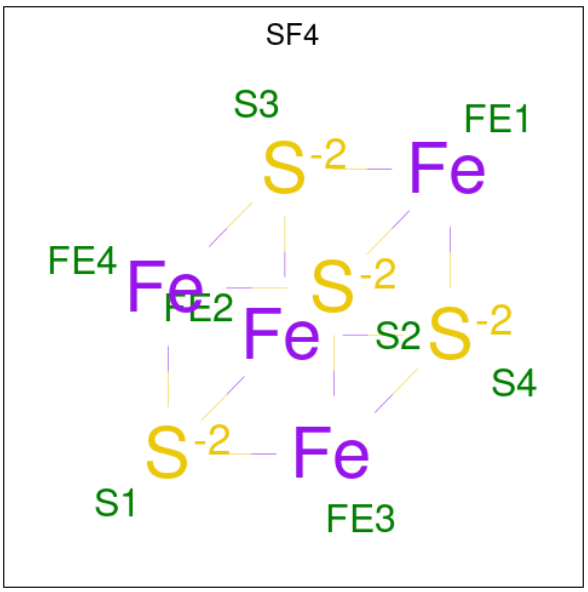
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	RN	3	3	3	0	0
56	RO	1	1	1	0	0
56	RP	2	2	2	0	0
56	RQ	4	4	4	0	0
56	RR	5	5	5	0	0
56	RT	3	3	3	0	0
56	RU	3	3	3	0	0
56	RV	4	4	4	0	0
56	RW	2	2	2	0	0
56	RX	1	1	1	0	0
56	RZ	1	1	1	0	0
56	R0	4	4	4	0	0
56	R1	3	3	3	0	0
56	R3	2	2	2	0	0
56	R4	1	1	1	0	0
56	R5	3	3	3	0	0
56	R7	2	2	2	0	0
56	R8	1	1	1	0	0
56	R9	2	2	2	0	0

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	YY	1	Total Zn 1 1	0	0
57	Y4	1	Total Zn 1 1	0	0
57	Y5	1	Total Zn 1 1	0	0
57	Y6	1	Total Zn 1 1	0	0
57	Y9	1	Total Zn 1 1	0	0
57	XN	1	Total Zn 1 1	0	0
57	QN	1	Total Zn 1 1	0	0
57	RY	1	Total Zn 1 1	0	0
57	R4	1	Total Zn 1 1	0	0
57	R5	1	Total Zn 1 1	0	0
57	R6	1	Total Zn 1 1	0	0
57	R9	1	Total Zn 1 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



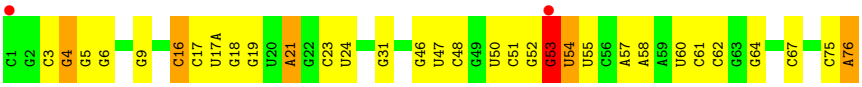
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
58	XD	1	8	4	4	0	0
			Total	Fe	S		
58	QD	1	8	4	4	0	0

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: P-site tRNA fMet

Chain QV:

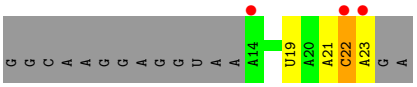


• Molecule 1: P-site tRNA fMet

Chain XV:

• Molecule 2: messenger RNA

Chain QX:

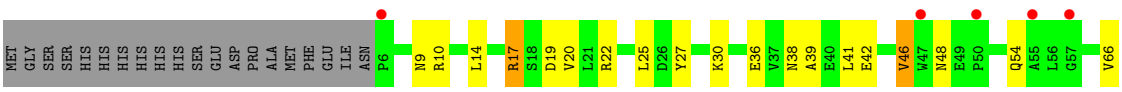


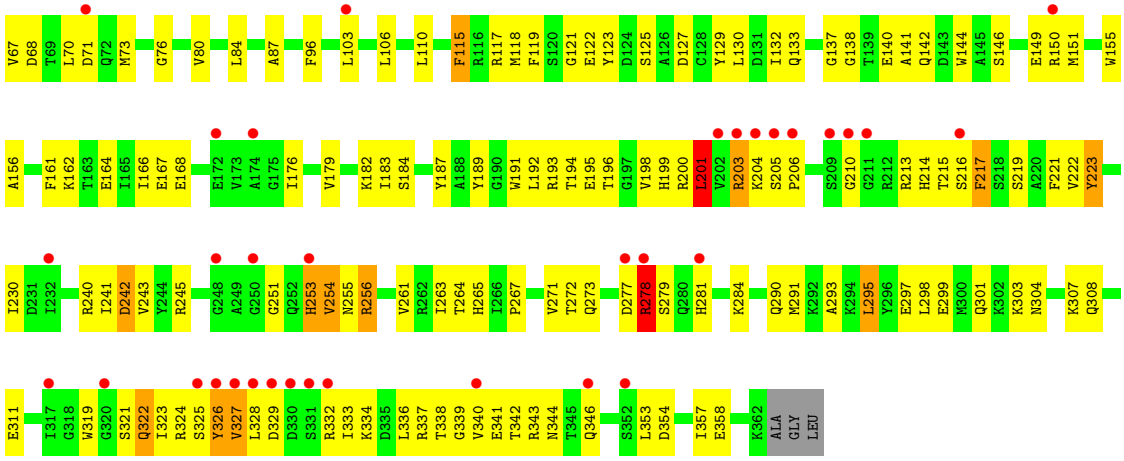
• Molecule 2: messenger RNA

Chain XX:

• Molecule 3: Peptide chain release factor 2

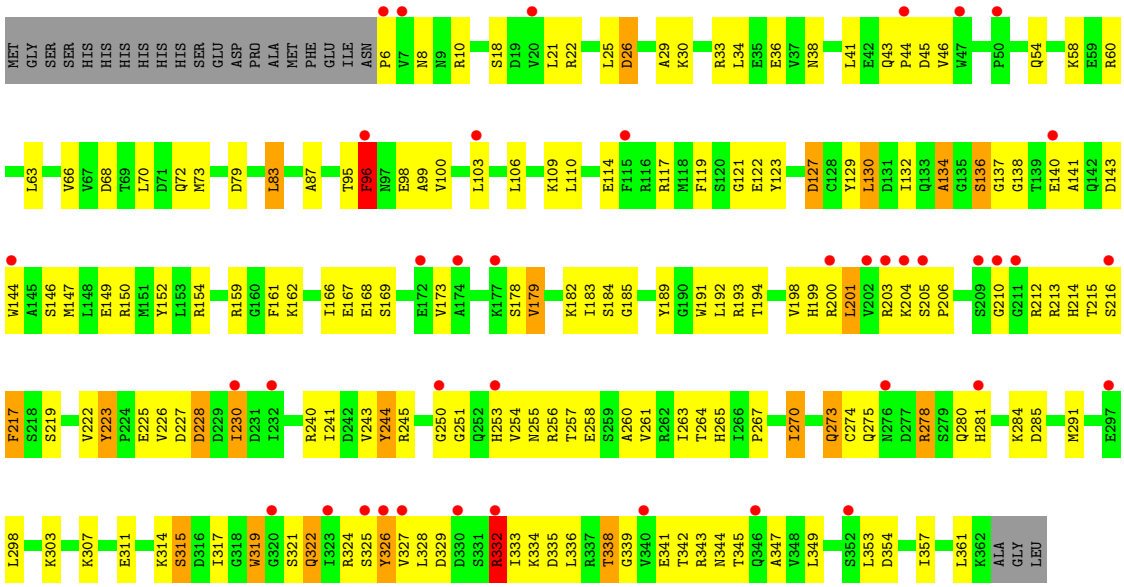
Chain QY:





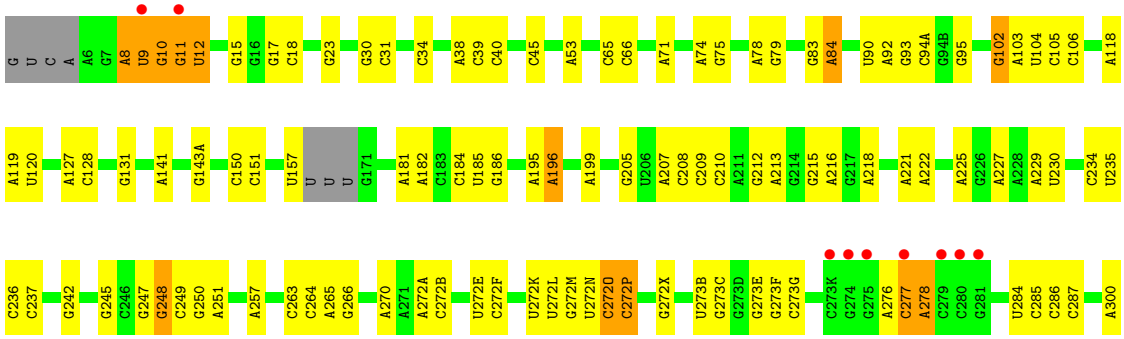
- Molecule 3: Peptide chain release factor 2

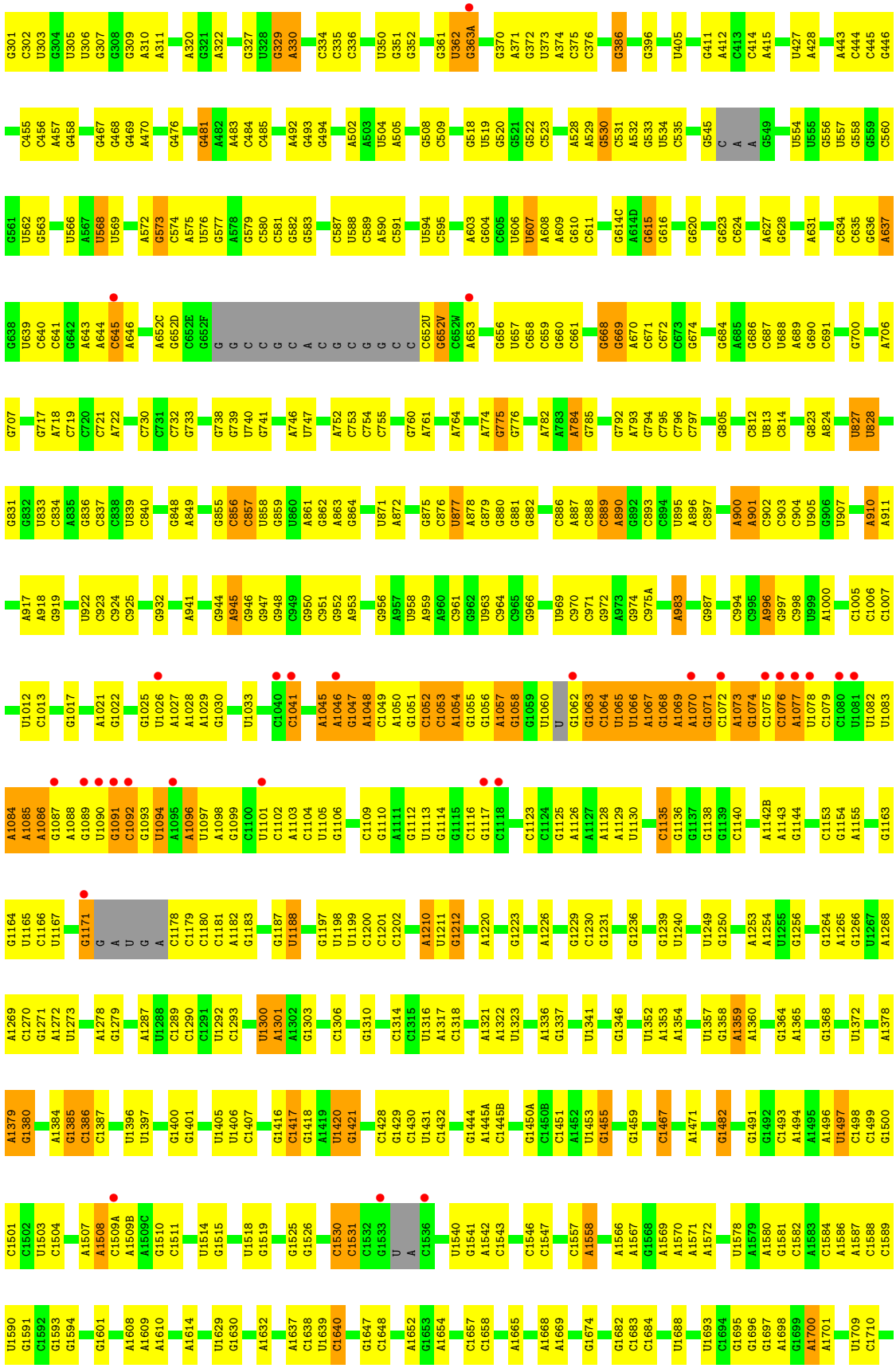
Chain XY:

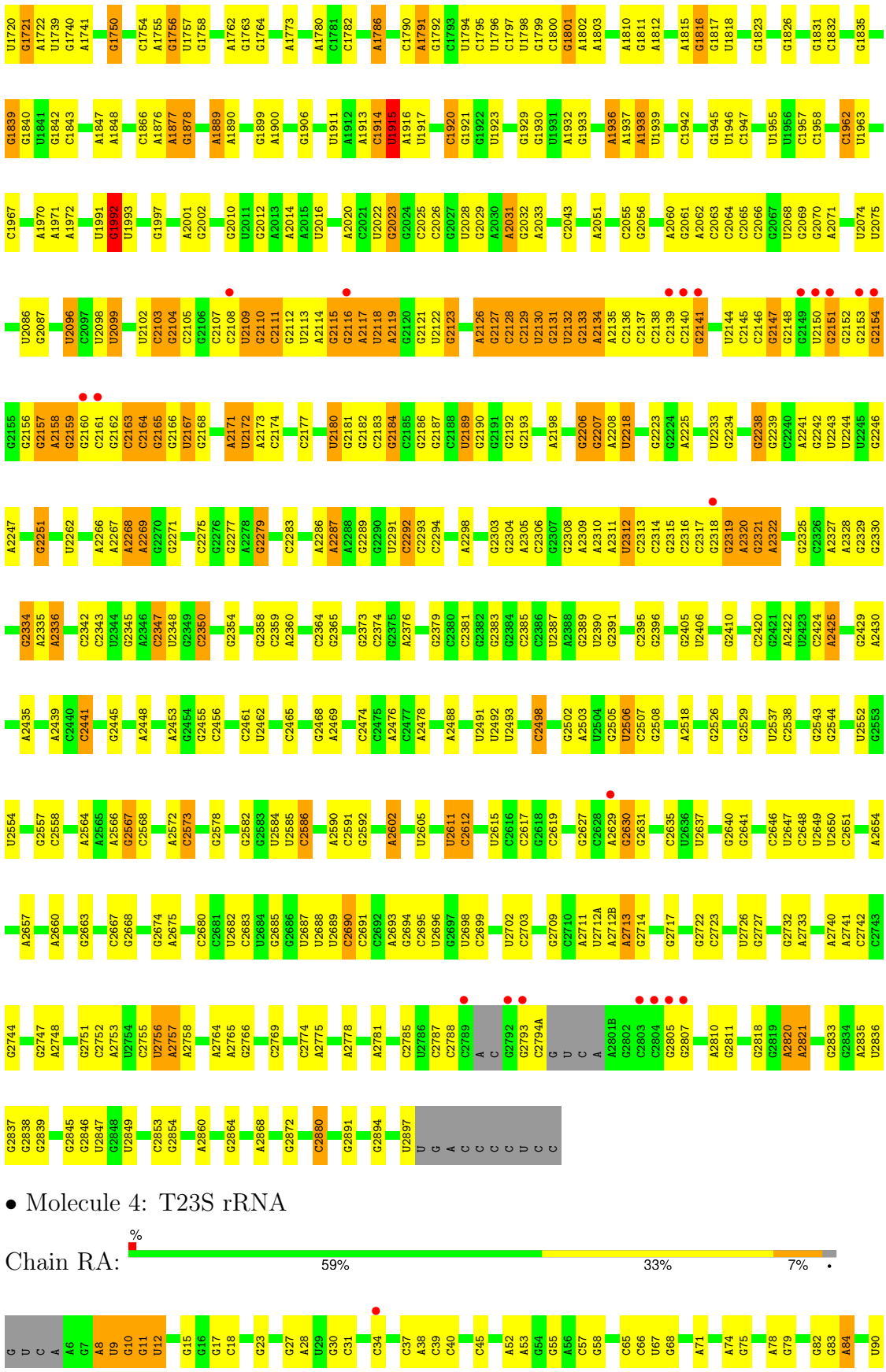


- Molecule 4: T23S rRNA

Chain YA:

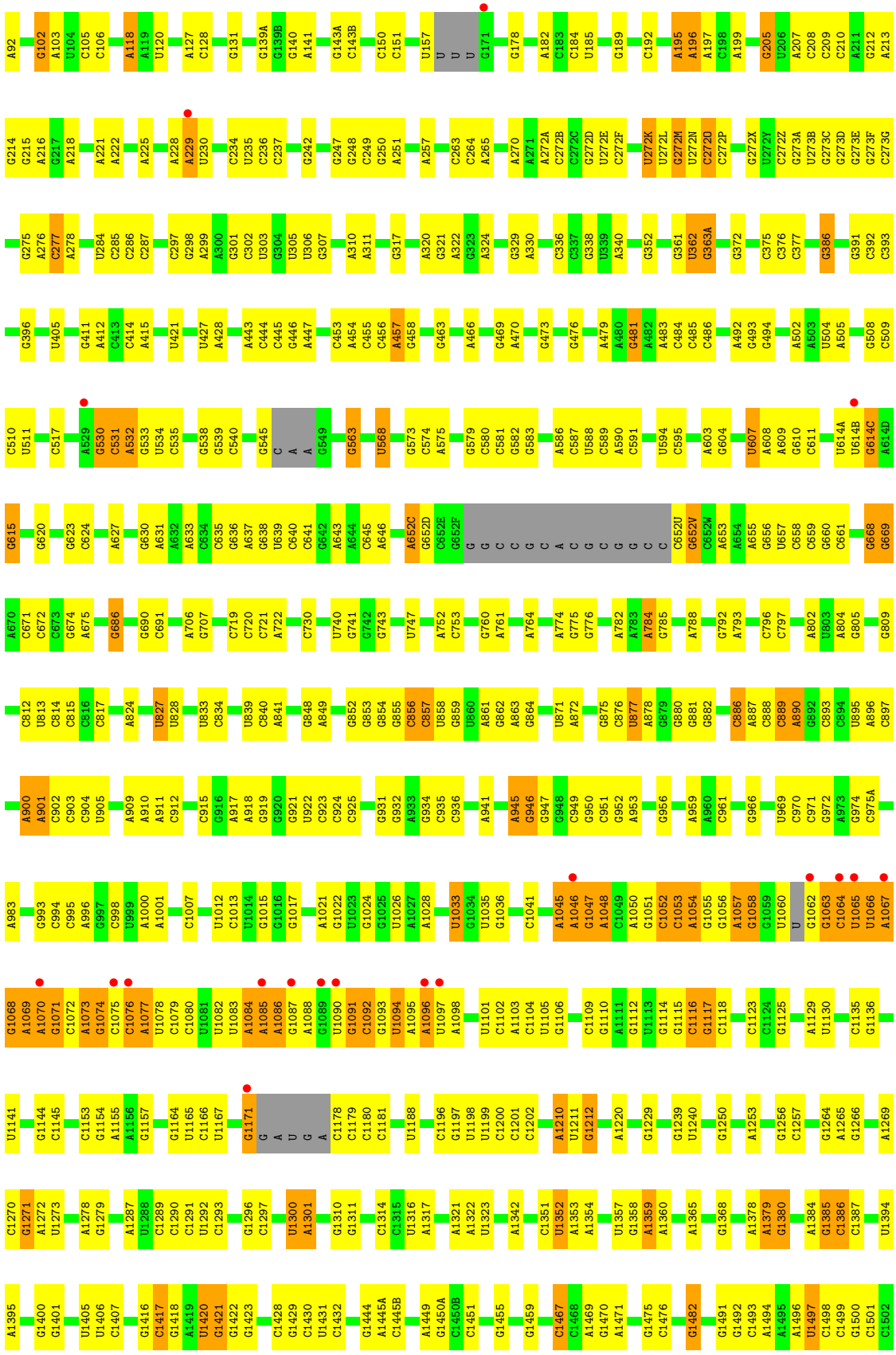


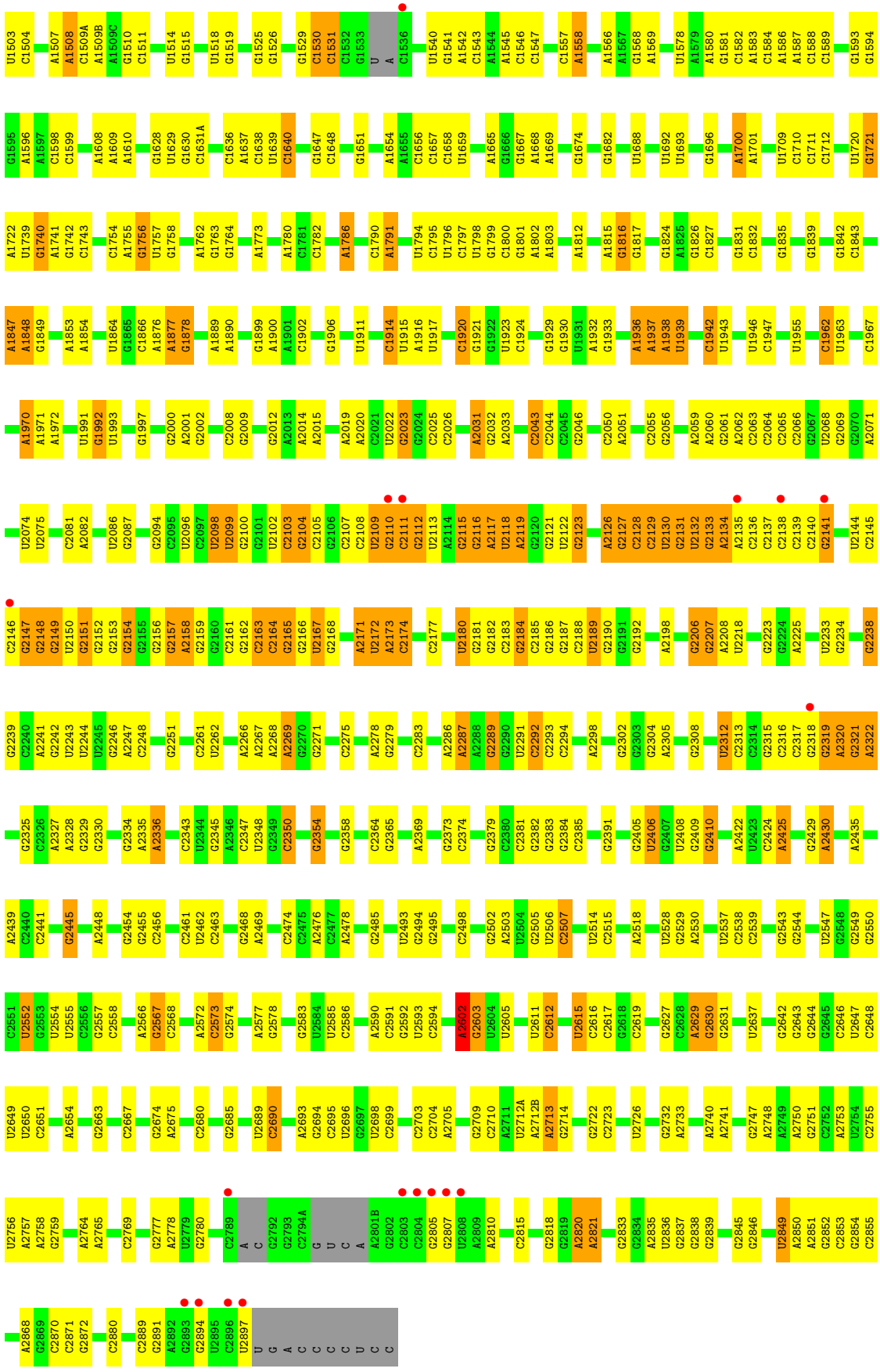

G301 C302 U303 G304 U305 U306 G307 G308 G309 A310 A311 A320 G321 A322 G327 U328 G329 A330 C334 C335 C336 U350 G351 G352 G361 U362 G363A G370 A371 G372 U373 A374 C375 C376 G386 G396 U405 G411 A412 C413 C414 A415 U427 A428 A443 C444 C445 G446
C455 C456 A457 G458 G467 G468 G469 A470 G476 G481 A482 A483 C484 C485 A492 G493 G494 A502 A503 U504 A505 G508 C509 G518 U519 G520 G521 U522 C523 A528 A529 G530 C531 A532 G533 U534 C535 G545 C A A G549 U554 U555 G556 U557 G558 G559 C560
G561 U562 G563 U566 A567 U568 U569 A572 G573 C574 A575 U576 G577 A578 G579 C580 C581 G582 G583 C587 U588 C589 A590 C591 U594 C595 A603 G604 C605 U606 U607 A608 A609 G610 C611 G614C A614D G615 G616 G620 G623 C624 A627 G628 A631 C634 C635 G636 A637
G638 U639 C640 C641 G642 A643 A644 C645 A646 A652C G652D G652E G652F G G G C C G C A C G G C G C C C652U G652V C652W A653 G656 U657 C658 G659 G660 C661 G668 G669 A670 C671 C672 G673 G674 G684 A685 G686 C687 U688 A689 G690 C691 G700 A706
G707 G717 A718 C719 C720 C721 A722 C730 C731 C732 G733 G738 G739 U740 G741 A746 U747 A752 C753 C754 C755 G760 A761 A764 A774 G775 G776 A782 A783 A784 G785 G792 A793 G794 C795 C796 C797 G805 C812 U813 C814 G823 A824 U827 U828
G831 G832 U833 C834 A835 G836 C837 G838 U839 C840 G848 A849 G855 C856 C857 U858 G859 U860 A861 G862 A863 G864 U871 A872 G875 C876 U877 A878 G879 G880 G881 G882 C886 A887 C888 C889 A890 G892 C893 C894 U895 A896 C897 A900 A901 C902 C903 C904 U905 G906 U907 A910 A911
A917 A918 G919 U922 C923 C924 C925 G932 A941 G944 A945 G946 G947 G948 C949 G950 C951 G952 A953 G956 A957 U958 A959 A960 C961 G962 U963 C964 C965 G966 U969 C970 C971 G972 A973 G974 C975A A983 G987 C994 C995 A996 G997 C998 U999 A1000 C1005 C1006 C1007
U1012 C1013 G1017 A1021 G1022 G1025 U1026 A1027 A1028 A1029 G1030 U1033 C1040 C1041 A1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 C1053 A1054 G1055 G1056 A1057 G1058 C1059 U1060 U G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 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 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 C1109 G1110 A1111 G1112 U1113 G1114 G1115 C1116 G1117 C1118 C1123 C1124 G1125 A1126 A1127 A1128 A1129 U1130 C1135 G1136 G1137 G1138 G1139 C1140 A1142B A1143 G1144 C1153 G1154 A1155 G1163
G1164 U1165 C1166 U1167 G1171 G A U G A C1178 C1179 C1180 C1181 A1182 G1183 G1187 U1188 G1197 U1198 U1199 C1200 C1201 C1202 A1210 U1211 G1212 A1220 G1223 A1226 G1229 C1230 G1231 G1236 G1239 U1240 U1249 G1250 A1253 A1254 U1255 G1256 G1264 A1265 G1266 U1267 A1268
A1269 C1270 G1271 A1272 U1273 A1278 G1279 A1287 U1288 C1289 C1290 G1291 U1292 C1293 U1300 A1301 A1302 G1303 C1306 G1310 C1314 C1315 U1316 A1317 C1318 A1321 A1322 U1323 A1336 G1337 U1341 G1346 U1352 A1353 A1354 U1357 G1358 A1359 A1360 G1364 A1365 G1368 U1372 A1378
A1379 G1380 A1384 G1385 C1386 C1387 U1396 U1397 G1400 G1401 U1405 U1406 C1407 G1416 C1417 G1418 A1419 U1420 G1421 C1428 G1429 C1430 U1431 C1432 G1444 A1445A C1445B G1450A C1450B C1451 A1452 U1453 G1455 G1459 C1467 A1471 G1482 G1491 G1492 C1493 A1494 A1495 A1496 U1497 C1498 C1499 G1500
C1501 C1502 U1503 C1504 A1507 A1508 C1509A A1509B A1509C G1510 C1511 U1514 G1515 U1518 G1519 G1525 G1526 C1530 C1531 C1532 G1533 U A C1536 U1540 G1541 A1542 C1543 C1546 C1547 C1557 A1558 A1566 A1567 G1568 A1569 A1570 A1571 A1572 U1578 A1579 A1580 G1581 C1582 A1583 C1584 A1586 A1587 C1588 C1589
U1590 G1591 C1592 G1593 G1594 G1601 A1608 A1609 A1610 A1614 U1629 G1630 A1632 A1637 C1638 U1639 C1640 G1647 C1648 A1652 G1653 A1654 C1657 C1658 A1665 A1668 A1669 G1674 G1682 C1683 C1684 U1688 U1693 C1694 G1695 G1696 G1697 A1698 G1699 A1700 A1701 U1709 C1710



• Molecule 4: T23S rRNA

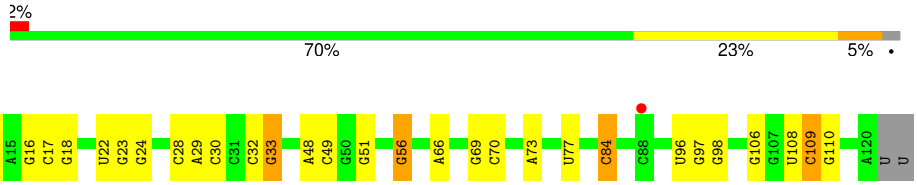
Chain RA:




U1503 C1504 A1507 A1508 C1509A A1509B A1509C G1510 C1511 U1514 G1515 U1518 G1519 G1525 G1526 G1529 C1530 C1531 C1532 G1533 U A C1536 U1540 G1541 A1542 C1543 A1544 A1545 C1546 C1547 C1557 A1558 A1566 A1567 G1568 A1569 U1578 A1579 A1580 G1581 C1582 A1583 C1584 A1586 A1587 C1588 C1589 G1593 G1594
G1595 A1596 A1597 C1598 C1599 A1608 A1609 A1610 G1628 U1629 G1630 C1631A C1636 A1637 C1638 U1639 C1640 G1647 C1648 G1651 A1654 A1655 C1656 C1657 C1658 U1659 A1665 G1666 G1667 A1668 A1669 G1674 G1682 U1688 U1692 U1693 G1696 A1700 A1701 U1709 C1710 C1711 C1712 U1720 G1721
A1722 U1739 G1740 A1741 G1742 C1743 C1754 A1755 G1756 U1757 G1758 A1762 G1763 G1764 A1773 A1780 C1781 C1782 A1786 C1790 A1791 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 A1812 A1815 G1816 G1817 G1824 A1825 G1826 C1827 G1831 C1832 G1835 G1839 G1842 C1843
A1847 A1848 G1849 A1853 A1854 U1864 G1865 C1866 A1876 A1877 G1878 A1889 A1890 G1899 A1900 A1901 C1902 G1906 U1911 C1914 U1915 A1916 U1917 C1920 G1921 G1922 U1923 C1924 G1929 G1930 U1931 A1932 G1933 A1936 A1937 A1938 U1939 C1942 U1943 U1946 C1947 U1955 C1962 U1963 C1967
A1970 A1971 A1972 U1991 G1992 U1993 G1997 G2000 A2001 G2002 C2008 G2009 G2012 A2013 A2014 A2015 A2019 A2020 C2021 U2022 G2023 G2024 C2025 C2026 A2031 G2032 A2033 C2043 C2044 C2045 G2046 C2050 A2051 C2055 G2056 A2059 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2067 U2068 G2069 G2070 A2071
U2074 U2075 C2081 A2082 U2086 G2087 G2094 C2095 U2096 C2097 U2098 U2099 G2100 C2101 U2102 C2103 G2104 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 A2126 G2127 G2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 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 A2171 U2172 A2173 C2174 C2177 U2180 G2181 G2182 C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2190 G2191 G2192 A2198 G2206 G2207 A2208 U2218 G2223 G2224 A2225 U2233 G2234 G2238
G2239 C2240 A2241 G2242 U2243 U2244 U2245 G2246 A2247 C2248 G2251 C2261 U2262 A2266 A2267 A2268 A2269 C2270 G2271 C2275 A2278 G2279 C2283 A2286 A2287 A2288 G2289 G2290 U2291 C2292 C2293 C2294 A2298 G2302 G2303 G2304 A2305 G2308 U2312 C2313 C2314 G2315 C2316 C2317 G2318 G2319 A2320 G2321 A2322
G2325 C2326 A2327 A2328 G2329 G2330 G2334 A2335 A2336 C2343 U2344 G2345 A2346 C2347 U2348 G2349 C2350 G2354 G2358 C2364 G2365 A2369 G2373 C2374 G2379 C2380 C2381 G2382 G2383 G2384 C2385 G2391 G2405 U2406 G2407 U2408 G2409 G2410 A2422 U2423 C2424 A2425 G2429 A2430 A2435
A2439 C2440 C2441 G2445 A2448 G2454 G2455 C2456 C2461 U2462 C2463 G2468 A2469 C2474 C2475 A2476 C2477 A2478 G2485 U2493 G2494 G2495 C2498 G2502 A2503 U2504 G2505 U2506 C2507 U2514 C2515 A2518 U2528 G2529 A2530 U2537 C2538 C2539 G2543 G2544 U2547 G2548 G2549 G2550
C2551 U2552 G2553 U2554 U2555 C2556 G2557 C2558 A2566 G2567 C2568 A2572 C2573 G2574 A2577 G2578 G2583 U2584 U2585 C2586 A2590 C2591 G2592 U2593 C2594 A2602 G2603 U2604 U2605 U2611 C2612 U2615 C2616 C2617 G2618 C2619 G2627 C2628 A2629 G2630 G2631 U2637 G2642 G2643 G2644 G2645 C2646 U2647 C2648
U2649 U2650 C2651 A2654 G2663 C2667 G2674 A2675 C2680 G2685 U2689 C2690 A2693 G2694 G2695 U2696 G2697 U2698 C2699 C2703 C2704 A2705 G2709 C2710 A2711 U2712A A2712B A2713 G2714 G2722 C2723 U2726 G2732 A2733 A2740 A2741 G2747 A2748 A2749 A2750 G2751 C2752 A2753 U2754 C2755
U2756 A2757 A2758 G2759 A2764 A2765 C2769 G2777 A2778 U2779 G2780 C2789 A C G2792 G2793 C2794A G C C C A A2801B G2802 C2803 C2804 C2805 G2807 U2808 A2809 A2810 C2815 G2818 G2819 A2820 A2821 G2833 G2834 A2835 U2836 G2837 G2838 G2839 G2845 G2846 U2849 A2850 A2851 C2852 C2853 G2854 C2855
A2868 G2869 C2870 C2871 G2872 C2880 C2889 G2891 A2892 G2893 G2894 U2895 C2896 U2897 U G A C C C C U C C

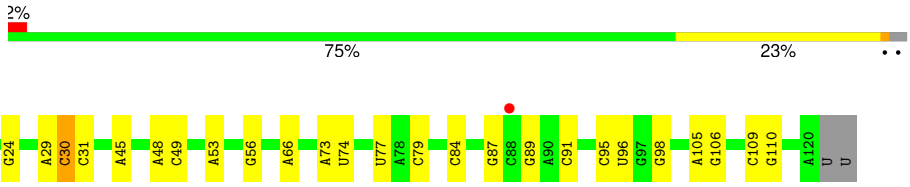
• Molecule 5: 5S rRNA

Chain YB:



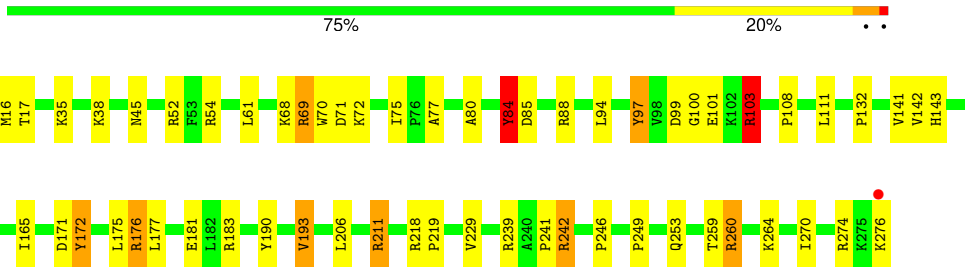
• Molecule 5: 5S rRNA

Chain RB:



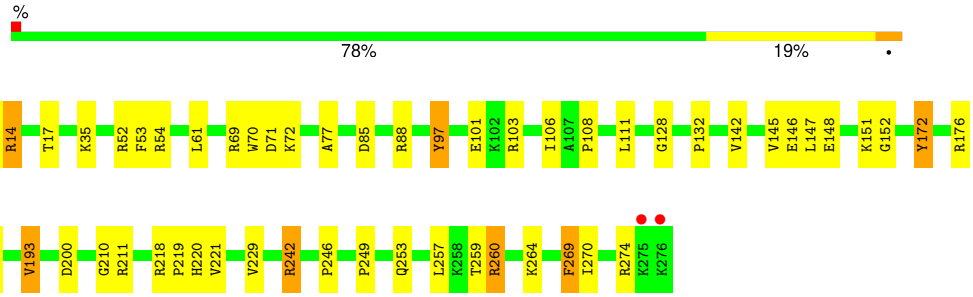
• Molecule 6: 50S ribosomal protein L2

Chain YD:



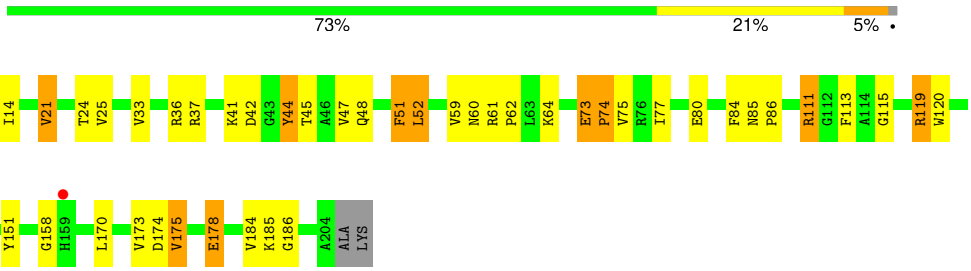
• Molecule 6: 50S ribosomal protein L2

Chain RD:



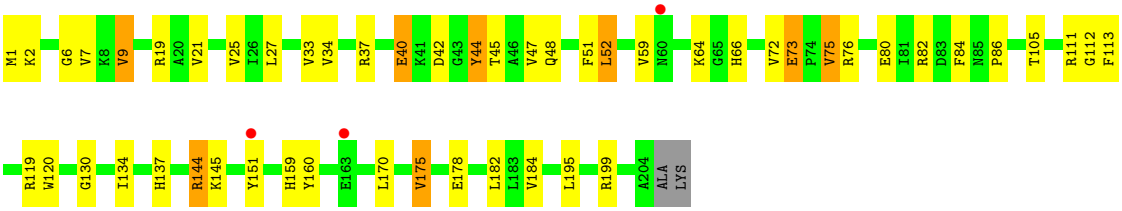
• Molecule 7: 50S ribosomal protein L3

Chain YE:



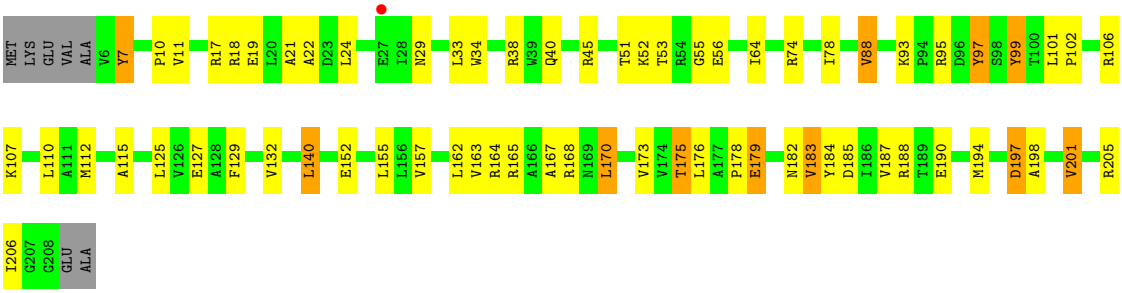
• Molecule 7: 50S ribosomal protein L3

Chain RE:



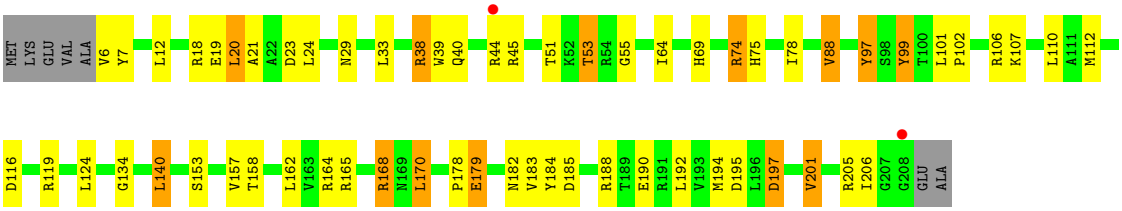
• Molecule 8: 50S ribosomal protein L4

Chain YF:



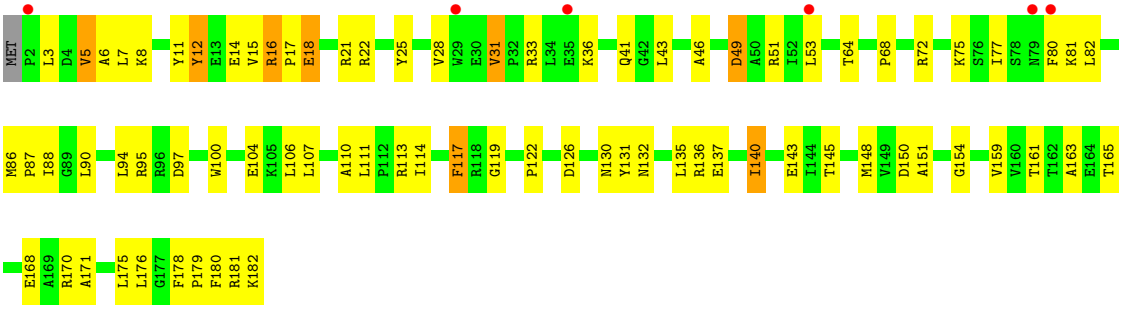
• Molecule 8: 50S ribosomal protein L4

Chain RF:



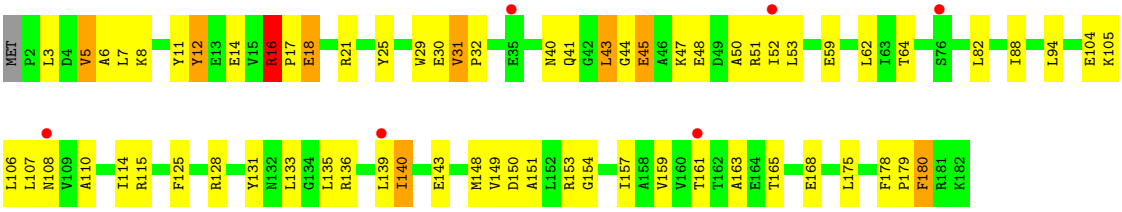
• Molecule 9: 50S ribosomal protein L5

Chain YG:



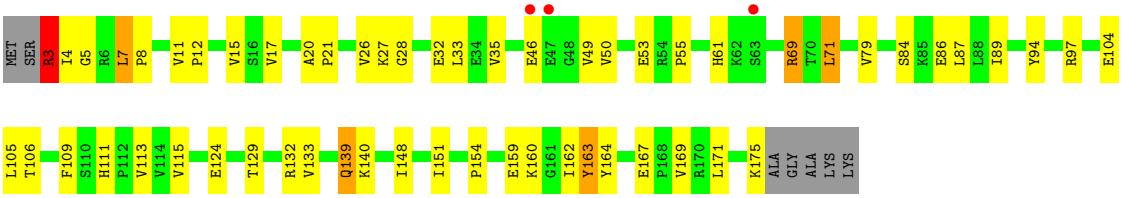
• Molecule 9: 50S ribosomal protein L5

Chain RG:



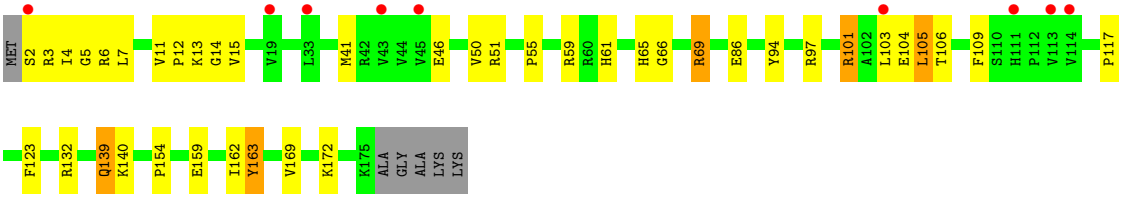
- Molecule 10: 50S ribosomal protein L6

Chain YH:



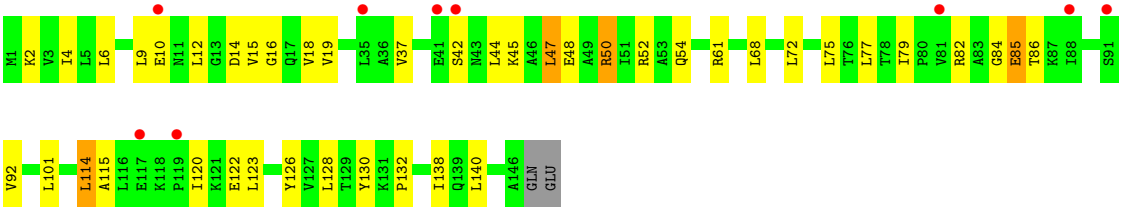
- Molecule 10: 50S ribosomal protein L6

Chain RH:



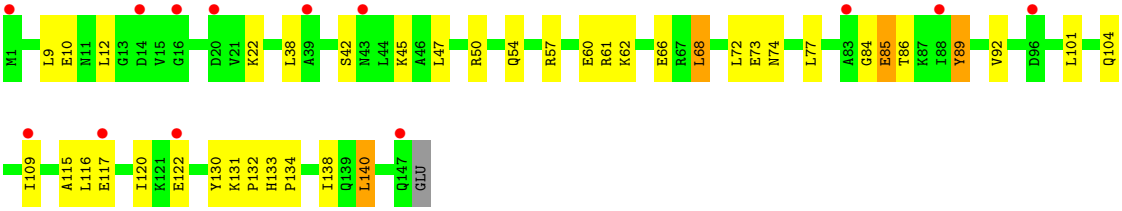
- Molecule 11: 50S ribosomal protein L9

Chain YI:



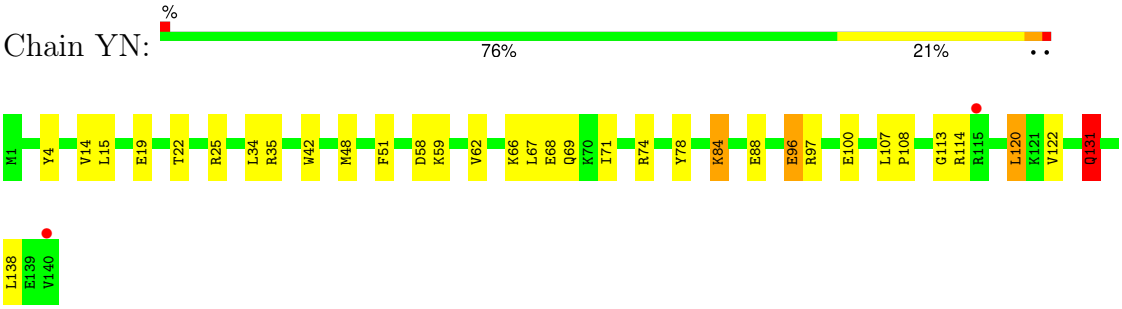
- Molecule 11: 50S ribosomal protein L9

Chain RI:



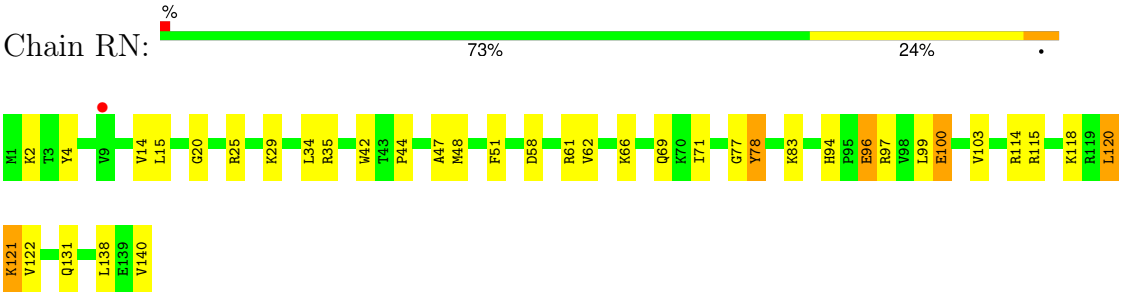
• Molecule 12: 50S ribosomal protein L13

Chain YN:



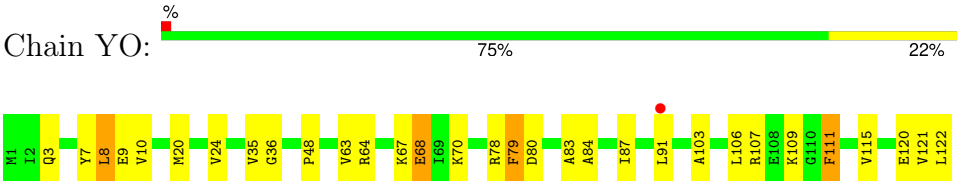
• Molecule 12: 50S ribosomal protein L13

Chain RN:



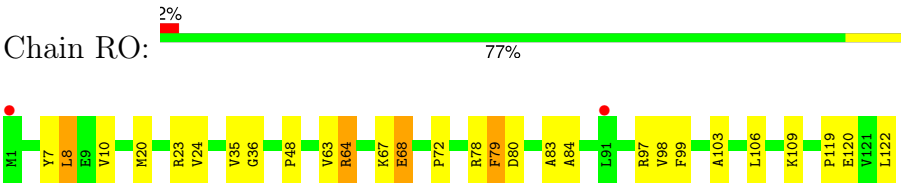
• Molecule 13: 50S ribosomal protein L14

Chain YO:



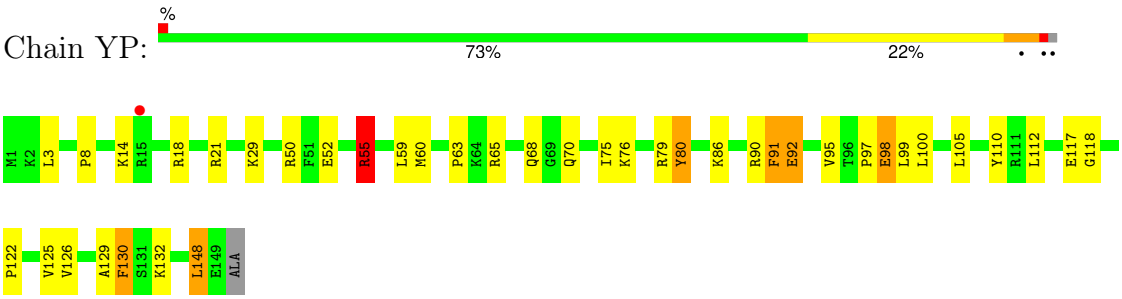
• Molecule 13: 50S ribosomal protein L14

Chain RO:



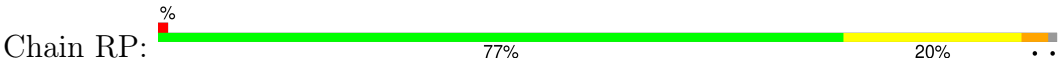
• Molecule 14: 50S ribosomal protein L15

Chain YP:



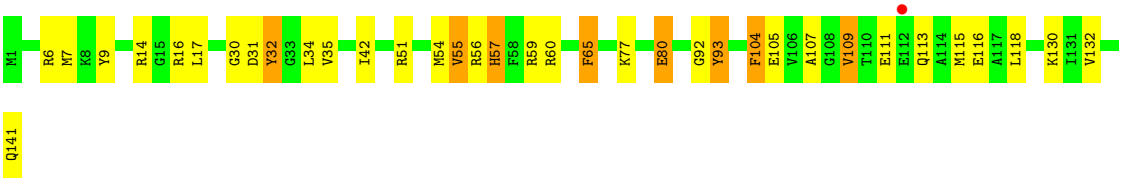
• Molecule 14: 50S ribosomal protein L15

Chain RP:



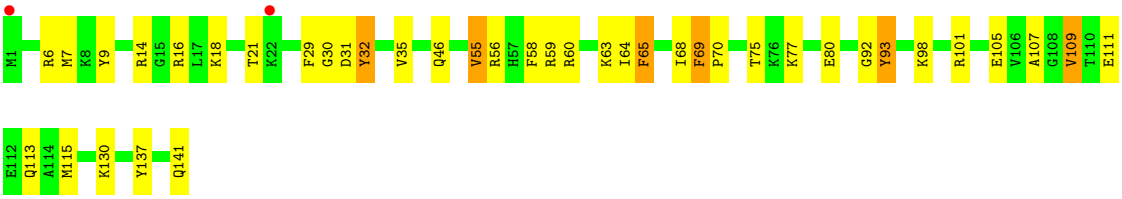
• Molecule 15: 50S ribosomal protein L16

Chain YQ:



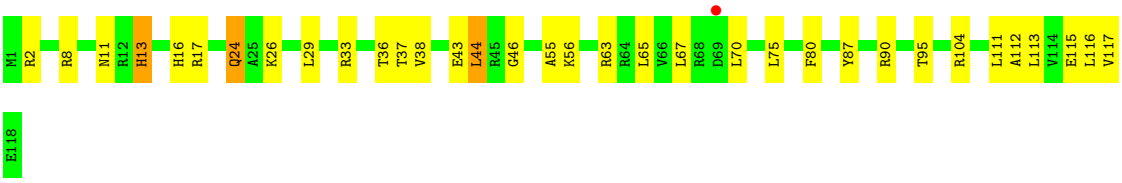
• Molecule 15: 50S ribosomal protein L16

Chain RQ:



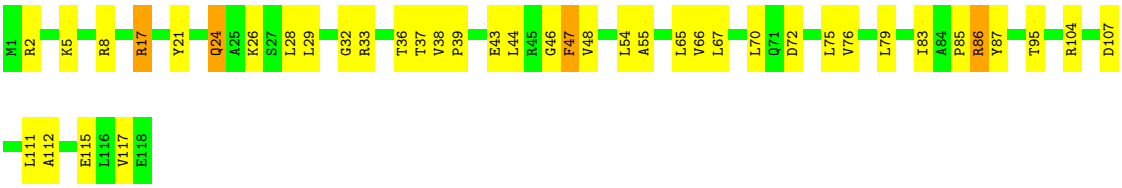
• Molecule 16: 50S ribosomal protein L17

Chain YR:



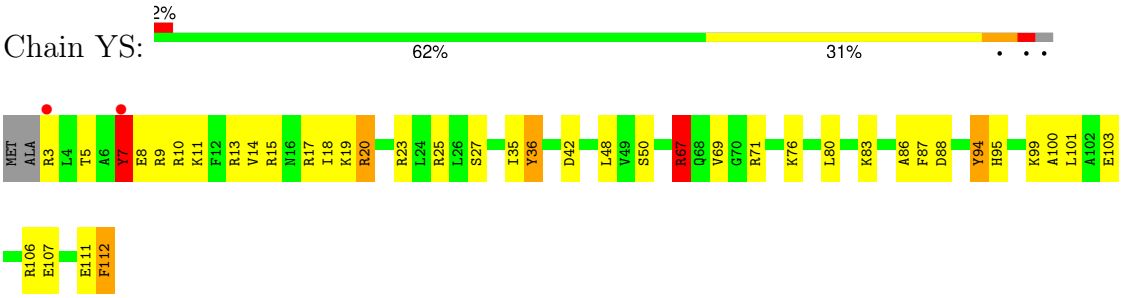
• Molecule 16: 50S ribosomal protein L17

Chain RR:



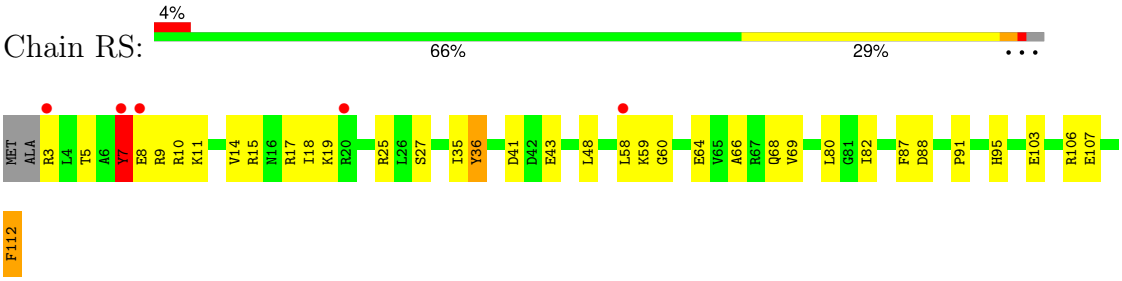
• Molecule 17: 50S ribosomal protein L18

Chain YS:



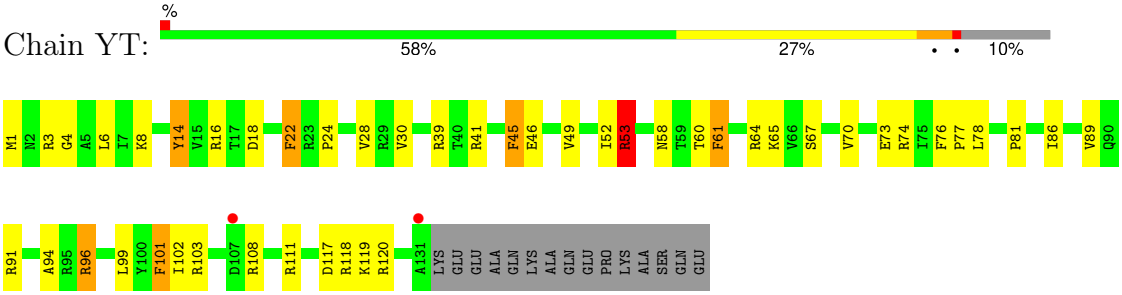
• Molecule 17: 50S ribosomal protein L18

Chain RS:



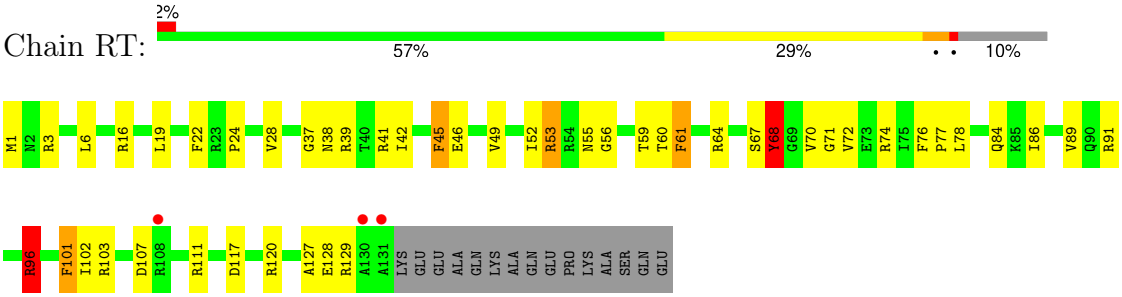
• Molecule 18: 50S ribosomal protein L19

Chain YT:



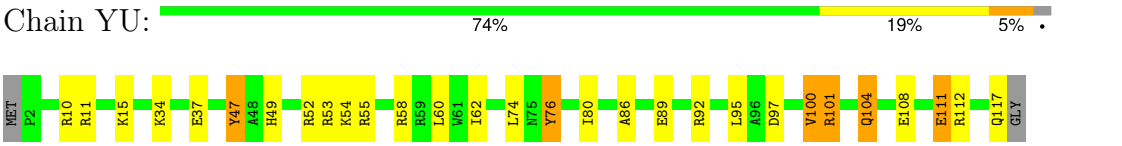
• Molecule 18: 50S ribosomal protein L19

Chain RT:



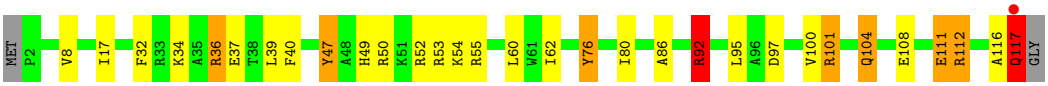
• Molecule 19: 50S ribosomal protein L20

Chain YU:



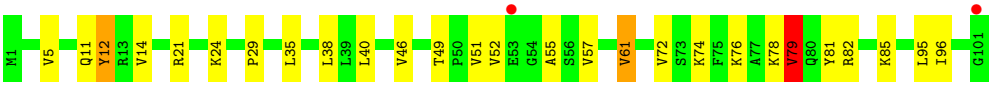
• Molecule 19: 50S ribosomal protein L20

Chain RU:



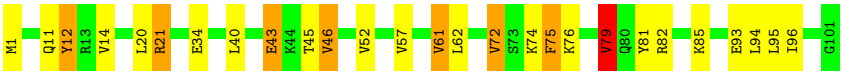
• Molecule 20: 50S ribosomal protein L21

Chain YV:



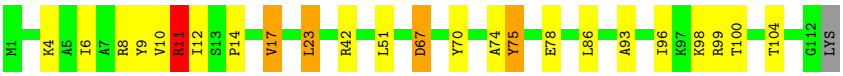
• Molecule 20: 50S ribosomal protein L21

Chain RV:



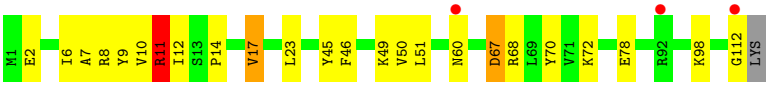
• Molecule 21: 50S ribosomal protein L22

Chain YW:



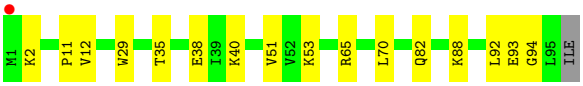
• Molecule 21: 50S ribosomal protein L22

Chain RW:



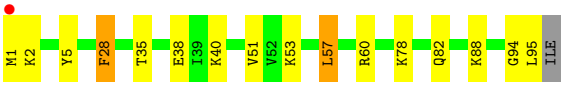
• Molecule 22: 50S ribosomal protein L23

Chain YX:



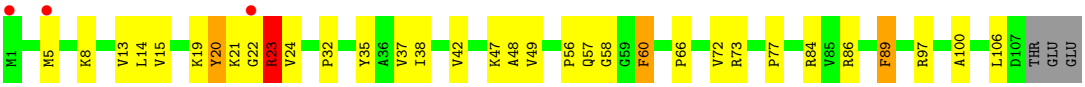
• Molecule 22: 50S ribosomal protein L23

Chain RX:



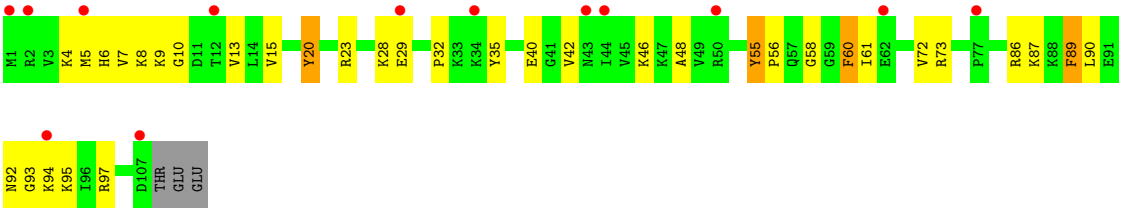
• Molecule 23: 50S ribosomal protein L24

Chain YY:



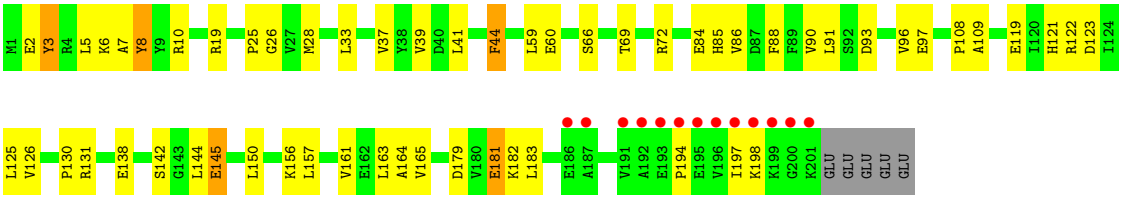
• Molecule 23: 50S ribosomal protein L24

Chain RY:



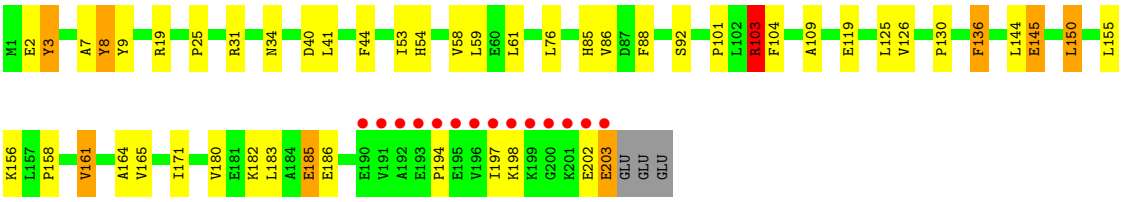
• Molecule 24: 50S ribosomal protein L25

Chain YZ:



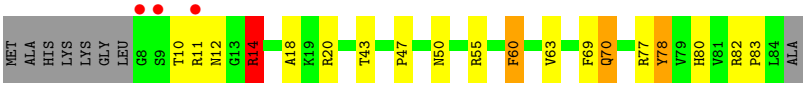
• Molecule 24: 50S ribosomal protein L25

Chain RZ:



• Molecule 25: 50S ribosomal protein L27

Chain Y0:

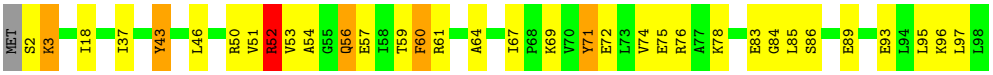


• Molecule 25: 50S ribosomal protein L27

Chain R0:

• Molecule 26: 50S ribosomal protein L28

Chain Y1:

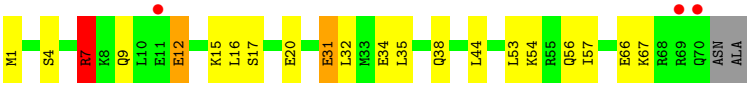


• Molecule 26: 50S ribosomal protein L28

Chain R1:

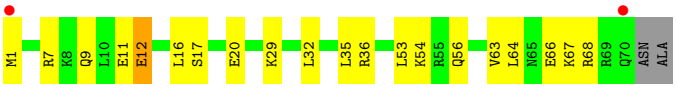
• Molecule 27: 50S ribosomal protein L29

Chain Y2:



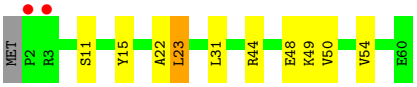
• Molecule 27: 50S ribosomal protein L29

Chain R2:



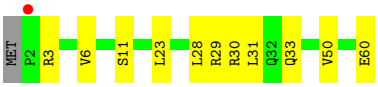
• Molecule 28: 50S ribosomal protein L30

Chain Y3:



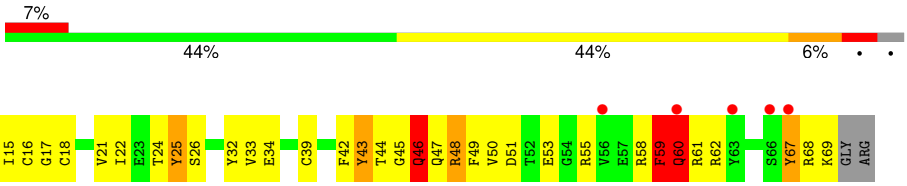
• Molecule 28: 50S ribosomal protein L30

Chain R3:



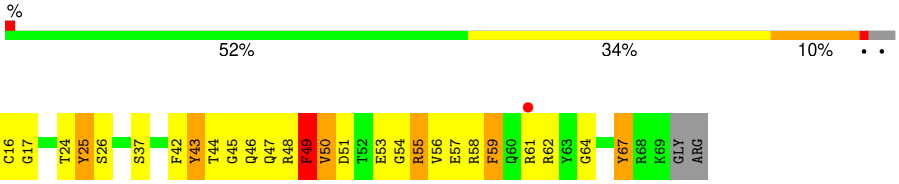
• Molecule 29: 50S ribosomal protein L31

Chain Y4:



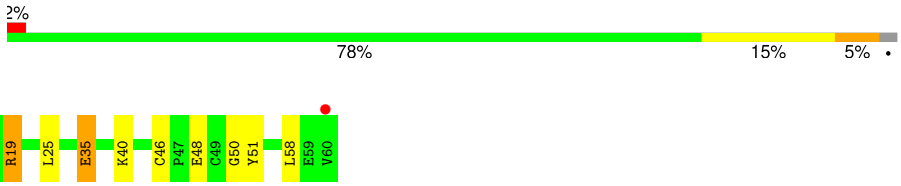
• Molecule 29: 50S ribosomal protein L31

Chain R4:



• Molecule 30: 50S ribosomal protein L32

Chain Y5:

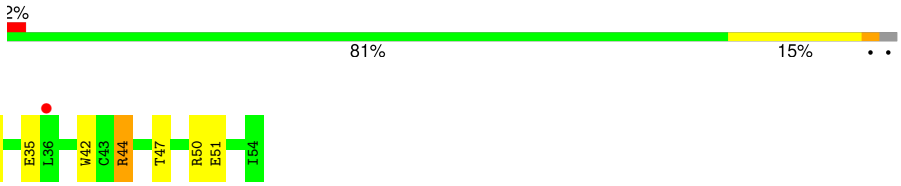


• Molecule 30: 50S ribosomal protein L32

Chain R5:

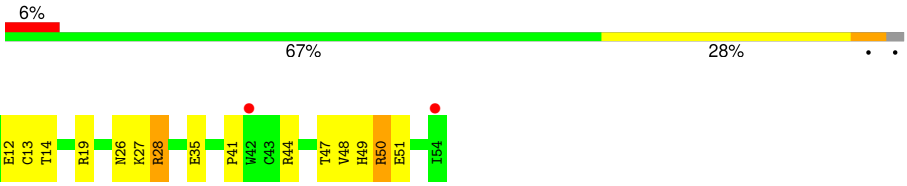
• Molecule 31: 50S ribosomal protein L33

Chain Y6:



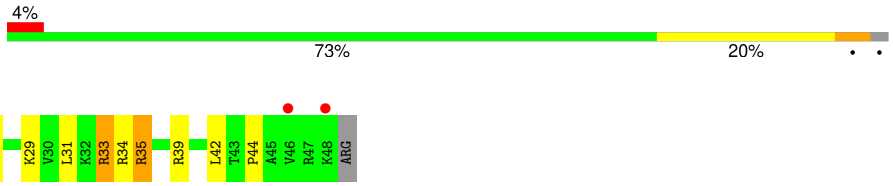
• Molecule 31: 50S ribosomal protein L33

Chain R6:



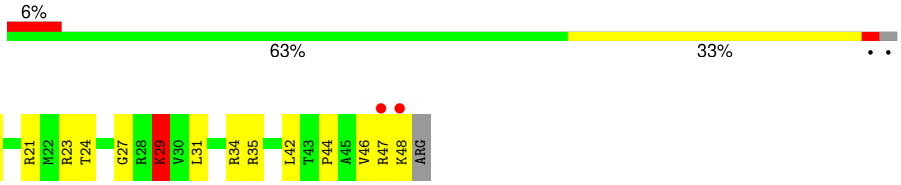
• Molecule 32: 50S ribosomal protein L34

Chain Y7:



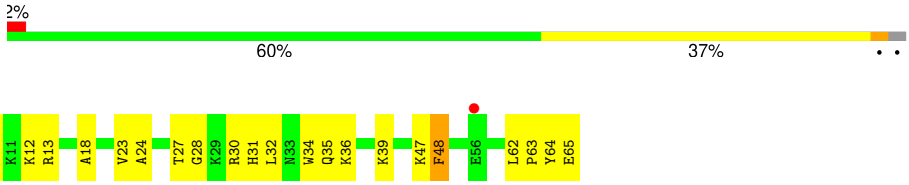
• Molecule 32: 50S ribosomal protein L34

Chain R7:



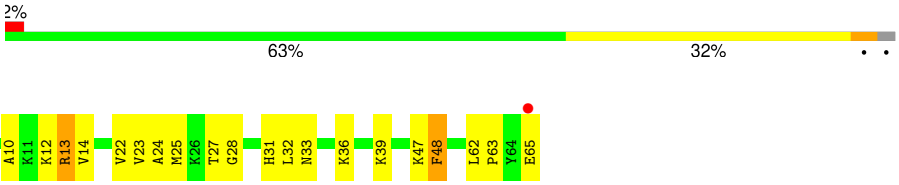
• Molecule 33: 50S ribosomal protein L35

Chain Y8:



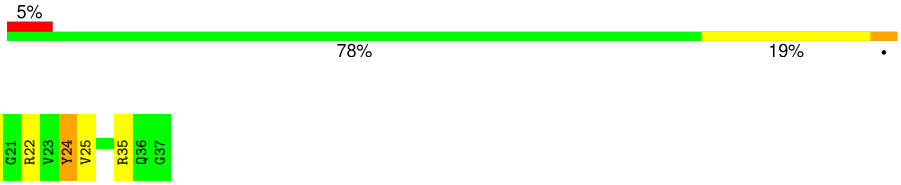
• Molecule 33: 50S ribosomal protein L35

Chain R8:



• Molecule 34: 50S ribosomal protein L36

Chain Y9:

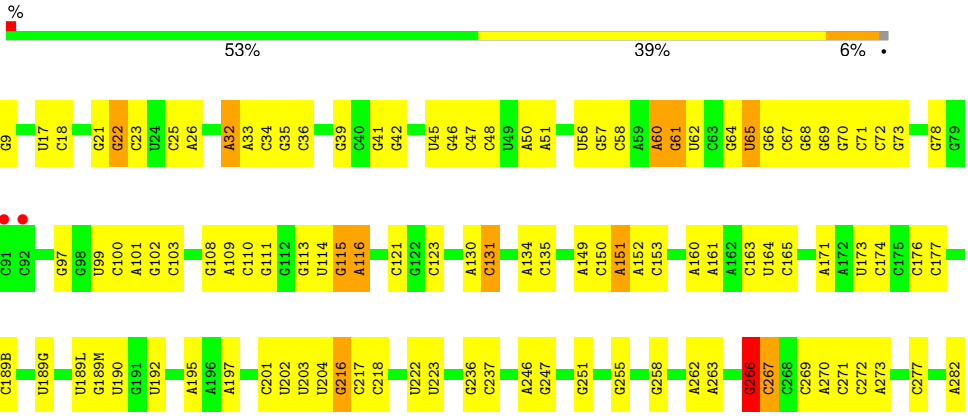


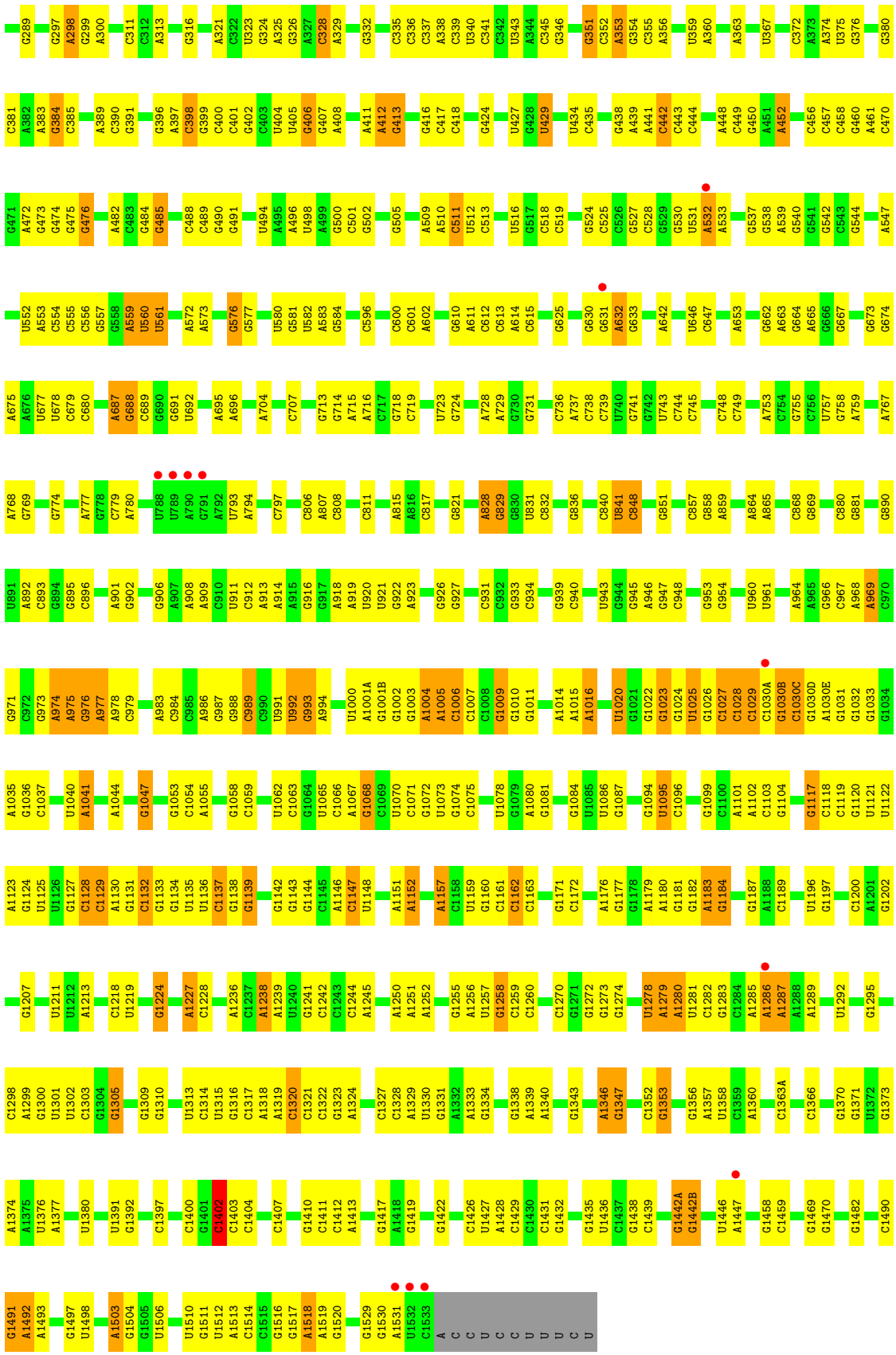
• Molecule 34: 50S ribosomal protein L36

Chain R9:

• Molecule 35: 16S rRNA

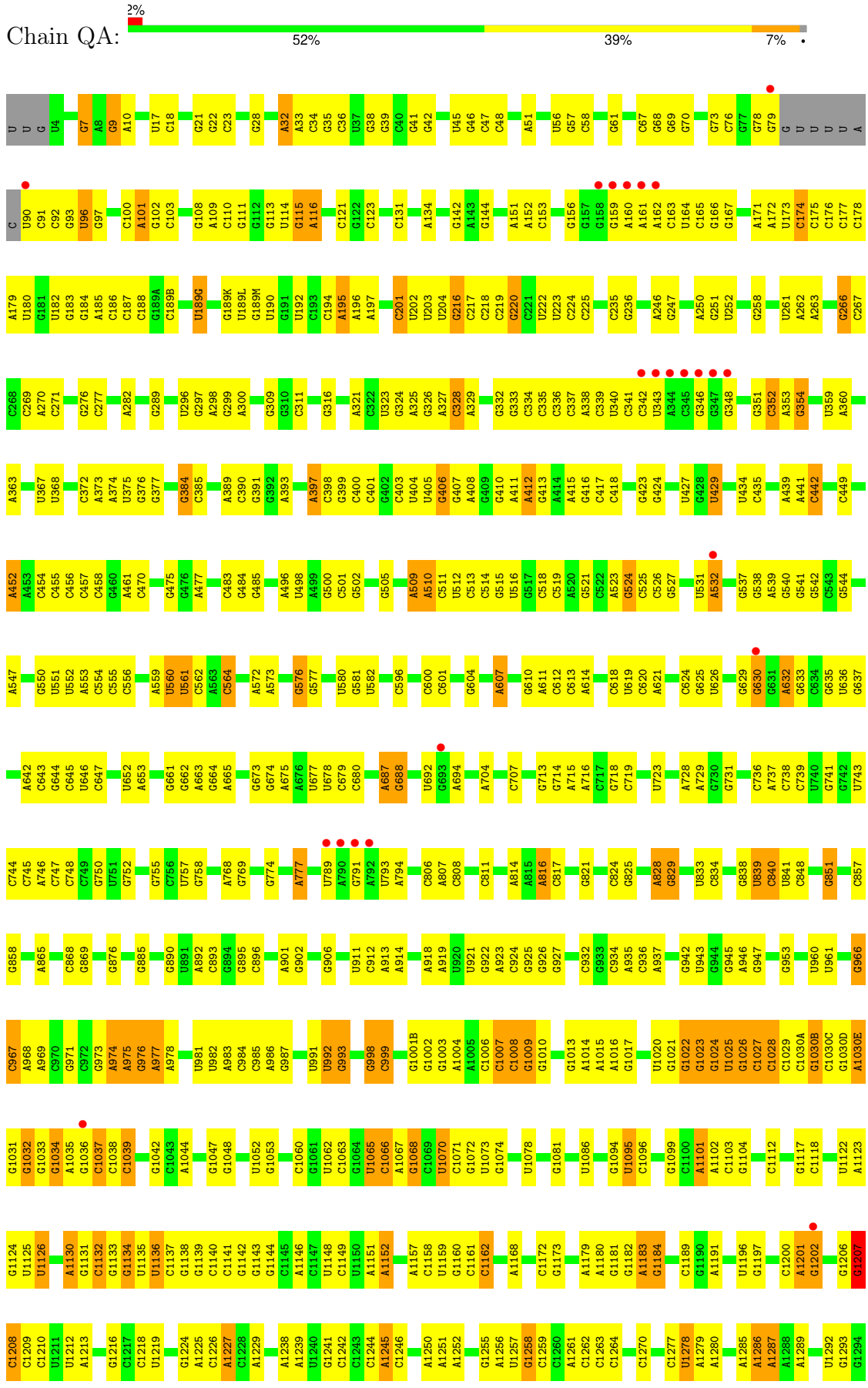
Chain XA:

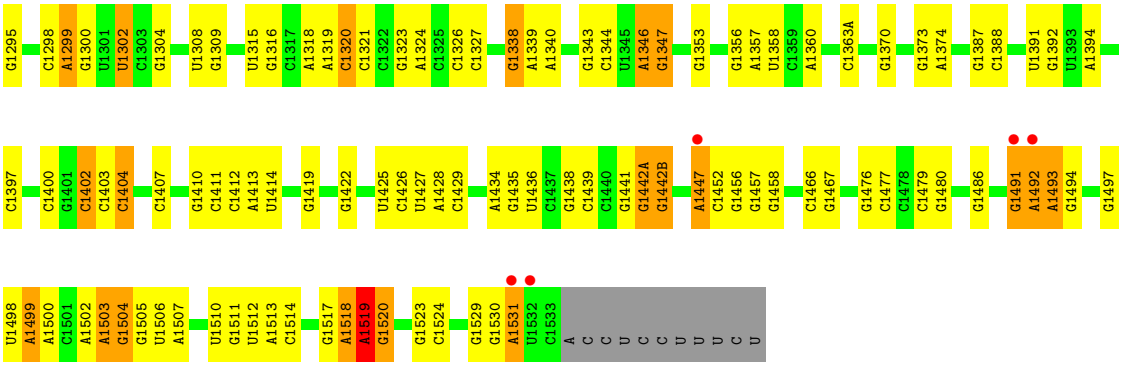




- Molecule 35: 16S rRNA

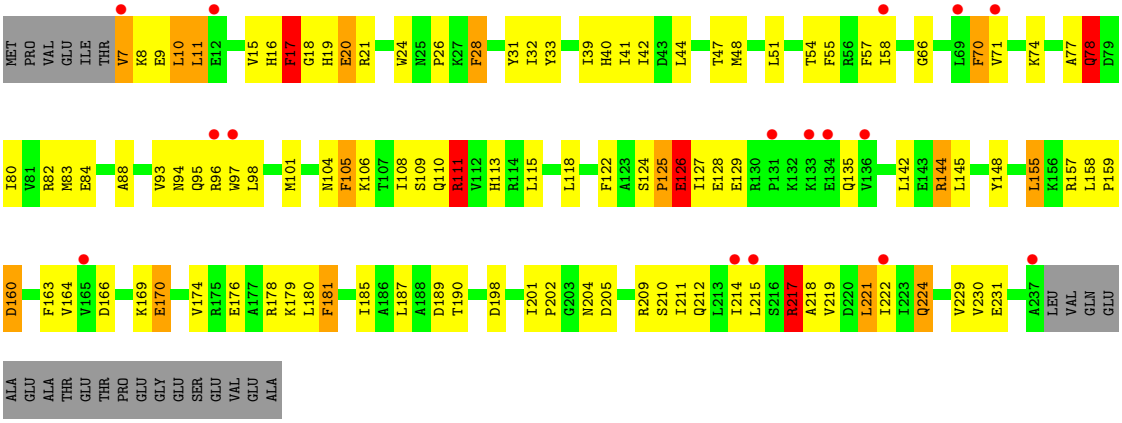
Chain QA:





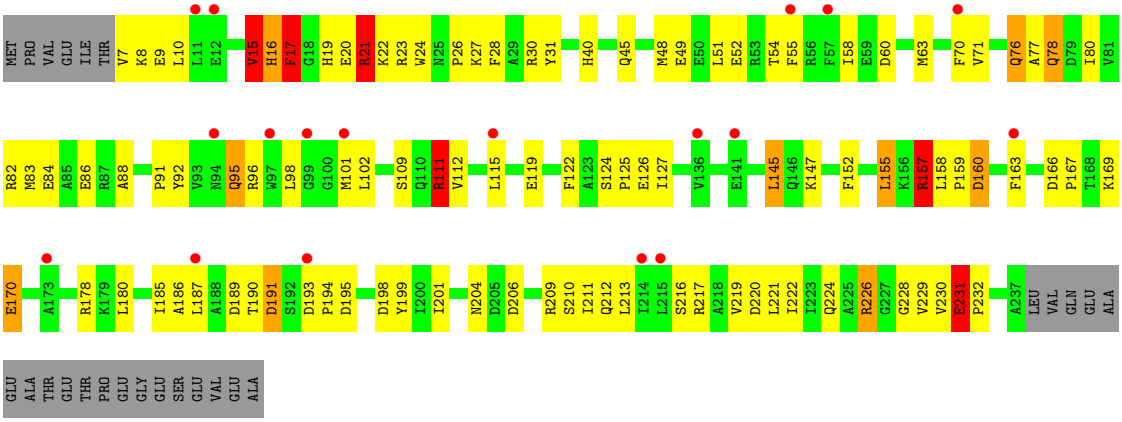
• Molecule 36: 30S ribosomal protein S2

Chain XB:



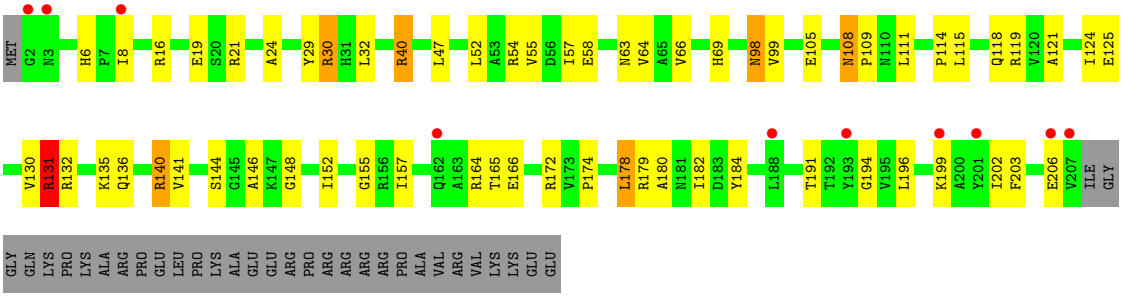
• Molecule 36: 30S ribosomal protein S2

Chain QB:



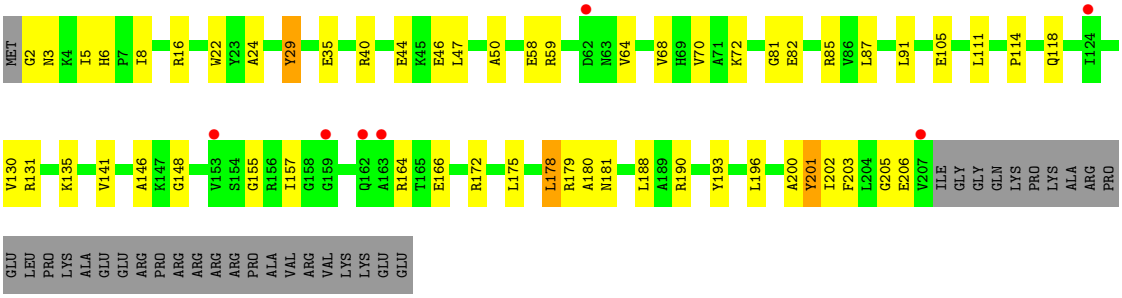
• Molecule 37: 30S ribosomal protein S3

Chain XC:



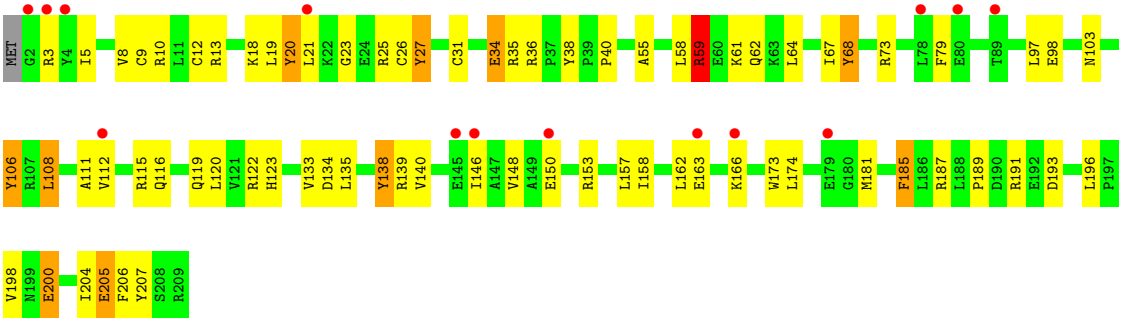
- Molecule 37: 30S ribosomal protein S3

Chain QC:



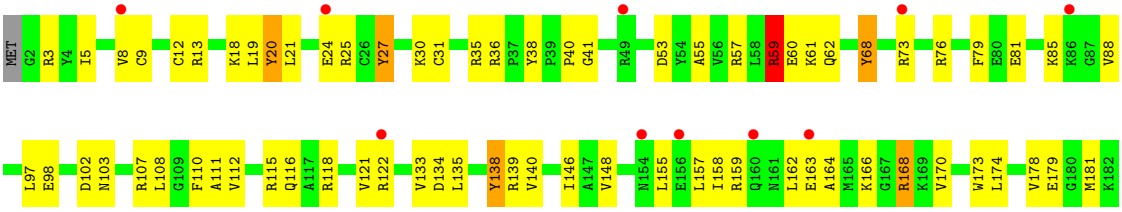
- Molecule 38: 30S ribosomal protein S4

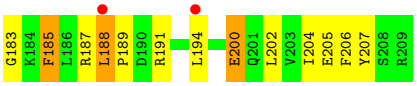
Chain XD:



- Molecule 38: 30S ribosomal protein S4

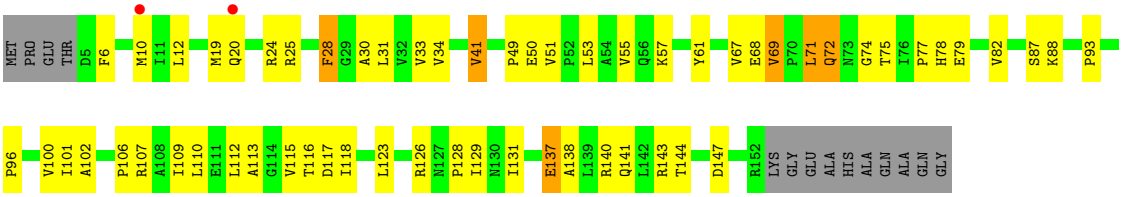
Chain QD:





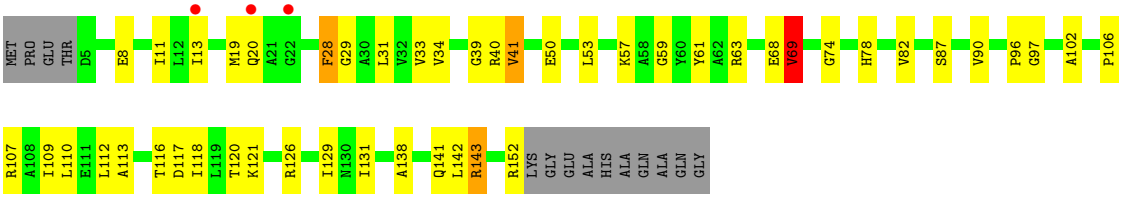
• Molecule 39: 30S ribosomal protein S5

Chain XE:



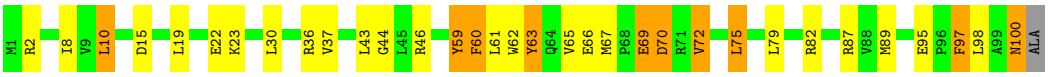
• Molecule 39: 30S ribosomal protein S5

Chain QE:



• Molecule 40: 30S ribosomal protein S6

Chain XF:

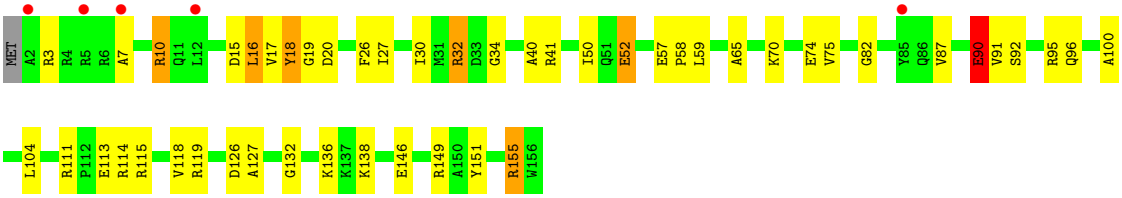


• Molecule 40: 30S ribosomal protein S6

Chain QF:

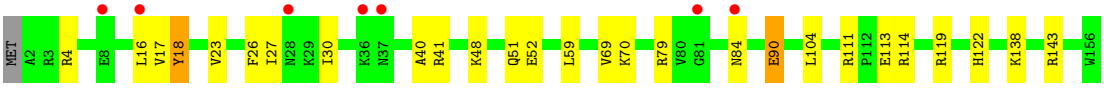
• Molecule 41: 30S ribosomal protein S7

Chain XG:



• Molecule 41: 30S ribosomal protein S7

Chain QG:

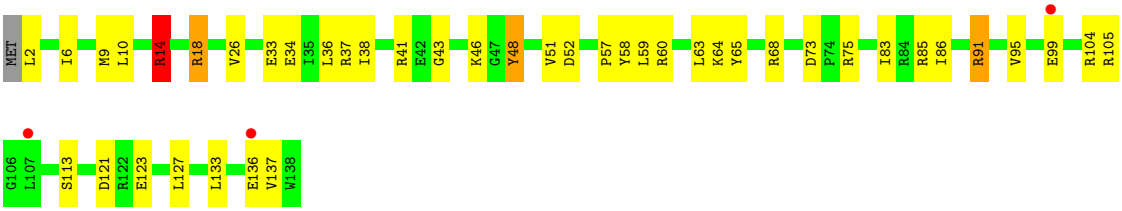


• Molecule 42: 30S ribosomal protein S8

Chain XH:

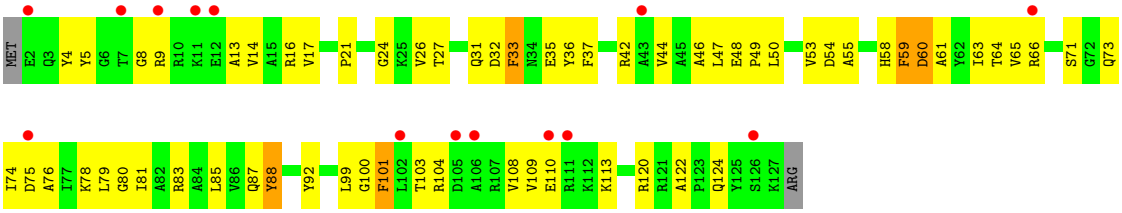
• Molecule 42: 30S ribosomal protein S8

Chain QH:



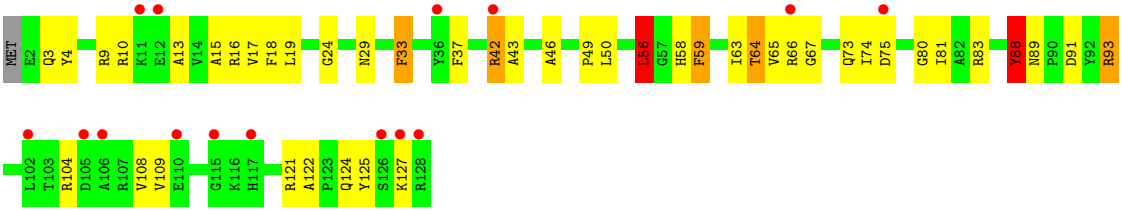
• Molecule 43: 30S ribosomal protein S9

Chain XI:



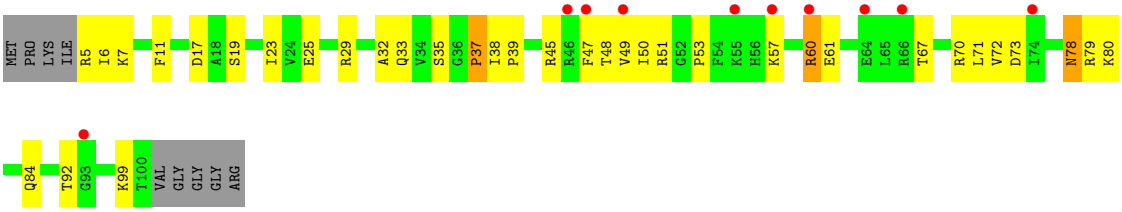
• Molecule 43: 30S ribosomal protein S9

Chain QI:



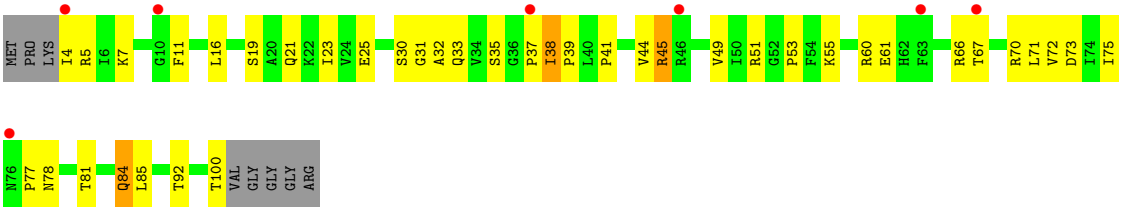
• Molecule 44: 30S ribosomal protein S10

Chain XJ:



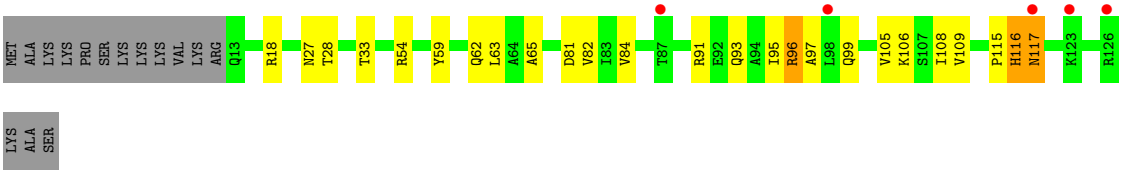
• Molecule 44: 30S ribosomal protein S10

Chain QJ:



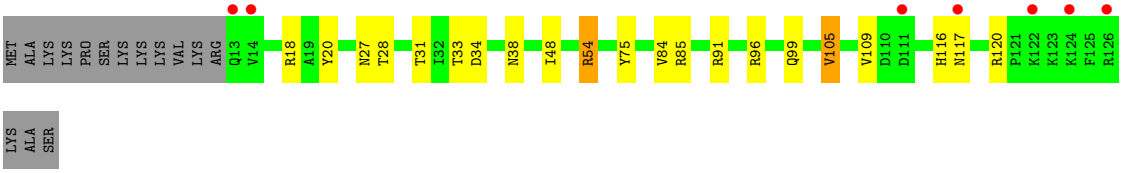
• Molecule 45: 30S ribosomal protein S11

Chain XK:



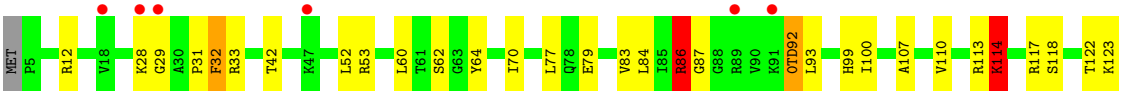
• Molecule 45: 30S ribosomal protein S11

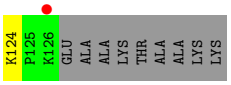
Chain QK:



• Molecule 46: 30S ribosomal protein S12

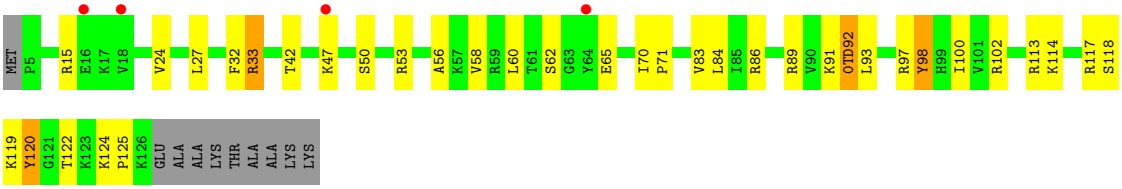
Chain XL:





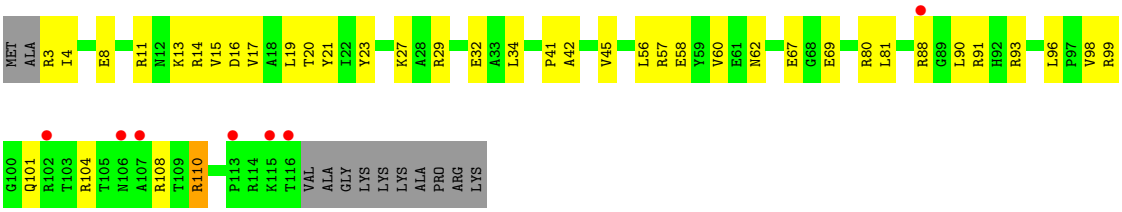
• Molecule 46: 30S ribosomal protein S12

Chain QL:



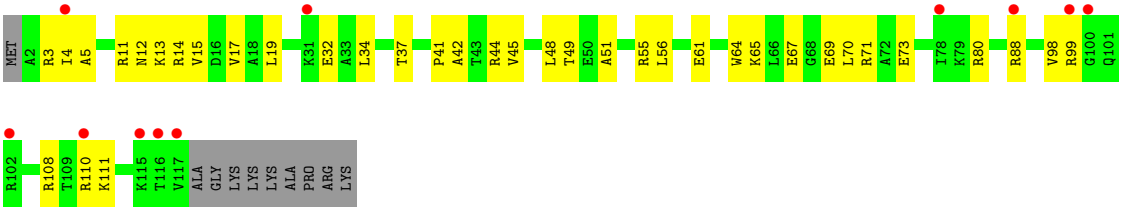
• Molecule 47: 30S ribosomal protein S13

Chain XM:



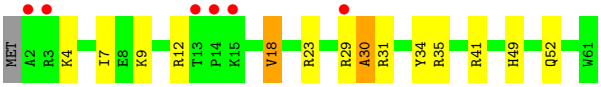
• Molecule 47: 30S ribosomal protein S13

Chain QM:



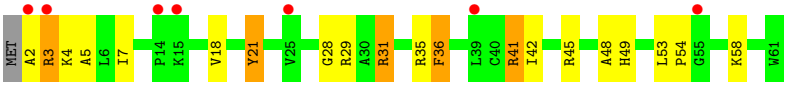
• Molecule 48: 30S ribosomal protein S14 type Z

Chain XN:



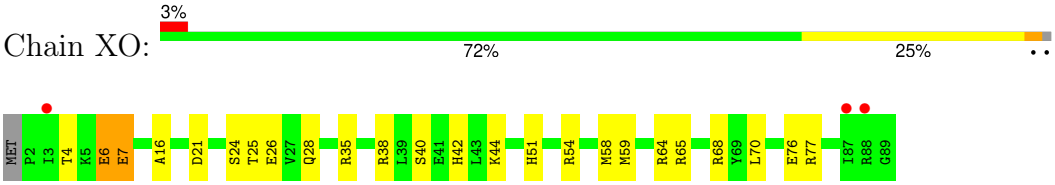
• Molecule 48: 30S ribosomal protein S14 type Z

Chain QN:



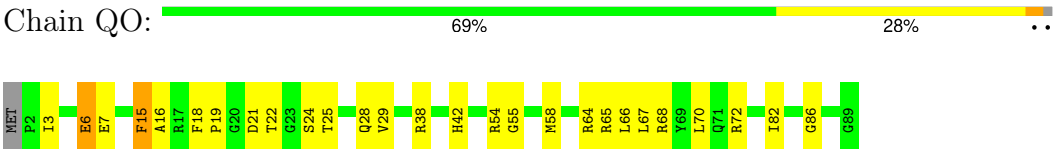
• Molecule 49: 30S ribosomal protein S15

Chain XO:



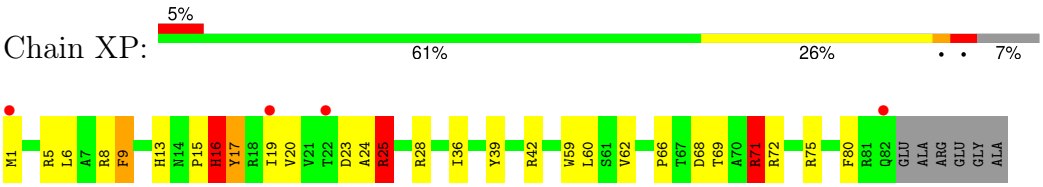
• Molecule 49: 30S ribosomal protein S15

Chain QO:



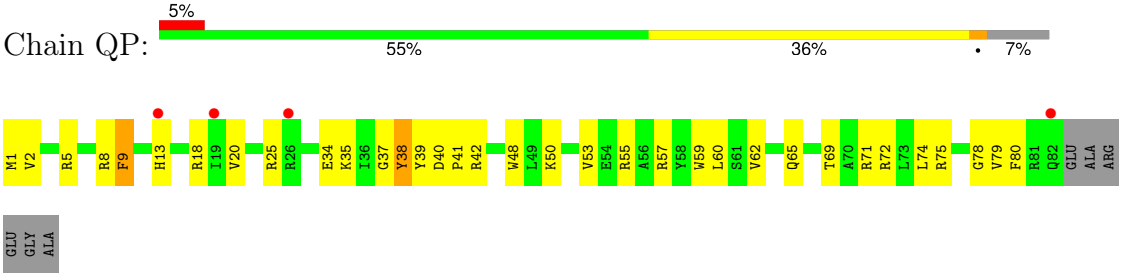
• Molecule 50: 30S ribosomal protein S16

Chain XP:



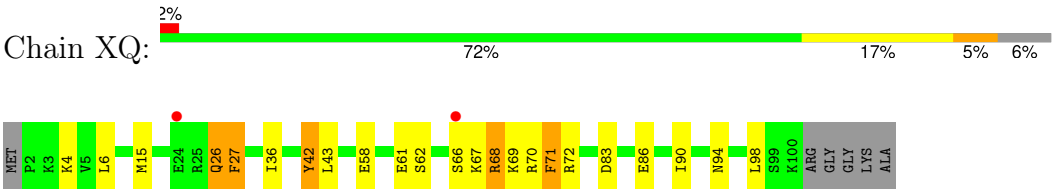
• Molecule 50: 30S ribosomal protein S16

Chain QP:



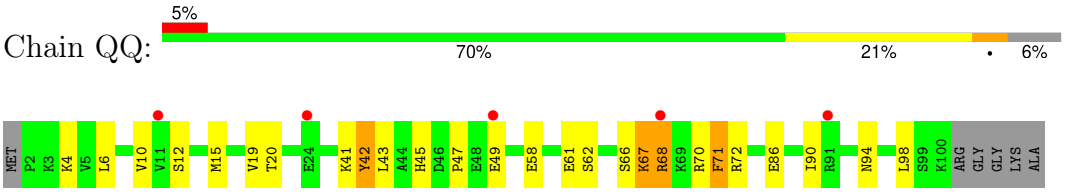
• Molecule 51: 30S ribosomal protein S17

Chain XQ:



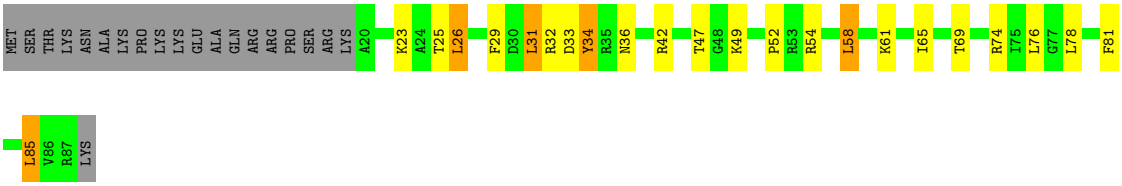
• Molecule 51: 30S ribosomal protein S17

Chain QQ:



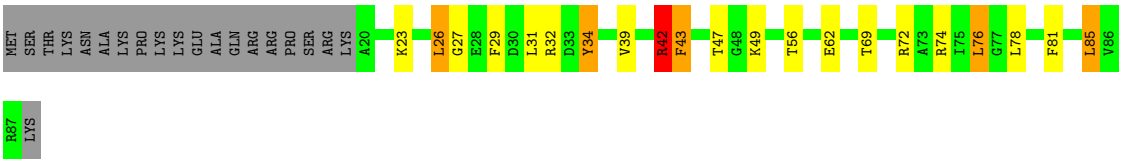
• Molecule 52: 30S ribosomal protein S18

Chain XR:



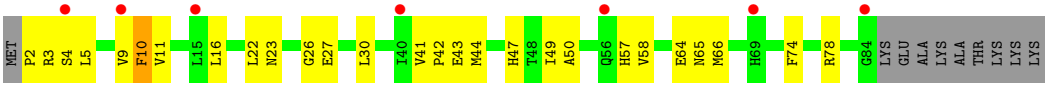
• Molecule 52: 30S ribosomal protein S18

Chain QR:



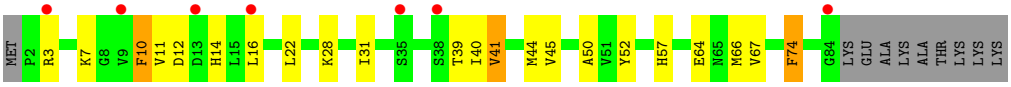
• Molecule 53: 30S ribosomal protein S19

Chain XS:



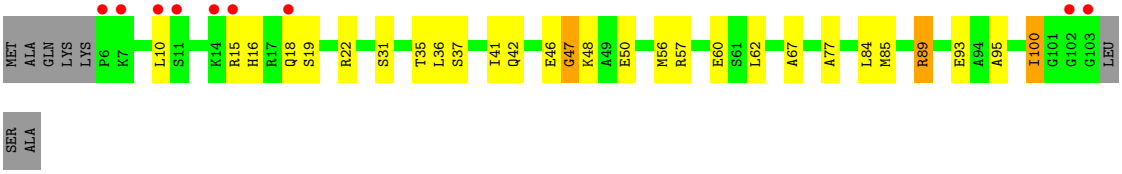
• Molecule 53: 30S ribosomal protein S19

Chain QS:



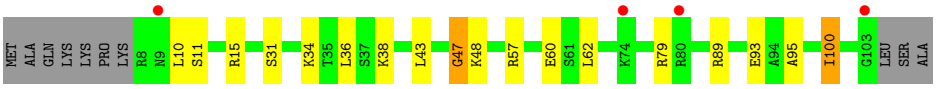
• Molecule 54: 30S ribosomal protein S20

Chain XT:



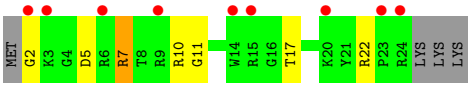
• Molecule 54: 30S ribosomal protein S20

Chain QT:



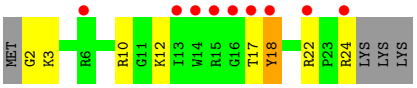
• Molecule 55: 30S ribosomal protein Thx

Chain XU:



- Molecule 55: 30S ribosomal protein Thx

Chain QU:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.48Å 450.41Å 622.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.88 – 3.10 49.88 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.88-3.10) 99.9 (49.88-3.10)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.196 , 0.227 0.195 , 0.226	Depositor DCC
R_{free} test set	49511 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å^2)	65.2	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 66.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	296662	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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: 7MG, 2MG, UR3, 0TD, 4OC, PSU, 5MU, OMG, MA6, SF4, MG, 2MA, 2MU, ZN, M2G, 5MC

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	QV	0.17	0/1836	0.38	1/2859 (0.0%)
1	XV	0.15	0/1836	0.33	0/2859
2	QX	0.15	0/241	0.39	0/373
2	XX	0.15	0/241	0.39	0/373
3	QY	0.37	1/2873 (0.0%)	0.79	6/3870 (0.2%)
3	XY	0.36	1/2873 (0.0%)	0.79	3/3870 (0.1%)
4	RA	0.15	0/68901	0.36	6/107544 (0.0%)
4	YA	0.16	0/68901	0.36	1/107544 (0.0%)
5	RB	0.13	0/2876	0.30	0/4486
5	YB	0.14	0/2878	0.32	0/4490
6	RD	0.33	1/2181 (0.0%)	0.69	1/2940 (0.0%)
6	YD	0.44	2/2186 (0.1%)	0.82	9/2944 (0.3%)
7	RE	0.30	0/1592	0.69	1/2149 (0.0%)
7	YE	0.50	1/1592 (0.1%)	0.71	2/2149 (0.1%)
8	RF	0.28	0/1619	0.68	0/2193
8	YF	0.26	0/1615	0.68	0/2188
9	RG	0.46	4/1451 (0.3%)	0.75	1/1961 (0.1%)
9	YG	0.31	0/1449	0.75	2/1957 (0.1%)
10	RH	0.25	0/1356	0.64	0/1834
10	YH	0.35	1/1350 (0.1%)	0.77	4/1826 (0.2%)
11	RI	0.35	1/1109 (0.1%)	0.73	0/1512
11	YI	0.37	1/1091 (0.1%)	0.75	4/1490 (0.3%)
12	RN	0.59	4/1148 (0.3%)	0.79	4/1547 (0.3%)
12	YN	0.39	1/1144 (0.1%)	0.69	1/1543 (0.1%)
13	RO	0.22	0/943	0.63	2/1269 (0.2%)
13	YO	0.31	0/943	0.68	1/1269 (0.1%)
14	RP	0.28	0/1152	0.73	1/1533 (0.1%)
14	YP	0.29	0/1152	0.74	1/1533 (0.1%)
15	RQ	0.30	0/1143	0.74	0/1527
15	YQ	0.34	0/1143	0.73	1/1527 (0.1%)
16	RR	0.42	0/982	0.85	5/1312 (0.4%)
16	YR	0.41	1/982 (0.1%)	0.79	4/1312 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	RS	0.34	0/887	0.78	1/1180 (0.1%)
17	YS	0.35	0/880	0.93	3/1172 (0.3%)
18	RT	0.34	0/1105	0.86	2/1477 (0.1%)
18	YT	0.30	0/1097	0.82	1/1468 (0.1%)
19	RU	0.61	3/977 (0.3%)	0.97	8/1301 (0.6%)
19	YU	0.61	2/977 (0.2%)	1.00	11/1301 (0.8%)
20	RV	0.45	1/786 (0.1%)	0.94	3/1053 (0.3%)
20	YV	0.33	0/782	0.77	1/1049 (0.1%)
21	RW	0.25	0/897	0.63	1/1205 (0.1%)
21	YW	0.25	0/897	0.64	1/1205 (0.1%)
22	RX	0.22	0/764	0.62	0/1025
22	YX	0.20	0/764	0.59	0/1025
23	RY	0.23	0/823	0.68	0/1099
23	YY	0.44	0/823	0.86	4/1100 (0.4%)
24	RZ	0.31	0/1620	0.76	5/2200 (0.2%)
24	YZ	0.35	0/1590	0.72	0/2162
25	R0	0.46	1/616 (0.2%)	0.97	5/821 (0.6%)
25	Y0	0.45	1/616 (0.2%)	0.86	1/821 (0.1%)
26	R1	0.27	0/761	0.72	1/1013 (0.1%)
26	Y1	0.75	3/766 (0.4%)	0.81	2/1018 (0.2%)
27	R2	0.32	0/590	0.73	0/781
27	Y2	0.54	1/594 (0.2%)	0.81	3/785 (0.4%)
28	R3	0.35	0/474	0.63	0/635
28	Y3	0.23	0/469	0.61	0/630
29	R4	0.67	3/559 (0.5%)	1.15	4/754 (0.5%)
29	Y4	0.62	2/549 (0.4%)	1.19	7/741 (0.9%)
30	R5	1.14	1/473 (0.2%)	1.14	3/639 (0.5%)
30	Y5	0.43	0/469	0.75	0/635
31	R6	0.67	3/460 (0.7%)	0.99	5/613 (0.8%)
31	Y6	0.26	0/456	0.64	0/608
32	R7	0.58	1/426 (0.2%)	0.94	0/561
32	Y7	0.33	0/426	0.83	1/561 (0.2%)
33	R8	0.26	0/525	0.68	0/691
33	Y8	0.24	0/525	0.60	0/691
34	R9	0.49	1/310 (0.3%)	0.97	2/407 (0.5%)
34	Y9	0.22	0/310	0.64	0/407
35	QA	0.14	0/35795	0.33	2/55864 (0.0%)
35	XA	0.14	1/35890 (0.0%)	0.33	2/56012 (0.0%)
36	QB	0.42	0/1876	0.94	6/2533 (0.2%)
36	XB	0.46	1/1860 (0.1%)	0.99	8/2518 (0.3%)
37	QC	0.30	0/1582	0.62	0/2137
37	XC	0.41	1/1566 (0.1%)	0.84	3/2119 (0.1%)
38	QD	0.30	0/1695	0.83	4/2274 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	XD	0.34	0/1698	0.81	1/2277 (0.0%)
39	QE	0.32	1/1149 (0.1%)	0.67	2/1548 (0.1%)
39	XE	0.35	1/1149 (0.1%)	0.66	1/1548 (0.1%)
40	QF	0.41	0/827	0.81	1/1120 (0.1%)
40	XF	0.33	0/829	0.81	1/1123 (0.1%)
41	QG	0.27	0/1254	0.67	0/1683
41	XG	0.46	1/1248 (0.1%)	0.86	4/1676 (0.2%)
42	QH	0.42	3/1118 (0.3%)	0.76	4/1506 (0.3%)
42	XH	0.37	0/1108	0.75	4/1494 (0.3%)
43	QI	0.63	1/1005 (0.1%)	0.85	4/1351 (0.3%)
43	XI	0.29	0/985	0.71	0/1329
44	QJ	0.37	0/732	0.78	3/993 (0.3%)
44	XJ	0.21	0/723	0.59	0/984
45	QK	0.30	0/849	0.74	4/1150 (0.3%)
45	XK	0.29	0/848	0.61	1/1149 (0.1%)
46	QL	0.27	0/937	0.66	1/1260 (0.1%)
46	XL	0.43	2/937 (0.2%)	0.75	2/1260 (0.2%)
47	QM	0.29	0/924	0.71	0/1242
47	XM	0.22	0/905	0.68	1/1217 (0.1%)
48	QN	0.36	0/501	0.87	1/664 (0.2%)
48	XN	0.35	0/501	0.90	5/664 (0.8%)
49	QO	0.50	0/739	1.09	9/985 (0.9%)
49	XO	0.35	0/739	0.80	1/985 (0.1%)
50	QP	0.30	0/697	0.69	0/939
50	XP	0.64	3/693 (0.4%)	1.03	6/935 (0.6%)
51	QQ	0.25	0/836	0.67	0/1117
51	XQ	0.43	1/836 (0.1%)	0.66	1/1117 (0.1%)
52	QR	0.31	0/560	0.85	1/746 (0.1%)
52	XR	0.24	0/560	0.65	0/746
53	QS	0.53	1/663 (0.2%)	0.73	1/895 (0.1%)
53	XS	0.24	0/660	0.56	0/893
54	QT	0.35	0/734	0.69	0/969
54	XT	0.40	1/736 (0.1%)	0.65	0/976
55	QU	0.29	0/203	0.77	0/266
55	XU	0.27	0/203	0.65	0/266
All	All	0.25	60/318172 (0.0%)	0.51	220/475147 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	QY	0	3
8	RF	0	1
11	YI	0	1
17	RS	0	1
19	RU	0	1
25	R0	0	1
26	Y1	0	1
29	R4	0	1
29	Y4	0	1
31	R6	0	1
34	R9	0	1
36	QB	0	2
36	XB	0	2
37	QC	0	1
44	QJ	0	1
44	XJ	0	1
45	XK	0	1
46	XL	0	2
48	XN	0	1
51	XQ	0	1
All	All	0	25

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	R5	27	PRO	CA-C	22.46	1.64	1.51
43	QI	93	ARG	CB-CG	-16.11	1.04	1.52
7	YE	143	ASN	CA-C	-13.14	1.35	1.52
26	Y1	52	ARG	CZ-NH2	10.37	1.47	1.33
53	QS	28	LYS	CD-CE	-9.61	1.23	1.52

The worst 5 of 220 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	R5	27	PRO	O-C-N	18.09	129.63	121.31
37	XC	131	ARG	CG-CD-NE	-15.39	78.13	112.00
36	XB	217	ARG	NE-CZ-NH2	-14.76	105.92	119.20
20	RV	21	ARG	NE-CZ-NH2	-14.15	106.47	119.20
4	RA	2603	G	O5'-P-OP1	-13.41	67.78	108.00

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	QY	115	PHE	Peptide
3	QY	201	LEU	Peptide
3	QY	48	ASN	Sidechain
26	Y1	52	ARG	Sidechain
11	YI	84	GLY	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	QV	1644	0	836	29	0
1	XV	1644	0	836	18	0
2	QX	215	0	109	3	0
2	XX	215	0	108	6	0
3	QY	2833	0	2729	143	0
3	XY	2833	0	2729	164	0
4	RA	61758	0	31149	806	0
4	YA	61758	0	31152	802	0
5	RB	2572	0	1305	18	0
5	YB	2573	0	1306	17	0
6	RD	2131	0	2207	66	0
6	YD	2136	0	2217	66	0
7	RE	1559	0	1618	43	0
7	YE	1559	0	1618	45	0
8	RF	1584	0	1625	57	0
8	YF	1580	0	1619	69	0
9	RG	1426	0	1445	55	0
9	YG	1424	0	1441	62	0
10	RH	1330	0	1407	32	0
10	YH	1324	0	1402	43	0
11	RI	1094	0	1127	34	0
11	YI	1076	0	1094	24	0
12	RN	1121	0	1195	29	0
12	YN	1117	0	1184	23	0
13	RO	933	0	996	28	0
13	YO	933	0	996	27	0
14	RP	1135	0	1212	35	0
14	YP	1135	0	1212	47	0
15	RQ	1122	0	1179	47	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	YQ	1122	0	1179	44	0
16	RR	968	0	1033	32	0
16	YR	968	0	1033	22	0
17	RS	877	0	938	38	0
17	YS	870	0	923	42	0
18	RT	1091	0	1151	47	0
18	YT	1083	0	1136	55	0
19	RU	959	0	1019	32	0
19	YU	959	0	1019	30	0
20	RV	775	0	841	25	0
20	YV	771	0	830	23	0
21	RW	886	0	940	19	0
21	YW	886	0	940	21	0
22	RX	750	0	814	14	0
22	YX	750	0	814	8	0
23	RY	810	0	892	35	0
23	YY	810	0	887	34	0
24	RZ	1587	0	1598	51	0
24	YZ	1557	0	1564	57	0
25	R0	608	0	622	19	0
25	Y0	608	0	622	21	0
26	R1	754	0	823	17	0
26	Y1	759	0	837	27	0
27	R2	588	0	643	14	0
27	Y2	592	0	654	17	0
28	R3	469	0	518	8	0
28	Y3	464	0	514	5	0
29	R4	546	0	522	40	0
29	Y4	536	0	514	48	0
30	R5	459	0	476	13	0
30	Y5	455	0	465	9	0
31	R6	453	0	473	9	0
31	Y6	449	0	469	6	0
32	R7	418	0	467	16	0
32	Y7	418	0	467	11	0
33	R8	517	0	582	22	0
33	Y8	517	0	582	26	0
34	R9	307	0	335	9	0
34	Y9	307	0	335	6	0
35	QA	32246	0	16294	529	0
35	XA	32331	0	16339	491	0
36	QB	1842	0	1862	94	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	XB	1825	0	1828	107	0
37	QC	1558	0	1557	51	0
37	XC	1542	0	1517	49	0
38	QD	1665	0	1688	88	0
38	XD	1668	0	1704	76	0
39	QE	1133	0	1191	35	0
39	XE	1133	0	1191	44	0
40	QF	814	0	808	48	0
40	XF	816	0	808	35	0
41	QG	1235	0	1249	24	0
41	XG	1229	0	1238	36	0
42	QH	1098	0	1143	34	0
42	XH	1088	0	1126	28	0
43	QI	986	0	990	50	0
43	XI	966	0	953	68	0
44	QJ	719	0	672	35	0
44	XJ	710	0	661	29	0
45	QK	834	0	838	13	0
45	XK	833	0	836	21	0
46	QL	932	0	981	38	0
46	XL	932	0	981	31	0
47	QM	914	0	954	36	0
47	XM	895	0	920	34	0
48	QN	492	0	529	29	0
48	XN	492	0	529	16	0
49	QO	728	0	760	17	0
49	XO	728	0	760	18	0
50	QP	681	0	697	30	0
50	XP	677	0	686	33	0
51	QQ	823	0	891	23	0
51	XQ	823	0	891	20	0
52	QR	555	0	618	24	0
52	XR	555	0	618	21	0
53	QS	648	0	658	22	0
53	XS	645	0	635	27	0
54	QT	732	0	809	14	0
54	XT	733	0	795	20	0
55	QU	199	0	208	11	0
55	XU	199	0	208	5	0
56	QA	279	0	0	0	0
56	QB	1	0	0	0	0
56	QD	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	QE	2	0	0	0	0
56	QF	1	0	0	0	0
56	QG	3	0	0	0	0
56	QH	2	0	0	0	0
56	QI	1	0	0	0	0
56	QL	3	0	0	0	0
56	QM	1	0	0	0	0
56	QN	2	0	0	0	0
56	QO	1	0	0	0	0
56	QQ	2	0	0	0	0
56	QR	1	0	0	0	0
56	QT	1	0	0	0	0
56	QU	1	0	0	0	0
56	QV	2	0	0	0	0
56	QY	3	0	0	0	0
56	R0	4	0	0	0	0
56	R1	3	0	0	0	0
56	R3	2	0	0	0	0
56	R4	1	0	0	0	0
56	R5	3	0	0	0	0
56	R7	2	0	0	0	0
56	R8	1	0	0	0	0
56	R9	2	0	0	0	0
56	RA	1066	0	0	0	0
56	RB	29	0	0	0	0
56	RD	13	0	0	0	0
56	RE	6	0	0	0	0
56	RF	12	0	0	0	0
56	RG	4	0	0	0	0
56	RH	2	0	0	0	0
56	RN	3	0	0	0	0
56	RO	1	0	0	0	0
56	RP	2	0	0	0	0
56	RQ	4	0	0	0	0
56	RR	5	0	0	0	0
56	RT	3	0	0	0	0
56	RU	3	0	0	0	0
56	RV	4	0	0	0	0
56	RW	2	0	0	0	0
56	RX	1	0	0	0	0
56	RZ	1	0	0	0	0
56	XA	190	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	XE	2	0	0	0	0
56	XF	4	0	0	0	0
56	XH	1	0	0	0	0
56	XJ	1	0	0	0	0
56	XK	1	0	0	0	0
56	XL	1	0	0	0	0
56	XR	1	0	0	0	0
56	XT	1	0	0	0	0
56	XX	1	0	0	0	0
56	Y0	1	0	0	0	0
56	Y1	1	0	0	0	0
56	Y5	1	0	0	0	0
56	Y7	1	0	0	0	0
56	Y8	2	0	0	0	0
56	YA	760	0	0	0	0
56	YB	19	0	0	0	0
56	YD	10	0	0	0	0
56	YE	7	0	0	0	0
56	YF	3	0	0	0	0
56	YG	3	0	0	0	0
56	YI	1	0	0	0	0
56	YN	1	0	0	0	0
56	YO	1	0	0	0	0
56	YP	1	0	0	0	0
56	YQ	2	0	0	0	0
56	YR	1	0	0	0	0
56	YT	3	0	0	0	0
56	YV	1	0	0	0	0
56	YW	2	0	0	0	0
56	YX	1	0	0	0	0
57	QN	1	0	0	0	0
57	R4	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R9	1	0	0	0	0
57	RY	1	0	0	0	0
57	XN	1	0	0	0	0
57	Y4	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YY	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
All	All	296662	0	200145	5505	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 5505 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)
12:RN:121:LYS:CD	12:RN:121:LYS:CE	1.75	1.59
4:YA:2012:G:OP1	21:YW:11:ARG:NH2	1.88	1.07
36:QB:15:VAL:HG23	36:QB:209:ARG:HB3	1.36	1.06
35:XA:1003:G:H2'	35:XA:1004:A:H4'	1.33	1.05
3:XY:281:HIS:HE1	4:YA:2493:U:H1'	1.22	1.04

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	QY	355/380 (93%)	304 (86%)	43 (12%)	8 (2%)	5 23
3	XY	355/380 (93%)	310 (87%)	33 (9%)	12 (3%)	3 16
6	RD	273/276 (99%)	258 (94%)	15 (6%)	0	100 100
6	YD	273/276 (99%)	257 (94%)	15 (6%)	1 (0%)	30 61
7	RE	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24 57
7	YE	202/206 (98%)	192 (95%)	8 (4%)	2 (1%)	12 41
8	RF	201/210 (96%)	197 (98%)	4 (2%)	0	100 100
8	YF	201/210 (96%)	197 (98%)	4 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	RG	179/182 (98%)	166 (93%)	10 (6%)	3 (2%)	7	30
9	YG	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	21	52
10	RH	172/180 (96%)	163 (95%)	9 (5%)	0	100	100
10	YH	171/180 (95%)	159 (93%)	12 (7%)	0	100	100
11	RI	145/148 (98%)	130 (90%)	13 (9%)	2 (1%)	9	34
11	YI	144/148 (97%)	136 (94%)	6 (4%)	2 (1%)	9	34
12	RN	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
12	YN	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	18	49
13	RO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
13	YO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
14	RP	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
14	YP	147/150 (98%)	137 (93%)	8 (5%)	2 (1%)	9	34
15	RQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
15	YQ	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	18	49
16	RR	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
16	YR	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
17	RS	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
17	YS	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
18	RT	129/146 (88%)	120 (93%)	7 (5%)	2 (2%)	7	30
18	YT	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
19	RU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
19	YU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
20	RV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12	41
20	YV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12	41
21	RW	110/113 (97%)	110 (100%)	0	0	100	100
21	YW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
22	RX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
22	YX	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11	39
23	RY	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
23	YY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
24	RZ	201/206 (98%)	192 (96%)	9 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	YZ	199/206 (97%)	188 (94%)	11 (6%)	0	100	100
25	R0	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
25	Y0	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
26	R1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	39
26	Y1	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11	39
27	R2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
27	Y2	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
28	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
29	R4	67/71 (94%)	52 (78%)	10 (15%)	5 (8%)	1	4
29	Y4	67/71 (94%)	57 (85%)	7 (10%)	3 (4%)	2	12
30	R5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
30	Y5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
31	R6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
31	Y6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
32	R7	46/49 (94%)	46 (100%)	0	0	100	100
32	Y7	46/49 (94%)	46 (100%)	0	0	100	100
33	R8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
33	Y8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
34	R9	35/37 (95%)	35 (100%)	0	0	100	100
34	Y9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
36	QB	229/256 (90%)	197 (86%)	20 (9%)	12 (5%)	1	10
36	XB	229/256 (90%)	198 (86%)	24 (10%)	7 (3%)	3	18
37	QC	204/239 (85%)	195 (96%)	9 (4%)	0	100	100
37	XC	204/239 (85%)	193 (95%)	9 (4%)	2 (1%)	12	41
38	QD	206/209 (99%)	190 (92%)	15 (7%)	1 (0%)	24	57
38	XD	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	24	57
39	QE	146/162 (90%)	143 (98%)	3 (2%)	0	100	100
39	XE	146/162 (90%)	141 (97%)	5 (3%)	0	100	100
40	QF	98/101 (97%)	90 (92%)	6 (6%)	2 (2%)	6	25
40	XF	98/101 (97%)	93 (95%)	3 (3%)	2 (2%)	6	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	QG	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
41	XG	153/156 (98%)	147 (96%)	4 (3%)	2 (1%)	9	35
42	QH	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	18	49
42	XH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
43	QI	125/128 (98%)	117 (94%)	7 (6%)	1 (1%)	16	47
43	XI	124/128 (97%)	113 (91%)	9 (7%)	2 (2%)	7	30
44	QJ	95/105 (90%)	84 (88%)	8 (8%)	3 (3%)	3	18
44	XJ	94/105 (90%)	82 (87%)	9 (10%)	3 (3%)	3	18
45	QK	112/129 (87%)	108 (96%)	3 (3%)	1 (1%)	14	44
45	XK	112/129 (87%)	110 (98%)	2 (2%)	0	100	100
46	QL	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
46	XL	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
47	QM	114/126 (90%)	106 (93%)	7 (6%)	1 (1%)	14	44
47	XM	112/126 (89%)	104 (93%)	7 (6%)	1 (1%)	14	44
48	QN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
48	XN	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
49	QO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
49	XO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
50	QP	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
50	XP	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
51	QQ	97/105 (92%)	91 (94%)	4 (4%)	2 (2%)	5	25
51	XQ	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
52	QR	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
52	XR	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
53	QS	81/93 (87%)	75 (93%)	6 (7%)	0	100	100
53	XS	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
54	QT	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	3	18
54	XT	96/106 (91%)	91 (95%)	2 (2%)	3 (3%)	3	18
55	QU	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	11
55	XU	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	11
All	All	12150/12888 (94%)	11432 (94%)	615 (5%)	103 (1%)	16	47

5 of 103 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	QY	254	VAL
3	XY	122	GLU
3	XY	230	ILE
3	XY	315	SER
9	YG	81	LYS

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	QY	304/324 (94%)	291 (96%)	13 (4%)	26	57
3	XY	304/324 (94%)	288 (95%)	16 (5%)	20	51
6	RD	214/218 (98%)	205 (96%)	9 (4%)	26	58
6	YD	215/218 (99%)	205 (95%)	10 (5%)	23	55
7	RE	164/166 (99%)	156 (95%)	8 (5%)	22	53
7	YE	164/166 (99%)	154 (94%)	10 (6%)	17	46
8	RF	160/166 (96%)	144 (90%)	16 (10%)	7	29
8	YF	159/166 (96%)	146 (92%)	13 (8%)	10	36
9	RG	144/156 (92%)	135 (94%)	9 (6%)	16	45
9	YG	142/156 (91%)	134 (94%)	8 (6%)	19	49
10	RH	144/148 (97%)	139 (96%)	5 (4%)	32	62
10	YH	143/148 (97%)	135 (94%)	8 (6%)	19	49
11	RI	111/124 (90%)	105 (95%)	6 (5%)	20	50
11	YI	108/124 (87%)	104 (96%)	4 (4%)	30	61
12	RN	119/119 (100%)	111 (93%)	8 (7%)	15	43
12	YN	118/119 (99%)	111 (94%)	7 (6%)	18	48
13	RO	100/100 (100%)	94 (94%)	6 (6%)	17	47
13	YO	100/100 (100%)	94 (94%)	6 (6%)	17	47
14	RP	115/116 (99%)	110 (96%)	5 (4%)	26	57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	YP	115/116 (99%)	108 (94%)	7 (6%)	17	46
15	RQ	111/111 (100%)	104 (94%)	7 (6%)	16	45
15	YQ	111/111 (100%)	103 (93%)	8 (7%)	13	40
16	RR	101/101 (100%)	99 (98%)	2 (2%)	48	72
16	YR	101/101 (100%)	98 (97%)	3 (3%)	36	65
17	RS	87/88 (99%)	83 (95%)	4 (5%)	24	55
17	YS	85/88 (97%)	77 (91%)	8 (9%)	8	31
18	RT	115/127 (91%)	105 (91%)	10 (9%)	9	34
18	YT	113/127 (89%)	102 (90%)	11 (10%)	8	30
19	RU	93/94 (99%)	83 (89%)	10 (11%)	6	25
19	YU	93/94 (99%)	86 (92%)	7 (8%)	12	39
20	RV	81/82 (99%)	73 (90%)	8 (10%)	7	29
20	YV	80/82 (98%)	74 (92%)	6 (8%)	12	39
21	RW	90/92 (98%)	85 (94%)	5 (6%)	19	49
21	YW	90/92 (98%)	83 (92%)	7 (8%)	11	38
22	RX	77/78 (99%)	75 (97%)	2 (3%)	40	68
22	YX	77/78 (99%)	77 (100%)	0	100	100
23	RY	86/91 (94%)	80 (93%)	6 (7%)	14	41
23	YY	86/91 (94%)	82 (95%)	4 (5%)	23	55
24	RZ	169/179 (94%)	158 (94%)	11 (6%)	15	44
24	YZ	165/179 (92%)	159 (96%)	6 (4%)	31	62
25	R0	61/67 (91%)	56 (92%)	5 (8%)	10	36
25	Y0	61/67 (91%)	57 (93%)	4 (7%)	15	43
26	R1	79/83 (95%)	76 (96%)	3 (4%)	29	60
26	Y1	81/83 (98%)	77 (95%)	4 (5%)	22	53
27	R2	65/67 (97%)	64 (98%)	1 (2%)	57	75
27	Y2	66/67 (98%)	61 (92%)	5 (8%)	12	39
28	R3	51/52 (98%)	51 (100%)	0	100	100
28	Y3	50/52 (96%)	48 (96%)	2 (4%)	28	60
29	R4	58/63 (92%)	52 (90%)	6 (10%)	7	27
29	Y4	54/63 (86%)	46 (85%)	8 (15%)	3	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	R5	51/52 (98%)	50 (98%)	1 (2%)	48	72
30	Y5	50/52 (96%)	46 (92%)	4 (8%)	11	37
31	R6	51/52 (98%)	50 (98%)	1 (2%)	48	72
31	Y6	50/52 (96%)	49 (98%)	1 (2%)	48	72
32	R7	41/42 (98%)	40 (98%)	1 (2%)	43	69
32	Y7	41/42 (98%)	40 (98%)	1 (2%)	43	69
33	R8	54/55 (98%)	52 (96%)	2 (4%)	30	61
33	Y8	54/55 (98%)	53 (98%)	1 (2%)	50	73
34	R9	34/34 (100%)	32 (94%)	2 (6%)	18	48
34	Y9	34/34 (100%)	33 (97%)	1 (3%)	37	66
36	QB	191/220 (87%)	180 (94%)	11 (6%)	18	48
36	XB	187/220 (85%)	170 (91%)	17 (9%)	9	32
37	QC	144/188 (77%)	141 (98%)	3 (2%)	47	71
37	XC	140/188 (74%)	135 (96%)	5 (4%)	31	62
38	QD	171/181 (94%)	162 (95%)	9 (5%)	20	51
38	XD	172/181 (95%)	159 (92%)	13 (8%)	12	39
39	QE	114/123 (93%)	111 (97%)	3 (3%)	40	68
39	XE	114/123 (93%)	110 (96%)	4 (4%)	32	62
40	QF	85/90 (94%)	79 (93%)	6 (7%)	13	41
40	XF	85/90 (94%)	78 (92%)	7 (8%)	10	36
41	QG	120/127 (94%)	116 (97%)	4 (3%)	33	63
41	XG	119/127 (94%)	114 (96%)	5 (4%)	26	58
42	QH	116/119 (98%)	110 (95%)	6 (5%)	21	51
42	XH	114/119 (96%)	112 (98%)	2 (2%)	51	73
43	QI	91/99 (92%)	84 (92%)	7 (8%)	12	38
43	XI	88/99 (89%)	83 (94%)	5 (6%)	18	49
44	QJ	68/92 (74%)	66 (97%)	2 (3%)	37	66
44	XJ	68/92 (74%)	67 (98%)	1 (2%)	57	75
45	QK	83/99 (84%)	81 (98%)	2 (2%)	43	69
45	XK	83/99 (84%)	82 (99%)	1 (1%)	63	78
46	QL	96/108 (89%)	93 (97%)	3 (3%)	35	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	XL	96/108 (89%)	88 (92%)	8 (8%)	10	35
47	QM	90/101 (89%)	89 (99%)	1 (1%)	65	78
47	XM	87/101 (86%)	86 (99%)	1 (1%)	65	78
48	QN	49/50 (98%)	43 (88%)	6 (12%)	5	20
48	XN	49/50 (98%)	47 (96%)	2 (4%)	27	59
49	QO	78/80 (98%)	75 (96%)	3 (4%)	29	60
49	XO	78/80 (98%)	76 (97%)	2 (3%)	40	68
50	QP	69/74 (93%)	65 (94%)	4 (6%)	18	48
50	XP	68/74 (92%)	62 (91%)	6 (9%)	9	33
51	QQ	94/97 (97%)	91 (97%)	3 (3%)	34	64
51	XQ	94/97 (97%)	91 (97%)	3 (3%)	34	64
52	QR	59/77 (77%)	53 (90%)	6 (10%)	7	28
52	XR	59/77 (77%)	54 (92%)	5 (8%)	10	35
53	QS	68/80 (85%)	65 (96%)	3 (4%)	25	56
53	XS	67/80 (84%)	64 (96%)	3 (4%)	24	56
54	QT	71/82 (87%)	71 (100%)	0	100	100
54	XT	70/82 (85%)	70 (100%)	0	100	100
55	QU	18/22 (82%)	17 (94%)	1 (6%)	19	49
55	XU	18/22 (82%)	18 (100%)	0	100	100
All	All	9971/10712 (93%)	9446 (95%)	525 (5%)	20	51

5 of 525 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	RU	47	TYR
20	RV	72	VAL
19	RU	36	ARG
32	R7	29	LYS
36	XB	17	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
53	QS	47	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	RU	117	GLN
54	QT	75	ASN
14	RP	9	ASN
27	R2	9	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QV	76/77 (98%)	17 (22%)	1 (1%)
1	XV	76/77 (98%)	16 (21%)	1 (1%)
2	QX	9/25 (36%)	3 (33%)	0
2	XX	9/25 (36%)	4 (44%)	0
35	QA	1497/1521 (98%)	230 (15%)	14 (0%)
35	XA	1501/1521 (98%)	227 (15%)	18 (1%)
4	RA	2858/2915 (98%)	452 (15%)	28 (0%)
4	YA	2858/2915 (98%)	456 (15%)	26 (0%)
5	RB	119/122 (97%)	9 (7%)	0
5	YB	119/122 (97%)	14 (11%)	0
All	All	9122/9320 (97%)	1428 (15%)	88 (0%)

5 of 1428 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QV	4	G
1	QV	5	G
1	QV	6	G
1	QV	9	G
1	QV	16	C

5 of 88 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	QA	1207	2MG
4	RA	1065	U
35	QA	1442(A)	G
4	RA	827	U
4	RA	1210	A

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

48 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	$\#\|Z\| > 2$
4	5MC	YA	1962	4,56	19,22,23	1.64	3 (15%)	26,32,35	1.13	2 (7%)
4	2MA	YA	2503	4,56	22,25,26	1.50	4 (18%)	32,37,40	2.33	7 (21%)
4	OMG	RA	2251	4,56,1	23,26,27	1.19	3 (13%)	32,38,41	1.99	6 (18%)
4	PSU	YA	2605	4	18,21,22	1.36	2 (11%)	21,30,33	2.00	4 (19%)
35	5MC	QA	1404	35	19,22,23	1.66	2 (10%)	26,32,35	1.07	2 (7%)
4	5MU	RA	1939	4	19,22,23	1.38	4 (21%)	27,32,35	2.13	6 (22%)
35	5MC	QA	967	35	19,22,23	1.66	3 (15%)	26,32,35	1.10	2 (7%)
4	2MU	RA	2552	4,56	19,22,24	1.25	3 (15%)	25,31,36	1.89	5 (20%)
46	0TD	QL	92	46	8,9,10	2.37	1 (12%)	6,11,13	2.36	3 (50%)
4	PSU	RA	1911	4	18,21,22	1.36	2 (11%)	21,30,33	2.04	4 (19%)
35	5MC	QA	1407	35	19,22,23	1.64	3 (15%)	26,32,35	1.16	3 (11%)
4	OMG	YA	2251	4,56,1	23,26,27	1.23	3 (13%)	32,38,41	2.00	6 (18%)
35	2MG	QA	1207	35,56	23,26,27	1.26	4 (17%)	33,38,41	2.29	7 (21%)
4	PSU	YA	1911	4	18,21,22	1.39	2 (11%)	21,30,33	2.03	4 (19%)
35	5MC	QA	1400	35	19,22,23	1.69	3 (15%)	26,32,35	1.12	2 (7%)
4	5MC	RA	1962	4,56	19,22,23	1.65	3 (15%)	26,32,35	1.10	2 (7%)
35	MA6	XA	1518	35	23,26,27	1.52	4 (17%)	33,38,41	2.31	13 (39%)
35	7MG	QA	527	35,56	23,26,27	1.30	3 (13%)	27,39,42	2.66	7 (25%)
35	UR3	QA	1498	35	19,22,23	1.00	1 (5%)	26,32,35	1.74	2 (7%)
4	PSU	RA	2605	4	18,21,22	1.35	2 (11%)	21,30,33	2.03	4 (19%)
35	MA6	QA	1518	35	23,26,27	1.57	5 (21%)	33,38,41	2.25	13 (39%)
35	7MG	XA	527	35	23,26,27	1.34	3 (13%)	27,39,42	2.62	7 (25%)
4	PSU	RA	1917	4	18,21,22	1.39	2 (11%)	21,30,33	1.97	3 (14%)
35	PSU	XA	516	35	18,21,22	1.36	2 (11%)	21,30,33	2.02	5 (23%)
35	MA6	QA	1519	35	23,26,27	1.55	5 (21%)	33,38,41	2.30	13 (39%)
4	5MU	YA	1939	4,56	19,22,23	1.41	6 (31%)	27,32,35	2.20	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
46	0TD	XL	92	46	8,9,10	2.52	2 (25%)	6,11,13	2.14	3 (50%)
35	5MC	XA	1407	35	19,22,23	1.58	3 (15%)	26,32,35	1.14	3 (11%)
35	PSU	QA	516	35,56	18,21,22	1.37	2 (11%)	21,30,33	2.01	4 (19%)
4	5MU	RA	1915	4,56	19,22,23	1.43	5 (26%)	27,32,35	2.20	8 (29%)
4	5MC	RA	1942	4,56	19,22,23	1.64	3 (15%)	26,32,35	1.08	2 (7%)
35	2MG	XA	1207	35	23,26,27	1.24	4 (17%)	33,38,41	2.22	6 (18%)
4	PSU	YA	1917	4	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
35	4OC	XA	1402	35	20,23,24	0.76	0	25,32,35	0.97	1 (4%)
35	UR3	XA	1498	35,56	19,22,23	1.02	2 (10%)	26,32,35	1.74	2 (7%)
4	5MC	YA	1942	4	19,22,23	1.55	3 (15%)	26,32,35	1.09	2 (7%)
35	M2G	XA	966	35	24,27,28	1.28	4 (16%)	33,40,43	1.86	6 (18%)
35	M2G	QA	966	35	24,27,28	1.29	4 (16%)	33,40,43	1.84	6 (18%)
4	5MU	YA	1915	4	19,22,23	1.48	5 (26%)	27,32,35	2.11	8 (29%)
35	5MC	XA	1400	35	19,22,23	1.61	3 (15%)	26,32,35	1.16	3 (11%)
4	2MU	YA	2552	4,56	19,22,24	1.25	3 (15%)	25,31,36	1.91	6 (24%)
35	5MC	XA	1404	35	19,22,23	1.66	3 (15%)	26,32,35	1.12	2 (7%)
35	4OC	QA	1402	35	20,23,24	0.77	0	25,32,35	0.96	1 (4%)
4	4OC	RA	1920	4	19,22,24	0.80	0	25,31,35	0.98	1 (4%)
35	5MC	XA	967	35	19,22,23	1.67	3 (15%)	26,32,35	1.12	2 (7%)
4	4OC	YA	1920	4	19,22,24	0.78	0	25,31,35	0.91	1 (4%)
35	MA6	XA	1519	35	23,26,27	1.55	3 (13%)	33,38,41	2.38	13 (39%)
4	2MA	RA	2503	4,56	22,25,26	1.48	4 (18%)	32,37,40	2.31	9 (28%)

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
4	5MC	YA	1962	4,56	-	0/7/25/26	0/2/2/2
4	2MA	YA	2503	4,56	-	1/7/25/26	0/3/3/3
4	OMG	RA	2251	4,56,1	-	0/9/27/28	0/3/3/3
4	PSU	YA	2605	4	-	0/7/25/26	0/2/2/2
35	5MC	QA	1404	35	-	0/7/25/26	0/2/2/2
4	5MU	RA	1939	4	-	0/7/25/26	0/2/2/2
35	5MC	QA	967	35	-	0/7/25/26	0/2/2/2
4	2MU	RA	2552	4,56	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	0TD	QL	92	46	-	1/7/12/14	-
4	PSU	RA	1911	4	-	0/7/25/26	0/2/2/2
35	5MC	QA	1407	35	-	0/7/25/26	0/2/2/2
4	OMG	YA	2251	4,56,1	-	0/9/27/28	0/3/3/3
35	2MG	QA	1207	35,56	-	0/9/27/28	0/3/3/3
4	PSU	YA	1911	4	-	0/7/25/26	0/2/2/2
35	5MC	QA	1400	35	-	1/7/25/26	0/2/2/2
4	5MC	RA	1962	4,56	-	0/7/25/26	0/2/2/2
35	MA6	XA	1518	35	-	1/11/29/30	0/3/3/3
35	7MG	QA	527	35,56	-	3/7/37/38	0/3/3/3
35	UR3	QA	1498	35	-	0/7/25/26	0/2/2/2
4	PSU	RA	2605	4	-	0/7/25/26	0/2/2/2
35	MA6	QA	1518	35	-	2/11/29/30	0/3/3/3
35	7MG	XA	527	35	-	2/7/37/38	0/3/3/3
4	PSU	RA	1917	4	-	0/7/25/26	0/2/2/2
35	PSU	XA	516	35	-	0/7/25/26	0/2/2/2
35	MA6	QA	1519	35	-	3/11/29/30	0/3/3/3
4	5MU	YA	1939	4,56	-	0/7/25/26	0/2/2/2
46	0TD	XL	92	46	-	3/7/12/14	-
35	5MC	XA	1407	35	-	0/7/25/26	0/2/2/2
35	PSU	QA	516	35,56	-	0/7/25/26	0/2/2/2
4	5MU	RA	1915	4,56	-	2/7/25/26	0/2/2/2
4	5MC	RA	1942	4,56	-	0/7/25/26	0/2/2/2
35	2MG	XA	1207	35	-	0/9/27/28	0/3/3/3
4	PSU	YA	1917	4	-	0/7/25/26	0/2/2/2
35	4OC	XA	1402	35	-	3/9/29/30	0/2/2/2
35	UR3	XA	1498	35,56	-	0/7/25/26	0/2/2/2
4	5MC	YA	1942	4	-	0/7/25/26	0/2/2/2
35	M2G	XA	966	35	-	0/11/29/30	0/3/3/3
35	M2G	QA	966	35	-	0/11/29/30	0/3/3/3
4	5MU	YA	1915	4	-	4/7/25/26	0/2/2/2
35	5MC	XA	1400	35	-	0/7/25/26	0/2/2/2
4	2MU	YA	2552	4,56	-	0/9/27/28	0/2/2/2
35	5MC	XA	1404	35	-	0/7/25/26	0/2/2/2
35	4OC	QA	1402	35	-	2/9/29/30	0/2/2/2
4	4OC	RA	1920	4	-	1/9/27/30	0/2/2/2
35	5MC	XA	967	35	-	0/7/25/26	0/2/2/2
4	4OC	YA	1920	4	-	2/9/27/30	0/2/2/2
35	MA6	XA	1519	35	-	5/11/29/30	0/3/3/3
4	2MA	RA	2503	4,56	-	0/7/25/26	0/3/3/3

The worst 5 of 136 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	XL	92	0TD	CB-CA	-6.39	1.52	1.54
35	QA	1400	5MC	C5-C4	6.20	1.48	1.44
35	QA	1404	5MC	C5-C4	6.09	1.48	1.44
35	XA	967	5MC	C5-C4	6.08	1.48	1.44
46	QL	92	0TD	CB-CA	-6.06	1.52	1.54

The worst 5 of 231 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	QA	527	7MG	N9-C4-N3	9.17	138.90	125.46
35	XA	527	7MG	N9-C4-N3	8.92	138.53	125.46
4	RA	2503	2MA	C5-C4-N3	-8.37	118.36	127.18
4	YA	2503	2MA	C5-C4-N3	-8.28	118.46	127.18
35	QA	1207	2MG	C2-N3-C4	7.36	121.20	112.00

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	YA	1915	5MU	O4'-C1'-N1-C2
4	YA	1915	5MU	O4'-C1'-N1-C6
35	XA	1519	MA6	C5-C6-N6-C10
46	XL	92	0TD	O-C-CA-CB
35	QA	1519	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

20 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	YA	1962	5MC	1	0
35	QA	1404	5MC	1	0
4	RA	1939	5MU	1	0
35	QA	967	5MC	1	0
4	RA	2552	2MU	1	0
46	QL	92	0TD	2	0
4	YA	2251	OMG	1	0
35	QA	1207	2MG	2	0
4	RA	1962	5MC	1	0
35	XA	1518	MA6	1	0
35	QA	1518	MA6	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	QA	1519	MA6	2	0
46	XL	92	0TD	1	0
4	RA	1942	5MC	2	0
35	XA	1402	4OC	1	0
35	QA	966	M2G	1	0
4	YA	1915	5MU	4	0
35	QA	1402	4OC	1	0
4	RA	1920	4OC	1	0
4	YA	1920	4OC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2527 ligands modelled in this entry, 2525 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	SF4	XD	301	38	0,12,12	-	-	-		
58	SF4	QD	302	38	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
58	SF4	XD	301	38	-	-	0/6/5/5
58	SF4	QD	302	38	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	QV	77/77 (100%)	-0.18	2 (2%)	57	36	57, 94, 173, 210	0
1	XV	77/77 (100%)	-0.30	2 (2%)	57	36	49, 84, 141, 212	0
2	QX	10/25 (40%)	1.43	3 (30%)	1	1	69, 105, 168, 212	0
2	XX	10/25 (40%)	1.30	3 (30%)	1	1	52, 112, 150, 183	0
3	QY	357/380 (93%)	0.85	39 (10%)	10	5	77, 135, 202, 220	0
3	XY	357/380 (93%)	0.92	40 (11%)	10	5	73, 132, 203, 228	0
4	RA	2856/2915 (97%)	-0.53	38 (1%)	75	56	22, 55, 177, 347	0
4	YA	2856/2915 (97%)	-0.60	59 (2%)	63	42	14, 41, 183, 343	0
5	RB	120/122 (98%)	-0.18	2 (1%)	69	48	56, 91, 116, 152	0
5	YB	120/122 (98%)	-0.52	2 (1%)	69	48	39, 63, 85, 130	0
6	RD	275/276 (99%)	-0.08	2 (0%)	84	68	25, 47, 71, 109	0
6	YD	275/276 (99%)	-0.27	1 (0%)	88	76	16, 39, 69, 132	0
7	RE	204/206 (99%)	-0.07	3 (1%)	72	52	26, 53, 85, 119	0
7	YE	204/206 (99%)	-0.17	1 (0%)	87	73	19, 46, 86, 135	0
8	RF	203/210 (96%)	0.02	2 (0%)	79	61	29, 67, 110, 133	0
8	YF	203/210 (96%)	-0.16	1 (0%)	87	73	15, 45, 89, 139	0
9	RG	181/182 (99%)	0.55	6 (3%)	49	29	76, 103, 134, 155	0
9	YG	181/182 (99%)	0.30	6 (3%)	49	29	55, 78, 121, 184	0
10	RH	174/180 (96%)	0.62	9 (5%)	33	17	74, 111, 147, 158	0
10	YH	173/180 (96%)	0.15	3 (1%)	69	48	40, 64, 95, 139	0
11	RI	147/148 (99%)	0.89	13 (8%)	15	9	59, 103, 135, 164	0
11	YI	146/148 (98%)	0.73	9 (6%)	26	14	51, 92, 127, 150	0
12	RN	140/140 (100%)	0.00	1 (0%)	84	68	40, 62, 101, 140	0
12	YN	140/140 (100%)	-0.12	2 (1%)	73	53	27, 47, 87, 129	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	RO	122/122 (100%)	-0.10	2 (1%)	70	49	33, 52, 78, 113	0
13	YO	122/122 (100%)	-0.23	1 (0%)	82	65	27, 45, 71, 83	0
14	RP	149/150 (99%)	0.22	2 (1%)	75	56	29, 72, 109, 138	0
14	YP	149/150 (99%)	0.00	1 (0%)	84	68	18, 52, 84, 115	0
15	RQ	141/141 (100%)	0.13	2 (1%)	73	53	43, 67, 88, 112	0
15	YQ	141/141 (100%)	-0.03	1 (0%)	84	68	30, 48, 74, 124	0
16	RR	118/118 (100%)	-0.00	0	100	100	31, 50, 77, 93	0
16	YR	118/118 (100%)	-0.09	1 (0%)	82	65	28, 43, 67, 89	0
17	RS	110/112 (98%)	0.47	5 (4%)	38	20	66, 89, 113, 133	0
17	YS	110/112 (98%)	0.07	2 (1%)	67	47	47, 62, 89, 106	0
18	RT	131/146 (89%)	-0.00	3 (2%)	61	39	37, 59, 105, 155	0
18	YT	131/146 (89%)	0.02	2 (1%)	72	52	36, 53, 98, 122	0
19	RU	116/118 (98%)	0.10	1 (0%)	81	63	33, 57, 91, 113	0
19	YU	116/118 (98%)	-0.25	0	100	100	23, 37, 67, 104	0
20	RV	101/101 (100%)	-0.05	0	100	100	37, 74, 100, 122	0
20	YV	101/101 (100%)	-0.25	2 (1%)	65	44	21, 50, 88, 109	0
21	RW	112/113 (99%)	0.02	3 (2%)	56	35	34, 48, 81, 122	0
21	YW	112/113 (99%)	-0.19	0	100	100	25, 37, 68, 143	0
22	RX	95/96 (98%)	0.26	1 (1%)	78	59	45, 60, 87, 120	0
22	YX	95/96 (98%)	-0.11	1 (1%)	78	59	28, 42, 80, 115	0
23	RY	107/110 (97%)	1.01	13 (12%)	8	5	57, 83, 131, 176	0
23	YY	107/110 (97%)	0.41	3 (2%)	55	34	38, 64, 107, 150	0
24	RZ	203/206 (98%)	0.58	14 (6%)	23	12	71, 100, 156, 194	0
24	YZ	201/206 (97%)	0.38	13 (6%)	25	13	50, 77, 135, 178	0
25	R0	77/85 (90%)	0.18	2 (2%)	57	36	50, 62, 90, 109	0
25	Y0	77/85 (90%)	-0.01	3 (3%)	43	24	31, 45, 80, 110	0
26	R1	97/98 (98%)	0.20	3 (3%)	51	30	33, 58, 89, 111	0
26	Y1	97/98 (98%)	-0.11	0	100	100	27, 47, 95, 114	0
27	R2	70/72 (97%)	0.26	2 (2%)	53	32	53, 74, 106, 130	0
27	Y2	70/72 (97%)	0.32	3 (4%)	40	22	34, 55, 82, 142	0
28	R3	59/60 (98%)	0.09	1 (1%)	69	48	42, 63, 107, 148	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	Y3	59/60 (98%)	0.06	2 (3%) 48 28	28, 43, 106, 122	0
29	R4	69/71 (97%)	0.64	1 (1%) 73 53	99, 136, 177, 184	0
29	Y4	69/71 (97%)	0.71	5 (7%) 21 11	75, 124, 168, 178	0
30	R5	59/60 (98%)	-0.15	0 100 100	29, 51, 94, 160	0
30	Y5	59/60 (98%)	-0.28	1 (1%) 69 48	18, 42, 91, 141	0
31	R6	53/54 (98%)	0.81	3 (5%) 29 16	82, 102, 143, 150	0
31	Y6	53/54 (98%)	0.64	1 (1%) 66 45	75, 88, 116, 130	0
32	R7	48/49 (97%)	0.02	3 (6%) 26 14	28, 42, 83, 120	0
32	Y7	48/49 (97%)	-0.11	2 (4%) 40 22	17, 31, 69, 115	0
33	R8	64/65 (98%)	0.08	1 (1%) 70 49	39, 54, 73, 107	0
33	Y8	64/65 (98%)	-0.08	1 (1%) 70 49	24, 38, 58, 71	0
34	R9	37/37 (100%)	0.75	0 100 100	58, 77, 101, 112	0
34	Y9	37/37 (100%)	0.52	2 (5%) 31 17	49, 61, 81, 93	0
35	QA	1488/1521 (97%)	-0.11	28 (1%) 66 45	42, 86, 173, 260	0
35	XA	1492/1521 (98%)	-0.19	19 (1%) 75 56	32, 84, 168, 253	0
36	QB	231/256 (90%)	0.70	18 (7%) 19 10	85, 122, 153, 178	0
36	XB	231/256 (90%)	0.58	16 (6%) 23 12	80, 110, 143, 161	0
37	QC	206/239 (86%)	0.43	7 (3%) 48 28	88, 115, 144, 168	0
37	XC	206/239 (86%)	0.49	10 (4%) 35 18	80, 104, 134, 167	0
38	QD	208/209 (99%)	0.59	12 (5%) 29 16	62, 91, 125, 150	0
38	XD	208/209 (99%)	0.73	14 (6%) 24 13	68, 96, 133, 152	0
39	QE	148/162 (91%)	0.13	3 (2%) 65 44	64, 86, 114, 143	0
39	XE	148/162 (91%)	0.11	2 (1%) 73 53	62, 78, 114, 139	0
40	QF	100/101 (99%)	0.27	3 (3%) 52 31	70, 95, 118, 132	0
40	XF	100/101 (99%)	-0.00	0 100 100	62, 81, 109, 124	0
41	QG	155/156 (99%)	0.47	7 (4%) 38 20	82, 109, 137, 157	0
41	XG	155/156 (99%)	0.43	5 (3%) 50 30	78, 100, 130, 155	0
42	QH	137/138 (99%)	0.39	3 (2%) 62 41	55, 86, 114, 123	0
42	XH	137/138 (99%)	0.35	1 (0%) 84 68	60, 86, 113, 120	0
43	QI	127/128 (99%)	1.12	15 (11%) 9 5	78, 123, 151, 175	0
43	XI	126/128 (98%)	0.91	14 (11%) 10 5	68, 111, 139, 165	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	QJ	97/105 (92%)	0.91	7 (7%) 21 11	90, 121, 149, 161	0
44	XJ	96/105 (91%)	0.92	10 (10%) 11 6	78, 116, 144, 146	0
45	QK	114/129 (88%)	0.35	7 (6%) 27 15	63, 86, 113, 138	0
45	XK	114/129 (88%)	0.25	5 (4%) 39 21	47, 75, 105, 132	0
46	QL	121/132 (91%)	0.45	4 (3%) 49 29	47, 66, 90, 105	0
46	XL	121/132 (91%)	0.39	7 (5%) 29 16	48, 66, 94, 116	0
47	QM	116/126 (92%)	0.71	11 (9%) 14 7	85, 114, 138, 148	0
47	XM	114/126 (90%)	0.65	7 (6%) 27 15	84, 107, 128, 144	0
48	QN	60/61 (98%)	1.10	7 (11%) 9 5	88, 111, 129, 146	0
48	XN	60/61 (98%)	0.89	6 (10%) 12 6	73, 92, 115, 127	0
49	QO	88/89 (98%)	0.41	0 100 100	60, 80, 109, 121	0
49	XO	88/89 (98%)	0.43	3 (3%) 48 28	48, 80, 112, 123	0
50	QP	82/88 (93%)	0.59	4 (4%) 35 18	58, 76, 104, 114	0
50	XP	82/88 (93%)	0.72	4 (4%) 35 18	71, 93, 118, 141	0
51	QQ	99/105 (94%)	0.44	5 (5%) 33 18	53, 78, 114, 138	0
51	XQ	99/105 (94%)	0.41	2 (2%) 65 44	59, 78, 101, 126	0
52	QR	68/88 (77%)	0.38	0 100 100	72, 90, 119, 139	0
52	XR	68/88 (77%)	0.24	0 100 100	56, 83, 114, 124	0
53	QS	83/93 (89%)	0.83	7 (8%) 17 9	87, 120, 146, 161	0
53	XS	83/93 (89%)	1.01	7 (8%) 17 9	89, 118, 142, 183	0
54	QT	96/106 (90%)	0.71	4 (4%) 40 22	54, 80, 116, 120	0
54	XT	98/106 (92%)	0.74	9 (9%) 14 8	65, 88, 120, 128	0
55	QU	23/27 (85%)	1.65	9 (39%) 1 0	88, 103, 130, 145	0
55	XU	23/27 (85%)	1.69	9 (39%) 1 0	81, 102, 117, 119	0
All	All	21456/22208 (96%)	0.02	669 (3%) 51 30	14, 73, 148, 347	0

The worst 5 of 669 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	RY	1	MET	9.6
43	QI	128	ARG	7.7
24	YZ	193	GLU	7.4
24	RZ	199	LYS	7.1
23	YY	1	MET	6.8

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
4	5MU	RA	1915	21/22	0.81	0.12	92,100,114,117	0
35	2MG	QA	1207	24/25	0.88	0.10	101,124,131,134	0
35	2MG	XA	1207	24/25	0.88	0.11	85,98,106,107	0
4	PSU	RA	1917	20/21	0.88	0.10	53,73,89,103	0
46	0TD	XL	92	10/11	0.89	0.13	58,67,84,87	0
46	0TD	QL	92	10/11	0.89	0.13	59,72,74,78	0
4	PSU	YA	1917	20/21	0.90	0.09	51,62,88,91	0
4	5MU	YA	1915	21/22	0.91	0.10	52,76,85,87	0
35	PSU	QA	516	20/21	0.91	0.08	71,77,87,88	0
35	PSU	XA	516	20/21	0.92	0.08	75,86,95,95	0
35	M2G	QA	966	25/26	0.92	0.12	71,80,92,93	0
35	M2G	XA	966	25/26	0.93	0.13	56,75,94,105	0
35	7MG	QA	527	24/25	0.93	0.12	51,70,76,76	0
35	5MC	XA	967	21/22	0.93	0.11	62,75,84,92	0
35	5MC	QA	967	21/22	0.93	0.11	71,84,95,99	0
35	4OC	XA	1402	22/23	0.94	0.11	45,57,67,81	0
4	PSU	YA	1911	20/21	0.94	0.08	45,57,62,63	0
4	4OC	RA	1920	21/23	0.94	0.10	55,62,85,94	0
35	5MC	XA	1400	21/22	0.95	0.10	50,65,74,85	0
35	7MG	XA	527	24/25	0.95	0.09	54,63,74,79	0
35	5MC	XA	1404	21/22	0.95	0.11	34,45,58,63	0
35	4OC	QA	1402	22/23	0.95	0.10	55,67,72,74	0
4	PSU	RA	1911	20/21	0.96	0.07	55,66,73,74	0
35	5MC	XA	1407	21/22	0.96	0.09	46,49,58,59	0
35	MA6	QA	1518	24/25	0.96	0.09	48,58,67,72	0
35	5MC	QA	1400	21/22	0.96	0.10	66,75,85,88	0
4	5MU	YA	1939	21/22	0.97	0.07	15,27,36,48	0
35	5MC	QA	1404	21/22	0.97	0.09	55,62,67,73	0
4	5MC	YA	1942	21/22	0.97	0.07	25,38,47,50	0
35	MA6	QA	1519	24/25	0.97	0.12	41,56,68,79	0
4	OMG	YA	2251	24/25	0.97	0.07	13,25,35,41	0
4	4OC	YA	1920	21/23	0.97	0.07	40,47,55,60	0
35	UR3	XA	1498	21/22	0.97	0.07	34,43,57,66	0
35	MA6	XA	1518	24/25	0.97	0.09	31,41,46,52	0
35	MA6	XA	1519	24/25	0.97	0.08	28,45,53,54	0
4	5MU	RA	1939	21/22	0.97	0.07	23,37,44,52	0
4	5MC	RA	1942	21/22	0.97	0.08	41,50,62,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	5MC	YA	1962	21/22	0.98	0.06	25,33,47,55	0
35	5MC	QA	1407	21/22	0.98	0.06	44,51,62,68	0
35	UR3	QA	1498	21/22	0.98	0.07	44,57,69,72	0
4	2MA	YA	2503	23/24	0.98	0.06	8,22,36,38	0
4	2MU	YA	2552	21/23	0.98	0.06	19,28,42,46	0
4	PSU	YA	2605	20/21	0.98	0.07	10,25,42,59	0
4	5MC	RA	1962	21/22	0.98	0.06	39,46,52,62	0
4	OMG	RA	2251	24/25	0.98	0.07	31,38,50,55	0
4	2MA	RA	2503	23/24	0.98	0.06	16,24,31,37	0
4	2MU	RA	2552	21/23	0.98	0.05	19,33,40,48	0
4	PSU	RA	2605	20/21	0.98	0.07	19,36,47,48	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
56	MG	XA	1673	1/1	-0.17	0.18	103,103,103,103	0
56	MG	QA	1647	1/1	-0.15	0.26	134,134,134,134	0
56	MG	QA	1612	1/1	-0.07	0.37	97,97,97,97	0
56	MG	QA	1839	1/1	-0.06	0.21	93,93,93,93	0
56	MG	XA	1773	1/1	-0.05	0.65	96,96,96,96	0
56	MG	QA	1698	1/1	-0.04	0.28	100,100,100,100	0
56	MG	QG	203	1/1	-0.03	0.17	100,100,100,100	0
56	MG	QA	1799	1/1	-0.01	0.24	83,83,83,83	0
56	MG	QA	1858	1/1	0.01	1.04	115,115,115,115	0
56	MG	QA	1751	1/1	0.01	0.28	83,83,83,83	0
56	MG	XA	1669	1/1	0.04	0.21	103,103,103,103	0
56	MG	QA	1683	1/1	0.05	0.18	112,112,112,112	0
56	MG	RA	3112	1/1	0.06	0.27	117,117,117,117	0
56	MG	Y1	101	1/1	0.09	0.18	104,104,104,104	0
56	MG	RA	3994	1/1	0.09	0.31	88,88,88,88	0
56	MG	YA	3637	1/1	0.12	0.67	101,101,101,101	0
56	MG	QA	1736	1/1	0.14	0.40	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
56	MG	YA	3344	1/1	0.16	0.26	80,80,80,80	0
56	MG	QI	201	1/1	0.16	0.26	106,106,106,106	0
56	MG	RH	201	1/1	0.16	0.12	88,88,88,88	0
56	MG	QY	401	1/1	0.17	0.38	111,111,111,111	0
56	MG	XA	1783	1/1	0.18	0.41	99,99,99,99	0
56	MG	RA	3983	1/1	0.18	0.20	84,84,84,84	0
56	MG	XA	1725	1/1	0.19	0.48	87,87,87,87	0
56	MG	XA	1727	1/1	0.19	0.26	84,84,84,84	0
56	MG	RA	3546	1/1	0.19	0.33	111,111,111,111	0
56	MG	YA	3185	1/1	0.22	0.41	105,105,105,105	0
56	MG	RG	201	1/1	0.22	0.12	121,121,121,121	0
56	MG	QA	1785	1/1	0.22	0.36	84,84,84,84	0
56	MG	QA	1686	1/1	0.23	0.21	103,103,103,103	0
56	MG	QA	1783	1/1	0.24	0.19	77,77,77,77	0
56	MG	QA	1603	1/1	0.25	0.32	105,105,105,105	0
56	MG	RA	3196	1/1	0.25	0.32	104,104,104,104	0
56	MG	QD	304	1/1	0.25	0.35	111,111,111,111	0
56	MG	RA	3727	1/1	0.25	0.51	108,108,108,108	0
56	MG	QA	1757	1/1	0.26	0.32	86,86,86,86	0
56	MG	RA	3951	1/1	0.26	0.43	87,87,87,87	0
56	MG	QA	1685	1/1	0.26	0.34	91,91,91,91	0
56	MG	RA	3875	1/1	0.27	0.34	90,90,90,90	0
56	MG	QA	1829	1/1	0.27	0.21	94,94,94,94	0
56	MG	QA	1657	1/1	0.28	0.45	98,98,98,98	0
56	MG	XA	1637	1/1	0.29	0.22	89,89,89,89	0
56	MG	RB	208	1/1	0.30	0.24	90,90,90,90	0
56	MG	QU	101	1/1	0.31	0.21	81,81,81,81	0
56	MG	QA	1768	1/1	0.31	0.26	91,91,91,91	0
56	MG	RB	223	1/1	0.32	0.41	102,102,102,102	0
56	MG	QA	1693	1/1	0.32	0.24	88,88,88,88	0
56	MG	QA	1764	1/1	0.32	0.31	101,101,101,101	0
56	MG	XE	201	1/1	0.33	0.31	79,79,79,79	0
56	MG	XF	203	1/1	0.33	0.31	109,109,109,109	0
56	MG	XA	1753	1/1	0.34	0.42	99,99,99,99	0
56	MG	RA	3115	1/1	0.34	0.39	92,92,92,92	0
56	MG	QA	1867	1/1	0.34	0.16	99,99,99,99	0
56	MG	RA	3410	1/1	0.34	0.28	76,76,76,76	0
56	MG	RA	3452	1/1	0.34	0.28	78,78,78,78	0
56	MG	XA	1662	1/1	0.35	0.25	80,80,80,80	0
56	MG	YA	3270	1/1	0.35	0.29	83,83,83,83	0
56	MG	QE	202	1/1	0.35	0.16	91,91,91,91	0
56	MG	RH	202	1/1	0.35	0.12	96,96,96,96	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3524	1/1	0.36	0.25	96,96,96,96	0
56	MG	QA	1871	1/1	0.37	0.18	100,100,100,100	0
56	MG	RA	3358	1/1	0.37	0.18	99,99,99,99	0
56	MG	YN	201	1/1	0.37	0.18	87,87,87,87	0
56	MG	YA	3459	1/1	0.38	0.30	85,85,85,85	0
56	MG	YG	201	1/1	0.38	0.24	116,116,116,116	0
56	MG	YI	201	1/1	0.38	0.14	110,110,110,110	0
56	MG	QA	1633	1/1	0.38	0.11	95,95,95,95	0
56	MG	QA	1780	1/1	0.38	0.23	92,92,92,92	0
56	MG	YA	3628	1/1	0.39	0.36	105,105,105,105	0
56	MG	XA	1639	1/1	0.39	0.32	98,98,98,98	0
56	MG	RA	3058	1/1	0.39	0.70	88,88,88,88	0
56	MG	QD	301	1/1	0.39	0.30	90,90,90,90	0
56	MG	RA	3271	1/1	0.40	0.22	93,93,93,93	0
56	MG	XA	1692	1/1	0.40	0.39	75,75,75,75	0
56	MG	RA	3961	1/1	0.40	0.33	114,114,114,114	0
56	MG	RA	3572	1/1	0.40	0.42	83,83,83,83	0
56	MG	YA	3491	1/1	0.40	0.36	53,53,53,53	0
56	MG	RA	3011	1/1	0.41	0.24	84,84,84,84	0
56	MG	QA	1731	1/1	0.41	0.33	71,71,71,71	0
56	MG	QA	1832	1/1	0.41	0.29	92,92,92,92	0
56	MG	YA	3467	1/1	0.41	0.55	82,82,82,82	0
56	MG	RA	3654	1/1	0.41	0.39	87,87,87,87	0
56	MG	QA	1712	1/1	0.41	0.22	87,87,87,87	0
56	MG	QA	1715	1/1	0.41	0.29	77,77,77,77	0
56	MG	QA	1725	1/1	0.41	0.63	90,90,90,90	0
56	MG	QA	1682	1/1	0.42	0.25	93,93,93,93	0
56	MG	QA	1727	1/1	0.42	0.18	100,100,100,100	0
56	MG	RA	3105	1/1	0.42	0.14	71,71,71,71	0
56	MG	YA	3177	1/1	0.43	0.22	71,71,71,71	0
56	MG	RA	3100	1/1	0.43	0.30	93,93,93,93	0
56	MG	RA	3987	1/1	0.43	0.39	80,80,80,80	0
56	MG	YA	3505	1/1	0.44	0.39	88,88,88,88	0
56	MG	QA	1842	1/1	0.44	0.24	84,84,84,84	0
56	MG	YA	3174	1/1	0.44	0.25	95,95,95,95	0
56	MG	RA	3439	1/1	0.44	0.20	89,89,89,89	0
56	MG	QA	1674	1/1	0.45	0.21	85,85,85,85	0
56	MG	RB	217	1/1	0.45	0.26	94,94,94,94	0
56	MG	XA	1754	1/1	0.45	0.58	86,86,86,86	0
56	MG	XA	1711	1/1	0.46	0.30	92,92,92,92	0
56	MG	RA	3982	1/1	0.46	0.36	83,83,83,83	0
56	MG	RA	3519	1/1	0.46	0.28	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
56	MG	RA	3523	1/1	0.46	0.26	64,64,64,64	0
56	MG	YA	3193	1/1	0.46	0.37	101,101,101,101	0
56	MG	YB	209	1/1	0.46	0.44	102,102,102,102	0
56	MG	RA	3635	1/1	0.46	0.17	112,112,112,112	0
56	MG	QA	1789	1/1	0.46	0.39	99,99,99,99	0
56	MG	RA	3099	1/1	0.46	0.33	102,102,102,102	0
56	MG	QA	1848	1/1	0.46	0.34	68,68,68,68	0
56	MG	QA	1748	1/1	0.46	0.28	92,92,92,92	0
56	MG	R9	101	1/1	0.46	0.40	92,92,92,92	0
56	MG	XA	1609	1/1	0.47	0.51	88,88,88,88	0
56	MG	RA	3922	1/1	0.47	0.30	70,70,70,70	0
56	MG	QA	1844	1/1	0.47	0.22	80,80,80,80	0
56	MG	RA	3062	1/1	0.47	0.19	82,82,82,82	0
56	MG	RA	3733	1/1	0.47	0.47	96,96,96,96	0
56	MG	XA	1608	1/1	0.48	0.25	76,76,76,76	0
56	MG	XA	1787	1/1	0.48	0.56	84,84,84,84	0
56	MG	RA	3780	1/1	0.48	0.47	74,74,74,74	0
56	MG	RA	3198	1/1	0.48	0.15	84,84,84,84	0
56	MG	YA	3415	1/1	0.48	0.35	84,84,84,84	0
56	MG	YA	3488	1/1	0.48	0.18	105,105,105,105	0
56	MG	RA	3634	1/1	0.48	0.18	81,81,81,81	0
56	MG	YA	3028	1/1	0.48	0.23	51,51,51,51	0
56	MG	XA	1654	1/1	0.48	0.33	89,89,89,89	0
56	MG	QA	1812	1/1	0.49	0.41	68,68,68,68	0
56	MG	QA	1713	1/1	0.49	0.29	79,79,79,79	0
56	MG	YA	3662	1/1	0.49	0.56	91,91,91,91	0
56	MG	YA	3379	1/1	0.49	0.32	70,70,70,70	0
56	MG	RA	4004	1/1	0.49	0.56	93,93,93,93	0
56	MG	R4	102	1/1	0.49	0.12	88,88,88,88	0
56	MG	QA	1608	1/1	0.49	0.21	110,110,110,110	0
57	ZN	Y4	101	1/1	0.49	0.14	305,305,305,305	0
56	MG	RA	3553	1/1	0.50	0.38	87,87,87,87	0
56	MG	QA	1798	1/1	0.50	0.33	119,119,119,119	0
56	MG	RA	3511	1/1	0.50	0.41	62,62,62,62	0
56	MG	YA	3057	1/1	0.50	0.38	99,99,99,99	0
56	MG	RA	3942	1/1	0.50	0.26	104,104,104,104	0
56	MG	YA	3632	1/1	0.50	0.27	62,62,62,62	0
56	MG	YA	3421	1/1	0.50	0.30	75,75,75,75	0
56	MG	RA	3552	1/1	0.51	0.23	97,97,97,97	0
56	MG	XA	1709	1/1	0.51	0.26	72,72,72,72	0
56	MG	QA	1601	1/1	0.51	0.72	129,129,129,129	0
56	MG	YA	3293	1/1	0.51	0.36	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
56	MG	RA	3437	1/1	0.51	0.26	77,77,77,77	0
56	MG	RA	3540	1/1	0.51	0.28	73,73,73,73	0
56	MG	QA	1606	1/1	0.51	0.24	93,93,93,93	0
56	MG	RA	3993	1/1	0.52	0.26	86,86,86,86	0
56	MG	YA	3528	1/1	0.52	0.56	104,104,104,104	0
56	MG	RA	3752	1/1	0.52	0.43	102,102,102,102	0
56	MG	QA	1756	1/1	0.52	0.36	114,114,114,114	0
56	MG	RB	215	1/1	0.52	0.25	91,91,91,91	0
56	MG	RA	3293	1/1	0.52	0.12	128,128,128,128	0
56	MG	YA	3396	1/1	0.52	0.36	94,94,94,94	0
56	MG	XA	1651	1/1	0.52	0.21	90,90,90,90	0
56	MG	YA	3414	1/1	0.52	0.50	83,83,83,83	0
56	MG	YA	3242	1/1	0.52	0.53	88,88,88,88	0
56	MG	YA	3253	1/1	0.52	0.28	98,98,98,98	0
56	MG	R5	104	1/1	0.52	0.15	67,67,67,67	0
56	MG	QA	1738	1/1	0.52	0.29	98,98,98,98	0
56	MG	YA	3037	1/1	0.52	0.29	88,88,88,88	0
56	MG	XJ	201	1/1	0.53	0.17	97,97,97,97	0
56	MG	RA	3786	1/1	0.53	0.17	87,87,87,87	0
56	MG	YA	3347	1/1	0.53	0.35	99,99,99,99	0
56	MG	RA	3481	1/1	0.53	0.18	81,81,81,81	0
56	MG	RA	3595	1/1	0.53	0.23	84,84,84,84	0
56	MG	QA	1876	1/1	0.53	0.13	84,84,84,84	0
56	MG	QA	1651	1/1	0.54	0.32	89,89,89,89	0
56	MG	RB	211	1/1	0.54	0.19	95,95,95,95	0
56	MG	QA	1745	1/1	0.54	0.32	98,98,98,98	0
56	MG	XA	1660	1/1	0.54	0.17	99,99,99,99	0
56	MG	QY	403	1/1	0.54	0.45	81,81,81,81	0
56	MG	RD	310	1/1	0.54	0.23	94,94,94,94	0
56	MG	RA	3688	1/1	0.54	0.24	90,90,90,90	0
56	MG	QA	1697	1/1	0.54	0.25	76,76,76,76	0
56	MG	YA	3058	1/1	0.54	0.17	75,75,75,75	0
56	MG	YA	3462	1/1	0.54	0.38	75,75,75,75	0
56	MG	RA	3563	1/1	0.54	0.29	66,66,66,66	0
56	MG	RA	3781	1/1	0.54	0.27	60,60,60,60	0
56	MG	RA	3490	1/1	0.54	0.33	86,86,86,86	0
56	MG	QM	201	1/1	0.55	0.20	85,85,85,85	0
56	MG	RA	3525	1/1	0.55	0.29	65,65,65,65	0
56	MG	QA	1840	1/1	0.55	0.32	89,89,89,89	0
56	MG	QA	1875	1/1	0.55	0.25	75,75,75,75	0
56	MG	QA	1665	1/1	0.55	0.27	102,102,102,102	0
56	MG	YE	303	1/1	0.55	0.58	103,103,103,103	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3728	1/1	0.55	0.47	74,74,74,74	0
56	MG	RA	3399	1/1	0.55	0.28	117,117,117,117	0
56	MG	RA	3158	1/1	0.55	0.30	67,67,67,67	0
56	MG	RA	3339	1/1	0.56	0.30	68,68,68,68	0
56	MG	RA	3179	1/1	0.56	0.25	77,77,77,77	0
56	MG	XA	1758	1/1	0.56	0.29	60,60,60,60	0
56	MG	RD	313	1/1	0.56	0.36	82,82,82,82	0
56	MG	RA	3065	1/1	0.56	0.27	89,89,89,89	0
56	MG	RA	3412	1/1	0.56	0.39	71,71,71,71	0
56	MG	YA	3465	1/1	0.56	0.47	82,82,82,82	0
56	MG	RA	3277	1/1	0.56	0.31	94,94,94,94	0
56	MG	RA	3683	1/1	0.56	0.19	96,96,96,96	0
56	MG	QA	1763	1/1	0.56	0.28	100,100,100,100	0
56	MG	RA	3463	1/1	0.56	0.38	78,78,78,78	0
56	MG	XA	1682	1/1	0.57	0.43	86,86,86,86	0
56	MG	YA	3311	1/1	0.57	0.52	94,94,94,94	0
56	MG	QA	1653	1/1	0.57	0.28	85,85,85,85	0
56	MG	QA	1735	1/1	0.57	0.25	107,107,107,107	0
56	MG	XA	1624	1/1	0.57	0.17	76,76,76,76	0
56	MG	RA	3237	1/1	0.57	0.54	100,100,100,100	0
56	MG	RA	3247	1/1	0.57	0.33	88,88,88,88	0
56	MG	YA	3547	1/1	0.57	0.23	80,80,80,80	0
56	MG	RA	3067	1/1	0.57	0.21	83,83,83,83	0
56	MG	XA	1666	1/1	0.57	0.22	63,63,63,63	0
56	MG	RA	3322	1/1	0.57	0.34	90,90,90,90	0
56	MG	YF	302	1/1	0.57	0.54	85,85,85,85	0
56	MG	YA	3475	1/1	0.57	0.23	84,84,84,84	0
56	MG	QA	1793	1/1	0.57	0.41	82,82,82,82	0
56	MG	RA	3724	1/1	0.58	0.15	67,67,67,67	0
56	MG	YA	3448	1/1	0.58	0.27	81,81,81,81	0
56	MG	XA	1785	1/1	0.58	0.28	81,81,81,81	0
56	MG	XA	1652	1/1	0.58	0.25	78,78,78,78	0
56	MG	XA	1671	1/1	0.58	0.36	108,108,108,108	0
56	MG	RA	3361	1/1	0.58	0.20	76,76,76,76	0
56	MG	YA	3400	1/1	0.58	0.24	74,74,74,74	0
56	MG	RA	3784	1/1	0.58	0.23	94,94,94,94	0
56	MG	RB	229	1/1	0.58	0.22	108,108,108,108	0
56	MG	RA	3175	1/1	0.58	0.30	70,70,70,70	0
56	MG	XA	1675	1/1	0.58	0.30	82,82,82,82	0
56	MG	YA	3545	1/1	0.58	0.32	99,99,99,99	0
56	MG	YA	3092	1/1	0.58	0.14	113,113,113,113	0
56	MG	XA	1705	1/1	0.58	0.27	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	QA	1759	1/1	0.58	0.23	78,78,78,78	0
56	MG	QA	1814	1/1	0.58	0.20	97,97,97,97	0
56	MG	XA	1781	1/1	0.58	0.51	110,110,110,110	0
56	MG	RA	3289	1/1	0.58	0.22	83,83,83,83	0
56	MG	RA	3401	1/1	0.59	0.12	44,44,44,44	0
56	MG	RA	3828	1/1	0.59	0.15	94,94,94,94	0
56	MG	RA	3847	1/1	0.59	0.21	102,102,102,102	0
56	MG	RA	3851	1/1	0.59	0.22	91,91,91,91	0
56	MG	QD	303	1/1	0.59	0.16	79,79,79,79	0
56	MG	YA	3370	1/1	0.59	0.33	67,67,67,67	0
56	MG	QA	1690	1/1	0.59	0.15	72,72,72,72	0
56	MG	YB	205	1/1	0.59	0.24	89,89,89,89	0
56	MG	QA	1694	1/1	0.59	0.40	97,97,97,97	0
56	MG	QA	1720	1/1	0.59	0.43	97,97,97,97	0
56	MG	RA	3217	1/1	0.59	0.18	88,88,88,88	0
56	MG	RN	202	1/1	0.59	0.18	98,98,98,98	0
56	MG	RA	3777	1/1	0.59	0.52	93,93,93,93	0
56	MG	QA	1878	1/1	0.59	0.34	108,108,108,108	0
56	MG	RA	3367	1/1	0.59	0.40	74,74,74,74	0
56	MG	YA	3501	1/1	0.59	0.52	115,115,115,115	0
56	MG	QA	1826	1/1	0.60	0.20	74,74,74,74	0
56	MG	XA	1703	1/1	0.60	0.22	60,60,60,60	0
56	MG	XA	1610	1/1	0.60	0.30	79,79,79,79	0
56	MG	QA	1837	1/1	0.60	0.28	69,69,69,69	0
56	MG	RA	3031	1/1	0.60	0.34	75,75,75,75	0
56	MG	QA	1664	1/1	0.60	0.34	92,92,92,92	0
56	MG	RA	3611	1/1	0.60	0.22	80,80,80,80	0
56	MG	YA	3561	1/1	0.60	0.26	45,45,45,45	0
56	MG	YA	3455	1/1	0.60	0.48	79,79,79,79	0
56	MG	RW	202	1/1	0.60	0.38	89,89,89,89	0
56	MG	YA	3120	1/1	0.60	0.21	72,72,72,72	0
56	MG	QA	1652	1/1	0.60	0.20	83,83,83,83	0
56	MG	QA	1816	1/1	0.60	0.44	76,76,76,76	0
56	MG	RA	3249	1/1	0.60	0.69	94,94,94,94	0
56	MG	RA	3625	1/1	0.61	0.44	91,91,91,91	0
56	MG	RA	3756	1/1	0.61	0.29	83,83,83,83	0
56	MG	RA	3375	1/1	0.61	0.27	73,73,73,73	0
56	MG	QA	1739	1/1	0.61	0.17	87,87,87,87	0
56	MG	YA	3466	1/1	0.61	0.38	80,80,80,80	0
56	MG	RA	3782	1/1	0.61	0.48	94,94,94,94	0
56	MG	XA	1721	1/1	0.61	0.39	86,86,86,86	0
56	MG	YA	3261	1/1	0.61	0.17	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
56	MG	RA	3701	1/1	0.61	0.36	64,64,64,64	0
56	MG	RA	3429	1/1	0.61	0.21	89,89,89,89	0
56	MG	RA	3589	1/1	0.61	0.22	100,100,100,100	0
56	MG	QA	1856	1/1	0.61	0.30	89,89,89,89	0
56	MG	YA	3364	1/1	0.61	0.35	67,67,67,67	0
56	MG	RA	3422	1/1	0.62	0.33	84,84,84,84	0
56	MG	QA	1675	1/1	0.62	0.19	94,94,94,94	0
56	MG	RA	3577	1/1	0.62	0.29	94,94,94,94	0
56	MG	RA	3431	1/1	0.62	0.35	88,88,88,88	0
56	MG	QA	1805	1/1	0.62	0.15	76,76,76,76	0
56	MG	QA	1810	1/1	0.62	0.29	69,69,69,69	0
56	MG	YA	3478	1/1	0.62	0.23	67,67,67,67	0
56	MG	RA	3823	1/1	0.62	0.32	97,97,97,97	0
56	MG	YA	3131	1/1	0.62	0.31	88,88,88,88	0
56	MG	QL	201	1/1	0.62	0.17	66,66,66,66	0
56	MG	YD	302	1/1	0.62	0.30	71,71,71,71	0
56	MG	RF	312	1/1	0.62	0.18	62,62,62,62	0
56	MG	QA	1822	1/1	0.62	0.36	65,65,65,65	0
56	MG	XA	1719	1/1	0.62	0.41	95,95,95,95	0
56	MG	RA	3028	1/1	0.62	0.26	69,69,69,69	0
56	MG	RA	3943	1/1	0.62	0.31	86,86,86,86	0
56	MG	RT	203	1/1	0.62	0.11	88,88,88,88	0
56	MG	XA	1616	1/1	0.62	0.16	115,115,115,115	0
56	MG	RA	3203	1/1	0.62	0.43	97,97,97,97	0
56	MG	QA	1615	1/1	0.62	0.12	107,107,107,107	0
56	MG	XA	1603	1/1	0.62	0.23	76,76,76,76	0
56	MG	QA	1642	1/1	0.62	0.23	83,83,83,83	0
56	MG	RB	216	1/1	0.63	0.13	59,59,59,59	0
56	MG	RA	3878	1/1	0.63	0.40	81,81,81,81	0
56	MG	YA	3340	1/1	0.63	0.24	59,59,59,59	0
56	MG	QA	1752	1/1	0.63	0.24	77,77,77,77	0
56	MG	XA	1784	1/1	0.63	0.40	72,72,72,72	0
56	MG	RA	3154	1/1	0.63	0.23	88,88,88,88	0
56	MG	RA	3256	1/1	0.63	0.49	103,103,103,103	0
56	MG	QA	1861	1/1	0.63	0.31	75,75,75,75	0
56	MG	YB	218	1/1	0.63	0.21	80,80,80,80	0
56	MG	RA	3278	1/1	0.63	0.37	83,83,83,83	0
56	MG	QA	1726	1/1	0.63	0.38	81,81,81,81	0
56	MG	RA	3549	1/1	0.63	0.29	78,78,78,78	0
56	MG	RA	4001	1/1	0.63	0.34	58,58,58,58	0
56	MG	RA	3187	1/1	0.63	0.51	106,106,106,106	0
56	MG	XA	1648	1/1	0.63	0.18	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
56	MG	QA	1819	1/1	0.63	0.15	65,65,65,65	0
56	MG	YA	3099	1/1	0.63	0.23	106,106,106,106	0
56	MG	QA	1843	1/1	0.64	0.16	89,89,89,89	0
56	MG	RA	3675	1/1	0.64	0.31	75,75,75,75	0
56	MG	RA	3364	1/1	0.64	0.23	96,96,96,96	0
56	MG	YA	3544	1/1	0.64	0.40	81,81,81,81	0
56	MG	RA	3370	1/1	0.64	0.58	88,88,88,88	0
56	MG	RA	3036	1/1	0.64	0.19	69,69,69,69	0
56	MG	YA	3134	1/1	0.64	0.37	89,89,89,89	0
56	MG	RA	3205	1/1	0.64	0.22	76,76,76,76	0
56	MG	QA	1769	1/1	0.64	0.16	95,95,95,95	0
56	MG	RA	3746	1/1	0.64	0.38	112,112,112,112	0
56	MG	YA	3247	1/1	0.64	0.33	106,106,106,106	0
56	MG	QA	1750	1/1	0.64	0.24	67,67,67,67	0
56	MG	RA	3343	1/1	0.64	0.22	68,68,68,68	0
56	MG	YA	3427	1/1	0.64	0.24	75,75,75,75	0
56	MG	YA	3095	1/1	0.65	0.18	68,68,68,68	0
56	MG	QA	1708	1/1	0.65	0.26	77,77,77,77	0
56	MG	QA	1802	1/1	0.65	0.28	79,79,79,79	0
56	MG	YA	3302	1/1	0.65	0.38	72,72,72,72	0
56	MG	RA	3491	1/1	0.65	0.35	81,81,81,81	0
56	MG	QA	1849	1/1	0.65	0.47	81,81,81,81	0
56	MG	RF	302	1/1	0.65	0.20	73,73,73,73	0
56	MG	RA	3051	1/1	0.65	0.28	83,83,83,83	0
56	MG	RA	3404	1/1	0.65	0.18	81,81,81,81	0
56	MG	RA	3644	1/1	0.65	0.29	84,84,84,84	0
56	MG	QA	1831	1/1	0.65	0.43	93,93,93,93	0
56	MG	YA	3308	1/1	0.65	0.25	64,64,64,64	0
56	MG	YA	3740	1/1	0.65	0.23	52,52,52,52	0
56	MG	YA	3107	1/1	0.65	0.34	80,80,80,80	0
56	MG	RA	4019	1/1	0.65	0.43	87,87,87,87	0
56	MG	QA	1766	1/1	0.65	0.36	71,71,71,71	0
56	MG	QA	1874	1/1	0.65	0.27	74,74,74,74	0
56	MG	QN	103	1/1	0.65	0.49	80,80,80,80	0
56	MG	QA	1862	1/1	0.66	0.25	101,101,101,101	0
56	MG	QA	1835	1/1	0.66	0.29	89,89,89,89	0
56	MG	XA	1689	1/1	0.66	0.17	64,64,64,64	0
56	MG	YA	3439	1/1	0.66	0.27	80,80,80,80	0
56	MG	RA	3729	1/1	0.66	0.19	59,59,59,59	0
56	MG	QA	1777	1/1	0.66	0.14	81,81,81,81	0
56	MG	RA	3489	1/1	0.66	0.39	50,50,50,50	0
56	MG	RA	3122	1/1	0.66	0.35	92,92,92,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	QA	1668	1/1	0.66	0.26	102,102,102,102	0
56	MG	QA	1645	1/1	0.66	0.30	75,75,75,75	0
56	MG	RA	3515	1/1	0.66	0.39	67,67,67,67	0
56	MG	YA	3498	1/1	0.66	0.32	64,64,64,64	0
56	MG	RA	3641	1/1	0.66	0.23	65,65,65,65	0
56	MG	QA	1702	1/1	0.66	0.25	64,64,64,64	0
56	MG	RA	4002	1/1	0.66	0.40	83,83,83,83	0
56	MG	YA	3476	1/1	0.66	0.28	52,52,52,52	0
56	MG	YA	3655	1/1	0.66	0.51	86,86,86,86	0
56	MG	YA	3532	1/1	0.66	0.25	60,60,60,60	0
56	MG	YA	3582	1/1	0.66	0.40	101,101,101,101	0
56	MG	RA	3682	1/1	0.67	0.26	81,81,81,81	0
56	MG	RB	227	1/1	0.67	0.29	74,74,74,74	0
56	MG	QA	1650	1/1	0.67	0.11	72,72,72,72	0
56	MG	YA	3150	1/1	0.67	0.40	84,84,84,84	0
56	MG	YA	3406	1/1	0.67	0.38	80,80,80,80	0
56	MG	RA	3722	1/1	0.67	0.26	82,82,82,82	0
56	MG	RA	3191	1/1	0.67	0.23	69,69,69,69	0
56	MG	RA	3725	1/1	0.67	0.19	80,80,80,80	0
56	MG	RG	203	1/1	0.67	0.20	79,79,79,79	0
56	MG	XA	1615	1/1	0.67	0.15	63,63,63,63	0
56	MG	QA	1721	1/1	0.67	0.29	75,75,75,75	0
56	MG	QA	1762	1/1	0.67	0.62	93,93,93,93	0
56	MG	QA	1604	1/1	0.67	0.12	75,75,75,75	0
56	MG	RV	201	1/1	0.67	0.16	110,110,110,110	0
56	MG	RB	210	1/1	0.67	0.25	109,109,109,109	0
56	MG	YA	3233	1/1	0.67	0.23	95,95,95,95	0
56	MG	RA	3647	1/1	0.67	0.45	88,88,88,88	0
56	MG	QA	1820	1/1	0.67	0.13	79,79,79,79	0
56	MG	YA	3148	1/1	0.67	0.34	92,92,92,92	0
56	MG	YA	3159	1/1	0.68	0.36	91,91,91,91	0
56	MG	QA	1866	1/1	0.68	0.47	89,89,89,89	0
56	MG	YA	3508	1/1	0.68	0.35	102,102,102,102	0
56	MG	RA	3757	1/1	0.68	0.32	70,70,70,70	0
56	MG	XA	1672	1/1	0.68	0.09	91,91,91,91	0
56	MG	QY	402	1/1	0.68	0.34	111,111,111,111	0
56	MG	RB	212	1/1	0.68	0.12	74,74,74,74	0
56	MG	RA	3637	1/1	0.68	0.31	66,66,66,66	0
56	MG	XA	1674	1/1	0.68	0.11	73,73,73,73	0
56	MG	RA	3197	1/1	0.68	0.18	85,85,85,85	0
56	MG	RB	222	1/1	0.68	0.31	94,94,94,94	0
56	MG	QA	1734	1/1	0.68	0.37	85,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3735	1/1	0.68	0.37	71,71,71,71	0
56	MG	RA	3671	1/1	0.68	0.24	71,71,71,71	0
56	MG	RA	3672	1/1	0.68	0.21	75,75,75,75	0
56	MG	YA	3393	1/1	0.68	0.16	66,66,66,66	0
56	MG	YA	3265	1/1	0.68	0.22	64,64,64,64	0
56	MG	RA	3220	1/1	0.68	0.26	75,75,75,75	0
56	MG	QA	1644	1/1	0.68	0.23	108,108,108,108	0
56	MG	RA	3693	1/1	0.68	0.30	67,67,67,67	0
56	MG	YB	206	1/1	0.68	0.21	99,99,99,99	0
56	MG	YA	3175	1/1	0.68	0.12	123,123,123,123	0
56	MG	QA	1853	1/1	0.68	0.34	107,107,107,107	0
56	MG	RA	3969	1/1	0.68	0.39	98,98,98,98	0
56	MG	QA	1718	1/1	0.68	0.42	82,82,82,82	0
56	MG	RA	3571	1/1	0.68	0.40	94,94,94,94	0
56	MG	QA	1823	1/1	0.68	0.31	70,70,70,70	0
56	MG	RA	3131	1/1	0.68	0.14	67,67,67,67	0
56	MG	QA	1602	1/1	0.68	0.15	95,95,95,95	0
56	MG	RA	3734	1/1	0.68	0.35	70,70,70,70	0
56	MG	YA	3504	1/1	0.69	0.29	74,74,74,74	0
56	MG	QA	1732	1/1	0.69	0.26	96,96,96,96	0
56	MG	YA	3534	1/1	0.69	0.47	124,124,124,124	0
56	MG	YB	211	1/1	0.69	0.28	70,70,70,70	0
56	MG	XA	1788	1/1	0.69	0.34	62,62,62,62	0
56	MG	QA	1737	1/1	0.69	0.49	72,72,72,72	0
56	MG	RA	3863	1/1	0.69	0.32	87,87,87,87	0
56	MG	RA	3280	1/1	0.69	0.24	78,78,78,78	0
56	MG	QA	1623	1/1	0.69	0.21	74,74,74,74	0
56	MG	YA	3417	1/1	0.69	0.50	106,106,106,106	0
56	MG	RA	3314	1/1	0.69	0.36	58,58,58,58	0
56	MG	QA	1743	1/1	0.69	0.16	71,71,71,71	0
56	MG	YA	3349	1/1	0.69	0.29	49,49,49,49	0
56	MG	RA	3960	1/1	0.69	0.58	89,89,89,89	0
56	MG	RA	3617	1/1	0.69	0.30	83,83,83,83	0
56	MG	RA	3963	1/1	0.69	0.20	110,110,110,110	0
56	MG	QA	1681	1/1	0.69	0.15	85,85,85,85	0
56	MG	XH	201	1/1	0.69	0.15	78,78,78,78	0
56	MG	QA	1796	1/1	0.69	0.32	73,73,73,73	0
56	MG	RA	3499	1/1	0.69	0.33	77,77,77,77	0
56	MG	RA	3638	1/1	0.69	0.29	85,85,85,85	0
56	MG	YA	3510	1/1	0.69	0.35	80,80,80,80	0
56	MG	YA	3557	1/1	0.69	0.40	67,67,67,67	0
56	MG	YA	3449	1/1	0.69	0.33	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3747	1/1	0.69	0.45	108,108,108,108	0
56	MG	YA	3094	1/1	0.69	0.17	68,68,68,68	0
56	MG	RB	203	1/1	0.69	0.33	106,106,106,106	0
56	MG	RA	3798	1/1	0.70	0.39	99,99,99,99	0
56	MG	RA	3809	1/1	0.70	0.29	76,76,76,76	0
56	MG	RA	3150	1/1	0.70	0.14	74,74,74,74	0
56	MG	QA	1788	1/1	0.70	0.20	81,81,81,81	0
56	MG	RA	3035	1/1	0.70	0.24	97,97,97,97	0
56	MG	QA	1761	1/1	0.70	0.41	72,72,72,72	0
56	MG	RA	3040	1/1	0.70	0.40	76,76,76,76	0
56	MG	RA	3864	1/1	0.70	0.33	76,76,76,76	0
56	MG	RA	3872	1/1	0.70	0.45	78,78,78,78	0
56	MG	RA	3292	1/1	0.70	0.11	83,83,83,83	0
56	MG	YA	3060	1/1	0.70	0.20	62,62,62,62	0
56	MG	XA	1770	1/1	0.70	0.19	104,104,104,104	0
56	MG	RA	3935	1/1	0.70	0.24	91,91,91,91	0
56	MG	RA	3061	1/1	0.70	0.12	84,84,84,84	0
56	MG	YA	3136	1/1	0.70	0.16	59,59,59,59	0
56	MG	XA	1777	1/1	0.70	0.59	98,98,98,98	0
56	MG	RF	310	1/1	0.70	0.39	88,88,88,88	0
56	MG	RA	3199	1/1	0.70	0.18	68,68,68,68	0
56	MG	YA	3281	1/1	0.70	0.57	60,60,60,60	0
56	MG	YA	3578	1/1	0.70	0.31	95,95,95,95	0
56	MG	QA	1662	1/1	0.70	0.31	82,82,82,82	0
56	MG	RA	3368	1/1	0.70	0.56	76,76,76,76	0
56	MG	RA	3762	1/1	0.70	0.12	76,76,76,76	0
56	MG	QA	1811	1/1	0.70	0.14	83,83,83,83	0
56	MG	RA	3992	1/1	0.70	0.21	74,74,74,74	0
56	MG	QA	1838	1/1	0.70	0.23	85,85,85,85	0
56	MG	XA	1749	1/1	0.70	0.36	82,82,82,82	0
56	MG	YA	3246	1/1	0.70	0.42	118,118,118,118	0
56	MG	RA	3252	1/1	0.70	0.40	91,91,91,91	0
56	MG	YA	3443	1/1	0.70	0.32	81,81,81,81	0
56	MG	RA	3457	1/1	0.71	0.47	81,81,81,81	0
56	MG	RA	3659	1/1	0.71	0.33	62,62,62,62	0
56	MG	RA	3559	1/1	0.71	0.33	97,97,97,97	0
56	MG	RA	3763	1/1	0.71	0.26	61,61,61,61	0
56	MG	XA	1693	1/1	0.71	0.29	81,81,81,81	0
56	MG	QG	202	1/1	0.71	0.21	92,92,92,92	0
56	MG	RA	3201	1/1	0.71	0.20	70,70,70,70	0
56	MG	XA	1702	1/1	0.71	0.23	61,61,61,61	0
56	MG	RA	3976	1/1	0.71	0.19	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RF	301	1/1	0.71	0.48	101,101,101,101	0
56	MG	QA	1624	1/1	0.71	0.41	73,73,73,73	0
56	MG	YA	3100	1/1	0.71	0.14	87,87,87,87	0
56	MG	RA	3791	1/1	0.71	0.26	64,64,64,64	0
56	MG	XA	1683	1/1	0.71	0.28	69,69,69,69	0
56	MG	RA	3228	1/1	0.71	0.39	101,101,101,101	0
56	MG	RA	3620	1/1	0.71	0.18	90,90,90,90	0
56	MG	RA	3517	1/1	0.71	0.55	107,107,107,107	0
56	MG	QA	1754	1/1	0.71	0.28	108,108,108,108	0
56	MG	QA	1643	1/1	0.71	0.33	86,86,86,86	0
56	MG	YA	3729	1/1	0.71	0.29	61,61,61,61	0
56	MG	RA	3433	1/1	0.71	0.22	66,66,66,66	0
56	MG	YA	3267	1/1	0.71	0.37	100,100,100,100	0
56	MG	RA	3735	1/1	0.71	0.23	66,66,66,66	0
56	MG	R8	101	1/1	0.71	0.35	75,75,75,75	0
56	MG	QA	1609	1/1	0.71	0.19	106,106,106,106	0
56	MG	XA	1716	1/1	0.71	0.24	57,57,57,57	0
56	MG	YA	3432	1/1	0.72	0.45	84,84,84,84	0
56	MG	RA	3573	1/1	0.72	0.46	91,91,91,91	0
56	MG	QA	1863	1/1	0.72	0.23	80,80,80,80	0
56	MG	XA	1650	1/1	0.72	0.19	84,84,84,84	0
56	MG	XA	1751	1/1	0.72	0.27	59,59,59,59	0
56	MG	RA	3598	1/1	0.72	0.41	94,94,94,94	0
56	MG	XA	1706	1/1	0.72	0.30	67,67,67,67	0
56	MG	RA	3903	1/1	0.72	0.21	57,57,57,57	0
56	MG	RA	3497	1/1	0.72	0.28	82,82,82,82	0
56	MG	QV	102	1/1	0.72	0.21	45,45,45,45	0
56	MG	RA	3621	1/1	0.72	0.23	61,61,61,61	0
56	MG	QA	1746	1/1	0.72	0.24	65,65,65,65	0
56	MG	RA	3263	1/1	0.72	0.16	67,67,67,67	0
56	MG	RA	3953	1/1	0.72	0.21	86,86,86,86	0
56	MG	YA	3405	1/1	0.72	0.36	86,86,86,86	0
56	MG	XA	1759	1/1	0.72	0.15	56,56,56,56	0
56	MG	YA	3517	1/1	0.72	0.39	92,92,92,92	0
56	MG	QA	1782	1/1	0.72	0.23	69,69,69,69	0
56	MG	RA	3775	1/1	0.72	0.23	56,56,56,56	0
56	MG	RA	3527	1/1	0.72	0.44	67,67,67,67	0
56	MG	RA	3533	1/1	0.72	0.14	49,49,49,49	0
56	MG	RA	3538	1/1	0.72	0.13	80,80,80,80	0
56	MG	YA	3490	1/1	0.72	0.51	104,104,104,104	0
56	MG	XA	1697	1/1	0.72	0.37	70,70,70,70	0
56	MG	QA	1851	1/1	0.72	0.21	94,94,94,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	R3	101	1/1	0.72	0.55	95,95,95,95	0
56	MG	QA	1787	1/1	0.72	0.27	76,76,76,76	0
56	MG	RA	3319	1/1	0.72	0.29	54,54,54,54	0
56	MG	XA	1661	1/1	0.72	0.20	87,87,87,87	0
56	MG	XA	1726	1/1	0.72	0.23	74,74,74,74	0
56	MG	QA	1676	1/1	0.72	0.13	88,88,88,88	0
56	MG	YA	3123	1/1	0.73	0.20	86,86,86,86	0
56	MG	YA	3108	1/1	0.73	0.46	98,98,98,98	0
56	MG	RA	3754	1/1	0.73	0.28	92,92,92,92	0
56	MG	YA	3658	1/1	0.73	0.28	77,77,77,77	0
56	MG	RA	3933	1/1	0.73	0.28	76,76,76,76	0
56	MG	YA	3461	1/1	0.73	0.38	81,81,81,81	0
56	MG	QA	1821	1/1	0.73	0.31	90,90,90,90	0
56	MG	RB	225	1/1	0.73	0.09	76,76,76,76	0
56	MG	RB	226	1/1	0.73	0.16	99,99,99,99	0
56	MG	RA	3669	1/1	0.73	0.29	81,81,81,81	0
56	MG	QA	1640	1/1	0.73	0.17	75,75,75,75	0
56	MG	YA	3707	1/1	0.73	0.41	95,95,95,95	0
56	MG	YA	3727	1/1	0.73	0.30	59,59,59,59	0
56	MG	YA	3495	1/1	0.73	0.28	63,63,63,63	0
56	MG	YA	3102	1/1	0.73	0.25	60,60,60,60	0
56	MG	RA	3600	1/1	0.73	0.26	87,87,87,87	0
56	MG	RA	3076	1/1	0.73	0.41	83,83,83,83	0
56	MG	XA	1734	1/1	0.73	0.24	78,78,78,78	0
56	MG	YA	3227	1/1	0.73	0.15	64,64,64,64	0
56	MG	XA	1658	1/1	0.73	0.20	79,79,79,79	0
56	MG	RA	3990	1/1	0.73	0.27	109,109,109,109	0
56	MG	RA	3818	1/1	0.73	0.20	67,67,67,67	0
56	MG	QA	1610	1/1	0.73	0.16	105,105,105,105	0
56	MG	RA	3631	1/1	0.73	0.56	125,125,125,125	0
56	MG	RA	3834	1/1	0.73	0.25	80,80,80,80	0
56	MG	QA	1749	1/1	0.73	0.35	56,56,56,56	0
56	MG	RA	3023	1/1	0.73	0.22	73,73,73,73	0
56	MG	RA	3636	1/1	0.73	0.59	91,91,91,91	0
56	MG	XA	1708	1/1	0.73	0.44	78,78,78,78	0
56	MG	RA	3871	1/1	0.73	0.21	77,77,77,77	0
56	MG	RA	3239	1/1	0.73	0.53	112,112,112,112	0
56	MG	RA	3426	1/1	0.74	0.39	88,88,88,88	0
56	MG	YA	3603	1/1	0.74	0.58	100,100,100,100	0
56	MG	QA	1869	1/1	0.74	0.20	61,61,61,61	0
56	MG	YA	3236	1/1	0.74	0.45	106,106,106,106	0
56	MG	YA	3403	1/1	0.74	0.22	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	XA	1649	1/1	0.74	0.20	92,92,92,92	0
56	MG	RA	3077	1/1	0.74	0.17	70,70,70,70	0
56	MG	RA	3453	1/1	0.74	0.31	64,64,64,64	0
56	MG	RA	4015	1/1	0.74	0.51	89,89,89,89	0
56	MG	RA	3261	1/1	0.74	0.27	82,82,82,82	0
56	MG	YA	3260	1/1	0.74	0.31	71,71,71,71	0
56	MG	YA	3468	1/1	0.74	0.42	58,58,58,58	0
56	MG	RA	3272	1/1	0.74	0.14	83,83,83,83	0
56	MG	RA	3102	1/1	0.74	0.32	107,107,107,107	0
56	MG	XA	1686	1/1	0.74	0.25	68,68,68,68	0
56	MG	XA	1747	1/1	0.74	0.28	59,59,59,59	0
56	MG	RA	3283	1/1	0.74	0.33	101,101,101,101	0
56	MG	YA	3523	1/1	0.74	0.20	56,56,56,56	0
56	MG	RA	3839	1/1	0.74	0.13	72,72,72,72	0
56	MG	RA	3514	1/1	0.74	0.22	87,87,87,87	0
56	MG	YA	3198	1/1	0.74	0.19	80,80,80,80	0
56	MG	YB	215	1/1	0.74	0.27	92,92,92,92	0
56	MG	YA	3566	1/1	0.74	0.24	60,60,60,60	0
56	MG	YD	301	1/1	0.74	0.23	60,60,60,60	0
56	MG	YA	3167	1/1	0.74	0.36	88,88,88,88	0
56	MG	RA	3171	1/1	0.74	0.19	89,89,89,89	0
56	MG	XA	1663	1/1	0.74	0.23	107,107,107,107	0
56	MG	RA	3537	1/1	0.74	0.27	93,93,93,93	0
56	MG	RA	3916	1/1	0.74	0.28	72,72,72,72	0
56	MG	RA	3357	1/1	0.74	0.17	61,61,61,61	0
56	MG	XA	1620	1/1	0.74	0.14	63,63,63,63	0
56	MG	QT	201	1/1	0.74	0.38	65,65,65,65	0
56	MG	RA	3940	1/1	0.74	0.18	83,83,83,83	0
56	MG	QA	1808	1/1	0.74	0.28	54,54,54,54	0
56	MG	QA	1809	1/1	0.74	0.16	67,67,67,67	0
56	MG	RT	201	1/1	0.74	0.23	77,77,77,77	0
56	MG	RA	3015	1/1	0.74	0.23	72,72,72,72	0
56	MG	XA	1668	1/1	0.74	0.28	87,87,87,87	0
56	MG	QA	1854	1/1	0.74	0.23	67,67,67,67	0
56	MG	R0	102	1/1	0.74	0.18	84,84,84,84	0
56	MG	R0	104	1/1	0.74	0.30	90,90,90,90	0
56	MG	YA	3154	1/1	0.74	0.28	86,86,86,86	0
56	MG	XA	1625	1/1	0.74	0.19	74,74,74,74	0
56	MG	XA	1715	1/1	0.74	0.27	55,55,55,55	0
56	MG	QA	1733	1/1	0.74	0.25	60,60,60,60	0
56	MG	QA	1765	1/1	0.74	0.26	83,83,83,83	0
56	MG	QA	1636	1/1	0.74	0.27	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
57	ZN	R4	101	1/1	0.74	0.18	269,269,269,269	0
56	MG	RA	3731	1/1	0.75	0.23	83,83,83,83	0
56	MG	XL	201	1/1	0.75	0.36	85,85,85,85	0
56	MG	QA	1847	1/1	0.75	0.43	64,64,64,64	0
56	MG	XA	1647	1/1	0.75	0.31	92,92,92,92	0
56	MG	YA	3445	1/1	0.75	0.24	72,72,72,72	0
56	MG	QA	1818	1/1	0.75	0.19	63,63,63,63	0
56	MG	QA	1661	1/1	0.75	0.41	81,81,81,81	0
56	MG	QA	1784	1/1	0.75	0.24	64,64,64,64	0
56	MG	QA	1753	1/1	0.75	0.22	71,71,71,71	0
56	MG	QN	102	1/1	0.75	0.15	68,68,68,68	0
56	MG	YA	3657	1/1	0.75	0.26	34,34,34,34	0
56	MG	QA	1639	1/1	0.75	0.22	79,79,79,79	0
56	MG	RA	3957	1/1	0.75	0.13	66,66,66,66	0
56	MG	XA	1698	1/1	0.75	0.32	66,66,66,66	0
56	MG	RA	3126	1/1	0.75	0.28	79,79,79,79	0
56	MG	YA	3190	1/1	0.75	0.12	78,78,78,78	0
56	MG	RA	3542	1/1	0.75	0.34	76,76,76,76	0
56	MG	QA	1864	1/1	0.75	0.29	90,90,90,90	0
56	MG	RA	3785	1/1	0.75	0.21	56,56,56,56	0
56	MG	QA	1672	1/1	0.75	0.34	45,45,45,45	0
56	MG	QA	1709	1/1	0.75	0.30	53,53,53,53	0
56	MG	YA	3492	1/1	0.75	0.39	63,63,63,63	0
56	MG	XA	1704	1/1	0.75	0.17	83,83,83,83	0
56	MG	YA	3249	1/1	0.75	0.34	72,72,72,72	0
56	MG	RA	3039	1/1	0.75	0.27	76,76,76,76	0
56	MG	QA	1611	1/1	0.75	0.48	89,89,89,89	0
56	MG	RA	3193	1/1	0.75	0.42	94,94,94,94	0
56	MG	R1	102	1/1	0.75	0.43	71,71,71,71	0
56	MG	RA	3710	1/1	0.75	0.49	70,70,70,70	0
56	MG	RA	3312	1/1	0.75	0.12	124,124,124,124	0
56	MG	XA	1643	1/1	0.75	0.11	80,80,80,80	0
56	MG	RA	3057	1/1	0.75	0.24	93,93,93,93	0
56	MG	XA	1645	1/1	0.75	0.24	93,93,93,93	0
56	MG	RA	3331	1/1	0.75	0.42	73,73,73,73	0
56	MG	QA	1770	1/1	0.75	0.15	73,73,73,73	0
56	MG	RA	3507	1/1	0.76	0.26	109,109,109,109	0
56	MG	XA	1723	1/1	0.76	0.21	75,75,75,75	0
56	MG	XA	1724	1/1	0.76	0.29	65,65,65,65	0
56	MG	YA	3712	1/1	0.76	0.34	51,51,51,51	0
56	MG	RA	3997	1/1	0.76	0.07	98,98,98,98	0
56	MG	YA	3082	1/1	0.76	0.25	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3639	1/1	0.76	0.41	65,65,65,65	0
56	MG	RA	4003	1/1	0.76	0.22	51,51,51,51	0
56	MG	RA	3212	1/1	0.76	0.41	95,95,95,95	0
56	MG	RA	3789	1/1	0.76	0.20	95,95,95,95	0
56	MG	YA	3509	1/1	0.76	0.29	71,71,71,71	0
56	MG	RA	4035	1/1	0.76	0.44	116,116,116,116	0
56	MG	RA	4042	1/1	0.76	0.17	80,80,80,80	0
56	MG	RB	201	1/1	0.76	0.20	72,72,72,72	0
56	MG	RA	3795	1/1	0.76	0.20	75,75,75,75	0
56	MG	RA	3645	1/1	0.76	0.32	84,84,84,84	0
56	MG	RA	3800	1/1	0.76	0.31	102,102,102,102	0
56	MG	YA	3621	1/1	0.76	0.28	49,49,49,49	0
56	MG	Y7	101	1/1	0.76	0.35	75,75,75,75	0
56	MG	XA	1748	1/1	0.76	0.21	60,60,60,60	0
56	MG	RA	3387	1/1	0.76	0.17	50,50,50,50	0
56	MG	YA	3191	1/1	0.76	0.17	76,76,76,76	0
56	MG	RA	3103	1/1	0.76	0.36	104,104,104,104	0
56	MG	XA	1604	1/1	0.76	0.32	99,99,99,99	0
56	MG	YA	3435	1/1	0.76	0.27	36,36,36,36	0
56	MG	YB	201	1/1	0.76	0.21	89,89,89,89	0
56	MG	RA	3685	1/1	0.76	0.25	97,97,97,97	0
56	MG	YA	3550	1/1	0.76	0.38	76,76,76,76	0
56	MG	QA	1728	1/1	0.76	0.22	64,64,64,64	0
56	MG	RA	3694	1/1	0.76	0.58	107,107,107,107	0
56	MG	RA	3003	1/1	0.76	0.29	73,73,73,73	0
56	MG	RA	3132	1/1	0.76	0.10	63,63,63,63	0
56	MG	RA	3564	1/1	0.76	0.40	101,101,101,101	0
56	MG	YA	3642	1/1	0.76	0.35	58,58,58,58	0
56	MG	RA	3927	1/1	0.76	0.39	81,81,81,81	0
56	MG	XA	1769	1/1	0.76	0.31	64,64,64,64	0
56	MG	YA	3171	1/1	0.76	0.40	104,104,104,104	0
56	MG	RA	3446	1/1	0.76	0.33	63,63,63,63	0
56	MG	RA	3580	1/1	0.76	0.39	112,112,112,112	0
56	MG	RN	203	1/1	0.76	0.19	86,86,86,86	0
56	MG	RP	202	1/1	0.76	0.14	78,78,78,78	0
56	MG	YA	3559	1/1	0.76	0.30	54,54,54,54	0
56	MG	RA	3590	1/1	0.76	0.30	104,104,104,104	0
56	MG	YA	3239	1/1	0.76	0.48	94,94,94,94	0
56	MG	RA	3954	1/1	0.76	0.29	77,77,77,77	0
56	MG	RA	3177	1/1	0.76	0.36	72,72,72,72	0
56	MG	YA	3160	1/1	0.76	0.44	67,67,67,67	0
56	MG	XA	1634	1/1	0.76	0.14	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3674	1/1	0.76	0.34	74,74,74,74	0
56	MG	YA	3699	1/1	0.76	0.35	66,66,66,66	0
56	MG	YA	3206	1/1	0.76	0.32	100,100,100,100	0
56	MG	YA	3710	1/1	0.76	0.22	61,61,61,61	0
56	MG	RA	3630	1/1	0.76	0.52	90,90,90,90	0
56	MG	RA	3985	1/1	0.76	0.32	81,81,81,81	0
56	MG	XA	1789	1/1	0.76	0.09	58,58,58,58	0
56	MG	RA	3649	1/1	0.77	0.28	85,85,85,85	0
56	MG	RA	3936	1/1	0.77	0.26	74,74,74,74	0
56	MG	RA	3327	1/1	0.77	0.30	62,62,62,62	0
56	MG	QA	1607	1/1	0.77	0.30	71,71,71,71	0
56	MG	YA	3126	1/1	0.77	0.18	91,91,91,91	0
56	MG	RA	3948	1/1	0.77	0.31	89,89,89,89	0
56	MG	RA	3567	1/1	0.77	0.22	81,81,81,81	0
56	MG	RA	3222	1/1	0.77	0.11	72,72,72,72	0
56	MG	YA	3529	1/1	0.77	0.33	73,73,73,73	0
56	MG	QA	1872	1/1	0.77	0.11	85,85,85,85	0
56	MG	YA	3018	1/1	0.77	0.32	75,75,75,75	0
56	MG	RA	3139	1/1	0.77	0.16	72,72,72,72	0
56	MG	RA	3366	1/1	0.77	0.33	72,72,72,72	0
56	MG	YQ	202	1/1	0.77	0.21	59,59,59,59	0
56	MG	RE	304	1/1	0.77	0.34	75,75,75,75	0
56	MG	RA	3973	1/1	0.77	0.34	84,84,84,84	0
56	MG	RA	3974	1/1	0.77	0.37	70,70,70,70	0
56	MG	RF	304	1/1	0.77	0.35	63,63,63,63	0
56	MG	YA	3087	1/1	0.77	0.23	64,64,64,64	0
56	MG	Y5	101	1/1	0.77	0.15	63,63,63,63	0
56	MG	YA	3597	1/1	0.77	0.26	74,74,74,74	0
56	MG	QA	1666	1/1	0.77	0.11	74,74,74,74	0
56	MG	RA	3824	1/1	0.77	0.36	76,76,76,76	0
56	MG	XA	1750	1/1	0.77	0.26	87,87,87,87	0
56	MG	QA	1817	1/1	0.77	0.20	64,64,64,64	0
56	MG	QA	1850	1/1	0.77	0.32	51,51,51,51	0
56	MG	RA	3524	1/1	0.77	0.25	71,71,71,71	0
56	MG	YA	3689	1/1	0.77	0.32	67,67,67,67	0
56	MG	XF	204	1/1	0.77	0.20	101,101,101,101	0
56	MG	YA	3369	1/1	0.77	0.20	63,63,63,63	0
56	MG	YA	3613	1/1	0.77	0.25	53,53,53,53	0
56	MG	YB	217	1/1	0.77	0.27	77,77,77,77	0
56	MG	RA	4011	1/1	0.77	0.14	83,83,83,83	0
56	MG	YA	3164	1/1	0.77	0.45	87,87,87,87	0
56	MG	YA	3166	1/1	0.77	0.33	132,132,132,132	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3179	1/1	0.77	0.26	69,69,69,69	0
56	MG	YA	3223	1/1	0.77	0.28	91,91,91,91	0
56	MG	RA	4058	1/1	0.77	0.42	120,120,120,120	0
56	MG	RA	3550	1/1	0.77	0.28	70,70,70,70	0
56	MG	RA	3444	1/1	0.77	0.69	83,83,83,83	0
56	MG	YA	3469	1/1	0.77	0.42	88,88,88,88	0
56	MG	QB	301	1/1	0.78	0.18	91,91,91,91	0
56	MG	XA	1665	1/1	0.78	0.15	73,73,73,73	0
56	MG	RA	3825	1/1	0.78	0.18	98,98,98,98	0
56	MG	RB	224	1/1	0.78	0.28	78,78,78,78	0
56	MG	XA	1644	1/1	0.78	0.19	61,61,61,61	0
56	MG	YA	3678	1/1	0.78	0.30	50,50,50,50	0
56	MG	RA	3248	1/1	0.78	0.16	56,56,56,56	0
56	MG	YA	3745	1/1	0.78	0.33	67,67,67,67	0
56	MG	RA	3251	1/1	0.78	0.33	69,69,69,69	0
56	MG	XA	1731	1/1	0.78	0.22	65,65,65,65	0
56	MG	RA	3486	1/1	0.78	0.44	78,78,78,78	0
56	MG	YE	301	1/1	0.78	0.38	95,95,95,95	0
56	MG	XA	1744	1/1	0.78	0.27	59,59,59,59	0
56	MG	YA	3086	1/1	0.78	0.34	95,95,95,95	0
56	MG	RA	3265	1/1	0.78	0.08	111,111,111,111	0
56	MG	RA	3663	1/1	0.78	0.29	77,77,77,77	0
56	MG	RA	3374	1/1	0.78	0.78	92,92,92,92	0
56	MG	YA	3695	1/1	0.78	0.44	76,76,76,76	0
56	MG	RA	3924	1/1	0.78	0.20	65,65,65,65	0
56	MG	RA	3510	1/1	0.78	0.13	38,38,38,38	0
56	MG	QA	1797	1/1	0.78	0.30	95,95,95,95	0
56	MG	YA	3303	1/1	0.78	0.23	85,85,85,85	0
56	MG	RA	4024	1/1	0.78	0.29	59,59,59,59	0
56	MG	YA	3173	1/1	0.78	0.34	85,85,85,85	0
56	MG	QA	1616	1/1	0.78	0.10	92,92,92,92	0
56	MG	RU	202	1/1	0.78	0.19	78,78,78,78	0
56	MG	RA	4046	1/1	0.78	0.43	86,86,86,86	0
56	MG	RA	4049	1/1	0.78	0.14	92,92,92,92	0
56	MG	QA	1804	1/1	0.78	0.29	71,71,71,71	0
56	MG	QA	1621	1/1	0.78	0.12	71,71,71,71	0
56	MG	RA	3790	1/1	0.78	0.21	82,82,82,82	0
56	MG	YA	3474	1/1	0.78	0.30	72,72,72,72	0
56	MG	RB	209	1/1	0.78	0.08	92,92,92,92	0
56	MG	YA	3255	1/1	0.78	0.20	88,88,88,88	0
56	MG	YB	214	1/1	0.78	0.20	45,45,45,45	0
56	MG	YA	3070	1/1	0.78	0.16	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
56	MG	YA	3667	1/1	0.78	0.20	90,90,90,90	0
56	MG	YA	3085	1/1	0.78	0.14	86,86,86,86	0
56	MG	XA	1623	1/1	0.79	0.36	73,73,73,73	0
56	MG	QA	1667	1/1	0.79	0.12	67,67,67,67	0
56	MG	YA	3042	1/1	0.79	0.20	61,61,61,61	0
56	MG	RA	3653	1/1	0.79	0.19	75,75,75,75	0
56	MG	RA	3934	1/1	0.79	0.07	62,62,62,62	0
56	MG	RA	3768	1/1	0.79	0.32	76,76,76,76	0
56	MG	QA	1760	1/1	0.79	0.40	77,77,77,77	0
56	MG	RA	3142	1/1	0.79	0.13	76,76,76,76	0
56	MG	RA	3661	1/1	0.79	0.20	89,89,89,89	0
56	MG	QA	1813	1/1	0.79	0.36	83,83,83,83	0
56	MG	RA	3665	1/1	0.79	0.34	77,77,77,77	0
56	MG	YA	3005	1/1	0.79	0.25	63,63,63,63	0
56	MG	RA	3299	1/1	0.79	0.41	96,96,96,96	0
56	MG	RA	3302	1/1	0.79	0.16	92,92,92,92	0
56	MG	RA	3956	1/1	0.79	0.35	77,77,77,77	0
56	MG	QA	1744	1/1	0.79	0.22	65,65,65,65	0
56	MG	RB	228	1/1	0.79	0.09	93,93,93,93	0
56	MG	RA	3679	1/1	0.79	0.27	54,54,54,54	0
56	MG	RA	3591	1/1	0.79	0.36	77,77,77,77	0
56	MG	YA	3718	1/1	0.79	0.13	60,60,60,60	0
56	MG	RA	3596	1/1	0.79	0.17	83,83,83,83	0
56	MG	RA	3522	1/1	0.79	0.18	55,55,55,55	0
56	MG	RA	3316	1/1	0.79	0.38	84,84,84,84	0
56	MG	RA	3607	1/1	0.79	0.33	98,98,98,98	0
56	MG	RA	3977	1/1	0.79	0.31	62,62,62,62	0
56	MG	YA	3726	1/1	0.79	0.36	81,81,81,81	0
56	MG	RA	3706	1/1	0.79	0.26	58,58,58,58	0
56	MG	RA	3241	1/1	0.79	0.35	108,108,108,108	0
56	MG	QA	1730	1/1	0.79	0.27	49,49,49,49	0
56	MG	XA	1772	1/1	0.79	0.35	51,51,51,51	0
56	MG	RA	3181	1/1	0.79	0.15	90,90,90,90	0
56	MG	RA	3841	1/1	0.79	0.33	64,64,64,64	0
56	MG	RA	3845	1/1	0.79	0.27	94,94,94,94	0
56	MG	XA	1722	1/1	0.79	0.08	67,67,67,67	0
56	MG	YA	3069	1/1	0.79	0.24	78,78,78,78	0
56	MG	YA	3646	1/1	0.79	0.17	69,69,69,69	0
56	MG	RA	3456	1/1	0.79	0.22	58,58,58,58	0
56	MG	RA	3195	1/1	0.79	0.34	115,115,115,115	0
56	MG	QA	1773	1/1	0.79	0.11	71,71,71,71	0
56	MG	YA	3418	1/1	0.79	0.38	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
56	MG	RA	4018	1/1	0.79	0.29	70,70,70,70	0
56	MG	QA	1830	1/1	0.79	0.18	85,85,85,85	0
56	MG	RA	3883	1/1	0.79	0.30	93,93,93,93	0
56	MG	RA	3890	1/1	0.79	0.41	57,57,57,57	0
56	MG	RA	3898	1/1	0.79	0.11	48,48,48,48	0
56	MG	RA	3558	1/1	0.79	0.33	82,82,82,82	0
56	MG	RA	3907	1/1	0.79	0.32	78,78,78,78	0
56	MG	YA	3737	1/1	0.79	0.72	107,107,107,107	0
56	MG	QA	1637	1/1	0.80	0.28	93,93,93,93	0
56	MG	RA	3227	1/1	0.80	0.26	93,93,93,93	0
56	MG	RA	3346	1/1	0.80	0.38	72,72,72,72	0
56	MG	RA	3704	1/1	0.80	0.34	91,91,91,91	0
56	MG	RA	4038	1/1	0.80	0.26	66,66,66,66	0
56	MG	RA	3593	1/1	0.80	0.29	66,66,66,66	0
56	MG	YA	3698	1/1	0.80	0.46	77,77,77,77	0
56	MG	RA	3713	1/1	0.80	0.27	47,47,47,47	0
56	MG	RA	3715	1/1	0.80	0.30	76,76,76,76	0
56	MG	RA	3719	1/1	0.80	0.19	55,55,55,55	0
56	MG	RA	3498	1/1	0.80	0.25	58,58,58,58	0
56	MG	RB	207	1/1	0.80	0.13	82,82,82,82	0
56	MG	YA	3645	1/1	0.80	0.26	67,67,67,67	0
56	MG	RA	3891	1/1	0.80	0.25	59,59,59,59	0
56	MG	RA	3505	1/1	0.80	0.16	64,64,64,64	0
56	MG	QA	1767	1/1	0.80	0.20	90,90,90,90	0
56	MG	RA	3362	1/1	0.80	0.31	93,93,93,93	0
56	MG	RA	3912	1/1	0.80	0.78	76,76,76,76	0
56	MG	YA	3251	1/1	0.80	0.26	100,100,100,100	0
56	MG	RA	3512	1/1	0.80	0.41	80,80,80,80	0
56	MG	YA	3649	1/1	0.80	0.28	60,60,60,60	0
56	MG	XA	1601	1/1	0.80	0.28	75,75,75,75	0
56	MG	RA	3629	1/1	0.80	0.30	60,60,60,60	0
56	MG	RA	3741	1/1	0.80	0.12	61,61,61,61	0
56	MG	QA	1860	1/1	0.80	0.19	100,100,100,100	0
56	MG	YA	3653	1/1	0.80	0.32	55,55,55,55	0
56	MG	RA	3017	1/1	0.80	0.42	68,68,68,68	0
56	MG	YA	3204	1/1	0.80	0.13	42,42,42,42	0
56	MG	QA	1696	1/1	0.80	0.12	73,73,73,73	0
56	MG	YA	3599	1/1	0.80	0.31	70,70,70,70	0
56	MG	XA	1718	1/1	0.80	0.29	73,73,73,73	0
56	MG	RA	3764	1/1	0.80	0.28	60,60,60,60	0
56	MG	XA	1680	1/1	0.80	0.17	77,77,77,77	0
56	MG	RA	3038	1/1	0.80	0.25	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
56	MG	RA	3642	1/1	0.80	0.18	70,70,70,70	0
56	MG	YA	3052	1/1	0.80	0.18	45,45,45,45	0
56	MG	YA	3186	1/1	0.80	0.14	39,39,39,39	0
56	MG	RG	202	1/1	0.80	0.16	85,85,85,85	0
56	MG	RA	3646	1/1	0.80	0.34	92,92,92,92	0
56	MG	QA	1660	1/1	0.80	0.21	77,77,77,77	0
56	MG	XA	1775	1/1	0.80	0.43	72,72,72,72	0
56	MG	YA	3732	1/1	0.80	0.38	73,73,73,73	0
56	MG	QA	1795	1/1	0.80	0.33	61,61,61,61	0
56	MG	XA	1687	1/1	0.80	0.21	101,101,101,101	0
56	MG	YA	3456	1/1	0.80	0.38	68,68,68,68	0
56	MG	RA	3557	1/1	0.80	0.23	63,63,63,63	0
56	MG	XA	1619	1/1	0.80	0.10	74,74,74,74	0
56	MG	RA	3667	1/1	0.80	0.19	60,60,60,60	0
56	MG	RA	3801	1/1	0.80	0.15	74,74,74,74	0
56	MG	YA	3197	1/1	0.80	0.23	77,77,77,77	0
56	MG	R0	103	1/1	0.80	0.54	81,81,81,81	0
56	MG	RA	3812	1/1	0.80	0.22	106,106,106,106	0
56	MG	YA	3676	1/1	0.80	0.44	73,73,73,73	0
56	MG	YA	3228	1/1	0.80	0.14	75,75,75,75	0
56	MG	RA	3317	1/1	0.80	0.27	73,73,73,73	0
56	MG	RA	3207	1/1	0.80	0.31	69,69,69,69	0
56	MG	RA	3459	1/1	0.80	0.40	78,78,78,78	0
56	MG	YA	3020	1/1	0.80	0.45	80,80,80,80	0
56	MG	XA	1790	1/1	0.80	0.11	98,98,98,98	0
56	MG	YA	3314	1/1	0.80	0.32	55,55,55,55	0
56	MG	RA	3310	1/1	0.81	0.19	96,96,96,96	0
56	MG	YA	3463	1/1	0.81	0.14	47,47,47,47	0
56	MG	YA	3419	1/1	0.81	0.33	66,66,66,66	0
56	MG	RA	3995	1/1	0.81	0.37	111,111,111,111	0
56	MG	YA	3103	1/1	0.81	0.16	63,63,63,63	0
56	MG	RA	3998	1/1	0.81	0.25	87,87,87,87	0
56	MG	YA	3567	1/1	0.81	0.26	42,42,42,42	0
56	MG	RA	3182	1/1	0.81	0.47	85,85,85,85	0
56	MG	RA	3019	1/1	0.81	0.39	113,113,113,113	0
56	MG	QA	1859	1/1	0.81	0.29	50,50,50,50	0
56	MG	RA	4008	1/1	0.81	0.51	86,86,86,86	0
56	MG	YA	3424	1/1	0.81	0.08	27,27,27,27	0
56	MG	RA	3806	1/1	0.81	0.36	78,78,78,78	0
56	MG	XA	1712	1/1	0.81	0.27	61,61,61,61	0
56	MG	YA	3001	1/1	0.81	0.25	90,90,90,90	0
56	MG	YA	3511	1/1	0.81	0.39	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3694	1/1	0.81	0.43	80,80,80,80	0
56	MG	YA	3516	1/1	0.81	0.37	78,78,78,78	0
56	MG	QA	1774	1/1	0.81	0.27	77,77,77,77	0
56	MG	YA	3200	1/1	0.81	0.41	70,70,70,70	0
56	MG	YA	3312	1/1	0.81	0.28	73,73,73,73	0
56	MG	RA	4054	1/1	0.81	0.44	97,97,97,97	0
56	MG	RA	3206	1/1	0.81	0.36	97,97,97,97	0
56	MG	RA	4066	1/1	0.81	0.28	78,78,78,78	0
56	MG	YA	3163	1/1	0.81	0.19	52,52,52,52	0
56	MG	RA	3545	1/1	0.81	0.25	70,70,70,70	0
56	MG	RA	3846	1/1	0.81	0.36	80,80,80,80	0
56	MG	YA	3003	1/1	0.81	0.41	106,106,106,106	0
56	MG	QA	1688	1/1	0.81	0.23	62,62,62,62	0
56	MG	YD	307	1/1	0.81	0.28	64,64,64,64	0
56	MG	RA	3551	1/1	0.81	0.24	72,72,72,72	0
56	MG	YA	3341	1/1	0.81	0.25	42,42,42,42	0
56	MG	RA	3075	1/1	0.81	0.18	56,56,56,56	0
56	MG	YA	3220	1/1	0.81	0.37	87,87,87,87	0
56	MG	RA	3232	1/1	0.81	0.33	57,57,57,57	0
56	MG	RA	3402	1/1	0.81	0.24	71,71,71,71	0
56	MG	YA	3722	1/1	0.81	0.31	89,89,89,89	0
56	MG	RA	3081	1/1	0.81	0.37	91,91,91,91	0
56	MG	RA	3090	1/1	0.81	0.34	93,93,93,93	0
56	MG	YA	3723	1/1	0.81	0.34	67,67,67,67	0
56	MG	XA	1740	1/1	0.81	0.27	65,65,65,65	0
56	MG	YA	3411	1/1	0.81	0.23	83,83,83,83	0
56	MG	YA	3538	1/1	0.81	0.26	44,44,44,44	0
56	MG	YA	3412	1/1	0.81	0.43	72,72,72,72	0
56	MG	RA	3583	1/1	0.81	0.20	72,72,72,72	0
56	MG	RE	302	1/1	0.81	0.35	109,109,109,109	0
56	MG	RA	3926	1/1	0.81	0.41	83,83,83,83	0
56	MG	QH	202	1/1	0.81	0.10	77,77,77,77	0
56	MG	RA	3438	1/1	0.81	0.20	71,71,71,71	0
56	MG	YA	3279	1/1	0.81	0.18	61,61,61,61	0
56	MG	RA	3118	1/1	0.81	0.23	76,76,76,76	0
56	MG	RA	3594	1/1	0.81	0.21	67,67,67,67	0
56	MG	YA	3192	1/1	0.81	0.21	71,71,71,71	0
56	MG	RA	3941	1/1	0.81	0.14	69,69,69,69	0
56	MG	YA	3180	1/1	0.81	0.25	43,43,43,43	0
56	MG	RA	3740	1/1	0.81	0.30	76,76,76,76	0
56	MG	RA	3128	1/1	0.81	0.20	48,48,48,48	0
56	MG	RA	3744	1/1	0.81	0.27	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3275	1/1	0.81	0.38	72,72,72,72	0
56	MG	RA	3751	1/1	0.81	0.11	51,51,51,51	0
56	MG	RA	3955	1/1	0.81	0.20	74,74,74,74	0
56	MG	RA	3602	1/1	0.81	0.44	80,80,80,80	0
56	MG	RA	3604	1/1	0.81	0.33	91,91,91,91	0
56	MG	Y8	101	1/1	0.81	0.39	70,70,70,70	0
56	MG	RV	204	1/1	0.81	0.50	70,70,70,70	0
56	MG	YA	3196	1/1	0.81	0.36	109,109,109,109	0
56	MG	RA	3758	1/1	0.81	0.15	49,49,49,49	0
56	MG	QO	101	1/1	0.81	0.13	79,79,79,79	0
56	MG	RA	3472	1/1	0.81	0.21	51,51,51,51	0
56	MG	QQ	201	1/1	0.81	0.12	71,71,71,71	0
56	MG	RA	3284	1/1	0.81	0.34	97,97,97,97	0
56	MG	QQ	202	1/1	0.81	0.11	68,68,68,68	0
56	MG	QA	1663	1/1	0.81	0.15	73,73,73,73	0
56	MG	QA	1852	1/1	0.81	0.25	60,60,60,60	0
56	MG	RA	3162	1/1	0.81	0.30	72,72,72,72	0
56	MG	RA	3002	1/1	0.81	0.32	70,70,70,70	0
56	MG	RA	3304	1/1	0.81	0.16	39,39,39,39	0
56	MG	XA	1605	1/1	0.82	0.18	72,72,72,72	0
56	MG	RA	4014	1/1	0.82	0.30	83,83,83,83	0
56	MG	RA	3276	1/1	0.82	0.30	91,91,91,91	0
56	MG	RA	3157	1/1	0.82	0.26	72,72,72,72	0
56	MG	YA	3563	1/1	0.82	0.43	76,76,76,76	0
56	MG	RA	3858	1/1	0.82	0.27	80,80,80,80	0
56	MG	RA	4029	1/1	0.82	0.20	91,91,91,91	0
56	MG	YA	3203	1/1	0.82	0.29	84,84,84,84	0
56	MG	YA	3230	1/1	0.82	0.34	57,57,57,57	0
56	MG	YA	3720	1/1	0.82	0.32	83,83,83,83	0
56	MG	RA	3454	1/1	0.82	0.10	51,51,51,51	0
56	MG	RA	3286	1/1	0.82	0.29	118,118,118,118	0
56	MG	QA	1614	1/1	0.82	0.15	48,48,48,48	0
56	MG	RA	3880	1/1	0.82	0.21	54,54,54,54	0
56	MG	RA	4065	1/1	0.82	0.25	86,86,86,86	0
56	MG	RA	3037	1/1	0.82	0.25	88,88,88,88	0
56	MG	RA	3461	1/1	0.82	0.41	76,76,76,76	0
56	MG	YA	3336	1/1	0.82	0.35	71,71,71,71	0
56	MG	RB	206	1/1	0.82	0.16	74,74,74,74	0
56	MG	RA	3296	1/1	0.82	0.21	102,102,102,102	0
56	MG	YA	3530	1/1	0.82	0.38	59,59,59,59	0
56	MG	YA	3586	1/1	0.82	0.42	48,48,48,48	0
56	MG	QA	1824	1/1	0.82	0.52	127,127,127,127	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	QA	1622	1/1	0.82	0.16	62,62,62,62	0
56	MG	RA	3921	1/1	0.82	0.38	88,88,88,88	0
56	MG	XA	1622	1/1	0.82	0.12	42,42,42,42	0
56	MG	YA	3588	1/1	0.82	0.23	76,76,76,76	0
56	MG	YA	3122	1/1	0.82	0.29	60,60,60,60	0
56	MG	YA	3731	1/1	0.82	0.25	32,32,32,32	0
56	MG	RA	3929	1/1	0.82	0.28	65,65,65,65	0
56	MG	QA	1742	1/1	0.82	0.23	58,58,58,58	0
56	MG	XA	1627	1/1	0.82	0.20	62,62,62,62	0
56	MG	XA	1632	1/1	0.82	0.31	59,59,59,59	0
56	MG	YA	3046	1/1	0.82	0.30	75,75,75,75	0
56	MG	QA	1791	1/1	0.82	0.38	96,96,96,96	0
56	MG	RA	3340	1/1	0.82	0.31	52,52,52,52	0
56	MG	RA	3088	1/1	0.82	0.54	89,89,89,89	0
56	MG	YA	3507	1/1	0.82	0.25	44,44,44,44	0
56	MG	RA	3093	1/1	0.82	0.11	72,72,72,72	0
56	MG	YG	202	1/1	0.82	0.16	78,78,78,78	0
56	MG	XA	1685	1/1	0.82	0.23	65,65,65,65	0
56	MG	RA	3224	1/1	0.82	0.27	96,96,96,96	0
56	MG	YA	3078	1/1	0.82	0.29	60,60,60,60	0
56	MG	YA	3422	1/1	0.82	0.23	122,122,122,122	0
56	MG	QA	1648	1/1	0.82	0.11	67,67,67,67	0
56	MG	RA	3535	1/1	0.82	0.25	57,57,57,57	0
56	MG	YA	3742	1/1	0.82	0.22	36,36,36,36	0
56	MG	RA	3788	1/1	0.82	0.18	75,75,75,75	0
56	MG	RA	3968	1/1	0.82	0.29	66,66,66,66	0
56	MG	YA	3222	1/1	0.82	0.33	71,71,71,71	0
56	MG	RA	3240	1/1	0.82	0.27	92,92,92,92	0
56	MG	YA	3304	1/1	0.82	0.29	56,56,56,56	0
56	MG	RA	3794	1/1	0.82	0.44	86,86,86,86	0
56	MG	RA	3246	1/1	0.82	0.26	69,69,69,69	0
56	MG	RA	3397	1/1	0.82	0.35	65,65,65,65	0
56	MG	RA	3121	1/1	0.82	0.28	83,83,83,83	0
56	MG	YA	3755	1/1	0.82	0.19	80,80,80,80	0
56	MG	RV	202	1/1	0.82	0.14	55,55,55,55	0
56	MG	YA	3146	1/1	0.82	0.19	60,60,60,60	0
56	MG	YA	3130	1/1	0.82	0.38	65,65,65,65	0
56	MG	RZ	301	1/1	0.82	0.09	66,66,66,66	0
56	MG	RA	3130	1/1	0.82	0.14	69,69,69,69	0
56	MG	RA	3556	1/1	0.82	0.30	75,75,75,75	0
56	MG	QA	1857	1/1	0.82	0.44	71,71,71,71	0
56	MG	RA	3005	1/1	0.82	0.26	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
56	MG	YA	3700	1/1	0.82	0.28	71,71,71,71	0
56	MG	RA	3826	1/1	0.82	0.21	62,62,62,62	0
56	MG	RA	3827	1/1	0.82	0.30	57,57,57,57	0
56	MG	YA	3437	1/1	0.82	0.34	85,85,85,85	0
56	MG	QA	1723	1/1	0.82	0.17	50,50,50,50	0
56	MG	RA	3152	1/1	0.82	0.19	106,106,106,106	0
56	MG	RA	3569	1/1	0.82	0.30	64,64,64,64	0
56	MG	XA	1626	1/1	0.83	0.52	77,77,77,77	0
56	MG	RA	3584	1/1	0.83	0.13	45,45,45,45	0
56	MG	YR	201	1/1	0.83	0.21	66,66,66,66	0
56	MG	RA	3059	1/1	0.83	0.21	76,76,76,76	0
56	MG	YT	202	1/1	0.83	0.25	84,84,84,84	0
56	MG	RA	3592	1/1	0.83	0.32	56,56,56,56	0
56	MG	YT	203	1/1	0.83	0.19	78,78,78,78	0
56	MG	YB	207	1/1	0.83	0.48	110,110,110,110	0
56	MG	RA	3726	1/1	0.83	0.24	53,53,53,53	0
56	MG	RA	4047	1/1	0.83	0.45	117,117,117,117	0
56	MG	XA	1778	1/1	0.83	0.29	60,60,60,60	0
56	MG	RA	4052	1/1	0.83	0.17	90,90,90,90	0
56	MG	RA	3074	1/1	0.83	0.10	52,52,52,52	0
56	MG	QA	1825	1/1	0.83	0.26	74,74,74,74	0
56	MG	YA	3161	1/1	0.83	0.30	76,76,76,76	0
56	MG	QA	1776	1/1	0.83	0.29	80,80,80,80	0
56	MG	YA	3464	1/1	0.83	0.33	73,73,73,73	0
56	MG	RB	202	1/1	0.83	0.13	55,55,55,55	0
56	MG	YA	3208	1/1	0.83	0.29	60,60,60,60	0
56	MG	RA	3737	1/1	0.83	0.22	77,77,77,77	0
56	MG	YA	3687	1/1	0.83	0.23	75,75,75,75	0
56	MG	QA	1833	1/1	0.83	0.26	51,51,51,51	0
56	MG	RA	3354	1/1	0.83	0.19	61,61,61,61	0
56	MG	YA	3210	1/1	0.83	0.27	65,65,65,65	0
56	MG	RA	3747	1/1	0.83	0.38	96,96,96,96	0
56	MG	YA	3641	1/1	0.83	0.41	86,86,86,86	0
56	MG	YA	3733	1/1	0.83	0.17	62,62,62,62	0
56	MG	QL	203	1/1	0.83	0.14	60,60,60,60	0
56	MG	RA	3755	1/1	0.83	0.34	71,71,71,71	0
56	MG	RA	3518	1/1	0.83	0.32	82,82,82,82	0
56	MG	QA	1741	1/1	0.83	0.30	45,45,45,45	0
56	MG	XA	1728	1/1	0.83	0.19	101,101,101,101	0
56	MG	RA	3760	1/1	0.83	0.18	74,74,74,74	0
56	MG	YA	3214	1/1	0.83	0.25	111,111,111,111	0
56	MG	QA	1641	1/1	0.83	0.34	105,105,105,105	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3245	1/1	0.83	0.14	81,81,81,81	0
56	MG	RA	3526	1/1	0.83	0.30	51,51,51,51	0
56	MG	RD	304	1/1	0.83	0.35	86,86,86,86	0
56	MG	RA	3772	1/1	0.83	0.25	57,57,57,57	0
56	MG	XF	202	1/1	0.83	0.10	73,73,73,73	0
56	MG	XA	1691	1/1	0.83	0.30	60,60,60,60	0
56	MG	QA	1747	1/1	0.83	0.35	72,72,72,72	0
56	MG	YA	3263	1/1	0.83	0.50	81,81,81,81	0
56	MG	YD	310	1/1	0.83	0.11	64,64,64,64	0
56	MG	XA	1653	1/1	0.83	0.33	79,79,79,79	0
56	MG	RF	309	1/1	0.83	0.34	68,68,68,68	0
56	MG	QA	1801	1/1	0.83	0.23	78,78,78,78	0
56	MG	RA	3652	1/1	0.83	0.33	88,88,88,88	0
56	MG	XK	201	1/1	0.83	0.09	53,53,53,53	0
56	MG	QA	1703	1/1	0.83	0.13	60,60,60,60	0
56	MG	XA	1613	1/1	0.83	0.10	51,51,51,51	0
56	MG	QA	1806	1/1	0.83	0.17	73,73,73,73	0
56	MG	RA	3425	1/1	0.83	0.29	94,94,94,94	0
56	MG	YA	3104	1/1	0.83	0.35	85,85,85,85	0
56	MG	YA	3101	1/1	0.83	0.34	70,70,70,70	0
56	MG	RO	201	1/1	0.83	0.21	93,93,93,93	0
56	MG	YA	3053	1/1	0.83	0.36	77,77,77,77	0
56	MG	RA	3670	1/1	0.83	0.17	80,80,80,80	0
56	MG	RA	3805	1/1	0.83	0.33	98,98,98,98	0
56	MG	RA	3034	1/1	0.83	0.34	100,100,100,100	0
56	MG	RA	3166	1/1	0.83	0.28	68,68,68,68	0
56	MG	RA	3169	1/1	0.83	0.19	82,82,82,82	0
56	MG	RA	3816	1/1	0.83	0.34	102,102,102,102	0
56	MG	QA	1655	1/1	0.83	0.20	64,64,64,64	0
56	MG	YA	3138	1/1	0.83	0.23	61,61,61,61	0
56	MG	R0	101	1/1	0.83	0.27	94,94,94,94	0
56	MG	RA	3996	1/1	0.83	0.40	73,73,73,73	0
56	MG	YA	3065	1/1	0.83	0.27	88,88,88,88	0
56	MG	YA	3288	1/1	0.83	0.30	53,53,53,53	0
56	MG	YA	3292	1/1	0.83	0.64	81,81,81,81	0
56	MG	QA	1724	1/1	0.83	0.25	76,76,76,76	0
56	MG	RA	3042	1/1	0.83	0.19	80,80,80,80	0
56	MG	RA	3831	1/1	0.83	0.23	65,65,65,65	0
56	MG	RA	4005	1/1	0.83	0.19	58,58,58,58	0
56	MG	YA	3555	1/1	0.83	0.34	77,77,77,77	0
56	MG	RA	3702	1/1	0.83	0.25	67,67,67,67	0
56	MG	RA	3458	1/1	0.83	0.23	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
56	MG	XA	1602	1/1	0.84	0.27	86,86,86,86	0
56	MG	RA	3842	1/1	0.84	0.21	72,72,72,72	0
56	MG	RA	3294	1/1	0.84	0.23	61,61,61,61	0
56	MG	RA	4021	1/1	0.84	0.14	56,56,56,56	0
56	MG	YA	3295	1/1	0.84	0.23	44,44,44,44	0
56	MG	YA	3525	1/1	0.84	0.33	86,86,86,86	0
56	MG	RA	3587	1/1	0.84	0.39	53,53,53,53	0
56	MG	RA	3095	1/1	0.84	0.40	88,88,88,88	0
56	MG	RA	3862	1/1	0.84	0.24	79,79,79,79	0
56	MG	YA	3562	1/1	0.84	0.25	70,70,70,70	0
56	MG	XA	1606	1/1	0.84	0.06	95,95,95,95	0
56	MG	RA	3311	1/1	0.84	0.37	100,100,100,100	0
56	MG	YA	3050	1/1	0.84	0.16	85,85,85,85	0
56	MG	YA	3238	1/1	0.84	0.24	91,91,91,91	0
56	MG	RA	4056	1/1	0.84	0.39	70,70,70,70	0
56	MG	YA	3470	1/1	0.84	0.18	59,59,59,59	0
56	MG	RA	3485	1/1	0.84	0.51	65,65,65,65	0
56	MG	RA	3881	1/1	0.84	0.48	68,68,68,68	0
56	MG	RA	3111	1/1	0.84	0.30	106,106,106,106	0
56	MG	RA	3214	1/1	0.84	0.23	59,59,59,59	0
56	MG	RA	3601	1/1	0.84	0.54	87,87,87,87	0
56	MG	QA	1630	1/1	0.84	0.16	81,81,81,81	0
56	MG	RA	3739	1/1	0.84	0.31	78,78,78,78	0
56	MG	QA	1677	1/1	0.84	0.35	94,94,94,94	0
56	MG	YA	3570	1/1	0.84	0.36	59,59,59,59	0
56	MG	QA	1771	1/1	0.84	0.13	57,57,57,57	0
56	MG	YA	3531	1/1	0.84	0.25	66,66,66,66	0
56	MG	XA	1733	1/1	0.84	0.16	72,72,72,72	0
56	MG	YB	202	1/1	0.84	0.15	56,56,56,56	0
56	MG	RA	3925	1/1	0.84	0.30	83,83,83,83	0
56	MG	RA	3352	1/1	0.84	0.29	65,65,65,65	0
56	MG	RA	3628	1/1	0.84	0.25	65,65,65,65	0
56	MG	QA	1865	1/1	0.84	0.29	75,75,75,75	0
56	MG	XA	1739	1/1	0.84	0.34	61,61,61,61	0
56	MG	XA	1656	1/1	0.84	0.25	80,80,80,80	0
56	MG	RA	3134	1/1	0.84	0.28	83,83,83,83	0
56	MG	RA	3244	1/1	0.84	0.16	71,71,71,71	0
56	MG	RA	3939	1/1	0.84	0.27	58,58,58,58	0
56	MG	XA	1618	1/1	0.84	0.36	72,72,72,72	0
56	MG	RA	3365	1/1	0.84	0.26	61,61,61,61	0
56	MG	XA	1701	1/1	0.84	0.30	51,51,51,51	0
56	MG	RA	3143	1/1	0.84	0.11	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
56	MG	RA	3769	1/1	0.84	0.36	46,46,46,46	0
56	MG	RA	3949	1/1	0.84	0.18	80,80,80,80	0
56	MG	YA	3135	1/1	0.84	0.50	89,89,89,89	0
56	MG	QA	1827	1/1	0.84	0.21	52,52,52,52	0
56	MG	RA	3371	1/1	0.84	0.37	75,75,75,75	0
56	MG	RA	3779	1/1	0.84	0.31	86,86,86,86	0
56	MG	YA	3051	1/1	0.84	0.18	64,64,64,64	0
56	MG	YA	3351	1/1	0.84	0.30	51,51,51,51	0
56	MG	RA	3380	1/1	0.84	0.24	43,43,43,43	0
56	MG	XT	201	1/1	0.84	0.13	65,65,65,65	0
56	MG	RA	3396	1/1	0.84	0.31	58,58,58,58	0
56	MG	RG	204	1/1	0.84	0.16	67,67,67,67	0
56	MG	RA	3258	1/1	0.84	0.35	96,96,96,96	0
56	MG	YA	3257	1/1	0.84	0.36	84,84,84,84	0
56	MG	YA	3115	1/1	0.84	0.24	52,52,52,52	0
56	MG	QA	1792	1/1	0.84	0.22	69,69,69,69	0
56	MG	YX	101	1/1	0.84	0.25	31,31,31,31	0
56	MG	RP	201	1/1	0.84	0.50	72,72,72,72	0
56	MG	RA	3407	1/1	0.84	0.35	34,34,34,34	0
56	MG	Y0	101	1/1	0.84	0.40	65,65,65,65	0
56	MG	RT	202	1/1	0.84	0.17	65,65,65,65	0
56	MG	RA	3176	1/1	0.84	0.43	96,96,96,96	0
56	MG	QG	201	1/1	0.84	0.21	91,91,91,91	0
56	MG	RA	3555	1/1	0.84	0.55	68,68,68,68	0
56	MG	QA	1711	1/1	0.84	0.17	63,63,63,63	0
56	MG	RA	3180	1/1	0.84	0.22	75,75,75,75	0
56	MG	RA	3279	1/1	0.84	0.31	103,103,103,103	0
56	MG	RX	101	1/1	0.84	0.24	51,51,51,51	0
56	MG	YA	3133	1/1	0.84	0.28	91,91,91,91	0
56	MG	YA	3330	1/1	0.84	0.26	62,62,62,62	0
56	MG	YA	3616	1/1	0.84	0.38	53,53,53,53	0
56	MG	RA	3566	1/1	0.84	0.21	57,57,57,57	0
56	MG	RA	3689	1/1	0.84	0.45	70,70,70,70	0
56	MG	RA	3285	1/1	0.84	0.20	85,85,85,85	0
56	MG	R1	103	1/1	0.84	0.13	55,55,55,55	0
56	MG	XA	1771	1/1	0.84	0.32	62,62,62,62	0
56	MG	RA	3696	1/1	0.84	0.36	74,74,74,74	0
56	MG	YA	3248	1/1	0.84	0.21	105,105,105,105	0
56	MG	YA	3493	1/1	0.84	0.21	74,74,74,74	0
56	MG	RA	3703	1/1	0.84	0.33	71,71,71,71	0
56	MG	RA	3837	1/1	0.84	0.19	59,59,59,59	0
56	MG	RA	3448	1/1	0.84	0.28	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3865	1/1	0.85	0.30	51,51,51,51	0
56	MG	RA	3866	1/1	0.85	0.11	76,76,76,76	0
56	MG	RA	3867	1/1	0.85	0.17	63,63,63,63	0
56	MG	YA	3551	1/1	0.85	0.31	60,60,60,60	0
56	MG	RA	3603	1/1	0.85	0.38	101,101,101,101	0
56	MG	RA	3129	1/1	0.85	0.19	45,45,45,45	0
56	MG	XA	1713	1/1	0.85	0.24	49,49,49,49	0
56	MG	YA	3693	1/1	0.85	0.25	60,60,60,60	0
56	MG	YA	3359	1/1	0.85	0.25	72,72,72,72	0
56	MG	YA	3622	1/1	0.85	0.30	49,49,49,49	0
56	MG	RA	3136	1/1	0.85	0.29	84,84,84,84	0
56	MG	XA	1629	1/1	0.85	0.13	51,51,51,51	0
56	MG	XA	1720	1/1	0.85	0.33	63,63,63,63	0
56	MG	QA	1868	1/1	0.85	0.35	58,58,58,58	0
56	MG	YA	3519	1/1	0.85	0.44	79,79,79,79	0
56	MG	RA	3250	1/1	0.85	0.29	69,69,69,69	0
56	MG	RA	3151	1/1	0.85	0.27	59,59,59,59	0
56	MG	RA	3918	1/1	0.85	0.40	71,71,71,71	0
56	MG	YA	3420	1/1	0.85	0.13	39,39,39,39	0
56	MG	YA	3218	1/1	0.85	0.39	89,89,89,89	0
56	MG	RA	3759	1/1	0.85	0.26	67,67,67,67	0
56	MG	YB	208	1/1	0.85	0.15	81,81,81,81	0
56	MG	RA	3259	1/1	0.85	0.11	87,87,87,87	0
56	MG	RA	3377	1/1	0.85	0.29	42,42,42,42	0
56	MG	QA	1679	1/1	0.85	0.19	64,64,64,64	0
56	MG	RA	3528	1/1	0.85	0.31	76,76,76,76	0
56	MG	RA	3530	1/1	0.85	0.19	75,75,75,75	0
56	MG	QA	1632	1/1	0.85	0.15	70,70,70,70	0
56	MG	RA	3163	1/1	0.85	0.69	93,93,93,93	0
56	MG	RA	3536	1/1	0.85	0.30	64,64,64,64	0
56	MG	RA	3268	1/1	0.85	0.26	95,95,95,95	0
56	MG	RA	3650	1/1	0.85	0.32	69,69,69,69	0
56	MG	RA	3053	1/1	0.85	0.35	89,89,89,89	0
56	MG	QA	1877	1/1	0.85	0.19	94,94,94,94	0
56	MG	XA	1642	1/1	0.85	0.22	55,55,55,55	0
56	MG	YA	3497	1/1	0.85	0.21	63,63,63,63	0
56	MG	RA	3950	1/1	0.85	0.26	87,87,87,87	0
56	MG	YA	3450	1/1	0.85	0.36	79,79,79,79	0
56	MG	RA	3952	1/1	0.85	0.26	49,49,49,49	0
56	MG	YA	3565	1/1	0.85	0.34	85,85,85,85	0
56	MG	YA	3368	1/1	0.85	0.25	62,62,62,62	0
56	MG	RA	3415	1/1	0.85	0.28	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
56	MG	QE	201	1/1	0.85	0.27	84,84,84,84	0
56	MG	QA	1689	1/1	0.85	0.29	80,80,80,80	0
56	MG	YA	3502	1/1	0.85	0.29	79,79,79,79	0
56	MG	QA	1691	1/1	0.85	0.27	104,104,104,104	0
56	MG	YA	3176	1/1	0.85	0.22	102,102,102,102	0
56	MG	YA	3221	1/1	0.85	0.40	77,77,77,77	0
56	MG	RA	3290	1/1	0.85	0.27	74,74,74,74	0
56	MG	RA	3086	1/1	0.85	0.49	124,124,124,124	0
56	MG	YA	3375	1/1	0.85	0.36	55,55,55,55	0
56	MG	RA	3810	1/1	0.85	0.18	75,75,75,75	0
56	MG	RA	3440	1/1	0.85	0.32	57,57,57,57	0
56	MG	RA	3978	1/1	0.85	0.35	55,55,55,55	0
56	MG	RA	3981	1/1	0.85	0.08	69,69,69,69	0
56	MG	RA	3089	1/1	0.85	0.21	67,67,67,67	0
56	MG	YA	3124	1/1	0.85	0.26	54,54,54,54	0
56	MG	YA	3541	1/1	0.85	0.24	20,20,20,20	0
56	MG	QA	1700	1/1	0.85	0.26	66,66,66,66	0
56	MG	YA	3485	1/1	0.85	0.50	77,77,77,77	0
56	MG	RA	3305	1/1	0.85	0.17	98,98,98,98	0
56	MG	RA	3578	1/1	0.85	0.21	60,60,60,60	0
56	MG	XA	1655	1/1	0.85	0.28	84,84,84,84	0
56	MG	YA	3384	1/1	0.85	0.24	38,38,38,38	0
56	MG	YA	3043	1/1	0.85	0.28	62,62,62,62	0
56	MG	RA	3835	1/1	0.85	0.38	56,56,56,56	0
56	MG	RA	3208	1/1	0.85	0.15	70,70,70,70	0
56	MG	YA	3609	1/1	0.85	0.18	51,51,51,51	0
56	MG	YA	3682	1/1	0.85	0.13	37,37,37,37	0
56	MG	RA	3466	1/1	0.85	0.34	56,56,56,56	0
56	MG	QA	1758	1/1	0.85	0.36	76,76,76,76	0
56	MG	RA	3476	1/1	0.85	0.30	30,30,30,30	0
56	MG	YA	3683	1/1	0.85	0.30	39,39,39,39	0
56	MG	RA	3849	1/1	0.85	0.12	52,52,52,52	0
56	MG	RA	4013	1/1	0.85	0.22	76,76,76,76	0
56	MG	R5	101	1/1	0.85	0.37	105,105,105,105	0
56	MG	QA	1714	1/1	0.85	0.13	42,42,42,42	0
56	MG	RA	3329	1/1	0.85	0.16	86,86,86,86	0
56	MG	YA	3026	1/1	0.85	0.29	93,93,93,93	0
56	MG	XA	1760	1/1	0.85	0.30	71,71,71,71	0
56	MG	YA	3688	1/1	0.85	0.30	62,62,62,62	0
56	MG	YD	305	1/1	0.86	0.33	82,82,82,82	0
56	MG	YA	3264	1/1	0.86	0.21	88,88,88,88	0
56	MG	RA	3520	1/1	0.86	0.19	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	4051	1/1	0.86	0.25	63,63,63,63	0
56	MG	YA	3019	1/1	0.86	0.32	81,81,81,81	0
56	MG	RA	3018	1/1	0.86	0.28	89,89,89,89	0
56	MG	XA	1617	1/1	0.86	0.23	44,44,44,44	0
56	MG	YA	3032	1/1	0.86	0.34	80,80,80,80	0
56	MG	RA	3369	1/1	0.86	0.23	47,47,47,47	0
56	MG	YA	3596	1/1	0.86	0.24	39,39,39,39	0
56	MG	YA	3313	1/1	0.86	0.34	46,46,46,46	0
56	MG	XA	1667	1/1	0.86	0.10	77,77,77,77	0
56	MG	YA	3383	1/1	0.86	0.25	70,70,70,70	0
56	MG	QV	101	1/1	0.86	0.28	118,118,118,118	0
56	MG	YA	3429	1/1	0.86	0.34	67,67,67,67	0
56	MG	RA	3260	1/1	0.86	0.43	71,71,71,71	0
56	MG	YA	3271	1/1	0.86	0.23	70,70,70,70	0
56	MG	RA	3156	1/1	0.86	0.32	117,117,117,117	0
56	MG	YO	201	1/1	0.86	0.21	78,78,78,78	0
56	MG	QA	1704	1/1	0.86	0.24	74,74,74,74	0
56	MG	RA	3662	1/1	0.86	0.34	89,89,89,89	0
56	MG	YA	3434	1/1	0.86	0.23	55,55,55,55	0
56	MG	RA	3050	1/1	0.86	0.43	88,88,88,88	0
56	MG	RB	218	1/1	0.86	0.19	79,79,79,79	0
56	MG	RB	221	1/1	0.86	0.20	64,64,64,64	0
56	MG	RA	3274	1/1	0.86	0.29	101,101,101,101	0
56	MG	YA	3272	1/1	0.86	0.20	39,39,39,39	0
56	MG	YA	3038	1/1	0.86	0.28	48,48,48,48	0
56	MG	YA	3225	1/1	0.86	0.23	74,74,74,74	0
56	MG	YW	202	1/1	0.86	0.14	55,55,55,55	0
56	MG	YA	3757	1/1	0.86	0.21	70,70,70,70	0
56	MG	XA	1736	1/1	0.86	0.20	58,58,58,58	0
56	MG	QA	1656	1/1	0.86	0.25	58,58,58,58	0
56	MG	RA	3063	1/1	0.86	0.18	41,41,41,41	0
56	MG	RA	3432	1/1	0.86	0.14	58,58,58,58	0
56	MG	RA	3064	1/1	0.86	0.10	54,54,54,54	0
56	MG	RA	3814	1/1	0.86	0.37	63,63,63,63	0
56	MG	XR	101	1/1	0.86	0.23	89,89,89,89	0
56	MG	RA	3817	1/1	0.86	0.34	76,76,76,76	0
56	MG	RA	3970	1/1	0.86	0.32	31,31,31,31	0
56	MG	RA	3066	1/1	0.86	0.24	56,56,56,56	0
56	MG	XA	1641	1/1	0.86	0.25	61,61,61,61	0
56	MG	YA	3514	1/1	0.86	0.38	62,62,62,62	0
56	MG	RF	311	1/1	0.86	0.35	74,74,74,74	0
56	MG	YA	3635	1/1	0.86	0.25	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	QA	1772	1/1	0.86	0.36	79,79,79,79	0
56	MG	YA	3039	1/1	0.86	0.31	73,73,73,73	0
56	MG	YA	3140	1/1	0.86	0.35	65,65,65,65	0
56	MG	XA	1646	1/1	0.86	0.21	63,63,63,63	0
56	MG	XA	1696	1/1	0.86	0.23	67,67,67,67	0
56	MG	QA	1778	1/1	0.86	0.27	61,61,61,61	0
56	MG	RN	201	1/1	0.86	0.25	85,85,85,85	0
56	MG	YA	3706	1/1	0.86	0.28	79,79,79,79	0
56	MG	YA	3004	1/1	0.86	0.08	43,43,43,43	0
56	MG	QA	1669	1/1	0.86	0.29	71,71,71,71	0
56	MG	YA	3169	1/1	0.86	0.28	91,91,91,91	0
56	MG	QA	1673	1/1	0.86	0.13	52,52,52,52	0
56	MG	RQ	203	1/1	0.86	0.27	82,82,82,82	0
56	MG	RR	3203	1/1	0.86	0.32	84,84,84,84	0
56	MG	YA	3127	1/1	0.86	0.13	50,50,50,50	0
56	MG	YA	3713	1/1	0.86	0.50	67,67,67,67	0
56	MG	RA	3219	1/1	0.86	0.16	66,66,66,66	0
56	MG	RA	3104	1/1	0.86	0.17	57,57,57,57	0
56	MG	QA	1613	1/1	0.86	0.10	97,97,97,97	0
56	MG	YA	3716	1/1	0.86	0.27	65,65,65,65	0
56	MG	RA	3332	1/1	0.86	0.13	53,53,53,53	0
56	MG	RA	3334	1/1	0.86	0.26	46,46,46,46	0
56	MG	RA	4006	1/1	0.86	0.26	81,81,81,81	0
56	MG	RA	3338	1/1	0.86	0.36	38,38,38,38	0
56	MG	RA	4010	1/1	0.86	0.23	76,76,76,76	0
56	MG	QR	101	1/1	0.86	0.17	71,71,71,71	0
56	MG	XA	1764	1/1	0.86	0.33	52,52,52,52	0
56	MG	RA	3229	1/1	0.86	0.36	82,82,82,82	0
56	MG	RA	3344	1/1	0.86	0.29	51,51,51,51	0
56	MG	YA	3360	1/1	0.86	0.27	53,53,53,53	0
56	MG	RA	3351	1/1	0.86	0.18	70,70,70,70	0
56	MG	YA	3526	1/1	0.86	0.21	43,43,43,43	0
56	MG	YA	3056	1/1	0.86	0.26	81,81,81,81	0
56	MG	RA	3753	1/1	0.86	0.35	48,48,48,48	0
56	MG	YA	3097	1/1	0.86	0.20	37,37,37,37	0
56	MG	RA	3009	1/1	0.86	0.11	53,53,53,53	0
56	MG	RA	4040	1/1	0.86	0.29	69,69,69,69	0
56	MG	RA	3243	1/1	0.86	0.25	73,73,73,73	0
56	MG	RA	3342	1/1	0.87	0.33	60,60,60,60	0
56	MG	YA	3031	1/1	0.87	0.24	46,46,46,46	0
56	MG	RA	3859	1/1	0.87	0.31	72,72,72,72	0
56	MG	RA	3462	1/1	0.87	0.21	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
56	MG	RA	4026	1/1	0.87	0.25	71,71,71,71	0
56	MG	YA	3748	1/1	0.87	0.30	95,95,95,95	0
56	MG	RA	4031	1/1	0.87	0.29	102,102,102,102	0
56	MG	RA	4034	1/1	0.87	0.22	73,73,73,73	0
56	MG	QA	1836	1/1	0.87	0.27	89,89,89,89	0
56	MG	YA	3479	1/1	0.87	0.24	50,50,50,50	0
56	MG	RA	3475	1/1	0.87	0.40	46,46,46,46	0
56	MG	YA	3623	1/1	0.87	0.25	54,54,54,54	0
56	MG	RA	3868	1/1	0.87	0.25	48,48,48,48	0
56	MG	QH	201	1/1	0.87	0.28	76,76,76,76	0
56	MG	RA	3484	1/1	0.87	0.25	30,30,30,30	0
56	MG	RA	3599	1/1	0.87	0.22	66,66,66,66	0
56	MG	RA	3167	1/1	0.87	0.10	69,69,69,69	0
56	MG	RA	4053	1/1	0.87	0.20	74,74,74,74	0
56	MG	YA	3624	1/1	0.87	0.42	71,71,71,71	0
56	MG	RA	4055	1/1	0.87	0.25	86,86,86,86	0
56	MG	RA	3360	1/1	0.87	0.33	66,66,66,66	0
56	MG	YA	3482	1/1	0.87	0.29	65,65,65,65	0
56	MG	RA	3887	1/1	0.87	0.22	53,53,53,53	0
56	MG	XA	1681	1/1	0.87	0.19	106,106,106,106	0
56	MG	RA	3363	1/1	0.87	0.22	50,50,50,50	0
56	MG	YA	3372	1/1	0.87	0.33	49,49,49,49	0
56	MG	YA	3109	1/1	0.87	0.19	35,35,35,35	0
56	MG	RA	3178	1/1	0.87	0.28	79,79,79,79	0
56	MG	RA	3909	1/1	0.87	0.25	73,73,73,73	0
56	MG	RA	3911	1/1	0.87	0.18	46,46,46,46	0
56	MG	YA	3012	1/1	0.87	0.14	56,56,56,56	0
56	MG	RA	3914	1/1	0.87	0.25	56,56,56,56	0
56	MG	YA	3639	1/1	0.87	0.33	74,74,74,74	0
56	MG	RA	3083	1/1	0.87	0.25	80,80,80,80	0
56	MG	YA	3116	1/1	0.87	0.19	58,58,58,58	0
56	MG	YA	3231	1/1	0.87	0.21	59,59,59,59	0
56	MG	RA	3373	1/1	0.87	0.28	44,44,44,44	0
56	MG	QA	1699	1/1	0.87	0.15	65,65,65,65	0
56	MG	RB	220	1/1	0.87	0.36	47,47,47,47	0
56	MG	YB	213	1/1	0.87	0.28	57,57,57,57	0
56	MG	YA	3392	1/1	0.87	0.28	54,54,54,54	0
56	MG	RA	3379	1/1	0.87	0.33	44,44,44,44	0
56	MG	YA	3181	1/1	0.87	0.22	66,66,66,66	0
56	MG	RA	3386	1/1	0.87	0.23	26,26,26,26	0
56	MG	RA	3282	1/1	0.87	0.26	109,109,109,109	0
56	MG	RA	3389	1/1	0.87	0.24	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3390	1/1	0.87	0.26	27,27,27,27	0
56	MG	YA	3576	1/1	0.87	0.28	37,37,37,37	0
56	MG	YA	3183	1/1	0.87	0.14	47,47,47,47	0
56	MG	QA	1654	1/1	0.87	0.21	64,64,64,64	0
56	MG	RA	3648	1/1	0.87	0.28	82,82,82,82	0
56	MG	RE	301	1/1	0.87	0.42	81,81,81,81	0
56	MG	RA	3532	1/1	0.87	0.10	52,52,52,52	0
56	MG	RA	3008	1/1	0.87	0.08	46,46,46,46	0
56	MG	YA	3273	1/1	0.87	0.18	72,72,72,72	0
56	MG	XA	1700	1/1	0.87	0.23	43,43,43,43	0
56	MG	RF	303	1/1	0.87	0.32	80,80,80,80	0
56	MG	RA	3108	1/1	0.87	0.25	69,69,69,69	0
56	MG	YA	3584	1/1	0.87	0.21	56,56,56,56	0
56	MG	XA	1611	1/1	0.87	0.18	73,73,73,73	0
56	MG	RA	3413	1/1	0.87	0.20	34,34,34,34	0
56	MG	RA	3114	1/1	0.87	0.33	91,91,91,91	0
56	MG	RA	3797	1/1	0.87	0.32	84,84,84,84	0
56	MG	RA	3418	1/1	0.87	0.38	36,36,36,36	0
56	MG	RA	3421	1/1	0.87	0.12	42,42,42,42	0
56	MG	RA	3962	1/1	0.87	0.29	62,62,62,62	0
56	MG	YA	3118	1/1	0.87	0.17	91,91,91,91	0
56	MG	RA	3802	1/1	0.87	0.41	89,89,89,89	0
56	MG	RA	3215	1/1	0.87	0.29	98,98,98,98	0
56	MG	YA	3659	1/1	0.87	0.23	29,29,29,29	0
56	MG	RA	3807	1/1	0.87	0.30	70,70,70,70	0
56	MG	XA	1755	1/1	0.87	0.22	43,43,43,43	0
56	MG	YA	3661	1/1	0.87	0.38	63,63,63,63	0
56	MG	RA	3811	1/1	0.87	0.12	55,55,55,55	0
56	MG	YA	3404	1/1	0.87	0.29	13,13,13,13	0
56	MG	YA	3064	1/1	0.87	0.17	55,55,55,55	0
56	MG	RA	3434	1/1	0.87	0.32	61,61,61,61	0
56	MG	XA	1762	1/1	0.87	0.08	48,48,48,48	0
56	MG	RA	3687	1/1	0.87	0.17	57,57,57,57	0
56	MG	RA	3821	1/1	0.87	0.27	29,29,29,29	0
56	MG	YA	3671	1/1	0.87	0.27	37,37,37,37	0
56	MG	XA	1767	1/1	0.87	0.27	37,37,37,37	0
56	MG	RA	3690	1/1	0.87	0.46	74,74,74,74	0
56	MG	YA	3361	1/1	0.87	0.13	65,65,65,65	0
56	MG	YA	3071	1/1	0.87	0.23	77,77,77,77	0
56	MG	YA	3442	1/1	0.87	0.27	53,53,53,53	0
56	MG	RA	3829	1/1	0.87	0.51	65,65,65,65	0
56	MG	RA	3699	1/1	0.87	0.14	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	XA	1714	1/1	0.87	0.16	58,58,58,58	0
56	MG	RA	3450	1/1	0.87	0.48	53,53,53,53	0
56	MG	RA	3836	1/1	0.87	0.26	91,91,91,91	0
56	MG	YA	3316	1/1	0.87	0.17	53,53,53,53	0
56	MG	RA	3575	1/1	0.87	0.25	62,62,62,62	0
56	MG	RA	3840	1/1	0.87	0.16	83,83,83,83	0
56	MG	YA	3324	1/1	0.87	0.35	39,39,39,39	0
56	MG	R5	103	1/1	0.87	0.25	59,59,59,59	0
56	MG	RA	3052	1/1	0.87	0.26	85,85,85,85	0
56	MG	QA	1779	1/1	0.87	0.12	80,80,80,80	0
56	MG	YA	3447	1/1	0.87	0.26	68,68,68,68	0
56	MG	QA	1627	1/1	0.87	0.10	42,42,42,42	0
56	MG	RA	3586	1/1	0.87	0.26	73,73,73,73	0
56	MG	XA	1630	1/1	0.88	0.18	62,62,62,62	0
56	MG	QA	1705	1/1	0.88	0.21	37,37,37,37	0
56	MG	QA	1670	1/1	0.88	0.24	81,81,81,81	0
56	MG	YA	3454	1/1	0.88	0.49	52,52,52,52	0
56	MG	YA	3024	1/1	0.88	0.43	59,59,59,59	0
56	MG	RA	3732	1/1	0.88	0.11	54,54,54,54	0
56	MG	RD	301	1/1	0.88	0.41	76,76,76,76	0
56	MG	YA	3309	1/1	0.88	0.14	37,37,37,37	0
56	MG	RA	3428	1/1	0.88	0.16	60,60,60,60	0
56	MG	RD	311	1/1	0.88	0.24	70,70,70,70	0
56	MG	RD	312	1/1	0.88	0.18	76,76,76,76	0
56	MG	YA	3520	1/1	0.88	0.20	68,68,68,68	0
56	MG	RA	3815	1/1	0.88	0.11	68,68,68,68	0
56	MG	YA	3178	1/1	0.88	0.15	62,62,62,62	0
56	MG	RA	3085	1/1	0.88	0.17	76,76,76,76	0
56	MG	RE	306	1/1	0.88	0.17	59,59,59,59	0
56	MG	YA	3438	1/1	0.88	0.21	45,45,45,45	0
56	MG	RA	3819	1/1	0.88	0.19	33,33,33,33	0
56	MG	RA	3657	1/1	0.88	0.22	65,65,65,65	0
56	MG	RA	3742	1/1	0.88	0.12	81,81,81,81	0
56	MG	RA	3931	1/1	0.88	0.31	73,73,73,73	0
56	MG	RA	3223	1/1	0.88	0.14	63,63,63,63	0
56	MG	RA	3026	1/1	0.88	0.28	72,72,72,72	0
56	MG	QA	1815	1/1	0.88	0.24	65,65,65,65	0
56	MG	RA	3750	1/1	0.88	0.44	66,66,66,66	0
56	MG	XA	1786	1/1	0.88	0.13	72,72,72,72	0
56	MG	RA	3033	1/1	0.88	0.36	91,91,91,91	0
56	MG	RA	3164	1/1	0.88	0.25	87,87,87,87	0
56	MG	RA	3832	1/1	0.88	0.12	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
56	MG	XA	1695	1/1	0.88	0.34	52,52,52,52	0
56	MG	RA	3097	1/1	0.88	0.28	93,93,93,93	0
56	MG	RA	3449	1/1	0.88	0.20	45,45,45,45	0
56	MG	RA	4045	1/1	0.88	0.26	71,71,71,71	0
56	MG	RA	3295	1/1	0.88	0.12	73,73,73,73	0
56	MG	RA	3674	1/1	0.88	0.35	77,77,77,77	0
56	MG	YA	3017	1/1	0.88	0.33	60,60,60,60	0
56	MG	RQ	202	1/1	0.88	0.11	51,51,51,51	0
56	MG	YA	3709	1/1	0.88	0.24	58,58,58,58	0
56	MG	RR	3202	1/1	0.88	0.26	69,69,69,69	0
56	MG	RA	3101	1/1	0.88	0.21	68,68,68,68	0
56	MG	YA	3045	1/1	0.88	0.14	27,27,27,27	0
56	MG	YA	3040	1/1	0.88	0.20	66,66,66,66	0
56	MG	XE	202	1/1	0.88	0.10	67,67,67,67	0
56	MG	RA	3959	1/1	0.88	0.10	43,43,43,43	0
56	MG	QA	1619	1/1	0.88	0.12	75,75,75,75	0
56	MG	QL	202	1/1	0.88	0.16	68,68,68,68	0
56	MG	RA	3048	1/1	0.88	0.25	78,78,78,78	0
56	MG	RA	3612	1/1	0.88	0.33	64,64,64,64	0
56	MG	YA	3049	1/1	0.88	0.31	78,78,78,78	0
56	MG	RA	3695	1/1	0.88	0.14	52,52,52,52	0
56	MG	RA	3547	1/1	0.88	0.21	74,74,74,74	0
56	MG	YA	3378	1/1	0.88	0.22	53,53,53,53	0
56	MG	YA	3643	1/1	0.88	0.34	36,36,36,36	0
56	MG	QA	1794	1/1	0.88	0.22	79,79,79,79	0
56	MG	R1	101	1/1	0.88	0.27	82,82,82,82	0
56	MG	XA	1766	1/1	0.88	0.44	52,52,52,52	0
56	MG	RA	3480	1/1	0.88	0.28	42,42,42,42	0
56	MG	YA	3644	1/1	0.88	0.31	57,57,57,57	0
56	MG	R3	102	1/1	0.88	0.32	80,80,80,80	0
56	MG	RA	3709	1/1	0.88	0.25	75,75,75,75	0
56	MG	YA	3355	1/1	0.88	0.30	75,75,75,75	0
56	MG	YE	304	1/1	0.88	0.22	51,51,51,51	0
56	MG	YA	3084	1/1	0.88	0.20	66,66,66,66	0
56	MG	RA	3336	1/1	0.88	0.22	66,66,66,66	0
56	MG	QA	1635	1/1	0.88	0.10	58,58,58,58	0
57	ZN	YY	201	1/1	0.88	0.11	221,221,221,221	0
56	MG	YA	3068	1/1	0.88	0.12	65,65,65,65	0
57	ZN	RY	201	1/1	0.88	0.15	210,210,210,210	0
56	MG	YA	3535	1/1	0.88	0.35	75,75,75,75	0
56	MG	RA	3608	1/1	0.89	0.18	104,104,104,104	0
56	MG	RA	3270	1/1	0.89	0.33	103,103,103,103	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3882	1/1	0.89	0.25	77,77,77,77	0
56	MG	YA	3117	1/1	0.89	0.08	42,42,42,42	0
56	MG	QF	201	1/1	0.89	0.14	59,59,59,59	0
56	MG	YA	3187	1/1	0.89	0.17	40,40,40,40	0
56	MG	YA	3701	1/1	0.89	0.40	60,60,60,60	0
56	MG	RA	3896	1/1	0.89	0.34	59,59,59,59	0
56	MG	YA	3436	1/1	0.89	0.28	51,51,51,51	0
56	MG	YA	3232	1/1	0.89	0.30	104,104,104,104	0
56	MG	RA	4062	1/1	0.89	0.21	78,78,78,78	0
56	MG	RA	4063	1/1	0.89	0.37	68,68,68,68	0
56	MG	RA	3905	1/1	0.89	0.31	41,41,41,41	0
56	MG	YA	3188	1/1	0.89	0.36	94,94,94,94	0
56	MG	YA	3513	1/1	0.89	0.30	80,80,80,80	0
56	MG	RA	3384	1/1	0.89	0.31	21,21,21,21	0
56	MG	RA	3385	1/1	0.89	0.21	27,27,27,27	0
56	MG	YA	3471	1/1	0.89	0.29	58,58,58,58	0
56	MG	RA	3281	1/1	0.89	0.35	85,85,85,85	0
56	MG	QA	1834	1/1	0.89	0.14	43,43,43,43	0
56	MG	RA	3920	1/1	0.89	0.30	41,41,41,41	0
56	MG	RA	3521	1/1	0.89	0.32	81,81,81,81	0
56	MG	YA	3473	1/1	0.89	0.25	77,77,77,77	0
56	MG	YA	3715	1/1	0.89	0.24	58,58,58,58	0
56	MG	YA	3021	1/1	0.89	0.23	69,69,69,69	0
56	MG	YA	3648	1/1	0.89	0.19	40,40,40,40	0
56	MG	YA	3719	1/1	0.89	0.37	79,79,79,79	0
56	MG	RA	3776	1/1	0.89	0.30	73,73,73,73	0
56	MG	YE	302	1/1	0.89	0.25	79,79,79,79	0
56	MG	YA	3083	1/1	0.89	0.42	99,99,99,99	0
56	MG	RA	3406	1/1	0.89	0.16	60,60,60,60	0
56	MG	YA	3310	1/1	0.89	0.27	38,38,38,38	0
56	MG	YE	305	1/1	0.89	0.21	57,57,57,57	0
56	MG	QA	1845	1/1	0.89	0.35	77,77,77,77	0
56	MG	RA	3204	1/1	0.89	0.24	59,59,59,59	0
56	MG	RA	3297	1/1	0.89	0.12	39,39,39,39	0
56	MG	RA	3656	1/1	0.89	0.26	44,44,44,44	0
56	MG	RA	3416	1/1	0.89	0.23	60,60,60,60	0
56	MG	YA	3105	1/1	0.89	0.21	37,37,37,37	0
56	MG	RD	302	1/1	0.89	0.25	53,53,53,53	0
56	MG	RA	3301	1/1	0.89	0.38	66,66,66,66	0
56	MG	YA	3725	1/1	0.89	0.23	68,68,68,68	0
56	MG	YA	3446	1/1	0.89	0.34	71,71,71,71	0
56	MG	RA	3796	1/1	0.89	0.39	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3664	1/1	0.89	0.26	48,48,48,48	0
56	MG	YG	203	1/1	0.89	0.12	54,54,54,54	0
56	MG	RA	3548	1/1	0.89	0.25	38,38,38,38	0
56	MG	YA	3481	1/1	0.89	0.34	77,77,77,77	0
56	MG	RA	3107	1/1	0.89	0.36	109,109,109,109	0
56	MG	XA	1638	1/1	0.89	0.10	118,118,118,118	0
56	MG	YA	3269	1/1	0.89	0.15	78,78,78,78	0
56	MG	YA	3241	1/1	0.89	0.21	85,85,85,85	0
56	MG	YP	201	1/1	0.89	0.25	79,79,79,79	0
56	MG	RF	305	1/1	0.89	0.32	69,69,69,69	0
56	MG	XX	101	1/1	0.89	0.30	122,122,122,122	0
56	MG	RA	3967	1/1	0.89	0.34	61,61,61,61	0
56	MG	YA	3664	1/1	0.89	0.29	42,42,42,42	0
56	MG	RA	3024	1/1	0.89	0.28	74,74,74,74	0
56	MG	QA	1678	1/1	0.89	0.21	80,80,80,80	0
56	MG	RA	3560	1/1	0.89	0.27	23,23,23,23	0
56	MG	RA	3027	1/1	0.89	0.37	103,103,103,103	0
56	MG	RA	3127	1/1	0.89	0.22	52,52,52,52	0
56	MG	RA	3565	1/1	0.89	0.12	44,44,44,44	0
56	MG	RA	3691	1/1	0.89	0.16	64,64,64,64	0
56	MG	RA	3692	1/1	0.89	0.24	87,87,87,87	0
56	MG	XA	1763	1/1	0.89	0.39	49,49,49,49	0
56	MG	YA	3048	1/1	0.89	0.19	57,57,57,57	0
56	MG	YA	3059	1/1	0.89	0.39	79,79,79,79	0
56	MG	QA	1620	1/1	0.89	0.10	75,75,75,75	0
56	MG	YA	3278	1/1	0.89	0.17	38,38,38,38	0
56	MG	YA	3110	1/1	0.89	0.19	63,63,63,63	0
56	MG	YA	3611	1/1	0.89	0.20	31,31,31,31	0
56	MG	YA	3457	1/1	0.89	0.13	33,33,33,33	0
56	MG	YA	3423	1/1	0.89	0.31	59,59,59,59	0
56	MG	RA	3705	1/1	0.89	0.32	50,50,50,50	0
56	MG	YA	3684	1/1	0.89	0.36	39,39,39,39	0
56	MG	RA	3581	1/1	0.89	0.26	75,75,75,75	0
56	MG	RA	3460	1/1	0.89	0.36	51,51,51,51	0
56	MG	RU	203	1/1	0.89	0.53	64,64,64,64	0
56	MG	QA	1692	1/1	0.89	0.18	52,52,52,52	0
56	MG	XA	1774	1/1	0.89	0.31	59,59,59,59	0
56	MG	RA	3355	1/1	0.89	0.28	24,24,24,24	0
56	MG	RA	3588	1/1	0.89	0.12	63,63,63,63	0
56	MG	RA	3844	1/1	0.89	0.41	113,113,113,113	0
56	MG	RA	3464	1/1	0.89	0.31	71,71,71,71	0
56	MG	RA	3356	1/1	0.89	0.07	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3468	1/1	0.89	0.18	40,40,40,40	0
56	MG	YA	3199	1/1	0.89	0.25	102,102,102,102	0
56	MG	XA	1776	1/1	0.89	0.36	61,61,61,61	0
56	MG	YA	3499	1/1	0.89	0.14	38,38,38,38	0
56	MG	RA	3730	1/1	0.89	0.12	51,51,51,51	0
56	MG	RA	3861	1/1	0.89	0.08	43,43,43,43	0
56	MG	YA	3426	1/1	0.89	0.19	50,50,50,50	0
56	MG	XA	1779	1/1	0.89	0.38	60,60,60,60	0
56	MG	YA	3034	1/1	0.89	0.18	68,68,68,68	0
56	MG	YA	3055	1/1	0.89	0.25	45,45,45,45	0
56	MG	XA	1659	1/1	0.89	0.10	75,75,75,75	0
56	MG	RA	3736	1/1	0.89	0.18	74,74,74,74	0
56	MG	R7	101	1/1	0.89	0.15	66,66,66,66	0
56	MG	RA	3165	1/1	0.89	0.26	99,99,99,99	0
56	MG	RA	4037	1/1	0.89	0.28	69,69,69,69	0
56	MG	YA	3629	1/1	0.89	0.17	44,44,44,44	0
56	MG	YA	3229	1/1	0.89	0.20	71,71,71,71	0
56	MG	RA	3493	1/1	0.89	0.20	60,60,60,60	0
56	MG	RA	3495	1/1	0.89	0.36	43,43,43,43	0
56	MG	QA	1659	1/1	0.90	0.38	84,84,84,84	0
56	MG	RA	4025	1/1	0.90	0.15	32,32,32,32	0
56	MG	XA	1657	1/1	0.90	0.28	65,65,65,65	0
56	MG	YA	3332	1/1	0.90	0.25	28,28,28,28	0
56	MG	YA	3607	1/1	0.90	0.21	53,53,53,53	0
56	MG	RA	3697	1/1	0.90	0.30	55,55,55,55	0
56	MG	YA	3335	1/1	0.90	0.20	30,30,30,30	0
56	MG	YA	3428	1/1	0.90	0.15	44,44,44,44	0
56	MG	YB	203	1/1	0.90	0.22	72,72,72,72	0
56	MG	YA	3536	1/1	0.90	0.13	42,42,42,42	0
56	MG	RA	3055	1/1	0.90	0.33	85,85,85,85	0
56	MG	XA	1729	1/1	0.90	0.19	58,58,58,58	0
56	MG	YA	3294	1/1	0.90	0.22	52,52,52,52	0
56	MG	QA	1873	1/1	0.90	0.23	70,70,70,70	0
56	MG	QA	1807	1/1	0.90	0.23	65,65,65,65	0
56	MG	RA	3712	1/1	0.90	0.24	53,53,53,53	0
56	MG	YA	3500	1/1	0.90	0.28	53,53,53,53	0
56	MG	YA	3089	1/1	0.90	0.30	80,80,80,80	0
56	MG	YA	3184	1/1	0.90	0.18	80,80,80,80	0
56	MG	YA	3546	1/1	0.90	0.30	47,47,47,47	0
56	MG	RA	3723	1/1	0.90	0.22	68,68,68,68	0
56	MG	YA	3201	1/1	0.90	0.12	87,87,87,87	0
56	MG	RA	3183	1/1	0.90	0.35	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3441	1/1	0.90	0.17	61,61,61,61	0
56	MG	RA	4064	1/1	0.90	0.19	64,64,64,64	0
56	MG	RA	3185	1/1	0.90	0.30	94,94,94,94	0
56	MG	RA	3445	1/1	0.90	0.17	58,58,58,58	0
56	MG	XA	1743	1/1	0.90	0.32	44,44,44,44	0
56	MG	RA	3447	1/1	0.90	0.13	57,57,57,57	0
56	MG	RA	3582	1/1	0.90	0.34	72,72,72,72	0
56	MG	RA	3189	1/1	0.90	0.10	39,39,39,39	0
56	MG	RA	3892	1/1	0.90	0.35	55,55,55,55	0
56	MG	RA	3190	1/1	0.90	0.28	62,62,62,62	0
56	MG	RA	3308	1/1	0.90	0.13	64,64,64,64	0
56	MG	RA	3902	1/1	0.90	0.16	49,49,49,49	0
56	MG	RA	3451	1/1	0.90	0.27	27,27,27,27	0
56	MG	RA	3071	1/1	0.90	0.27	63,63,63,63	0
56	MG	RA	3192	1/1	0.90	0.26	92,92,92,92	0
56	MG	YA	3074	1/1	0.90	0.21	63,63,63,63	0
56	MG	YA	3307	1/1	0.90	0.31	73,73,73,73	0
56	MG	YA	3703	1/1	0.90	0.23	35,35,35,35	0
56	MG	RB	219	1/1	0.90	0.14	57,57,57,57	0
56	MG	YA	3634	1/1	0.90	0.42	48,48,48,48	0
56	MG	YA	3552	1/1	0.90	0.37	52,52,52,52	0
56	MG	YA	3636	1/1	0.90	0.15	45,45,45,45	0
56	MG	RA	3325	1/1	0.90	0.26	42,42,42,42	0
56	MG	RA	3200	1/1	0.90	0.29	99,99,99,99	0
56	MG	XA	1621	1/1	0.90	0.29	68,68,68,68	0
56	MG	QA	1684	1/1	0.90	0.17	97,97,97,97	0
56	MG	YD	303	1/1	0.90	0.25	44,44,44,44	0
56	MG	YA	3044	1/1	0.90	0.13	35,35,35,35	0
56	MG	RA	3471	1/1	0.90	0.22	42,42,42,42	0
56	MG	RA	3335	1/1	0.90	0.19	46,46,46,46	0
56	MG	QA	1687	1/1	0.90	0.14	97,97,97,97	0
56	MG	RA	3091	1/1	0.90	0.27	104,104,104,104	0
56	MG	RD	305	1/1	0.90	0.18	86,86,86,86	0
56	MG	RD	307	1/1	0.90	0.27	83,83,83,83	0
56	MG	RA	3478	1/1	0.90	0.26	34,34,34,34	0
56	MG	YA	3354	1/1	0.90	0.38	47,47,47,47	0
56	MG	YA	3472	1/1	0.90	0.28	23,23,23,23	0
56	MG	RA	3937	1/1	0.90	0.11	38,38,38,38	0
56	MG	YA	3441	1/1	0.90	0.23	34,34,34,34	0
56	MG	XA	1761	1/1	0.90	0.18	38,38,38,38	0
56	MG	RA	3766	1/1	0.90	0.23	29,29,29,29	0
56	MG	YA	3275	1/1	0.90	0.27	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
56	MG	YA	3276	1/1	0.90	0.33	67,67,67,67	0
56	MG	YA	3564	1/1	0.90	0.19	42,42,42,42	0
56	MG	YA	3262	1/1	0.90	0.27	88,88,88,88	0
56	MG	RA	3492	1/1	0.90	0.26	68,68,68,68	0
56	MG	QA	1629	1/1	0.90	0.11	51,51,51,51	0
56	MG	RF	308	1/1	0.90	0.27	74,74,74,74	0
56	MG	XA	1633	1/1	0.90	0.22	51,51,51,51	0
56	MG	RA	3496	1/1	0.90	0.20	16,16,16,16	0
56	MG	RA	3225	1/1	0.90	0.31	109,109,109,109	0
56	MG	YE	307	1/1	0.90	0.07	64,64,64,64	0
56	MG	XA	1636	1/1	0.90	0.06	60,60,60,60	0
56	MG	RA	3640	1/1	0.90	0.16	48,48,48,48	0
56	MG	YA	3149	1/1	0.90	0.21	56,56,56,56	0
56	MG	YA	3182	1/1	0.90	0.15	68,68,68,68	0
56	MG	RA	3509	1/1	0.90	0.35	69,69,69,69	0
56	MG	RA	3233	1/1	0.90	0.24	72,72,72,72	0
56	MG	RA	3234	1/1	0.90	0.12	64,64,64,64	0
56	MG	RA	3966	1/1	0.90	0.32	65,65,65,65	0
56	MG	RA	3113	1/1	0.90	0.30	65,65,65,65	0
56	MG	YA	3366	1/1	0.90	0.26	59,59,59,59	0
56	MG	QA	1841	1/1	0.90	0.20	28,28,28,28	0
56	MG	RA	3117	1/1	0.90	0.17	64,64,64,64	0
56	MG	RQ	201	1/1	0.90	0.12	47,47,47,47	0
56	MG	RA	3651	1/1	0.90	0.11	41,41,41,41	0
56	MG	YA	3573	1/1	0.90	0.35	38,38,38,38	0
56	MG	RA	3120	1/1	0.90	0.11	63,63,63,63	0
56	MG	QA	1775	1/1	0.90	0.27	72,72,72,72	0
56	MG	RR	3204	1/1	0.90	0.32	83,83,83,83	0
56	MG	RA	3013	1/1	0.90	0.37	71,71,71,71	0
56	MG	YA	3522	1/1	0.90	0.29	65,65,65,65	0
56	MG	YA	3577	1/1	0.90	0.36	53,53,53,53	0
56	MG	YA	3250	1/1	0.90	0.14	45,45,45,45	0
56	MG	YA	3660	1/1	0.90	0.21	34,34,34,34	0
56	MG	YA	3483	1/1	0.90	0.27	26,26,26,26	0
56	MG	RA	3989	1/1	0.90	0.07	39,39,39,39	0
56	MG	XA	1780	1/1	0.90	0.34	40,40,40,40	0
56	MG	YA	3315	1/1	0.90	0.34	62,62,62,62	0
56	MG	RA	3666	1/1	0.90	0.23	69,69,69,69	0
56	MG	RA	3529	1/1	0.90	0.27	77,77,77,77	0
56	MG	YT	201	1/1	0.90	0.12	57,57,57,57	0
56	MG	RA	3531	1/1	0.90	0.10	34,34,34,34	0
56	MG	YA	3291	1/1	0.90	0.28	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3029	1/1	0.90	0.33	66,66,66,66	0
56	MG	RA	3140	1/1	0.90	0.24	93,93,93,93	0
56	MG	YA	3323	1/1	0.90	0.18	37,37,37,37	0
56	MG	RA	3264	1/1	0.90	0.34	63,63,63,63	0
56	MG	RA	3680	1/1	0.90	0.21	46,46,46,46	0
56	MG	RA	3681	1/1	0.90	0.14	119,119,119,119	0
56	MG	YA	3741	1/1	0.90	0.20	57,57,57,57	0
56	MG	RA	3148	1/1	0.90	0.17	66,66,66,66	0
56	MG	RA	3149	1/1	0.90	0.08	39,39,39,39	0
56	MG	RA	3686	1/1	0.90	0.28	62,62,62,62	0
56	MG	RA	3544	1/1	0.90	0.36	78,78,78,78	0
56	MG	R7	102	1/1	0.90	0.24	72,72,72,72	0
56	MG	YA	3593	1/1	0.90	0.23	28,28,28,28	0
56	MG	YA	3266	1/1	0.90	0.33	70,70,70,70	0
56	MG	RA	4017	1/1	0.90	0.28	90,90,90,90	0
56	MG	YA	3377	1/1	0.90	0.35	52,52,52,52	0
56	MG	YA	3189	1/1	0.90	0.24	96,96,96,96	0
56	MG	YA	3751	1/1	0.90	0.14	39,39,39,39	0
56	MG	YA	3209	1/1	0.91	0.21	48,48,48,48	0
56	MG	YA	3738	1/1	0.91	0.11	68,68,68,68	0
56	MG	YA	3548	1/1	0.91	0.27	32,32,32,32	0
56	MG	YA	3407	1/1	0.91	0.32	18,18,18,18	0
56	MG	RA	3500	1/1	0.91	0.28	25,25,25,25	0
56	MG	RA	3504	1/1	0.91	0.32	38,38,38,38	0
56	MG	XA	1676	1/1	0.91	0.25	42,42,42,42	0
56	MG	YA	3007	1/1	0.91	0.17	63,63,63,63	0
56	MG	YA	3512	1/1	0.91	0.28	62,62,62,62	0
56	MG	RA	3708	1/1	0.91	0.18	54,54,54,54	0
56	MG	RA	3125	1/1	0.91	0.14	36,36,36,36	0
56	MG	RA	3300	1/1	0.91	0.31	68,68,68,68	0
56	MG	YA	3061	1/1	0.91	0.25	57,57,57,57	0
56	MG	RA	3958	1/1	0.91	0.32	104,104,104,104	0
56	MG	YA	3556	1/1	0.91	0.17	41,41,41,41	0
56	MG	RA	3303	1/1	0.91	0.41	79,79,79,79	0
56	MG	RA	3716	1/1	0.91	0.12	52,52,52,52	0
56	MG	RA	3218	1/1	0.91	0.15	65,65,65,65	0
56	MG	RA	3609	1/1	0.91	0.12	71,71,71,71	0
56	MG	RA	3830	1/1	0.91	0.15	66,66,66,66	0
56	MG	XA	1737	1/1	0.91	0.23	47,47,47,47	0
56	MG	QA	1649	1/1	0.91	0.15	50,50,50,50	0
56	MG	RA	3613	1/1	0.91	0.19	35,35,35,35	0
56	MG	XA	1684	1/1	0.91	0.29	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
56	MG	YA	3367	1/1	0.91	0.15	56,56,56,56	0
56	MG	YA	3558	1/1	0.91	0.09	25,25,25,25	0
56	MG	RA	3424	1/1	0.91	0.24	80,80,80,80	0
56	MG	YA	3287	1/1	0.91	0.36	35,35,35,35	0
56	MG	XA	1745	1/1	0.91	0.25	44,44,44,44	0
56	MG	RA	3427	1/1	0.91	0.29	78,78,78,78	0
56	MG	RA	3843	1/1	0.91	0.20	72,72,72,72	0
56	MG	YA	3758	1/1	0.91	0.19	76,76,76,76	0
56	MG	RE	305	1/1	0.91	0.13	33,33,33,33	0
56	MG	YA	3416	1/1	0.91	0.44	39,39,39,39	0
56	MG	YA	3234	1/1	0.91	0.15	76,76,76,76	0
56	MG	YA	3235	1/1	0.91	0.24	91,91,91,91	0
56	MG	YB	204	1/1	0.91	0.14	99,99,99,99	0
56	MG	RA	3991	1/1	0.91	0.18	73,73,73,73	0
56	MG	RA	3235	1/1	0.91	0.19	70,70,70,70	0
56	MG	RA	3852	1/1	0.91	0.14	47,47,47,47	0
56	MG	RA	3856	1/1	0.91	0.19	33,33,33,33	0
56	MG	RA	3436	1/1	0.91	0.31	56,56,56,56	0
56	MG	YA	3521	1/1	0.91	0.27	95,95,95,95	0
56	MG	YA	3145	1/1	0.91	0.22	59,59,59,59	0
56	MG	YA	3451	1/1	0.91	0.28	64,64,64,64	0
56	MG	RA	3643	1/1	0.91	0.36	71,71,71,71	0
56	MG	YA	3062	1/1	0.91	0.12	57,57,57,57	0
56	MG	RA	3748	1/1	0.91	0.12	61,61,61,61	0
56	MG	YA	3113	1/1	0.91	0.18	104,104,104,104	0
56	MG	RA	3541	1/1	0.91	0.22	74,74,74,74	0
56	MG	YA	3114	1/1	0.91	0.22	90,90,90,90	0
56	MG	RA	3072	1/1	0.91	0.43	93,93,93,93	0
56	MG	YA	3575	1/1	0.91	0.25	30,30,30,30	0
56	MG	RA	3873	1/1	0.91	0.27	31,31,31,31	0
56	MG	RA	3159	1/1	0.91	0.29	107,107,107,107	0
56	MG	QA	1781	1/1	0.91	0.24	54,54,54,54	0
56	MG	YA	3297	1/1	0.91	0.25	19,19,19,19	0
56	MG	QA	1729	1/1	0.91	0.27	50,50,50,50	0
56	MG	RA	3080	1/1	0.91	0.22	81,81,81,81	0
56	MG	RQ	204	1/1	0.91	0.25	72,72,72,72	0
56	MG	YA	3381	1/1	0.91	0.17	11,11,11,11	0
56	MG	RA	3253	1/1	0.91	0.14	66,66,66,66	0
56	MG	RA	3889	1/1	0.91	0.26	48,48,48,48	0
56	MG	RA	3658	1/1	0.91	0.47	95,95,95,95	0
56	MG	RA	3082	1/1	0.91	0.33	62,62,62,62	0
56	MG	RA	3554	1/1	0.91	0.30	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
56	MG	XA	1607	1/1	0.91	0.17	47,47,47,47	0
56	MG	RA	3084	1/1	0.91	0.23	79,79,79,79	0
56	MG	QA	1786	1/1	0.91	0.14	54,54,54,54	0
56	MG	XA	1707	1/1	0.91	0.25	58,58,58,58	0
56	MG	RA	3087	1/1	0.91	0.37	99,99,99,99	0
56	MG	YA	3425	1/1	0.91	0.15	49,49,49,49	0
56	MG	YA	3580	1/1	0.91	0.29	27,27,27,27	0
56	MG	QA	1617	1/1	0.91	0.11	61,61,61,61	0
56	MG	YA	3581	1/1	0.91	0.29	24,24,24,24	0
56	MG	YA	3029	1/1	0.91	0.37	57,57,57,57	0
56	MG	YA	3243	1/1	0.91	0.14	67,67,67,67	0
56	MG	RA	3470	1/1	0.91	0.23	34,34,34,34	0
56	MG	YA	3079	1/1	0.91	0.30	91,91,91,91	0
56	MG	RA	3098	1/1	0.91	0.07	12,12,12,12	0
56	MG	QA	1680	1/1	0.91	0.24	64,64,64,64	0
56	MG	YA	3226	1/1	0.91	0.35	75,75,75,75	0
56	MG	RA	3372	1/1	0.91	0.26	61,61,61,61	0
56	MG	RA	4057	1/1	0.91	0.23	77,77,77,77	0
56	MG	YA	3025	1/1	0.91	0.15	55,55,55,55	0
56	MG	QA	1625	1/1	0.91	0.17	61,61,61,61	0
56	MG	QA	1800	1/1	0.91	0.23	41,41,41,41	0
56	MG	YA	3010	1/1	0.91	0.14	41,41,41,41	0
56	MG	YA	3402	1/1	0.91	0.25	32,32,32,32	0
56	MG	YA	3119	1/1	0.91	0.27	78,78,78,78	0
56	MG	RA	3381	1/1	0.91	0.23	39,39,39,39	0
56	MG	YA	3027	1/1	0.91	0.19	45,45,45,45	0
56	MG	YA	3669	1/1	0.91	0.22	15,15,15,15	0
56	MG	YA	3252	1/1	0.91	0.32	70,70,70,70	0
56	MG	YA	3608	1/1	0.91	0.30	44,44,44,44	0
56	MG	YA	3554	1/1	0.92	0.21	44,44,44,44	0
56	MG	RA	3623	1/1	0.92	0.21	34,34,34,34	0
56	MG	RA	4050	1/1	0.92	0.30	59,59,59,59	0
56	MG	YA	3444	1/1	0.92	0.30	27,27,27,27	0
56	MG	RA	3626	1/1	0.92	0.10	68,68,68,68	0
56	MG	YA	3373	1/1	0.92	0.23	41,41,41,41	0
56	MG	YW	201	1/1	0.92	0.19	75,75,75,75	0
56	MG	YA	3121	1/1	0.92	0.27	47,47,47,47	0
56	MG	YA	3749	1/1	0.92	0.16	54,54,54,54	0
56	MG	RA	3632	1/1	0.92	0.26	55,55,55,55	0
56	MG	RA	3383	1/1	0.92	0.34	40,40,40,40	0
56	MG	YA	3376	1/1	0.92	0.22	58,58,58,58	0
56	MG	YA	3752	1/1	0.92	0.06	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
56	MG	YA	3147	1/1	0.92	0.19	84,84,84,84	0
56	MG	YA	3343	1/1	0.92	0.22	21,21,21,21	0
56	MG	YA	3280	1/1	0.92	0.24	14,14,14,14	0
56	MG	RA	3174	1/1	0.92	0.14	62,62,62,62	0
56	MG	RA	3392	1/1	0.92	0.22	28,28,28,28	0
56	MG	YA	3692	1/1	0.92	0.15	39,39,39,39	0
56	MG	RA	3915	1/1	0.92	0.20	41,41,41,41	0
56	MG	YA	3035	1/1	0.92	0.24	73,73,73,73	0
56	MG	YA	3630	1/1	0.92	0.20	32,32,32,32	0
56	MG	YA	3487	1/1	0.92	0.31	46,46,46,46	0
56	MG	YA	3633	1/1	0.92	0.32	47,47,47,47	0
56	MG	YA	3137	1/1	0.92	0.18	40,40,40,40	0
56	MG	YA	3489	1/1	0.92	0.24	15,15,15,15	0
56	MG	YA	3224	1/1	0.92	0.12	66,66,66,66	0
56	MG	RA	3408	1/1	0.92	0.23	24,24,24,24	0
56	MG	XA	1664	1/1	0.92	0.23	67,67,67,67	0
56	MG	YA	3386	1/1	0.92	0.26	23,23,23,23	0
56	MG	YA	3638	1/1	0.92	0.23	65,65,65,65	0
56	MG	RA	3288	1/1	0.92	0.24	95,95,95,95	0
56	MG	RA	3783	1/1	0.92	0.16	42,42,42,42	0
56	MG	YA	3387	1/1	0.92	0.28	37,37,37,37	0
56	MG	YA	3708	1/1	0.92	0.31	37,37,37,37	0
56	MG	XA	1614	1/1	0.92	0.17	60,60,60,60	0
56	MG	RA	3938	1/1	0.92	0.24	100,100,100,100	0
56	MG	RA	3787	1/1	0.92	0.48	105,105,105,105	0
56	MG	XA	1670	1/1	0.92	0.17	80,80,80,80	0
56	MG	YA	3458	1/1	0.92	0.30	46,46,46,46	0
56	MG	YA	3389	1/1	0.92	0.19	50,50,50,50	0
56	MG	QA	1755	1/1	0.92	0.21	69,69,69,69	0
56	MG	XA	1741	1/1	0.92	0.23	67,67,67,67	0
56	MG	RD	303	1/1	0.92	0.10	41,41,41,41	0
56	MG	XA	1742	1/1	0.92	0.25	52,52,52,52	0
56	MG	YA	3390	1/1	0.92	0.36	33,33,33,33	0
56	MG	YA	3289	1/1	0.92	0.25	38,38,38,38	0
56	MG	YA	3714	1/1	0.92	0.44	80,80,80,80	0
56	MG	RA	3202	1/1	0.92	0.21	92,92,92,92	0
56	MG	YA	3165	1/1	0.92	0.15	73,73,73,73	0
56	MG	XA	1678	1/1	0.92	0.18	81,81,81,81	0
56	MG	XA	1679	1/1	0.92	0.26	52,52,52,52	0
56	MG	YA	3268	1/1	0.92	0.28	73,73,73,73	0
56	MG	QA	1618	1/1	0.92	0.10	96,96,96,96	0
56	MG	YA	3080	1/1	0.92	0.37	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3313	1/1	0.92	0.17	21,21,21,21	0
56	MG	RA	3209	1/1	0.92	0.31	100,100,100,100	0
56	MG	RA	3211	1/1	0.92	0.14	88,88,88,88	0
56	MG	RA	3561	1/1	0.92	0.12	42,42,42,42	0
56	MG	RA	3110	1/1	0.92	0.16	70,70,70,70	0
56	MG	RA	3010	1/1	0.92	0.08	50,50,50,50	0
56	MG	RF	306	1/1	0.92	0.22	79,79,79,79	0
56	MG	RA	3320	1/1	0.92	0.21	14,14,14,14	0
56	MG	YA	3540	1/1	0.92	0.25	27,27,27,27	0
56	MG	RA	3216	1/1	0.92	0.23	77,77,77,77	0
56	MG	RA	3972	1/1	0.92	0.21	81,81,81,81	0
56	MG	YA	3650	1/1	0.92	0.30	48,48,48,48	0
56	MG	RA	3822	1/1	0.92	0.11	37,37,37,37	0
56	MG	RA	3975	1/1	0.92	0.14	63,63,63,63	0
56	MG	YA	3401	1/1	0.92	0.28	19,19,19,19	0
56	MG	YA	3036	1/1	0.92	0.17	55,55,55,55	0
56	MG	YA	3656	1/1	0.92	0.16	34,34,34,34	0
56	MG	RA	3980	1/1	0.92	0.17	49,49,49,49	0
56	MG	RA	3574	1/1	0.92	0.24	62,62,62,62	0
56	MG	XA	1628	1/1	0.92	0.16	56,56,56,56	0
56	MG	XA	1688	1/1	0.92	0.16	56,56,56,56	0
56	MG	YA	3589	1/1	0.92	0.21	31,31,31,31	0
56	MG	RA	3700	1/1	0.92	0.14	53,53,53,53	0
56	MG	XA	1690	1/1	0.92	0.29	53,53,53,53	0
56	MG	RA	3226	1/1	0.92	0.59	104,104,104,104	0
56	MG	YA	3590	1/1	0.92	0.15	41,41,41,41	0
56	MG	RA	3341	1/1	0.92	0.29	30,30,30,30	0
56	MG	XA	1765	1/1	0.92	0.34	49,49,49,49	0
56	MG	QA	1634	1/1	0.92	0.09	44,44,44,44	0
56	MG	RA	3707	1/1	0.92	0.32	69,69,69,69	0
56	MG	XA	1631	1/1	0.92	0.23	60,60,60,60	0
56	MG	RR	3205	1/1	0.92	0.15	60,60,60,60	0
56	MG	YF	301	1/1	0.92	0.19	54,54,54,54	0
56	MG	RA	3349	1/1	0.92	0.18	40,40,40,40	0
56	MG	RA	3350	1/1	0.92	0.18	65,65,65,65	0
56	MG	YA	3591	1/1	0.92	0.24	42,42,42,42	0
56	MG	QA	1638	1/1	0.92	0.14	41,41,41,41	0
56	MG	QA	1855	1/1	0.92	0.19	56,56,56,56	0
56	MG	RA	3717	1/1	0.92	0.28	38,38,38,38	0
56	MG	RV	203	1/1	0.92	0.18	55,55,55,55	0
56	MG	RA	3133	1/1	0.92	0.12	79,79,79,79	0
56	MG	YA	3730	1/1	0.92	0.29	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3254	1/1	0.92	0.20	67,67,67,67	0
56	MG	RA	3853	1/1	0.92	0.64	64,64,64,64	0
56	MG	RA	3242	1/1	0.92	0.11	54,54,54,54	0
56	MG	RA	3857	1/1	0.92	0.24	35,35,35,35	0
56	MG	YA	3329	1/1	0.92	0.23	19,19,19,19	0
56	MG	YA	3240	1/1	0.92	0.29	70,70,70,70	0
56	MG	QA	1716	1/1	0.92	0.14	81,81,81,81	0
56	MG	RA	3045	1/1	0.92	0.30	71,71,71,71	0
56	MG	RA	4020	1/1	0.92	0.21	88,88,88,88	0
56	MG	RA	3145	1/1	0.92	0.08	43,43,43,43	0
56	MG	QA	1717	1/1	0.92	0.26	29,29,29,29	0
56	MG	RA	3605	1/1	0.92	0.17	70,70,70,70	0
56	MG	RA	3606	1/1	0.92	0.45	53,53,53,53	0
56	MG	YA	3168	1/1	0.92	0.18	88,88,88,88	0
56	MG	XA	1640	1/1	0.92	0.18	66,66,66,66	0
56	MG	RA	3869	1/1	0.92	0.66	77,77,77,77	0
56	MG	YA	3549	1/1	0.92	0.20	34,34,34,34	0
56	MG	YA	3215	1/1	0.92	0.09	54,54,54,54	0
56	MG	YA	3030	1/1	0.92	0.18	39,39,39,39	0
56	MG	R9	103	1/1	0.92	0.18	67,67,67,67	0
56	MG	RA	3254	1/1	0.92	0.18	92,92,92,92	0
56	MG	RA	3876	1/1	0.92	0.44	54,54,54,54	0
56	MG	RA	3155	1/1	0.92	0.20	78,78,78,78	0
56	MG	YA	3338	1/1	0.92	0.31	16,16,16,16	0
56	MG	RA	3886	1/1	0.93	0.29	52,52,52,52	0
56	MG	RA	4041	1/1	0.93	0.36	77,77,77,77	0
56	MG	RA	3405	1/1	0.93	0.22	32,32,32,32	0
56	MG	RA	4043	1/1	0.93	0.15	86,86,86,86	0
56	MG	QA	1803	1/1	0.93	0.23	49,49,49,49	0
56	MG	XA	1756	1/1	0.93	0.20	27,27,27,27	0
56	MG	YA	3754	1/1	0.93	0.20	26,26,26,26	0
56	MG	RA	4048	1/1	0.93	0.20	81,81,81,81	0
56	MG	RA	3043	1/1	0.93	0.07	38,38,38,38	0
56	MG	RA	3411	1/1	0.93	0.21	31,31,31,31	0
56	MG	RA	3897	1/1	0.93	0.26	61,61,61,61	0
56	MG	YA	3162	1/1	0.93	0.12	27,27,27,27	0
56	MG	RA	3046	1/1	0.93	0.17	68,68,68,68	0
56	MG	RA	3414	1/1	0.93	0.22	34,34,34,34	0
56	MG	RA	3307	1/1	0.93	0.11	76,76,76,76	0
56	MG	YA	3756	1/1	0.93	0.22	80,80,80,80	0
56	MG	RA	3908	1/1	0.93	0.21	22,22,22,22	0
56	MG	YA	3585	1/1	0.93	0.26	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	4059	1/1	0.93	0.27	101,101,101,101	0
56	MG	RA	4061	1/1	0.93	0.20	96,96,96,96	0
56	MG	RA	3910	1/1	0.93	0.49	66,66,66,66	0
56	MG	YA	3348	1/1	0.93	0.17	17,17,17,17	0
56	MG	RA	3774	1/1	0.93	0.14	59,59,59,59	0
56	MG	YA	3155	1/1	0.93	0.22	65,65,65,65	0
56	MG	RA	3423	1/1	0.93	0.23	21,21,21,21	0
56	MG	RA	3137	1/1	0.93	0.26	97,97,97,97	0
56	MG	RA	3917	1/1	0.93	0.40	67,67,67,67	0
56	MG	YA	3318	1/1	0.93	0.24	26,26,26,26	0
56	MG	RA	3315	1/1	0.93	0.20	29,29,29,29	0
56	MG	RA	3054	1/1	0.93	0.22	78,78,78,78	0
56	MG	RA	3660	1/1	0.93	0.22	46,46,46,46	0
56	MG	YA	3298	1/1	0.93	0.23	19,19,19,19	0
56	MG	YA	3211	1/1	0.93	0.24	89,89,89,89	0
56	MG	RA	3144	1/1	0.93	0.30	84,84,84,84	0
56	MG	YA	3409	1/1	0.93	0.23	120,120,120,120	0
56	MG	RA	3230	1/1	0.93	0.44	81,81,81,81	0
56	MG	RA	3326	1/1	0.93	0.08	20,20,20,20	0
56	MG	RA	3932	1/1	0.93	0.28	61,61,61,61	0
56	MG	RA	3231	1/1	0.93	0.36	97,97,97,97	0
56	MG	RA	3328	1/1	0.93	0.16	34,34,34,34	0
56	MG	RA	3146	1/1	0.93	0.08	37,37,37,37	0
56	MG	RA	3330	1/1	0.93	0.14	41,41,41,41	0
56	MG	XA	1768	1/1	0.93	0.17	45,45,45,45	0
56	MG	YA	3594	1/1	0.93	0.21	35,35,35,35	0
56	MG	QA	1626	1/1	0.93	0.04	78,78,78,78	0
56	MG	RA	3678	1/1	0.93	0.21	31,31,31,31	0
56	MG	RA	3236	1/1	0.93	0.53	69,69,69,69	0
56	MG	YA	3410	1/1	0.93	0.24	31,31,31,31	0
56	MG	YA	3170	1/1	0.93	0.22	56,56,56,56	0
56	MG	RA	3945	1/1	0.93	0.21	25,25,25,25	0
56	MG	RA	3804	1/1	0.93	0.19	78,78,78,78	0
56	MG	YA	3598	1/1	0.93	0.21	49,49,49,49	0
56	MG	YA	3156	1/1	0.93	0.27	40,40,40,40	0
56	MG	RA	3684	1/1	0.93	0.29	71,71,71,71	0
56	MG	YA	3494	1/1	0.93	0.19	36,36,36,36	0
56	MG	YA	3413	1/1	0.93	0.30	36,36,36,36	0
56	MG	YA	3331	1/1	0.93	0.29	9,9,9,9	0
56	MG	YA	3217	1/1	0.93	0.14	75,75,75,75	0
56	MG	RA	3345	1/1	0.93	0.21	20,20,20,20	0
56	MG	YA	3717	1/1	0.93	0.13	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3610	1/1	0.93	0.22	20,20,20,20	0
56	MG	QA	1828	1/1	0.93	0.17	41,41,41,41	0
56	MG	YA	3111	1/1	0.93	0.26	58,58,58,58	0
56	MG	QA	1701	1/1	0.93	0.32	50,50,50,50	0
56	MG	YA	3142	1/1	0.93	0.17	58,58,58,58	0
56	MG	XA	1782	1/1	0.93	0.20	46,46,46,46	0
56	MG	YA	3721	1/1	0.93	0.17	65,65,65,65	0
56	MG	YA	3391	1/1	0.93	0.21	18,18,18,18	0
56	MG	YA	3619	1/1	0.93	0.24	38,38,38,38	0
56	MG	YA	3665	1/1	0.93	0.21	31,31,31,31	0
56	MG	QA	1646	1/1	0.93	0.26	46,46,46,46	0
56	MG	YA	3666	1/1	0.93	0.30	36,36,36,36	0
56	MG	YA	3207	1/1	0.93	0.27	70,70,70,70	0
56	MG	RA	3474	1/1	0.93	0.13	45,45,45,45	0
56	MG	YA	3139	1/1	0.93	0.28	66,66,66,66	0
56	MG	YA	3394	1/1	0.93	0.24	19,19,19,19	0
56	MG	XA	1732	1/1	0.93	0.37	44,44,44,44	0
56	MG	XA	1677	1/1	0.93	0.29	71,71,71,71	0
56	MG	RA	3184	1/1	0.93	0.18	60,60,60,60	0
56	MG	YA	3537	1/1	0.93	0.18	57,57,57,57	0
56	MG	RA	3186	1/1	0.93	0.17	77,77,77,77	0
56	MG	RA	3714	1/1	0.93	0.20	36,36,36,36	0
56	MG	RA	3984	1/1	0.93	0.23	41,41,41,41	0
56	MG	XA	1735	1/1	0.93	0.26	53,53,53,53	0
56	MG	RA	3986	1/1	0.93	0.33	79,79,79,79	0
56	MG	RA	3488	1/1	0.93	0.24	57,57,57,57	0
56	MG	RA	3988	1/1	0.93	0.27	75,75,75,75	0
56	MG	RA	3188	1/1	0.93	0.34	115,115,115,115	0
56	MG	YA	3626	1/1	0.93	0.22	25,25,25,25	0
56	MG	YA	3677	1/1	0.93	0.26	42,42,42,42	0
56	MG	YA	3574	1/1	0.93	0.27	30,30,30,30	0
56	MG	RA	3376	1/1	0.93	0.14	52,52,52,52	0
56	MG	RA	3494	1/1	0.93	0.38	55,55,55,55	0
56	MG	RA	3850	1/1	0.93	0.17	43,43,43,43	0
56	MG	QA	1658	1/1	0.93	0.10	94,94,94,94	0
56	MG	YA	3679	1/1	0.93	0.13	36,36,36,36	0
56	MG	YA	3680	1/1	0.93	0.39	50,50,50,50	0
56	MG	RA	4000	1/1	0.93	0.16	30,30,30,30	0
56	MG	RA	3854	1/1	0.93	0.25	47,47,47,47	0
56	MG	RU	201	1/1	0.93	0.18	70,70,70,70	0
56	MG	RA	3610	1/1	0.93	0.15	67,67,67,67	0
56	MG	RA	3021	1/1	0.93	0.30	101,101,101,101	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3395	1/1	0.93	0.18	17,17,17,17	0
56	MG	YA	3539	1/1	0.93	0.20	18,18,18,18	0
56	MG	RA	3860	1/1	0.93	0.23	25,25,25,25	0
56	MG	RA	4007	1/1	0.93	0.20	49,49,49,49	0
56	MG	RW	201	1/1	0.93	0.12	64,64,64,64	0
56	MG	RA	3614	1/1	0.93	0.27	32,32,32,32	0
56	MG	YA	3631	1/1	0.93	0.18	55,55,55,55	0
56	MG	YA	3244	1/1	0.93	0.25	39,39,39,39	0
56	MG	RA	4012	1/1	0.93	0.18	89,89,89,89	0
56	MG	YA	3746	1/1	0.93	0.15	35,35,35,35	0
56	MG	RA	3388	1/1	0.93	0.24	49,49,49,49	0
56	MG	YA	3477	1/1	0.93	0.34	70,70,70,70	0
56	MG	RA	4016	1/1	0.93	0.18	68,68,68,68	0
56	MG	YA	3258	1/1	0.93	0.22	68,68,68,68	0
56	MG	RA	3391	1/1	0.93	0.27	17,17,17,17	0
56	MG	YA	3690	1/1	0.93	0.16	31,31,31,31	0
56	MG	RA	3394	1/1	0.93	0.27	31,31,31,31	0
56	MG	YA	3750	1/1	0.93	0.27	22,22,22,22	0
56	MG	RA	4023	1/1	0.93	0.10	49,49,49,49	0
56	MG	XA	1752	1/1	0.93	0.24	51,51,51,51	0
56	MG	RA	3398	1/1	0.93	0.27	20,20,20,20	0
56	MG	RA	3749	1/1	0.93	0.15	63,63,63,63	0
56	MG	RA	4027	1/1	0.93	0.25	39,39,39,39	0
56	MG	YV	201	1/1	0.93	0.15	44,44,44,44	0
56	MG	YA	3453	1/1	0.93	0.12	35,35,35,35	0
56	MG	RA	4032	1/1	0.93	0.25	76,76,76,76	0
56	MG	YA	3245	1/1	0.93	0.30	107,107,107,107	0
56	MG	RA	3403	1/1	0.93	0.20	25,25,25,25	0
56	MG	RA	3210	1/1	0.93	0.23	67,67,67,67	0
56	MG	RA	3884	1/1	0.93	0.19	71,71,71,71	0
56	MG	RA	3930	1/1	0.94	0.29	54,54,54,54	0
56	MG	RA	3562	1/1	0.94	0.17	59,59,59,59	0
56	MG	RA	3677	1/1	0.94	0.38	61,61,61,61	0
56	MG	RA	3347	1/1	0.94	0.25	23,23,23,23	0
56	MG	RA	3161	1/1	0.94	0.15	72,72,72,72	0
56	MG	YA	3334	1/1	0.94	0.31	14,14,14,14	0
56	MG	YA	3704	1/1	0.94	0.25	29,29,29,29	0
56	MG	YA	3072	1/1	0.94	0.36	99,99,99,99	0
56	MG	RA	3568	1/1	0.94	0.21	27,27,27,27	0
56	MG	YA	3277	1/1	0.94	0.24	17,17,17,17	0
56	MG	RA	3078	1/1	0.94	0.34	70,70,70,70	0
56	MG	RB	204	1/1	0.94	0.23	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3553	1/1	0.94	0.33	58,58,58,58	0
56	MG	YA	3654	1/1	0.94	0.43	54,54,54,54	0
56	MG	YA	3216	1/1	0.94	0.19	25,25,25,25	0
56	MG	RA	3257	1/1	0.94	0.18	100,100,100,100	0
56	MG	RA	3947	1/1	0.94	0.07	20,20,20,20	0
56	MG	RA	3172	1/1	0.94	0.25	80,80,80,80	0
56	MG	RA	3173	1/1	0.94	0.09	50,50,50,50	0
56	MG	RB	213	1/1	0.94	0.43	58,58,58,58	0
56	MG	QA	1707	1/1	0.94	0.20	28,28,28,28	0
56	MG	YA	3711	1/1	0.94	0.32	47,47,47,47	0
56	MG	YA	3339	1/1	0.94	0.27	15,15,15,15	0
56	MG	QA	1710	1/1	0.94	0.18	28,28,28,28	0
56	MG	YA	3202	1/1	0.94	0.20	38,38,38,38	0
56	MG	YB	212	1/1	0.94	0.36	57,57,57,57	0
56	MG	YA	3081	1/1	0.94	0.34	71,71,71,71	0
56	MG	RA	3477	1/1	0.94	0.21	46,46,46,46	0
56	MG	YA	3219	1/1	0.94	0.16	60,60,60,60	0
56	MG	YA	3484	1/1	0.94	0.21	21,21,21,21	0
56	MG	RA	3007	1/1	0.94	0.11	61,61,61,61	0
56	MG	RA	3482	1/1	0.94	0.22	21,21,21,21	0
56	MG	YA	3153	1/1	0.94	0.07	37,37,37,37	0
56	MG	YA	3486	1/1	0.94	0.32	30,30,30,30	0
56	MG	RA	3965	1/1	0.94	0.13	45,45,45,45	0
56	MG	YA	3663	1/1	0.94	0.33	38,38,38,38	0
56	MG	YA	3345	1/1	0.94	0.19	39,39,39,39	0
56	MG	RA	3012	1/1	0.94	0.07	53,53,53,53	0
56	MG	YA	3073	1/1	0.94	0.12	67,67,67,67	0
56	MG	RA	3711	1/1	0.94	0.27	80,80,80,80	0
56	MG	YA	3620	1/1	0.94	0.20	34,34,34,34	0
56	MG	RD	308	1/1	0.94	0.41	80,80,80,80	0
56	MG	RD	309	1/1	0.94	0.15	78,78,78,78	0
56	MG	YA	3194	1/1	0.94	0.17	70,70,70,70	0
56	MG	YA	3668	1/1	0.94	0.20	28,28,28,28	0
56	MG	YA	3047	1/1	0.94	0.11	44,44,44,44	0
56	MG	RA	3106	1/1	0.94	0.17	102,102,102,102	0
56	MG	YA	3350	1/1	0.94	0.15	23,23,23,23	0
56	MG	RA	3287	1/1	0.94	0.22	83,83,83,83	0
56	MG	RA	3721	1/1	0.94	0.18	73,73,73,73	0
56	MG	YA	3672	1/1	0.94	0.39	26,26,26,26	0
56	MG	RA	3109	1/1	0.94	0.16	66,66,66,66	0
56	MG	YA	3075	1/1	0.94	0.09	43,43,43,43	0
56	MG	QA	1605	1/1	0.94	0.07	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3675	1/1	0.94	0.20	29,29,29,29	0
56	MG	RA	3393	1/1	0.94	0.20	14,14,14,14	0
56	MG	RA	3508	1/1	0.94	0.18	42,42,42,42	0
56	MG	YA	3066	1/1	0.94	0.24	50,50,50,50	0
56	MG	RA	3615	1/1	0.94	0.27	34,34,34,34	0
56	MG	YA	3098	1/1	0.94	0.10	49,49,49,49	0
56	MG	RA	3618	1/1	0.94	0.25	48,48,48,48	0
56	MG	YA	3734	1/1	0.94	0.27	41,41,41,41	0
56	MG	RA	3116	1/1	0.94	0.21	104,104,104,104	0
56	MG	RA	3298	1/1	0.94	0.11	24,24,24,24	0
56	MG	YF	303	1/1	0.94	0.27	85,85,85,85	0
56	MG	QA	1671	1/1	0.94	0.10	64,64,64,64	0
56	MG	RA	3738	1/1	0.94	0.29	53,53,53,53	0
56	MG	YA	3356	1/1	0.94	0.38	50,50,50,50	0
56	MG	YA	3213	1/1	0.94	0.24	67,67,67,67	0
56	MG	YA	3023	1/1	0.94	0.09	16,16,16,16	0
56	MG	RA	3124	1/1	0.94	0.06	46,46,46,46	0
56	MG	RA	3743	1/1	0.94	0.14	35,35,35,35	0
56	MG	QA	1740	1/1	0.94	0.28	55,55,55,55	0
56	MG	RA	3213	1/1	0.94	0.22	105,105,105,105	0
56	MG	YA	3397	1/1	0.94	0.34	68,68,68,68	0
56	MG	RA	3309	1/1	0.94	0.11	63,63,63,63	0
56	MG	YA	3579	1/1	0.94	0.22	36,36,36,36	0
56	MG	YA	3326	1/1	0.94	0.27	27,27,27,27	0
56	MG	QA	1870	1/1	0.94	0.26	47,47,47,47	0
56	MG	RR	3201	1/1	0.94	0.28	62,62,62,62	0
56	MG	RA	3044	1/1	0.94	0.08	29,29,29,29	0
56	MG	YA	3743	1/1	0.94	0.29	43,43,43,43	0
56	MG	XA	1699	1/1	0.94	0.32	44,44,44,44	0
56	MG	YQ	201	1/1	0.94	0.13	33,33,33,33	0
56	MG	YA	3744	1/1	0.94	0.27	33,33,33,33	0
56	MG	RA	3534	1/1	0.94	0.11	44,44,44,44	0
56	MG	RA	3135	1/1	0.94	0.13	77,77,77,77	0
56	MG	YA	3328	1/1	0.94	0.20	15,15,15,15	0
56	MG	RA	3321	1/1	0.94	0.17	19,19,19,19	0
56	MG	YA	3365	1/1	0.94	0.23	48,48,48,48	0
56	MG	RA	4022	1/1	0.94	0.12	73,73,73,73	0
56	MG	RA	3539	1/1	0.94	0.31	39,39,39,39	0
56	MG	RA	3138	1/1	0.94	0.21	53,53,53,53	0
56	MG	YA	3583	1/1	0.94	0.23	29,29,29,29	0
56	MG	RA	3767	1/1	0.94	0.28	37,37,37,37	0
56	MG	RA	3899	1/1	0.94	0.16	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
56	MG	RA	3900	1/1	0.94	0.16	30,30,30,30	0
56	MG	YA	3274	1/1	0.94	0.21	48,48,48,48	0
56	MG	QA	1879	1/1	0.94	0.26	78,78,78,78	0
56	MG	YA	3691	1/1	0.94	0.23	38,38,38,38	0
56	MG	YA	3543	1/1	0.94	0.22	36,36,36,36	0
56	MG	YA	3640	1/1	0.94	0.30	40,40,40,40	0
56	MG	YA	3299	1/1	0.94	0.25	10,10,10,10	0
56	MG	RA	3333	1/1	0.94	0.29	24,24,24,24	0
56	MG	YA	3753	1/1	0.94	0.18	54,54,54,54	0
56	MG	YA	3506	1/1	0.94	0.14	53,53,53,53	0
56	MG	RA	3913	1/1	0.94	0.27	43,43,43,43	0
56	MG	YA	3301	1/1	0.94	0.20	42,42,42,42	0
56	MG	RA	3238	1/1	0.94	0.25	106,106,106,106	0
56	MG	YA	3259	1/1	0.94	0.23	66,66,66,66	0
56	MG	YA	3333	1/1	0.94	0.24	26,26,26,26	0
56	MG	YA	3408	1/1	0.94	0.24	17,17,17,17	0
56	MG	RA	3668	1/1	0.94	0.24	49,49,49,49	0
56	MG	RA	3068	1/1	0.94	0.19	79,79,79,79	0
56	MG	RA	3069	1/1	0.94	0.10	55,55,55,55	0
56	MG	XA	1717	1/1	0.94	0.28	59,59,59,59	0
56	MG	YA	3760	1/1	0.94	0.18	85,85,85,85	0
56	MG	RA	3673	1/1	0.94	0.22	45,45,45,45	0
56	MG	RA	3792	1/1	0.94	0.21	35,35,35,35	0
56	MG	RA	3073	1/1	0.94	0.20	64,64,64,64	0
56	MG	RA	3622	1/1	0.95	0.19	20,20,20,20	0
56	MG	RA	3141	1/1	0.95	0.47	93,93,93,93	0
56	MG	RA	3255	1/1	0.95	0.22	100,100,100,100	0
56	MG	XA	1757	1/1	0.95	0.16	30,30,30,30	0
56	MG	RA	3627	1/1	0.95	0.26	76,76,76,76	0
56	MG	YA	3724	1/1	0.95	0.28	51,51,51,51	0
56	MG	YA	3014	1/1	0.95	0.07	39,39,39,39	0
56	MG	RA	3793	1/1	0.95	0.28	38,38,38,38	0
56	MG	YA	3571	1/1	0.95	0.21	23,23,23,23	0
56	MG	YA	3430	1/1	0.95	0.05	20,20,20,20	0
56	MG	YA	3144	1/1	0.95	0.22	57,57,57,57	0
56	MG	RA	3262	1/1	0.95	0.20	80,80,80,80	0
56	MG	RA	3893	1/1	0.95	0.28	34,34,34,34	0
56	MG	YA	3286	1/1	0.95	0.08	35,35,35,35	0
56	MG	RA	3799	1/1	0.95	0.16	54,54,54,54	0
56	MG	YA	3157	1/1	0.95	0.14	44,44,44,44	0
56	MG	RA	3999	1/1	0.95	0.13	21,21,21,21	0
56	MG	RA	3096	1/1	0.95	0.12	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
56	MG	RA	3266	1/1	0.95	0.14	74,74,74,74	0
56	MG	RA	3803	1/1	0.95	0.11	64,64,64,64	0
56	MG	RA	3267	1/1	0.95	0.11	47,47,47,47	0
56	MG	RA	3718	1/1	0.95	0.18	62,62,62,62	0
56	MG	YA	3618	1/1	0.95	0.18	24,24,24,24	0
56	MG	RA	3269	1/1	0.95	0.11	74,74,74,74	0
56	MG	RA	3483	1/1	0.95	0.23	21,21,21,21	0
56	MG	YA	3237	1/1	0.95	0.20	69,69,69,69	0
56	MG	RA	4009	1/1	0.95	0.11	70,70,70,70	0
56	MG	YA	3518	1/1	0.95	0.22	16,16,16,16	0
56	MG	YA	3357	1/1	0.95	0.20	39,39,39,39	0
56	MG	RA	3813	1/1	0.95	0.23	23,23,23,23	0
56	MG	YB	216	1/1	0.95	0.26	45,45,45,45	0
56	MG	RA	3409	1/1	0.95	0.17	33,33,33,33	0
56	MG	YA	3736	1/1	0.95	0.10	39,39,39,39	0
56	MG	RF	307	1/1	0.95	0.26	65,65,65,65	0
56	MG	YA	3158	1/1	0.95	0.29	49,49,49,49	0
56	MG	YA	3076	1/1	0.95	0.19	4,4,4,4	0
56	MG	RA	3919	1/1	0.95	0.27	47,47,47,47	0
56	MG	YA	3440	1/1	0.95	0.14	29,29,29,29	0
56	MG	RA	3820	1/1	0.95	0.14	28,28,28,28	0
56	MG	YA	3702	1/1	0.95	0.13	30,30,30,30	0
56	MG	RA	3923	1/1	0.95	0.25	79,79,79,79	0
56	MG	XA	1730	1/1	0.95	0.14	47,47,47,47	0
56	MG	YA	3625	1/1	0.95	0.19	19,19,19,19	0
56	MG	RA	3417	1/1	0.95	0.11	42,42,42,42	0
56	MG	RA	3221	1/1	0.95	0.24	63,63,63,63	0
56	MG	RA	3928	1/1	0.95	0.30	59,59,59,59	0
56	MG	YA	3077	1/1	0.95	0.09	35,35,35,35	0
56	MG	YA	3705	1/1	0.95	0.17	32,32,32,32	0
56	MG	RA	3502	1/1	0.95	0.19	20,20,20,20	0
56	MG	RA	3503	1/1	0.95	0.16	21,21,21,21	0
56	MG	YA	3212	1/1	0.95	0.14	62,62,62,62	0
56	MG	RA	3353	1/1	0.95	0.21	35,35,35,35	0
56	MG	RA	3506	1/1	0.95	0.14	26,26,26,26	0
56	MG	RA	4039	1/1	0.95	0.16	73,73,73,73	0
56	MG	RA	3170	1/1	0.95	0.14	66,66,66,66	0
56	MG	YA	3054	1/1	0.95	0.14	27,27,27,27	0
56	MG	YA	3033	1/1	0.95	0.07	13,13,13,13	0
56	MG	YA	3587	1/1	0.95	0.14	31,31,31,31	0
56	MG	YA	3125	1/1	0.95	0.14	58,58,58,58	0
56	MG	RA	3359	1/1	0.95	0.12	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3513	1/1	0.95	0.07	14,14,14,14	0
56	MG	YE	306	1/1	0.95	0.21	13,13,13,13	0
56	MG	RA	3001	1/1	0.95	0.17	68,68,68,68	0
56	MG	QA	1719	1/1	0.95	0.28	32,32,32,32	0
56	MG	YA	3002	1/1	0.95	0.12	64,64,64,64	0
56	MG	YA	3342	1/1	0.95	0.17	20,20,20,20	0
56	MG	RA	3006	1/1	0.95	0.10	33,33,33,33	0
56	MG	RA	3848	1/1	0.95	0.30	50,50,50,50	0
56	MG	QA	1722	1/1	0.95	0.24	61,61,61,61	0
56	MG	YA	3319	1/1	0.95	0.21	20,20,20,20	0
56	MG	YA	3399	1/1	0.95	0.29	36,36,36,36	0
56	MG	YA	3371	1/1	0.95	0.21	14,14,14,14	0
56	MG	YA	3321	1/1	0.95	0.26	29,29,29,29	0
56	MG	YA	3088	1/1	0.95	0.07	42,42,42,42	0
56	MG	RA	3765	1/1	0.95	0.29	40,40,40,40	0
56	MG	YA	3009	1/1	0.95	0.13	37,37,37,37	0
56	MG	XF	201	1/1	0.95	0.11	39,39,39,39	0
56	MG	RA	3306	1/1	0.95	0.34	66,66,66,66	0
56	MG	RA	3016	1/1	0.95	0.34	77,77,77,77	0
56	MG	RA	3770	1/1	0.95	0.21	22,22,22,22	0
56	MG	RA	3771	1/1	0.95	0.08	45,45,45,45	0
56	MG	YA	3325	1/1	0.95	0.17	20,20,20,20	0
56	MG	YA	3759	1/1	0.95	0.38	64,64,64,64	0
56	MG	RA	3378	1/1	0.95	0.22	25,25,25,25	0
56	MG	YA	3602	1/1	0.95	0.22	16,16,16,16	0
56	MG	RA	3455	1/1	0.95	0.27	48,48,48,48	0
56	MG	YA	3205	1/1	0.95	0.21	58,58,58,58	0
56	MG	RA	3194	1/1	0.95	0.16	67,67,67,67	0
56	MG	RA	3870	1/1	0.95	0.23	24,24,24,24	0
56	MG	XA	1710	1/1	0.95	0.20	66,66,66,66	0
56	MG	YA	3604	1/1	0.95	0.23	11,11,11,11	0
56	MG	RA	3619	1/1	0.95	0.23	27,27,27,27	0
56	MG	RA	3874	1/1	0.95	0.24	25,25,25,25	0
56	MG	RA	3025	1/1	0.95	0.06	23,23,23,23	0
57	ZN	Y6	101	1/1	0.95	0.18	169,169,169,169	0
56	MG	YA	3569	1/1	0.95	0.29	32,32,32,32	0
56	MG	RA	3877	1/1	0.95	0.19	23,23,23,23	0
57	ZN	R6	101	1/1	0.95	0.15	160,160,160,160	0
56	MG	RA	3633	1/1	0.96	0.28	74,74,74,74	0
56	MG	RA	3778	1/1	0.96	0.28	41,41,41,41	0
56	MG	XA	1738	1/1	0.96	0.29	58,58,58,58	0
56	MG	YA	3011	1/1	0.96	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
56	MG	RA	3435	1/1	0.96	0.31	23,23,23,23	0
56	MG	YA	3686	1/1	0.96	0.20	15,15,15,15	0
56	MG	YA	3352	1/1	0.96	0.26	11,11,11,11	0
56	MG	RA	3047	1/1	0.96	0.04	12,12,12,12	0
56	MG	YA	3647	1/1	0.96	0.20	27,27,27,27	0
56	MG	RA	3570	1/1	0.96	0.13	35,35,35,35	0
56	MG	RA	3049	1/1	0.96	0.13	48,48,48,48	0
56	MG	YA	3172	1/1	0.96	0.17	69,69,69,69	0
56	MG	YA	3615	1/1	0.96	0.24	11,11,11,11	0
56	MG	RA	4030	1/1	0.96	0.25	71,71,71,71	0
56	MG	RA	3324	1/1	0.96	0.18	14,14,14,14	0
56	MG	RA	3160	1/1	0.96	0.28	83,83,83,83	0
56	MG	RA	4033	1/1	0.96	0.18	17,17,17,17	0
56	MG	RA	3576	1/1	0.96	0.21	43,43,43,43	0
56	MG	YA	3096	1/1	0.96	0.14	26,26,26,26	0
56	MG	RA	4036	1/1	0.96	0.23	85,85,85,85	0
56	MG	RA	3720	1/1	0.96	0.08	33,33,33,33	0
56	MG	YA	3617	1/1	0.96	0.13	17,17,17,17	0
56	MG	RA	3004	1/1	0.96	0.06	29,29,29,29	0
56	MG	YA	3063	1/1	0.96	0.10	35,35,35,35	0
56	MG	QA	1706	1/1	0.96	0.24	35,35,35,35	0
56	MG	YA	3152	1/1	0.96	0.14	50,50,50,50	0
56	MG	YA	3022	1/1	0.96	0.16	62,62,62,62	0
56	MG	RA	3060	1/1	0.96	0.06	21,21,21,21	0
56	MG	YA	3696	1/1	0.96	0.21	17,17,17,17	0
56	MG	RA	3879	1/1	0.96	0.14	29,29,29,29	0
56	MG	YA	3015	1/1	0.96	0.17	23,23,23,23	0
56	MG	YA	3090	1/1	0.96	0.18	54,54,54,54	0
56	MG	YA	3296	1/1	0.96	0.35	32,32,32,32	0
56	MG	YA	3533	1/1	0.96	0.16	48,48,48,48	0
56	MG	YA	3560	1/1	0.96	0.07	6,6,6,6	0
56	MG	RA	3885	1/1	0.96	0.20	66,66,66,66	0
56	MG	RA	3119	1/1	0.96	0.12	74,74,74,74	0
56	MG	RA	3400	1/1	0.96	0.28	21,21,21,21	0
56	MG	YA	3132	1/1	0.96	0.21	86,86,86,86	0
56	MG	YA	3627	1/1	0.96	0.28	38,38,38,38	0
56	MG	RA	3465	1/1	0.96	0.20	27,27,27,27	0
56	MG	YA	3006	1/1	0.96	0.11	18,18,18,18	0
56	MG	RA	3467	1/1	0.96	0.20	21,21,21,21	0
56	MG	RA	3894	1/1	0.96	0.23	23,23,23,23	0
56	MG	RA	3895	1/1	0.96	0.20	54,54,54,54	0
56	MG	RA	3070	1/1	0.96	0.24	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3469	1/1	0.96	0.35	40,40,40,40	0
56	MG	YA	3093	1/1	0.96	0.08	18,18,18,18	0
56	MG	YA	3592	1/1	0.96	0.23	28,28,28,28	0
56	MG	RA	3022	1/1	0.96	0.20	76,76,76,76	0
56	MG	RA	3901	1/1	0.96	0.16	16,16,16,16	0
56	MG	RA	3291	1/1	0.96	0.20	86,86,86,86	0
56	MG	YA	3300	1/1	0.96	0.18	40,40,40,40	0
56	MG	YA	3322	1/1	0.96	0.14	9,9,9,9	0
56	MG	RA	3906	1/1	0.96	0.19	20,20,20,20	0
56	MG	YA	3067	1/1	0.96	0.36	53,53,53,53	0
56	MG	YA	3283	1/1	0.96	0.18	36,36,36,36	0
56	MG	RA	3543	1/1	0.96	0.16	26,26,26,26	0
56	MG	RA	3479	1/1	0.96	0.24	19,19,19,19	0
56	MG	YA	3568	1/1	0.96	0.14	19,19,19,19	0
56	MG	RB	214	1/1	0.96	0.27	44,44,44,44	0
56	MG	RA	3079	1/1	0.96	0.11	64,64,64,64	0
56	MG	QA	1846	1/1	0.96	0.36	47,47,47,47	0
56	MG	RA	3616	1/1	0.96	0.17	33,33,33,33	0
56	MG	YA	3515	1/1	0.96	0.19	12,12,12,12	0
56	MG	RA	3030	1/1	0.96	0.39	113,113,113,113	0
56	MG	XA	1612	1/1	0.96	0.10	41,41,41,41	0
56	MG	RA	3761	1/1	0.96	0.17	22,22,22,22	0
56	MG	RA	3032	1/1	0.96	0.12	49,49,49,49	0
56	MG	RA	3487	1/1	0.96	0.06	17,17,17,17	0
56	MG	YA	3600	1/1	0.96	0.36	51,51,51,51	0
56	MG	YA	3398	1/1	0.96	0.16	25,25,25,25	0
56	MG	RA	3624	1/1	0.96	0.18	38,38,38,38	0
56	MG	YA	3285	1/1	0.96	0.29	25,25,25,25	0
56	MG	YA	3256	1/1	0.96	0.24	43,43,43,43	0
56	MG	YA	3606	1/1	0.96	0.27	25,25,25,25	0
56	MG	RA	3698	1/1	0.96	0.12	73,73,73,73	0
56	MG	YA	3327	1/1	0.96	0.22	7,7,7,7	0
56	MG	YA	3681	1/1	0.96	0.35	38,38,38,38	0
56	MG	YA	3305	1/1	0.96	0.08	19,19,19,19	0
56	MG	RA	3094	1/1	0.96	0.44	71,71,71,71	0
56	MG	YA	3496	1/1	0.96	0.22	18,18,18,18	0
56	MG	YA	3614	1/1	0.97	0.22	26,26,26,26	0
56	MG	RA	3473	1/1	0.97	0.15	26,26,26,26	0
56	MG	YA	3572	1/1	0.97	0.12	28,28,28,28	0
56	MG	RA	3382	1/1	0.97	0.14	20,20,20,20	0
56	MG	YA	3388	1/1	0.97	0.13	33,33,33,33	0
56	MG	RA	3944	1/1	0.97	0.04	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3431	1/1	0.97	0.12	57,57,57,57	0
56	MG	RA	3676	1/1	0.97	0.13	86,86,86,86	0
56	MG	RA	3430	1/1	0.97	0.12	9,9,9,9	0
56	MG	YD	306	1/1	0.97	0.14	53,53,53,53	0
56	MG	YA	3337	1/1	0.97	0.17	35,35,35,35	0
56	MG	YA	3433	1/1	0.97	0.14	19,19,19,19	0
56	MG	YA	3374	1/1	0.97	0.27	34,34,34,34	0
56	MG	YA	3128	1/1	0.97	0.06	26,26,26,26	0
56	MG	YA	3452	1/1	0.97	0.09	46,46,46,46	0
56	MG	RA	3147	1/1	0.97	0.15	39,39,39,39	0
56	MG	YA	3320	1/1	0.97	0.20	26,26,26,26	0
56	MG	RA	3585	1/1	0.97	0.30	59,59,59,59	0
56	MG	YA	3141	1/1	0.97	0.21	23,23,23,23	0
56	MG	YA	3129	1/1	0.97	0.06	31,31,31,31	0
56	MG	RA	3395	1/1	0.97	0.06	22,22,22,22	0
56	MG	RA	3904	1/1	0.97	0.10	24,24,24,24	0
56	MG	RA	3443	1/1	0.97	0.29	20,20,20,20	0
56	MG	Y8	102	1/1	0.97	0.28	41,41,41,41	0
56	MG	RA	3964	1/1	0.97	0.08	44,44,44,44	0
56	MG	YA	3670	1/1	0.97	0.19	12,12,12,12	0
56	MG	RA	3041	1/1	0.97	0.05	44,44,44,44	0
56	MG	RA	3745	1/1	0.97	0.13	21,21,21,21	0
56	MG	YA	3527	1/1	0.97	0.27	50,50,50,50	0
56	MG	RA	3855	1/1	0.97	0.45	62,62,62,62	0
56	MG	RA	3273	1/1	0.97	0.23	76,76,76,76	0
56	MG	RA	3971	1/1	0.97	0.20	19,19,19,19	0
56	MG	QA	1631	1/1	0.97	0.03	34,34,34,34	0
56	MG	YA	3605	1/1	0.97	0.18	19,19,19,19	0
56	MG	YA	3697	1/1	0.97	0.36	38,38,38,38	0
56	MG	YA	3091	1/1	0.97	0.06	36,36,36,36	0
56	MG	QA	1695	1/1	0.97	0.31	48,48,48,48	0
56	MG	RA	3501	1/1	0.97	0.32	22,22,22,22	0
56	MG	YA	3282	1/1	0.97	0.18	10,10,10,10	0
56	MG	RA	3979	1/1	0.97	0.16	37,37,37,37	0
56	MG	RA	3808	1/1	0.97	0.16	56,56,56,56	0
56	MG	RA	3014	1/1	0.97	0.12	38,38,38,38	0
56	MG	QA	1790	1/1	0.97	0.33	56,56,56,56	0
56	MG	YA	3290	1/1	0.97	0.24	47,47,47,47	0
56	MG	RA	4044	1/1	0.97	0.18	95,95,95,95	0
56	MG	RA	3655	1/1	0.97	0.16	25,25,25,25	0
56	MG	XA	1635	1/1	0.97	0.14	29,29,29,29	0
56	MG	YA	3106	1/1	0.97	0.06	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
56	MG	YA	3385	1/1	0.97	0.20	23,23,23,23	0
56	MG	RA	3168	1/1	0.97	0.10	71,71,71,71	0
56	MG	RA	3020	1/1	0.97	0.27	89,89,89,89	0
56	MG	RA	3092	1/1	0.97	0.15	79,79,79,79	0
56	MG	RA	3056	1/1	0.97	0.14	70,70,70,70	0
56	MG	XA	1694	1/1	0.97	0.26	30,30,30,30	0
56	MG	YA	3358	1/1	0.97	0.28	18,18,18,18	0
56	MG	RA	3420	1/1	0.97	0.07	19,19,19,19	0
56	MG	YA	3284	1/1	0.97	0.14	8,8,8,8	0
56	MG	YA	3728	1/1	0.97	0.12	8,8,8,8	0
56	MG	YB	219	1/1	0.97	0.23	31,31,31,31	0
56	MG	RA	3337	1/1	0.97	0.26	81,81,81,81	0
56	MG	RA	4060	1/1	0.97	0.20	82,82,82,82	0
58	SF4	XD	301	8/8	0.97	0.06	58,74,100,102	0
56	MG	RA	3323	1/1	0.98	0.07	38,38,38,38	0
56	MG	YA	3143	1/1	0.98	0.10	56,56,56,56	0
56	MG	YA	3542	1/1	0.98	0.17	21,21,21,21	0
56	MG	YA	3016	1/1	0.98	0.06	29,29,29,29	0
56	MG	YA	3151	1/1	0.98	0.03	8,8,8,8	0
56	MG	RA	4028	1/1	0.98	0.11	78,78,78,78	0
56	MG	YA	3041	1/1	0.98	0.05	35,35,35,35	0
56	MG	RA	3123	1/1	0.98	0.12	30,30,30,30	0
56	MG	RE	303	1/1	0.98	0.11	15,15,15,15	0
56	MG	YA	3503	1/1	0.98	0.10	18,18,18,18	0
56	MG	RB	205	1/1	0.98	0.07	47,47,47,47	0
56	MG	YA	3353	1/1	0.98	0.12	14,14,14,14	0
56	MG	RA	3597	1/1	0.98	0.12	19,19,19,19	0
56	MG	YB	210	1/1	0.98	0.36	57,57,57,57	0
56	MG	YA	3195	1/1	0.98	0.07	33,33,33,33	0
56	MG	YA	3685	1/1	0.98	0.24	19,19,19,19	0
56	MG	YA	3317	1/1	0.98	0.07	24,24,24,24	0
56	MG	YA	3595	1/1	0.98	0.27	12,12,12,12	0
56	MG	YA	3480	1/1	0.98	0.21	17,17,17,17	0
56	MG	RA	3888	1/1	0.98	0.28	24,24,24,24	0
56	MG	YA	3008	1/1	0.98	0.11	47,47,47,47	0
56	MG	YA	3013	1/1	0.98	0.06	23,23,23,23	0
56	MG	YA	3651	1/1	0.98	0.32	15,15,15,15	0
56	MG	YA	3652	1/1	0.98	0.29	24,24,24,24	0
56	MG	YA	3112	1/1	0.98	0.10	9,9,9,9	0
56	MG	YA	3673	1/1	0.98	0.15	13,13,13,13	0
56	MG	YA	3382	1/1	0.98	0.19	29,29,29,29	0
56	MG	YD	304	1/1	0.98	0.13	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
56	MG	YA	3601	1/1	0.98	0.30	29,29,29,29	0
56	MG	YA	3739	1/1	0.98	0.35	79,79,79,79	0
56	MG	RA	3579	1/1	0.98	0.15	24,24,24,24	0
56	MG	RA	3348	1/1	0.98	0.14	34,34,34,34	0
56	MG	XA	1746	1/1	0.98	0.30	35,35,35,35	0
56	MG	RA	3318	1/1	0.98	0.16	19,19,19,19	0
56	MG	YA	3460	1/1	0.98	0.10	28,28,28,28	0
56	MG	YD	308	1/1	0.98	0.10	71,71,71,71	0
56	MG	QA	1628	1/1	0.98	0.26	49,49,49,49	0
56	MG	YD	309	1/1	0.98	0.10	14,14,14,14	0
57	ZN	Y9	101	1/1	0.98	0.07	107,107,107,107	0
56	MG	RA	3833	1/1	0.98	0.20	29,29,29,29	0
56	MG	RA	3419	1/1	0.98	0.24	17,17,17,17	0
56	MG	RD	306	1/1	0.98	0.07	33,33,33,33	0
56	MG	RA	3946	1/1	0.98	0.04	18,18,18,18	0
58	SF4	QD	302	8/8	0.98	0.07	51,57,76,106	0
56	MG	YA	3612	1/1	0.99	0.09	23,23,23,23	0
56	MG	RA	3838	1/1	0.99	0.27	17,17,17,17	0
56	MG	RA	3516	1/1	0.99	0.23	13,13,13,13	0
56	MG	YA	3306	1/1	0.99	0.12	9,9,9,9	0
57	ZN	Y5	102	1/1	0.99	0.06	119,119,119,119	0
56	MG	YA	3362	1/1	0.99	0.25	18,18,18,18	0
56	MG	YA	3363	1/1	0.99	0.29	11,11,11,11	0
57	ZN	XN	101	1/1	0.99	0.02	94,94,94,94	0
57	ZN	QN	101	1/1	0.99	0.03	105,105,105,105	0
56	MG	YA	3380	1/1	0.99	0.14	7,7,7,7	0
56	MG	RA	3773	1/1	0.99	0.18	25,25,25,25	0
57	ZN	R5	102	1/1	0.99	0.03	119,119,119,119	0
56	MG	RA	3153	1/1	0.99	0.04	35,35,35,35	0
57	ZN	R9	102	1/1	0.99	0.07	92,92,92,92	0
56	MG	YA	3346	1/1	0.99	0.30	16,16,16,16	0
56	MG	RA	3442	1/1	0.99	0.26	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.