



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2016 – 12:28 AM GMT

PDB ID : 4YPB
Title : Precleavage 70S structure of the *P. vulgaris* HigB DeltaH92 toxin bound to the AAA codon
Authors : Schureck, M.A.; Dunkle, J.A.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2015-03-12
Resolution : 3.40 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

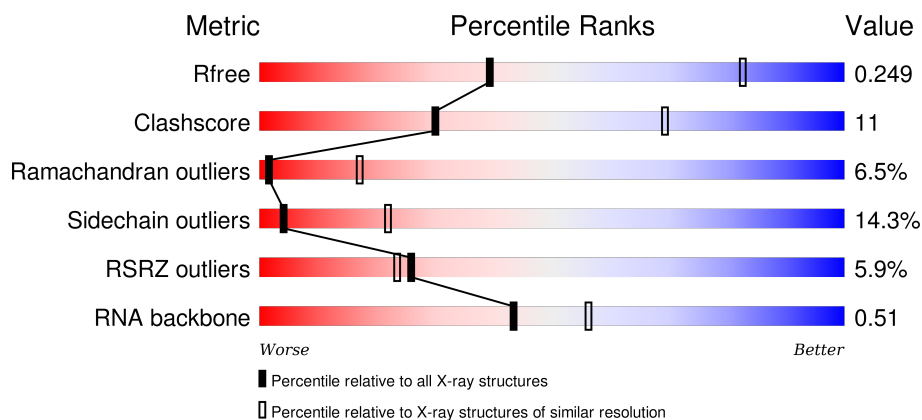
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)
RNA backbone	2183	1041 (4.00-2.80)

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

Mol	Chain	Length	Quality of chain
1	QA	1522	<div> <div>3%</div> <div>55% 33% 10% ..</div> </div>
1	XA	1522	<div> <div>3%</div> <div>55% 34% 9% ..</div> </div>
2	QB	256	<div> <div>11%</div> <div>52% 31% 8% . 8%</div> </div>
2	XB	256	<div> <div>8%</div> <div>50% 34% 8% 8%</div> </div>

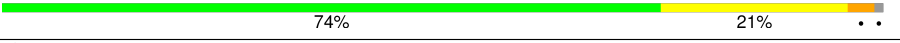





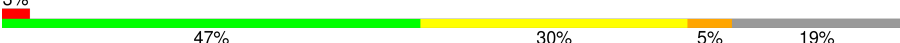
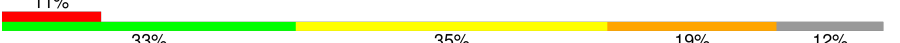
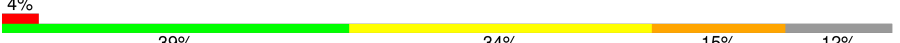


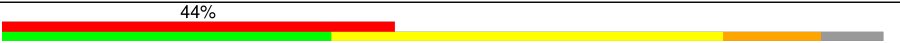
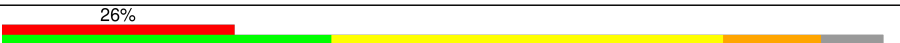








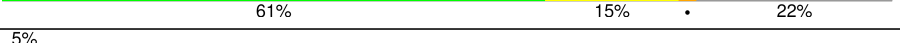



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	




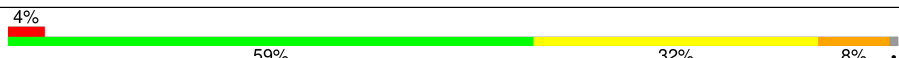
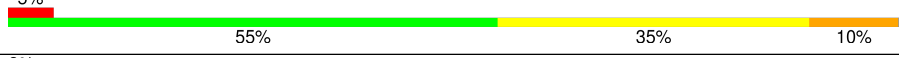

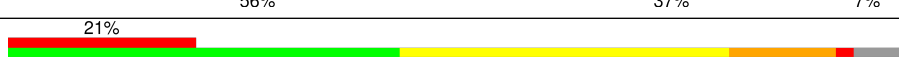
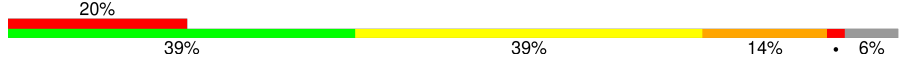


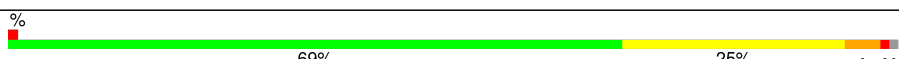


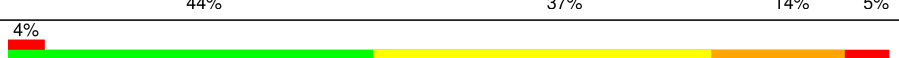
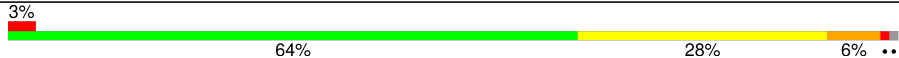

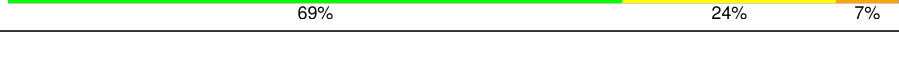


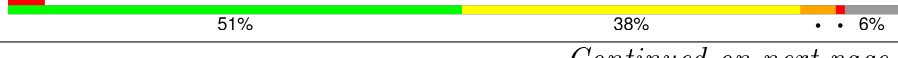



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	QW	77	
22	XV	77	
22	XW	77	
23	QX	25	
23	XX	25	
24	QY	117	
24	XY	117	
25	RA	2916	
25	YA	2916	
26	RB	124	
26	YB	124	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	RD	276	
27	YD	276	
28	RE	206	
28	YE	206	
29	RF	210	
29	YF	210	
30	RG	182	
30	YG	182	
31	RH	180	
31	YH	180	
32	RI	148	
32	YI	148	
33	RN	140	
33	YN	140	
34	RO	122	
34	YO	122	
35	RP	150	
35	YP	150	
36	RQ	141	
36	YQ	141	
37	RR	118	
37	YR	118	
38	RS	112	
38	YS	112	
39	RT	146	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
39	YT	146	
40	RU	118	
40	YU	118	
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	71	
51	R5	60	
51	Y5	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	R6	54	
52	Y6	54	
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	

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	1604	-	-	-	X
56	MG	QA	1605	-	-	-	X
56	MG	QA	1606	-	-	-	X
56	MG	QA	1608	-	-	-	X
56	MG	QA	1609	-	-	-	X
56	MG	QA	1619	-	-	-	X
56	MG	QA	1625	-	-	-	X
56	MG	QA	1632	-	-	-	X
56	MG	QA	1636	-	-	-	X
56	MG	QA	1637	-	-	-	X
56	MG	QA	1639	-	-	-	X
56	MG	QA	1640	-	-	-	X
56	MG	QA	1641	-	-	-	X
56	MG	QA	1643	-	-	-	X
56	MG	QA	1644	-	-	-	X
56	MG	QA	1645	-	-	-	X
56	MG	QA	1651	-	-	-	X
56	MG	QA	1656	-	-	-	X
56	MG	QA	1662	-	-	-	X
56	MG	QA	1668	-	-	-	X
56	MG	QA	1670	-	-	-	X
56	MG	QA	1681	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	QA	1682	-	-	-	X
56	MG	QA	1687	-	-	-	X
56	MG	QA	1699	-	-	-	X
56	MG	QA	1703	-	-	-	X
56	MG	QA	1719	-	-	-	X
56	MG	QA	1728	-	-	-	X
56	MG	QA	1729	-	-	-	X
56	MG	QA	1741	-	-	-	X
56	MG	R5	102	-	-	-	X
56	MG	RA	3001	-	-	-	X
56	MG	RA	3002	-	-	-	X
56	MG	RA	3004	-	-	-	X
56	MG	RA	3007	-	-	-	X
56	MG	RA	3011	-	-	-	X
56	MG	RA	3012	-	-	-	X
56	MG	RA	3013	-	-	-	X
56	MG	RA	3014	-	-	-	X
56	MG	RA	3018	-	-	-	X
56	MG	RA	3022	-	-	-	X
56	MG	RA	3026	-	-	-	X
56	MG	RA	3027	-	-	-	X
56	MG	RA	3028	-	-	-	X
56	MG	RA	3032	-	-	-	X
56	MG	RA	3033	-	-	-	X
56	MG	RA	3034	-	-	-	X
56	MG	RA	3037	-	-	-	X
56	MG	RA	3039	-	-	-	X
56	MG	RA	3045	-	-	-	X
56	MG	RA	3047	-	-	-	X
56	MG	RA	3048	-	-	-	X
56	MG	RA	3050	-	-	-	X
56	MG	RA	3051	-	-	-	X
56	MG	RA	3053	-	-	-	X
56	MG	RA	3055	-	-	-	X
56	MG	RA	3056	-	-	-	X
56	MG	RA	3057	-	-	-	X
56	MG	RA	3061	-	-	-	X
56	MG	RA	3063	-	-	-	X
56	MG	RA	3065	-	-	-	X
56	MG	RA	3066	-	-	-	X
56	MG	RA	3067	-	-	-	X
56	MG	RA	3071	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3072	-	-	-	X
56	MG	RA	3073	-	-	-	X
56	MG	RA	3074	-	-	-	X
56	MG	RA	3079	-	-	-	X
56	MG	RA	3080	-	-	-	X
56	MG	RA	3081	-	-	-	X
56	MG	RA	3082	-	-	-	X
56	MG	RA	3083	-	-	-	X
56	MG	RA	3094	-	-	-	X
56	MG	RA	3095	-	-	-	X
56	MG	RA	3099	-	-	-	X
56	MG	RA	3103	-	-	-	X
56	MG	RA	3104	-	-	-	X
56	MG	RA	3105	-	-	-	X
56	MG	RA	3107	-	-	-	X
56	MG	RA	3108	-	-	-	X
56	MG	RA	3110	-	-	-	X
56	MG	RA	3116	-	-	-	X
56	MG	RA	3125	-	-	-	X
56	MG	RA	3128	-	-	-	X
56	MG	RA	3131	-	-	-	X
56	MG	RA	3135	-	-	-	X
56	MG	RA	3140	-	-	-	X
56	MG	RA	3148	-	-	-	X
56	MG	RA	3149	-	-	-	X
56	MG	RA	3153	-	-	-	X
56	MG	RA	3155	-	-	-	X
56	MG	RA	3159	-	-	-	X
56	MG	RA	3165	-	-	-	X
56	MG	RA	3166	-	-	-	X
56	MG	RA	3173	-	-	-	X
56	MG	RA	3177	-	-	-	X
56	MG	RA	3184	-	-	-	X
56	MG	RA	3189	-	-	-	X
56	MG	RA	3193	-	-	-	X
56	MG	RA	3195	-	-	-	X
56	MG	RA	3197	-	-	-	X
56	MG	RA	3198	-	-	-	X
56	MG	RA	3202	-	-	-	X
56	MG	RA	3205	-	-	-	X
56	MG	RA	3206	-	-	-	X
56	MG	RA	3209	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3213	-	-	-	X
56	MG	RA	3222	-	-	-	X
56	MG	RA	3225	-	-	-	X
56	MG	RA	3228	-	-	-	X
56	MG	RA	3233	-	-	-	X
56	MG	RA	3244	-	-	-	X
56	MG	RA	3247	-	-	-	X
56	MG	RA	3251	-	-	-	X
56	MG	RA	3254	-	-	-	X
56	MG	RA	3259	-	-	-	X
56	MG	RA	3263	-	-	-	X
56	MG	RA	3264	-	-	-	X
56	MG	RA	3275	-	-	-	X
56	MG	RA	3291	-	-	-	X
56	MG	RA	3292	-	-	-	X
56	MG	RA	3295	-	-	-	X
56	MG	RA	3296	-	-	-	X
56	MG	RA	3306	-	-	-	X
56	MG	RA	3316	-	-	-	X
56	MG	RA	3318	-	-	-	X
56	MG	RA	3331	-	-	-	X
56	MG	RA	3339	-	-	-	X
56	MG	RA	3343	-	-	-	X
56	MG	RA	3350	-	-	-	X
56	MG	RA	3355	-	-	-	X
56	MG	RA	3357	-	-	-	X
56	MG	RA	3363	-	-	-	X
56	MG	RA	3365	-	-	-	X
56	MG	RA	3368	-	-	-	X
56	MG	RA	3369	-	-	-	X
56	MG	RA	3370	-	-	-	X
56	MG	RA	3376	-	-	-	X
56	MG	RA	3377	-	-	-	X
56	MG	RA	3385	-	-	-	X
56	MG	RA	3386	-	-	-	X
56	MG	RA	3405	-	-	-	X
56	MG	RA	3407	-	-	-	X
56	MG	RA	3411	-	-	-	X
56	MG	RA	3420	-	-	-	X
56	MG	RA	3425	-	-	-	X
56	MG	RA	3427	-	-	-	X
56	MG	RA	3430	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3431	-	-	-	X
56	MG	RA	3432	-	-	-	X
56	MG	RA	3434	-	-	-	X
56	MG	RA	3436	-	-	-	X
56	MG	RA	3438	-	-	-	X
56	MG	RD	302	-	-	-	X
56	MG	RQ	202	-	-	-	X
56	MG	XA	1601	-	-	-	X
56	MG	XA	1604	-	-	-	X
56	MG	XA	1605	-	-	-	X
56	MG	XA	1607	-	-	-	X
56	MG	XA	1611	-	-	-	X
56	MG	XA	1613	-	-	-	X
56	MG	XA	1618	-	-	-	X
56	MG	XA	1624	-	-	-	X
56	MG	XA	1625	-	-	-	X
56	MG	XA	1635	-	-	-	X
56	MG	XA	1638	-	-	-	X
56	MG	XA	1640	-	-	-	X
56	MG	XA	1643	-	-	-	X
56	MG	XA	1644	-	-	-	X
56	MG	XA	1650	-	-	-	X
56	MG	XA	1652	-	-	-	X
56	MG	XA	1659	-	-	-	X
56	MG	XA	1664	-	-	-	X
56	MG	XA	1667	-	-	-	X
56	MG	XA	1692	-	-	-	X
56	MG	XA	1695	-	-	-	X
56	MG	XA	1697	-	-	-	X
56	MG	XA	1701	-	-	-	X
56	MG	XA	1717	-	-	-	X
56	MG	XA	1742	-	-	-	X
56	MG	XA	1745	-	-	-	X
56	MG	XA	1754	-	-	-	X
56	MG	XA	1755	-	-	-	X
56	MG	Y1	101	-	-	-	X
56	MG	YA	3003	-	-	-	X
56	MG	YA	3006	-	-	-	X
56	MG	YA	3010	-	-	-	X
56	MG	YA	3011	-	-	-	X
56	MG	YA	3012	-	-	-	X
56	MG	YA	3013	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3017	-	-	-	X
56	MG	YA	3018	-	-	-	X
56	MG	YA	3025	-	-	-	X
56	MG	YA	3026	-	-	-	X
56	MG	YA	3027	-	-	-	X
56	MG	YA	3031	-	-	-	X
56	MG	YA	3033	-	-	-	X
56	MG	YA	3038	-	-	-	X
56	MG	YA	3042	-	-	-	X
56	MG	YA	3044	-	-	-	X
56	MG	YA	3049	-	-	-	X
56	MG	YA	3054	-	-	-	X
56	MG	YA	3055	-	-	-	X
56	MG	YA	3056	-	-	-	X
56	MG	YA	3060	-	-	-	X
56	MG	YA	3062	-	-	-	X
56	MG	YA	3064	-	-	-	X
56	MG	YA	3066	-	-	-	X
56	MG	YA	3070	-	-	-	X
56	MG	YA	3071	-	-	-	X
56	MG	YA	3072	-	-	-	X
56	MG	YA	3073	-	-	-	X
56	MG	YA	3078	-	-	-	X
56	MG	YA	3079	-	-	-	X
56	MG	YA	3080	-	-	-	X
56	MG	YA	3081	-	-	-	X
56	MG	YA	3082	-	-	-	X
56	MG	YA	3088	-	-	-	X
56	MG	YA	3092	-	-	-	X
56	MG	YA	3097	-	-	-	X
56	MG	YA	3099	-	-	-	X
56	MG	YA	3101	-	-	-	X
56	MG	YA	3102	-	-	-	X
56	MG	YA	3103	-	-	-	X
56	MG	YA	3106	-	-	-	X
56	MG	YA	3109	-	-	-	X
56	MG	YA	3111	-	-	-	X
56	MG	YA	3121	-	-	-	X
56	MG	YA	3122	-	-	-	X
56	MG	YA	3127	-	-	-	X
56	MG	YA	3130	-	-	-	X
56	MG	YA	3133	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3137	-	-	-	X
56	MG	YA	3146	-	-	-	X
56	MG	YA	3147	-	-	-	X
56	MG	YA	3151	-	-	-	X
56	MG	YA	3155	-	-	-	X
56	MG	YA	3156	-	-	-	X
56	MG	YA	3167	-	-	-	X
56	MG	YA	3170	-	-	-	X
56	MG	YA	3186	-	-	-	X
56	MG	YA	3190	-	-	-	X
56	MG	YA	3191	-	-	-	X
56	MG	YA	3192	-	-	-	X
56	MG	YA	3201	-	-	-	X
56	MG	YA	3203	-	-	-	X
56	MG	YA	3204	-	-	-	X
56	MG	YA	3208	-	-	-	X
56	MG	YA	3209	-	-	-	X
56	MG	YA	3210	-	-	-	X
56	MG	YA	3220	-	-	-	X
56	MG	YA	3221	-	-	-	X
56	MG	YA	3224	-	-	-	X
56	MG	YA	3227	-	-	-	X
56	MG	YA	3233	-	-	-	X
56	MG	YA	3234	-	-	-	X
56	MG	YA	3240	-	-	-	X
56	MG	YA	3249	-	-	-	X
56	MG	YA	3250	-	-	-	X
56	MG	YA	3255	-	-	-	X
56	MG	YA	3264	-	-	-	X
56	MG	YA	3276	-	-	-	X
56	MG	YA	3280	-	-	-	X
56	MG	YA	3282	-	-	-	X
56	MG	YA	3295	-	-	-	X
56	MG	YA	3305	-	-	-	X
56	MG	YA	3325	-	-	-	X
56	MG	YA	3335	-	-	-	X
56	MG	YA	3336	-	-	-	X
56	MG	YA	3338	-	-	-	X
56	MG	YA	3339	-	-	-	X
56	MG	YA	3340	-	-	-	X
56	MG	YA	3375	-	-	-	X
56	MG	YA	3392	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3407	-	-	-	X
56	MG	YA	3414	-	-	-	X
56	MG	YA	3416	-	-	-	X
56	MG	YA	3418	-	-	-	X
56	MG	YA	3424	-	-	-	X
56	MG	YA	3425	-	-	-	X
56	MG	YA	3426	-	-	-	X
56	MG	YA	3428	-	-	-	X
56	MG	YA	3431	-	-	-	X
56	MG	YA	3455	-	-	-	X
56	MG	YA	3459	-	-	-	X
56	MG	YA	3460	-	-	-	X
56	MG	YA	3463	-	-	-	X
56	MG	YA	3467	-	-	-	X
56	MG	YA	3472	-	-	-	X
56	MG	YA	3473	-	-	-	X
56	MG	YA	3484	-	-	-	X
56	MG	YA	3485	-	-	-	X
56	MG	YD	301	-	-	-	X
56	MG	YF	301	-	-	-	X
56	MG	YQ	201	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 297549 atoms, of which 18 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 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1511	Total	C	N	O	P	0	0	0
			32472	14453	6011	10497	1511			
1	XA	1508	Total	C	N	O	P	0	0	0
			32409	14425	6001	10475	1508			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	236	Total	C	N	O	S	0	0	0
			1915	1223	343	344	5			
2	XB	236	Total	C	N	O	S	0	0	0
			1915	1223	343	344	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	QC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
3	XC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	QD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	XD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	154	Total	C	N	O	S	0	0	0
			1178	743	221	210	4			
5	XE	154	Total	C	N	O	S	0	0	0
			1178	743	221	210	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	QF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	XF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	QG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	XG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	XH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	QI	128	Total	C	N	O	S	0	0	0
			1018	644	198	175	1			
9	XI	128	Total	C	N	O	S	0	0	0
			1018	644	198	175	1			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	QJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	XJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	121	Total	C	N	O	S	0	0	0
			901	560	171	167	3			
11	XK	121	Total	C	N	O	S	0	0	0
			901	560	171	167	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	QL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	XL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			
13	XM	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	XO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	QP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	XP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	QQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	XQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	71	Total	C	N	O	0	0	0
			585	373	116	96			
18	XR	71	Total	C	N	O	0	0	0
			585	373	116	96			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	82	Total	C	N	O	S	0	0	0
			656	419	121	114	2			
19	XS	82	Total	C	N	O	S	0	0	0
			656	419	121	114	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	XT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	QU	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	XU	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	QW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	QX	20	Total	C	H	N	O	P	0	0	0
			449	199	9	89	132	20			
23	XX	20	Total	C	H	N	O	P	0	0	0
			449	199	9	89	132	20			

- Molecule 24 is a protein called Host inhibition of growth B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	QY	91	Total	C	N	O	0	0	0
			746	478	131	137			
24	XY	91	Total	C	N	O	0	0	0
			746	478	131	137			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QY	0	MET	-	initiating methionine	UNP Q7A225
QY	1	GLY	-	expression tag	UNP Q7A225
QY	92	LYS	-	expression tag	UNP Q7A225
QY	93	LEU	-	expression tag	UNP Q7A225
QY	94	GLY	-	expression tag	UNP Q7A225
QY	95	PRO	-	expression tag	UNP Q7A225
QY	96	GLU	-	expression tag	UNP Q7A225

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
QY	97	GLN	-	expression tag	UNP Q7A225
QY	98	LYS	-	expression tag	UNP Q7A225
QY	99	LEU	-	expression tag	UNP Q7A225
QY	100	ILE	-	expression tag	UNP Q7A225
QY	101	SER	-	expression tag	UNP Q7A225
QY	102	GLU	-	expression tag	UNP Q7A225
QY	103	GLU	-	expression tag	UNP Q7A225
QY	104	ASP	-	expression tag	UNP Q7A225
QY	105	LEU	-	expression tag	UNP Q7A225
QY	106	ASN	-	expression tag	UNP Q7A225
QY	107	SER	-	expression tag	UNP Q7A225
QY	108	ALA	-	expression tag	UNP Q7A225
QY	109	VAL	-	expression tag	UNP Q7A225
QY	110	ASP	-	expression tag	UNP Q7A225
QY	111	HIS	-	expression tag	UNP Q7A225
QY	112	HIS	-	expression tag	UNP Q7A225
QY	113	HIS	-	expression tag	UNP Q7A225
QY	114	HIS	-	expression tag	UNP Q7A225
QY	115	HIS	-	expression tag	UNP Q7A225
QY	116	HIS	-	expression tag	UNP Q7A225
XY	0	MET	-	initiating methionine	UNP Q7A225
XY	1	GLY	-	expression tag	UNP Q7A225
XY	92	LYS	-	expression tag	UNP Q7A225
XY	93	LEU	-	expression tag	UNP Q7A225
XY	94	GLY	-	expression tag	UNP Q7A225
XY	95	PRO	-	expression tag	UNP Q7A225
XY	96	GLU	-	expression tag	UNP Q7A225
XY	97	GLN	-	expression tag	UNP Q7A225
XY	98	LYS	-	expression tag	UNP Q7A225
XY	99	LEU	-	expression tag	UNP Q7A225
XY	100	ILE	-	expression tag	UNP Q7A225
XY	101	SER	-	expression tag	UNP Q7A225
XY	102	GLU	-	expression tag	UNP Q7A225
XY	103	GLU	-	expression tag	UNP Q7A225
XY	104	ASP	-	expression tag	UNP Q7A225
XY	105	LEU	-	expression tag	UNP Q7A225
XY	106	ASN	-	expression tag	UNP Q7A225
XY	107	SER	-	expression tag	UNP Q7A225
XY	108	ALA	-	expression tag	UNP Q7A225
XY	109	VAL	-	expression tag	UNP Q7A225
XY	110	ASP	-	expression tag	UNP Q7A225
XY	111	HIS	-	expression tag	UNP Q7A225

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
XY	112	HIS	-	expression tag	UNP Q7A225
XY	113	HIS	-	expression tag	UNP Q7A225
XY	114	HIS	-	expression tag	UNP Q7A225
XY	115	HIS	-	expression tag	UNP Q7A225
XY	116	HIS	-	expression tag	UNP Q7A225

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	RA	2891	Total	C	N	O	P	0	0	0
			62269	27713	11649	20016	2891			
25	YA	2875	Total	C	N	O	P	0	0	0
			61924	27560	11583	19906	2875			

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	RB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
26	YB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
27	YD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
28	YE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	RF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			
29	YF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	RG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
30	YG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	RH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
31	YH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	RI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
32	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	RN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
33	YN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

Continued on next page...

Continued from previous page...

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
35	YP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RQ	140	Total	C	N	O	S	0	0	0
			1112	710	210	185	7			
36	YQ	139	Total	C	N	O	S	0	0	0
			1107	707	209	184	7			

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RR	117	Total	C	N	O		0	0	0
			960	599	202	159				
37	YR	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RS	111	Total	C	N	O		0	0	0
			882	556	176	150				
38	YS	111	Total	C	N	O		0	0	0
			882	556	176	150				

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
39	YT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
40	YU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
41	YV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
42	YW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	RX	92	Total	C	N	O	0	0	0
			725	471	131	123			
43	YX	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
44	YY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RZ	176	Total	C	N	O	S	0	0	0
			1404	897	252	252	3			
45	YZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R0	83	Total	C	N	O	S	0	0	0
			657	407	139	110	1			
46	Y0	83	Total	C	N	O	S	0	0	0
			657	407	139	110	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
47	Y1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
48	Y2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	R3	59	Total	C	N	O	0	0	0
			469	298	90	81			
49	Y3	59	Total	C	N	O	0	0	0
			469	298	90	81			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	R4	70	Total	C	N	O	S	0	0	0
			573	359	107	103	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	Y4	70	Total	C	N	O	S	0	0	0
			573	359	107	103	4			

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
51	Y5	57	Total	C	N	O	S	0	0	0
			442	278	88	71	5			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	R6	48	Total	C	N	O	S	0	0	0
			417	259	86	68	4			
52	Y6	48	Total	C	N	O	S	0	0	0
			417	259	86	68	4			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	R7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
53	Y7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

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

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	R9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
55	Y9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	150	Total 150	Mg 150	0	0
56	YV	1	Total 1	Mg 1	0	0
56	RP	3	Total 3	Mg 3	0	0
56	QX	1	Total 1	Mg 1	0	0
56	YA	487	Total 487	Mg 487	0	0
56	Y5	3	Total 3	Mg 3	0	0
56	YH	1	Total 1	Mg 1	0	0
56	RT	1	Total 1	Mg 1	0	0
56	QD	2	Total 2	Mg 2	0	0
56	XS	1	Total 1	Mg 1	0	0
56	Y1	1	Total 1	Mg 1	0	0
56	YD	1	Total 1	Mg 1	0	0
56	QV	4	Total 4	Mg 4	0	0
56	YO	1	Total 1	Mg 1	0	0
56	XA	163	Total 163	Mg 163	0	0
56	YY	1	Total 1	Mg 1	0	0
56	RQ	2	Total 2	Mg 2	0	0
56	R0	3	Total 3	Mg 3	0	0
56	QL	1	Total 1	Mg 1	0	0
56	Y0	3	Total 3	Mg 3	0	0
56	YG	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	YQ	2	Total 2	Mg 2	0	0
56	RY	1	Total 1	Mg 1	0	0
56	YN	1	Total 1	Mg 1	0	0
56	XF	1	Total 1	Mg 1	0	0
56	RR	1	Total 1	Mg 1	0	0
56	RD	2	Total 2	Mg 2	0	0
56	R1	1	Total 1	Mg 1	0	0
56	XL	1	Total 1	Mg 1	0	0
56	Y7	1	Total 1	Mg 1	0	0
56	RV	1	Total 1	Mg 1	0	0
56	R5	3	Total 3	Mg 3	0	0
56	RA	441	Total 441	Mg 441	0	0
56	YF	1	Total 1	Mg 1	0	0
56	YP	1	Total 1	Mg 1	0	0
56	RE	1	Total 1	Mg 1	0	0
56	R2	1	Total 1	Mg 1	0	0
56	YB	6	Total 6	Mg 6	0	0
56	YW	1	Total 1	Mg 1	0	0
56	XV	3	Total 3	Mg 3	0	0
56	RB	4	Total 4	Mg 4	0	0
56	XD	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	RF	1	Total	Mg	0	0
			1	1		
56	YE	1	Total	Mg	0	0
			1	1		

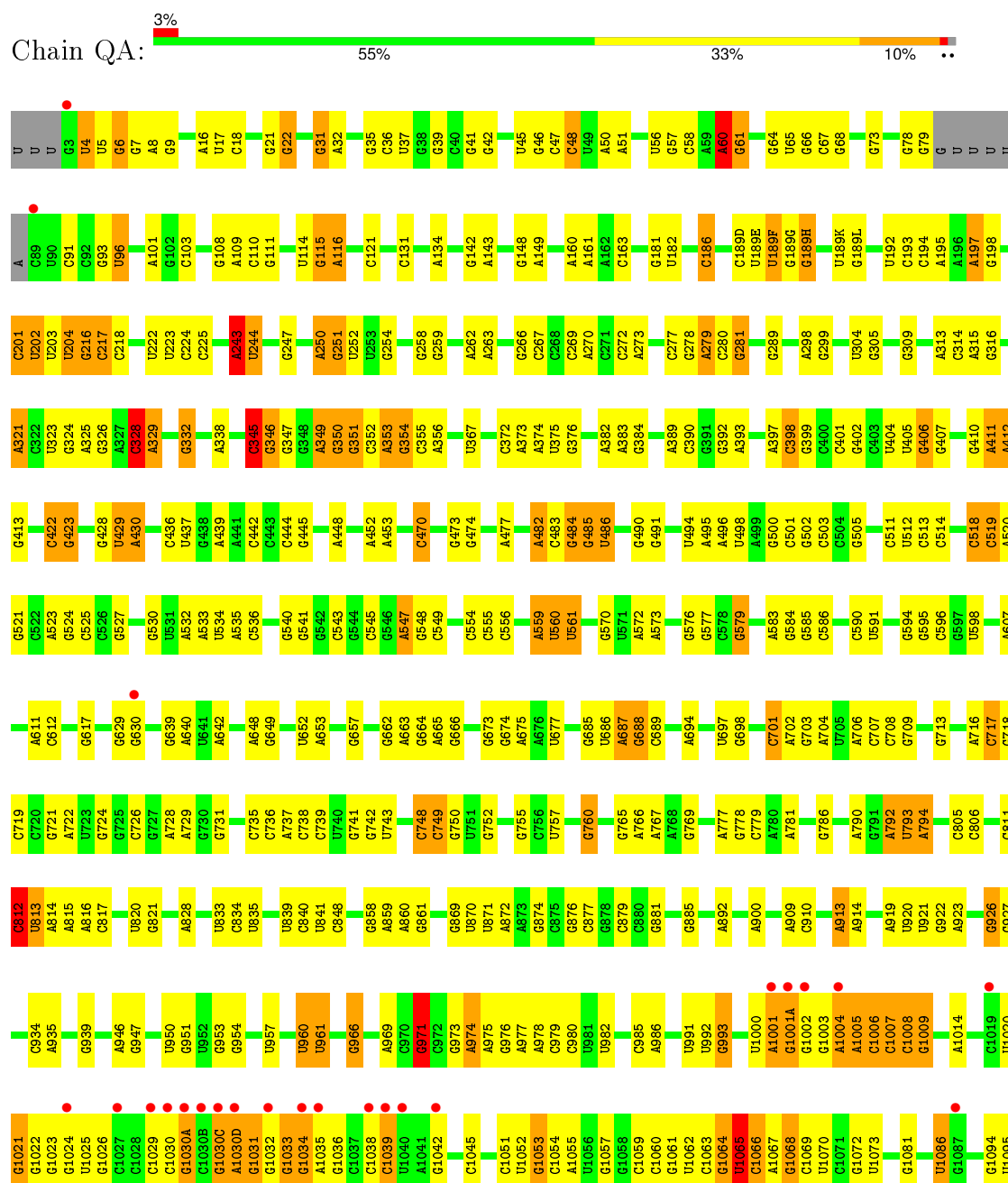
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

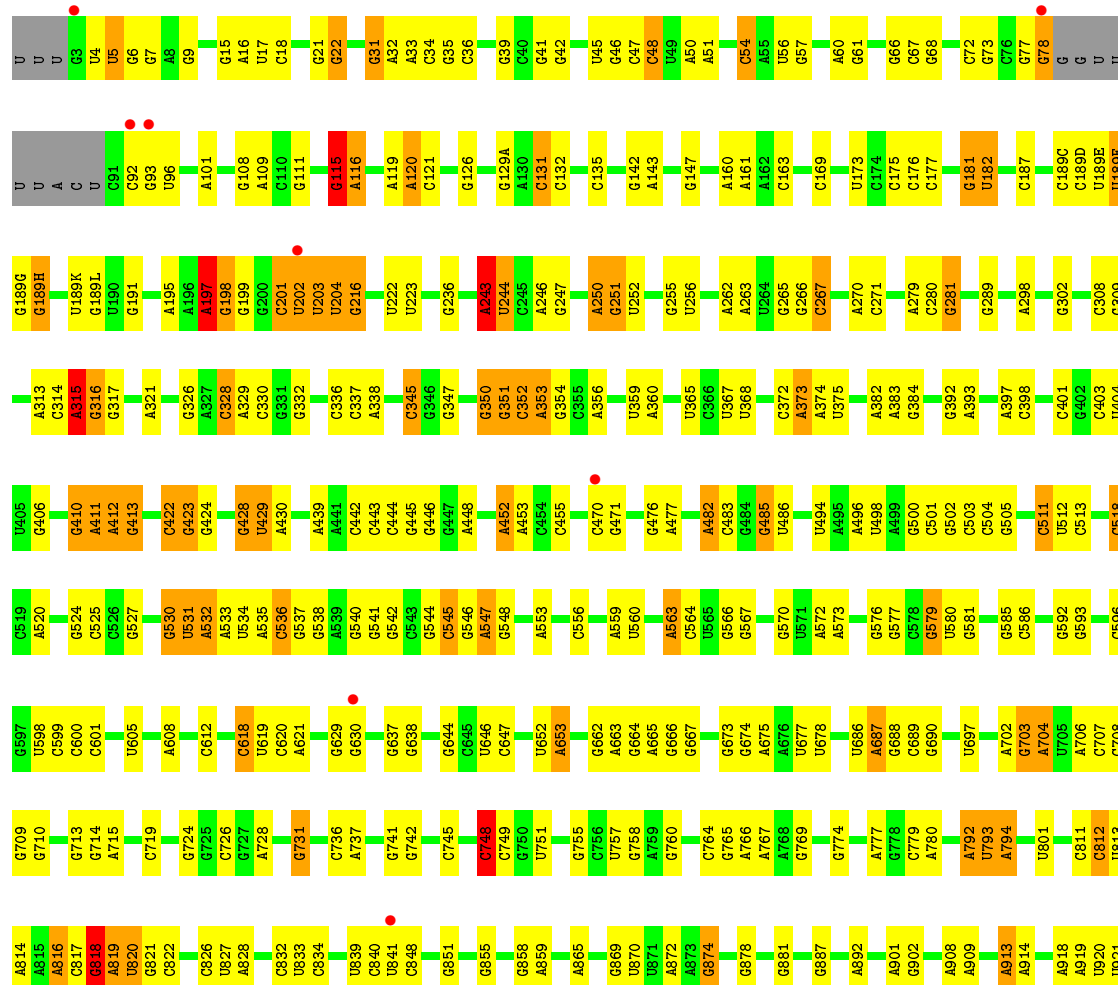
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	XD	1	Total	Zn	0	0
			1	1		
57	QD	1	Total	Zn	0	0
			1	1		
57	QN	1	Total	Zn	0	0
			1	1		
57	XN	1	Total	Zn	0	0
			1	1		

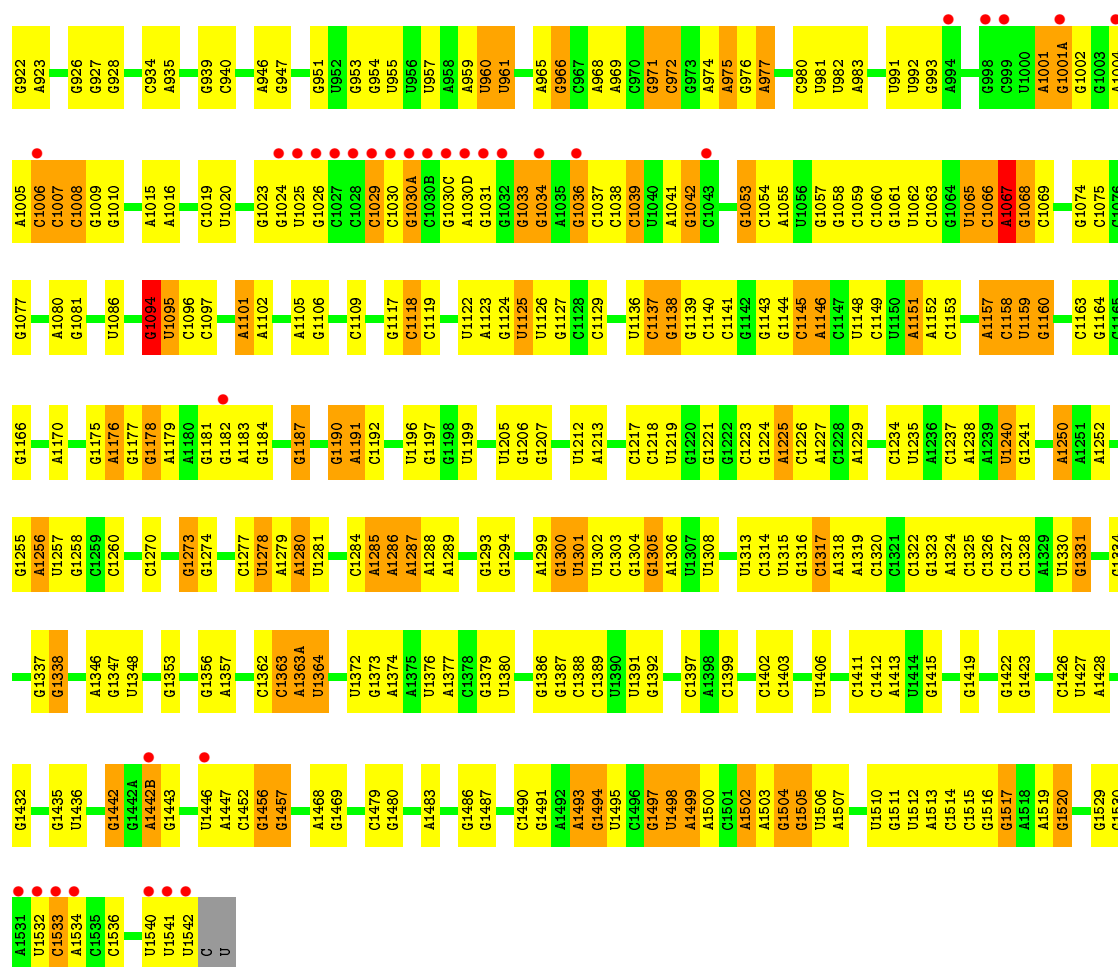
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

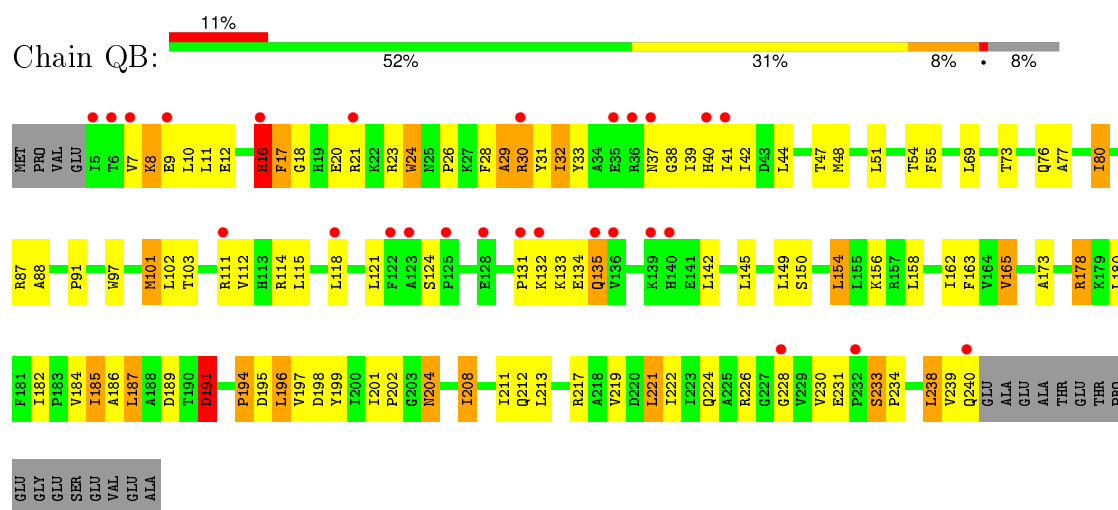
• Molecule 1: 16S rRNA





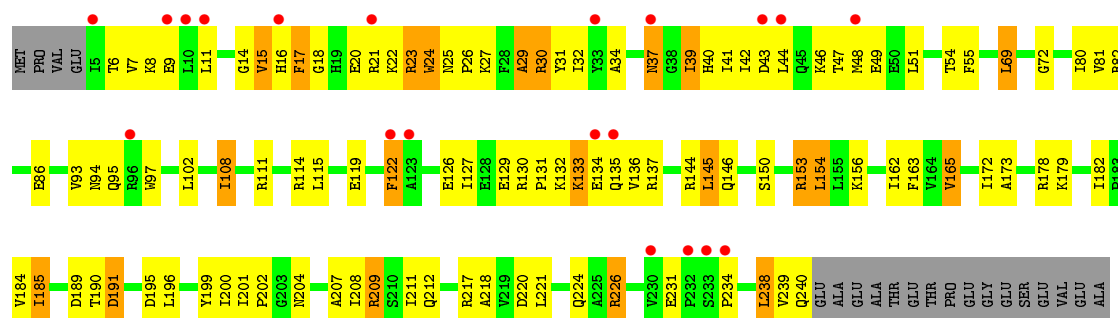


• Molecule 2: 30S ribosomal protein S2

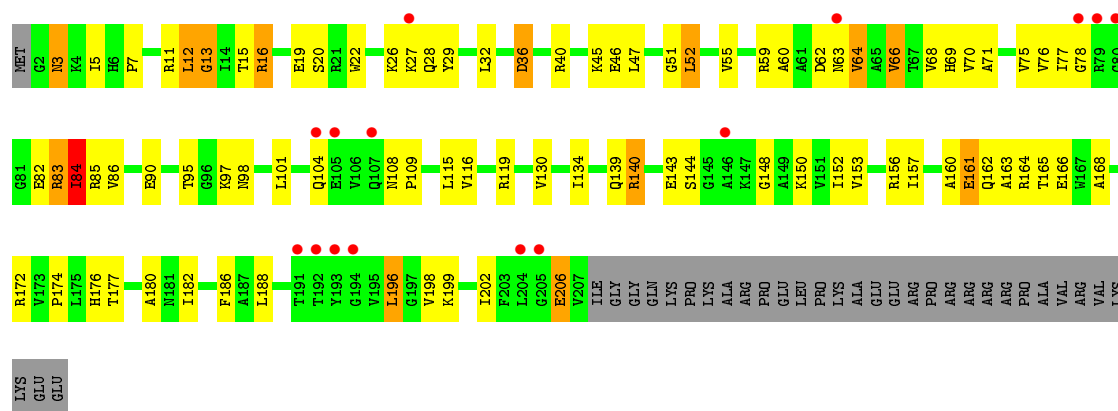


• Molecule 2: 30S ribosomal protein S2

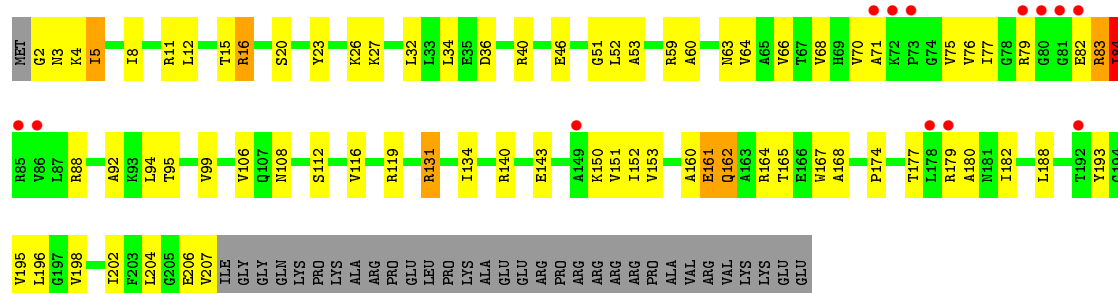




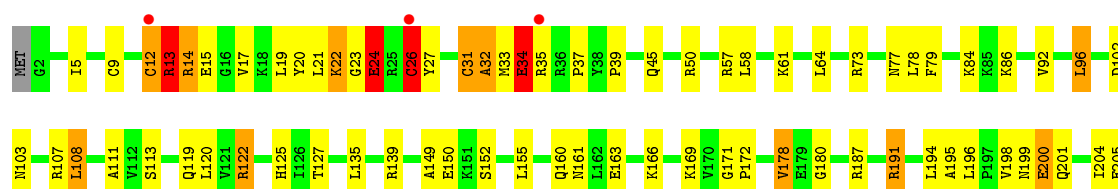
• Molecule 3: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S3

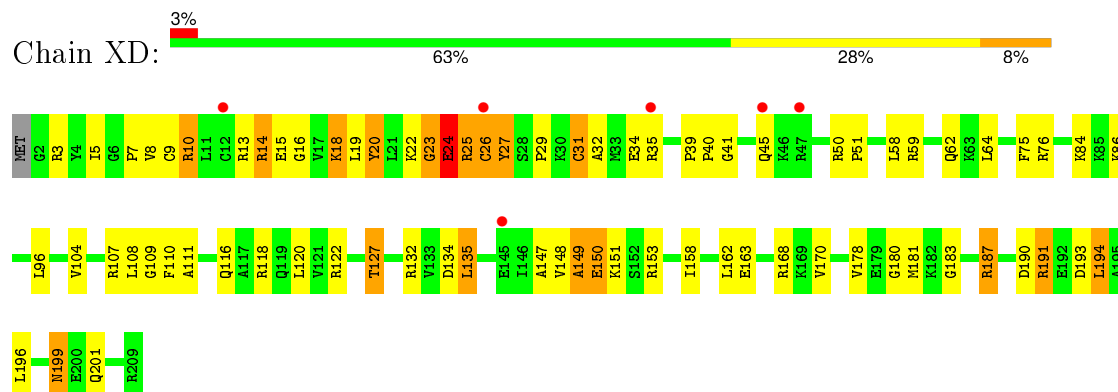


• Molecule 4: 30S ribosomal protein S4

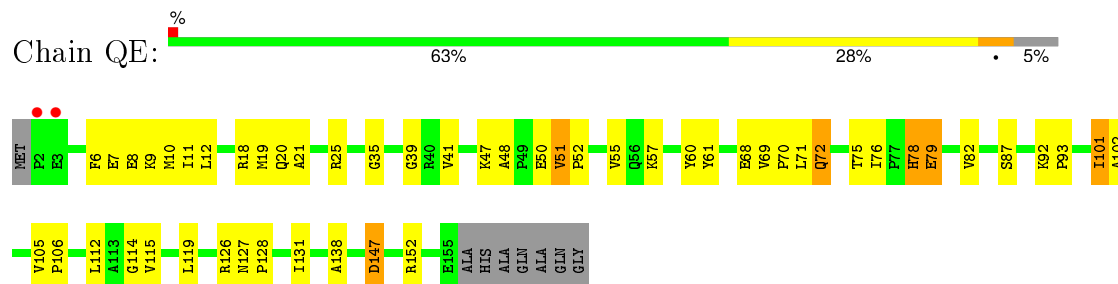




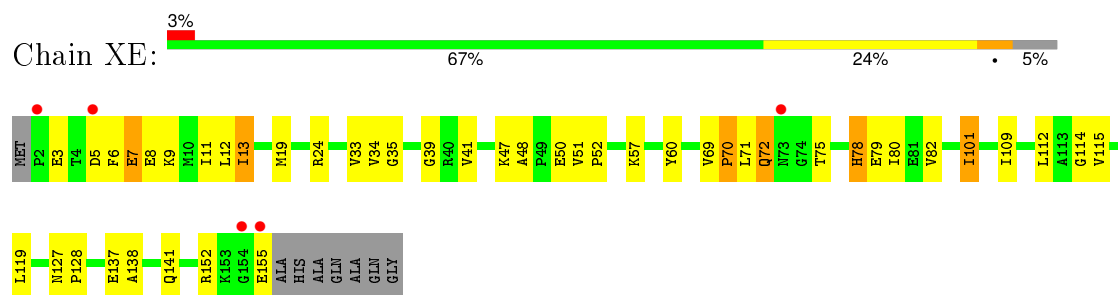
• Molecule 4: 30S ribosomal protein S4



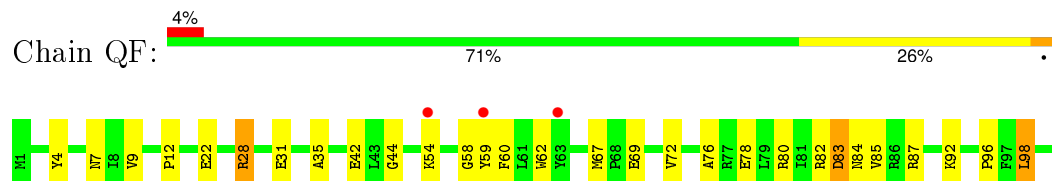
• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6



• Molecule 6: 30S ribosomal protein S6

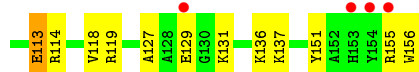




- Molecule 7: 30S ribosomal protein S7



- Molecule 7: 30S ribosomal protein S7



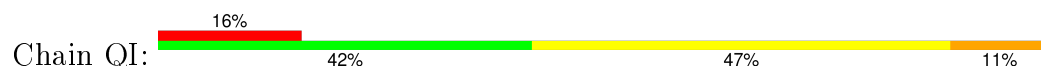
- Molecule 8: 30S ribosomal protein S8

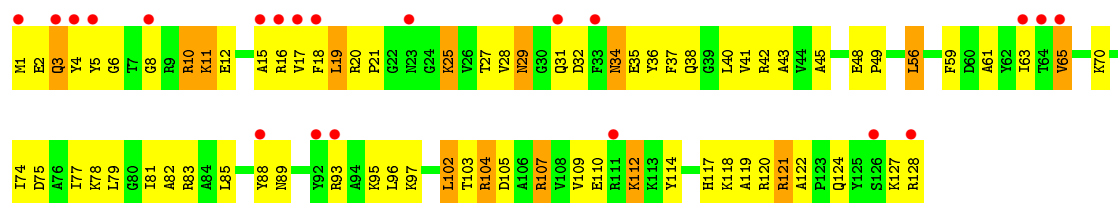


- Molecule 8: 30S ribosomal protein S8

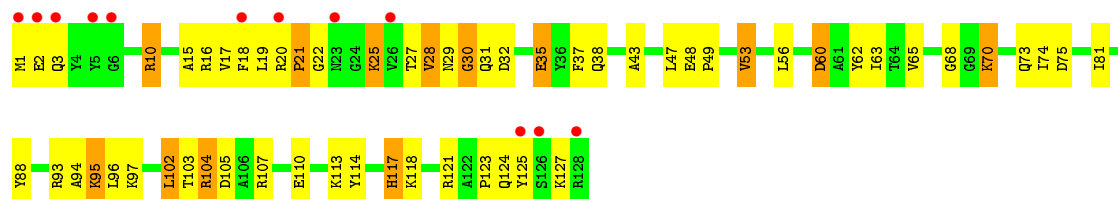


- Molecule 9: 30S ribosomal protein S9

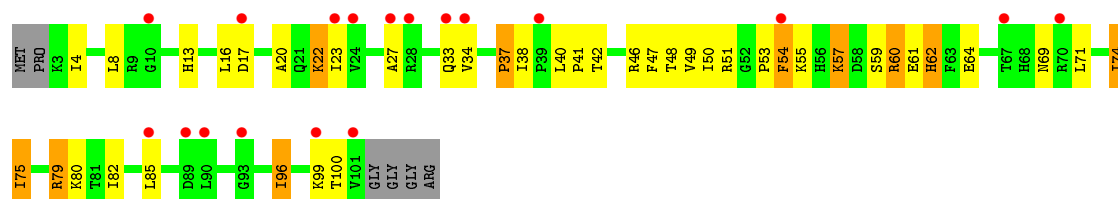




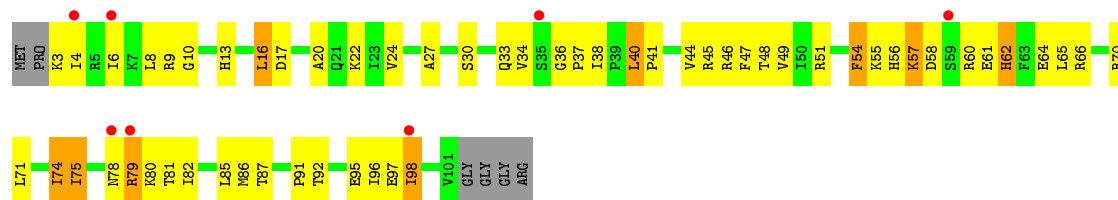
• Molecule 9: 30S ribosomal protein S9



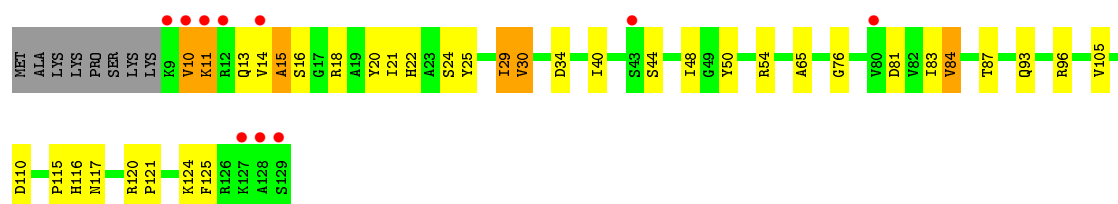
• Molecule 10: 30S ribosomal protein S10



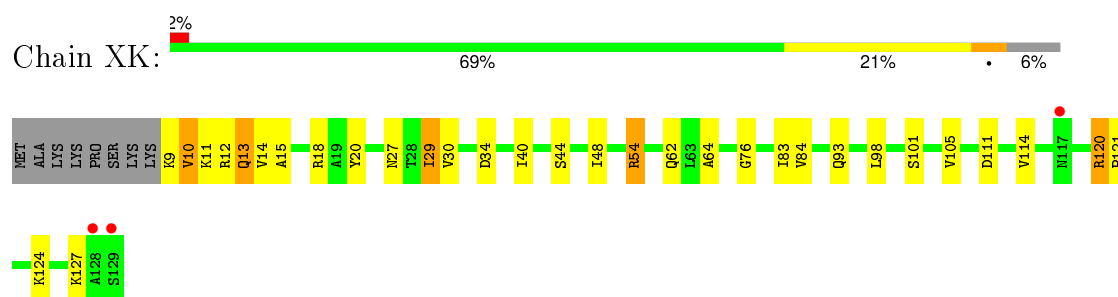
• Molecule 10: 30S ribosomal protein S10



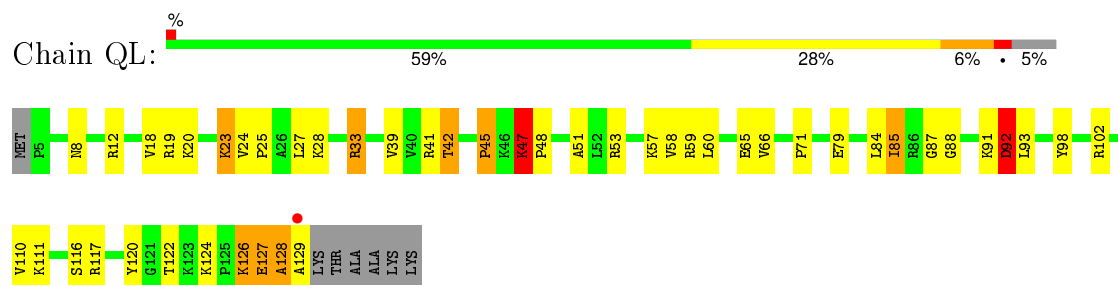
• Molecule 11: 30S ribosomal protein S11



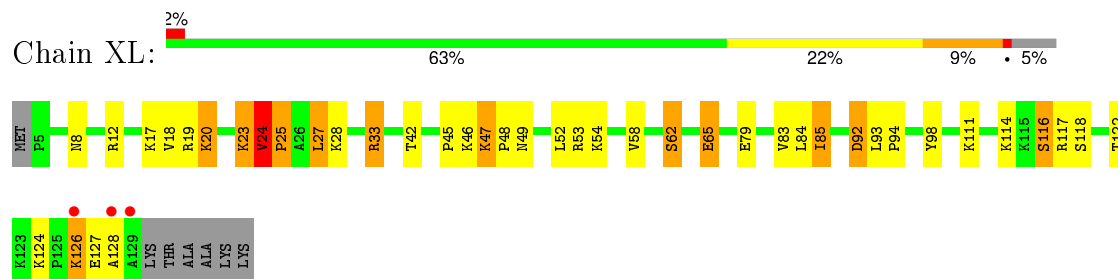
• Molecule 11: 30S ribosomal protein S11



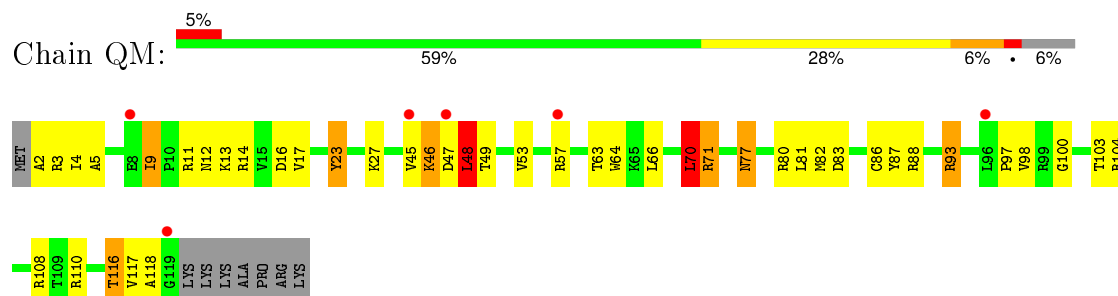
- Molecule 12: 30S ribosomal protein S12



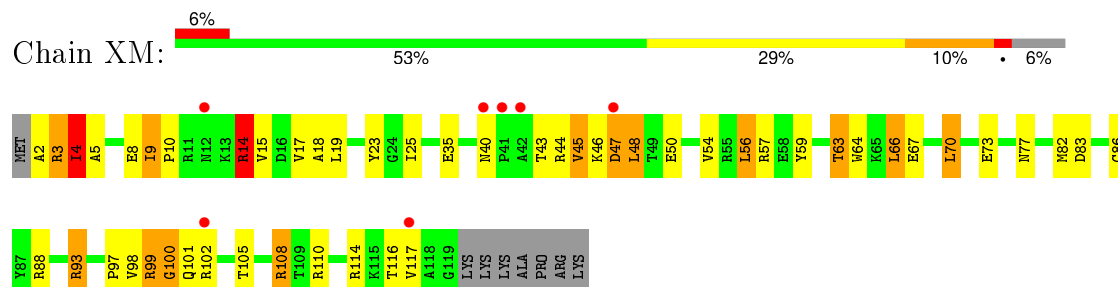
- Molecule 12: 30S ribosomal protein S12



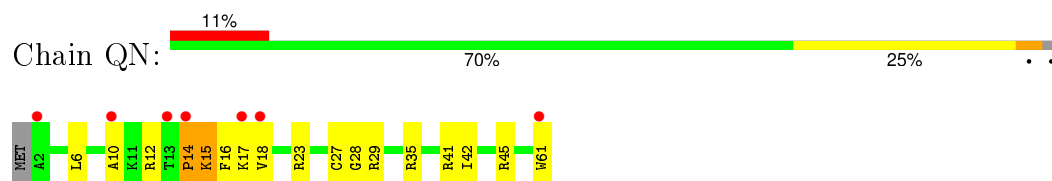
- Molecule 13: 30S ribosomal protein S13



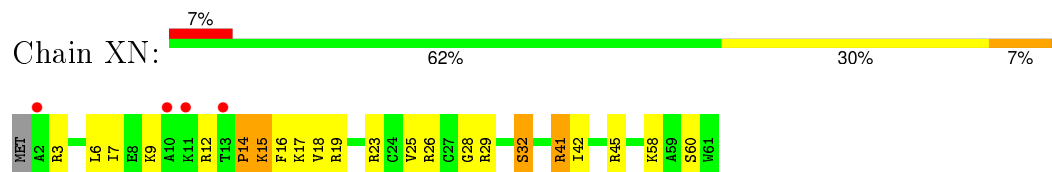
- Molecule 13: 30S ribosomal protein S13



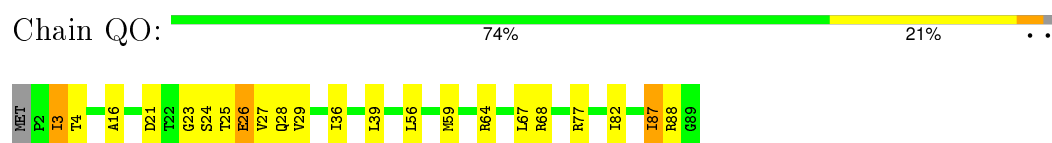
- Molecule 14: 30S ribosomal protein S14



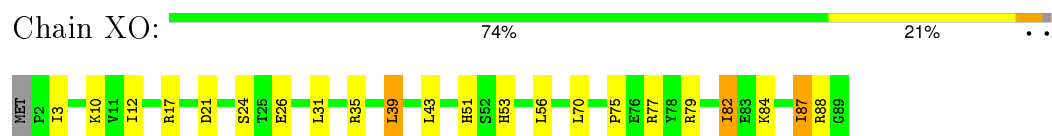
- Molecule 14: 30S ribosomal protein S14



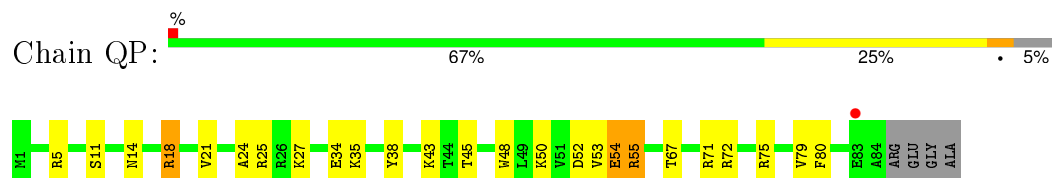
- Molecule 15: 30S ribosomal protein S15



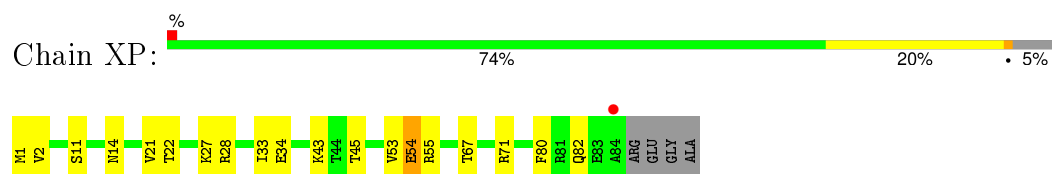
- Molecule 15: 30S ribosomal protein S15



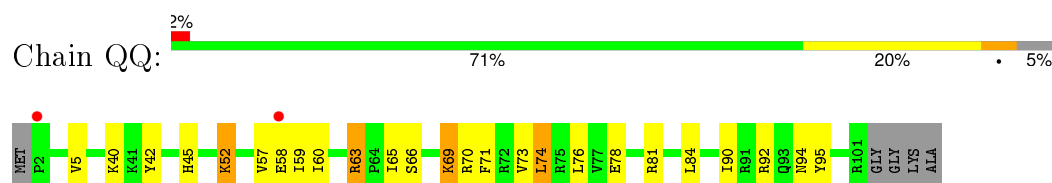
- Molecule 16: 30S ribosomal protein S16



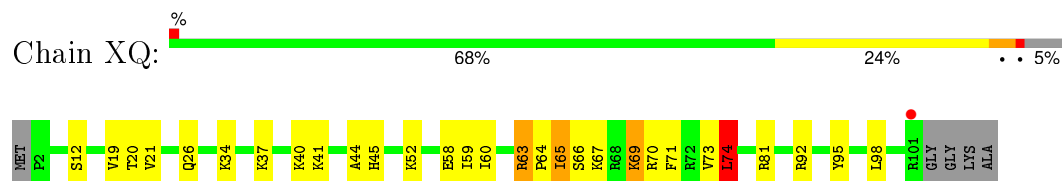
- Molecule 16: 30S ribosomal protein S16



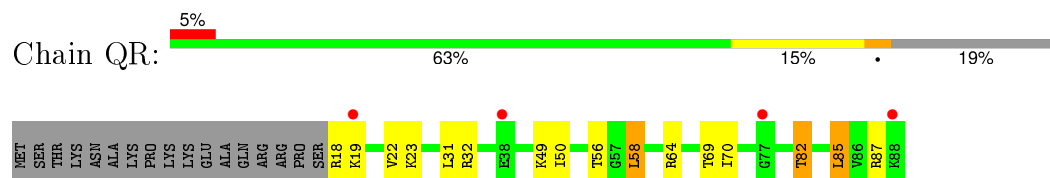
- Molecule 17: 30S ribosomal protein S17



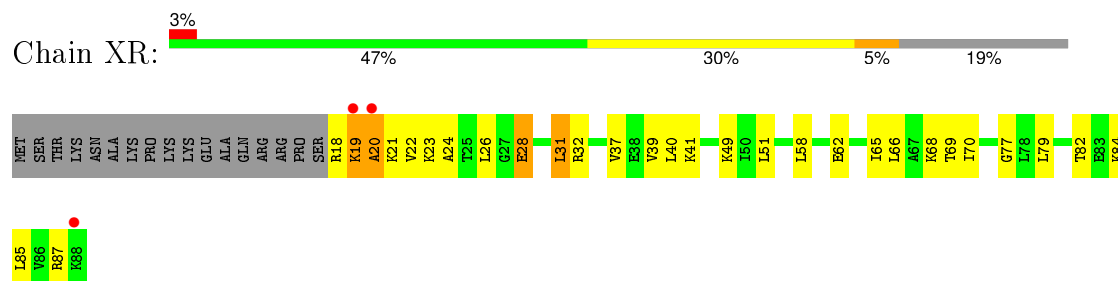
- Molecule 17: 30S ribosomal protein S17



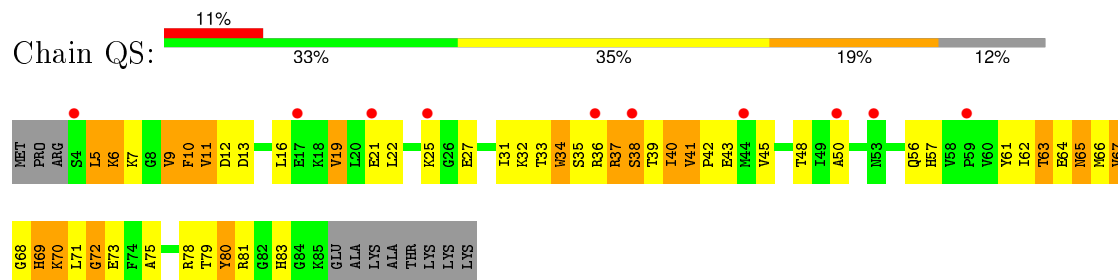
- Molecule 18: 30S ribosomal protein S18



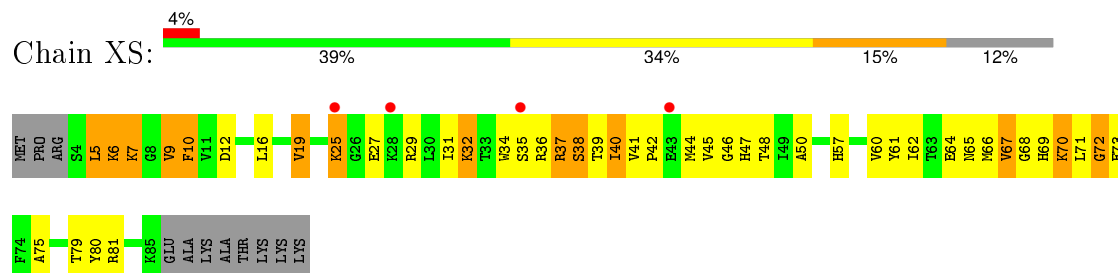
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19

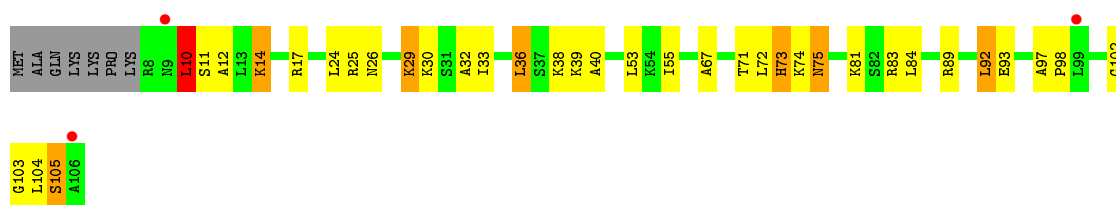


- Molecule 19: 30S ribosomal protein S19

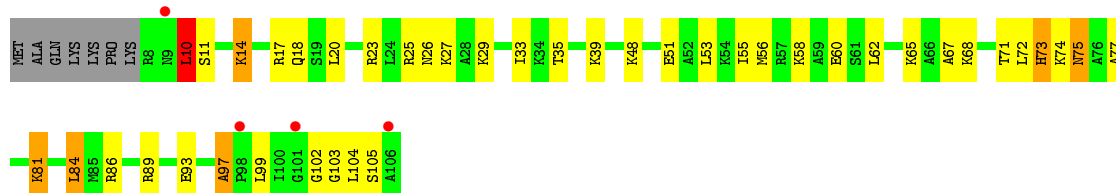


- Molecule 20: 30S ribosomal protein S20

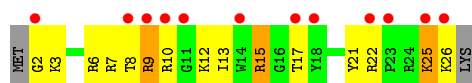
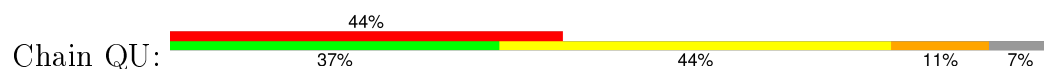




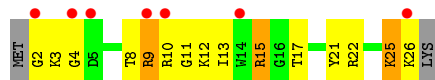
- Molecule 20: 30S ribosomal protein S20



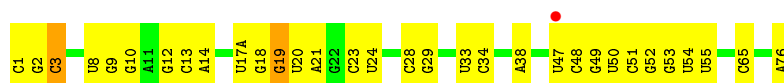
- Molecule 21: 30S ribosomal protein Thx



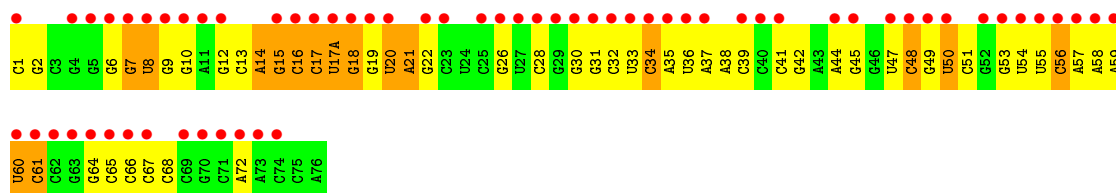
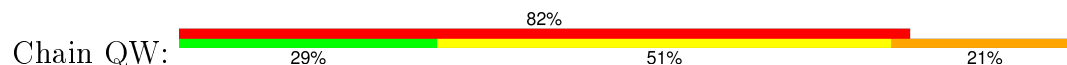
- Molecule 21: 30S ribosomal protein Thx



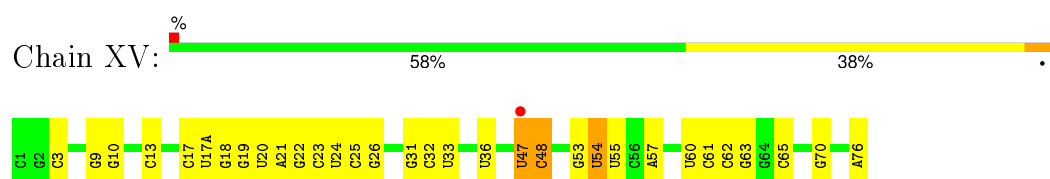
- Molecule 22: tRNA fMet



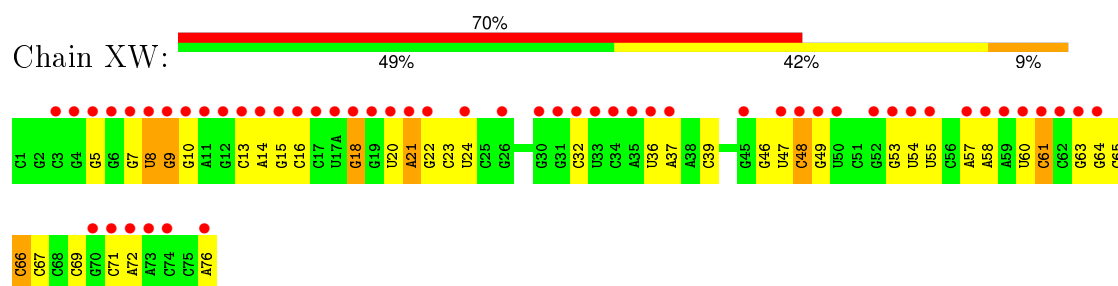
- Molecule 22: tRNA fMet



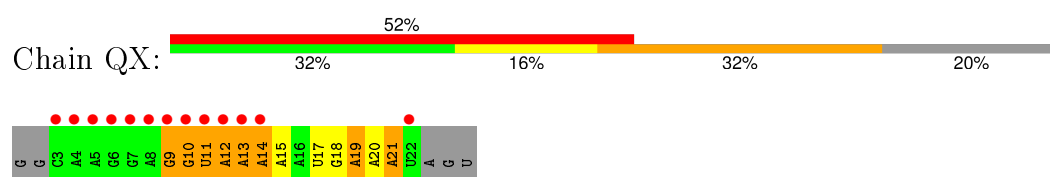
- Molecule 22: tRNA fMet



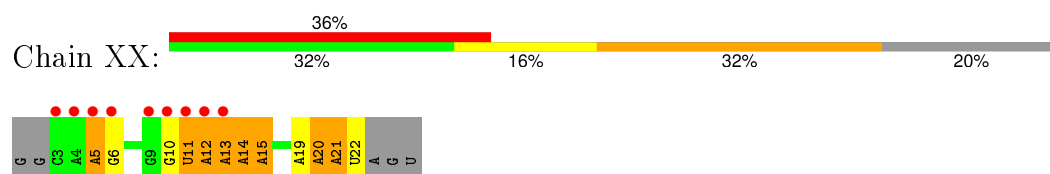
- Molecule 22: tRNA fMet



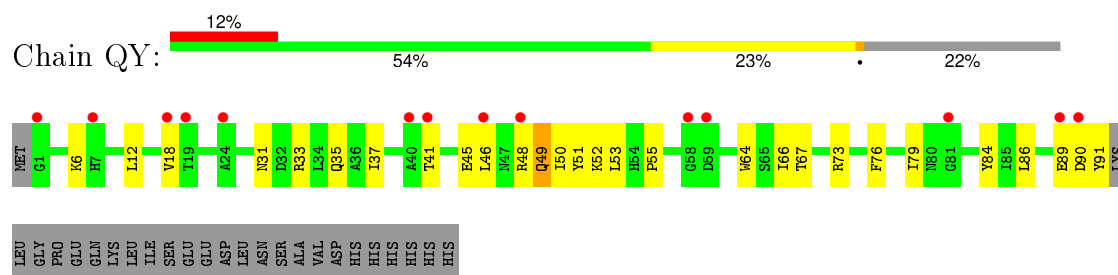
- Molecule 23: messenger RNA



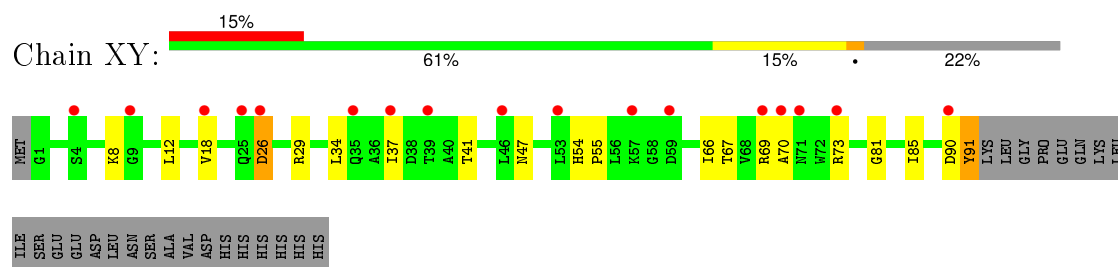
- Molecule 23: messenger RNA



- Molecule 24: Host inhibition of growth B



- Molecule 24: Host inhibition of growth B



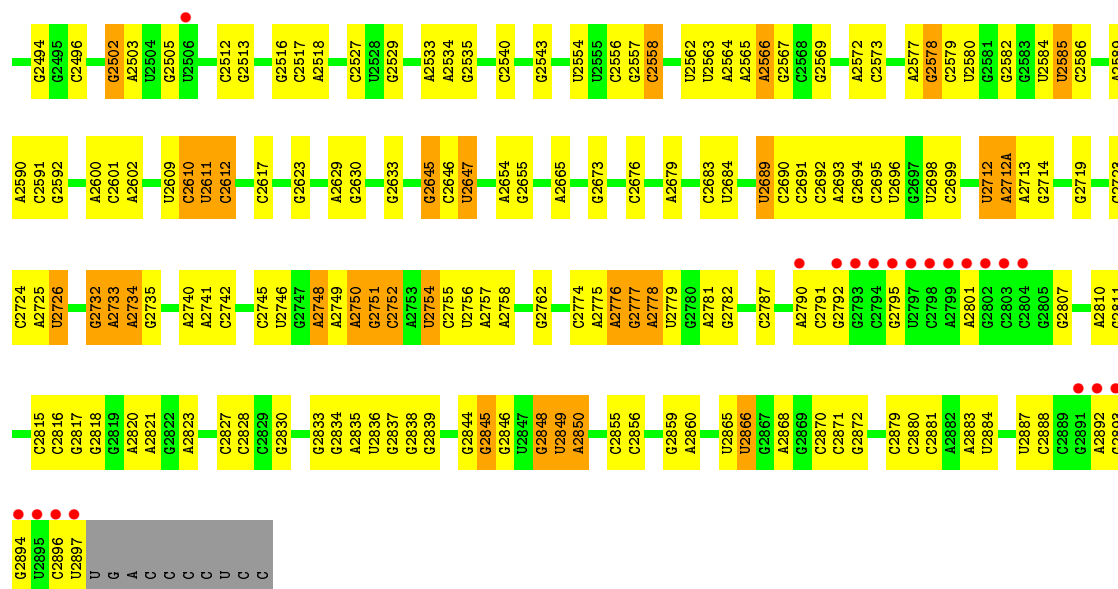
- Molecule 25: 23S rRNA



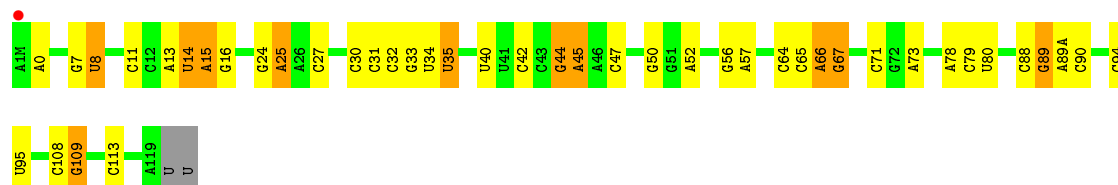
A2600	G2515	G2421	A2320	A2295	C2145	C2078	A1970	G1865	G1774	A1654	C1547	C1445A	G1358	A1268
C2601	A2518	A2422	G2325	C2226	C2147	C2082	A1971	C1866	U1775	C1657	C1548	C1445A	A1359	A1269
A2602	U2519	A2424	G2326	U2231	G2148	A2082	A1972	A1877	A1780	C1658	C1549	C1445A	A1360	G1271
U2604		A2425	A2327	U2233	U2150	G2083	G1980	G1879	A1766	A1667	C1550	C1445A	C1362	U1272
U2609	C2527	G2429	A2328	G2234	G2151	G2087	G1982	C1880	A1681	A1668	A1584	C1445A	G1363	U1273
U2628	U2528	A2430	G2329	G2238	G2152	U2091	C1988	C1882	C1790	G1674	C1557	C1445A	A1365	A1275
C2610	A2530	A2434	G2330	G2239	G2153	U2092	G1989	C1883	A1791	A1674	C1558	C1445A	A1366	A1278
C2612		A2435	G2331	U2245	G2155	G2093	C1990	G1883	C1792	A1675	A1558	C1445A	A1367	
U2615	G2535	U2438	G2334	U2243	G2156	U2096	G1991	G1888	U1794	G1681	A1562	C1445A	G1374	U1282
G2536	A2541	A2439	A2335	U2244	G2157	U2097	G1992	A1889	C1795	G1563	G1465	C1445A	C1375	U1282
U2537	G2542	A2440	A2336	U2245	A2158	C2097	U1993	A1890	U1796	G1566	G1466	C1445A	C1376	
C2538	C2343	G2441	G2337	G2246	G2159	U2098	C1999	G1899	U1797	A1567	C1467	C1445A	A1379	A1286
A2541	U2344	G2445	G2340	G2249	C2161	U2099	C1999	A1900	U1798	A1689	C1467	C1445A	G1379	
A2542	G2345	U2446	G2341	G2250	C2162	U2102	G2010	A1901	G1799	U1681	A1471	C1445A	U1281	U1282
G2543	A2346	G2447	A2347	C2262	C2163	C2103	G2011	G1902	C1800	A1570	C1475	C1445A	A1384	
G2544	G2347	G2448	G2348	C2263	G2164	G2104	A2015	G1903	G1801	A1571	C1476	C1445A	G1385	U1300
G2545	G2348	A2449	G2349	A2267	G2165	C2105	G2016	G1904	G1802	A1572	C1477	C1445A	A1386	A1301
U2546	G2349	U2450	G2350	A2268	G2166	G2106	G2017	G1905	U1805	A1573	C1478	C1445A	A1387	A1302
	G2351	G2451	G2351	A2269	G2167	C2107	G2018	G1906	A1809	U1576	C1479	C1445A	A1388	
G2552	G2352	G2452	G2352	A2270	G2168	C2108	A2019	G1907	A1810	U1577	C1480	C1445A	U1396	
G2553	G2353	G2453	G2353	G2271	A2170	U2109	C2021	G1908	G1811	U1578	C1481	C1445A	U1397	
U2554	G2354	G2454	G2354	G2272	A2171	G2110	U2022	C1908	A1812		C1482	C1445A	A1392	
A2555	G2355	G2455	G2355	G2273	U2172	C2111	G2023	U1911	G1813	G1581	C1483	C1445A	U1393	
G2556	G2356	G2456	G2356	C2275	C2173	G2112	G2024	A1912	G1814	C1582	C1484	C1445A	U1394	
G2557	G2357	G2457	A2369	G2276	C2174	U2113	G2025	A1913	C1815	C1583	C1485	C1445A	A1389	
G2558	G2358	G2458	G2374	G2277	C2175	A2114	G2026	U1914	G1816	U1584	C1486	C1445A	U1390	
G2559	G2359	G2459	G2375	A2278	G2176	G2115	A2030	U1915	A1817	U1585	C1487	C1445A	U1391	
G2560	G2360	G2460	G2376	G2279	C2177	G2116	G2031	U1916	A1818	U1586	C1488	C1445A	U1392	
A2561	G2361	G2461	G2377	G2280	C2178	A2117	G2032	U1917	U1819	U1587	C1489	C1445A	U1393	
U2562	G2362	G2462	A2377	G2281	C2179	U2118	G2033	U1918	U1820	C1588	C1490	C1445A	U1394	
A2564	G2363	G2463	G2381	G2282	U2180	A2119	A2034	U1919	C1827	C1589	C1491	C1445A	U1395	
G2565	G2364	G2464	G2382	C2283	C2183	G2120	G2037	C1920	G1828	C1590	C1492	C1445A	U1396	
G2566	G2365	G2465	G2383	A2286	C2184	U2121	G2038	U1923	A1829	C1591	C1493	C1445A	U1397	
G2567	G2366	G2466	G2384	A2287	C2185	U2122	C1924	C1924	G1830	C1592	C1494	C1445A	U1398	
G2568	G2367	G2467	G2385	A2288	G2186	G2123	A2042	G1929	G1831	C1593	C1495	C1445A	U1399	
G2569	G2368	G2468	G2386	G2289	G2187	G2124	C2043	G1930	C1832	U1602	C1496	C1445A	U1400	
A2572	G2369	G2469	G2387	U2291	C2188	G2125	G2052	U1931	G1835	C1594	C1497	C1445A	U1401	
C2573	U2390	G2470	G2388	G2292	U2189	A2126	G2053	A1936	G1839	C1595	C1498	C1445A	U1402	
	G2391	G2471	G2389	G2293	G2190	C2127	C2054	A1937	U1847	C1596	C1499	C1445A	U1403	
G2577	G2392	G2472	G2390	G2294	G2191	C2128	G2055	A1938	A1853	C1597	C1500	C1445A	U1404	
G2578	A2393	G2473	G2391	G2295	G2192	C2129	G2056	A1939	A1854	C1598	C1501	C1445A	U1405	
C2579	G2394	G2474	G2392	U2296	G2193	U2130	A2059	U1939	G1847	C1599	C1502	C1445A	U1406	
U2580	G2402	G2475	G2393	A2305	U2197	U2131	G2061	G1948	A1853	C1600	C1503	C1445A	U1407	
	G2405	G2476	G2394	G2306	A2198	U2132	G2062	G1949	A1854	C1601	C1504	C1445A	U1408	
G2583	U2406	G2477	G2395	G2307	A2199	U2133	C2063	A1952	G1857	C1602	C1505	C1445A	U1409	
U2584	G2407	G2478	G2396	G2308	C2200	C2136	C2064	A1953	G1858	C1603	C1506	C1445A	U1410	
U2585	G2408	G2479	G2397	G2309	U2203	C2137	C2065	A1954	G1859	C1604	C1507	C1445A	U1411	
C2586	G2409	G2480	G2398	A2310	C2204	C2138	C2066	U1955	A1860	C1605	C1508	C1445A	U1412	
U2590	G2410	G2481	G2399	G2312	U2205	C2139	G2067	U1956	G1861	C1606	C1509	C1445A	U1413	
G2591	A2411	G2482	G2402	U2312	C2206	C2140	G2068	G1963	G1862	C1607	C1510	C1445A	U1414	
U2592	G2412	G2483	G2403	G2313	G2207	G2141	G2069	U1964	G1863	C1608	C1511	C1445A	U1415	
U2593	G2413	G2484	G2404	G2314	A2208	C2142	G2070	U1965	G1864	C1609	C1512	C1445A	U1416	
G2594	G2414	G2485	G2405	G2315	U2218	U2143	U2071	U1966	G1865	C1610	C1513	C1445A	U1417	
	G2415	G2486	G2406	G2316	C2219	U2144	U2072	U1967	U1866	C1611	C1514	C1445A	U1418	
	G2416	G2487	G2407	G2317	U2220	U2145	U2073		U1867	C1612	C1515	C1445A	U1419	
	G2417	G2488	G2408	G2318	C2221	U2146	U2074		U1868	C1613	C1516	C1445A	U1420	
	G2418	G2489	G2409	G2319	U2222	U2147	U2075		U1869	C1614	C1517	C1445A	U1421	
	G2419	G2490	G2410	G2320	U2223	U2148	U2076		U1870	C1615	C1518	C1445A	U1422	
	G2420	G2491	G2411	G2321	C2224	U2149	U2077		U1871	C1616	C1519	C1445A	U1423	
	G2421	G2492	G2412	G2322	U2225	U2150	U2078		U1872	C1617	C1520	C1445A	U1424	
	G2422	G2493	G2413	G2323	U2226	U2151	U2079		U1873	C1618	C1521	C1445A	U1425	
	G2423	G2494	G2414	G2324	U2227	U2152	U2080		U1874	C1619	C1522	C1445A	U1426	
	G2424	G2495	G2415	G2325	U2228	U2153	U2081		U1875	C1620	C1523	C1445A	U1427	
	G2425	G2496	G2416	G2326	U2229	U2154	U2082		U1876	C1621	C1524	C1445A	U1428	
	G2426	G2497	G2417	G2327	U2230	U2155	U2083		U1877	C1622	C1525	C1445A	U1429	
	G2427	G2498	G2418	G2328	U2231	U2156	U2084		U1878	C1623	C1526	C1445A	U1430	
	G2428	G2499	G2419	G2329	U2232	U2157	U2085		U1879	C1624	C1527	C1445A	U1431	
	G2429	G2500	G2420	G2330	U2233	U2158	U2086		U1880	C1625	C1528	C1445A	U1432	
	G2430	G2501	G2421	G2331	U2234	U2159	U2087		U1881	C1626	C1529	C1445A	U1433	
	G2431	G2502	G2422	G2332	U2235	U2160	U2088		U1882	C1627	C1530	C1445A	U1434	
	G2432	G2503	G2423	G2333	U2236	U2161	U2089		U1883	C1628	C1531	C1445A	U1435	
	G2433	G2504	G2424	G2334	U2237	U2162	U2090		U1884	C1629	C1532	C1445A	U1436	
	G2434	G2505	G2425	G2335	U2238	U2163	U2091		U1885	C1630	C1533	C1445A	U1437	
	G2435	G2506	G2426	G2336	U2239	U2164	U2092		U1886	C1631	C1534	C1445A	U1438	
	G2436	G2507	G2427	G2337	U2240	U2165	U2093		U1887	C1632	C1535	C1445A	U1439	
	G2437	G2508	G2428	G2338	U2241	U2166	U2094		U1888	C1633	C1536	C1445A	U1440	
	G2438	G2509	G2429	G2339	U2242	U2167	U2095		U1889	C1634	C1537	C1445A	U1441	
	G2439	G2510	G2430	G2340	U2243	U2168	U2096		U1890	C1635	C1538	C1445A	U1442	
	G2440	G2511	G2431	G2341	U2244	U2169	U2097		U1891	C1636	C1539	C1445A	U1443	
	G2441	G2512	G2432	G2342	U2245	U2170	U2098		U1892	C1637	C1540	C1445A	U1444	
	G2442	G2513	G2433	G2343	U2246	U2171	U2099		U1893	C1638	C1541	C1445A	U1445	
	G2443	G2514	G2434	G2344	U2247	U2172	U2100		U1894	C1639	C1542	C1445A	U1446	
	G2444	G2515	G2435	G2345	U2248	U2173	U2101		U1895	C1640	C1543	C1445A	U1447	
	G2445	G2516	G2436	G2346	U2249	U2174	U2102		U1896	C1641	C1544	C1445A	U1448	
	G2446	G2517	G2437	G2347	U2250	U2175	U2103		U1897	C1642	C1545	C1445A	U1449	
	G2447	G2518	G2438	G2348	U2251	U2176	U2104		U1898	C1643	C1546	C1445A	U1450	
	G2448	G2519	G2439	G2349	U2252	U2177	U2105		U1899	C1644	C1547	C1445A	U1451	
	G2449	G2520	G2440	G2350	U2253	U2178	U2106		U1900	C1645	C1548	C1445A	U1452	
	G2450	G2521	G2441	G2351	U2254	U2179	U2107		U1901	C1646	C1549	C1445A	U1453	
	G2451	G2522	G2442	G2352	U2255	U2180	U2108		U1902	C1647	C1550	C1445A	U1454	
	G2452	G2523	G2443	G2353	U2256	U2181	U2109		U1903	C1648	C1551	C1445A	U	



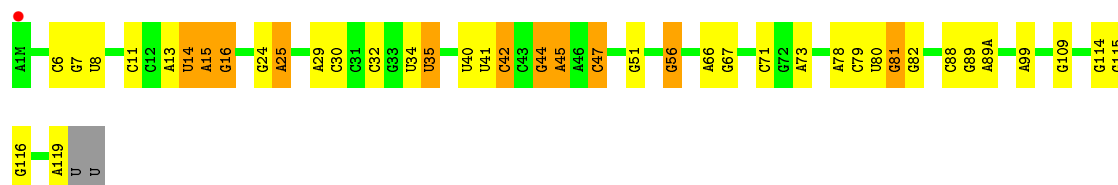
G2410	G2411	G2307	A2198	U2130	U2041	A1936	C1843	A1732	A1614	U1514	C1428	U1313	C1218	C1053
G2414	G2415	A2309	U2208	U2132	C2043	A1938	G1844	G1733	C1615	C1515	A1434	C1314	G1219	G1125
G2415			G2209	G2133			G1845	C1734	A1616	G1519	A1434	G1319	A1220	G1055
G2420	G2421	G2312	G2210	A2134	G2046	U1946	A1847	C1741	A1617	C1522	C1437	C1225		G1056
G2421	G2422	G2313	A2212	A2135		G1947	A1848	C1742	A1618			A1322	C1225	G1057
G2422	A2423	G2315	U2213	C2136	G2049	G1948	U1851	G1750	C1625	G1525	G1441	C1230	G1230	G1058
G2423	G2424	G2319	G2215	C2138	C2055	A1952	G1858	G1754	G1627	G1527	C1445	U1329	G1231	U1060
G2424	C2424	A2320	G2219	C2139	G2056	U1955	G1861	G1756	G1628	A1528	C1446	C1330	G1236	U1061
A2425			G2224	G2141	A2059	C1958			A1634	G1534	A1449	C1333	G1239	G1063
A2428			A2225	C2142	A2060		G1869	C1761	U1639	U1535	G1449A	A1336	U1240	C1064
G2428	G2429	A2327	C2226	U2143	G2061	U1963	C1870	A1762	U1639	A1536	C1450	G1337	A1241	U1065
A2430		A2328	G2228	C2145	A2062	G1964	A1871	G1763	C1640	C1537	C1451	G1338	A1247	U1066
G2432		G2329		C2146	G2069	C1967	A1872	G1764			A1453	G1338	U1248	G1068
A2434			U2232	G2147	G2070		G1878	G1765	C1648	U1541	U1454	U1352	U1249	A1069
A2435		A2336	G2233	G2148	A2071		C1881	U1766	G1649	G1542	G1455	G1250	U1250	A1142A
			U2234	C2149		A1970	C1882	U1767		A1543	G1455		G1251	A1143
U2438	A2438	G2341	G2238	U2150	U2074	A1971	C1883	U1768	G1653	A1543	C1458	U1357	C1251	G1071
A2439	A2439	C2342	G2239	G2151	U2075	A1972	G1884	U1769	A1654	A1545	G1459	C1358	G1252	C1072
C2440		U2344		G2152		C1973	A1884	A1773	G1657	C1547	A1460	A1359	A1253	G1073
C2441		G2345	U2245	G2153	G2080	C1974	A1885		C1657		G1461	A1360	U1254	C1074
G2442	G2443	A2346	G2246	G2154			C1886	A1779	C1658				U1255	C1075
G2444	G2444	C2347	A2247	G2156	U2086	A1981	C1887	U1779	G1666	A1554	G1465	A1365	G1256	C1076
G2445	G2446		C2248	G2157	G2083	U1991	A1889	A1784	G1667	A1558	C1467	A1368	U1262	U1077
G2447		C2350	G2252	A2158		U1992	C1895	A1785	A1668	G1559	A1471	A1379	U1263	G1078
A2448		G2354	G2253	G2160	U2099	U1993	G1896	A1786	A1669			G1380	U1264	U1081
U2449	C2355	C2356	C2261	C2161			C1895	A1786	G1674	A1566	G1475	A1384	U1266	C1080
A2450		U2357		G2162	C2103	C1999	A1900	A1791	C1675	A1569	A1477	G1385	G1270	A1084
			A2267	C2163	C2104	G2010	G1903		G1681			U1391	G1271	A1086
G2458		G2365	A2268	G2164	C2105	U2011	G1904	C1797	C1686	G1573	U1482	U1396	U1272	G1087
C2465	G2466	G2370	A2269	G2165	C2106	G2012	G1905		U1805	U1578	U1489	C1403	U1273	A1088
G2467	G2467	G2371	C2275	U2167	C2107	U2016	G1906	C1800	G1687	A1579	A1490	U1404	A1274	C1089
G2468			G2276	G2168	C2108	U2016	G1907	G1301	U1688	C1575	A1490	U1405	A1275	G1092
A2469		C2374	G2277	A2169	U2109	U2016	C1908	A1802	U1693	U1576	G1488	C1402	G1277	G1093
			A2278	A2170	G2110	A2019			U1694	C1577	C1478	C1401	G1278	U1094
			A2279	A2171	C2111	A2020	A1912	U1805	C1694	U1578	U1489	C1403	G1279	A1095
G2472	U2472	C2381	C2281	U2172	G2112	C2021	A1913	C2021	G1695	A1579	A1490	U1404	G1280	A1096
A2473	G2473	G2382	C2281	U2173	G2113	U2022	C1914	G1813	G1696	A1580		U1405	G1281	U1097
G2474	C2474	G2383	G2282	C2174	A2114	G2023	U1915	G1814	G1696	C1581	C1493	U1406	U1282	A1098
C2475	G2475	G2384	C2283	C2175	G2115	G2024	A1916	A1815	A1700	C1585	A1496	C1407	G1283	U1188
G2476		C2385		A2176	G2116	G2025	U1917	G1816	G1702	A1586	U1497	C1408	A1284	A1189
C2477			A2287	C2177	A2117	G2026	A1918		G1703	A1587			G1285	G1099
		A2393	A2288	C2178	U2118	G2027	A1919	A1819	C1703	A1587				A1103
A2478		C2394		U2119	C2119	U2028	U1926	U1820	C1711	C1588	G1500	G1416	C1289	C1104
G2481	G2481	C2395	U2291	C2183	G2120	G2029	U1926	A1821	C1711	C1588	G1500	G1417	C1289	G1105
G2482	G2482	G2396	C2292	G2184	A2030	A2030	A1927	G1822	C1712	C1592	C1502	U1420	C1297	G1106
C2483	C2483		C2293	G2185	U2122	A2031	A1928	G1822						C1201
G2484		U2401	C2294	G2186	G2123	G2032	G1829	A1829	G1725	G1595	C1505	G1421	U1300	G1109
G2485	C2403	C2403		G2187	G2124	A2033	G1930	G1835	U1726		C1506	G1422	A1301	G1110
G2486	G2404	G2404	A2298	U2189	G2125	U2034	U1931	G1835	U1727	C1598	A1507	G1423	A1302	A1111
G2487	G2405	G2405	G2299	G2190	A2126	G2035	A1932	G1838	G1728	A1508	A1508	G1424	G1303	G1112
A2488				G2191	G2127	G2035	G1933	C1838	A1729	C1509	C1509	G1425	G1303	G1114
G2489		U2406	C2305	G2192	C2128	C2039	C1934	G1839	U1730	A1609	A1510	G1426	G1309	G1122
			G2306	C2193	C2129	C2040	G1935	G1839	C1731	A1610		A1427		G1123



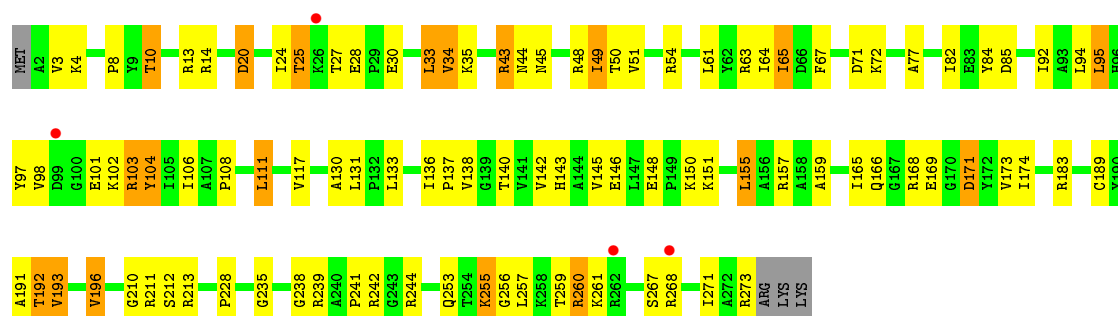
- Molecule 26: 5S rRNA



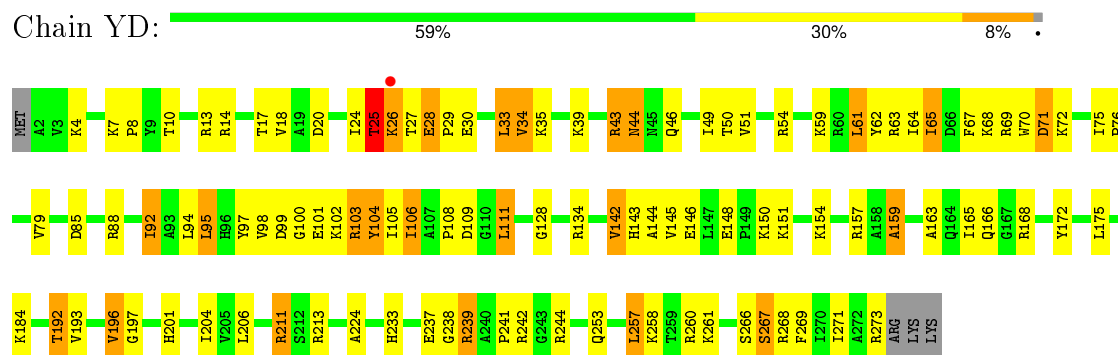
- Molecule 26: 5S rRNA



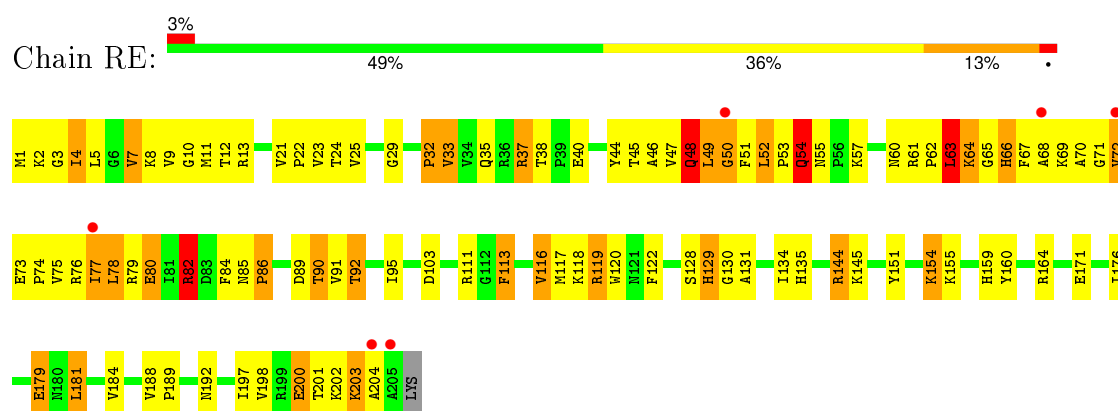
- Molecule 27: 50S ribosomal protein L2



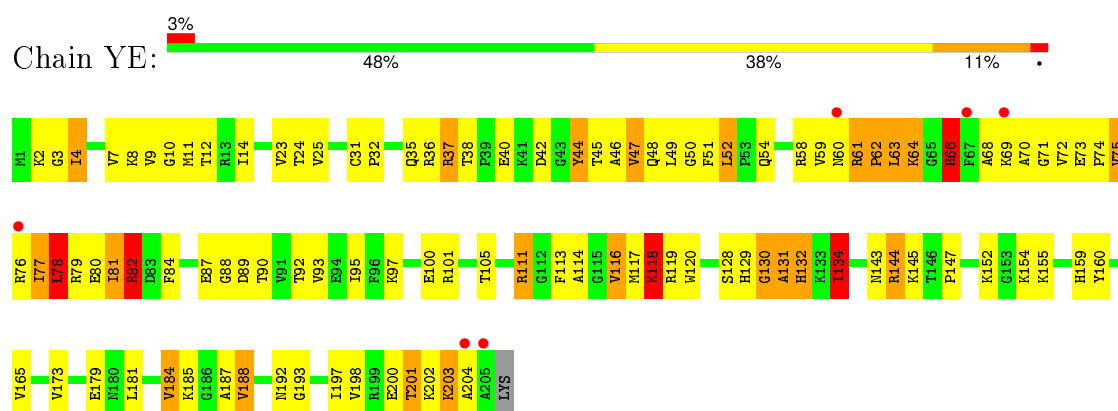
- Molecule 27: 50S ribosomal protein L2



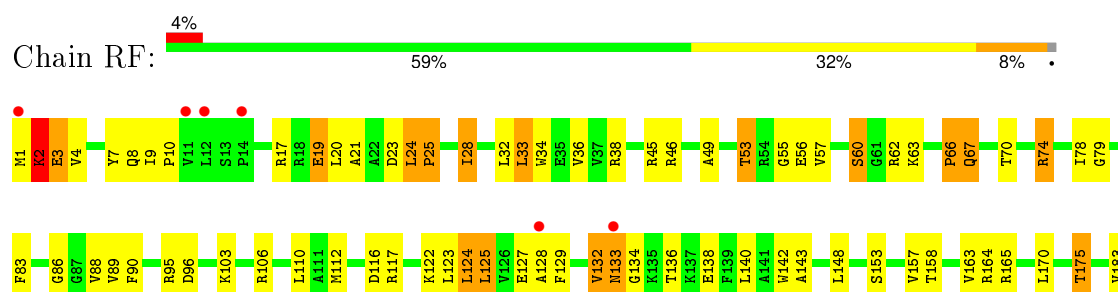
- Molecule 28: 50S ribosomal protein L3

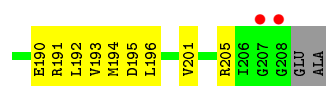


- Molecule 28: 50S ribosomal protein L3

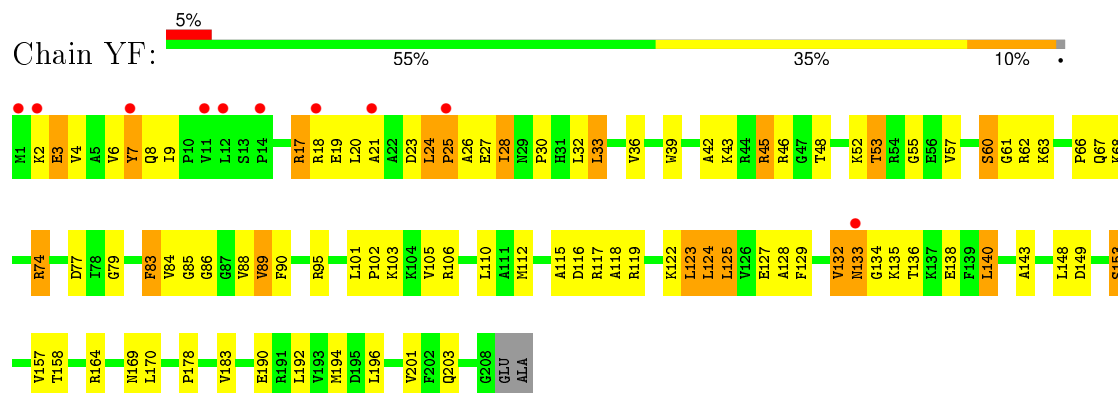


- Molecule 29: 50S ribosomal protein L4

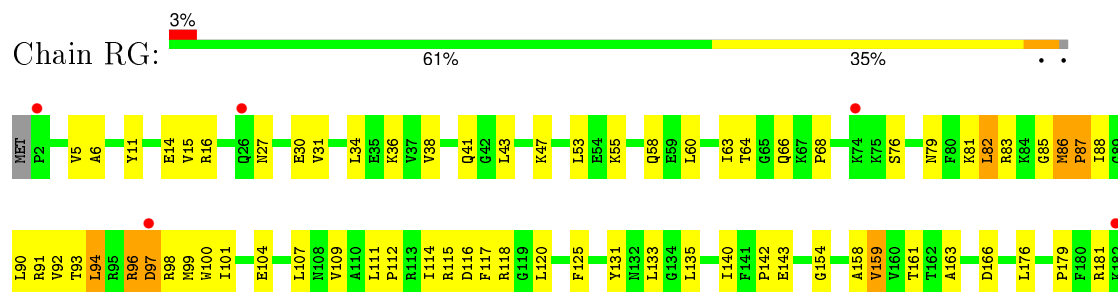




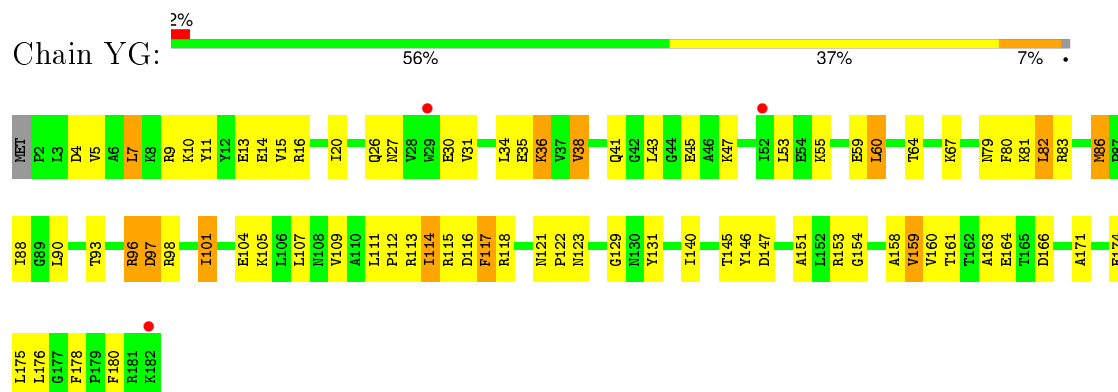
- Molecule 29: 50S ribosomal protein L4



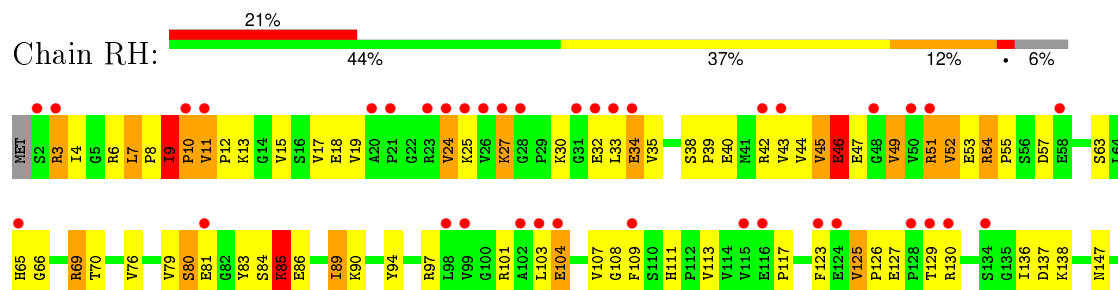
- Molecule 30: 50S ribosomal protein L5

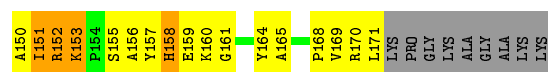


- Molecule 30: 50S ribosomal protein L5

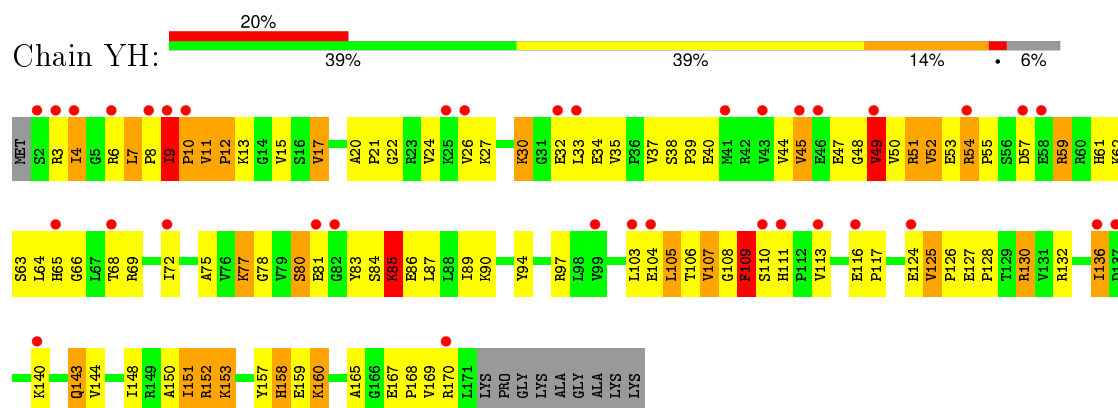


- Molecule 31: 50S ribosomal protein L6

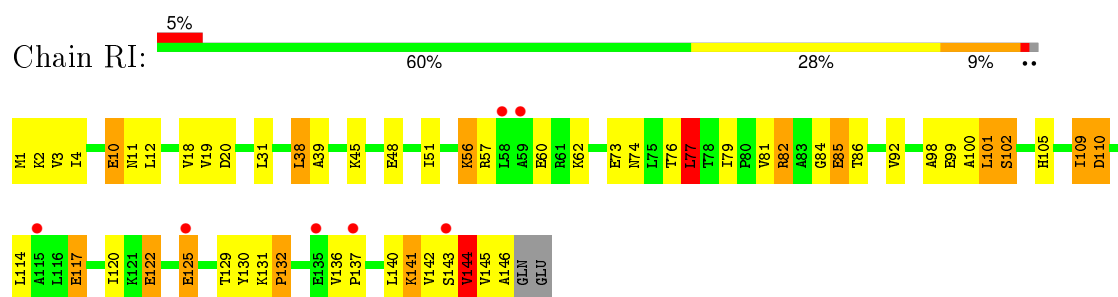




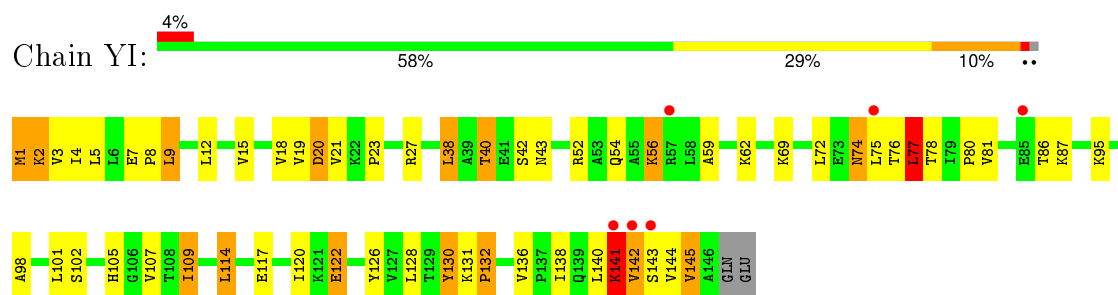
• Molecule 31: 50S ribosomal protein L6



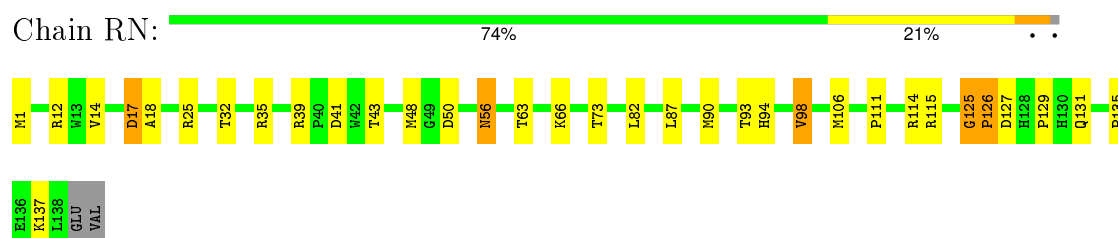
• Molecule 32: 50S ribosomal protein L9



• Molecule 32: 50S ribosomal protein L9

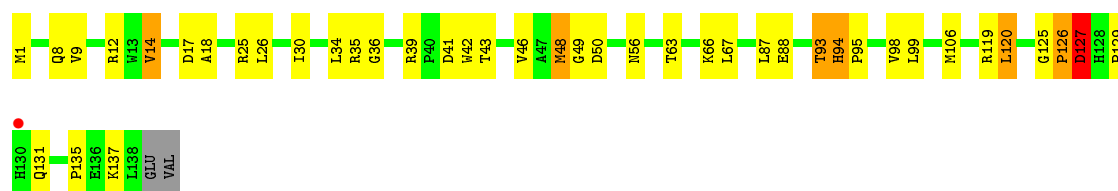


• Molecule 33: 50S ribosomal protein L13

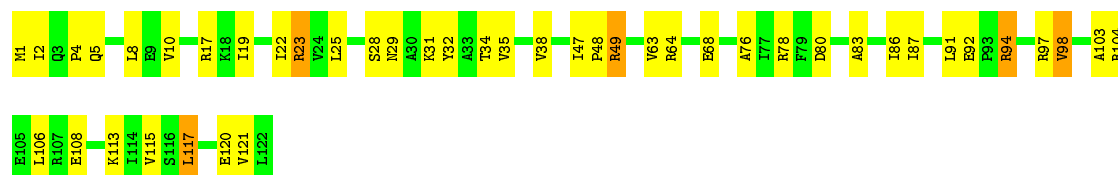


• Molecule 33: 50S ribosomal protein L13

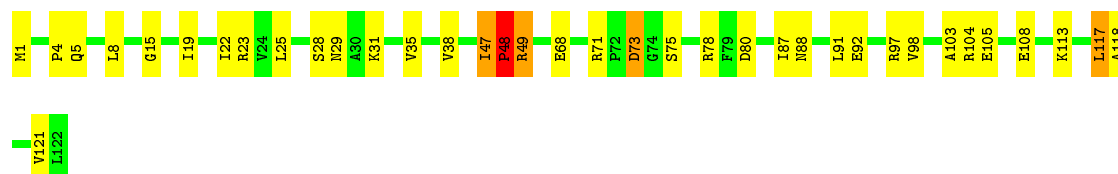




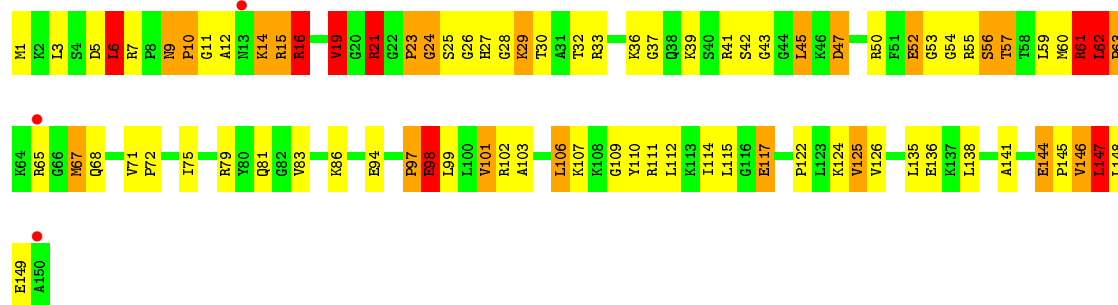
- Molecule 34: 50S ribosomal protein L14



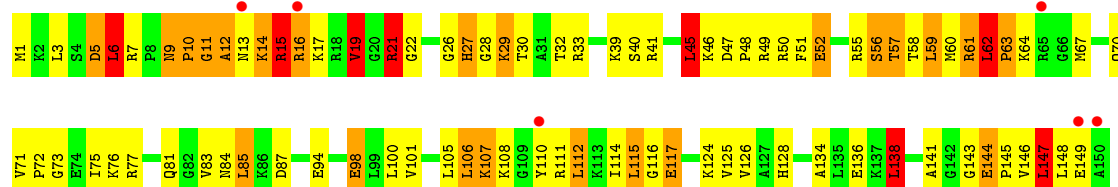
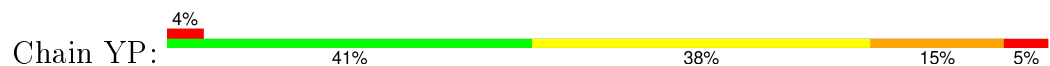
- Molecule 34: 50S ribosomal protein L14



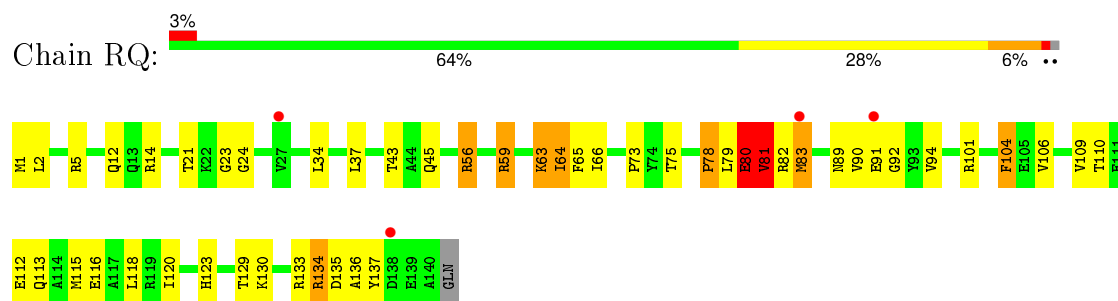
- Molecule 35: 50S ribosomal protein L15



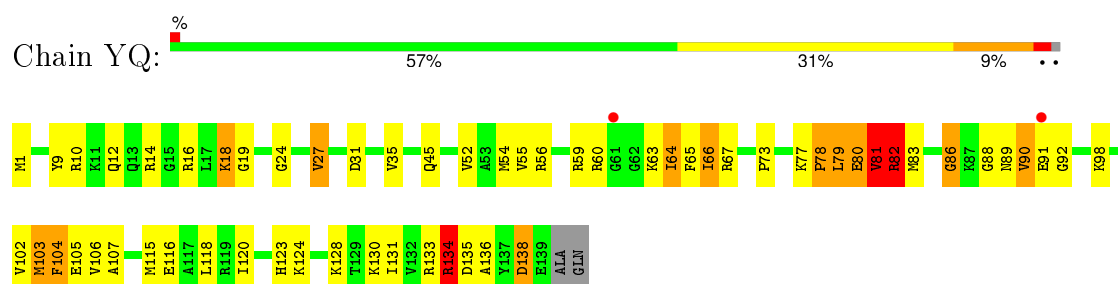
- Molecule 35: 50S ribosomal protein L15



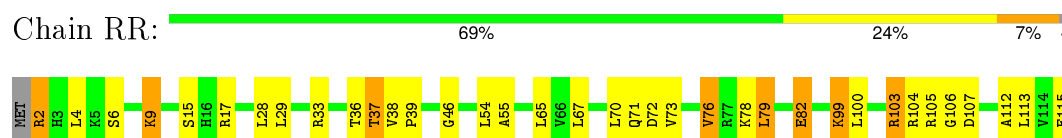
- Molecule 36: 50S ribosomal protein L16



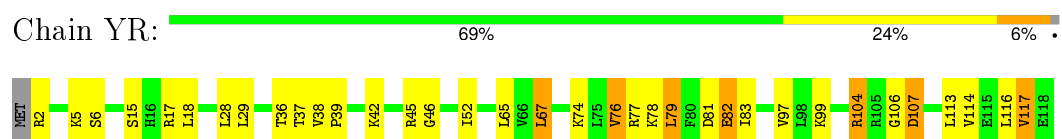
- Molecule 36: 50S ribosomal protein L16



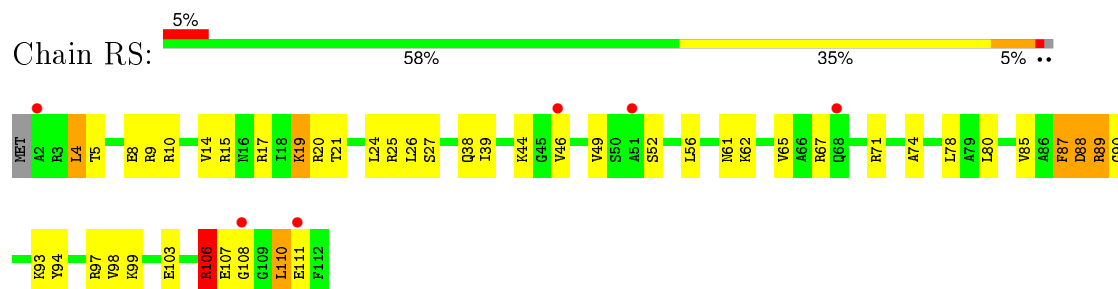
- Molecule 37: 50S ribosomal protein L17



- Molecule 37: 50S ribosomal protein L17



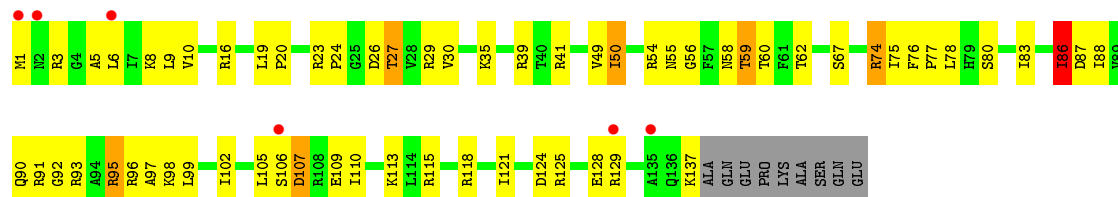
- Molecule 38: 50S ribosomal protein L18



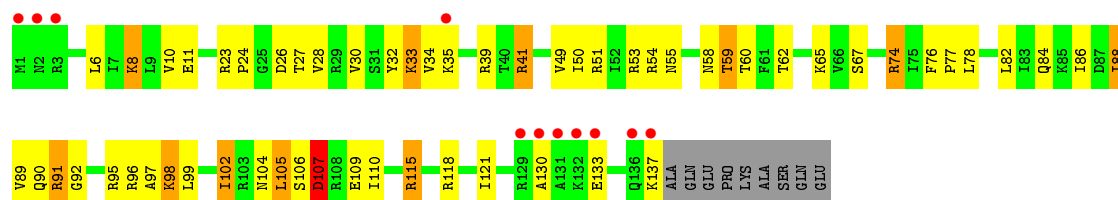
- Molecule 38: 50S ribosomal protein L18



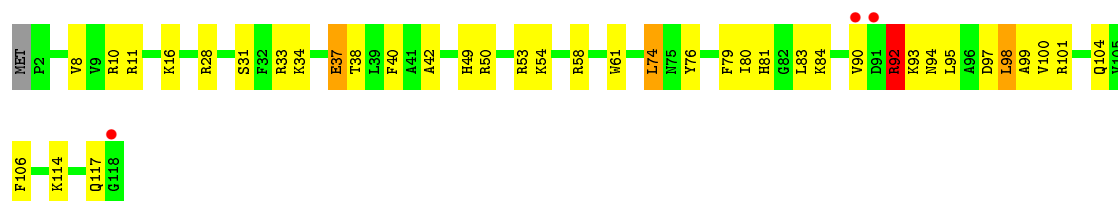
- Molecule 39: 50S ribosomal protein L19



- Molecule 39: 50S ribosomal protein L19



- Molecule 40: 50S ribosomal protein L20

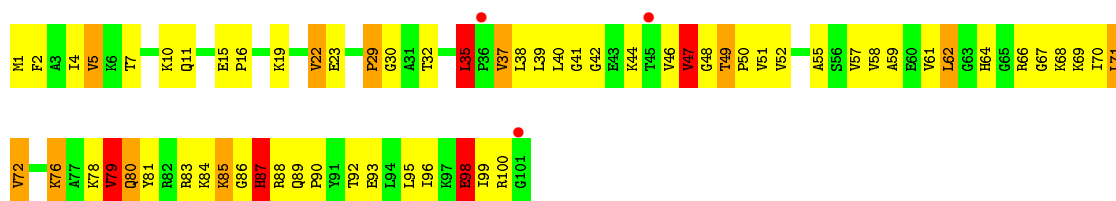


- Molecule 40: 50S ribosomal protein L20

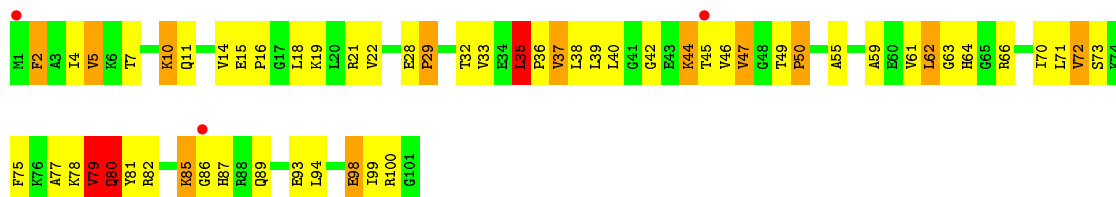
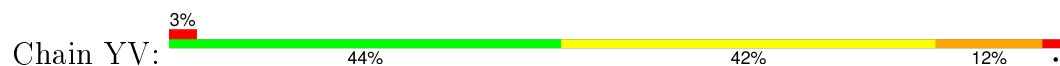


- Molecule 41: 50S ribosomal protein L21

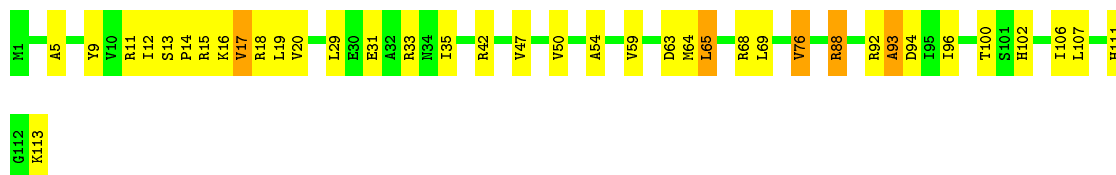




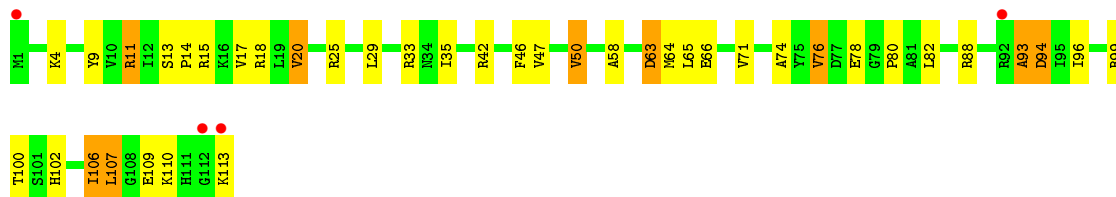
- Molecule 41: 50S ribosomal protein L21



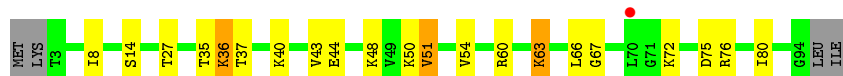
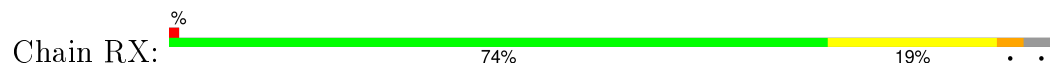
- Molecule 42: 50S ribosomal protein L22



- Molecule 42: 50S ribosomal protein L22

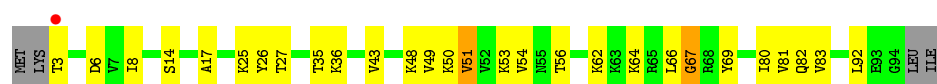


- Molecule 43: 50S ribosomal protein L23



- Molecule 43: 50S ribosomal protein L23

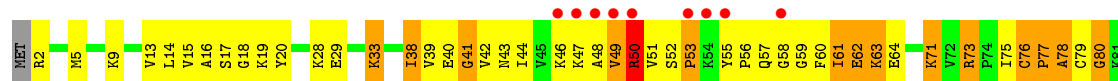




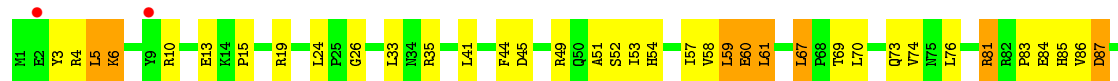
- Molecule 44: 50S ribosomal protein L24



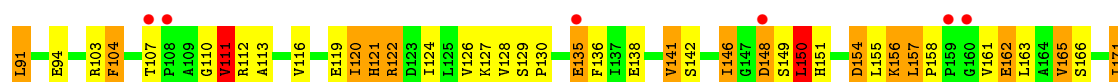
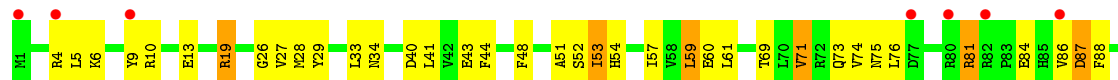
- Molecule 44: 50S ribosomal protein L24

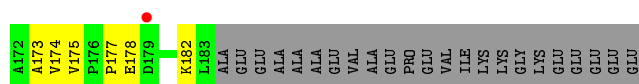


- Molecule 45: 50S ribosomal protein L25



- Molecule 45: 50S ribosomal protein L25





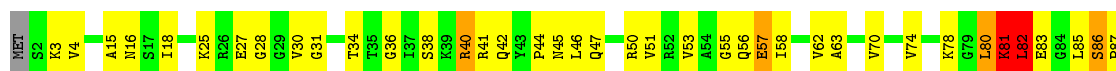
- Molecule 46: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L27



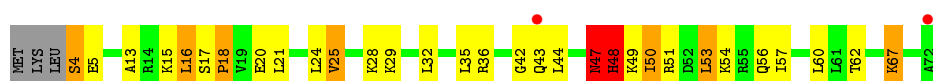
- Molecule 47: 50S ribosomal protein L28



- Molecule 47: 50S ribosomal protein L28

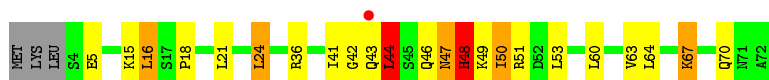


- Molecule 48: 50S ribosomal protein L29



- Molecule 48: 50S ribosomal protein L29





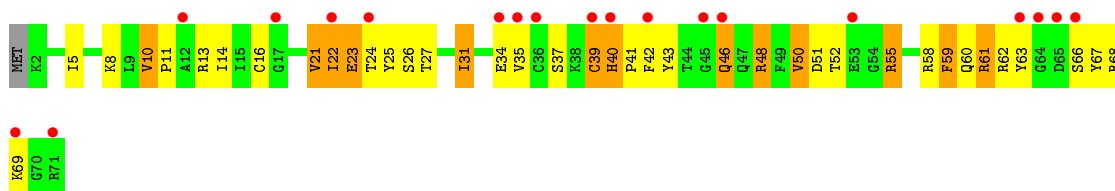
- Molecule 49: 50S ribosomal protein L30



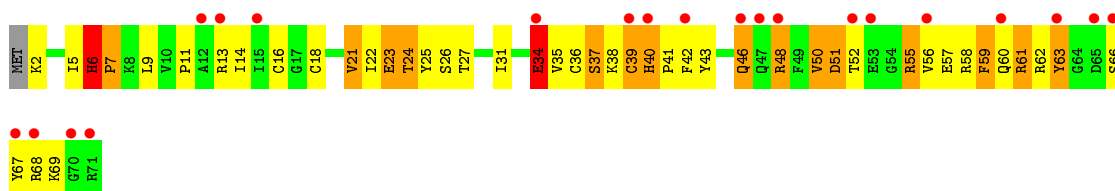
- Molecule 49: 50S ribosomal protein L30



- Molecule 50: 50S ribosomal protein L31



- Molecule 50: 50S ribosomal protein L31

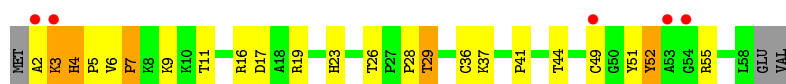


- Molecule 51: 50S ribosomal protein L32

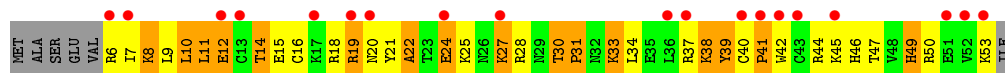
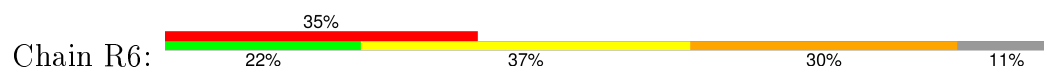


- Molecule 51: 50S ribosomal protein L32

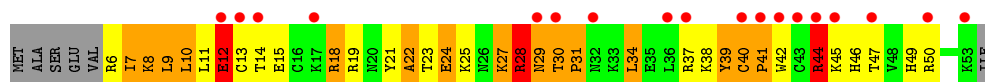
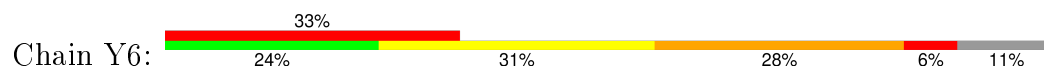




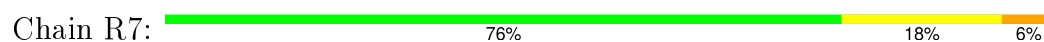
- Molecule 52: 50S ribosomal protein L33



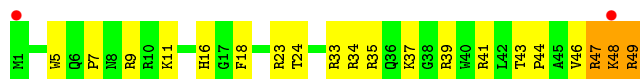
- Molecule 52: 50S ribosomal protein L33



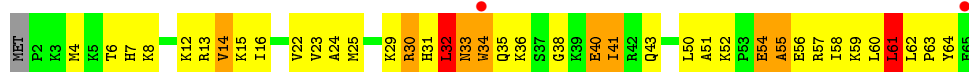
- Molecule 53: 50S ribosomal protein L34



- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35

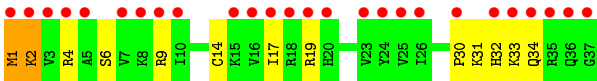


- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36





● Molecule 55: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	214.11Å 453.88Å 607.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.93 – 3.40 34.99 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (34.93-3.40) 98.9 (34.99-3.20)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.202 , 0.234 0.216 , 0.249	Depositor DCC
R_{free} test set	36504 reflections (4.82%)	DCC
Wilson B-factor (Å ²)	72.8	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 76.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 951681 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	297549	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, A2M

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	QA	0.30	1/36346 (0.0%)	0.79	15/56724 (0.0%)
1	XA	0.31	0/36276	0.80	19/56615 (0.0%)
2	QB	0.25	0/1950	0.49	0/2630
2	XB	0.26	0/1950	0.49	1/2630 (0.0%)
3	QC	0.24	0/1636	0.47	0/2205
3	XC	0.27	0/1636	0.48	0/2205
4	QD	0.28	0/1733	0.50	0/2318
4	XD	0.28	0/1733	0.50	0/2318
5	QE	0.28	0/1195	0.48	0/1609
5	XE	0.29	0/1195	0.48	0/1609
6	QF	0.25	0/856	0.45	0/1154
6	XF	0.28	0/856	0.45	0/1154
7	QG	0.24	0/1276	0.45	0/1709
7	XG	0.26	0/1276	0.45	0/1709
8	QH	0.25	0/1136	0.47	0/1527
8	XH	0.27	0/1136	0.45	0/1527
9	QI	0.25	0/1037	0.48	0/1389
9	XI	0.26	0/1037	0.48	0/1389
10	QJ	0.24	0/814	0.45	0/1095
10	XJ	0.24	0/814	0.46	0/1095
11	QK	0.27	0/916	0.44	0/1234
11	XK	0.28	0/916	0.48	0/1234
12	QL	0.31	0/991	0.52	1/1327 (0.1%)
12	XL	0.36	1/991 (0.1%)	0.56	1/1327 (0.1%)
13	QM	0.26	0/947	0.53	1/1270 (0.1%)
13	XM	0.25	0/947	0.52	0/1270
14	QN	0.25	0/501	0.47	0/664
14	XN	0.29	0/501	0.49	0/664
15	QO	0.24	0/745	0.39	0/992
15	XO	0.27	0/745	0.43	0/992
16	QP	0.27	0/721	0.46	0/970
16	XP	0.25	0/721	0.45	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.26	0/847	0.46	0/1131
17	XQ	0.30	0/847	0.47	0/1131
18	QR	0.25	0/590	0.48	0/782
18	XR	0.27	0/590	0.51	0/782
19	QS	0.27	0/670	0.53	0/901
19	XS	0.29	0/670	0.52	0/901
20	QT	0.25	0/765	0.49	1/1007 (0.1%)
20	XT	0.25	0/765	0.48	0/1007
21	QU	0.23	0/221	0.46	0/288
21	XU	0.25	0/221	0.44	0/288
22	QV	0.28	0/1832	0.77	0/2855
22	QW	0.20	0/1832	0.75	0/2855
22	XV	0.31	0/1832	0.80	0/2855
22	XW	0.19	0/1832	0.77	0/2855
23	QX	0.44	0/417	0.87	0/649
23	XX	0.43	0/417	0.96	0/649
24	QY	0.31	0/762	0.45	0/1028
24	XY	0.26	0/762	0.42	0/1028
25	RA	0.39	4/69742 (0.0%)	0.85	22/108874 (0.0%)
25	YA	0.39	1/69356 (0.0%)	0.86	21/108271 (0.0%)
26	RB	0.28	0/2928	0.79	0/4568
26	YB	0.30	0/2928	0.80	0/4568
27	RD	0.34	0/2165	0.56	0/2919
27	YD	0.37	0/2165	0.60	0/2919
28	RE	0.33	0/1601	0.58	0/2160
28	YE	0.33	0/1601	0.58	0/2160
29	RF	0.35	0/1662	0.58	0/2249
29	YF	0.31	0/1662	0.58	0/2249
30	RG	0.25	0/1499	0.46	0/2016
30	YG	0.25	0/1499	0.46	0/2016
31	RH	0.25	0/1332	0.60	1/1802 (0.1%)
31	YH	0.29	0/1332	0.67	1/1802 (0.1%)
32	RI	0.24	0/1151	0.54	0/1558
32	YI	0.28	0/1151	0.58	0/1558
33	RN	0.28	0/1131	0.50	0/1525
33	YN	0.29	0/1131	0.51	0/1525
34	RO	0.32	0/943	0.51	0/1269
34	YO	0.33	0/943	0.53	0/1269
35	RP	0.34	0/1162	0.66	0/1544
35	YP	0.35	0/1162	0.70	2/1544 (0.1%)
36	RQ	0.34	0/1133	0.57	0/1515
36	YQ	0.35	0/1128	0.58	1/1508 (0.1%)
37	RR	0.27	0/974	0.51	0/1302

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	YR	0.30	0/974	0.53	0/1302
38	RS	0.25	0/892	0.48	0/1187
38	YS	0.29	0/892	0.54	0/1187
39	RT	0.27	0/1155	0.46	0/1542
39	YT	0.30	0/1155	0.47	0/1542
40	RU	0.32	0/982	0.53	0/1306
40	YU	0.33	0/982	0.52	0/1306
41	RV	0.37	0/790	0.69	1/1057 (0.1%)
41	YV	0.35	0/790	0.68	1/1057 (0.1%)
42	RW	0.30	0/911	0.51	0/1220
42	YW	0.31	0/911	0.52	0/1220
43	RX	0.32	0/739	0.51	0/993
43	YX	0.35	0/739	0.52	0/993
44	RY	0.33	0/798	0.61	0/1064
44	YY	0.31	0/798	0.59	0/1064
45	RZ	0.33	0/1435	0.58	1/1947 (0.1%)
45	YZ	0.30	0/1493	0.60	0/2026
46	R0	0.32	0/666	0.52	0/885
46	Y0	0.32	0/666	0.58	0/885
47	R1	0.31	0/770	0.57	0/1022
47	Y1	0.36	0/770	0.59	0/1022
48	R2	0.28	0/583	0.58	0/771
48	Y2	0.33	0/583	0.59	1/771 (0.1%)
49	R3	0.29	0/474	0.44	0/635
49	Y3	0.28	0/474	0.47	0/635
50	R4	0.24	0/586	0.46	0/785
50	Y4	0.30	0/586	0.50	0/785
51	R5	0.30	0/473	0.58	1/639 (0.2%)
51	Y5	0.30	0/456	0.57	0/617
52	R6	0.29	0/424	0.67	0/565
52	Y6	0.46	0/424	0.80	0/565
53	R7	0.33	0/438	0.49	0/575
53	Y7	0.35	0/438	0.53	0/575
54	R8	0.42	0/525	0.75	0/691
54	Y8	0.39	0/525	0.66	0/691
55	R9	0.26	0/310	0.43	0/407
55	Y9	0.24	0/302	0.41	0/397
All	All	0.34	7/321792 (0.0%)	0.76	92/481138 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	RA	1035	U	O3'-P	-5.77	1.54	1.61
25	RA	1034	G	O3'-P	-5.46	1.54	1.61
25	YA	1545	A	O3'-P	5.37	1.67	1.61
25	RA	371	A	O3'-P	-5.36	1.54	1.61
25	RA	2092	U	O3'-P	-5.31	1.54	1.61

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	YH	9	ILE	C-N-CD	-11.87	94.49	120.60
1	XA	315	A	P-O3'-C3'	7.69	128.93	119.70
25	RA	614(A)	U	P-O3'-C3'	7.53	128.74	119.70
1	QA	345	C	C2-N1-C1'	7.50	127.05	118.80
1	QA	328	C	P-O3'-C3'	6.46	127.45	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32472	0	16393	490	0
1	XA	32409	0	16361	449	0
2	QB	1915	0	1969	56	0
2	XB	1915	0	1969	60	0
3	QC	1612	0	1677	51	0
3	XC	1612	0	1677	50	0
4	QD	1703	0	1765	47	0
4	XD	1703	0	1765	43	0
5	QE	1178	0	1234	29	0
5	XE	1178	0	1234	22	0
6	QF	843	0	857	18	0
6	XF	843	0	857	22	0
7	QG	1257	0	1296	30	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	35	0
8	QH	1116	0	1177	30	0
8	XH	1116	0	1177	27	0
9	QI	1018	0	1049	52	0
9	XI	1018	0	1049	45	0
10	QJ	801	0	849	35	0
10	XJ	801	0	849	46	0
11	QK	901	0	926	27	0
11	XK	901	0	926	23	0
12	QL	975	0	1062	27	0
12	XL	975	0	1062	24	0
13	QM	937	0	995	27	0
13	XM	937	0	995	56	0
14	QN	492	0	528	15	0
14	XN	492	0	528	20	0
15	QO	734	0	771	14	0
15	XO	734	0	771	14	0
16	QP	705	0	725	15	0
16	XP	705	0	725	9	0
17	QQ	834	0	904	16	0
17	XQ	834	0	904	19	0
18	QR	585	0	657	11	0
18	XR	585	0	657	19	0
19	QS	656	0	678	47	0
19	XS	656	0	678	42	0
20	QT	763	0	861	23	0
20	XT	763	0	861	28	0
21	QU	217	0	234	12	0
21	XU	217	0	234	16	0
22	QV	1640	0	837	29	0
22	QW	1640	0	837	46	0
22	XV	1640	0	837	18	0
22	XW	1640	0	837	23	0
23	QX	440	9	224	18	0
23	XX	440	9	224	15	0
24	QY	746	0	742	16	0
24	XY	746	0	742	17	0
25	RA	62269	0	31392	818	0
25	YA	61924	0	31213	687	0
26	RB	2617	0	1328	29	0
26	YB	2617	0	1328	33	0
27	RD	2115	0	2195	66	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	YD	2115	0	2195	83	0
28	RE	1568	0	1634	123	0
28	YE	1568	0	1634	79	0
29	RF	1627	0	1680	50	0
29	YF	1627	0	1680	58	0
30	RG	1474	0	1535	49	0
30	YG	1474	0	1535	51	0
31	RH	1307	0	1382	89	0
31	YH	1307	0	1382	66	0
32	RI	1136	0	1223	32	0
32	YI	1136	0	1223	62	0
33	RN	1104	0	1180	14	0
33	YN	1104	0	1180	24	0
34	RO	933	0	996	32	0
34	YO	933	0	996	26	0
35	RP	1145	0	1228	91	0
35	YP	1145	0	1228	97	0
36	RQ	1112	0	1170	33	0
36	YQ	1107	0	1166	40	0
37	RR	960	0	1021	17	0
37	YR	960	0	1021	23	0
38	RS	882	0	943	30	0
38	YS	882	0	943	35	0
39	RT	1141	0	1202	46	0
39	YT	1141	0	1202	36	0
40	RU	964	0	1022	41	0
40	YU	964	0	1022	30	0
41	RV	779	0	852	63	0
41	YV	779	0	852	54	0
42	RW	900	0	964	24	0
42	YW	900	0	964	21	0
43	RX	725	0	778	14	0
43	YX	725	0	778	16	0
44	RY	785	0	878	54	0
44	YY	785	0	878	54	0
45	RZ	1404	0	1437	80	0
45	YZ	1461	0	1493	47	0
46	R0	657	0	683	17	0
46	Y0	657	0	683	25	0
47	R1	763	0	848	31	0
47	Y1	763	0	848	23	0
48	R2	581	0	629	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	Y2	581	0	629	14	0
49	R3	469	0	518	10	0
49	Y3	469	0	518	9	0
50	R4	573	0	565	25	0
50	Y4	573	0	565	45	0
51	R5	459	0	480	10	0
51	Y5	442	0	465	24	0
52	R6	417	0	441	27	0
52	Y6	417	0	441	46	0
53	R7	430	0	480	6	0
53	Y7	430	0	480	12	0
54	R8	517	0	582	42	0
54	Y8	517	0	582	37	0
55	R9	307	0	338	11	0
55	Y9	299	0	326	6	0
56	QA	150	0	0	0	0
56	QD	2	0	0	0	0
56	QL	1	0	0	0	0
56	QV	4	0	0	0	0
56	QX	1	0	0	0	0
56	R0	3	0	0	0	0
56	R1	1	0	0	0	0
56	R2	1	0	0	0	0
56	R5	3	0	0	0	0
56	RA	441	0	0	0	0
56	RB	4	0	0	0	0
56	RD	2	0	0	0	0
56	RE	1	0	0	0	0
56	RF	1	0	0	0	0
56	RP	3	0	0	0	0
56	RQ	2	0	0	0	0
56	RR	1	0	0	0	0
56	RT	1	0	0	0	0
56	RV	1	0	0	0	0
56	RY	1	0	0	0	0
56	XA	163	0	0	0	0
56	XD	1	0	0	0	0
56	XF	1	0	0	0	0
56	XL	1	0	0	0	0
56	XS	1	0	0	0	0
56	XV	3	0	0	0	0
56	Y0	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	Y1	1	0	0	0	0
56	Y5	3	0	0	0	0
56	Y7	1	0	0	0	0
56	YA	487	0	0	0	0
56	YB	6	0	0	0	0
56	YD	1	0	0	0	0
56	YE	1	0	0	0	0
56	YF	1	0	0	0	0
56	YG	1	0	0	0	0
56	YH	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	YV	1	0	0	0	0
56	YW	1	0	0	0	0
56	YY	1	0	0	0	0
57	QD	1	0	0	0	0
57	QN	1	0	0	0	0
57	XD	1	0	0	0	0
57	XN	1	0	0	0	0
All	All	297531	18	201516	5344	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 5344 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)
41:YV:49:THR:CG2	41:YV:50:PRO:HD3	1.35	1.56
44:RY:76:CYS:SG	44:RY:77:PRO:HD2	1.44	1.55
31:RH:9:ILE:CG2	31:RH:10:PRO:HA	1.36	1.51
41:RV:49:THR:CG2	41:RV:50:PRO:HD3	1.50	1.41
32:YI:77:LEU:HB2	32:YI:142:VAL:CG2	1.54	1.37

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	234/256 (91%)	186 (80%)	29 (12%)	19 (8%)	1	11
2	XB	234/256 (91%)	189 (81%)	27 (12%)	18 (8%)	1	12
3	QC	204/239 (85%)	162 (79%)	26 (13%)	16 (8%)	1	12
3	XC	204/239 (85%)	159 (78%)	33 (16%)	12 (6%)	2	19
4	QD	206/209 (99%)	169 (82%)	26 (13%)	11 (5%)	2	22
4	XD	206/209 (99%)	168 (82%)	24 (12%)	14 (7%)	1	16
5	QE	152/162 (94%)	136 (90%)	12 (8%)	4 (3%)	7	42
5	XE	152/162 (94%)	137 (90%)	10 (7%)	5 (3%)	5	37
6	QF	99/101 (98%)	89 (90%)	10 (10%)	0	100	100
6	XF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
7	QG	153/156 (98%)	136 (89%)	13 (8%)	4 (3%)	7	42
7	XG	153/156 (98%)	134 (88%)	15 (10%)	4 (3%)	7	42
8	QH	136/138 (99%)	126 (93%)	7 (5%)	3 (2%)	8	46
8	XH	136/138 (99%)	123 (90%)	10 (7%)	3 (2%)	8	46
9	QI	126/128 (98%)	94 (75%)	24 (19%)	8 (6%)	2	18
9	XI	126/128 (98%)	96 (76%)	23 (18%)	7 (6%)	2	21
10	QJ	97/105 (92%)	80 (82%)	13 (13%)	4 (4%)	3	30
10	XJ	97/105 (92%)	81 (84%)	11 (11%)	5 (5%)	2	23
11	QK	119/129 (92%)	100 (84%)	14 (12%)	5 (4%)	3	29
11	XK	119/129 (92%)	105 (88%)	10 (8%)	4 (3%)	5	36
12	QL	123/132 (93%)	99 (80%)	16 (13%)	8 (6%)	1	17
12	XL	123/132 (93%)	97 (79%)	18 (15%)	8 (6%)	1	17
13	QM	116/126 (92%)	88 (76%)	17 (15%)	11 (10%)	1	8
13	XM	116/126 (92%)	88 (76%)	17 (15%)	11 (10%)	1	8
14	QN	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	2	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	XN	58/61 (95%)	50 (86%)	5 (9%)	3 (5%)	2	23
15	QO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
15	XO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
16	QP	82/88 (93%)	72 (88%)	10 (12%)	0	100	100
16	XP	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
17	QQ	98/105 (93%)	90 (92%)	7 (7%)	1 (1%)	19	63
17	XQ	98/105 (93%)	89 (91%)	7 (7%)	2 (2%)	9	48
18	QR	69/88 (78%)	61 (88%)	8 (12%)	0	100	100
18	XR	69/88 (78%)	62 (90%)	6 (9%)	1 (1%)	14	55
19	QS	80/93 (86%)	52 (65%)	18 (22%)	10 (12%)	0	4
19	XS	80/93 (86%)	52 (65%)	18 (22%)	10 (12%)	0	4
20	QT	97/106 (92%)	79 (81%)	15 (16%)	3 (3%)	5	39
20	XT	97/106 (92%)	80 (82%)	14 (14%)	3 (3%)	5	39
21	QU	23/27 (85%)	17 (74%)	5 (22%)	1 (4%)	3	29
21	XU	23/27 (85%)	18 (78%)	3 (13%)	2 (9%)	1	10
24	QY	89/117 (76%)	80 (90%)	9 (10%)	0	100	100
24	XY	89/117 (76%)	84 (94%)	5 (6%)	0	100	100
27	RD	270/276 (98%)	224 (83%)	38 (14%)	8 (3%)	5	39
27	YD	270/276 (98%)	229 (85%)	31 (12%)	10 (4%)	4	33
28	RE	203/206 (98%)	141 (70%)	36 (18%)	26 (13%)	0	4
28	YE	203/206 (98%)	133 (66%)	37 (18%)	33 (16%)	0	2
29	RF	206/210 (98%)	167 (81%)	26 (13%)	13 (6%)	2	18
29	YF	206/210 (98%)	168 (82%)	22 (11%)	16 (8%)	1	12
30	RG	179/182 (98%)	141 (79%)	26 (14%)	12 (7%)	1	16
30	YG	179/182 (98%)	147 (82%)	21 (12%)	11 (6%)	2	18
31	RH	168/180 (93%)	104 (62%)	37 (22%)	27 (16%)	0	2
31	YH	168/180 (93%)	98 (58%)	42 (25%)	28 (17%)	0	2
32	RI	144/148 (97%)	110 (76%)	28 (19%)	6 (4%)	3	29
32	YI	144/148 (97%)	116 (81%)	22 (15%)	6 (4%)	3	29
33	RN	136/140 (97%)	116 (85%)	13 (10%)	7 (5%)	2	24
33	YN	136/140 (97%)	110 (81%)	19 (14%)	7 (5%)	2	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	RO	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	24	67
34	YO	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	24	67
35	RP	148/150 (99%)	99 (67%)	23 (16%)	26 (18%)	0	2
35	YP	148/150 (99%)	103 (70%)	22 (15%)	23 (16%)	0	2
36	RQ	138/141 (98%)	110 (80%)	17 (12%)	11 (8%)	1	12
36	YQ	137/141 (97%)	111 (81%)	15 (11%)	11 (8%)	1	12
37	RR	115/118 (98%)	107 (93%)	4 (4%)	4 (4%)	4	35
37	YR	115/118 (98%)	109 (95%)	3 (3%)	3 (3%)	7	42
38	RS	109/112 (97%)	84 (77%)	17 (16%)	8 (7%)	1	14
38	YS	109/112 (97%)	85 (78%)	13 (12%)	11 (10%)	1	7
39	RT	135/146 (92%)	108 (80%)	25 (18%)	2 (2%)	13	54
39	YT	135/146 (92%)	113 (84%)	17 (13%)	5 (4%)	4	33
40	RU	115/118 (98%)	107 (93%)	6 (5%)	2 (2%)	11	51
40	YU	115/118 (98%)	103 (90%)	9 (8%)	3 (3%)	7	42
41	RV	99/101 (98%)	71 (72%)	13 (13%)	15 (15%)	0	2
41	YV	99/101 (98%)	70 (71%)	15 (15%)	14 (14%)	0	3
42	RW	111/113 (98%)	107 (96%)	1 (1%)	3 (3%)	6	41
42	YW	111/113 (98%)	104 (94%)	3 (3%)	4 (4%)	4	34
43	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	8	46
43	YX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	8	46
44	RY	100/110 (91%)	57 (57%)	28 (28%)	15 (15%)	0	2
44	YY	100/110 (91%)	58 (58%)	26 (26%)	16 (16%)	0	2
45	RZ	174/206 (84%)	119 (68%)	33 (19%)	22 (13%)	0	4
45	YZ	181/206 (88%)	122 (67%)	42 (23%)	17 (9%)	1	8
46	R0	81/85 (95%)	73 (90%)	5 (6%)	3 (4%)	4	33
46	Y0	81/85 (95%)	67 (83%)	11 (14%)	3 (4%)	4	33
47	R1	95/98 (97%)	71 (75%)	12 (13%)	12 (13%)	0	4
47	Y1	95/98 (97%)	76 (80%)	13 (14%)	6 (6%)	2	18
48	R2	67/72 (93%)	54 (81%)	8 (12%)	5 (8%)	1	13
48	Y2	67/72 (93%)	56 (84%)	5 (8%)	6 (9%)	1	9
49	R3	57/60 (95%)	51 (90%)	6 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	Y3	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
50	R4	68/71 (96%)	43 (63%)	12 (18%)	13 (19%)	0	1
50	Y4	68/71 (96%)	37 (54%)	15 (22%)	16 (24%)	0	1
51	R5	57/60 (95%)	46 (81%)	9 (16%)	2 (4%)	4	35
51	Y5	55/60 (92%)	48 (87%)	3 (6%)	4 (7%)	1	14
52	R6	46/54 (85%)	22 (48%)	15 (33%)	9 (20%)	0	1
52	Y6	46/54 (85%)	16 (35%)	17 (37%)	13 (28%)	0	0
53	R7	47/49 (96%)	47 (100%)	0	0	100	100
53	Y7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
54	R8	62/65 (95%)	48 (77%)	7 (11%)	7 (11%)	0	6
54	Y8	62/65 (95%)	48 (77%)	7 (11%)	7 (11%)	0	6
55	R9	35/37 (95%)	34 (97%)	0	1 (3%)	6	40
55	Y9	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
All	All	11647/12362 (94%)	9400 (81%)	1486 (13%)	761 (6%)	1	17

5 of 761 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	29	ALA
2	QB	165	VAL
2	QB	195	ASP
2	QB	238	LEU
3	QC	64	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	204/220 (93%)	174 (85%)	30 (15%)	4	20
2	XB	204/220 (93%)	176 (86%)	28 (14%)	4	23
3	QC	160/188 (85%)	142 (89%)	18 (11%)	7	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	XC	160/188 (85%)	142 (89%)	18 (11%)	7	32
4	QD	180/181 (99%)	156 (87%)	24 (13%)	5	24
4	XD	180/181 (99%)	157 (87%)	23 (13%)	5	26
5	QE	119/123 (97%)	103 (87%)	16 (13%)	5	24
5	XE	119/123 (97%)	106 (89%)	13 (11%)	8	34
6	QF	90/90 (100%)	85 (94%)	5 (6%)	26	66
6	XF	90/90 (100%)	76 (84%)	14 (16%)	3	18
7	QG	126/127 (99%)	112 (89%)	14 (11%)	8	33
7	XG	126/127 (99%)	109 (86%)	17 (14%)	5	24
8	QH	119/119 (100%)	109 (92%)	10 (8%)	14	49
8	XH	119/119 (100%)	106 (89%)	13 (11%)	8	34
9	QI	99/99 (100%)	79 (80%)	20 (20%)	1	7
9	XI	99/99 (100%)	80 (81%)	19 (19%)	2	9
10	QJ	89/92 (97%)	77 (86%)	12 (14%)	5	24
10	XJ	89/92 (97%)	75 (84%)	14 (16%)	3	18
11	QK	92/99 (93%)	82 (89%)	10 (11%)	8	34
11	XK	92/99 (93%)	83 (90%)	9 (10%)	10	40
12	QL	104/109 (95%)	89 (86%)	15 (14%)	4	21
12	XL	104/109 (95%)	87 (84%)	17 (16%)	3	16
13	QM	94/101 (93%)	80 (85%)	14 (15%)	4	20
13	XM	94/101 (93%)	82 (87%)	12 (13%)	5	26
14	QN	49/50 (98%)	48 (98%)	1 (2%)	63	87
14	XN	49/50 (98%)	43 (88%)	6 (12%)	6	28
15	QO	79/80 (99%)	74 (94%)	5 (6%)	22	62
15	XO	79/80 (99%)	74 (94%)	5 (6%)	22	62
16	QP	72/74 (97%)	64 (89%)	8 (11%)	8	33
16	XP	72/74 (97%)	64 (89%)	8 (11%)	8	33
17	QQ	95/97 (98%)	90 (95%)	5 (5%)	28	67
17	XQ	95/97 (98%)	88 (93%)	7 (7%)	17	55
18	QR	62/77 (80%)	56 (90%)	6 (10%)	10	40
18	XR	62/77 (80%)	54 (87%)	8 (13%)	5	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	QS	71/80 (89%)	54 (76%)	17 (24%)	1	4
19	XS	71/80 (89%)	58 (82%)	13 (18%)	2	10
20	QT	76/82 (93%)	62 (82%)	14 (18%)	2	10
20	XT	76/82 (93%)	66 (87%)	10 (13%)	5	25
21	QU	20/22 (91%)	18 (90%)	2 (10%)	9	38
21	XU	20/22 (91%)	18 (90%)	2 (10%)	9	38
24	QY	78/102 (76%)	75 (96%)	3 (4%)	40	76
24	XY	78/102 (76%)	74 (95%)	4 (5%)	29	69
27	RD	214/218 (98%)	178 (83%)	36 (17%)	2	14
27	YD	214/218 (98%)	180 (84%)	34 (16%)	3	17
28	RE	165/166 (99%)	137 (83%)	28 (17%)	2	14
28	YE	165/166 (99%)	138 (84%)	27 (16%)	3	15
29	RF	165/166 (99%)	139 (84%)	26 (16%)	3	17
29	YF	165/166 (99%)	142 (86%)	23 (14%)	4	23
30	RG	155/156 (99%)	148 (96%)	7 (4%)	34	73
30	YG	155/156 (99%)	138 (89%)	17 (11%)	8	34
31	RH	142/148 (96%)	123 (87%)	19 (13%)	5	24
31	YH	142/148 (96%)	117 (82%)	25 (18%)	2	12
32	RI	122/124 (98%)	98 (80%)	24 (20%)	1	8
32	YI	122/124 (98%)	99 (81%)	23 (19%)	2	9
33	RN	117/119 (98%)	107 (92%)	10 (8%)	13	48
33	YN	117/119 (98%)	104 (89%)	13 (11%)	8	33
34	RO	100/100 (100%)	91 (91%)	9 (9%)	12	45
34	YO	100/100 (100%)	90 (90%)	10 (10%)	9	38
35	RP	116/116 (100%)	83 (72%)	33 (28%)	0	2
35	YP	116/116 (100%)	84 (72%)	32 (28%)	0	3
36	RQ	110/111 (99%)	93 (84%)	17 (16%)	3	18
36	YQ	110/111 (99%)	93 (84%)	17 (16%)	3	18
37	RR	100/101 (99%)	82 (82%)	18 (18%)	2	11
37	YR	100/101 (99%)	87 (87%)	13 (13%)	5	25
38	RS	87/88 (99%)	80 (92%)	7 (8%)	15	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	YS	87/88 (99%)	73 (84%)	14 (16%)	3	16
39	RT	120/127 (94%)	99 (82%)	21 (18%)	2	13
39	YT	120/127 (94%)	98 (82%)	22 (18%)	2	10
40	RU	93/94 (99%)	85 (91%)	8 (9%)	13	48
40	YU	93/94 (99%)	85 (91%)	8 (9%)	13	48
41	RV	82/82 (100%)	65 (79%)	17 (21%)	1	7
41	YV	82/82 (100%)	64 (78%)	18 (22%)	1	5
42	RW	92/92 (100%)	82 (89%)	10 (11%)	8	34
42	YW	92/92 (100%)	79 (86%)	13 (14%)	4	22
43	RX	74/78 (95%)	65 (88%)	9 (12%)	6	28
43	YX	74/78 (95%)	68 (92%)	6 (8%)	15	51
44	RY	85/91 (93%)	65 (76%)	20 (24%)	1	4
44	YY	85/91 (93%)	61 (72%)	24 (28%)	0	2
45	RZ	155/179 (87%)	127 (82%)	28 (18%)	2	11
45	YZ	162/179 (90%)	134 (83%)	28 (17%)	2	13
46	R0	66/67 (98%)	62 (94%)	4 (6%)	23	63
46	Y0	66/67 (98%)	58 (88%)	8 (12%)	6	28
47	R1	82/83 (99%)	68 (83%)	14 (17%)	2	14
47	Y1	82/83 (99%)	72 (88%)	10 (12%)	6	28
48	R2	64/67 (96%)	52 (81%)	12 (19%)	2	9
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	8	34
49	R3	51/52 (98%)	44 (86%)	7 (14%)	4	23
49	Y3	51/52 (98%)	47 (92%)	4 (8%)	16	52
50	R4	62/63 (98%)	47 (76%)	15 (24%)	1	4
50	Y4	62/63 (98%)	44 (71%)	18 (29%)	0	2
51	R5	51/52 (98%)	40 (78%)	11 (22%)	1	6
51	Y5	49/52 (94%)	43 (88%)	6 (12%)	6	28
52	R6	47/52 (90%)	32 (68%)	15 (32%)	0	2
52	Y6	47/52 (90%)	30 (64%)	17 (36%)	0	1
53	R7	42/42 (100%)	35 (83%)	7 (17%)	3	14
53	Y7	42/42 (100%)	35 (83%)	7 (17%)	3	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	R8	54/55 (98%)	44 (82%)	10 (18%)	2	10
54	Y8	54/55 (98%)	44 (82%)	10 (18%)	2	10
55	R9	34/34 (100%)	32 (94%)	2 (6%)	24	64
55	Y9	33/34 (97%)	33 (100%)	0	100	100
All	All	9854/10270 (96%)	8447 (86%)	1407 (14%)	4	22

5 of 1407 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	R4	21	VAL
6	XF	85	VAL
45	YZ	71	VAL
51	R5	48	GLU
2	XB	185	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
45	RZ	118	GLN
3	XC	3	ASN
37	YR	3	HIS
40	RU	81	HIS
50	Y4	6	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1509/1522 (99%)	295 (19%)	46 (3%)
1	XA	1506/1522 (98%)	290 (19%)	38 (2%)
22	QV	76/77 (98%)	13 (17%)	0
22	QW	76/77 (98%)	20 (26%)	2 (2%)
22	XV	76/77 (98%)	12 (15%)	1 (1%)
22	XW	76/77 (98%)	18 (23%)	0
23	QX	19/25 (76%)	8 (42%)	2 (10%)
23	XX	19/25 (76%)	9 (47%)	1 (5%)
25	RA	2888/2916 (99%)	590 (20%)	42 (1%)
25	YA	2872/2916 (98%)	567 (19%)	41 (1%)
26	RB	121/124 (97%)	20 (16%)	1 (0%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	YB	121/124 (97%)	21 (17%)	1 (0%)
All	All	9359/9482 (98%)	1863 (19%)	175 (1%)

5 of 1863 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	4	U
1	QA	5	U
1	QA	6	G
1	QA	9	G
1	QA	22	G

5 of 175 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2191	G
1	XA	115	G
25	YA	2191	G
25	RA	2275	C
25	RA	2776	A

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

6 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
23	A2M	QX	19	23	18,25,26	1.01	1 (5%)	18,36,39	2.22	3 (16%)
23	A2M	QX	20	23	18,25,26	1.13	1 (5%)	18,36,39	1.66	1 (5%)
23	A2M	QX	21	1,23	18,25,26	1.06	1 (5%)	18,36,39	2.06	1 (5%)
23	A2M	XX	19	56,23	18,25,26	1.03	1 (5%)	18,36,39	2.32	5 (27%)
23	A2M	XX	20	23	18,25,26	1.10	2 (11%)	18,36,39	2.03	2 (11%)
23	A2M	XX	21	1,23	18,25,26	1.01	1 (5%)	18,36,39	2.35	6 (33%)

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
23	A2M	QX	19	23	-	0/5/27/28	0/3/3/3
23	A2M	QX	20	23	-	0/5/27/28	0/3/3/3
23	A2M	QX	21	1,23	-	0/5/27/28	0/3/3/3
23	A2M	XX	19	56,23	-	0/5/27/28	0/3/3/3
23	A2M	XX	20	23	-	0/5/27/28	0/3/3/3
23	A2M	XX	21	1,23	-	0/5/27/28	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	XX	20	A2M	O4'-C1'	2.34	1.44	1.41
23	QX	19	A2M	C5-C4	2.87	1.47	1.40
23	XX	20	A2M	C5-C4	2.91	1.47	1.40
23	XX	21	A2M	C5-C4	2.93	1.47	1.40
23	QX	21	A2M	C5-C4	3.00	1.47	1.40

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	QX	19	A2M	N3-C2-N1	-7.43	123.04	128.87
23	QX	21	A2M	N3-C2-N1	-7.00	123.37	128.87
23	XX	20	A2M	N3-C2-N1	-6.81	123.52	128.87
23	XX	21	A2M	N3-C2-N1	-6.67	123.63	128.87
23	XX	19	A2M	N3-C2-N1	-6.53	123.74	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	QX	19	A2M	1	0
23	QX	21	A2M	2	0
23	XX	20	A2M	2	0
23	XX	21	A2M	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1312 ligands modelled in this entry, 1312 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1511/1522 (99%)	-0.00	42 (2%) 56 52	39, 80, 190, 435	0
1	XA	1508/1522 (99%)	-0.02	40 (2%) 58 53	27, 78, 175, 487	0
2	QB	236/256 (92%)	0.55	27 (11%) 7 7	58, 138, 241, 336	0
2	XB	236/256 (92%)	0.31	20 (8%) 13 13	52, 119, 215, 332	0
3	QC	206/239 (86%)	0.41	15 (7%) 18 17	61, 111, 200, 469	0
3	XC	206/239 (86%)	0.25	13 (6%) 23 22	44, 103, 197, 564	0
4	QD	208/209 (99%)	-0.18	3 (1%) 78 73	35, 66, 119, 173	0
4	XD	208/209 (99%)	0.04	6 (2%) 55 50	41, 82, 132, 198	0
5	QE	154/162 (95%)	-0.08	2 (1%) 79 74	34, 74, 138, 244	0
5	XE	154/162 (95%)	-0.02	5 (3%) 51 47	31, 68, 144, 340	0
6	QF	101/101 (100%)	0.35	4 (3%) 42 37	58, 117, 161, 183	0
6	XF	101/101 (100%)	-0.15	0 100 100	29, 68, 110, 175	0
7	QG	155/156 (99%)	0.31	13 (8%) 14 13	80, 130, 214, 347	0
7	XG	155/156 (99%)	0.16	9 (5%) 26 24	54, 101, 179, 252	0
8	QH	138/138 (100%)	-0.20	1 (0%) 89 85	41, 81, 119, 179	0
8	XH	138/138 (100%)	-0.08	0 100 100	48, 79, 128, 182	0
9	QI	128/128 (100%)	0.89	21 (16%) 2 2	78, 156, 267, 359	0
9	XI	128/128 (100%)	0.54	12 (9%) 11 11	61, 115, 202, 350	0
10	QJ	99/105 (94%)	1.01	18 (18%) 2 2	74, 149, 278, 339	0
10	XJ	99/105 (94%)	0.64	7 (7%) 19 18	63, 133, 253, 371	0
11	QK	121/129 (93%)	0.53	10 (8%) 14 13	43, 102, 182, 301	0
11	XK	121/129 (93%)	0.05	3 (2%) 61 55	32, 71, 159, 258	0
12	QL	125/132 (94%)	-0.06	1 (0%) 87 83	27, 62, 103, 271	0
12	XL	125/132 (94%)	-0.04	3 (2%) 62 57	30, 64, 103, 263	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	118/126 (93%)	0.56	6 (5%) 32 28	75, 133, 248, 348	0
13	XM	118/126 (93%)	0.36	7 (5%) 26 23	64, 114, 183, 467	0
14	QN	60/61 (98%)	0.80	7 (11%) 6 6	79, 110, 169, 205	0
14	XN	60/61 (98%)	0.55	4 (6%) 21 20	60, 93, 133, 240	0
15	QO	88/89 (98%)	0.05	0 100 100	37, 86, 136, 170	0
15	XO	88/89 (98%)	-0.11	0 100 100	34, 74, 110, 161	0
16	QP	84/88 (95%)	-0.22	1 (1%) 81 75	38, 68, 111, 260	0
16	XP	84/88 (95%)	0.26	1 (1%) 81 75	63, 90, 138, 347	0
17	QQ	100/105 (95%)	0.01	2 (2%) 68 62	33, 79, 110, 133	0
17	XQ	100/105 (95%)	0.12	1 (1%) 84 79	35, 82, 118, 188	0
18	QR	71/88 (80%)	0.33	4 (5%) 28 25	64, 114, 191, 248	0
18	XR	71/88 (80%)	0.13	3 (4%) 40 35	33, 66, 181, 270	0
19	QS	82/93 (88%)	0.73	10 (12%) 5 5	78, 148, 306, 418	0
19	XS	82/93 (88%)	0.63	4 (4%) 33 29	57, 126, 215, 401	0
20	QT	99/106 (93%)	0.15	3 (3%) 54 49	54, 85, 160, 222	0
20	XT	99/106 (93%)	0.29	4 (4%) 42 37	61, 107, 176, 212	0
21	QU	25/27 (92%)	1.99	12 (48%) 0 0	94, 130, 197, 278	0
21	XU	25/27 (92%)	1.38	7 (28%) 1 1	74, 113, 170, 194	0
22	QV	77/77 (100%)	0.28	1 (1%) 79 74	46, 83, 132, 187	0
22	QW	77/77 (100%)	3.43	63 (81%) 0 0	86, 279, 383, 409	0
22	XV	77/77 (100%)	-0.13	1 (1%) 79 74	42, 79, 123, 172	0
22	XW	77/77 (100%)	3.19	54 (70%) 0 0	115, 271, 335, 411	0
23	QX	17/25 (68%)	2.50	13 (76%) 0 0	53, 218, 306, 334	0
23	XX	17/25 (68%)	2.30	9 (52%) 0 0	45, 237, 354, 390	0
24	QY	91/117 (77%)	1.08	14 (15%) 3 3	83, 126, 163, 188	0
24	XY	91/117 (77%)	1.25	17 (18%) 2 2	82, 127, 165, 185	0
25	RA	2891/2916 (99%)	0.11	159 (5%) 29 26	20, 56, 239, 588	0
25	YA	2875/2916 (98%)	0.05	150 (5%) 31 28	20, 54, 248, 583	0
26	RB	122/124 (98%)	0.05	1 (0%) 87 83	46, 96, 148, 214	0
26	YB	122/124 (98%)	-0.01	1 (0%) 87 83	55, 86, 136, 215	0
27	RD	272/276 (98%)	-0.11	4 (1%) 76 71	17, 54, 102, 322	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	YD	272/276 (98%)	-0.27	1 (0%) 93 91	12, 35, 83, 212	0
28	RE	205/206 (99%)	0.12	6 (2%) 55 50	25, 73, 159, 362	0
28	YE	205/206 (99%)	0.11	6 (2%) 55 50	26, 73, 168, 563	0
29	RF	208/210 (99%)	-0.12	8 (3%) 44 39	13, 44, 168, 316	0
29	YF	208/210 (99%)	0.03	10 (4%) 34 31	22, 67, 240, 535	0
30	RG	181/182 (99%)	0.26	5 (2%) 56 52	62, 110, 161, 194	0
30	YG	181/182 (99%)	0.13	3 (1%) 73 67	42, 97, 165, 199	0
31	RH	170/180 (94%)	1.34	38 (22%) 1 1	59, 182, 468, 582	0
31	YH	170/180 (94%)	0.95	36 (21%) 1 1	58, 146, 370, 574	0
32	RI	146/148 (98%)	0.47	7 (4%) 34 31	51, 113, 183, 290	0
32	YI	146/148 (98%)	0.35	6 (4%) 41 36	36, 92, 188, 341	0
33	RN	138/140 (98%)	-0.15	0 100 100	25, 75, 121, 188	0
33	YN	138/140 (98%)	-0.05	1 (0%) 89 85	26, 81, 141, 196	0
34	RO	122/122 (100%)	-0.38	0 100 100	26, 58, 90, 120	0
34	YO	122/122 (100%)	-0.37	0 100 100	27, 58, 91, 116	0
35	RP	150/150 (100%)	0.02	3 (2%) 68 62	19, 68, 152, 324	0
35	YP	150/150 (100%)	0.14	6 (4%) 42 37	27, 66, 149, 278	0
36	RQ	140/141 (99%)	0.02	4 (2%) 55 50	30, 70, 115, 294	0
36	YQ	139/141 (98%)	0.04	2 (1%) 78 73	35, 70, 127, 273	0
37	RR	117/118 (99%)	-0.20	0 100 100	26, 65, 100, 156	0
37	YR	117/118 (99%)	-0.12	0 100 100	33, 65, 115, 161	0
38	RS	111/112 (99%)	0.29	6 (5%) 29 27	59, 112, 201, 486	0
38	YS	111/112 (99%)	0.28	3 (2%) 58 53	54, 93, 171, 315	0
39	RT	137/146 (93%)	-0.10	6 (4%) 38 34	36, 78, 172, 561	0
39	YT	137/146 (93%)	0.28	11 (8%) 15 14	29, 80, 263, 460	0
40	RU	117/118 (99%)	-0.18	3 (2%) 59 54	20, 56, 126, 223	0
40	YU	117/118 (99%)	0.06	2 (1%) 73 67	32, 74, 147, 342	0
41	RV	101/101 (100%)	-0.08	3 (2%) 54 49	23, 79, 142, 406	0
41	YV	101/101 (100%)	0.34	3 (2%) 54 49	27, 102, 149, 576	0
42	RW	113/113 (100%)	-0.15	0 100 100	23, 53, 113, 248	0
42	YW	113/113 (100%)	-0.00	4 (3%) 48 42	26, 61, 118, 368	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	RX	92/96 (95%)	-0.04	1 (1%) 82 77	37, 69, 114, 140	0
43	YX	92/96 (95%)	-0.18	1 (1%) 82 77	26, 55, 107, 126	0
44	RY	102/110 (92%)	0.77	13 (12%) 5 5	33, 78, 230, 539	0
44	YY	102/110 (92%)	0.77	16 (15%) 3 3	40, 95, 248, 579	0
45	RZ	176/206 (85%)	0.45	13 (7%) 17 17	54, 109, 230, 333	0
45	YZ	183/206 (88%)	0.37	14 (7%) 16 16	55, 111, 190, 333	0
46	R0	83/85 (97%)	0.26	6 (7%) 18 17	30, 69, 179, 363	0
46	Y0	83/85 (97%)	0.28	4 (4%) 34 31	29, 70, 166, 209	0
47	R1	97/98 (98%)	0.39	5 (5%) 31 28	27, 64, 206, 399	0
47	Y1	97/98 (98%)	0.20	8 (8%) 14 13	17, 46, 207, 422	0
48	R2	69/72 (95%)	0.11	2 (2%) 55 50	35, 87, 189, 288	0
48	Y2	69/72 (95%)	-0.20	1 (1%) 78 73	28, 69, 119, 233	0
49	R3	59/60 (98%)	0.15	2 (3%) 49 44	36, 63, 116, 167	0
49	Y3	59/60 (98%)	0.05	1 (1%) 73 67	39, 80, 135, 184	0
50	R4	70/71 (98%)	1.29	19 (27%) 1 1	105, 280, 598, 608	0
50	Y4	70/71 (98%)	1.53	21 (30%) 1 1	92, 189, 571, 588	0
51	R5	59/60 (98%)	0.36	6 (10%) 9 9	21, 60, 201, 299	0
51	Y5	57/60 (95%)	0.37	5 (8%) 12 12	15, 71, 193, 303	0
52	R6	48/54 (88%)	1.83	19 (39%) 0 0	71, 128, 199, 285	0
52	Y6	48/54 (88%)	1.66	18 (37%) 0 1	60, 111, 181, 219	0
53	R7	49/49 (100%)	-0.19	0 100 100	15, 36, 127, 208	0
53	Y7	49/49 (100%)	-0.14	2 (4%) 41 36	10, 29, 97, 215	0
54	R8	64/65 (98%)	0.10	2 (3%) 52 48	22, 50, 116, 225	0
54	Y8	64/65 (98%)	0.30	3 (4%) 35 32	22, 52, 96, 236	0
55	R9	37/37 (100%)	3.11	26 (70%) 0 0	99, 140, 190, 246	0
55	Y9	36/37 (97%)	4.31	33 (91%) 0 0	88, 155, 219, 248	0
All	All	21218/21844 (97%)	0.19	1262 (5%) 26 23	10, 78, 219, 608	0

The worst 5 of 1262 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	RA	2801(A)	A	18.9
25	RA	1075	C	13.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
25	RA	2801	A	13.7
25	RA	2169	A	13.4
25	YA	2798	C	13.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
23	A2M	QX	19	23/24	0.85	0.36	-	108,108,108,108	0
23	A2M	XX	20	23/24	0.90	0.25	-	107,107,108,108	0
23	A2M	QX	21	23/24	0.84	0.31	-	108,155,155,155	0
23	A2M	QX	20	23/24	0.90	0.26	-	108,114,114,114	0
23	A2M	XX	21	23/24	0.84	0.30	-	108,164,164,164	0
23	A2M	XX	19	23/24	0.88	0.26	-	99,99,108,108	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
56	MG	RA	3244	1/1	0.89	0.46	64.82	16,16,16,16	0
56	MG	RA	3263	1/1	0.88	0.81	62.70	31,31,31,31	0
56	MG	YA	3080	1/1	0.94	0.49	48.60	15,15,15,15	0
56	MG	RA	3063	1/1	0.98	0.63	47.99	29,29,29,29	0
56	MG	YA	3049	1/1	0.99	0.47	46.52	12,12,12,12	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3375	1/1	0.91	0.52	41.60	51,51,51,51	0
56	MG	RA	3275	1/1	0.87	0.83	39.18	48,48,48,48	0
56	MG	RA	3411	1/1	0.84	0.82	39.08	29,29,29,29	0
56	MG	YA	3054	1/1	0.98	0.48	38.85	1,1,1,1	0
56	MG	RA	3165	1/1	0.92	0.55	36.19	25,25,25,25	0
56	MG	XA	1652	1/1	0.93	0.73	33.96	48,48,48,48	0
56	MG	RA	3363	1/1	0.95	0.65	33.27	34,34,34,34	0
56	MG	YA	3335	1/1	0.95	0.50	32.82	16,16,16,16	0
56	MG	YA	3025	1/1	0.98	0.63	31.54	16,16,16,16	0
56	MG	YA	3280	1/1	0.90	0.73	30.79	40,40,40,40	0
56	MG	QA	1640	1/1	0.99	0.38	30.48	53,53,53,53	0
56	MG	RA	3002	1/1	0.79	0.63	29.98	42,42,42,42	0
56	MG	YA	3472	1/1	0.78	0.54	29.52	69,69,69,69	0
56	MG	YA	3190	1/1	0.91	0.74	29.30	22,22,22,22	0
56	MG	YA	3081	1/1	0.98	0.49	28.76	7,7,7,7	0
56	MG	RA	3292	1/1	0.95	0.71	28.72	31,31,31,31	0
56	MG	YA	3295	1/1	0.91	0.39	28.53	52,52,52,52	0
56	MG	RA	3079	1/1	0.98	0.47	27.59	10,10,10,10	0
56	MG	RA	3331	1/1	0.78	0.32	27.17	69,69,69,69	0
56	MG	RA	3012	1/1	0.96	0.76	26.88	29,29,29,29	0
56	MG	YA	3460	1/1	0.89	0.61	26.63	35,35,35,35	0
56	MG	RA	3081	1/1	0.97	0.34	26.54	4,4,4,4	0
56	MG	RA	3369	1/1	0.96	0.54	25.84	38,38,38,38	0
56	MG	YA	3325	1/1	0.98	0.37	25.28	14,14,14,14	0
56	MG	YA	3192	1/1	0.84	0.64	24.84	23,23,23,23	0
56	MG	RA	3055	1/1	0.97	0.51	24.33	10,10,10,10	0
56	MG	YA	3455	1/1	0.94	0.47	23.91	42,42,42,42	0
56	MG	RA	3173	1/1	0.99	0.44	23.58	5,5,5,5	0
56	MG	RA	3082	1/1	0.99	0.45	23.48	0,0,0,0	0
56	MG	XA	1701	1/1	0.96	0.34	23.45	42,42,42,42	0
56	MG	RA	3195	1/1	0.98	0.61	23.16	29,29,29,29	0
56	MG	RA	3189	1/1	0.98	0.46	22.85	6,6,6,6	0
56	MG	YA	3338	1/1	0.95	0.47	22.83	15,15,15,15	0
56	MG	YA	3092	1/1	0.93	0.90	22.21	52,52,52,52	0
56	MG	XA	1650	1/1	0.98	0.44	22.17	16,16,16,16	0
56	MG	QA	1681	1/1	0.86	0.42	21.54	37,37,37,37	0
56	MG	YA	3031	1/1	0.82	0.45	20.84	26,26,26,26	0
56	MG	RA	3405	1/1	0.82	0.31	20.79	43,43,43,43	0
56	MG	RA	3026	1/1	0.97	0.54	20.33	24,24,24,24	0
56	MG	YA	3103	1/1	0.97	0.36	20.02	17,17,17,17	0
56	MG	YA	3425	1/1	0.71	0.84	19.53	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3122	1/1	0.96	0.49	19.32	14,14,14,14	0
56	MG	RA	3128	1/1	0.84	0.41	19.31	43,43,43,43	0
56	MG	YA	3255	1/1	0.93	0.61	19.20	33,33,33,33	0
56	MG	YA	3078	1/1	0.99	0.43	19.14	9,9,9,9	0
56	MG	RA	3022	1/1	0.94	0.36	18.75	17,17,17,17	0
56	MG	RA	3149	1/1	0.98	0.62	18.74	2,2,2,2	0
56	MG	RA	3073	1/1	0.93	0.63	18.62	35,35,35,35	0
56	MG	RA	3377	1/1	0.93	0.50	18.49	24,24,24,24	0
56	MG	RA	3048	1/1	0.99	0.49	18.29	5,5,5,5	0
56	MG	YA	3201	1/1	0.98	0.42	18.24	20,20,20,20	0
56	MG	RA	3316	1/1	0.78	0.60	17.84	57,57,57,57	0
56	MG	RA	3370	1/1	0.92	0.52	17.47	43,43,43,43	0
56	MG	YA	3003	1/1	0.97	0.44	17.46	4,4,4,4	0
56	MG	YA	3224	1/1	0.94	0.47	16.77	22,22,22,22	0
56	MG	YA	3017	1/1	0.96	0.70	16.73	30,30,30,30	0
56	MG	RA	3209	1/1	0.91	0.47	16.56	19,19,19,19	0
56	MG	RA	3425	1/1	0.90	0.40	16.51	38,38,38,38	0
56	MG	RA	3135	1/1	0.91	0.31	16.47	32,32,32,32	0
56	MG	YA	3336	1/1	0.98	0.45	16.46	17,17,17,17	0
56	MG	YA	3250	1/1	0.96	0.45	16.44	27,27,27,27	0
56	MG	YA	3240	1/1	0.89	0.35	16.39	17,17,17,17	0
56	MG	RA	3050	1/1	0.94	0.37	16.32	6,6,6,6	0
56	MG	YA	3414	1/1	0.95	0.68	16.22	29,29,29,29	0
56	MG	YA	3006	1/1	0.98	0.49	16.00	32,32,32,32	0
56	MG	YA	3233	1/1	0.72	0.41	15.93	49,49,49,49	0
56	MG	RA	3037	1/1	0.74	0.67	15.91	24,24,24,24	0
56	MG	RA	3295	1/1	0.75	0.41	15.91	46,46,46,46	0
56	MG	RA	3291	1/1	0.98	0.33	15.68	31,31,31,31	0
56	MG	RA	3104	1/1	0.96	0.46	15.60	28,28,28,28	0
56	MG	YA	3167	1/1	0.94	0.32	15.53	30,30,30,30	0
56	MG	RA	3094	1/1	0.96	0.66	15.16	35,35,35,35	0
56	MG	RA	3233	1/1	0.87	0.40	15.12	25,25,25,25	0
56	MG	QA	1741	1/1	0.92	0.44	14.84	37,37,37,37	0
56	MG	YA	3467	1/1	0.70	0.45	14.66	68,68,68,68	0
56	MG	QA	1606	1/1	0.90	0.30	14.42	18,18,18,18	0
56	MG	RA	3213	1/1	0.89	0.42	14.19	21,21,21,21	0
56	MG	YA	3101	1/1	0.93	0.38	14.19	25,25,25,25	0
56	MG	RA	3103	1/1	0.93	0.43	14.10	43,43,43,43	0
56	MG	YA	3170	1/1	0.97	0.41	14.09	7,7,7,7	0
56	MG	YA	3428	1/1	0.93	0.56	14.08	55,55,55,55	0
56	MG	RA	3193	1/1	0.98	0.33	14.03	0,0,0,0	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3099	1/1	0.91	0.49	14.03	25,25,25,25	0
56	MG	RA	3095	1/1	0.91	0.52	13.88	45,45,45,45	0
56	MG	YA	3459	1/1	0.71	0.51	13.84	43,43,43,43	0
56	MG	RA	3028	1/1	0.97	0.49	13.35	10,10,10,10	0
56	MG	QA	1656	1/1	0.99	0.46	13.10	26,26,26,26	0
56	MG	YA	3392	1/1	0.81	0.56	13.00	60,60,60,60	0
56	MG	RA	3110	1/1	0.97	0.44	12.90	8,8,8,8	0
56	MG	YA	3186	1/1	0.97	0.39	12.71	1,1,1,1	0
56	MG	YA	3426	1/1	0.84	0.35	12.64	34,34,34,34	0
56	MG	RA	3228	1/1	0.98	0.42	12.40	18,18,18,18	0
56	MG	YA	3072	1/1	0.97	0.36	12.33	19,19,19,19	0
56	MG	RA	3376	1/1	0.96	0.32	12.09	5,5,5,5	0
56	MG	RA	3430	1/1	0.82	0.70	12.05	50,50,50,50	0
56	MG	RA	3318	1/1	0.84	0.32	11.98	32,32,32,32	0
56	MG	XA	1643	1/1	0.95	0.35	11.97	23,23,23,23	0
56	MG	QA	1637	1/1	0.91	0.47	11.77	53,53,53,53	0
56	MG	QA	1608	1/1	0.92	0.55	11.77	25,25,25,25	0
56	MG	QA	1682	1/1	0.83	0.61	11.75	51,51,51,51	0
56	MG	RA	3007	1/1	0.99	0.30	11.42	5,5,5,5	0
56	MG	YF	301	1/1	0.88	0.65	11.13	37,37,37,37	0
56	MG	QA	1719	1/1	0.74	0.47	10.98	70,70,70,70	0
56	MG	RA	3065	1/1	0.97	0.41	10.94	10,10,10,10	0
56	MG	XA	1742	1/1	0.95	0.43	10.87	73,73,73,73	0
56	MG	RA	3125	1/1	0.92	0.31	10.86	26,26,26,26	0
56	MG	YA	3111	1/1	0.93	0.25	10.84	53,53,53,53	0
56	MG	YA	3127	1/1	0.88	0.33	10.78	51,51,51,51	0
56	MG	YA	3340	1/1	0.94	0.53	10.78	29,29,29,29	0
56	MG	RA	3177	1/1	0.99	0.31	10.77	16,16,16,16	0
56	MG	RA	3067	1/1	0.98	0.41	10.73	28,28,28,28	0
56	MG	RA	3057	1/1	0.97	0.52	10.62	2,2,2,2	0
56	MG	YA	3038	1/1	0.91	0.59	10.58	45,45,45,45	0
56	MG	YA	3056	1/1	0.98	0.47	10.56	1,1,1,1	0
56	MG	RA	3247	1/1	0.92	0.34	10.49	26,26,26,26	0
56	MG	RA	3066	1/1	0.99	0.35	10.47	31,31,31,31	0
56	MG	YA	3044	1/1	0.98	0.33	10.30	12,12,12,12	0
56	MG	RA	3264	1/1	0.86	0.33	10.13	42,42,42,42	0
56	MG	RA	3032	1/1	0.99	0.28	10.09	5,5,5,5	0
56	MG	RQ	202	1/1	0.75	0.52	10.08	48,48,48,48	0
56	MG	RA	3083	1/1	0.76	0.26	10.05	5,5,5,5	0
56	MG	RA	3051	1/1	0.73	0.37	10.02	62,62,62,62	0
56	MG	XA	1664	1/1	0.98	0.40	10.00	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3416	1/1	0.48	0.27	9.92	9,9,9,9	0
56	MG	YA	3027	1/1	0.97	0.42	9.90	14,14,14,14	0
56	MG	YA	3282	1/1	0.93	0.55	9.86	49,49,49,49	0
56	MG	XA	1667	1/1	0.92	0.32	9.82	30,30,30,30	0
56	MG	RA	3027	1/1	0.97	0.42	9.74	2,2,2,2	0
56	MG	RA	3018	1/1	0.95	0.44	9.68	10,10,10,10	0
56	MG	YA	3203	1/1	0.96	0.25	9.66	30,30,30,30	0
56	MG	QA	1670	1/1	0.92	0.37	9.58	48,48,48,48	0
56	MG	RA	3001	1/1	0.96	0.34	9.45	41,41,41,41	0
56	MG	XA	1605	1/1	0.98	0.26	9.43	6,6,6,6	0
56	MG	RA	3045	1/1	0.98	0.37	9.22	4,4,4,4	0
56	MG	YA	3064	1/1	0.99	0.33	9.15	5,5,5,5	0
56	MG	XA	1635	1/1	0.97	0.53	9.14	36,36,36,36	0
56	MG	QA	1639	1/1	0.93	0.30	9.06	48,48,48,48	0
56	MG	RA	3432	1/1	0.89	0.29	9.01	91,91,91,91	0
56	MG	RA	3222	1/1	0.75	0.43	8.99	45,45,45,45	0
56	MG	YA	3070	1/1	0.96	0.34	8.97	3,3,3,3	0
56	MG	RA	3108	1/1	0.78	0.61	8.90	33,33,33,33	0
56	MG	RA	3033	1/1	0.98	0.35	8.84	8,8,8,8	0
56	MG	YA	3227	1/1	0.72	0.37	8.77	53,53,53,53	0
56	MG	RA	3116	1/1	0.89	0.32	8.74	18,18,18,18	0
56	MG	QA	1619	1/1	0.98	0.41	8.54	12,12,12,12	0
56	MG	XA	1611	1/1	0.85	0.46	8.46	46,46,46,46	0
56	MG	YA	3305	1/1	0.94	0.30	8.42	21,21,21,21	0
56	MG	YA	3208	1/1	0.95	0.50	8.37	27,27,27,27	0
56	MG	YA	3013	1/1	0.86	0.26	8.31	0,0,0,0	0
56	MG	YA	3147	1/1	0.95	0.59	8.29	1,1,1,1	0
56	MG	XA	1625	1/1	0.25	0.29	8.29	80,80,80,80	0
56	MG	QA	1643	1/1	0.90	0.27	8.10	35,35,35,35	0
56	MG	RA	3074	1/1	0.97	0.44	8.00	27,27,27,27	0
56	MG	XA	1613	1/1	0.91	0.24	7.91	22,22,22,22	0
56	MG	RA	3385	1/1	0.98	0.35	7.89	2,2,2,2	0
56	MG	RA	3004	1/1	0.96	0.43	7.85	16,16,16,16	0
56	MG	RA	3431	1/1	0.89	0.29	7.84	40,40,40,40	0
56	MG	YA	3010	1/1	0.98	0.25	7.83	4,4,4,4	0
56	MG	QA	1728	1/1	0.70	0.25	7.82	48,48,48,48	0
56	MG	YA	3055	1/1	0.96	0.25	7.82	12,12,12,12	0
56	MG	YA	3082	1/1	0.82	0.27	7.80	20,20,20,20	0
56	MG	QA	1641	1/1	0.96	0.46	7.77	32,32,32,32	0
56	MG	YA	3011	1/1	0.97	0.51	7.76	0,0,0,0	0
56	MG	XA	1754	1/1	0.90	0.36	7.74	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	XA	1624	1/1	0.91	0.37	7.72	59,59,59,59	0
56	MG	YA	3146	1/1	0.95	0.38	7.66	24,24,24,24	0
56	MG	YA	3102	1/1	0.92	0.40	7.64	22,22,22,22	0
56	MG	YA	3249	1/1	0.85	0.41	7.62	34,34,34,34	0
56	MG	YA	3234	1/1	0.91	0.25	7.58	30,30,30,30	0
56	MG	YA	3209	1/1	0.99	0.30	7.56	9,9,9,9	0
56	MG	RA	3368	1/1	0.84	0.36	7.46	46,46,46,46	0
56	MG	YA	3407	1/1	0.96	0.34	7.43	4,4,4,4	0
56	MG	RA	3140	1/1	0.97	0.31	7.23	34,34,34,34	0
56	MG	RA	3034	1/1	0.99	0.35	7.17	9,9,9,9	0
56	MG	YA	3109	1/1	0.97	0.44	7.16	14,14,14,14	0
56	MG	RA	3365	1/1	0.87	0.34	7.11	21,21,21,21	0
56	MG	QA	1609	1/1	0.95	0.31	7.04	27,27,27,27	0
56	MG	YA	3026	1/1	0.92	0.39	6.85	30,30,30,30	0
56	MG	RA	3357	1/1	0.75	0.28	6.83	51,51,51,51	0
56	MG	YA	3099	1/1	0.59	0.52	6.80	68,68,68,68	0
56	MG	RA	3013	1/1	0.99	0.31	6.30	0,0,0,0	0
56	MG	YA	3191	1/1	0.97	0.40	6.29	9,9,9,9	0
56	MG	RA	3386	1/1	0.94	0.23	6.26	17,17,17,17	0
56	MG	RA	3148	1/1	0.83	0.23	6.16	19,19,19,19	0
56	MG	RA	3159	1/1	0.99	0.36	6.12	5,5,5,5	0
56	MG	XA	1618	1/1	0.94	0.31	6.09	15,15,15,15	0
56	MG	RA	3296	1/1	0.91	0.20	6.09	29,29,29,29	0
56	MG	RA	3039	1/1	0.99	0.29	6.02	21,21,21,21	0
56	MG	QA	1632	1/1	0.96	0.45	5.99	57,57,57,57	0
56	MG	RA	3184	1/1	0.85	0.22	5.87	24,24,24,24	0
56	MG	RA	3061	1/1	0.98	0.24	5.79	17,17,17,17	0
56	MG	YA	3033	1/1	0.98	0.26	5.68	10,10,10,10	0
56	MG	YA	3097	1/1	0.93	0.32	5.67	21,21,21,21	0
56	MG	RA	3198	1/1	0.96	0.28	5.65	26,26,26,26	0
56	MG	QA	1636	1/1	0.74	0.43	5.58	56,56,56,56	0
56	MG	XA	1604	1/1	0.97	0.28	5.51	9,9,9,9	0
56	MG	XA	1607	1/1	0.89	0.52	5.49	43,43,43,43	0
56	MG	RA	3105	1/1	0.90	0.32	5.47	33,33,33,33	0
56	MG	RA	3014	1/1	0.90	0.27	5.41	3,3,3,3	0
56	MG	YA	3204	1/1	0.95	0.20	5.38	10,10,10,10	0
56	MG	YA	3071	1/1	0.95	0.20	5.34	17,17,17,17	0
56	MG	RA	3427	1/1	0.86	0.40	5.31	35,35,35,35	0
56	MG	RA	3071	1/1	0.97	0.28	5.31	9,9,9,9	0
56	MG	XA	1692	1/1	0.96	0.25	5.30	36,36,36,36	0
56	MG	YA	3012	1/1	0.96	0.28	5.24	14,14,14,14	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3062	1/1	0.99	0.26	5.14	0,0,0,0	0
56	MG	YA	3210	1/1	0.91	0.28	4.99	25,25,25,25	0
56	MG	RD	302	1/1	0.98	0.35	4.97	9,9,9,9	0
56	MG	QA	1605	1/1	0.98	0.28	4.95	31,31,31,31	0
56	MG	R5	102	1/1	0.93	0.38	4.95	53,53,53,53	0
56	MG	RA	3343	1/1	0.72	0.40	4.91	61,61,61,61	0
56	MG	YA	3221	1/1	0.93	0.22	4.78	16,16,16,16	0
56	MG	RA	3107	1/1	0.95	0.26	4.73	20,20,20,20	0
56	MG	RA	3306	1/1	0.92	0.67	4.72	63,63,63,63	0
56	MG	YA	3424	1/1	0.91	0.24	4.67	46,46,46,46	0
56	MG	YA	3276	1/1	0.89	0.34	4.57	31,31,31,31	0
56	MG	XA	1640	1/1	0.99	0.34	4.49	29,29,29,29	0
56	MG	YA	3042	1/1	0.96	0.38	4.31	7,7,7,7	0
56	MG	RA	3072	1/1	0.94	0.34	4.25	32,32,32,32	0
56	MG	RA	3407	1/1	0.98	0.31	4.23	4,4,4,4	0
56	MG	RA	3350	1/1	0.96	0.24	4.22	45,45,45,45	0
56	MG	YA	3018	1/1	0.98	0.22	4.14	18,18,18,18	0
56	MG	QA	1651	1/1	0.97	0.19	4.01	29,29,29,29	0
56	MG	YA	3339	1/1	0.87	0.25	3.96	62,62,62,62	0
56	MG	RA	3155	1/1	0.98	0.24	3.96	12,12,12,12	0
56	MG	YA	3066	1/1	0.97	0.29	3.94	27,27,27,27	0
56	MG	QA	1699	1/1	0.77	0.28	3.94	55,55,55,55	0
56	MG	YA	3073	1/1	0.97	0.34	3.93	15,15,15,15	0
56	MG	RA	3153	1/1	0.89	0.23	3.92	25,25,25,25	0
56	MG	YA	3485	1/1	0.74	0.29	3.91	22,22,22,22	0
56	MG	YA	3151	1/1	0.91	0.22	3.90	26,26,26,26	0
56	MG	YA	3137	1/1	0.92	0.22	3.88	5,5,5,5	0
56	MG	QA	1601	1/1	0.98	0.25	3.82	17,17,17,17	0
56	MG	QA	1729	1/1	0.84	0.27	3.76	31,31,31,31	0
56	MG	YA	3473	1/1	0.88	0.20	3.70	30,30,30,30	0
56	MG	YA	3106	1/1	0.93	0.27	3.70	15,15,15,15	0
56	MG	RA	3225	1/1	0.90	0.33	3.60	40,40,40,40	0
56	MG	QA	1625	1/1	0.97	0.32	3.55	66,66,66,66	0
56	MG	RA	3434	1/1	0.92	0.21	3.54	37,37,37,37	0
56	MG	YA	3130	1/1	0.91	0.21	3.51	37,37,37,37	0
56	MG	YA	3431	1/1	0.95	0.18	3.49	52,52,52,52	0
56	MG	YA	3121	1/1	0.81	0.23	3.42	52,52,52,52	0
56	MG	YA	3060	1/1	0.98	0.27	3.41	3,3,3,3	0
56	MG	RA	3206	1/1	0.82	0.24	3.41	18,18,18,18	0
56	MG	YA	3079	1/1	0.96	0.24	3.40	34,34,34,34	0
56	MG	QA	1604	1/1	0.98	0.27	3.40	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3339	1/1	0.91	0.26	3.39	44,44,44,44	0
56	MG	RA	3205	1/1	0.95	0.23	3.38	19,19,19,19	0
56	MG	RA	3080	1/1	1.00	0.27	3.31	17,17,17,17	0
56	MG	YA	3155	1/1	0.78	0.24	3.30	41,41,41,41	0
56	MG	Y1	101	1/1	0.95	0.37	3.22	24,24,24,24	0
56	MG	QA	1644	1/1	0.97	0.24	3.18	23,23,23,23	0
56	MG	XA	1638	1/1	0.95	0.33	3.13	34,34,34,34	0
56	MG	XA	1745	1/1	0.86	0.23	3.07	45,45,45,45	0
56	MG	YA	3463	1/1	0.75	0.37	3.01	53,53,53,53	0
56	MG	QA	1687	1/1	0.95	0.25	2.95	52,52,52,52	0
56	MG	YA	3220	1/1	0.88	0.16	2.93	33,33,33,33	0
56	MG	YA	3088	1/1	0.95	0.21	2.93	5,5,5,5	0
56	MG	YQ	201	1/1	0.84	0.31	2.91	44,44,44,44	0
56	MG	YA	3484	1/1	0.80	0.30	2.86	24,24,24,24	0
56	MG	RA	3056	1/1	0.98	0.20	2.83	14,14,14,14	0
56	MG	RA	3436	1/1	0.95	0.30	2.80	8,8,8,8	0
56	MG	XA	1695	1/1	0.94	0.24	2.79	52,52,52,52	0
56	MG	RA	3202	1/1	0.93	0.21	2.79	22,22,22,22	0
56	MG	XA	1755	1/1	0.54	0.30	2.72	68,68,68,68	0
56	MG	YA	3418	1/1	0.94	0.17	2.71	16,16,16,16	0
56	MG	XA	1697	1/1	0.92	0.25	2.71	42,42,42,42	0
56	MG	XA	1659	1/1	0.97	0.42	2.68	27,27,27,27	0
56	MG	RA	3254	1/1	0.94	0.20	2.66	46,46,46,46	0
56	MG	YA	3133	1/1	0.90	0.18	2.60	25,25,25,25	0
56	MG	RA	3420	1/1	0.94	0.22	2.59	35,35,35,35	0
56	MG	RA	3011	1/1	0.99	0.19	2.59	1,1,1,1	0
56	MG	QA	1703	1/1	0.80	0.21	2.58	47,47,47,47	0
56	MG	RA	3438	1/1	0.89	0.23	2.54	23,23,23,23	0
56	MG	RA	3047	1/1	0.98	0.23	2.54	25,25,25,25	0
56	MG	RA	3166	1/1	0.76	0.23	2.51	31,31,31,31	0
56	MG	XA	1717	1/1	0.84	0.45	2.50	46,46,46,46	0
56	MG	YA	3156	1/1	0.96	0.36	2.49	15,15,15,15	0
56	MG	RA	3131	1/1	0.88	0.24	2.42	78,78,78,78	0
56	MG	RA	3197	1/1	0.90	0.21	2.42	30,30,30,30	0
56	MG	RA	3355	1/1	0.47	0.30	2.41	58,58,58,58	0
56	MG	QA	1645	1/1	0.96	0.25	2.40	41,41,41,41	0
56	MG	XA	1601	1/1	0.99	0.22	2.39	8,8,8,8	0
56	MG	XA	1644	1/1	0.94	0.22	2.38	25,25,25,25	0
56	MG	QA	1662	1/1	0.83	0.23	2.35	40,40,40,40	0
56	MG	YA	3264	1/1	0.97	0.29	2.28	16,16,16,16	0
56	MG	QA	1668	1/1	0.91	0.21	2.26	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3251	1/1	0.88	0.24	2.16	63,63,63,63	0
56	MG	YD	301	1/1	0.98	0.44	2.15	2,2,2,2	0
56	MG	RA	3259	1/1	0.79	0.24	2.11	46,46,46,46	0
56	MG	RA	3053	1/1	0.95	0.18	2.08	21,21,21,21	0
56	MG	QA	1614	1/1	0.92	0.19	1.92	38,38,38,38	0
56	MG	XA	1741	1/1	0.87	0.23	1.83	55,55,55,55	0
56	MG	YA	3093	1/1	0.98	0.23	1.70	17,17,17,17	0
56	MG	RA	3111	1/1	0.84	0.21	1.60	40,40,40,40	0
56	MG	YA	3050	1/1	0.93	0.19	1.59	24,24,24,24	0
56	MG	YA	3136	1/1	0.92	0.21	1.58	22,22,22,22	0
56	MG	RA	3172	1/1	0.89	0.18	1.57	28,28,28,28	0
56	MG	RA	3240	1/1	0.92	0.20	1.55	26,26,26,26	0
56	MG	XA	1748	1/1	0.94	0.23	1.54	66,66,66,66	0
56	MG	YA	3090	1/1	0.86	0.21	1.49	43,43,43,43	0
56	MG	YA	3298	1/1	0.94	0.21	1.48	21,21,21,21	0
56	MG	YA	3005	1/1	0.96	0.23	1.45	1,1,1,1	0
56	MG	YA	3327	1/1	0.97	0.17	1.36	54,54,54,54	0
56	MG	RA	3164	1/1	0.93	0.23	1.32	51,51,51,51	0
56	MG	YA	3347	1/1	0.89	0.27	1.30	29,29,29,29	0
56	MG	YA	3046	1/1	0.90	0.24	1.27	14,14,14,14	0
56	MG	XA	1736	1/1	0.93	0.20	1.25	23,23,23,23	0
56	MG	QA	1738	1/1	0.92	0.16	1.24	32,32,32,32	0
56	MG	YA	3444	1/1	0.96	0.27	1.17	5,5,5,5	0
56	MG	RA	3030	1/1	0.95	0.20	1.13	13,13,13,13	0
56	MG	YA	3286	1/1	0.97	0.18	0.99	20,20,20,20	0
56	MG	YA	3032	1/1	0.97	0.23	0.94	16,16,16,16	0
56	MG	QA	1626	1/1	0.80	0.17	0.91	46,46,46,46	0
56	MG	YA	3228	1/1	0.97	0.17	0.89	25,25,25,25	0
56	MG	QA	1693	1/1	0.76	0.17	0.88	66,66,66,66	0
56	MG	XA	1603	1/1	0.98	0.20	0.88	24,24,24,24	0
57	ZN	XD	301	1/1	0.88	0.37	0.85	48,48,48,48	0
56	MG	YA	3356	1/1	0.97	0.19	0.84	30,30,30,30	0
56	MG	RR	201	1/1	0.89	0.28	0.78	31,31,31,31	0
57	ZN	QD	301	1/1	0.97	0.33	0.74	29,29,29,29	0
56	MG	YA	3471	1/1	0.87	0.21	0.62	28,28,28,28	0
56	MG	XA	1743	1/1	0.90	0.16	0.61	53,53,53,53	0
56	MG	RA	3059	1/1	0.99	0.20	0.56	24,24,24,24	0
56	MG	YA	3434	1/1	0.94	0.19	0.52	42,42,42,42	0
56	MG	XA	1614	1/1	0.96	0.22	0.46	19,19,19,19	0
56	MG	YA	3456	1/1	0.81	0.21	0.43	28,28,28,28	0
56	MG	RA	3237	1/1	0.93	0.18	0.41	23,23,23,23	0
56	MG	XS	300	1/1	0.95	0.31	0.38	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	QA	1673	1/1	0.88	0.33	0.37	70,70,70,70	0
56	MG	XA	1656	1/1	0.70	0.17	0.36	45,45,45,45	0
56	MG	YA	3131	1/1	0.96	0.17	0.35	11,11,11,11	0
56	MG	YA	3164	1/1	0.85	0.16	0.35	38,38,38,38	0
56	MG	XA	1761	1/1	0.87	0.20	0.26	23,23,23,23	0
56	MG	QA	1628	1/1	0.82	0.24	0.26	68,68,68,68	0
56	MG	RA	3060	1/1	0.83	0.15	0.20	14,14,14,14	0
56	MG	RA	3235	1/1	0.92	0.20	0.18	28,28,28,28	0
56	MG	YA	3021	1/1	0.96	0.20	0.16	17,17,17,17	0
56	MG	XA	1732	1/1	0.97	0.14	0.16	32,32,32,32	0
56	MG	YA	3161	1/1	0.92	0.19	0.15	39,39,39,39	0
56	MG	XV	101	1/1	0.97	0.20	0.14	39,39,39,39	0
56	MG	XA	1634	1/1	0.92	0.20	0.12	46,46,46,46	0
56	MG	RA	3298	1/1	0.80	0.17	0.11	52,52,52,52	0
56	MG	QA	1725	1/1	0.85	0.18	0.08	64,64,64,64	0
56	MG	RA	3439	1/1	0.82	0.26	0.08	50,50,50,50	0
56	MG	QA	1654	1/1	0.98	0.22	0.05	20,20,20,20	0
56	MG	RD	301	1/1	0.92	0.21	0.03	24,24,24,24	0
56	MG	RA	3424	1/1	0.96	0.16	-0.03	26,26,26,26	0
56	MG	RP	201	1/1	0.96	0.25	-0.03	21,21,21,21	0
56	MG	QA	1750	1/1	0.71	0.23	-0.04	68,68,68,68	0
56	MG	RA	3157	1/1	0.76	0.19	-0.04	43,43,43,43	0
56	MG	XA	1642	1/1	0.98	0.18	-0.05	39,39,39,39	0
56	MG	RA	3283	1/1	0.94	0.18	-0.07	18,18,18,18	0
56	MG	YA	3008	1/1	0.99	0.17	-0.12	2,2,2,2	0
56	MG	RA	3162	1/1	0.85	0.20	-0.15	49,49,49,49	0
56	MG	QA	1744	1/1	0.93	0.16	-0.20	56,56,56,56	0
56	MG	RA	3351	1/1	0.83	0.21	-0.20	75,75,75,75	0
56	MG	RA	3281	1/1	0.84	0.16	-0.25	57,57,57,57	0
56	MG	YA	3128	1/1	0.86	0.17	-0.27	37,37,37,37	0
56	MG	YA	3244	1/1	0.86	0.17	-0.31	54,54,54,54	0
56	MG	QD	303	1/1	0.13	0.16	-0.40	69,69,69,69	0
56	MG	QV	104	1/1	0.96	0.17	-0.44	58,58,58,58	0
56	MG	RA	3437	1/1	0.95	0.18	-0.46	24,24,24,24	0
56	MG	XA	1653	1/1	0.97	0.14	-0.48	35,35,35,35	0
56	MG	YA	3284	1/1	0.98	0.17	-0.49	14,14,14,14	0
56	MG	YA	3104	1/1	0.98	0.16	-0.49	47,47,47,47	0
56	MG	RA	3009	1/1	0.97	0.15	-0.50	6,6,6,6	0
56	MG	YA	3420	1/1	0.89	0.17	-0.52	23,23,23,23	0
56	MG	YA	3108	1/1	0.92	0.17	-0.55	33,33,33,33	0
56	MG	RA	3132	1/1	0.90	0.17	-0.62	20,20,20,20	0
56	MG	QA	1742	1/1	0.88	0.15	-0.62	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	QA	1666	1/1	0.94	0.13	-0.63	23,23,23,23	0
56	MG	QA	1678	1/1	0.92	0.15	-0.65	29,29,29,29	0
56	MG	RA	3337	1/1	0.97	0.14	-0.68	41,41,41,41	0
56	MG	YA	3218	1/1	0.92	0.13	-0.73	36,36,36,36	0
56	MG	XA	1679	1/1	0.97	0.13	-0.75	37,37,37,37	0
56	MG	YA	3429	1/1	0.92	0.14	-0.80	38,38,38,38	0
56	MG	YA	3294	1/1	0.82	0.13	-0.82	56,56,56,56	0
56	MG	XA	1627	1/1	0.83	0.17	-0.85	57,57,57,57	0
56	MG	RA	3279	1/1	0.87	0.17	-0.90	26,26,26,26	0
56	MG	XF	201	1/1	0.86	0.18	-0.91	39,39,39,39	0
56	MG	QA	1615	1/1	0.93	0.14	-0.95	29,29,29,29	0
56	MG	YA	3206	1/1	0.95	0.15	-0.97	12,12,12,12	0
56	MG	YA	3474	1/1	0.96	0.13	-1.01	23,23,23,23	0
56	MG	XD	302	1/1	0.65	0.14	-1.04	85,85,85,85	0
56	MG	XA	1762	1/1	0.96	0.17	-1.11	53,53,53,53	0
56	MG	RA	3085	1/1	0.99	0.12	-1.12	13,13,13,13	0
56	MG	YG	201	1/1	0.64	0.14	-1.14	56,56,56,56	0
56	MG	Y5	103	1/1	0.97	0.15	-1.17	41,41,41,41	0
56	MG	RP	202	1/1	0.92	0.17	-1.24	18,18,18,18	0
56	MG	YA	3200	1/1	0.97	0.11	-1.24	1,1,1,1	0
56	MG	QA	1730	1/1	0.97	0.15	-1.28	58,58,58,58	0
57	ZN	XN	101	1/1	0.93	0.13	-1.31	67,67,67,67	0
56	MG	QA	1749	1/1	0.93	0.13	-1.32	41,41,41,41	0
57	ZN	QN	101	1/1	0.95	0.14	-1.33	76,76,76,76	0
56	MG	XA	1620	1/1	0.79	0.15	-1.34	21,21,21,21	0
56	MG	XA	1763	1/1	0.83	0.15	-1.34	52,52,52,52	0
56	MG	RA	3129	1/1	0.95	0.13	-1.36	14,14,14,14	0
56	MG	XA	1690	1/1	0.98	0.13	-1.40	65,65,65,65	0
56	MG	XA	1623	1/1	0.95	0.12	-1.46	20,20,20,20	0
56	MG	YA	3248	1/1	0.88	0.10	-1.56	30,30,30,30	0
56	MG	RA	3440	1/1	0.86	0.11	-1.57	12,12,12,12	0
56	MG	XA	1734	1/1	0.90	0.10	-1.72	27,27,27,27	0
56	MG	YA	3212	1/1	0.97	0.10	-1.73	32,32,32,32	0
56	MG	YP	201	1/1	0.97	0.13	-1.84	7,7,7,7	0
56	MG	YA	3486	1/1	0.94	0.10	-1.84	19,19,19,19	0
56	MG	YB	205	1/1	0.95	0.12	-1.86	48,48,48,48	0
56	MG	QV	101	1/1	0.91	0.12	-1.86	31,31,31,31	0
56	MG	R5	103	1/1	0.93	0.10	-1.89	25,25,25,25	0
56	MG	QA	1685	1/1	0.93	0.10	-2.04	11,11,11,11	0
56	MG	RP	203	1/1	0.95	0.17	-2.08	4,4,4,4	0
56	MG	RA	3174	1/1	0.91	0.10	-2.10	26,26,26,26	0
56	MG	YA	3059	1/1	0.90	0.14	-2.12	15,15,15,15	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	XA	1672	1/1	0.87	0.13	-2.28	44,44,44,44	0
56	MG	YA	3421	1/1	0.80	0.09	-2.36	68,68,68,68	0
56	MG	YN	201	1/1	0.93	0.14	-2.54	34,34,34,34	0
56	MG	RA	3121	1/1	0.88	0.12	-2.56	45,45,45,45	0
56	MG	YA	3029	1/1	0.86	0.12	-2.63	15,15,15,15	0
56	MG	RB	204	1/1	0.82	0.09	-2.78	47,47,47,47	0
56	MG	YA	3462	1/1	0.93	0.09	-2.98	48,48,48,48	0
56	MG	RA	3238	1/1	0.98	0.10	-3.09	11,11,11,11	0
56	MG	XA	1682	1/1	0.94	0.07	-3.13	26,26,26,26	0
56	MG	RA	3243	1/1	0.97	0.12	-3.25	37,37,37,37	0
56	MG	QA	1726	1/1	0.97	0.10	-3.45	23,23,23,23	0
56	MG	YA	3237	1/1	0.98	0.11	-3.80	37,37,37,37	0
56	MG	QA	1624	1/1	0.98	0.11	-4.04	31,31,31,31	0
56	MG	RF	301	1/1	0.93	0.10	-4.11	24,24,24,24	0
56	MG	RA	3141	1/1	0.81	0.09	-4.14	31,31,31,31	0
56	MG	QA	1688	1/1	0.94	0.10	-4.19	31,31,31,31	0
56	MG	YA	3084	1/1	0.88	0.09	-4.28	11,11,11,11	0
56	MG	YA	3058	1/1	0.99	0.06	-4.57	34,34,34,34	0
56	MG	XA	1609	1/1	0.98	0.06	-5.26	79,79,79,79	0
56	MG	YA	3238	1/1	0.93	0.12	-5.48	14,14,14,14	0
56	MG	YA	3138	1/1	0.96	0.05	-5.56	18,18,18,18	0
56	MG	RA	3161	1/1	0.93	0.16	-5.87	39,39,39,39	0
56	MG	RA	3006	1/1	0.97	0.07	-6.36	0,0,0,0	0
56	MG	YA	3171	1/1	0.94	0.09	-6.81	26,26,26,26	0
56	MG	YQ	202	1/1	0.93	0.29	-	27,27,27,27	0
56	MG	YA	3016	1/1	0.96	0.07	-	2,2,2,2	0
56	MG	RA	3163	1/1	0.98	0.25	-	34,34,34,34	0
56	MG	XA	1723	1/1	0.91	0.38	-	58,58,58,58	0
56	MG	QA	1613	1/1	0.87	0.25	-	51,51,51,51	0
56	MG	YA	3401	1/1	0.75	0.59	-	43,43,43,43	0
56	MG	YA	3239	1/1	0.84	0.33	-	40,40,40,40	0
56	MG	XA	1731	1/1	0.82	0.15	-	47,47,47,47	0
56	MG	QL	201	1/1	0.89	0.26	-	38,38,38,38	0
56	MG	YA	3397	1/1	0.92	0.57	-	58,58,58,58	0
56	MG	QA	1611	1/1	0.93	0.24	-	28,28,28,28	0
56	MG	QA	1717	1/1	0.94	0.77	-	33,33,33,33	0
56	MG	RA	3016	1/1	0.98	0.30	-	6,6,6,6	0
56	MG	QV	103	1/1	0.86	0.26	-	45,45,45,45	0
56	MG	RA	3133	1/1	0.96	0.33	-	52,52,52,52	0
56	MG	YA	3442	1/1	0.97	0.28	-	42,42,42,42	0
56	MG	YA	3413	1/1	0.95	0.26	-	7,7,7,7	0
56	MG	RA	3052	1/1	0.97	0.26	-	4,4,4,4	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3367	1/1	0.94	0.16	-	46,46,46,46	0
56	MG	RA	3203	1/1	0.96	0.25	-	26,26,26,26	0
56	MG	QA	1667	1/1	0.99	0.22	-	27,27,27,27	0
56	MG	RA	3310	1/1	0.97	0.39	-	17,17,17,17	0
56	MG	QA	1712	1/1	0.90	0.32	-	46,46,46,46	0
56	MG	RA	3341	1/1	0.95	0.16	-	31,31,31,31	0
56	MG	RA	3398	1/1	0.82	0.29	-	45,45,45,45	0
56	MG	RA	3070	1/1	0.92	0.32	-	25,25,25,25	0
56	MG	R5	101	1/1	0.95	0.32	-	14,14,14,14	0
56	MG	YA	3321	1/1	0.83	0.27	-	60,60,60,60	0
56	MG	YA	3215	1/1	0.58	0.29	-	79,79,79,79	0
56	MG	RA	3204	1/1	0.68	0.36	-	52,52,52,52	0
56	MG	YA	3482	1/1	0.73	0.42	-	69,69,69,69	0
56	MG	RA	3353	1/1	0.90	0.50	-	30,30,30,30	0
56	MG	QA	1748	1/1	0.92	0.37	-	47,47,47,47	0
56	MG	RA	3284	1/1	0.96	0.33	-	48,48,48,48	0
56	MG	RA	3101	1/1	0.87	0.35	-	37,37,37,37	0
56	MG	XA	1689	1/1	0.98	0.41	-	31,31,31,31	0
56	MG	YA	3074	1/1	0.96	0.54	-	21,21,21,21	0
56	MG	YA	3009	1/1	0.98	0.33	-	7,7,7,7	0
56	MG	XA	1760	1/1	0.94	0.28	-	47,47,47,47	0
56	MG	RA	3261	1/1	0.92	0.41	-	45,45,45,45	0
56	MG	YA	3223	1/1	0.71	0.37	-	60,60,60,60	0
56	MG	YA	3411	1/1	0.90	0.49	-	63,63,63,63	0
56	MG	YA	3267	1/1	0.94	0.16	-	32,32,32,32	0
56	MG	RA	3435	1/1	0.91	0.55	-	64,64,64,64	0
56	MG	YA	3402	1/1	0.75	0.25	-	70,70,70,70	0
56	MG	RA	3087	1/1	0.99	0.23	-	20,20,20,20	0
56	MG	RA	3260	1/1	0.97	0.37	-	22,22,22,22	0
56	MG	RA	3176	1/1	0.93	0.18	-	34,34,34,34	0
56	MG	RA	3273	1/1	0.96	0.18	-	44,44,44,44	0
56	MG	XA	1706	1/1	0.85	0.26	-	37,37,37,37	0
56	MG	RA	3378	1/1	0.98	0.37	-	2,2,2,2	0
56	MG	QA	1721	1/1	0.70	0.20	-	41,41,41,41	0
56	MG	YA	3040	1/1	0.93	0.29	-	25,25,25,25	0
56	MG	QA	1602	1/1	0.95	0.47	-	35,35,35,35	0
56	MG	XA	1630	1/1	0.73	0.20	-	40,40,40,40	0
56	MG	QA	1686	1/1	0.86	0.70	-	72,72,72,72	0
56	MG	YA	3364	1/1	0.92	0.80	-	50,50,50,50	0
56	MG	YA	3450	1/1	0.95	0.23	-	43,43,43,43	0
56	MG	QA	1627	1/1	0.61	0.80	-	72,72,72,72	0
56	MG	XA	1750	1/1	0.72	0.27	-	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3454	1/1	0.86	0.37	-	44,44,44,44	0
56	MG	QA	1649	1/1	0.95	0.23	-	31,31,31,31	0
56	MG	RA	3069	1/1	0.94	0.46	-	23,23,23,23	0
56	MG	XA	1615	1/1	0.96	0.31	-	37,37,37,37	0
56	MG	RA	3394	1/1	0.91	0.62	-	36,36,36,36	0
56	MG	QA	1705	1/1	0.92	0.24	-	37,37,37,37	0
56	MG	RA	3042	1/1	0.98	0.24	-	7,7,7,7	0
56	MG	YA	3257	1/1	0.94	0.24	-	36,36,36,36	0
56	MG	YB	203	1/1	0.92	0.33	-	27,27,27,27	0
56	MG	RA	3188	1/1	0.78	0.25	-	51,51,51,51	0
56	MG	YA	3160	1/1	0.96	0.27	-	25,25,25,25	0
56	MG	RA	3271	1/1	0.95	0.10	-	23,23,23,23	0
56	MG	QA	1633	1/1	0.98	0.42	-	23,23,23,23	0
56	MG	RA	3109	1/1	0.97	0.62	-	18,18,18,18	0
56	MG	RA	3257	1/1	0.96	0.13	-	25,25,25,25	0
56	MG	YA	3189	1/1	0.99	0.21	-	12,12,12,12	0
56	MG	XA	1649	1/1	0.99	0.14	-	12,12,12,12	0
56	MG	YE	301	1/1	0.98	0.15	-	4,4,4,4	0
56	MG	YA	3323	1/1	0.83	0.34	-	37,37,37,37	0
56	MG	YA	3346	1/1	0.92	0.13	-	54,54,54,54	0
56	MG	RA	3023	1/1	0.84	0.39	-	47,47,47,47	0
56	MG	YA	3039	1/1	0.98	0.51	-	14,14,14,14	0
56	MG	XA	1677	1/1	0.91	0.11	-	36,36,36,36	0
56	MG	YA	3281	1/1	0.91	0.13	-	27,27,27,27	0
56	MG	RA	3373	1/1	0.84	0.47	-	31,31,31,31	0
56	MG	XA	1722	1/1	0.90	0.15	-	38,38,38,38	0
56	MG	YA	3405	1/1	0.83	0.41	-	47,47,47,47	0
56	MG	RA	3214	1/1	0.84	0.33	-	33,33,33,33	0
56	MG	YA	3370	1/1	0.98	0.33	-	24,24,24,24	0
56	MG	XA	1756	1/1	0.86	0.25	-	61,61,61,61	0
56	MG	RA	3187	1/1	0.88	0.52	-	48,48,48,48	0
56	MG	QA	1689	1/1	0.93	0.45	-	42,42,42,42	0
56	MG	RA	3375	1/1	0.94	0.32	-	25,25,25,25	0
56	MG	XA	1727	1/1	0.79	1.21	-	78,78,78,78	0
56	MG	RA	3315	1/1	0.92	0.31	-	30,30,30,30	0
56	MG	YA	3395	1/1	0.77	0.20	-	46,46,46,46	0
56	MG	RA	3091	1/1	0.90	0.22	-	27,27,27,27	0
56	MG	RA	3015	1/1	0.96	0.28	-	9,9,9,9	0
56	MG	RA	3307	1/1	0.75	0.32	-	49,49,49,49	0
56	MG	YA	3182	1/1	0.73	0.28	-	58,58,58,58	0
56	MG	RA	3324	1/1	0.83	0.24	-	45,45,45,45	0
56	MG	YA	3057	1/1	0.99	0.33	-	3,3,3,3	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3216	1/1	0.92	0.28	-	13,13,13,13	0
56	MG	YA	3447	1/1	0.84	0.27	-	38,38,38,38	0
56	MG	YA	3125	1/1	0.97	0.22	-	13,13,13,13	0
56	MG	YA	3386	1/1	0.76	0.45	-	54,54,54,54	0
56	MG	RA	3255	1/1	0.96	0.27	-	38,38,38,38	0
56	MG	XA	1641	1/1	0.94	0.16	-	51,51,51,51	0
56	MG	YA	3188	1/1	0.80	0.36	-	38,38,38,38	0
56	MG	YA	3304	1/1	0.86	0.19	-	71,71,71,71	0
56	MG	YA	3085	1/1	0.96	0.36	-	17,17,17,17	0
56	MG	YA	3019	1/1	0.92	0.36	-	14,14,14,14	0
56	MG	XA	1705	1/1	0.89	0.63	-	38,38,38,38	0
56	MG	RA	3379	1/1	0.92	0.23	-	26,26,26,26	0
56	MG	YA	3117	1/1	0.93	0.35	-	14,14,14,14	0
56	MG	RA	3117	1/1	0.94	0.31	-	28,28,28,28	0
56	MG	QA	1694	1/1	0.92	0.22	-	27,27,27,27	0
56	MG	XA	1670	1/1	0.90	0.33	-	36,36,36,36	0
56	MG	YA	3087	1/1	0.98	0.20	-	14,14,14,14	0
56	MG	YA	3245	1/1	0.90	0.31	-	33,33,33,33	0
56	MG	RA	3299	1/1	0.51	0.44	-	48,48,48,48	0
56	MG	YA	3270	1/1	0.88	0.27	-	49,49,49,49	0
56	MG	RA	3422	1/1	0.74	0.29	-	43,43,43,43	0
56	MG	RA	3219	1/1	0.96	0.16	-	9,9,9,9	0
56	MG	YA	3273	1/1	0.97	0.18	-	24,24,24,24	0
56	MG	YA	3246	1/1	0.92	0.44	-	29,29,29,29	0
56	MG	RA	3421	1/1	0.86	0.21	-	59,59,59,59	0
56	MG	YA	3243	1/1	0.95	0.18	-	38,38,38,38	0
56	MG	YA	3178	1/1	0.93	0.17	-	36,36,36,36	0
56	MG	QA	1630	1/1	0.75	0.33	-	64,64,64,64	0
56	MG	RA	3327	1/1	0.96	0.12	-	46,46,46,46	0
56	MG	XA	1749	1/1	0.92	0.22	-	39,39,39,39	0
56	MG	YA	3251	1/1	0.93	0.16	-	54,54,54,54	0
56	MG	YA	3069	1/1	0.90	0.18	-	14,14,14,14	0
56	MG	YA	3043	1/1	0.97	0.24	-	9,9,9,9	0
56	MG	YA	3368	1/1	0.89	0.18	-	59,59,59,59	0
56	MG	R2	101	1/1	0.89	0.25	-	62,62,62,62	0
56	MG	XA	1676	1/1	0.96	0.15	-	32,32,32,32	0
56	MG	RA	3416	1/1	0.85	0.72	-	58,58,58,58	0
56	MG	QA	1610	1/1	0.95	0.12	-	60,60,60,60	0
56	MG	QX	101	1/1	0.97	0.23	-	17,17,17,17	0
56	MG	YA	3362	1/1	0.86	0.42	-	66,66,66,66	0
56	MG	RA	3305	1/1	0.76	0.35	-	42,42,42,42	0
56	MG	RA	3191	1/1	0.81	0.15	-	15,15,15,15	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3220	1/1	0.58	0.47	-	43,43,43,43	0
56	MG	YA	3366	1/1	0.83	0.19	-	64,64,64,64	0
56	MG	YA	3154	1/1	0.95	0.15	-	16,16,16,16	0
56	MG	YA	3438	1/1	0.86	0.22	-	68,68,68,68	0
56	MG	RA	3371	1/1	0.94	0.40	-	51,51,51,51	0
56	MG	YA	3409	1/1	0.99	0.39	-	10,10,10,10	0
56	MG	YA	3475	1/1	0.96	0.17	-	49,49,49,49	0
56	MG	RA	3190	1/1	0.92	0.37	-	19,19,19,19	0
56	MG	YA	3334	1/1	0.89	0.87	-	52,52,52,52	0
56	MG	RA	3029	1/1	0.96	0.24	-	16,16,16,16	0
56	MG	RA	3008	1/1	0.95	0.96	-	23,23,23,23	0
56	MG	RA	3212	1/1	0.95	0.34	-	18,18,18,18	0
56	MG	QA	1623	1/1	0.92	0.74	-	35,35,35,35	0
56	MG	R0	103	1/1	0.98	0.19	-	19,19,19,19	0
56	MG	QA	1646	1/1	0.93	0.37	-	36,36,36,36	0
56	MG	XA	1608	1/1	0.93	0.44	-	30,30,30,30	0
56	MG	RA	3403	1/1	0.94	0.29	-	43,43,43,43	0
56	MG	RA	3277	1/1	0.69	0.51	-	67,67,67,67	0
56	MG	RA	3113	1/1	0.97	0.11	-	17,17,17,17	0
56	MG	RA	3419	1/1	0.97	0.10	-	31,31,31,31	0
56	MG	YA	3367	1/1	0.96	0.29	-	30,30,30,30	0
56	MG	RA	3075	1/1	0.42	0.46	-	35,35,35,35	0
56	MG	RB	202	1/1	0.93	0.35	-	29,29,29,29	0
56	MG	RA	3340	1/1	0.86	0.43	-	72,72,72,72	0
56	MG	Y7	101	1/1	0.68	0.40	-	45,45,45,45	0
56	MG	YA	3142	1/1	0.94	0.32	-	14,14,14,14	0
56	MG	YA	3119	1/1	0.96	0.15	-	10,10,10,10	0
56	MG	YA	3441	1/1	0.85	0.18	-	49,49,49,49	0
56	MG	RA	3290	1/1	0.83	0.31	-	40,40,40,40	0
56	MG	RA	3267	1/1	0.90	0.21	-	28,28,28,28	0
56	MG	QA	1747	1/1	0.62	0.37	-	61,61,61,61	0
56	MG	XA	1710	1/1	0.88	0.28	-	48,48,48,48	0
56	MG	YA	3271	1/1	0.89	0.17	-	32,32,32,32	0
56	MG	RA	3313	1/1	0.93	0.42	-	20,20,20,20	0
56	MG	YA	3063	1/1	0.96	0.18	-	20,20,20,20	0
56	MG	QA	1665	1/1	0.79	0.14	-	51,51,51,51	0
56	MG	XA	1616	1/1	0.97	0.25	-	25,25,25,25	0
56	MG	QA	1697	1/1	0.93	0.53	-	30,30,30,30	0
56	MG	YA	3014	1/1	0.94	0.31	-	18,18,18,18	0
56	MG	YA	3145	1/1	0.92	0.13	-	68,68,68,68	0
56	MG	YA	3427	1/1	0.90	0.26	-	30,30,30,30	0
56	MG	YA	3385	1/1	0.92	0.40	-	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3288	1/1	0.74	0.26	-	54,54,54,54	0
56	MG	RA	3412	1/1	0.86	0.37	-	34,34,34,34	0
56	MG	YA	3262	1/1	0.92	0.33	-	36,36,36,36	0
56	MG	YA	3219	1/1	0.92	0.31	-	39,39,39,39	0
56	MG	YA	3285	1/1	0.81	0.36	-	26,26,26,26	0
56	MG	YA	3435	1/1	0.98	0.07	-	22,22,22,22	0
56	MG	QA	1713	1/1	0.92	0.28	-	38,38,38,38	0
56	MG	XA	1694	1/1	0.96	0.14	-	38,38,38,38	0
56	MG	YA	3383	1/1	0.86	0.26	-	34,34,34,34	0
56	MG	RA	3253	1/1	0.78	0.59	-	59,59,59,59	0
56	MG	XA	1696	1/1	0.61	0.34	-	71,71,71,71	0
56	MG	QA	1734	1/1	0.65	0.41	-	52,52,52,52	0
56	MG	YA	3015	1/1	0.96	0.27	-	9,9,9,9	0
56	MG	YA	3315	1/1	0.80	0.39	-	53,53,53,53	0
56	MG	RA	3093	1/1	0.85	0.11	-	27,27,27,27	0
56	MG	YA	3120	1/1	0.96	0.54	-	33,33,33,33	0
56	MG	XA	1746	1/1	0.92	0.15	-	47,47,47,47	0
56	MG	XA	1703	1/1	0.94	0.39	-	46,46,46,46	0
56	MG	YA	3047	1/1	0.91	0.42	-	10,10,10,10	0
56	MG	RA	3210	1/1	0.94	0.50	-	50,50,50,50	0
56	MG	YA	3076	1/1	0.98	0.17	-	26,26,26,26	0
56	MG	YA	3333	1/1	0.85	0.36	-	47,47,47,47	0
56	MG	RA	3147	1/1	0.89	0.21	-	41,41,41,41	0
56	MG	QA	1704	1/1	0.96	0.56	-	31,31,31,31	0
56	MG	YA	3297	1/1	0.95	0.45	-	35,35,35,35	0
56	MG	QA	1642	1/1	0.97	0.14	-	39,39,39,39	0
56	MG	XA	1685	1/1	0.93	0.50	-	38,38,38,38	0
56	MG	YA	3096	1/1	0.96	0.30	-	40,40,40,40	0
56	MG	YA	3393	1/1	0.92	0.49	-	21,21,21,21	0
56	MG	YA	3065	1/1	0.95	0.24	-	29,29,29,29	0
56	MG	YA	3328	1/1	0.86	0.46	-	38,38,38,38	0
56	MG	YA	3371	1/1	0.87	0.60	-	57,57,57,57	0
56	MG	RA	3297	1/1	0.95	0.34	-	47,47,47,47	0
56	MG	RA	3031	1/1	0.95	0.33	-	6,6,6,6	0
56	MG	QA	1647	1/1	0.74	0.27	-	55,55,55,55	0
56	MG	YA	3176	1/1	0.95	0.40	-	17,17,17,17	0
56	MG	Y5	102	1/1	0.57	0.55	-	47,47,47,47	0
56	MG	RA	3136	1/1	0.93	0.34	-	28,28,28,28	0
56	MG	YA	3172	1/1	0.88	0.13	-	53,53,53,53	0
56	MG	YA	3306	1/1	0.99	0.20	-	22,22,22,22	0
56	MG	YA	3112	1/1	0.95	0.14	-	14,14,14,14	0
56	MG	RA	3134	1/1	0.50	0.79	-	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	XA	1686	1/1	0.91	1.10	-	64,64,64,64	0
56	MG	YA	3265	1/1	0.91	0.26	-	40,40,40,40	0
56	MG	RA	3062	1/1	0.99	0.35	-	5,5,5,5	0
56	MG	YA	3252	1/1	0.94	0.50	-	47,47,47,47	0
56	MG	YA	3105	1/1	0.91	0.21	-	50,50,50,50	0
56	MG	RA	3323	1/1	0.94	0.07	-	38,38,38,38	0
56	MG	RA	3404	1/1	0.95	0.39	-	48,48,48,48	0
56	MG	RA	3344	1/1	0.96	0.13	-	15,15,15,15	0
56	MG	RA	3151	1/1	0.83	0.35	-	52,52,52,52	0
56	MG	YV	201	1/1	0.89	0.29	-	22,22,22,22	0
56	MG	QA	1698	1/1	0.94	0.13	-	41,41,41,41	0
56	MG	RA	3216	1/1	0.95	0.32	-	36,36,36,36	0
56	MG	RA	3252	1/1	0.89	0.26	-	21,21,21,21	0
56	MG	YA	3180	1/1	0.94	0.23	-	58,58,58,58	0
56	MG	RA	3395	1/1	0.97	0.40	-	27,27,27,27	0
56	MG	YA	3410	1/1	0.92	0.11	-	28,28,28,28	0
56	MG	YA	3384	1/1	0.78	0.40	-	64,64,64,64	0
56	MG	RA	3282	1/1	0.95	0.07	-	42,42,42,42	0
56	MG	YA	3229	1/1	0.86	0.49	-	43,43,43,43	0
56	MG	QA	1710	1/1	0.88	0.32	-	46,46,46,46	0
56	MG	XA	1651	1/1	0.95	0.21	-	25,25,25,25	0
56	MG	QA	1723	1/1	0.98	0.66	-	46,46,46,46	0
56	MG	YA	3098	1/1	0.90	0.23	-	47,47,47,47	0
56	MG	YA	3232	1/1	0.80	0.25	-	38,38,38,38	0
56	MG	YA	3114	1/1	0.94	0.20	-	20,20,20,20	0
56	MG	RA	3118	1/1	0.98	0.32	-	31,31,31,31	0
56	MG	RA	3285	1/1	0.91	0.32	-	28,28,28,28	0
56	MG	RA	3142	1/1	0.96	0.23	-	24,24,24,24	0
56	MG	RA	3224	1/1	0.94	0.19	-	19,19,19,19	0
56	MG	XA	1747	1/1	0.90	0.12	-	45,45,45,45	0
56	MG	YA	3247	1/1	0.94	0.29	-	41,41,41,41	0
56	MG	YA	3378	1/1	0.74	0.28	-	52,52,52,52	0
56	MG	RA	3396	1/1	0.91	0.24	-	37,37,37,37	0
56	MG	RA	3227	1/1	0.94	0.12	-	53,53,53,53	0
56	MG	RA	3158	1/1	0.79	0.28	-	61,61,61,61	0
56	MG	YA	3382	1/1	0.94	0.40	-	37,37,37,37	0
56	MG	YA	3048	1/1	0.90	0.28	-	22,22,22,22	0
56	MG	YA	3134	1/1	0.98	0.33	-	32,32,32,32	0
56	MG	YA	3351	1/1	0.86	0.24	-	42,42,42,42	0
56	MG	QA	1607	1/1	0.98	0.28	-	12,12,12,12	0
56	MG	QA	1652	1/1	0.91	0.19	-	23,23,23,23	0
56	MG	YA	3261	1/1	0.93	0.22	-	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3041	1/1	0.89	0.26	-	7,7,7,7	0
56	MG	RA	3246	1/1	0.92	0.24	-	25,25,25,25	0
56	MG	YA	3478	1/1	0.86	0.15	-	46,46,46,46	0
56	MG	XA	1626	1/1	0.96	0.34	-	22,22,22,22	0
56	MG	YA	3150	1/1	0.90	0.40	-	9,9,9,9	0
56	MG	RA	3302	1/1	0.92	0.14	-	46,46,46,46	0
56	MG	RA	3096	1/1	0.82	0.10	-	44,44,44,44	0
56	MG	XA	1654	1/1	0.89	0.49	-	42,42,42,42	0
56	MG	YA	3226	1/1	0.91	0.19	-	19,19,19,19	0
56	MG	QA	1677	1/1	0.81	0.12	-	60,60,60,60	0
56	MG	XA	1735	1/1	0.97	0.26	-	16,16,16,16	0
56	MG	XA	1619	1/1	0.98	0.15	-	12,12,12,12	0
56	MG	RA	3020	1/1	0.96	0.30	-	11,11,11,11	0
56	MG	YA	3307	1/1	0.86	0.34	-	46,46,46,46	0
56	MG	RA	3086	1/1	0.96	0.25	-	7,7,7,7	0
56	MG	RA	3146	1/1	0.82	0.21	-	26,26,26,26	0
56	MG	RA	3270	1/1	0.96	0.33	-	51,51,51,51	0
56	MG	RA	3010	1/1	0.97	0.41	-	14,14,14,14	0
56	MG	XA	1639	1/1	0.97	0.39	-	48,48,48,48	0
56	MG	RA	3097	1/1	0.91	0.31	-	48,48,48,48	0
56	MG	QA	1674	1/1	0.93	0.55	-	27,27,27,27	0
56	MG	RA	3169	1/1	0.89	0.31	-	47,47,47,47	0
56	MG	YA	3389	1/1	0.85	0.17	-	49,49,49,49	0
56	MG	YA	3124	1/1	0.97	0.23	-	8,8,8,8	0
56	MG	XA	1684	1/1	0.92	0.14	-	33,33,33,33	0
56	MG	RA	3276	1/1	0.85	0.25	-	50,50,50,50	0
56	MG	XA	1699	1/1	0.98	0.17	-	78,78,78,78	0
56	MG	QA	1621	1/1	0.91	0.16	-	29,29,29,29	0
56	MG	RA	3185	1/1	0.81	0.50	-	54,54,54,54	0
56	MG	YA	3089	1/1	0.97	0.51	-	7,7,7,7	0
56	MG	RA	3406	1/1	0.77	0.52	-	59,59,59,59	0
56	MG	YA	3279	1/1	0.92	0.13	-	54,54,54,54	0
56	MG	XA	1714	1/1	0.84	0.29	-	55,55,55,55	0
56	MG	YA	3390	1/1	0.85	0.16	-	54,54,54,54	0
56	MG	XA	1680	1/1	0.94	0.22	-	24,24,24,24	0
56	MG	RA	3356	1/1	0.84	0.10	-	39,39,39,39	0
56	MG	RA	3215	1/1	0.88	0.39	-	41,41,41,41	0
56	MG	XA	1724	1/1	0.83	0.20	-	33,33,33,33	0
56	MG	YW	201	1/1	0.93	0.53	-	52,52,52,52	0
56	MG	RA	3245	1/1	0.73	0.18	-	34,34,34,34	0
56	MG	RA	3391	1/1	0.58	0.43	-	19,19,19,19	0
56	MG	QA	1635	1/1	0.97	0.40	-	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3300	1/1	0.73	0.26	-	40,40,40,40	0
56	MG	RA	3429	1/1	0.94	0.25	-	50,50,50,50	0
56	MG	YA	3464	1/1	0.87	0.17	-	56,56,56,56	0
56	MG	XA	1737	1/1	0.94	0.47	-	14,14,14,14	0
56	MG	XA	1758	1/1	0.81	0.76	-	51,51,51,51	0
56	MG	RV	201	1/1	0.89	0.33	-	4,4,4,4	0
56	MG	RA	3236	1/1	0.94	0.43	-	45,45,45,45	0
56	MG	YA	3291	1/1	0.93	0.28	-	33,33,33,33	0
56	MG	XA	1657	1/1	0.97	0.23	-	31,31,31,31	0
56	MG	YA	3430	1/1	0.91	0.17	-	55,55,55,55	0
56	MG	RA	3044	1/1	0.96	0.32	-	1,1,1,1	0
56	MG	RA	3336	1/1	0.83	0.14	-	48,48,48,48	0
56	MG	YA	3036	1/1	0.97	0.38	-	10,10,10,10	0
56	MG	XA	1728	1/1	0.88	0.57	-	52,52,52,52	0
56	MG	RA	3335	1/1	0.94	0.34	-	52,52,52,52	0
56	MG	YA	3324	1/1	0.85	0.30	-	75,75,75,75	0
56	MG	YA	3374	1/1	0.96	0.18	-	28,28,28,28	0
56	MG	YA	3185	1/1	0.91	0.19	-	35,35,35,35	0
56	MG	QA	1695	1/1	0.81	0.54	-	47,47,47,47	0
56	MG	RA	3266	1/1	0.93	0.46	-	31,31,31,31	0
56	MG	RA	3268	1/1	0.82	0.58	-	48,48,48,48	0
56	MG	RA	3139	1/1	0.97	0.17	-	41,41,41,41	0
56	MG	RA	3239	1/1	0.89	0.58	-	45,45,45,45	0
56	MG	YA	3283	1/1	0.73	0.14	-	37,37,37,37	0
56	MG	XA	1655	1/1	0.95	0.18	-	39,39,39,39	0
56	MG	RA	3359	1/1	0.95	0.16	-	16,16,16,16	0
56	MG	RA	3054	1/1	0.95	0.36	-	11,11,11,11	0
56	MG	YA	3159	1/1	0.93	0.27	-	28,28,28,28	0
56	MG	YA	3453	1/1	0.84	0.19	-	35,35,35,35	0
56	MG	RA	3364	1/1	0.88	0.27	-	39,39,39,39	0
56	MG	QA	1746	1/1	0.61	0.49	-	56,56,56,56	0
56	MG	YA	3403	1/1	0.87	0.19	-	42,42,42,42	0
56	MG	RA	3171	1/1	0.52	0.40	-	51,51,51,51	0
56	MG	RA	3347	1/1	0.71	0.74	-	83,83,83,83	0
56	MG	YA	3110	1/1	0.88	0.14	-	29,29,29,29	0
56	MG	RA	3280	1/1	0.99	0.25	-	17,17,17,17	0
56	MG	YA	3278	1/1	0.82	0.46	-	52,52,52,52	0
56	MG	QA	1653	1/1	0.98	0.14	-	20,20,20,20	0
56	MG	QA	1731	1/1	0.79	0.13	-	34,34,34,34	0
56	MG	RA	3362	1/1	0.91	0.09	-	52,52,52,52	0
56	MG	YA	3322	1/1	0.53	0.45	-	55,55,55,55	0
56	MG	RA	3384	1/1	0.99	0.09	-	8,8,8,8	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3353	1/1	0.95	0.38	-	8,8,8,8	0
56	MG	RA	3397	1/1	0.82	0.22	-	49,49,49,49	0
56	MG	YA	3423	1/1	0.99	0.25	-	23,23,23,23	0
56	MG	YA	3345	1/1	0.83	0.42	-	38,38,38,38	0
56	MG	YA	3391	1/1	0.90	0.35	-	44,44,44,44	0
56	MG	QA	1708	1/1	0.92	0.60	-	42,42,42,42	0
56	MG	QA	1684	1/1	0.98	0.25	-	32,32,32,32	0
56	MG	RA	3200	1/1	0.96	0.46	-	31,31,31,31	0
56	MG	XA	1740	1/1	0.96	0.32	-	44,44,44,44	0
56	MG	RA	3167	1/1	0.92	0.21	-	54,54,54,54	0
56	MG	RA	3289	1/1	0.98	0.26	-	23,23,23,23	0
56	MG	RA	3168	1/1	0.45	0.72	-	54,54,54,54	0
56	MG	RA	3232	1/1	0.87	0.37	-	45,45,45,45	0
56	MG	RA	3106	1/1	0.94	0.20	-	57,57,57,57	0
56	MG	YA	3437	1/1	0.82	0.58	-	89,89,89,89	0
56	MG	YA	3357	1/1	0.45	0.74	-	53,53,53,53	0
56	MG	YA	3381	1/1	0.88	0.27	-	48,48,48,48	0
56	MG	QA	1629	1/1	0.89	0.46	-	26,26,26,26	0
56	MG	QA	1660	1/1	0.98	0.19	-	14,14,14,14	0
56	MG	YA	3360	1/1	0.84	0.33	-	44,44,44,44	0
56	MG	YA	3260	1/1	0.81	0.27	-	32,32,32,32	0
56	MG	YA	3317	1/1	0.76	0.56	-	48,48,48,48	0
56	MG	YA	3205	1/1	0.91	0.46	-	43,43,43,43	0
56	MG	XA	1729	1/1	0.91	0.34	-	47,47,47,47	0
56	MG	QA	1622	1/1	0.94	0.23	-	29,29,29,29	0
56	MG	YA	3086	1/1	0.94	0.18	-	23,23,23,23	0
56	MG	QA	1617	1/1	0.95	0.17	-	33,33,33,33	0
56	MG	YA	3177	1/1	0.94	0.35	-	35,35,35,35	0
56	MG	XA	1718	1/1	0.92	0.18	-	31,31,31,31	0
56	MG	YA	3166	1/1	0.92	0.40	-	24,24,24,24	0
56	MG	QA	1618	1/1	0.93	0.26	-	29,29,29,29	0
56	MG	XA	1702	1/1	0.85	0.66	-	46,46,46,46	0
56	MG	RT	201	1/1	0.95	0.13	-	44,44,44,44	0
56	MG	QA	1733	1/1	0.81	0.29	-	86,86,86,86	0
56	MG	RA	3293	1/1	0.97	0.39	-	58,58,58,58	0
56	MG	YA	3379	1/1	0.46	0.57	-	53,53,53,53	0
56	MG	XA	1629	1/1	0.86	0.25	-	53,53,53,53	0
56	MG	YA	3292	1/1	0.86	0.49	-	35,35,35,35	0
56	MG	XA	1698	1/1	0.94	0.11	-	44,44,44,44	0
56	MG	QA	1716	1/1	0.90	0.21	-	36,36,36,36	0
56	MG	RA	3249	1/1	0.73	0.24	-	47,47,47,47	0
56	MG	XA	1726	1/1	0.86	0.99	-	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	R1	101	1/1	0.91	0.42	-	46,46,46,46	0
56	MG	RA	3329	1/1	0.91	0.20	-	46,46,46,46	0
56	MG	RA	3401	1/1	0.84	0.19	-	41,41,41,41	0
56	MG	QV	102	1/1	0.90	0.26	-	28,28,28,28	0
56	MG	YA	3095	1/1	0.87	0.45	-	52,52,52,52	0
56	MG	RA	3414	1/1	0.91	0.30	-	54,54,54,54	0
56	MG	R0	102	1/1	0.95	0.61	-	39,39,39,39	0
56	MG	YA	3293	1/1	0.79	0.41	-	68,68,68,68	0
56	MG	QD	302	1/1	0.93	0.29	-	23,23,23,23	0
56	MG	QA	1736	1/1	0.96	0.19	-	33,33,33,33	0
56	MG	RA	3123	1/1	0.94	0.43	-	31,31,31,31	0
56	MG	RA	3144	1/1	0.95	0.21	-	10,10,10,10	0
56	MG	XA	1730	1/1	0.82	0.78	-	47,47,47,47	0
56	MG	RA	3248	1/1	0.94	0.37	-	38,38,38,38	0
56	MG	RA	3229	1/1	0.82	0.10	-	44,44,44,44	0
56	MG	XA	1733	1/1	0.70	0.17	-	47,47,47,47	0
56	MG	XA	1713	1/1	0.83	0.14	-	48,48,48,48	0
56	MG	XV	103	1/1	0.89	0.32	-	47,47,47,47	0
56	MG	RA	3077	1/1	0.98	0.35	-	16,16,16,16	0
56	MG	RA	3286	1/1	0.94	0.33	-	20,20,20,20	0
56	MG	YA	3242	1/1	0.90	0.53	-	42,42,42,42	0
56	MG	RA	3181	1/1	0.97	0.17	-	40,40,40,40	0
56	MG	YA	3187	1/1	0.89	0.32	-	19,19,19,19	0
56	MG	YA	3202	1/1	0.97	0.26	-	15,15,15,15	0
56	MG	YA	3068	1/1	0.71	0.46	-	32,32,32,32	0
56	MG	YA	3468	1/1	0.97	0.76	-	47,47,47,47	0
56	MG	XA	1751	1/1	0.92	0.31	-	70,70,70,70	0
56	MG	RA	3428	1/1	0.91	0.19	-	33,33,33,33	0
56	MG	YA	3135	1/1	0.98	0.20	-	14,14,14,14	0
56	MG	RA	3342	1/1	0.50	0.47	-	61,61,61,61	0
56	MG	YA	3020	1/1	0.98	0.22	-	18,18,18,18	0
56	MG	RA	3250	1/1	0.90	0.23	-	22,22,22,22	0
56	MG	RA	3345	1/1	0.59	0.31	-	42,42,42,42	0
56	MG	YA	3181	1/1	0.92	0.35	-	33,33,33,33	0
56	MG	YA	3398	1/1	0.79	0.28	-	55,55,55,55	0
56	MG	YA	3157	1/1	0.86	0.34	-	32,32,32,32	0
56	MG	QA	1720	1/1	0.81	0.28	-	53,53,53,53	0
56	MG	QA	1715	1/1	0.97	0.38	-	72,72,72,72	0
56	MG	RA	3294	1/1	0.95	0.12	-	10,10,10,10	0
56	MG	XV	102	1/1	0.92	0.22	-	34,34,34,34	0
56	MG	RA	3182	1/1	0.86	0.34	-	58,58,58,58	0
56	MG	RA	3201	1/1	0.95	0.07	-	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	XA	1720	1/1	0.98	0.17	-	44,44,44,44	0
56	MG	QA	1612	1/1	0.93	0.23	-	25,25,25,25	0
56	MG	RA	3231	1/1	0.97	0.15	-	50,50,50,50	0
56	MG	YA	3337	1/1	0.95	0.14	-	23,23,23,23	0
56	MG	YA	3301	1/1	0.85	0.26	-	34,34,34,34	0
56	MG	RA	3274	1/1	0.72	0.31	-	44,44,44,44	0
56	MG	RA	3143	1/1	0.92	0.14	-	58,58,58,58	0
56	MG	RA	3360	1/1	0.60	0.51	-	51,51,51,51	0
56	MG	YA	3053	1/1	0.97	0.49	-	27,27,27,27	0
56	MG	YA	3217	1/1	0.96	0.28	-	23,23,23,23	0
56	MG	RA	3124	1/1	0.96	0.24	-	32,32,32,32	0
56	MG	RA	3115	1/1	0.97	0.31	-	46,46,46,46	0
56	MG	YA	3417	1/1	0.95	0.47	-	22,22,22,22	0
56	MG	YA	3400	1/1	0.87	0.10	-	36,36,36,36	0
56	MG	YA	3034	1/1	0.98	0.33	-	21,21,21,21	0
56	MG	YA	3476	1/1	0.89	0.21	-	45,45,45,45	0
56	MG	YA	3023	1/1	0.99	0.44	-	2,2,2,2	0
56	MG	QA	1701	1/1	0.74	0.18	-	42,42,42,42	0
56	MG	XA	1602	1/1	0.97	0.44	-	8,8,8,8	0
56	MG	YA	3211	1/1	0.92	0.19	-	22,22,22,22	0
56	MG	RA	3043	1/1	0.95	0.35	-	17,17,17,17	0
56	MG	YA	3361	1/1	0.61	0.52	-	68,68,68,68	0
56	MG	YA	3326	1/1	0.92	0.60	-	51,51,51,51	0
56	MG	RA	3393	1/1	0.95	0.21	-	38,38,38,38	0
56	MG	XA	1647	1/1	0.94	0.20	-	47,47,47,47	0
56	MG	YA	3256	1/1	0.91	0.17	-	29,29,29,29	0
56	MG	RA	3230	1/1	0.90	0.43	-	20,20,20,20	0
56	MG	RA	3426	1/1	0.68	0.93	-	65,65,65,65	0
56	MG	YA	3061	1/1	0.98	0.37	-	0,0,0,0	0
56	MG	XA	1687	1/1	0.89	0.26	-	30,30,30,30	0
56	MG	RA	3119	1/1	0.96	0.17	-	8,8,8,8	0
56	MG	QA	1739	1/1	0.94	0.44	-	42,42,42,42	0
56	MG	YA	3140	1/1	0.83	0.21	-	58,58,58,58	0
56	MG	RA	3311	1/1	0.93	0.63	-	55,55,55,55	0
56	MG	XA	1712	1/1	0.98	0.33	-	34,34,34,34	0
56	MG	RA	3409	1/1	0.96	0.21	-	69,69,69,69	0
56	MG	YA	3344	1/1	0.72	0.51	-	35,35,35,35	0
56	MG	YA	3469	1/1	0.94	0.20	-	68,68,68,68	0
56	MG	RA	3354	1/1	0.88	0.31	-	34,34,34,34	0
56	MG	QA	1683	1/1	0.84	0.50	-	46,46,46,46	0
56	MG	YA	3480	1/1	0.83	0.15	-	65,65,65,65	0
56	MG	YA	3452	1/1	0.86	0.17	-	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3024	1/1	0.98	0.28	-	13,13,13,13	0
56	MG	YA	3207	1/1	0.98	0.19	-	13,13,13,13	0
56	MG	YB	202	1/1	0.85	0.27	-	38,38,38,38	0
56	MG	RA	3137	1/1	0.92	0.18	-	48,48,48,48	0
56	MG	YA	3045	1/1	0.95	0.23	-	3,3,3,3	0
56	MG	YA	3235	1/1	0.91	0.63	-	27,27,27,27	0
56	MG	YA	3487	1/1	0.97	0.34	-	18,18,18,18	0
56	MG	RA	3076	1/1	0.94	0.38	-	15,15,15,15	0
56	MG	YA	3272	1/1	0.93	0.26	-	26,26,26,26	0
56	MG	RA	3035	1/1	0.99	0.16	-	17,17,17,17	0
56	MG	XA	1752	1/1	0.97	0.14	-	44,44,44,44	0
56	MG	RA	3038	1/1	0.98	0.23	-	2,2,2,2	0
56	MG	XA	1725	1/1	0.85	0.31	-	44,44,44,44	0
56	MG	YA	3028	1/1	0.96	0.27	-	18,18,18,18	0
56	MG	QA	1634	1/1	0.86	0.20	-	41,41,41,41	0
56	MG	YA	3116	1/1	0.95	0.27	-	16,16,16,16	0
56	MG	YA	3477	1/1	0.94	0.35	-	38,38,38,38	0
56	MG	YA	3052	1/1	0.97	0.30	-	1,1,1,1	0
56	MG	RA	3333	1/1	0.90	0.30	-	35,35,35,35	0
56	MG	RA	3208	1/1	0.96	0.30	-	35,35,35,35	0
56	MG	RA	3389	1/1	0.90	0.10	-	22,22,22,22	0
56	MG	YA	3173	1/1	0.89	0.39	-	52,52,52,52	0
56	MG	RA	3272	1/1	0.93	0.12	-	46,46,46,46	0
56	MG	RA	3068	1/1	0.95	0.40	-	13,13,13,13	0
56	MG	RA	3199	1/1	0.84	0.65	-	39,39,39,39	0
56	MG	RA	3122	1/1	0.97	0.39	-	8,8,8,8	0
56	MG	XA	1678	1/1	0.92	0.34	-	41,41,41,41	0
56	MG	RA	3338	1/1	0.68	0.43	-	67,67,67,67	0
56	MG	RA	3241	1/1	0.93	0.31	-	27,27,27,27	0
56	MG	RA	3003	1/1	0.99	0.26	-	8,8,8,8	0
56	MG	YA	3376	1/1	0.83	0.20	-	38,38,38,38	0
56	MG	YA	3380	1/1	0.86	0.41	-	31,31,31,31	0
56	MG	YA	3196	1/1	0.67	0.27	-	35,35,35,35	0
56	MG	XA	1738	1/1	0.78	0.18	-	45,45,45,45	0
56	MG	RA	3256	1/1	0.85	0.41	-	93,93,93,93	0
56	MG	XA	1673	1/1	0.96	0.10	-	44,44,44,44	0
56	MG	YA	3277	1/1	0.90	0.31	-	38,38,38,38	0
56	MG	RA	3183	1/1	0.94	0.23	-	21,21,21,21	0
56	MG	RA	3392	1/1	0.82	0.28	-	36,36,36,36	0
56	MG	RA	3046	1/1	0.97	0.44	-	7,7,7,7	0
56	MG	YA	3350	1/1	0.90	0.15	-	22,22,22,22	0
56	MG	YA	3162	1/1	0.84	0.45	-	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3449	1/1	0.93	0.47	-	36,36,36,36	0
56	MG	QA	1672	1/1	0.95	0.65	-	54,54,54,54	0
56	MG	RA	3317	1/1	0.95	0.22	-	40,40,40,40	0
56	MG	QA	1743	1/1	0.85	0.10	-	57,57,57,57	0
56	MG	YA	3051	1/1	0.85	0.69	-	38,38,38,38	0
56	MG	YA	3254	1/1	0.95	0.40	-	26,26,26,26	0
56	MG	RA	3242	1/1	0.96	0.08	-	30,30,30,30	0
56	MG	RA	3100	1/1	0.83	0.30	-	52,52,52,52	0
56	MG	XA	1744	1/1	0.85	0.61	-	36,36,36,36	0
56	MG	YA	3290	1/1	0.68	0.37	-	82,82,82,82	0
56	MG	RA	3374	1/1	0.96	0.32	-	51,51,51,51	0
56	MG	RA	3036	1/1	0.96	0.30	-	26,26,26,26	0
56	MG	YA	3193	1/1	0.94	0.17	-	18,18,18,18	0
56	MG	RA	3194	1/1	0.97	0.38	-	21,21,21,21	0
56	MG	RA	3049	1/1	0.95	0.37	-	19,19,19,19	0
56	MG	YA	3269	1/1	0.93	0.33	-	30,30,30,30	0
56	MG	RA	3309	1/1	0.96	0.74	-	45,45,45,45	0
56	MG	YA	3126	1/1	0.98	0.27	-	10,10,10,10	0
56	MG	QA	1707	1/1	0.85	0.61	-	57,57,57,57	0
56	MG	YA	3194	1/1	0.97	0.28	-	17,17,17,17	0
56	MG	QA	1648	1/1	0.90	0.12	-	58,58,58,58	0
56	MG	RA	3304	1/1	0.95	0.35	-	37,37,37,37	0
56	MG	RA	3415	1/1	0.90	0.18	-	53,53,53,53	0
56	MG	YY	201	1/1	0.94	0.20	-	31,31,31,31	0
56	MG	RA	3217	1/1	0.98	0.19	-	27,27,27,27	0
56	MG	YA	3197	1/1	0.96	0.38	-	22,22,22,22	0
56	MG	RA	3423	1/1	0.89	0.38	-	42,42,42,42	0
56	MG	QA	1650	1/1	0.88	0.44	-	19,19,19,19	0
56	MG	Y0	103	1/1	0.87	0.33	-	27,27,27,27	0
56	MG	QA	1692	1/1	0.81	0.45	-	65,65,65,65	0
56	MG	XA	1621	1/1	0.86	0.22	-	38,38,38,38	0
56	MG	YA	3174	1/1	0.98	0.15	-	15,15,15,15	0
56	MG	XL	201	1/1	0.84	0.17	-	45,45,45,45	0
56	MG	XA	1660	1/1	0.95	0.38	-	37,37,37,37	0
56	MG	YA	3287	1/1	0.83	0.36	-	47,47,47,47	0
56	MG	YA	3343	1/1	0.90	0.21	-	64,64,64,64	0
56	MG	YA	3412	1/1	0.87	0.16	-	61,61,61,61	0
56	MG	XA	1693	1/1	0.83	0.14	-	36,36,36,36	0
56	MG	RA	3330	1/1	0.94	0.15	-	43,43,43,43	0
56	MG	RA	3223	1/1	0.95	0.25	-	26,26,26,26	0
56	MG	RA	3078	1/1	0.97	0.41	-	14,14,14,14	0
56	MG	XA	1759	1/1	0.72	0.66	-	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3199	1/1	0.91	0.29	-	45,45,45,45	0
56	MG	QA	1700	1/1	0.97	0.56	-	31,31,31,31	0
56	MG	RA	3418	1/1	0.92	0.35	-	28,28,28,28	0
56	MG	RA	3098	1/1	0.94	0.38	-	44,44,44,44	0
56	MG	YA	3077	1/1	0.97	0.42	-	16,16,16,16	0
56	MG	XA	1681	1/1	0.97	0.35	-	22,22,22,22	0
56	MG	RA	3130	1/1	0.98	0.29	-	12,12,12,12	0
56	MG	RA	3387	1/1	0.97	0.42	-	16,16,16,16	0
56	MG	YA	3129	1/1	0.93	0.35	-	41,41,41,41	0
56	MG	YB	204	1/1	0.92	0.09	-	49,49,49,49	0
56	MG	QA	1657	1/1	0.98	0.17	-	20,20,20,20	0
56	MG	QA	1732	1/1	0.94	0.08	-	54,54,54,54	0
56	MG	XA	1688	1/1	0.84	0.59	-	41,41,41,41	0
56	MG	YA	3094	1/1	0.91	0.08	-	43,43,43,43	0
56	MG	RA	3381	1/1	0.98	0.46	-	0,0,0,0	0
56	MG	YA	3332	1/1	0.90	0.47	-	25,25,25,25	0
56	MG	YA	3001	1/1	0.70	0.94	-	73,73,73,73	0
56	MG	Y5	101	1/1	0.97	0.17	-	22,22,22,22	0
56	MG	QA	1631	1/1	0.95	0.38	-	33,33,33,33	0
56	MG	XA	1661	1/1	0.97	0.30	-	23,23,23,23	0
56	MG	YA	3481	1/1	0.90	0.50	-	44,44,44,44	0
56	MG	RA	3319	1/1	0.94	0.14	-	50,50,50,50	0
56	MG	RA	3388	1/1	0.96	0.47	-	15,15,15,15	0
56	MG	RA	3402	1/1	0.87	0.53	-	57,57,57,57	0
56	MG	XA	1716	1/1	0.98	0.37	-	25,25,25,25	0
56	MG	RA	3019	1/1	0.98	0.27	-	17,17,17,17	0
56	MG	RA	3383	1/1	0.91	0.78	-	44,44,44,44	0
56	MG	XA	1709	1/1	0.99	0.50	-	23,23,23,23	0
56	MG	RA	3287	1/1	0.97	0.09	-	17,17,17,17	0
56	MG	YA	3258	1/1	0.93	0.09	-	46,46,46,46	0
56	MG	XA	1711	1/1	0.91	0.45	-	39,39,39,39	0
56	MG	RA	3312	1/1	0.92	0.49	-	26,26,26,26	0
56	MG	RA	3361	1/1	0.96	0.55	-	52,52,52,52	0
56	MG	XA	1674	1/1	0.96	0.24	-	32,32,32,32	0
56	MG	RA	3058	1/1	0.99	0.29	-	1,1,1,1	0
56	MG	QA	1690	1/1	0.98	0.09	-	27,27,27,27	0
56	MG	RA	3234	1/1	0.96	0.15	-	23,23,23,23	0
56	MG	YA	3479	1/1	0.92	0.13	-	52,52,52,52	0
56	MG	YA	3309	1/1	0.91	0.16	-	30,30,30,30	0
56	MG	RA	3303	1/1	0.89	0.24	-	34,34,34,34	0
56	MG	YA	3299	1/1	0.96	0.29	-	23,23,23,23	0
56	MG	YA	3148	1/1	0.98	0.31	-	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3118	1/1	0.88	0.34	-	27,27,27,27	0
56	MG	QA	1658	1/1	0.94	0.91	-	46,46,46,46	0
56	MG	YA	3465	1/1	0.95	0.09	-	41,41,41,41	0
56	MG	RA	3400	1/1	0.90	0.24	-	30,30,30,30	0
56	MG	YA	3483	1/1	0.96	0.96	-	58,58,58,58	0
56	MG	RA	3089	1/1	0.91	0.29	-	18,18,18,18	0
56	MG	QA	1661	1/1	0.94	0.12	-	23,23,23,23	0
56	MG	RA	3278	1/1	0.95	0.42	-	46,46,46,46	0
56	MG	YA	3213	1/1	0.94	0.38	-	33,33,33,33	0
56	MG	QA	1638	1/1	0.94	0.39	-	64,64,64,64	0
56	MG	RA	3308	1/1	0.94	0.28	-	47,47,47,47	0
56	MG	XA	1606	1/1	0.99	0.29	-	14,14,14,14	0
56	MG	YA	3404	1/1	0.99	0.35	-	20,20,20,20	0
56	MG	XA	1739	1/1	0.84	0.26	-	51,51,51,51	0
56	MG	XA	1610	1/1	0.98	0.22	-	15,15,15,15	0
56	MG	YA	3230	1/1	0.97	0.32	-	38,38,38,38	0
56	MG	XA	1668	1/1	0.98	0.44	-	20,20,20,20	0
56	MG	RA	3114	1/1	0.61	0.31	-	19,19,19,19	0
56	MG	XA	1637	1/1	0.94	0.17	-	49,49,49,49	0
56	MG	XA	1715	1/1	0.87	0.43	-	52,52,52,52	0
56	MG	RA	3092	1/1	0.87	0.45	-	41,41,41,41	0
56	MG	XA	1631	1/1	0.93	0.36	-	14,14,14,14	0
56	MG	XA	1622	1/1	0.90	0.76	-	37,37,37,37	0
56	MG	RA	3349	1/1	0.86	0.60	-	55,55,55,55	0
56	MG	RA	3192	1/1	0.99	0.47	-	15,15,15,15	0
56	MG	YA	3310	1/1	0.94	0.44	-	28,28,28,28	0
56	MG	RA	3090	1/1	0.96	0.42	-	4,4,4,4	0
56	MG	YA	3169	1/1	0.88	0.25	-	20,20,20,20	0
56	MG	YA	3179	1/1	0.94	0.40	-	41,41,41,41	0
56	MG	QA	1722	1/1	0.86	0.14	-	52,52,52,52	0
56	MG	RA	3301	1/1	0.96	0.18	-	41,41,41,41	0
56	MG	YA	3198	1/1	0.94	0.27	-	17,17,17,17	0
56	MG	RA	3352	1/1	0.81	0.48	-	62,62,62,62	0
56	MG	QA	1745	1/1	0.81	0.27	-	44,44,44,44	0
56	MG	RA	3262	1/1	0.95	0.12	-	48,48,48,48	0
56	MG	YA	3433	1/1	0.93	0.20	-	34,34,34,34	0
56	MG	RA	3211	1/1	0.86	0.14	-	11,11,11,11	0
56	MG	RA	3258	1/1	0.86	0.33	-	51,51,51,51	0
56	MG	XA	1612	1/1	0.94	0.14	-	39,39,39,39	0
56	MG	YH	201	1/1	0.15	0.61	-	118,118,118,118	0
56	MG	YA	3139	1/1	0.96	0.28	-	36,36,36,36	0
56	MG	RA	3320	1/1	0.73	0.62	-	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3143	1/1	0.96	0.19	-	23,23,23,23	0
56	MG	YA	3377	1/1	0.95	0.22	-	47,47,47,47	0
56	MG	YA	3037	1/1	0.99	0.36	-	10,10,10,10	0
56	MG	XA	1628	1/1	0.97	0.49	-	44,44,44,44	0
56	MG	YA	3296	1/1	0.91	0.23	-	51,51,51,51	0
56	MG	RA	3180	1/1	0.88	0.26	-	53,53,53,53	0
56	MG	RA	3410	1/1	0.91	0.36	-	70,70,70,70	0
56	MG	YA	3107	1/1	0.94	0.42	-	14,14,14,14	0
56	MG	RA	3413	1/1	0.75	0.38	-	63,63,63,63	0
56	MG	XA	1636	1/1	0.94	0.26	-	57,57,57,57	0
56	MG	YA	3007	1/1	0.96	1.05	-	38,38,38,38	0
56	MG	YA	3396	1/1	0.68	0.27	-	54,54,54,54	0
56	MG	XA	1662	1/1	0.90	0.28	-	44,44,44,44	0
56	MG	YA	3358	1/1	0.92	0.33	-	27,27,27,27	0
56	MG	XA	1757	1/1	0.84	0.61	-	60,60,60,60	0
56	MG	YA	3163	1/1	0.63	0.55	-	40,40,40,40	0
56	MG	YA	3419	1/1	0.98	0.23	-	2,2,2,2	0
56	MG	XA	1721	1/1	0.87	0.21	-	52,52,52,52	0
56	MG	YA	3348	1/1	0.94	0.23	-	30,30,30,30	0
56	MG	XA	1671	1/1	0.96	0.11	-	0,0,0,0	0
56	MG	RA	3433	1/1	0.92	0.22	-	39,39,39,39	0
56	MG	QA	1664	1/1	0.98	0.21	-	17,17,17,17	0
56	MG	YA	3067	1/1	0.98	0.38	-	19,19,19,19	0
56	MG	YA	3313	1/1	0.85	0.48	-	25,25,25,25	0
56	MG	RA	3160	1/1	0.94	0.39	-	31,31,31,31	0
56	MG	YA	3222	1/1	0.92	0.35	-	25,25,25,25	0
56	MG	YA	3149	1/1	0.78	0.40	-	54,54,54,54	0
56	MG	YA	3436	1/1	0.80	0.58	-	51,51,51,51	0
56	MG	RA	3186	1/1	0.81	0.19	-	45,45,45,45	0
56	MG	XA	1632	1/1	0.94	0.27	-	46,46,46,46	0
56	MG	RA	3196	1/1	0.95	0.39	-	18,18,18,18	0
56	MG	RA	3408	1/1	0.87	0.44	-	53,53,53,53	0
56	MG	XA	1665	1/1	0.93	0.40	-	26,26,26,26	0
56	MG	RA	3156	1/1	0.94	0.09	-	30,30,30,30	0
56	MG	YA	3115	1/1	0.95	0.36	-	40,40,40,40	0
56	MG	XA	1704	1/1	0.91	0.13	-	46,46,46,46	0
56	MG	YA	3153	1/1	0.71	0.40	-	37,37,37,37	0
56	MG	XA	1646	1/1	0.84	0.49	-	64,64,64,64	0
56	MG	YA	3432	1/1	0.69	0.58	-	78,78,78,78	0
56	MG	YA	3266	1/1	0.95	0.25	-	42,42,42,42	0
56	MG	YA	3363	1/1	0.87	0.52	-	56,56,56,56	0
56	MG	XA	1707	1/1	0.94	0.67	-	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	QA	1669	1/1	0.77	0.18	-	71,71,71,71	0
56	MG	YA	3330	1/1	0.91	0.23	-	31,31,31,31	0
56	MG	RA	3314	1/1	0.93	0.33	-	19,19,19,19	0
56	MG	RA	3328	1/1	0.82	0.37	-	42,42,42,42	0
56	MG	YA	3329	1/1	0.85	0.48	-	45,45,45,45	0
56	MG	RA	3152	1/1	0.90	0.44	-	19,19,19,19	0
56	MG	Y0	102	1/1	0.90	0.11	-	37,37,37,37	0
56	MG	YA	3446	1/1	0.99	0.26	-	20,20,20,20	0
56	MG	RA	3145	1/1	0.97	0.25	-	9,9,9,9	0
56	MG	RA	3322	1/1	0.93	0.12	-	15,15,15,15	0
56	MG	YA	3241	1/1	0.95	0.25	-	33,33,33,33	0
56	MG	YA	3349	1/1	0.89	0.34	-	24,24,24,24	0
56	MG	YA	3231	1/1	0.83	0.20	-	30,30,30,30	0
56	MG	RA	3207	1/1	0.98	0.21	-	18,18,18,18	0
56	MG	RA	3380	1/1	0.67	0.20	-	61,61,61,61	0
56	MG	YA	3141	1/1	0.89	0.26	-	24,24,24,24	0
56	MG	YA	3004	1/1	0.91	0.36	-	12,12,12,12	0
56	MG	XA	1700	1/1	0.82	0.45	-	79,79,79,79	0
56	MG	RA	3064	1/1	0.99	0.23	-	18,18,18,18	0
56	MG	YA	3132	1/1	0.77	0.65	-	60,60,60,60	0
56	MG	XA	1719	1/1	0.82	0.24	-	50,50,50,50	0
56	MG	RA	3021	1/1	0.97	0.21	-	4,4,4,4	0
56	MG	YA	3319	1/1	0.83	0.21	-	47,47,47,47	0
56	MG	RA	3005	1/1	0.98	0.66	-	32,32,32,32	0
56	MG	YA	3022	1/1	0.95	0.53	-	49,49,49,49	0
56	MG	YO	201	1/1	0.83	0.24	-	49,49,49,49	0
56	MG	YA	3308	1/1	0.86	0.38	-	26,26,26,26	0
56	MG	YA	3123	1/1	0.95	0.36	-	30,30,30,30	0
56	MG	RA	3120	1/1	0.84	0.89	-	40,40,40,40	0
56	MG	YA	3195	1/1	0.90	0.17	-	51,51,51,51	0
56	MG	R0	101	1/1	0.84	0.44	-	44,44,44,44	0
56	MG	YA	3288	1/1	0.97	0.19	-	25,25,25,25	0
56	MG	QA	1680	1/1	0.86	0.31	-	48,48,48,48	0
56	MG	RA	3084	1/1	0.92	0.19	-	27,27,27,27	0
56	MG	XA	1658	1/1	0.76	0.15	-	35,35,35,35	0
56	MG	RA	3372	1/1	0.95	0.20	-	7,7,7,7	0
56	MG	RA	3138	1/1	0.95	0.29	-	10,10,10,10	0
56	MG	XA	1663	1/1	0.94	0.24	-	30,30,30,30	0
56	MG	XA	1666	1/1	0.91	0.26	-	39,39,39,39	0
56	MG	RA	3332	1/1	0.74	0.31	-	40,40,40,40	0
56	MG	YA	3311	1/1	0.89	0.27	-	74,74,74,74	0
56	MG	YA	3408	1/1	0.82	0.14	-	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	Y0	101	1/1	0.97	0.13	-	18,18,18,18	0
56	MG	XA	1648	1/1	0.90	0.24	-	53,53,53,53	0
56	MG	YA	3415	1/1	0.49	0.52	-	68,68,68,68	0
56	MG	YA	3100	1/1	0.98	0.28	-	3,3,3,3	0
56	MG	RA	3325	1/1	0.86	0.28	-	46,46,46,46	0
56	MG	YA	3083	1/1	0.89	0.24	-	58,58,58,58	0
56	MG	YA	3331	1/1	0.94	0.20	-	24,24,24,24	0
56	MG	QA	1620	1/1	0.95	0.15	-	13,13,13,13	0
56	MG	QA	1616	1/1	0.94	0.19	-	29,29,29,29	0
56	MG	QA	1679	1/1	0.93	0.20	-	34,34,34,34	0
56	MG	QA	1718	1/1	0.93	0.34	-	47,47,47,47	0
56	MG	YA	3302	1/1	0.76	0.30	-	51,51,51,51	0
56	MG	RA	3441	1/1	0.96	0.28	-	14,14,14,14	0
56	MG	RA	3126	1/1	0.95	0.20	-	31,31,31,31	0
56	MG	YA	3470	1/1	0.95	0.27	-	35,35,35,35	0
56	MG	RA	3366	1/1	0.93	0.24	-	67,67,67,67	0
56	MG	YA	3274	1/1	0.98	0.41	-	35,35,35,35	0
56	MG	RA	3399	1/1	0.86	0.60	-	47,47,47,47	0
56	MG	YA	3184	1/1	0.84	0.30	-	28,28,28,28	0
56	MG	YA	3352	1/1	0.92	0.13	-	35,35,35,35	0
56	MG	QA	1655	1/1	0.98	0.44	-	31,31,31,31	0
56	MG	YA	3113	1/1	0.98	0.28	-	25,25,25,25	0
56	MG	YA	3300	1/1	0.97	0.33	-	48,48,48,48	0
56	MG	XA	1708	1/1	0.97	0.27	-	32,32,32,32	0
56	MG	YA	3448	1/1	0.70	0.40	-	51,51,51,51	0
56	MG	QA	1714	1/1	0.98	0.13	-	25,25,25,25	0
56	MG	QA	1727	1/1	0.87	0.35	-	43,43,43,43	0
56	MG	RA	3088	1/1	0.97	0.20	-	27,27,27,27	0
56	MG	RA	3417	1/1	0.57	0.36	-	66,66,66,66	0
56	MG	YA	3466	1/1	0.89	0.43	-	49,49,49,49	0
56	MG	YA	3158	1/1	0.98	0.28	-	40,40,40,40	0
56	MG	QA	1696	1/1	0.75	0.91	-	67,67,67,67	0
56	MG	YA	3443	1/1	0.92	0.14	-	17,17,17,17	0
56	MG	RA	3127	1/1	0.86	0.62	-	52,52,52,52	0
56	MG	YA	3152	1/1	0.65	0.33	-	54,54,54,54	0
56	MG	QA	1675	1/1	0.88	0.12	-	42,42,42,42	0
56	MG	RA	3334	1/1	0.92	0.65	-	40,40,40,40	0
56	MG	RA	3102	1/1	0.73	0.34	-	10,10,10,10	0
56	MG	YA	3355	1/1	0.81	0.49	-	63,63,63,63	0
56	MG	XA	1669	1/1	0.94	0.30	-	29,29,29,29	0
56	MG	YA	3002	1/1	0.95	0.15	-	0,0,0,0	0
56	MG	QA	1603	1/1	0.78	0.23	-	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3259	1/1	0.84	0.44	-	46,46,46,46	0
56	MG	XA	1675	1/1	0.81	0.91	-	46,46,46,46	0
56	MG	YA	3225	1/1	0.77	0.23	-	17,17,17,17	0
56	MG	YA	3439	1/1	0.85	0.11	-	43,43,43,43	0
56	MG	RA	3178	1/1	0.96	0.21	-	32,32,32,32	0
56	MG	YA	3365	1/1	0.96	0.40	-	22,22,22,22	0
56	MG	YA	3253	1/1	0.88	0.28	-	19,19,19,19	0
56	MG	RA	3226	1/1	0.88	0.39	-	33,33,33,33	0
56	MG	YA	3175	1/1	0.96	0.08	-	30,30,30,30	0
56	MG	RA	3218	1/1	0.95	0.21	-	13,13,13,13	0
56	MG	YA	3451	1/1	0.97	0.17	-	38,38,38,38	0
56	MG	YA	3075	1/1	0.92	0.29	-	8,8,8,8	0
56	MG	RA	3025	1/1	0.98	0.21	-	12,12,12,12	0
56	MG	YA	3168	1/1	0.96	0.30	-	19,19,19,19	0
56	MG	XA	1617	1/1	0.92	0.39	-	49,49,49,49	0
56	MG	RA	3382	1/1	0.95	0.27	-	28,28,28,28	0
56	MG	YA	3320	1/1	0.96	0.12	-	38,38,38,38	0
56	MG	XA	1645	1/1	0.93	0.31	-	35,35,35,35	0
56	MG	RA	3358	1/1	0.90	0.16	-	45,45,45,45	0
56	MG	RY	201	1/1	0.75	0.43	-	43,43,43,43	0
56	MG	QA	1724	1/1	0.62	0.20	-	63,63,63,63	0
56	MG	YA	3183	1/1	0.74	0.24	-	49,49,49,49	0
56	MG	RA	3040	1/1	0.97	0.47	-	4,4,4,4	0
56	MG	XA	1683	1/1	0.82	0.29	-	31,31,31,31	0
56	MG	YA	3369	1/1	0.94	0.16	-	35,35,35,35	0
56	MG	RA	3265	1/1	0.83	0.23	-	29,29,29,29	0
56	MG	YA	3457	1/1	0.91	0.20	-	49,49,49,49	0
56	MG	YA	3165	1/1	0.92	0.29	-	34,34,34,34	0
56	MG	YA	3422	1/1	0.73	0.14	-	58,58,58,58	0
56	MG	YA	3388	1/1	0.87	0.28	-	28,28,28,28	0
56	MG	YA	3314	1/1	0.95	0.14	-	47,47,47,47	0
56	MG	RB	203	1/1	0.89	0.32	-	37,37,37,37	0
56	MG	YA	3359	1/1	0.93	0.15	-	42,42,42,42	0
56	MG	QA	1706	1/1	0.72	0.36	-	52,52,52,52	0
56	MG	YA	3399	1/1	0.96	0.08	-	57,57,57,57	0
56	MG	RA	3112	1/1	0.98	0.08	-	22,22,22,22	0
56	MG	YA	3458	1/1	0.92	0.14	-	51,51,51,51	0
56	MG	YA	3030	1/1	0.97	0.31	-	3,3,3,3	0
56	MG	YA	3144	1/1	0.93	0.17	-	24,24,24,24	0
56	MG	QA	1737	1/1	0.87	0.25	-	43,43,43,43	0
56	MG	RE	301	1/1	0.98	0.28	-	1,1,1,1	0
56	MG	RA	3269	1/1	0.95	0.40	-	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3406	1/1	0.63	0.56	-	60,60,60,60	0
56	MG	RB	201	1/1	0.87	0.35	-	28,28,28,28	0
56	MG	RA	3170	1/1	0.85	0.42	-	26,26,26,26	0
56	MG	RA	3321	1/1	0.96	0.27	-	33,33,33,33	0
56	MG	YA	3236	1/1	0.97	0.33	-	14,14,14,14	0
56	MG	YA	3035	1/1	0.93	0.15	-	29,29,29,29	0
56	MG	QA	1676	1/1	0.96	0.31	-	31,31,31,31	0
56	MG	YA	3341	1/1	0.74	0.75	-	71,71,71,71	0
56	MG	QA	1740	1/1	0.93	0.51	-	49,49,49,49	0
56	MG	YA	3394	1/1	0.74	0.26	-	64,64,64,64	0
56	MG	YA	3268	1/1	0.89	0.75	-	49,49,49,49	0
56	MG	RA	3221	1/1	0.97	0.28	-	22,22,22,22	0
56	MG	XA	1633	1/1	0.96	0.33	-	25,25,25,25	0
56	MG	YA	3354	1/1	0.75	0.34	-	50,50,50,50	0
56	MG	QA	1663	1/1	0.81	1.39	-	68,68,68,68	0
56	MG	YA	3318	1/1	0.83	0.54	-	43,43,43,43	0
56	MG	QA	1659	1/1	0.93	0.28	-	25,25,25,25	0
56	MG	RA	3017	1/1	0.92	0.12	-	17,17,17,17	0
56	MG	QA	1671	1/1	0.87	0.38	-	43,43,43,43	0
56	MG	RA	3175	1/1	0.80	0.20	-	46,46,46,46	0
56	MG	RA	3024	1/1	0.98	0.47	-	7,7,7,7	0
56	MG	YB	206	1/1	0.88	0.13	-	48,48,48,48	0
56	MG	QA	1702	1/1	0.76	0.30	-	81,81,81,81	0
56	MG	YB	201	1/1	0.99	0.36	-	31,31,31,31	0
56	MG	QA	1691	1/1	0.94	0.33	-	20,20,20,20	0
56	MG	QA	1709	1/1	0.82	0.42	-	36,36,36,36	0
56	MG	RA	3154	1/1	0.90	0.21	-	41,41,41,41	0
56	MG	YA	3303	1/1	0.86	0.45	-	69,69,69,69	0
56	MG	YA	3342	1/1	0.82	0.52	-	66,66,66,66	0
56	MG	YA	3372	1/1	0.91	0.17	-	37,37,37,37	0
56	MG	YA	3041	1/1	0.94	0.31	-	30,30,30,30	0
56	MG	QA	1711	1/1	0.91	0.37	-	53,53,53,53	0
56	MG	YA	3373	1/1	0.96	0.26	-	35,35,35,35	0
56	MG	RA	3390	1/1	0.95	0.32	-	49,49,49,49	0
56	MG	YA	3387	1/1	0.87	0.21	-	27,27,27,27	0
56	MG	XA	1691	1/1	0.83	0.18	-	50,50,50,50	0
56	MG	RA	3150	1/1	0.95	0.40	-	40,40,40,40	0
56	MG	RA	3348	1/1	0.98	0.34	-	45,45,45,45	0
56	MG	YA	3289	1/1	0.94	0.25	-	44,44,44,44	0
56	MG	YA	3091	1/1	0.89	0.20	-	19,19,19,19	0
56	MG	YA	3445	1/1	0.97	0.10	-	19,19,19,19	0
56	MG	RQ	201	1/1	0.82	0.40	-	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3312	1/1	0.97	0.39	-	63,63,63,63	0
56	MG	QA	1735	1/1	0.90	0.56	-	66,66,66,66	0
56	MG	RA	3179	1/1	0.96	0.40	-	30,30,30,30	0
56	MG	YA	3214	1/1	0.88	0.71	-	53,53,53,53	0
56	MG	YA	3263	1/1	0.77	0.34	-	41,41,41,41	0
56	MG	YA	3440	1/1	0.83	0.30	-	62,62,62,62	0
56	MG	RA	3346	1/1	0.93	0.34	-	37,37,37,37	0
56	MG	YA	3461	1/1	0.93	0.15	-	37,37,37,37	0
56	MG	RA	3326	1/1	0.72	0.42	-	56,56,56,56	0
56	MG	XA	1753	1/1	0.94	0.28	-	70,70,70,70	0
56	MG	YA	3275	1/1	0.94	0.34	-	41,41,41,41	0
56	MG	YA	3316	1/1	0.98	0.11	-	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.