



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 6, 2023 – 12:37 AM EST

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

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

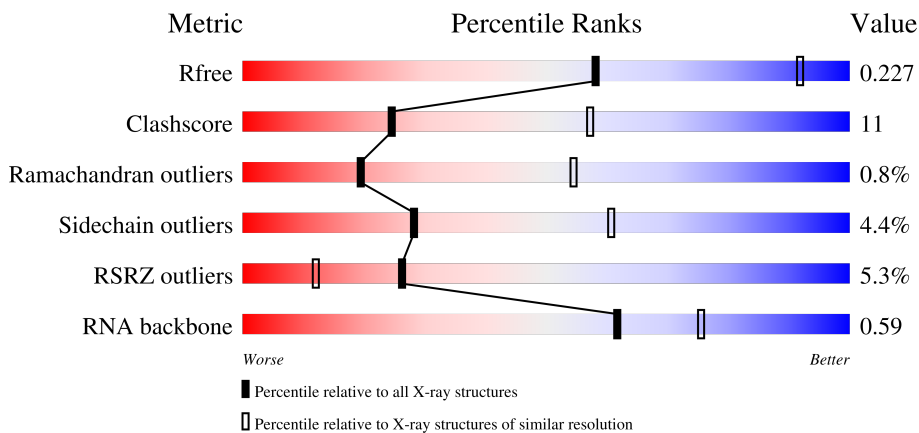
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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

Mol	Chain	Length	Quality of chain
1	QV	77	
1	XV	77	
2	QX	25	
2	XX	25	

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Mol	Chain	Length	Quality of chain
3	QY	380	43% 53% 36% 6%
3	XY	380	42% 51% 38% 5% 6%
4	RA	2915	5% 58% 33% 7%
4	YA	2915	4% 58% 33% 6%
5	RB	122	75% 22%
5	YB	122	70% 23% 5%
6	RD	276	79% 18%
6	YD	276	76% 20%
7	RE	206	75% 22%
7	YE	206	73% 23%
8	RF	210	68% 24%
8	YF	210	64% 30%
9	RG	182	3% 64% 34%
9	YG	182	2% 59% 38%
10	RH	180	15% 75% 19%
10	YH	180	66% 28%
11	RI	148	10% 72% 26%
11	YI	148	3% 70% 25%
12	RN	140	3% 76% 22%
12	YN	140	% 77% 19%
13	RO	122	78% 19%
13	YO	122	77% 20%
14	RP	150	2% 78% 19%
14	YP	150	% 75% 19%
15	RQ	141	72% 24%

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Mol	Chain	Length	Quality of chain
15	YQ	141	77% 19%
16	RR	118	67% 30%
16	YR	118	75% 23%
17	RS	112	2% 66% 28%
17	YS	112	62% 31%
18	RT	146	60% 25% 10%
18	YT	146	61% 24% 10%
19	RU	118	72% 19% 7%
19	YU	118	76% 17%
20	RV	101	76% 18%
20	YV	101	76% 21%
21	RW	113	80% 17%
21	YW	113	78% 18%
22	RX	96	2% 84% 12%
22	YX	96	82% 17%
23	RY	110	14% 67% 26%
23	YY	110	2% 68% 25%
24	RZ	206	9% 76% 18%
24	YZ	206	7% 70% 25%
25	R0	85	2% 72% 14% 9%
25	Y0	85	68% 18% 9%
26	R1	98	2% 76% 19%
26	Y1	98	63% 30% 5%
27	R2	72	71% 26%
27	Y2	72	69% 25%

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Mol	Chain	Length	Quality of chain
28	R3	60	5% 78% 20% .
28	Y3	60	2% 82% 15% ..
29	R4	71	10% 55% 34% 7% ..
29	Y4	71	11% 48% 39% 6% ..
30	R5	60	2% 75% 22% ..
30	Y5	60	78% 15% 5% .
31	R6	54	50% 69% 26% ...
31	Y6	54	30% 81% 15% ..
32	R7	49	2% 61% 33% ..
32	Y7	49	73% 18% ...
33	R8	65	66% 29% ...
33	Y8	65	60% 37% ..
34	R9	37	8% 70% 24% ..
34	Y9	37	3% 78% 19% .
35	QA	1521	2% 52% 39% 7% .
35	XA	1521	3% 53% 39% 6% ..
36	QB	256	6% 51% 33% 10%
36	XB	256	4% 48% 34% 5% 10%
37	QC	239	3% 63% 21% 14%
37	XC	239	3% 60% 23% 14%
38	QD	209	59% 36% ..
38	XD	209	65% 31% ..
39	QE	162	63% 25% 9%
39	XE	162	% 56% 32% 9%
40	QF	101	2% 63% 26% 10% .

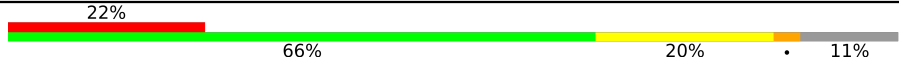

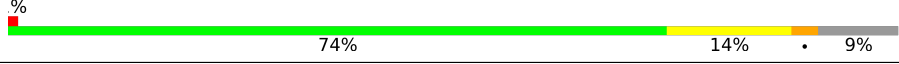

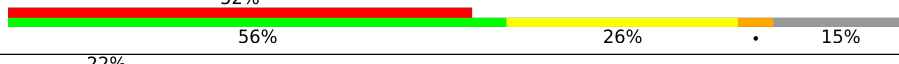
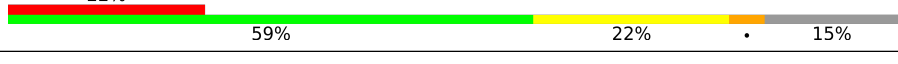
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Mol	Chain	Length	Quality of chain
40	XF	101	68% 23% 7% ..
41	QG	156	10% 83% 15% ..
41	XG	156	6% 69% 26% ...
42	QH	138	3% 71% 25% ...
42	XH	138	16% 70% 28% ..
43	QI	128	5% 63% 30% ...
43	XI	128	15% 50% 45% ..
44	QJ	105	10% 54% 35% • 8%
44	XJ	105	3% 60% 29% • 9%
45	QK	129	2% 72% 16% • 12%
45	XK	129	66% 19% • 12%
46	QL	132	2% 66% 23% • 8%
46	XL	132	68% 22% • 8%
47	QM	126	6% 63% 29% 8%
47	XM	126	6% 59% 32% 10%
48	QN	61	10% 66% 25% 7% ..
48	XN	61	2% 77% 20% ..
49	QO	89	72% 25% ..
49	XO	89	2% 73% 22% ..
50	QP	88	3% 56% 35% • 7%
50	XP	88	7% 61% 26% • • 7%
51	QQ	105	2% 72% 19% • 6%
51	XQ	105	75% 14% • • 6%
52	QR	88	10% 55% 16% 6% • 23%
52	XR	88	52% 22% • 23%

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Mol	Chain	Length	Quality of chain
53	QS	93	
53	XS	93	
54	QT	106	
54	XT	106	
55	QU	27	
55	XU	27	

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	1603	-	-	-	X
56	MG	QA	1608	-	-	-	X
56	MG	QA	1609	-	-	-	X
56	MG	QA	1611	-	-	-	X
56	MG	QA	1612	-	-	-	X
56	MG	QA	1624	-	-	-	X
56	MG	QA	1630	-	-	-	X
56	MG	QA	1632	-	-	-	X
56	MG	QA	1637	-	-	-	X
56	MG	QA	1640	-	-	-	X
56	MG	QA	1641	-	-	-	X
56	MG	QA	1642	-	-	-	X
56	MG	QA	1644	-	-	-	X
56	MG	QA	1646	-	-	-	X
56	MG	QA	1647	-	-	-	X
56	MG	QA	1652	-	-	-	X
56	MG	QA	1653	-	-	-	X
56	MG	QA	1657	-	-	-	X
56	MG	QA	1661	-	-	-	X
56	MG	QA	1662	-	-	-	X
56	MG	QA	1664	-	-	-	X
56	MG	QA	1665	-	-	-	X
56	MG	QA	1668	-	-	-	X
56	MG	QA	1669	-	-	-	X
56	MG	QA	1670	-	-	-	X
56	MG	QA	1672	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	QA	1675	-	-	-	X
56	MG	QA	1676	-	-	-	X
56	MG	QA	1677	-	-	-	X
56	MG	QA	1681	-	-	-	X
56	MG	QA	1685	-	-	-	X
56	MG	QA	1686	-	-	-	X
56	MG	QA	1691	-	-	-	X
56	MG	QA	1698	-	-	-	X
56	MG	QA	1699	-	-	-	X
56	MG	QA	1700	-	-	-	X
56	MG	QA	1704	-	-	-	X
56	MG	QA	1712	-	-	-	X
56	MG	QA	1713	-	-	-	X
56	MG	QA	1715	-	-	-	X
56	MG	QA	1718	-	-	-	X
56	MG	QA	1720	-	-	-	X
56	MG	QA	1721	-	-	-	X
56	MG	QA	1725	-	-	-	X
56	MG	QA	1727	-	-	-	X
56	MG	QA	1731	-	-	-	X
56	MG	QA	1732	-	-	-	X
56	MG	QA	1733	-	-	-	X
56	MG	QA	1734	-	-	-	X
56	MG	QA	1735	-	-	-	X
56	MG	QA	1736	-	-	-	X
56	MG	QA	1737	-	-	-	X
56	MG	QA	1738	-	-	-	X
56	MG	QA	1741	-	-	-	X
56	MG	QA	1745	-	-	-	X
56	MG	QA	1747	-	-	-	X
56	MG	QA	1748	-	-	-	X
56	MG	QA	1749	-	-	-	X
56	MG	QA	1753	-	-	-	X
56	MG	QA	1754	-	-	-	X
56	MG	QA	1755	-	-	-	X
56	MG	QA	1756	-	-	-	X
56	MG	QA	1757	-	-	-	X
56	MG	QA	1758	-	-	-	X
56	MG	QA	1760	-	-	-	X
56	MG	QA	1761	-	-	-	X
56	MG	QA	1762	-	-	-	X
56	MG	QA	1763	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	QA	1766	-	-	-	X
56	MG	QA	1769	-	-	-	X
56	MG	QA	1772	-	-	-	X
56	MG	QA	1774	-	-	-	X
56	MG	QA	1775	-	-	-	X
56	MG	QA	1778	-	-	-	X
56	MG	QA	1784	-	-	-	X
56	MG	QA	1785	-	-	-	X
56	MG	QA	1787	-	-	-	X
56	MG	QA	1788	-	-	-	X
56	MG	QA	1791	-	-	-	X
56	MG	QA	1792	-	-	-	X
56	MG	QA	1793	-	-	-	X
56	MG	QA	1794	-	-	-	X
56	MG	QA	1796	-	-	-	X
56	MG	QA	1797	-	-	-	X
56	MG	QA	1798	-	-	-	X
56	MG	QA	1799	-	-	-	X
56	MG	QA	1804	-	-	-	X
56	MG	QA	1808	-	-	-	X
56	MG	QA	1812	-	-	-	X
56	MG	QA	1813	-	-	-	X
56	MG	QA	1814	-	-	-	X
56	MG	QA	1816	-	-	-	X
56	MG	QA	1819	-	-	-	X
56	MG	QA	1821	-	-	-	X
56	MG	QA	1822	-	-	-	X
56	MG	QA	1823	-	-	-	X
56	MG	QA	1824	-	-	-	X
56	MG	QA	1826	-	-	-	X
56	MG	QA	1829	-	-	-	X
56	MG	QA	1831	-	-	-	X
56	MG	QA	1832	-	-	-	X
56	MG	QA	1835	-	-	-	X
56	MG	QA	1836	-	-	-	X
56	MG	QA	1837	-	-	-	X
56	MG	QA	1839	-	-	-	X
56	MG	QA	1840	-	-	-	X
56	MG	QA	1845	-	-	-	X
56	MG	QA	1847	-	-	-	X
56	MG	QA	1848	-	-	-	X
56	MG	QA	1850	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	QA	1851	-	-	-	X
56	MG	QA	1853	-	-	-	X
56	MG	QA	1856	-	-	-	X
56	MG	QA	1857	-	-	-	X
56	MG	QA	1858	-	-	-	X
56	MG	QA	1860	-	-	-	X
56	MG	QA	1861	-	-	-	X
56	MG	QA	1862	-	-	-	X
56	MG	QA	1864	-	-	-	X
56	MG	QA	1865	-	-	-	X
56	MG	QA	1866	-	-	-	X
56	MG	QA	1867	-	-	-	X
56	MG	QA	1871	-	-	-	X
56	MG	QA	1873	-	-	-	X
56	MG	QA	1878	-	-	-	X
56	MG	QA	1879	-	-	-	X
56	MG	QD	301	-	-	-	X
56	MG	QD	303	-	-	-	X
56	MG	QE	202	-	-	-	X
56	MG	QG	201	-	-	-	X
56	MG	QG	203	-	-	-	X
56	MG	QH	201	-	-	-	X
56	MG	QH	202	-	-	-	X
56	MG	QI	201	-	-	-	X
56	MG	QM	201	-	-	-	X
56	MG	QN	103	-	-	-	X
56	MG	QO	101	-	-	-	X
56	MG	QT	201	-	-	-	X
56	MG	QU	101	-	-	-	X
56	MG	QV	101	-	-	-	X
56	MG	QY	401	-	-	-	X
56	MG	QY	402	-	-	-	X
56	MG	QY	403	-	-	-	X
56	MG	R0	103	-	-	-	X
56	MG	R0	104	-	-	-	X
56	MG	R1	101	-	-	-	X
56	MG	R1	102	-	-	-	X
56	MG	R3	101	-	-	-	X
56	MG	R3	102	-	-	-	X
56	MG	R7	102	-	-	-	X
56	MG	R8	101	-	-	-	X
56	MG	RA	3003	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3005	-	-	-	X
56	MG	RA	3011	-	-	-	X
56	MG	RA	3013	-	-	-	X
56	MG	RA	3016	-	-	-	X
56	MG	RA	3031	-	-	-	X
56	MG	RA	3034	-	-	-	X
56	MG	RA	3035	-	-	-	X
56	MG	RA	3036	-	-	-	X
56	MG	RA	3039	-	-	-	X
56	MG	RA	3040	-	-	-	X
56	MG	RA	3051	-	-	-	X
56	MG	RA	3057	-	-	-	X
56	MG	RA	3058	-	-	-	X
56	MG	RA	3065	-	-	-	X
56	MG	RA	3066	-	-	-	X
56	MG	RA	3068	-	-	-	X
56	MG	RA	3076	-	-	-	X
56	MG	RA	3078	-	-	-	X
56	MG	RA	3081	-	-	-	X
56	MG	RA	3085	-	-	-	X
56	MG	RA	3086	-	-	-	X
56	MG	RA	3090	-	-	-	X
56	MG	RA	3100	-	-	-	X
56	MG	RA	3102	-	-	-	X
56	MG	RA	3103	-	-	-	X
56	MG	RA	3104	-	-	-	X
56	MG	RA	3105	-	-	-	X
56	MG	RA	3112	-	-	-	X
56	MG	RA	3115	-	-	-	X
56	MG	RA	3122	-	-	-	X
56	MG	RA	3126	-	-	-	X
56	MG	RA	3134	-	-	-	X
56	MG	RA	3138	-	-	-	X
56	MG	RA	3142	-	-	-	X
56	MG	RA	3144	-	-	-	X
56	MG	RA	3152	-	-	-	X
56	MG	RA	3162	-	-	-	X
56	MG	RA	3164	-	-	-	X
56	MG	RA	3166	-	-	-	X
56	MG	RA	3171	-	-	-	X
56	MG	RA	3177	-	-	-	X
56	MG	RA	3179	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3187	-	-	-	X
56	MG	RA	3193	-	-	-	X
56	MG	RA	3195	-	-	-	X
56	MG	RA	3197	-	-	-	X
56	MG	RA	3198	-	-	-	X
56	MG	RA	3200	-	-	-	X
56	MG	RA	3202	-	-	-	X
56	MG	RA	3203	-	-	-	X
56	MG	RA	3205	-	-	-	X
56	MG	RA	3206	-	-	-	X
56	MG	RA	3207	-	-	-	X
56	MG	RA	3211	-	-	-	X
56	MG	RA	3212	-	-	-	X
56	MG	RA	3224	-	-	-	X
56	MG	RA	3225	-	-	-	X
56	MG	RA	3226	-	-	-	X
56	MG	RA	3227	-	-	-	X
56	MG	RA	3228	-	-	-	X
56	MG	RA	3229	-	-	-	X
56	MG	RA	3236	-	-	-	X
56	MG	RA	3237	-	-	-	X
56	MG	RA	3239	-	-	-	X
56	MG	RA	3240	-	-	-	X
56	MG	RA	3245	-	-	-	X
56	MG	RA	3246	-	-	-	X
56	MG	RA	3249	-	-	-	X
56	MG	RA	3250	-	-	-	X
56	MG	RA	3251	-	-	-	X
56	MG	RA	3252	-	-	-	X
56	MG	RA	3256	-	-	-	X
56	MG	RA	3258	-	-	-	X
56	MG	RA	3261	-	-	-	X
56	MG	RA	3264	-	-	-	X
56	MG	RA	3271	-	-	-	X
56	MG	RA	3275	-	-	-	X
56	MG	RA	3276	-	-	-	X
56	MG	RA	3277	-	-	-	X
56	MG	RA	3279	-	-	-	X
56	MG	RA	3282	-	-	-	X
56	MG	RA	3283	-	-	-	X
56	MG	RA	3285	-	-	-	X
56	MG	RA	3289	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3291	-	-	-	X
56	MG	RA	3296	-	-	-	X
56	MG	RA	3302	-	-	-	X
56	MG	RA	3303	-	-	-	X
56	MG	RA	3309	-	-	-	X
56	MG	RA	3311	-	-	-	X
56	MG	RA	3312	-	-	-	X
56	MG	RA	3314	-	-	-	X
56	MG	RA	3316	-	-	-	X
56	MG	RA	3322	-	-	-	X
56	MG	RA	3327	-	-	-	X
56	MG	RA	3331	-	-	-	X
56	MG	RA	3339	-	-	-	X
56	MG	RA	3340	-	-	-	X
56	MG	RA	3351	-	-	-	X
56	MG	RA	3358	-	-	-	X
56	MG	RA	3360	-	-	-	X
56	MG	RA	3365	-	-	-	X
56	MG	RA	3367	-	-	-	X
56	MG	RA	3368	-	-	-	X
56	MG	RA	3370	-	-	-	X
56	MG	RA	3372	-	-	-	X
56	MG	RA	3375	-	-	-	X
56	MG	RA	3399	-	-	-	X
56	MG	RA	3402	-	-	-	X
56	MG	RA	3422	-	-	-	X
56	MG	RA	3425	-	-	-	X
56	MG	RA	3426	-	-	-	X
56	MG	RA	3427	-	-	-	X
56	MG	RA	3432	-	-	-	X
56	MG	RA	3436	-	-	-	X
56	MG	RA	3437	-	-	-	X
56	MG	RA	3439	-	-	-	X
56	MG	RA	3441	-	-	-	X
56	MG	RA	3446	-	-	-	X
56	MG	RA	3448	-	-	-	X
56	MG	RA	3457	-	-	-	X
56	MG	RA	3459	-	-	-	X
56	MG	RA	3461	-	-	-	X
56	MG	RA	3463	-	-	-	X
56	MG	RA	3466	-	-	-	X
56	MG	RA	3489	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3490	-	-	-	X
56	MG	RA	3491	-	-	-	X
56	MG	RA	3499	-	-	-	X
56	MG	RA	3511	-	-	-	X
56	MG	RA	3512	-	-	-	X
56	MG	RA	3515	-	-	-	X
56	MG	RA	3517	-	-	-	X
56	MG	RA	3518	-	-	-	X
56	MG	RA	3519	-	-	-	X
56	MG	RA	3521	-	-	-	X
56	MG	RA	3523	-	-	-	X
56	MG	RA	3524	-	-	-	X
56	MG	RA	3525	-	-	-	X
56	MG	RA	3527	-	-	-	X
56	MG	RA	3530	-	-	-	X
56	MG	RA	3537	-	-	-	X
56	MG	RA	3541	-	-	-	X
56	MG	RA	3542	-	-	-	X
56	MG	RA	3544	-	-	-	X
56	MG	RA	3545	-	-	-	X
56	MG	RA	3546	-	-	-	X
56	MG	RA	3549	-	-	-	X
56	MG	RA	3553	-	-	-	X
56	MG	RA	3556	-	-	-	X
56	MG	RA	3557	-	-	-	X
56	MG	RA	3558	-	-	-	X
56	MG	RA	3564	-	-	-	X
56	MG	RA	3571	-	-	-	X
56	MG	RA	3573	-	-	-	X
56	MG	RA	3577	-	-	-	X
56	MG	RA	3580	-	-	-	X
56	MG	RA	3583	-	-	-	X
56	MG	RA	3586	-	-	-	X
56	MG	RA	3589	-	-	-	X
56	MG	RA	3590	-	-	-	X
56	MG	RA	3591	-	-	-	X
56	MG	RA	3595	-	-	-	X
56	MG	RA	3596	-	-	-	X
56	MG	RA	3600	-	-	-	X
56	MG	RA	3602	-	-	-	X
56	MG	RA	3603	-	-	-	X
56	MG	RA	3608	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3617	-	-	-	X
56	MG	RA	3620	-	-	-	X
56	MG	RA	3625	-	-	-	X
56	MG	RA	3626	-	-	-	X
56	MG	RA	3628	-	-	-	X
56	MG	RA	3630	-	-	-	X
56	MG	RA	3631	-	-	-	X
56	MG	RA	3634	-	-	-	X
56	MG	RA	3636	-	-	-	X
56	MG	RA	3637	-	-	-	X
56	MG	RA	3639	-	-	-	X
56	MG	RA	3641	-	-	-	X
56	MG	RA	3644	-	-	-	X
56	MG	RA	3645	-	-	-	X
56	MG	RA	3646	-	-	-	X
56	MG	RA	3652	-	-	-	X
56	MG	RA	3654	-	-	-	X
56	MG	RA	3659	-	-	-	X
56	MG	RA	3662	-	-	-	X
56	MG	RA	3663	-	-	-	X
56	MG	RA	3669	-	-	-	X
56	MG	RA	3672	-	-	-	X
56	MG	RA	3681	-	-	-	X
56	MG	RA	3683	-	-	-	X
56	MG	RA	3684	-	-	-	X
56	MG	RA	3691	-	-	-	X
56	MG	RA	3693	-	-	-	X
56	MG	RA	3694	-	-	-	X
56	MG	RA	3699	-	-	-	X
56	MG	RA	3701	-	-	-	X
56	MG	RA	3703	-	-	-	X
56	MG	RA	3704	-	-	-	X
56	MG	RA	3706	-	-	-	X
56	MG	RA	3710	-	-	-	X
56	MG	RA	3719	-	-	-	X
56	MG	RA	3725	-	-	-	X
56	MG	RA	3727	-	-	-	X
56	MG	RA	3729	-	-	-	X
56	MG	RA	3733	-	-	-	X
56	MG	RA	3735	-	-	-	X
56	MG	RA	3740	-	-	-	X
56	MG	RA	3742	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3746	-	-	-	X
56	MG	RA	3747	-	-	-	X
56	MG	RA	3752	-	-	-	X
56	MG	RA	3754	-	-	-	X
56	MG	RA	3755	-	-	-	X
56	MG	RA	3768	-	-	-	X
56	MG	RA	3772	-	-	-	X
56	MG	RA	3774	-	-	-	X
56	MG	RA	3781	-	-	-	X
56	MG	RA	3782	-	-	-	X
56	MG	RA	3786	-	-	-	X
56	MG	RA	3787	-	-	-	X
56	MG	RA	3790	-	-	-	X
56	MG	RA	3796	-	-	-	X
56	MG	RA	3797	-	-	-	X
56	MG	RA	3798	-	-	-	X
56	MG	RA	3800	-	-	-	X
56	MG	RA	3807	-	-	-	X
56	MG	RA	3809	-	-	-	X
56	MG	RA	3810	-	-	-	X
56	MG	RA	3812	-	-	-	X
56	MG	RA	3817	-	-	-	X
56	MG	RA	3818	-	-	-	X
56	MG	RA	3822	-	-	-	X
56	MG	RA	3823	-	-	-	X
56	MG	RA	3824	-	-	-	X
56	MG	RA	3825	-	-	-	X
56	MG	RA	3828	-	-	-	X
56	MG	RA	3829	-	-	-	X
56	MG	RA	3834	-	-	-	X
56	MG	RA	3836	-	-	-	X
56	MG	RA	3839	-	-	-	X
56	MG	RA	3840	-	-	-	X
56	MG	RA	3842	-	-	-	X
56	MG	RA	3845	-	-	-	X
56	MG	RA	3846	-	-	-	X
56	MG	RA	3847	-	-	-	X
56	MG	RA	3849	-	-	-	X
56	MG	RA	3858	-	-	-	X
56	MG	RA	3862	-	-	-	X
56	MG	RA	3863	-	-	-	X
56	MG	RA	3868	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3871	-	-	-	X
56	MG	RA	3872	-	-	-	X
56	MG	RA	3875	-	-	-	X
56	MG	RA	3878	-	-	-	X
56	MG	RA	3880	-	-	-	X
56	MG	RA	3882	-	-	-	X
56	MG	RA	3890	-	-	-	X
56	MG	RA	3891	-	-	-	X
56	MG	RA	3892	-	-	-	X
56	MG	RA	3896	-	-	-	X
56	MG	RA	3909	-	-	-	X
56	MG	RA	3910	-	-	-	X
56	MG	RA	3912	-	-	-	X
56	MG	RA	3916	-	-	-	X
56	MG	RA	3921	-	-	-	X
56	MG	RA	3924	-	-	-	X
56	MG	RA	3926	-	-	-	X
56	MG	RA	3933	-	-	-	X
56	MG	RA	3935	-	-	-	X
56	MG	RA	3940	-	-	-	X
56	MG	RA	3942	-	-	-	X
56	MG	RA	3948	-	-	-	X
56	MG	RA	3949	-	-	-	X
56	MG	RA	3950	-	-	-	X
56	MG	RA	3951	-	-	-	X
56	MG	RA	3954	-	-	-	X
56	MG	RA	3958	-	-	-	X
56	MG	RA	3960	-	-	-	X
56	MG	RA	3961	-	-	-	X
56	MG	RA	3962	-	-	-	X
56	MG	RA	3963	-	-	-	X
56	MG	RA	3967	-	-	-	X
56	MG	RA	3968	-	-	-	X
56	MG	RA	3969	-	-	-	X
56	MG	RA	3973	-	-	-	X
56	MG	RA	3974	-	-	-	X
56	MG	RA	3976	-	-	-	X
56	MG	RA	3977	-	-	-	X
56	MG	RA	3982	-	-	-	X
56	MG	RA	3983	-	-	-	X
56	MG	RA	3985	-	-	-	X
56	MG	RA	3986	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3987	-	-	-	X
56	MG	RA	3988	-	-	-	X
56	MG	RA	3991	-	-	-	X
56	MG	RA	3993	-	-	-	X
56	MG	RA	3994	-	-	-	X
56	MG	RA	3998	-	-	-	X
56	MG	RA	4011	-	-	-	X
56	MG	RA	4015	-	-	-	X
56	MG	RA	4018	-	-	-	X
56	MG	RA	4019	-	-	-	X
56	MG	RA	4031	-	-	-	X
56	MG	RA	4041	-	-	-	X
56	MG	RA	4046	-	-	-	X
56	MG	RA	4047	-	-	-	X
56	MG	RA	4052	-	-	-	X
56	MG	RA	4053	-	-	-	X
56	MG	RA	4054	-	-	-	X
56	MG	RA	4055	-	-	-	X
56	MG	RA	4058	-	-	-	X
56	MG	RA	4059	-	-	-	X
56	MG	RA	4065	-	-	-	X
56	MG	RA	4066	-	-	-	X
56	MG	RB	203	-	-	-	X
56	MG	RB	210	-	-	-	X
56	MG	RB	217	-	-	-	X
56	MG	RB	222	-	-	-	X
56	MG	RB	223	-	-	-	X
56	MG	RB	224	-	-	-	X
56	MG	RB	225	-	-	-	X
56	MG	RB	226	-	-	-	X
56	MG	RB	227	-	-	-	X
56	MG	RB	228	-	-	-	X
56	MG	RB	229	-	-	-	X
56	MG	RD	304	-	-	-	X
56	MG	RD	308	-	-	-	X
56	MG	RD	310	-	-	-	X
56	MG	RD	311	-	-	-	X
56	MG	RD	312	-	-	-	X
56	MG	RD	313	-	-	-	X
56	MG	RE	304	-	-	-	X
56	MG	RF	301	-	-	-	X
56	MG	RF	302	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RF	310	-	-	-	X
56	MG	RF	311	-	-	-	X
56	MG	RF	312	-	-	-	X
56	MG	RG	201	-	-	-	X
56	MG	RH	201	-	-	-	X
56	MG	RH	202	-	-	-	X
56	MG	RN	201	-	-	-	X
56	MG	RN	202	-	-	-	X
56	MG	RO	201	-	-	-	X
56	MG	RQ	203	-	-	-	X
56	MG	RR	3204	-	-	-	X
56	MG	RR	3205	-	-	-	X
56	MG	RT	201	-	-	-	X
56	MG	RT	203	-	-	-	X
56	MG	RV	201	-	-	-	X
56	MG	RV	204	-	-	-	X
56	MG	RW	202	-	-	-	X
56	MG	XA	1603	-	-	-	X
56	MG	XA	1604	-	-	-	X
56	MG	XA	1605	-	-	-	X
56	MG	XA	1607	-	-	-	X
56	MG	XA	1608	-	-	-	X
56	MG	XA	1609	-	-	-	X
56	MG	XA	1616	-	-	-	X
56	MG	XA	1618	-	-	-	X
56	MG	XA	1621	-	-	-	X
56	MG	XA	1623	-	-	-	X
56	MG	XA	1624	-	-	-	X
56	MG	XA	1626	-	-	-	X
56	MG	XA	1632	-	-	-	X
56	MG	XA	1634	-	-	-	X
56	MG	XA	1637	-	-	-	X
56	MG	XA	1639	-	-	-	X
56	MG	XA	1645	-	-	-	X
56	MG	XA	1648	-	-	-	X
56	MG	XA	1650	-	-	-	X
56	MG	XA	1651	-	-	-	X
56	MG	XA	1652	-	-	-	X
56	MG	XA	1654	-	-	-	X
56	MG	XA	1655	-	-	-	X
56	MG	XA	1666	-	-	-	X
56	MG	XA	1668	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	XA	1669	-	-	-	X
56	MG	XA	1671	-	-	-	X
56	MG	XA	1672	-	-	-	X
56	MG	XA	1673	-	-	-	X
56	MG	XA	1675	-	-	-	X
56	MG	XA	1682	-	-	-	X
56	MG	XA	1692	-	-	-	X
56	MG	XA	1693	-	-	-	X
56	MG	XA	1697	-	-	-	X
56	MG	XA	1698	-	-	-	X
56	MG	XA	1700	-	-	-	X
56	MG	XA	1702	-	-	-	X
56	MG	XA	1703	-	-	-	X
56	MG	XA	1711	-	-	-	X
56	MG	XA	1715	-	-	-	X
56	MG	XA	1718	-	-	-	X
56	MG	XA	1719	-	-	-	X
56	MG	XA	1721	-	-	-	X
56	MG	XA	1725	-	-	-	X
56	MG	XA	1727	-	-	-	X
56	MG	XA	1728	-	-	-	X
56	MG	XA	1735	-	-	-	X
56	MG	XA	1748	-	-	-	X
56	MG	XA	1751	-	-	-	X
56	MG	XA	1753	-	-	-	X
56	MG	XA	1769	-	-	-	X
56	MG	XA	1773	-	-	-	X
56	MG	XA	1781	-	-	-	X
56	MG	XA	1783	-	-	-	X
56	MG	XA	1784	-	-	-	X
56	MG	XA	1785	-	-	-	X
56	MG	XA	1788	-	-	-	X
56	MG	XE	201	-	-	-	X
56	MG	XF	202	-	-	-	X
56	MG	XF	203	-	-	-	X
56	MG	XF	204	-	-	-	X
56	MG	XH	201	-	-	-	X
56	MG	XR	101	-	-	-	X
56	MG	XX	101	-	-	-	X
56	MG	Y0	101	-	-	-	X
56	MG	Y1	101	-	-	-	X
56	MG	Y8	101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3003	-	-	-	X
56	MG	YA	3018	-	-	-	X
56	MG	YA	3027	-	-	-	X
56	MG	YA	3037	-	-	-	X
56	MG	YA	3039	-	-	-	X
56	MG	YA	3051	-	-	-	X
56	MG	YA	3053	-	-	-	X
56	MG	YA	3056	-	-	-	X
56	MG	YA	3057	-	-	-	X
56	MG	YA	3059	-	-	-	X
56	MG	YA	3060	-	-	-	X
56	MG	YA	3061	-	-	-	X
56	MG	YA	3065	-	-	-	X
56	MG	YA	3069	-	-	-	X
56	MG	YA	3070	-	-	-	X
56	MG	YA	3075	-	-	-	X
56	MG	YA	3083	-	-	-	X
56	MG	YA	3086	-	-	-	X
56	MG	YA	3094	-	-	-	X
56	MG	YA	3099	-	-	-	X
56	MG	YA	3107	-	-	-	X
56	MG	YA	3108	-	-	-	X
56	MG	YA	3110	-	-	-	X
56	MG	YA	3111	-	-	-	X
56	MG	YA	3119	-	-	-	X
56	MG	YA	3134	-	-	-	X
56	MG	YA	3139	-	-	-	X
56	MG	YA	3148	-	-	-	X
56	MG	YA	3150	-	-	-	X
56	MG	YA	3155	-	-	-	X
56	MG	YA	3161	-	-	-	X
56	MG	YA	3164	-	-	-	X
56	MG	YA	3165	-	-	-	X
56	MG	YA	3166	-	-	-	X
56	MG	YA	3167	-	-	-	X
56	MG	YA	3169	-	-	-	X
56	MG	YA	3170	-	-	-	X
56	MG	YA	3173	-	-	-	X
56	MG	YA	3174	-	-	-	X
56	MG	YA	3176	-	-	-	X
56	MG	YA	3178	-	-	-	X
56	MG	YA	3179	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3184	-	-	-	X
56	MG	YA	3185	-	-	-	X
56	MG	YA	3186	-	-	-	X
56	MG	YA	3193	-	-	-	X
56	MG	YA	3198	-	-	-	X
56	MG	YA	3203	-	-	-	X
56	MG	YA	3206	-	-	-	X
56	MG	YA	3208	-	-	-	X
56	MG	YA	3211	-	-	-	X
56	MG	YA	3214	-	-	-	X
56	MG	YA	3222	-	-	-	X
56	MG	YA	3226	-	-	-	X
56	MG	YA	3233	-	-	-	X
56	MG	YA	3234	-	-	-	X
56	MG	YA	3237	-	-	-	X
56	MG	YA	3241	-	-	-	X
56	MG	YA	3246	-	-	-	X
56	MG	YA	3247	-	-	-	X
56	MG	YA	3248	-	-	-	X
56	MG	YA	3253	-	-	-	X
56	MG	YA	3260	-	-	-	X
56	MG	YA	3262	-	-	-	X
56	MG	YA	3265	-	-	-	X
56	MG	YA	3267	-	-	-	X
56	MG	YA	3269	-	-	-	X
56	MG	YA	3270	-	-	-	X
56	MG	YA	3273	-	-	-	X
56	MG	YA	3302	-	-	-	X
56	MG	YA	3311	-	-	-	X
56	MG	YA	3312	-	-	-	X
56	MG	YA	3314	-	-	-	X
56	MG	YA	3330	-	-	-	X
56	MG	YA	3336	-	-	-	X
56	MG	YA	3364	-	-	-	X
56	MG	YA	3368	-	-	-	X
56	MG	YA	3375	-	-	-	X
56	MG	YA	3396	-	-	-	X
56	MG	YA	3400	-	-	-	X
56	MG	YA	3403	-	-	-	X
56	MG	YA	3406	-	-	-	X
56	MG	YA	3414	-	-	-	X
56	MG	YA	3415	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3417	-	-	-	X
56	MG	YA	3418	-	-	-	X
56	MG	YA	3419	-	-	-	X
56	MG	YA	3421	-	-	-	X
56	MG	YA	3422	-	-	-	X
56	MG	YA	3426	-	-	-	X
56	MG	YA	3427	-	-	-	X
56	MG	YA	3431	-	-	-	X
56	MG	YA	3432	-	-	-	X
56	MG	YA	3437	-	-	-	X
56	MG	YA	3439	-	-	-	X
56	MG	YA	3443	-	-	-	X
56	MG	YA	3445	-	-	-	X
56	MG	YA	3446	-	-	-	X
56	MG	YA	3449	-	-	-	X
56	MG	YA	3450	-	-	-	X
56	MG	YA	3455	-	-	-	X
56	MG	YA	3456	-	-	-	X
56	MG	YA	3461	-	-	-	X
56	MG	YA	3462	-	-	-	X
56	MG	YA	3464	-	-	-	X
56	MG	YA	3465	-	-	-	X
56	MG	YA	3466	-	-	-	X
56	MG	YA	3467	-	-	-	X
56	MG	YA	3468	-	-	-	X
56	MG	YA	3473	-	-	-	X
56	MG	YA	3475	-	-	-	X
56	MG	YA	3477	-	-	-	X
56	MG	YA	3478	-	-	-	X
56	MG	YA	3479	-	-	-	X
56	MG	YA	3481	-	-	-	X
56	MG	YA	3485	-	-	-	X
56	MG	YA	3490	-	-	-	X
56	MG	YA	3491	-	-	-	X
56	MG	YA	3497	-	-	-	X
56	MG	YA	3500	-	-	-	X
56	MG	YA	3501	-	-	-	X
56	MG	YA	3502	-	-	-	X
56	MG	YA	3505	-	-	-	X
56	MG	YA	3510	-	-	-	X
56	MG	YA	3511	-	-	-	X
56	MG	YA	3512	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3517	-	-	-	X
56	MG	YA	3519	-	-	-	X
56	MG	YA	3522	-	-	-	X
56	MG	YA	3528	-	-	-	X
56	MG	YA	3529	-	-	-	X
56	MG	YA	3534	-	-	-	X
56	MG	YA	3535	-	-	-	X
56	MG	YA	3544	-	-	-	X
56	MG	YA	3545	-	-	-	X
56	MG	YA	3547	-	-	-	X
56	MG	YA	3550	-	-	-	X
56	MG	YA	3551	-	-	-	X
56	MG	YA	3557	-	-	-	X
56	MG	YA	3565	-	-	-	X
56	MG	YA	3577	-	-	-	X
56	MG	YA	3578	-	-	-	X
56	MG	YA	3582	-	-	-	X
56	MG	YA	3584	-	-	-	X
56	MG	YA	3599	-	-	-	X
56	MG	YA	3603	-	-	-	X
56	MG	YA	3624	-	-	-	X
56	MG	YA	3628	-	-	-	X
56	MG	YA	3635	-	-	-	X
56	MG	YA	3637	-	-	-	X
56	MG	YA	3641	-	-	-	X
56	MG	YA	3655	-	-	-	X
56	MG	YA	3662	-	-	-	X
56	MG	YA	3667	-	-	-	X
56	MG	YA	3676	-	-	-	X
56	MG	YA	3694	-	-	-	X
56	MG	YA	3695	-	-	-	X
56	MG	YA	3698	-	-	-	X
56	MG	YA	3707	-	-	-	X
56	MG	YA	3715	-	-	-	X
56	MG	YA	3722	-	-	-	X
56	MG	YA	3726	-	-	-	X
56	MG	YA	3727	-	-	-	X
56	MG	YA	3729	-	-	-	X
56	MG	YA	3737	-	-	-	X
56	MG	YA	3738	-	-	-	X
56	MG	YA	3745	-	-	-	X
56	MG	YA	3747	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YB	201	-	-	-	X
56	MG	YB	204	-	-	-	X
56	MG	YB	205	-	-	-	X
56	MG	YB	206	-	-	-	X
56	MG	YB	207	-	-	-	X
56	MG	YB	209	-	-	-	X
56	MG	YB	218	-	-	-	X
56	MG	YD	301	-	-	-	X
56	MG	YD	305	-	-	-	X
56	MG	YD	307	-	-	-	X
56	MG	YD	310	-	-	-	X
56	MG	YE	301	-	-	-	X
56	MG	YE	302	-	-	-	X
56	MG	YE	303	-	-	-	X
56	MG	YF	302	-	-	-	X
56	MG	YG	201	-	-	-	X
56	MG	YN	201	-	-	-	X
56	MG	YP	201	-	-	-	X
56	MG	YT	201	-	-	-	X
56	MG	YT	202	-	-	-	X
57	ZN	Y4	101	-	-	-	X

## 2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 296662 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called P-site tRNA fMet.

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

- Molecule 2 is a RNA chain called messenger RNA.

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

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

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

There are 30 discrepancies between the modelled and reference sequences:

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

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

- Molecule 4 is a RNA chain called T23S rRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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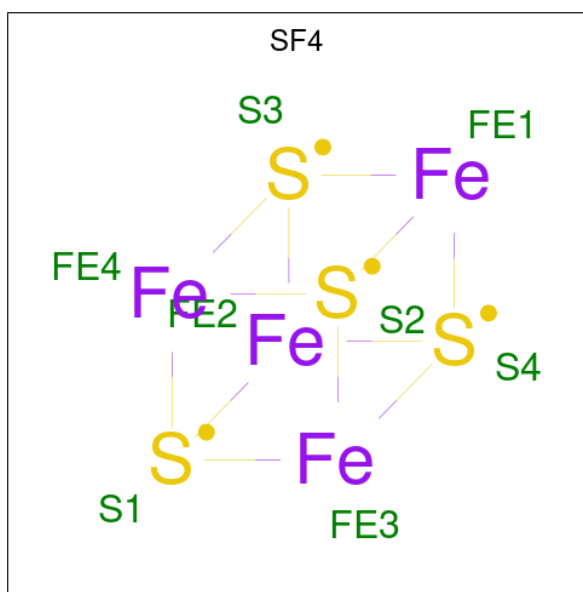
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	RN	3	Total Mg 3 3	0	0
56	RO	1	Total Mg 1 1	0	0
56	RP	2	Total Mg 2 2	0	0
56	RQ	4	Total Mg 4 4	0	0
56	RR	5	Total Mg 5 5	0	0
56	RT	3	Total Mg 3 3	0	0
56	RU	3	Total Mg 3 3	0	0
56	RV	4	Total Mg 4 4	0	0
56	RW	2	Total Mg 2 2	0	0
56	RX	1	Total Mg 1 1	0	0
56	RZ	1	Total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

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



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

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).

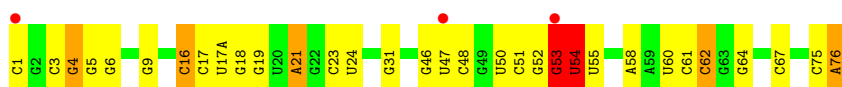


<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>			<b>ZeroOcc</b>	<b>AltConf</b>
58	XD	1	Total 8	Fe 4	S 4	0	0
58	QD	1	Total 8	Fe 4	S 4	0	0

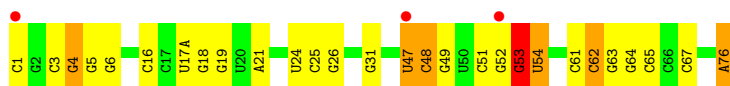
### 3 Residue-property plots [i](#)

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

- Molecule 1: P-site tRNA fMet



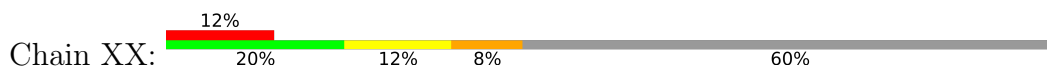
- Molecule 1: P-site tRNA fMet



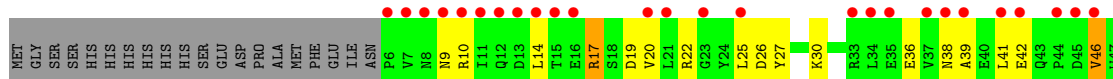
- Molecule 2: messenger RNA

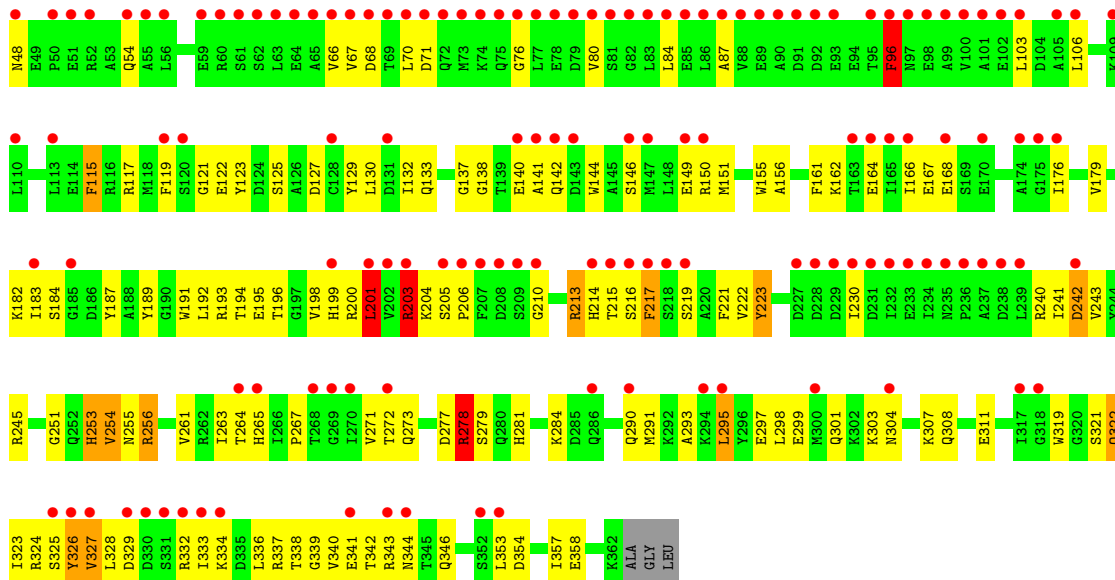


- Molecule 2: messenger RNA

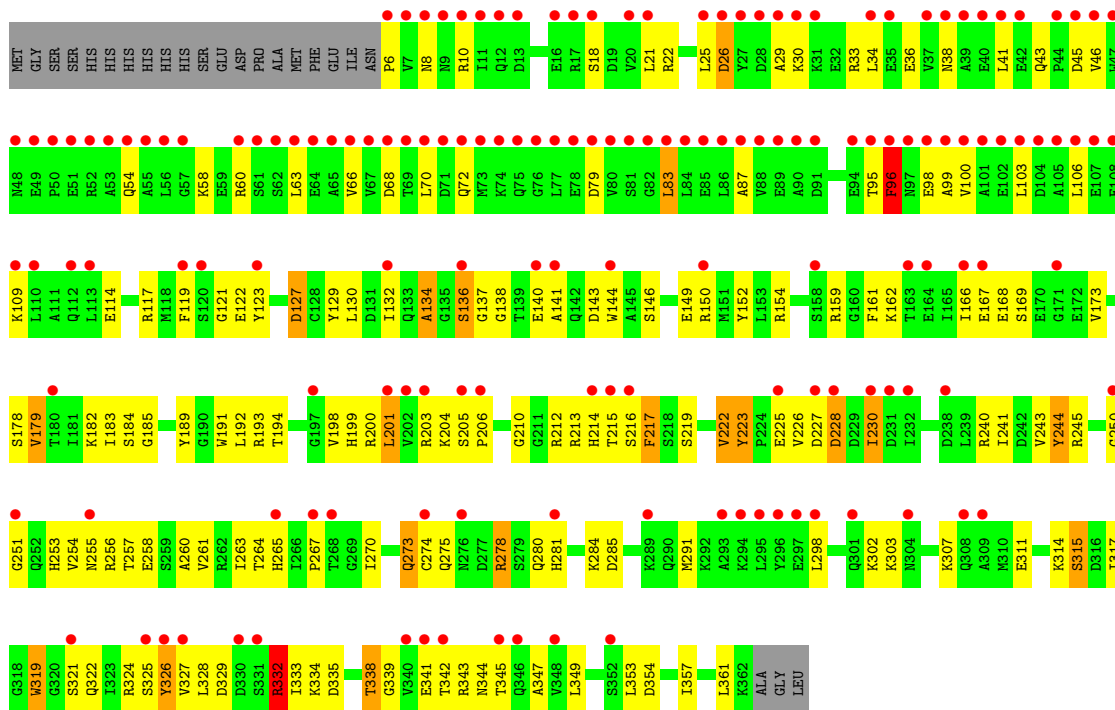
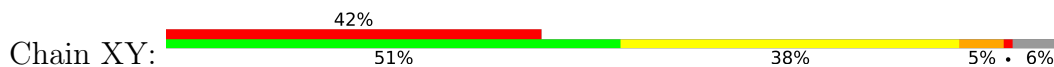


- Molecule 3: Peptide chain release factor 2



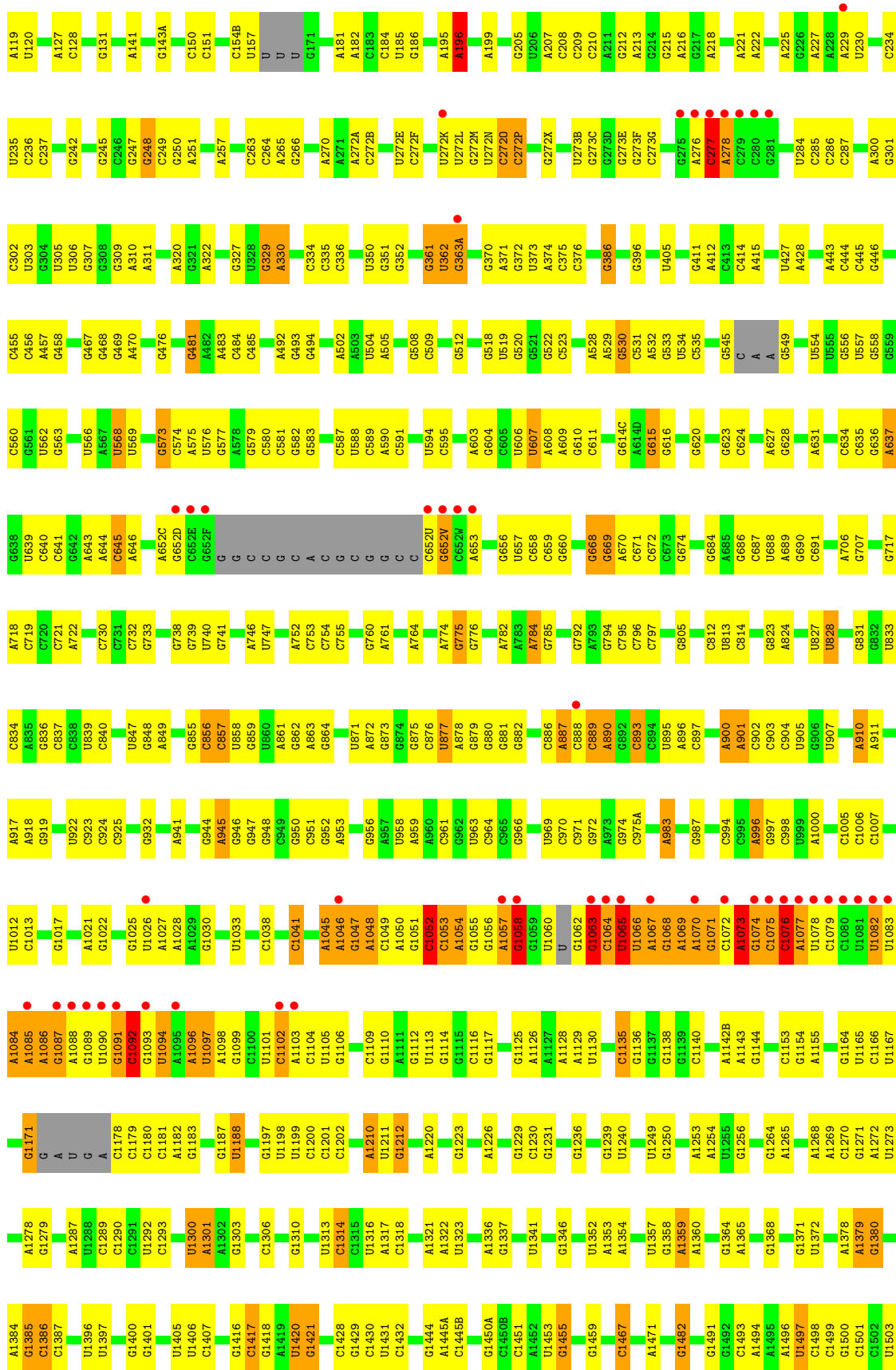


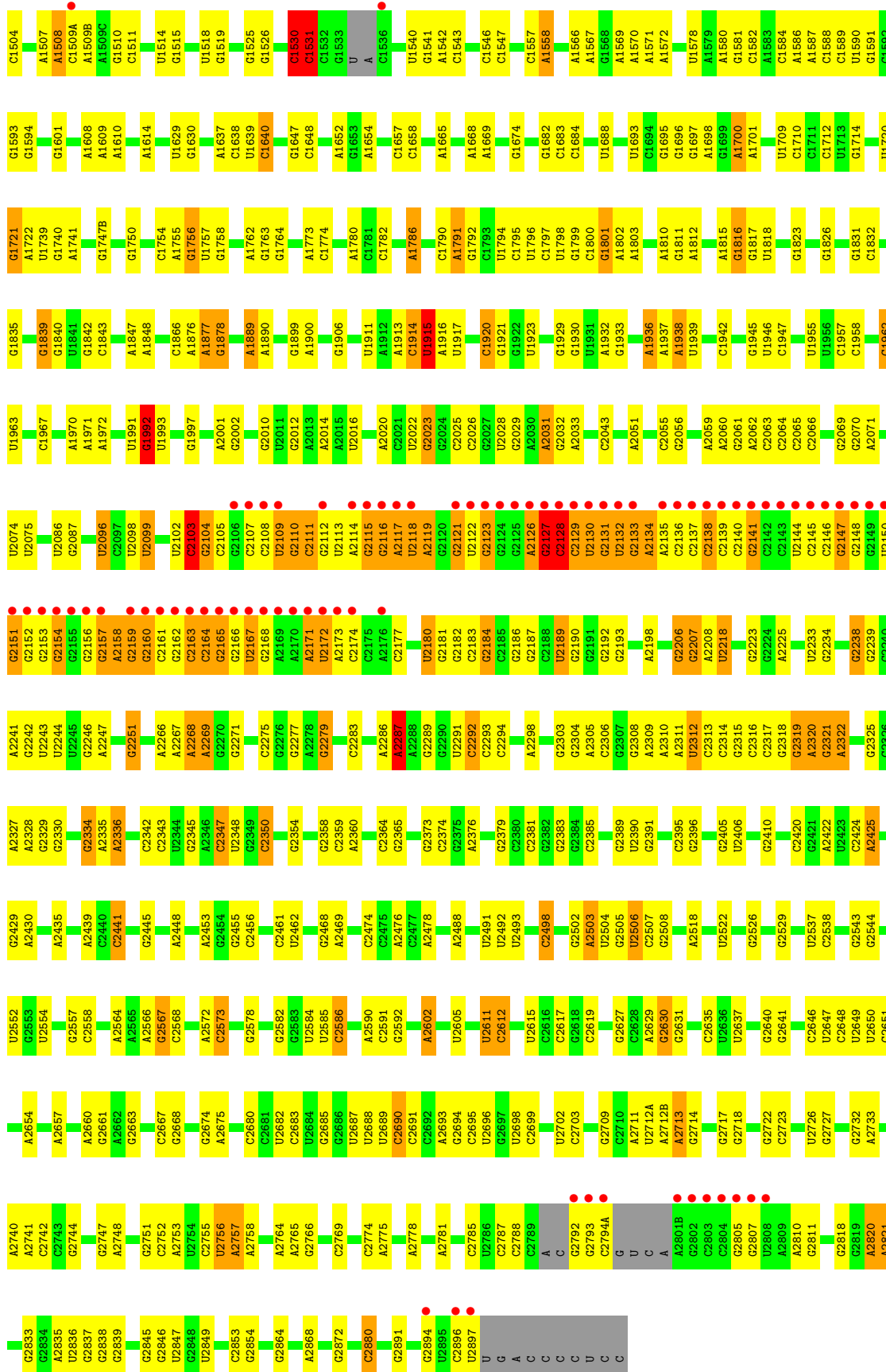
• Molecule 3: Peptide chain release factor 2



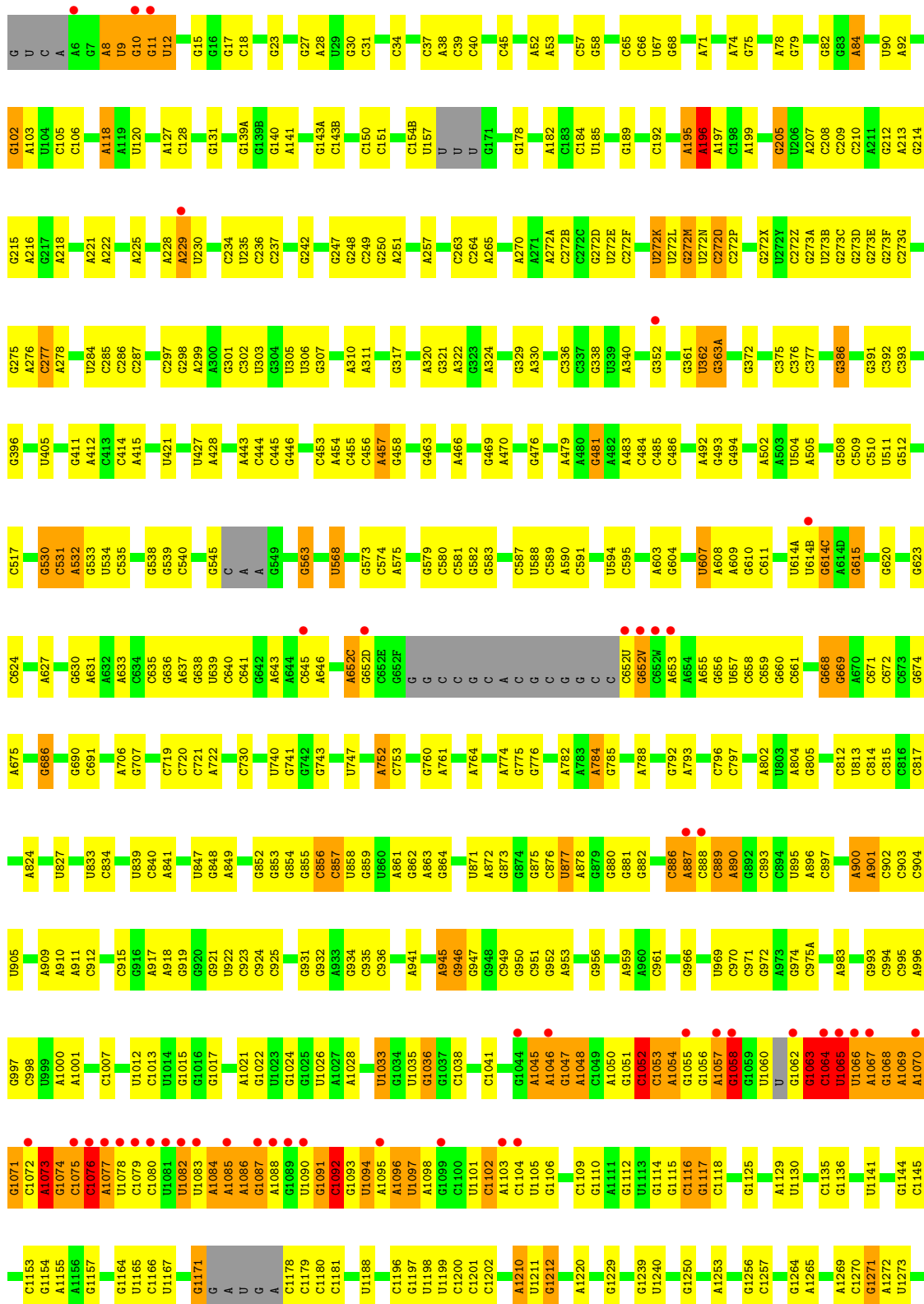
• Molecule 4: T23S rRNA





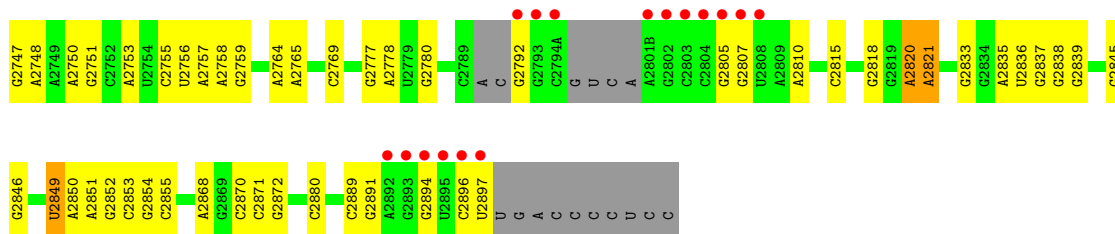


● Molecule 4: T23S rRNA





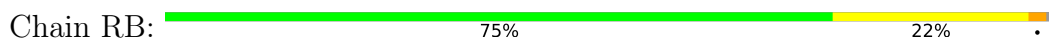




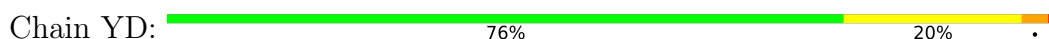
• Molecule 5: 5S rRNA



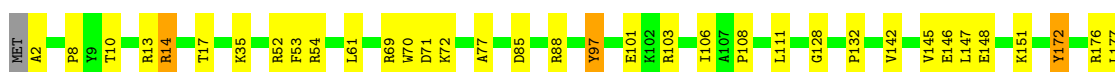
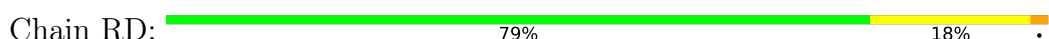
• Molecule 5: 5S rRNA



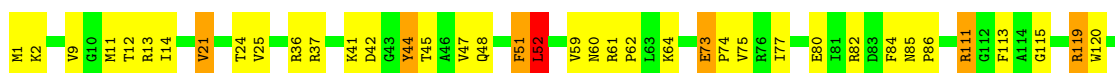
• Molecule 6: 50S ribosomal protein L2



• Molecule 6: 50S ribosomal protein L2



• Molecule 7: 50S ribosomal protein L3





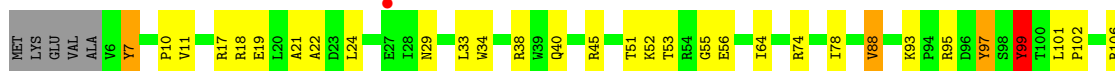
- Molecule 7: 50S ribosomal protein L3

Chain RE: 75% 22% ..



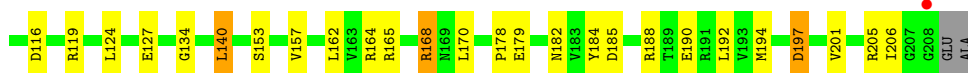
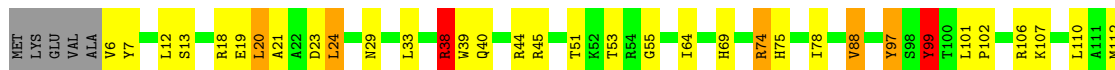
- Molecule 8: 50S ribosomal protein L4

Chain YF: 64% 30% ..



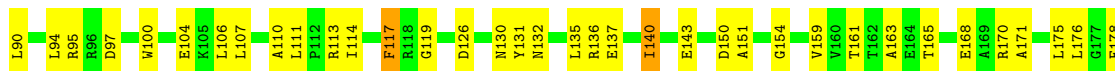
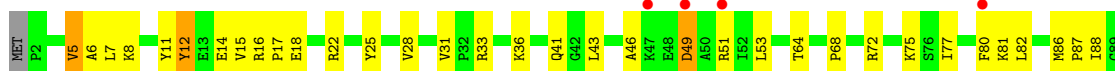
- Molecule 8: 50S ribosomal protein L4

Chain RF: 68% 24% ..

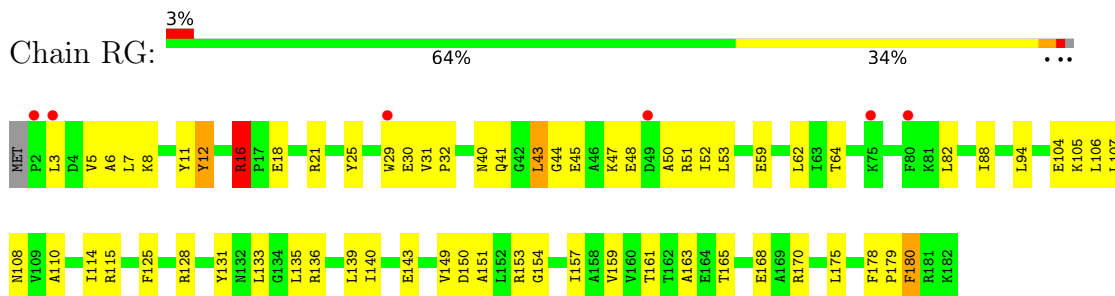


- Molecule 9: 50S ribosomal protein L5

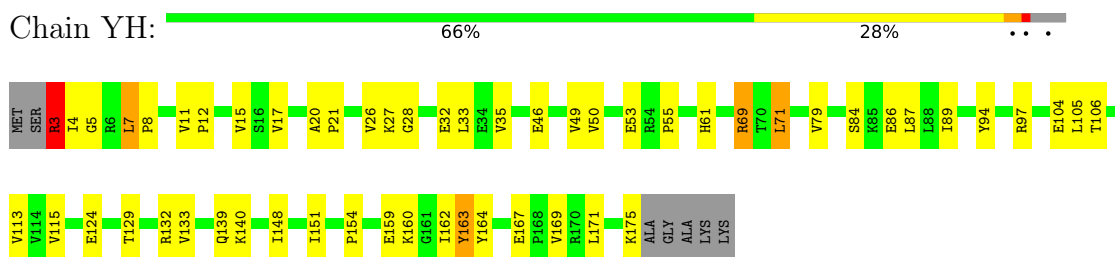
Chain YG: 2% 59% 38% ..



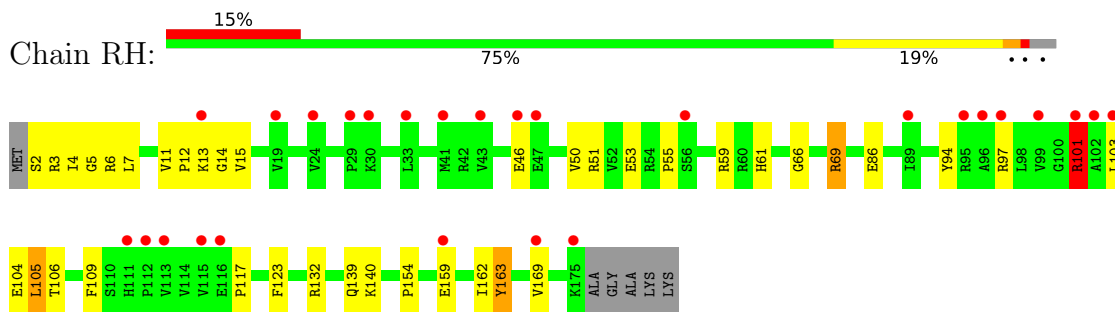
- Molecule 9: 50S ribosomal protein L5



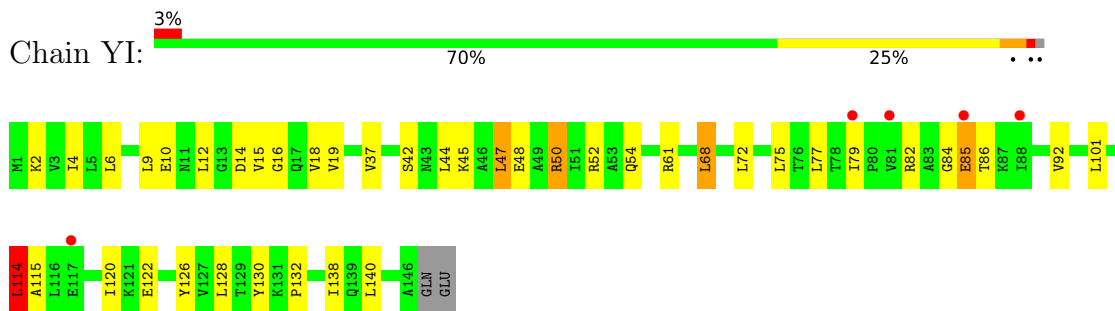
- Molecule 10: 50S ribosomal protein L6



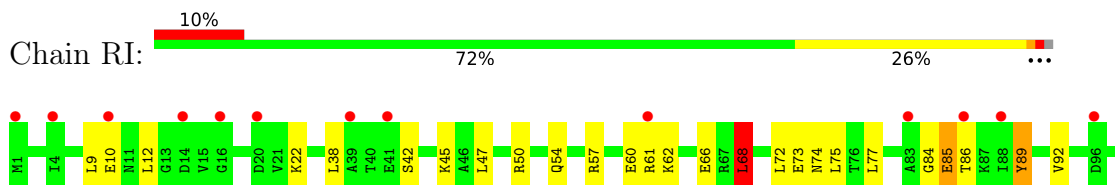
- Molecule 10: 50S ribosomal protein L6



- Molecule 11: 50S ribosomal protein L9

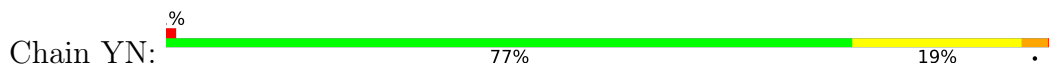


- Molecule 11: 50S ribosomal protein L9

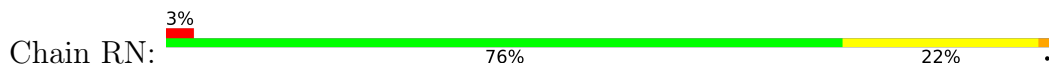




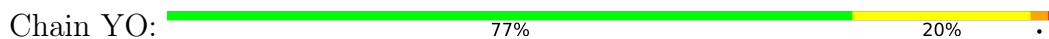
- Molecule 12: 50S ribosomal protein L13



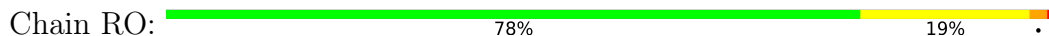
- Molecule 12: 50S ribosomal protein L13



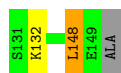
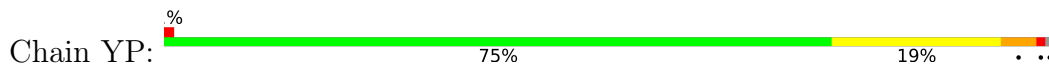
- Molecule 13: 50S ribosomal protein L14



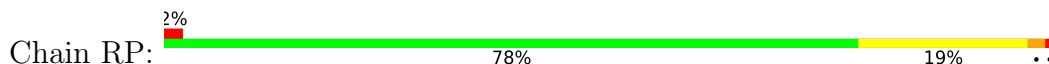
- Molecule 13: 50S ribosomal protein L14

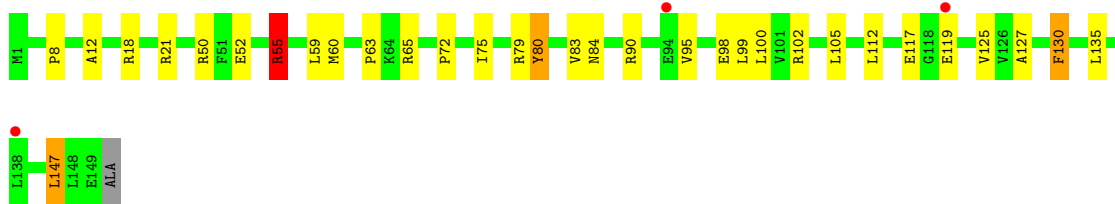


- Molecule 14: 50S ribosomal protein L15



- Molecule 14: 50S ribosomal protein L15





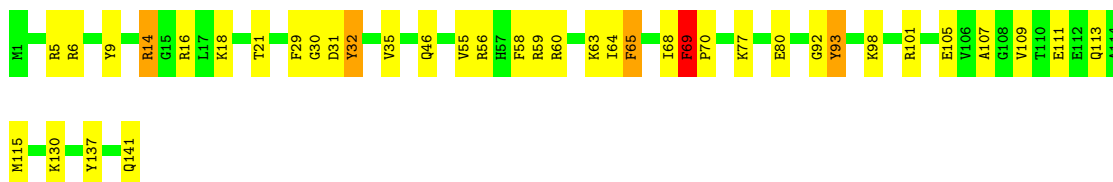
- Molecule 15: 50S ribosomal protein L16

Chain YQ: 77% 19%



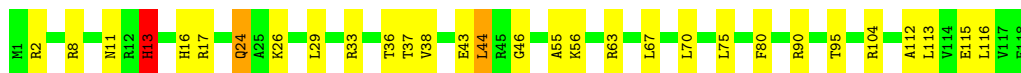
- Molecule 15: 50S ribosomal protein L16

Chain RQ: 72% 24%



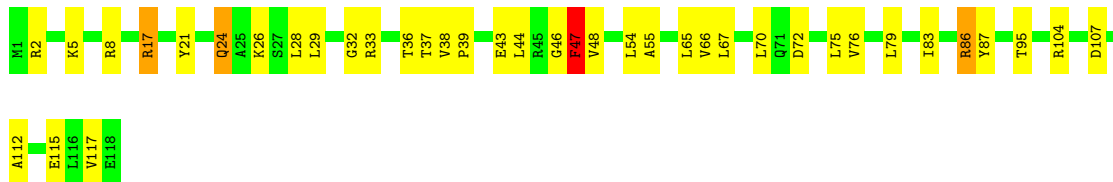
- Molecule 16: 50S ribosomal protein L17

Chain YR: 75% 23%



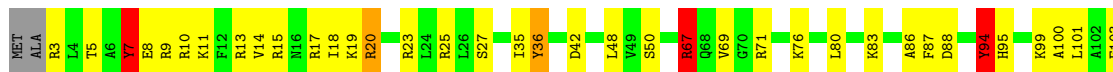
- Molecule 16: 50S ribosomal protein L17

Chain RR: 67% 30%



- Molecule 17: 50S ribosomal protein L18

Chain YS: 62% 31%

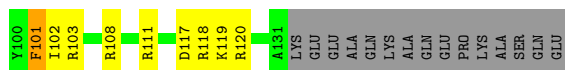
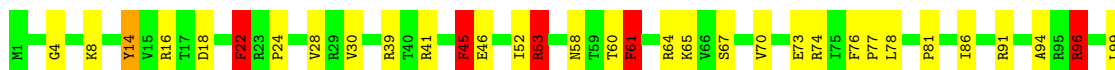




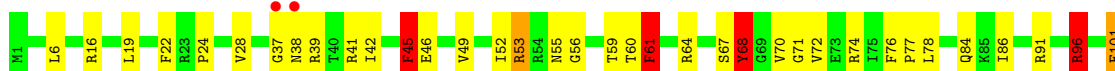
- Molecule 17: 50S ribosomal protein L18



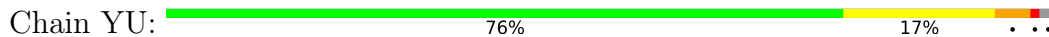
- Molecule 18: 50S ribosomal protein L19



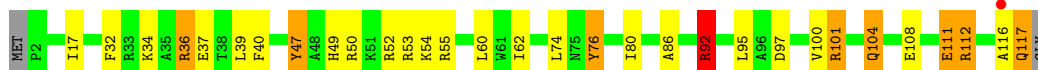
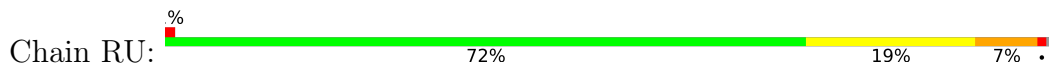
- Molecule 18: 50S ribosomal protein L19



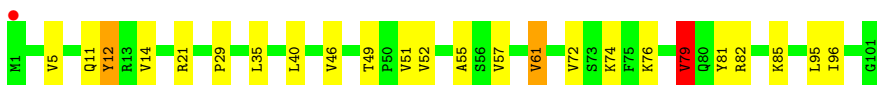
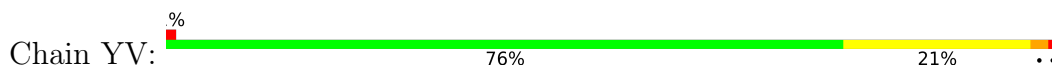
- Molecule 19: 50S ribosomal protein L20



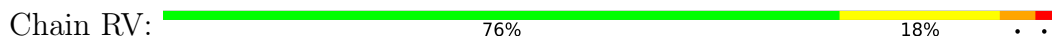
- Molecule 19: 50S ribosomal protein L20



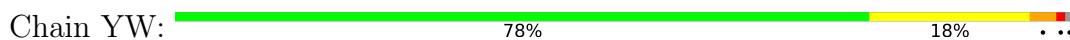
- Molecule 20: 50S ribosomal protein L21



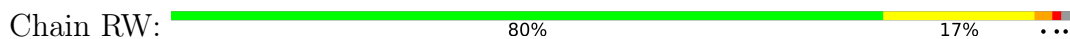
- Molecule 20: 50S ribosomal protein L21



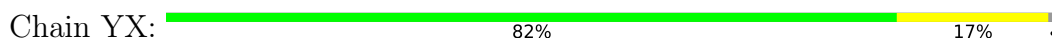
- Molecule 21: 50S ribosomal protein L22



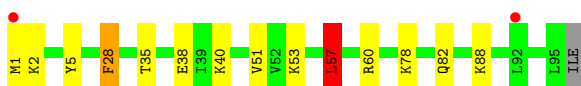
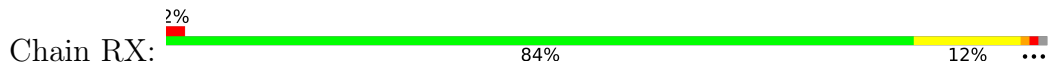
- Molecule 21: 50S ribosomal protein L22



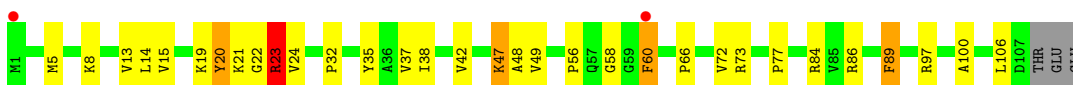
- Molecule 22: 50S ribosomal protein L23



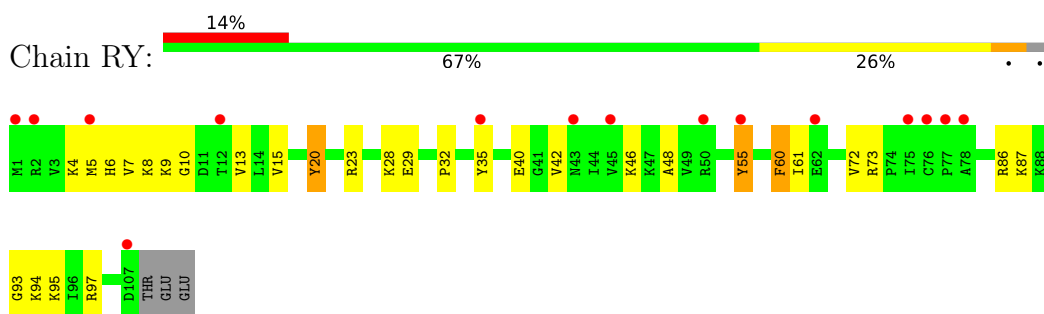
- Molecule 22: 50S ribosomal protein L23



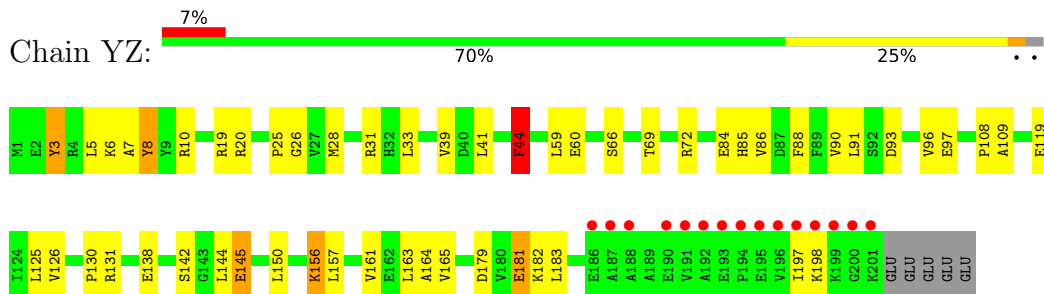
- Molecule 23: 50S ribosomal protein L24



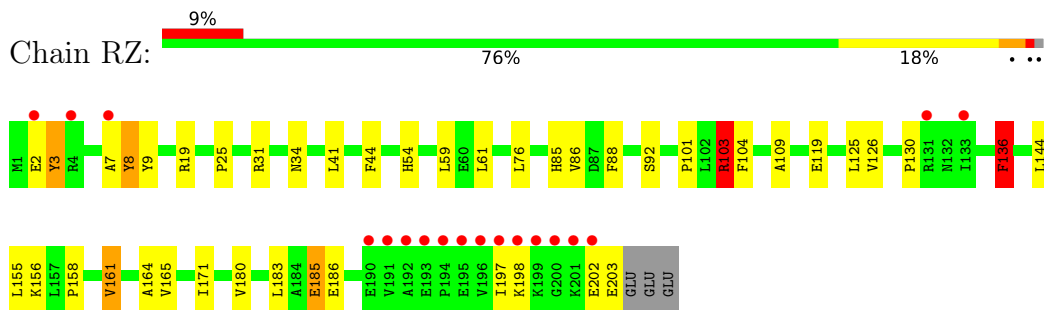
- Molecule 23: 50S ribosomal protein L24



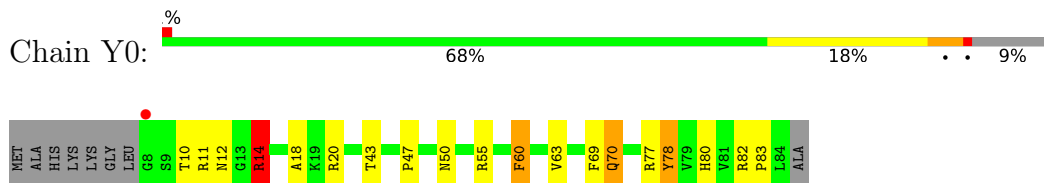
• Molecule 24: 50S ribosomal protein L25



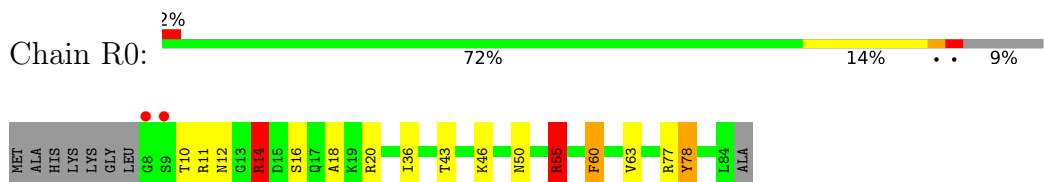
• Molecule 24: 50S ribosomal protein L25



• Molecule 25: 50S ribosomal protein L27



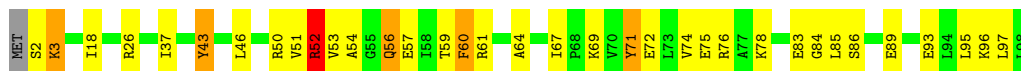
• Molecule 25: 50S ribosomal protein L27



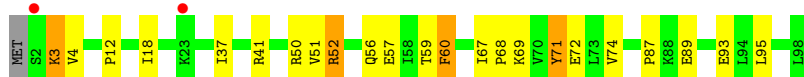
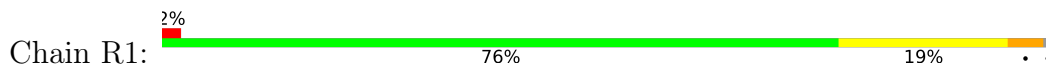
• Molecule 26: 50S ribosomal protein L28



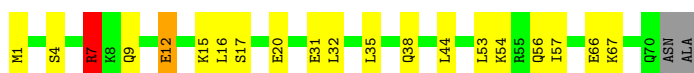




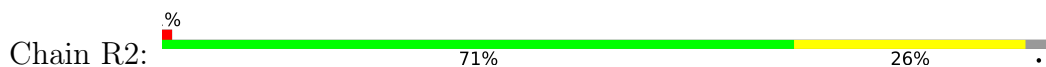
- Molecule 26: 50S ribosomal protein L28



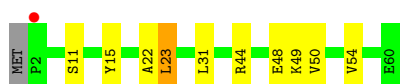
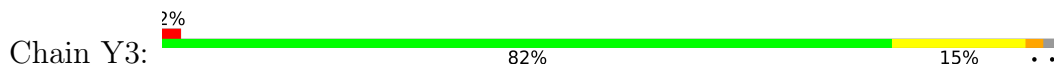
- Molecule 27: 50S ribosomal protein L29



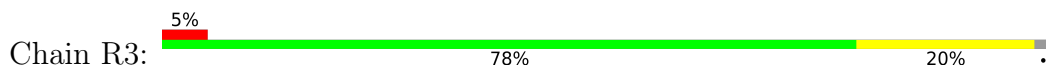
- Molecule 27: 50S ribosomal protein L29



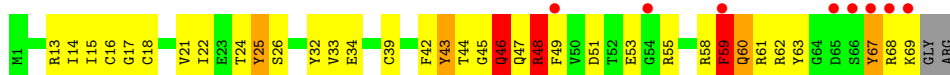
- Molecule 28: 50S ribosomal protein L30



- Molecule 28: 50S ribosomal protein L30



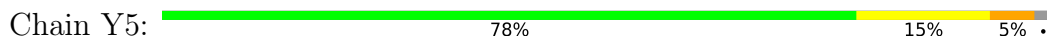
- Molecule 29: 50S ribosomal protein L31



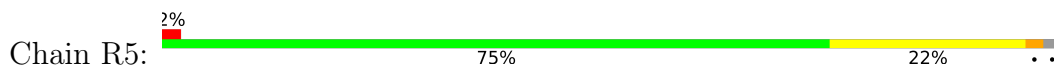
- Molecule 29: 50S ribosomal protein L31



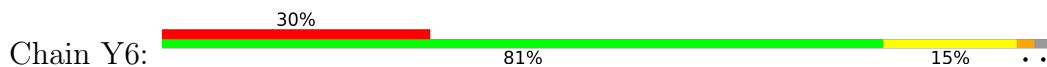
- Molecule 30: 50S ribosomal protein L32



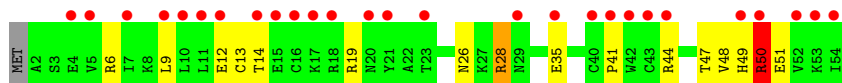
- Molecule 30: 50S ribosomal protein L32



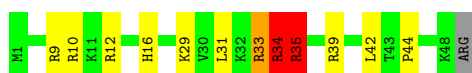
- Molecule 31: 50S ribosomal protein L33



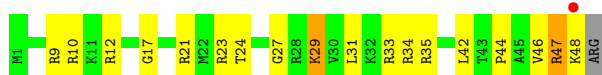
- Molecule 31: 50S ribosomal protein L33



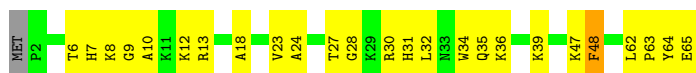
- Molecule 32: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L34



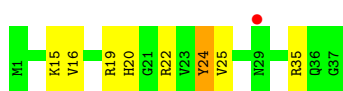
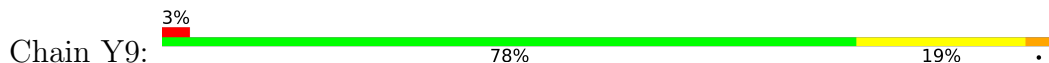
- Molecule 33: 50S ribosomal protein L35



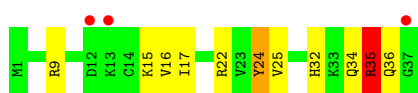
- Molecule 33: 50S ribosomal protein L35



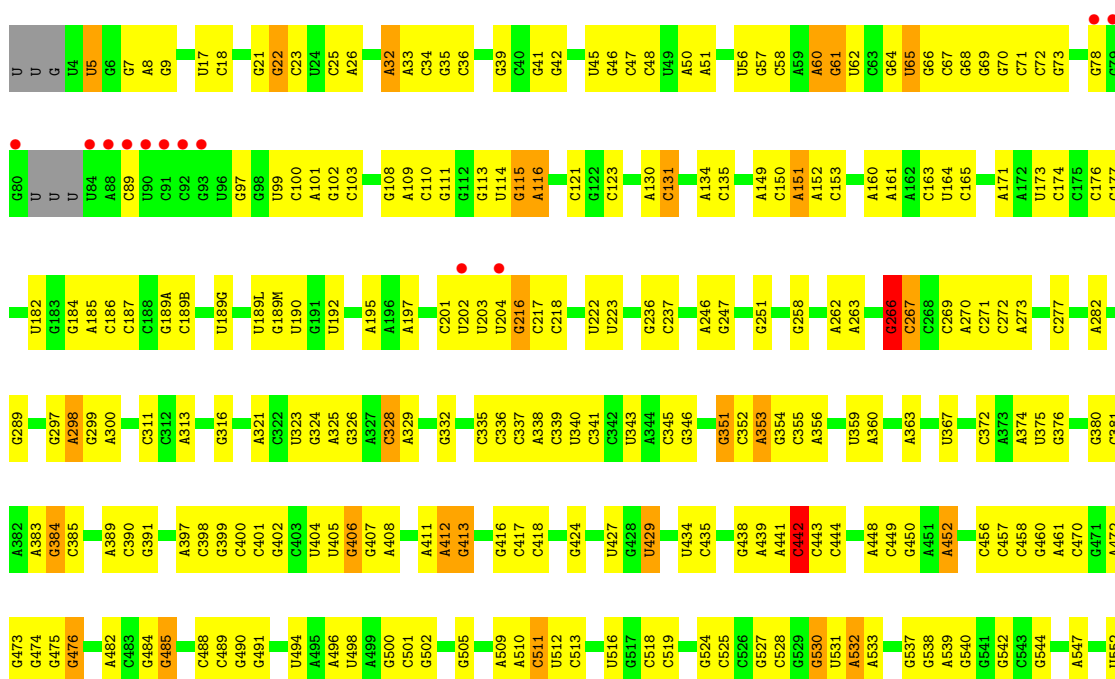
- Molecule 34: 50S ribosomal protein L36

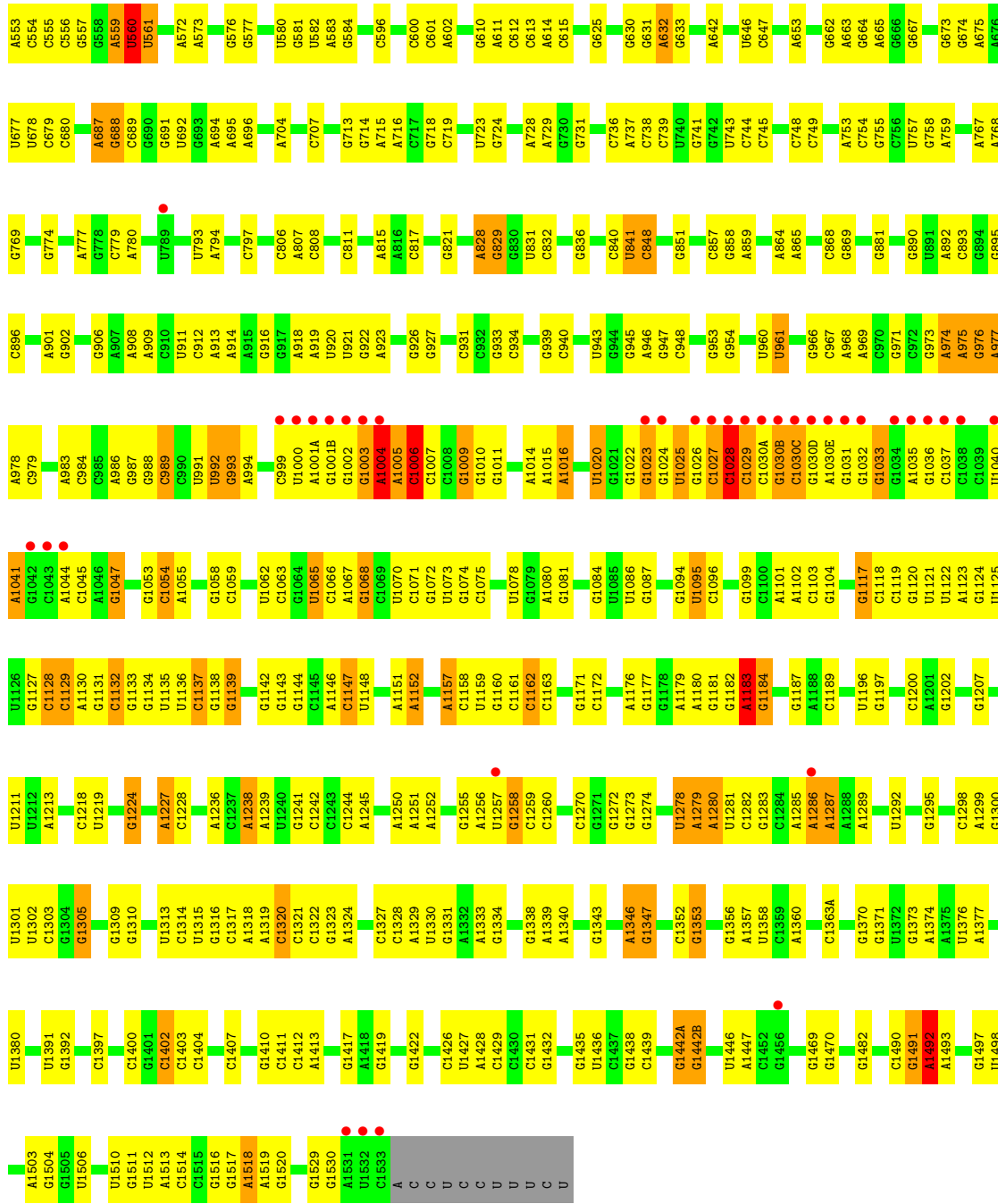


- Molecule 34: 50S ribosomal protein L36

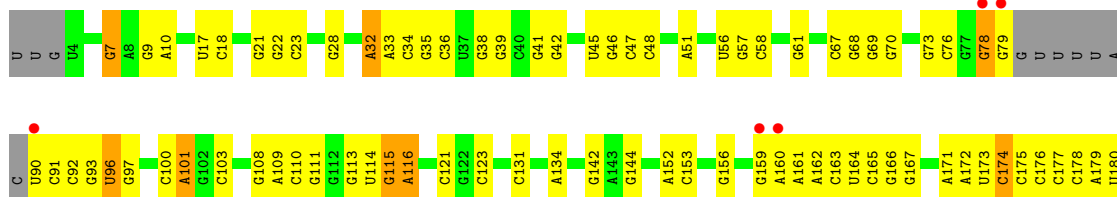


- Molecule 35: 16S rRNA

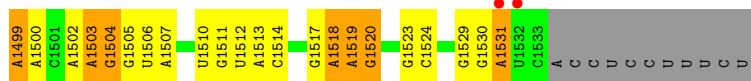




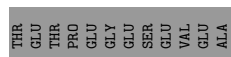
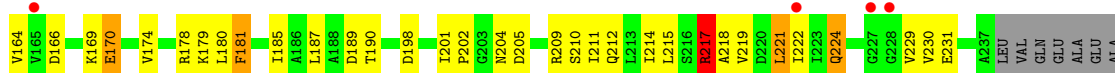
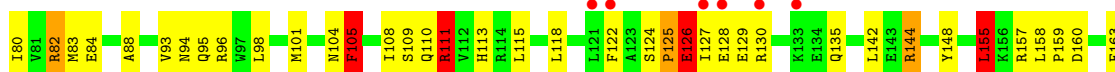
• Molecule 35: 16S rRNA



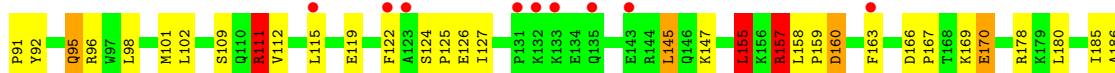
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C1298	A1299	C1300	U1301	C1302	C1303	G1304	U1308	C1309	G1310	U1315	G1316	G1317	A1318	A1319	C1320	C1321	C1322	G1323	A1324	C1325	C1326	C1327	G1338	A1339	A1340	G1343	C1344	U1345	A1346	G1347	G1353	G1356	A1357	U1358	C1359	A1360	C1363A	G1370	A1373	A1374	G1387	C1388	U1391	G1392	U1393	A1394	C1397							
U1211	U1212	A1213	G1216	G1217	C1218	U1219	G1224	A1225	C1226	C1227	G1228	A1229	A1238	U1239	U1240	G1241	C1243	C1244	A1245	C1246	A1250	A1251	A1252	G1255	A1256	U1257	C1258	C1259	G1260	A1261	C1262	C1263	C1264	C1270	C1277	U1278	A1279	A1280	U1281	A1285	A1286	A1287	A1288	A1289	U1292	G1293	C1294	G1295						
G1131	C1132	G1133	G1134	U1135	U1136	C1137	G1138	G1139	C1140	C1141	G1142	G1143	G1144	C1145	A1146	C1147	U1148	C1149	U1150	A1151	A1152	A1157	U1158	U1159	G1160	A1161	C1162	A1168	C1172	G1173	G1177	G1178	A1179	A1180	G1181	G1182	A1183	G1184	C1189	G1190	A1191	U1196	G1197	C1200	A1201	G1202	G1206	G1207	C1208	C1209	C1210			
G1036	C1037	C1039	G1042	C1043	A1044	G1047	G1048	C984	C985	U1052	G1053	C1060	U1061	U1062	C1063	U1064	C1066	A1067	U1068	U1070	C1071	G1072	U1073	G1074	U1078	G1081	U1086	G1088	U1094	U1096	G1099	C1100	A1101	C1103	G1104	C1112	G1117	C1118	U1122	A1123	G1124	U1125	U1126	A1130										
G973	A974	A975	G976	A977	A978	U981	U982	A983	C984	C985	A986	G987	U991	U992	G993	G998	C999	U1000	A1001A	G1001B	G1002	G1003	A1004	A1005	A1006	C1007	U1008	G1009	G1010	G1013	A1014	A1015	A1016	G1017	U1020	G1022	G1023	U1025	G1026	C1027	C1028	C1029	C1030A	G1030B	C1030C	G1030D	G966	C967	A968	A969	G970	G971	C972	
A865	C868	C869	G876	G885	A892	C893	G894	G895	C896	A901	C902	U911	C912	A913	A914	G791	U793	A794	G774	A777	G791	C806	A807	U677	U678	U679	C680	A687	G688	U692	C600	C601	G604	A607	G610	A611	C612	A613	A614	C618	U619	C620	A621	C624	G625	U626	G629	G630	G631	A632	G633	C634	G635	U636
C744	C745	A746	C747	C748	C749	G750	U751	G752	A753	C754	G755	C756	U757	G758	A768	G769	G774	A675	A676	U677	U678	C679	C680	A687	G688	U692	C600	C601	G604	A704	C707	G713	G714	A715	A716	C717	C718	C719	A828	G829	U833	C834	G838	U839	C840	U841	C848	C851	C857	G858	U743			
A637	A642	C643	G644	C645	U646	C647	U652	A653	G661	G662	A663	A664	A665	G673	A675	A676	U677	U678	C679	C680	A687	G688	U692	C600	C601	G604	A704	C707	G713	G714	A715	A716	C717	C718	C719	A828	G829	U833	C834	G838	U839	C840	U841	C848	C851	C857	G858	U743						
U567	U568	C372	A373	A374	U375	G376	G377	G384	C385	G388	A389	C390	G391	G392	A393	G396	A397	C398	G399	C400	C401	G402	C403	U404	U405	G406	G407	G408	G409	C410	A411	C412	G413	A414	G521	C522	A523	G524	C525	C526	G527	U531	A532	G537	G538	A539	G540	A439	A441	C442	C449			
A452	A453	C454	C455	C456	C457	C458	G460	A461	C470	G475	G476	A477	C483	C484	G485	A496	U498	A499	G500	C501	G502	G505	A509	A510	C511	U512	C513	C514	G515	U516	G517	C518	G521	C522	A523	G524	C525	C526	G527	U531	A532	G537	G538	A539	G540	A439	A441	C442	C449					
A270	C271	G276	C277	A282	G289	U296	G297	A298	G299	A300	G309	G310	C311	G316	A321	C322	U323	C324	A325	G326	A327	U328	A329	G332	G333	C334	C335	U336	C337	A338	C339	U340	C341	C342	U343	A344	C345	U347	G347	G348	G351	C352	A353	G354	A439	A441	C442	C449						
U182	G183	G184	A185	C186	C187	C188	G189A	C189B	U189G	G189K	U189L	G189M	U190	G191	U192	C193	C194	A195	A196	A197	C201	U202	U203	U204	G216	C217	C218	C219	G220	U222	U223	C224	C225	C235	C236	A246	G247	A250	G251	U252	G258	U261	A262	A263	G268	C267	C269							



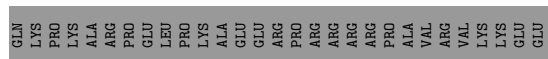
• Molecule 36: 30S ribosomal protein S2



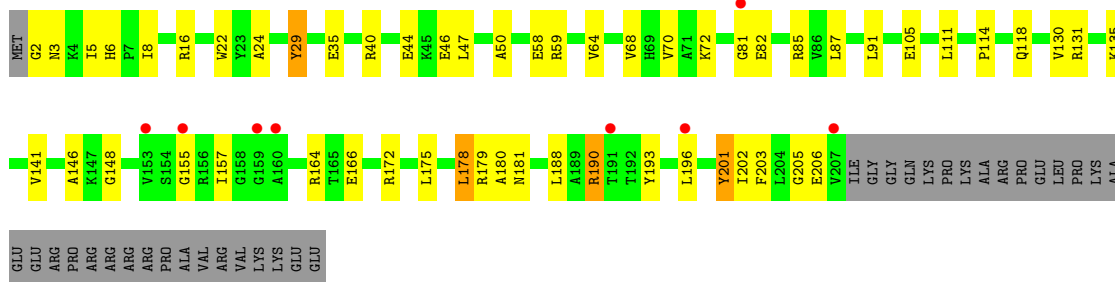
• Molecule 36: 30S ribosomal protein S2



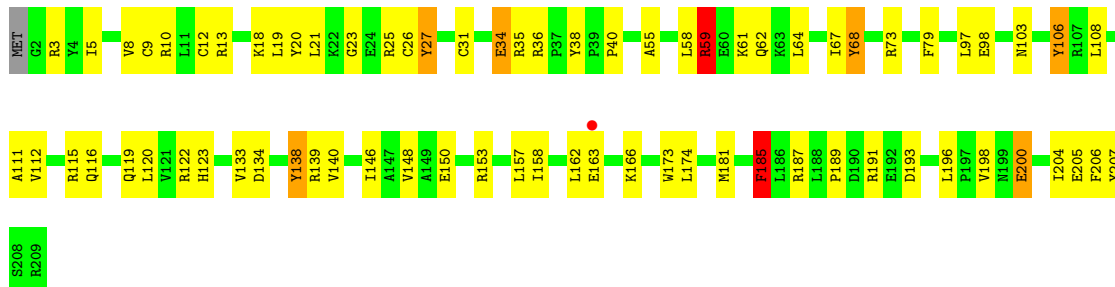
• Molecule 37: 30S ribosomal protein S3



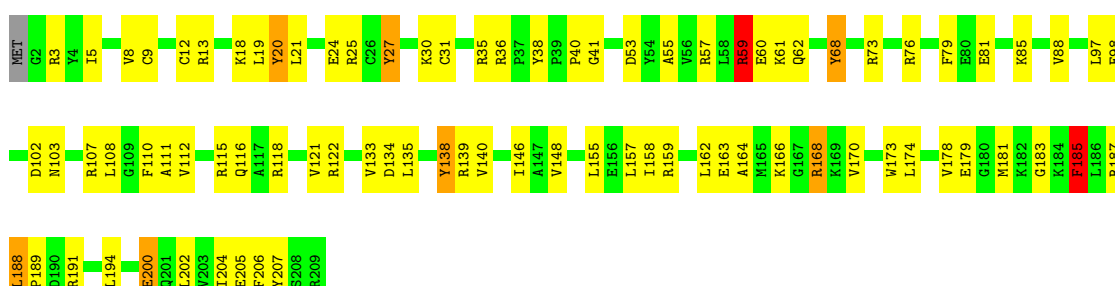
• Molecule 37: 30S ribosomal protein S3



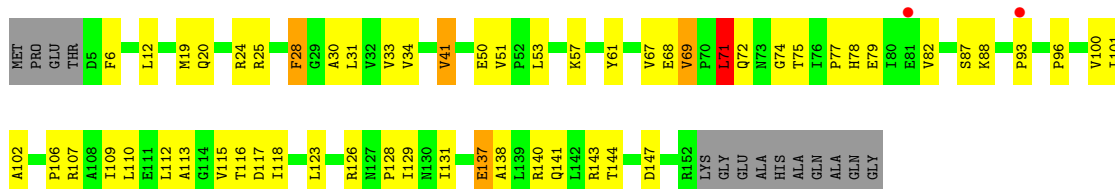
• Molecule 38: 30S ribosomal protein S4



• Molecule 38: 30S ribosomal protein S4

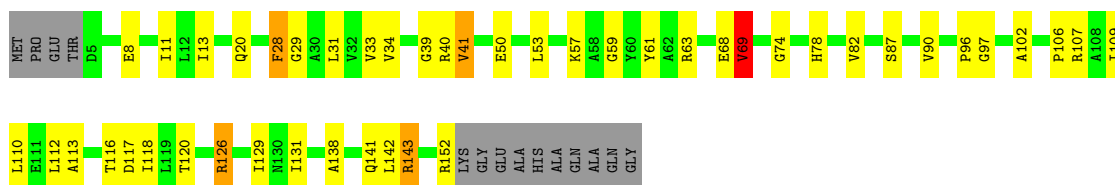


• Molecule 39: 30S ribosomal protein S5



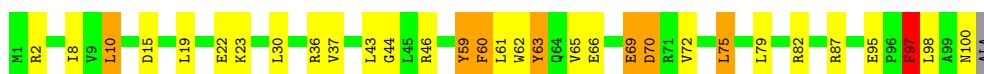
- Molecule 39: 30S ribosomal protein S5

Chain QE:  63% 25% 9%



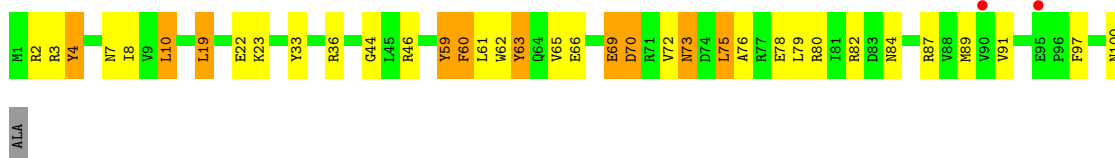
- Molecule 40: 30S ribosomal protein S6

Chain XF:  68% 23% 7% ..



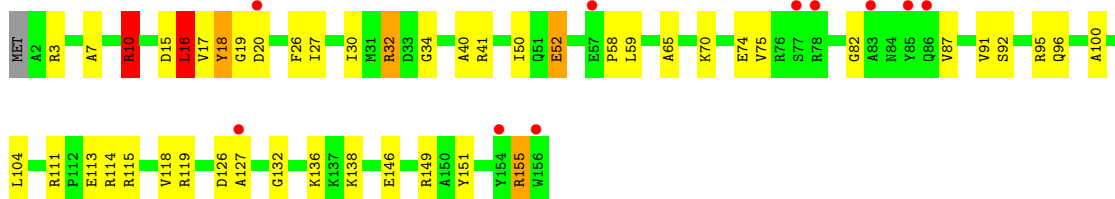
- Molecule 40: 30S ribosomal protein S6

Chain QF:  63% 26% 10% ..




- Molecule 41: 30S ribosomal protein S7

Chain XG:  6% 69% 26% ..



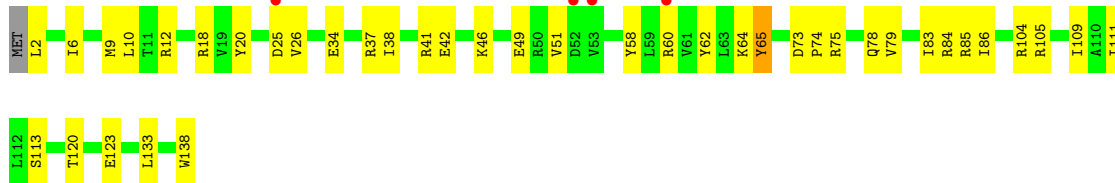
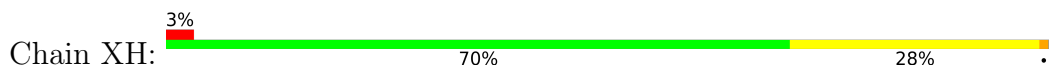
- Molecule 41: 30S ribosomal protein S7

Chain QG:  10% 83% 15% ..

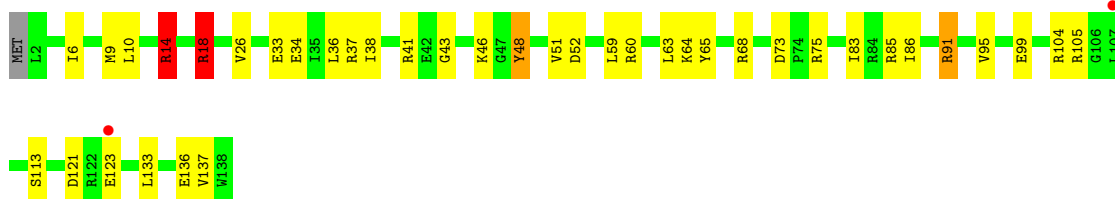
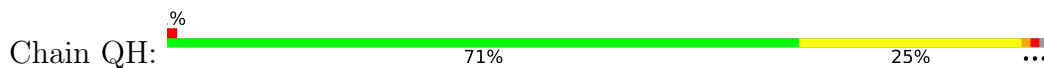


- Molecule 42: 30S ribosomal protein S8

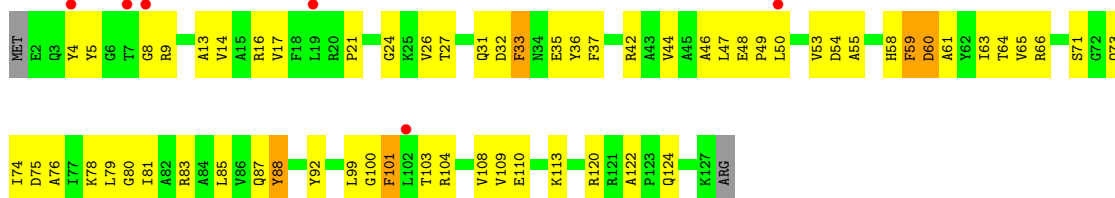




- Molecule 42: 30S ribosomal protein S8



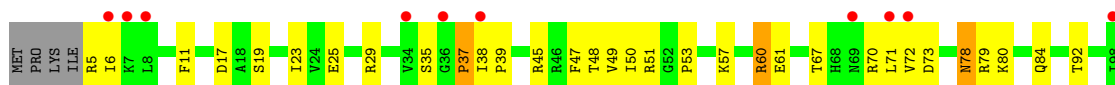
- Molecule 43: 30S ribosomal protein S9



- Molecule 43: 30S ribosomal protein S9

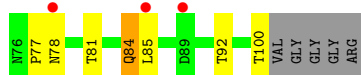
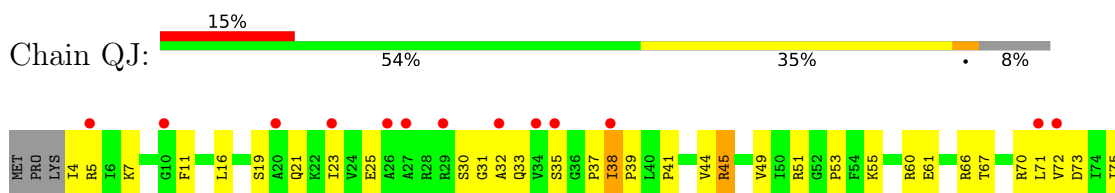


- Molecule 44: 30S ribosomal protein S10

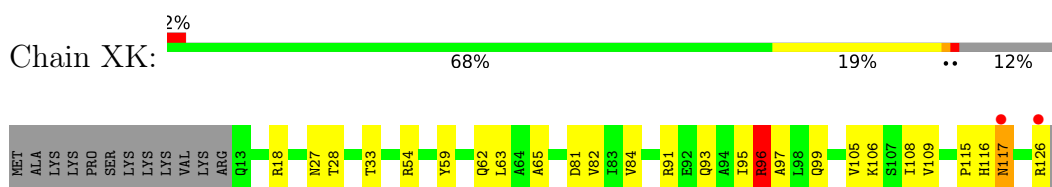




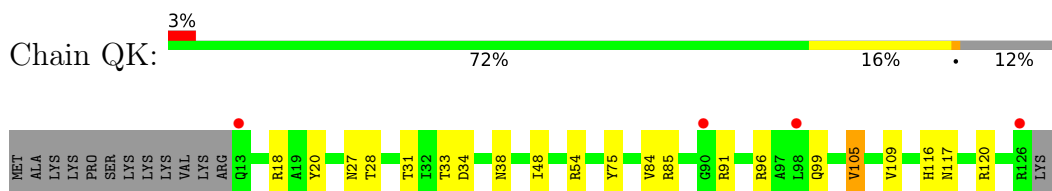
- Molecule 44: 30S ribosomal protein S10



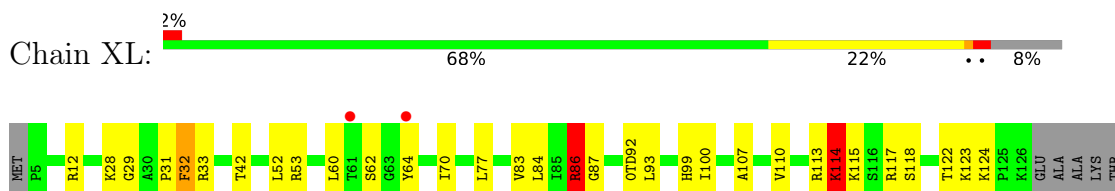
- Molecule 45: 30S ribosomal protein S11



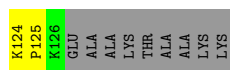
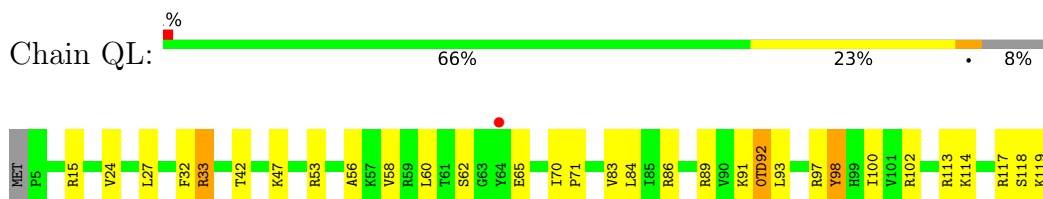
- Molecule 45: 30S ribosomal protein S11



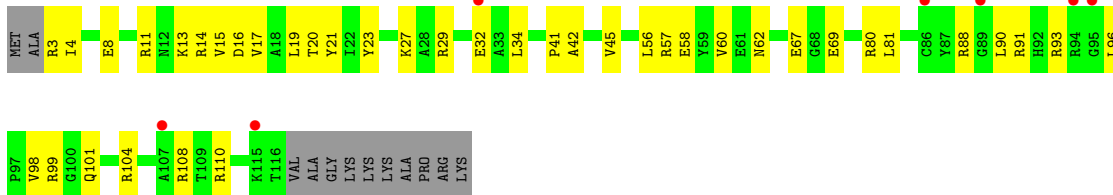
- Molecule 46: 30S ribosomal protein S12



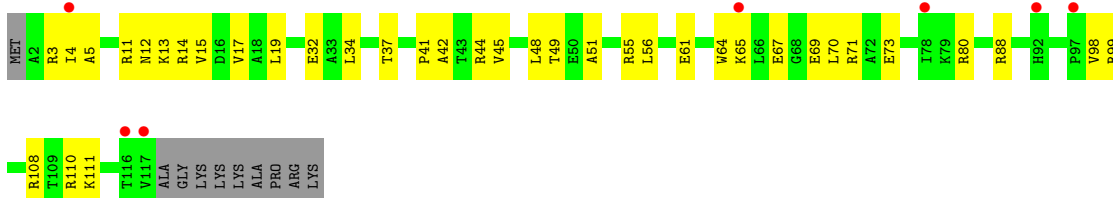
- Molecule 46: 30S ribosomal protein S12



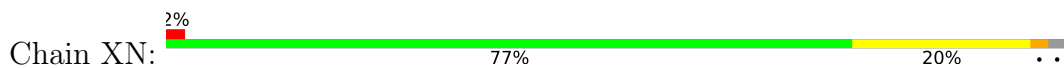
- Molecule 47: 30S ribosomal protein S13



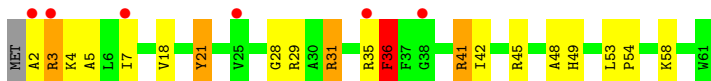
- Molecule 47: 30S ribosomal protein S13



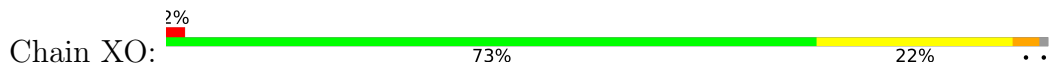
- Molecule 48: 30S ribosomal protein S14 type Z



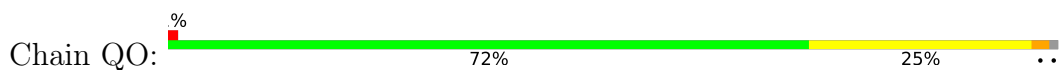
- Molecule 48: 30S ribosomal protein S14 type Z



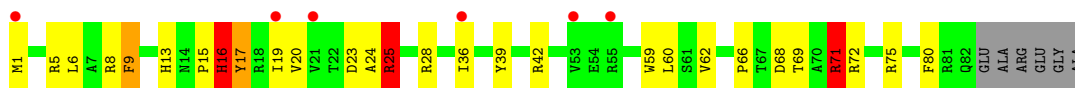
- Molecule 49: 30S ribosomal protein S15



- Molecule 49: 30S ribosomal protein S15



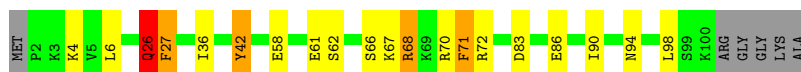
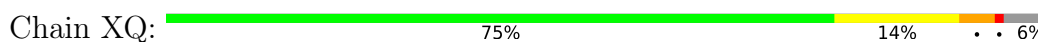
• Molecule 50: 30S ribosomal protein S16



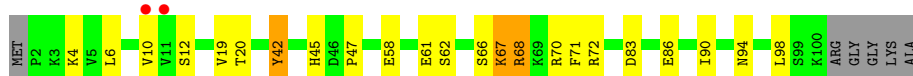
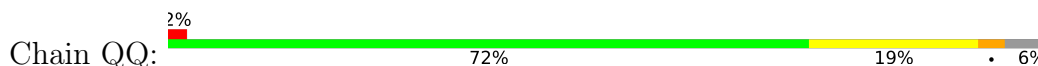
• Molecule 50: 30S ribosomal protein S16



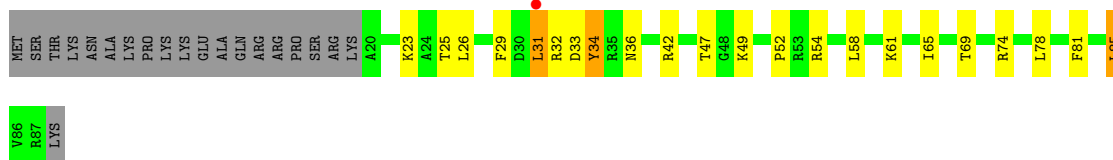
• Molecule 51: 30S ribosomal protein S17



• Molecule 51: 30S ribosomal protein S17



• Molecule 52: 30S ribosomal protein S18

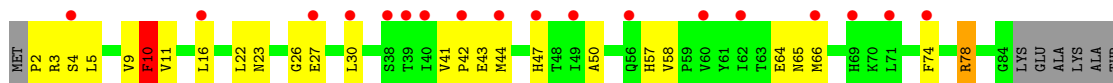


• Molecule 52: 30S ribosomal protein S18

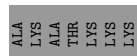
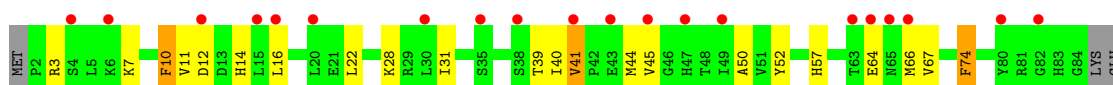




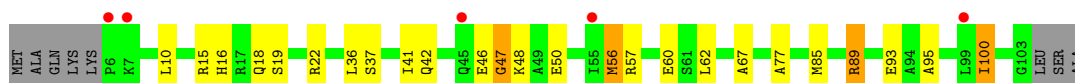
- Molecule 53: 30S ribosomal protein S19



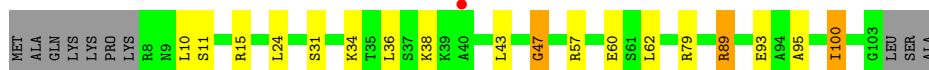
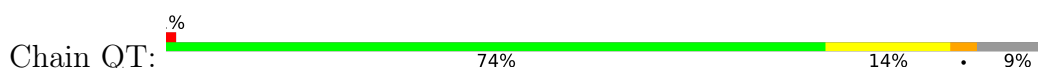
- Molecule 53: 30S ribosomal protein S19



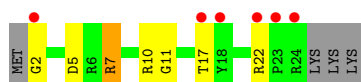
- Molecule 54: 30S ribosomal protein S20



- Molecule 54: 30S ribosomal protein S20

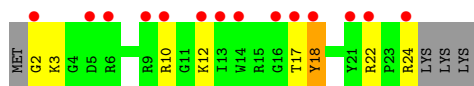


- Molecule 55: 30S ribosomal protein Thx



- Molecule 55: 30S ribosomal protein Thx





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.48Å 450.41Å 622.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.88 – 3.10 49.88 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.88-3.10) 100.0 (49.88-3.10)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.196 , 0.227 0.196 , 0.227	Depositor DCC
$R_{free}$ test set	49511 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.2	Xtrriage
Anisotropy	0.251	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 70.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	296662	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 2MU, SF4, OMG, 4OC, MA6, 5MU, 2MA, UR3, 0TD, ZN, 5MC, 2MG, PSU, 7MG, M2G, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	QV	0.39	1/1836 (0.1%)	0.88	5/2859 (0.2%)
1	XV	0.35	1/1836 (0.1%)	0.81	2/2859 (0.1%)
2	QX	0.31	0/241	0.88	0/373
2	XX	0.29	0/241	0.85	0/373
3	QY	0.39	1/2873 (0.0%)	0.88	12/3870 (0.3%)
3	XY	0.38	1/2873 (0.0%)	0.77	9/3870 (0.2%)
4	RA	0.28	0/68901	0.90	93/107544 (0.1%)
4	YA	0.30	0/68901	0.88	81/107544 (0.1%)
5	RB	0.24	0/2876	0.85	0/4486
5	YB	0.27	0/2878	0.88	0/4490
6	RD	0.39	1/2181 (0.0%)	0.71	2/2940 (0.1%)
6	YD	0.47	2/2186 (0.1%)	0.88	9/2944 (0.3%)
7	RE	0.35	0/1592	0.68	0/2149
7	YE	0.48	3/1592 (0.2%)	0.74	4/2149 (0.2%)
8	RF	0.34	0/1619	0.75	4/2193 (0.2%)
8	YF	0.33	0/1615	0.71	2/2188 (0.1%)
9	RG	0.49	1/1451 (0.1%)	0.75	3/1961 (0.2%)
9	YG	0.36	0/1449	0.75	0/1957
10	RH	0.35	1/1356 (0.1%)	0.68	1/1834 (0.1%)
10	YH	0.40	1/1350 (0.1%)	0.79	5/1826 (0.3%)
11	RI	0.39	1/1109 (0.1%)	0.75	2/1512 (0.1%)
11	YI	0.41	1/1091 (0.1%)	0.82	6/1490 (0.4%)
12	RN	0.62	3/1148 (0.3%)	0.77	2/1547 (0.1%)
12	YN	0.44	1/1144 (0.1%)	0.71	3/1543 (0.2%)
13	RO	0.32	0/943	0.67	3/1269 (0.2%)
13	YO	0.38	1/943 (0.1%)	0.69	2/1269 (0.2%)
14	RP	0.35	0/1152	0.81	3/1533 (0.2%)
14	YP	0.36	0/1152	0.82	3/1533 (0.2%)
15	RQ	0.37	0/1143	0.78	5/1527 (0.3%)
15	YQ	0.39	0/1143	0.70	1/1527 (0.1%)
16	RR	0.42	1/982 (0.1%)	0.87	6/1312 (0.5%)
16	YR	0.41	1/982 (0.1%)	0.75	2/1312 (0.2%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	RS	0.39	0/887	0.78	3/1180 (0.3%)
17	YS	0.40	0/880	0.96	4/1172 (0.3%)
18	RT	0.37	0/1105	0.87	6/1477 (0.4%)
18	YT	0.36	0/1097	0.90	7/1468 (0.5%)
19	RU	0.61	3/977 (0.3%)	1.20	9/1301 (0.7%)
19	YU	0.66	3/977 (0.3%)	1.09	8/1301 (0.6%)
20	RV	0.51	1/786 (0.1%)	1.31	5/1053 (0.5%)
20	YV	0.39	0/782	0.80	2/1049 (0.2%)
21	RW	0.31	0/897	0.71	3/1205 (0.2%)
21	YW	0.32	0/897	0.72	3/1205 (0.2%)
22	RX	0.31	0/764	0.66	1/1025 (0.1%)
22	YX	0.30	0/764	0.62	0/1025
23	RY	0.32	0/823	0.67	0/1099
23	YY	0.51	1/823 (0.1%)	0.92	4/1100 (0.4%)
24	RZ	0.36	0/1620	0.77	5/2200 (0.2%)
24	YZ	0.40	1/1590 (0.1%)	0.78	6/2162 (0.3%)
25	R0	0.46	0/616	1.07	5/821 (0.6%)
25	Y0	0.48	1/616 (0.2%)	0.87	2/821 (0.2%)
26	R1	0.33	0/761	0.75	2/1013 (0.2%)
26	Y1	0.73	5/766 (0.7%)	0.85	5/1018 (0.5%)
27	R2	0.35	0/590	0.70	0/781
27	Y2	0.56	2/594 (0.3%)	0.82	3/785 (0.4%)
28	R3	0.41	1/474 (0.2%)	0.63	0/635
28	Y3	0.28	0/469	0.61	0/630
29	R4	0.68	3/559 (0.5%)	1.06	4/754 (0.5%)
29	Y4	0.64	2/549 (0.4%)	1.05	6/741 (0.8%)
30	R5	0.54	1/473 (0.2%)	0.87	2/639 (0.3%)
30	Y5	0.52	0/469	0.73	0/635
31	R6	0.69	2/460 (0.4%)	1.23	5/613 (0.8%)
31	Y6	0.34	0/456	0.62	0/608
32	R7	0.59	2/426 (0.5%)	0.97	2/561 (0.4%)
32	Y7	0.37	0/426	0.92	4/561 (0.7%)
33	R8	0.33	0/525	0.87	2/691 (0.3%)
33	Y8	0.31	0/525	0.66	0/691
34	R9	0.48	1/310 (0.3%)	1.08	4/407 (1.0%)
34	Y9	0.29	0/310	0.69	0/407
35	QA	0.25	0/35795	0.86	32/55864 (0.1%)
35	XA	0.26	0/35890	0.88	34/56012 (0.1%)
36	QB	0.43	1/1876 (0.1%)	0.93	12/2533 (0.5%)
36	XB	0.47	1/1860 (0.1%)	1.14	14/2518 (0.6%)
37	QC	0.36	0/1582	0.69	1/2137 (0.0%)
37	XC	0.43	1/1566 (0.1%)	0.87	6/2119 (0.3%)
38	QD	0.36	0/1695	0.82	6/2274 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	XD	0.41	0/1698	0.79	2/2277 (0.1%)
39	QE	0.40	1/1149 (0.1%)	0.79	6/1548 (0.4%)
39	XE	0.41	1/1149 (0.1%)	0.65	1/1548 (0.1%)
40	QF	0.46	0/827	0.87	3/1120 (0.3%)
40	XF	0.39	0/829	0.83	1/1123 (0.1%)
41	QG	0.33	0/1254	0.66	1/1683 (0.1%)
41	XG	0.50	0/1248	0.84	7/1676 (0.4%)
42	QH	0.45	3/1118 (0.3%)	1.03	6/1506 (0.4%)
42	XH	0.41	0/1108	0.79	4/1494 (0.3%)
43	QI	0.71	1/1005 (0.1%)	0.92	5/1351 (0.4%)
43	XI	0.36	0/985	0.76	0/1329
44	QJ	0.36	0/732	0.80	3/993 (0.3%)
44	XJ	0.28	0/723	0.59	0/984
45	QK	0.34	0/849	0.71	2/1150 (0.2%)
45	XK	0.33	0/848	0.70	2/1149 (0.2%)
46	QL	0.34	0/937	0.71	1/1260 (0.1%)
46	XL	0.47	1/937 (0.1%)	0.74	2/1260 (0.2%)
47	QM	0.34	0/924	0.68	0/1242
47	XM	0.29	0/905	0.65	0/1217
48	QN	0.44	0/501	0.97	5/664 (0.8%)
48	XN	0.38	0/501	0.83	4/664 (0.6%)
49	QO	0.49	0/739	1.17	9/985 (0.9%)
49	XO	0.37	0/739	0.76	2/985 (0.2%)
50	QP	0.37	0/697	0.73	0/939
50	XP	0.60	1/693 (0.1%)	1.37	6/935 (0.6%)
51	QQ	0.34	0/836	0.69	0/1117
51	XQ	0.44	1/836 (0.1%)	0.68	1/1117 (0.1%)
52	QR	0.34	0/560	0.92	3/746 (0.4%)
52	XR	0.30	0/560	0.71	0/746
53	QS	0.61	2/663 (0.3%)	0.74	1/895 (0.1%)
53	XS	0.30	0/660	0.69	3/893 (0.3%)
54	QT	0.37	1/734 (0.1%)	0.65	1/969 (0.1%)
54	XT	0.41	1/736 (0.1%)	0.68	3/976 (0.3%)
55	QU	0.35	0/203	0.75	0/266
55	XU	0.32	0/203	0.68	0/266
All	All	0.33	67/318172 (0.0%)	0.86	571/475147 (0.1%)

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

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

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	QI	93	ARG	CB-CG	-17.94	1.04	1.52
53	QS	28	LYS	CD-CE	-11.05	1.23	1.51
26	Y1	52	ARG	CZ-NH2	10.67	1.47	1.33
1	QV	1	C	OP3-P	-10.63	1.48	1.61
1	XV	1	C	OP3-P	-10.63	1.48	1.61

The worst 5 of 571 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	RA	2603	G	O5'-P-OP1	-35.76	67.78	110.70
36	XB	217	ARG	NE-CZ-NH2	-28.77	105.92	120.30
20	RV	21	ARG	NE-CZ-NH2	-27.66	106.47	120.30
50	XP	71	ARG	NE-CZ-NH2	-21.01	109.79	120.30
42	QH	14	ARG	NE-CZ-NH1	19.41	130.01	120.30

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	QY	115	PHE	Peptide
3	QY	201	LEU	Peptide
3	QY	48	ASN	Sidechain
26	Y1	52	ARG	Sidechain
11	YI	84	GLY	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QV	1644	0	836	29	0
1	XV	1644	0	836	19	0
2	QX	215	0	109	3	0
2	XX	215	0	108	6	0
3	QY	2833	0	2729	139	0
3	XY	2833	0	2729	155	0
4	RA	61758	0	31149	799	0
4	YA	61758	0	31152	795	0
5	RB	2572	0	1305	19	0
5	YB	2573	0	1306	17	0
6	RD	2131	0	2207	63	0
6	YD	2136	0	2217	65	0
7	RE	1559	0	1618	41	0
7	YE	1559	0	1618	43	0
8	RF	1584	0	1625	58	0
8	YF	1580	0	1619	68	0
9	RG	1426	0	1445	51	0
9	YG	1424	0	1441	60	0
10	RH	1330	0	1407	30	0
10	YH	1324	0	1402	43	0
11	RI	1094	0	1127	34	0
11	YI	1076	0	1094	24	0
12	RN	1121	0	1195	27	0
12	YN	1117	0	1184	22	0
13	RO	933	0	996	28	0
13	YO	933	0	996	26	0
14	RP	1135	0	1212	33	0
14	YP	1135	0	1212	44	0
15	RQ	1122	0	1179	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	YQ	1122	0	1179	38	0
16	RR	968	0	1033	32	0
16	YR	968	0	1033	21	0
17	RS	877	0	938	38	0
17	YS	870	0	923	41	0
18	RT	1091	0	1151	44	0
18	YT	1083	0	1136	54	0
19	RU	959	0	1019	31	0
19	YU	959	0	1019	27	0
20	RV	775	0	841	23	0
20	YV	771	0	830	21	0
21	RW	886	0	940	18	0
21	YW	886	0	940	21	0
22	RX	750	0	814	13	0
22	YX	750	0	814	8	0
23	RY	810	0	892	35	0
23	YY	810	0	887	34	0
24	RZ	1587	0	1598	48	0
24	YZ	1557	0	1564	53	0
25	R0	608	0	622	19	0
25	Y0	608	0	622	21	0
26	R1	754	0	823	17	0
26	Y1	759	0	837	27	0
27	R2	588	0	643	13	0
27	Y2	592	0	654	17	0
28	R3	469	0	518	8	0
28	Y3	464	0	514	5	0
29	R4	546	0	522	37	0
29	Y4	536	0	514	45	0
30	R5	459	0	476	13	0
30	Y5	455	0	465	9	0
31	R6	453	0	473	9	0
31	Y6	449	0	469	6	0
32	R7	418	0	467	16	0
32	Y7	418	0	467	11	0
33	R8	517	0	582	21	0
33	Y8	517	0	582	26	0
34	R9	307	0	335	9	0
34	Y9	307	0	335	6	0
35	QA	32246	0	16294	525	0
35	XA	32331	0	16339	485	0
36	QB	1842	0	1862	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	XB	1825	0	1828	104	0
37	QC	1558	0	1557	50	0
37	XC	1542	0	1517	49	0
38	QD	1665	0	1688	86	0
38	XD	1668	0	1704	75	0
39	QE	1133	0	1191	33	0
39	XE	1133	0	1191	41	0
40	QF	814	0	808	44	0
40	XF	816	0	808	32	0
41	QG	1235	0	1249	23	0
41	XG	1229	0	1238	34	0
42	QH	1098	0	1143	33	0
42	XH	1088	0	1126	28	0
43	QI	986	0	990	50	0
43	XI	966	0	953	65	0
44	QJ	719	0	672	35	0
44	XJ	710	0	661	27	0
45	QK	834	0	838	13	0
45	XK	833	0	836	21	0
46	QL	932	0	981	36	0
46	XL	932	0	981	31	0
47	QM	914	0	954	36	0
47	XM	895	0	920	34	0
48	QN	492	0	529	29	0
48	XN	492	0	529	16	0
49	QO	728	0	760	16	0
49	XO	728	0	760	17	0
50	QP	681	0	697	30	0
50	XP	677	0	686	33	0
51	QQ	823	0	891	22	0
51	XQ	823	0	891	18	0
52	QR	555	0	618	22	0
52	XR	555	0	618	20	0
53	QS	648	0	658	22	0
53	XS	645	0	635	27	0
54	QT	732	0	809	13	0
54	XT	733	0	795	16	0
55	QU	199	0	208	10	0
55	XU	199	0	208	5	0
56	QA	279	0	0	0	0
56	QB	1	0	0	0	0
56	QD	3	0	0	0	0

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
All	All	296662	0	200145	5370	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 5370 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:RN:121:LYS:CD	12:RN:121:LYS:CE	1.75	1.59
4:YA:2012:G:OP1	21:YW:11:ARG:NH2	1.88	1.07
36:QB:15:VAL:HG23	36:QB:209:ARG:HB3	1.36	1.06
35:XA:1003:G:H2'	35:XA:1004:A:H4'	1.33	1.05
3:XY:281:HIS:HE1	4:YA:2493:U:H1'	1.22	1.04

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	QY	355/380 (93%)	304 (86%)	43 (12%)	8 (2%)	6	28
3	XY	355/380 (93%)	310 (87%)	33 (9%)	12 (3%)	3	21
6	RD	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
6	YD	273/276 (99%)	257 (94%)	15 (6%)	1 (0%)	34	69
7	RE	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29	64
7	YE	202/206 (98%)	192 (95%)	8 (4%)	2 (1%)	15	49
8	RF	201/210 (96%)	197 (98%)	4 (2%)	0	100	100
8	YF	201/210 (96%)	197 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	RG	179/182 (98%)	166 (93%)	10 (6%)	3 (2%)	9	36
9	YG	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	25	59
10	RH	172/180 (96%)	163 (95%)	9 (5%)	0	100	100
10	YH	171/180 (95%)	159 (93%)	12 (7%)	0	100	100
11	RI	145/148 (98%)	130 (90%)	13 (9%)	2 (1%)	11	40
11	YI	144/148 (97%)	136 (94%)	6 (4%)	2 (1%)	11	40
12	RN	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
12	YN	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	22	57
13	RO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
13	YO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
14	RP	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
14	YP	147/150 (98%)	137 (93%)	8 (5%)	2 (1%)	11	40
15	RQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
15	YQ	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	22	57
16	RR	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
16	YR	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
17	RS	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
17	YS	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
18	RT	129/146 (88%)	120 (93%)	7 (5%)	2 (2%)	9	37
18	YT	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
19	RU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
19	YU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
20	RV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	49
20	YV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	49
21	RW	110/113 (97%)	110 (100%)	0	0	100	100
21	YW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
22	RX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
22	YX	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	14	46
23	RY	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
23	YY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
24	RZ	201/206 (98%)	192 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	YZ	199/206 (97%)	188 (94%)	11 (6%)	0	100	100
25	R0	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
25	Y0	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
26	R1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	46
26	Y1	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	14	46
27	R2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
27	Y2	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
28	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
29	R4	67/71 (94%)	52 (78%)	10 (15%)	5 (8%)	1	6
29	Y4	67/71 (94%)	57 (85%)	7 (10%)	3 (4%)	2	15
30	R5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
30	Y5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
31	R6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
31	Y6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
32	R7	46/49 (94%)	46 (100%)	0	0	100	100
32	Y7	46/49 (94%)	46 (100%)	0	0	100	100
33	R8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
33	Y8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
34	R9	35/37 (95%)	35 (100%)	0	0	100	100
34	Y9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
36	QB	229/256 (90%)	197 (86%)	20 (9%)	12 (5%)	2	12
36	XB	229/256 (90%)	198 (86%)	24 (10%)	7 (3%)	4	23
37	QC	204/239 (85%)	195 (96%)	9 (4%)	0	100	100
37	XC	204/239 (85%)	193 (95%)	9 (4%)	2 (1%)	15	49
38	QD	206/209 (99%)	190 (92%)	15 (7%)	1 (0%)	29	64
38	XD	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	29	64
39	QE	146/162 (90%)	143 (98%)	3 (2%)	0	100	100
39	XE	146/162 (90%)	141 (97%)	5 (3%)	0	100	100
40	QF	98/101 (97%)	90 (92%)	6 (6%)	2 (2%)	7	31
40	XF	98/101 (97%)	93 (95%)	3 (3%)	2 (2%)	7	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	QG	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
41	XG	153/156 (98%)	147 (96%)	4 (3%)	2 (1%)	12	42
42	QH	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	22	57
42	XH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
43	QI	125/128 (98%)	117 (94%)	7 (6%)	1 (1%)	19	54
43	XI	124/128 (97%)	113 (91%)	9 (7%)	2 (2%)	9	37
44	QJ	95/105 (90%)	84 (88%)	8 (8%)	3 (3%)	4	22
44	XJ	94/105 (90%)	82 (87%)	9 (10%)	3 (3%)	4	22
45	QK	112/129 (87%)	108 (96%)	3 (3%)	1 (1%)	17	52
45	XK	112/129 (87%)	110 (98%)	2 (2%)	0	100	100
46	QL	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
46	XL	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
47	QM	114/126 (90%)	106 (93%)	7 (6%)	1 (1%)	17	52
47	XM	112/126 (89%)	104 (93%)	7 (6%)	1 (1%)	17	52
48	QN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
48	XN	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
49	QO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
49	XO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
50	QP	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
50	XP	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
51	QQ	97/105 (92%)	91 (94%)	4 (4%)	2 (2%)	7	30
51	XQ	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
52	QR	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
52	XR	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
53	QS	81/93 (87%)	75 (93%)	6 (7%)	0	100	100
53	XS	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
54	QT	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	4	22
54	XT	96/106 (91%)	91 (95%)	2 (2%)	3 (3%)	4	23
55	QU	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	14
55	XU	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	14
All	All	12150/12888 (94%)	11432 (94%)	615 (5%)	103 (1%)	19	54

5 of 103 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	QY	304/324 (94%)	290 (95%)	14 (5%)	27	59
3	XY	304/324 (94%)	292 (96%)	12 (4%)	32	65
6	RD	214/218 (98%)	206 (96%)	8 (4%)	34	66
6	YD	215/218 (99%)	208 (97%)	7 (3%)	38	69
7	RE	164/166 (99%)	158 (96%)	6 (4%)	34	66
7	YE	164/166 (99%)	156 (95%)	8 (5%)	25	57
8	RF	160/166 (96%)	149 (93%)	11 (7%)	15	45
8	YF	159/166 (96%)	152 (96%)	7 (4%)	28	61
9	RG	144/156 (92%)	139 (96%)	5 (4%)	36	68
9	YG	142/156 (91%)	137 (96%)	5 (4%)	36	68
10	RH	144/148 (97%)	140 (97%)	4 (3%)	43	73
10	YH	143/148 (97%)	136 (95%)	7 (5%)	25	57
11	RI	111/124 (90%)	105 (95%)	6 (5%)	22	53
11	YI	108/124 (87%)	105 (97%)	3 (3%)	43	73
12	RN	119/119 (100%)	114 (96%)	5 (4%)	30	62
12	YN	118/119 (99%)	111 (94%)	7 (6%)	19	50
13	RO	100/100 (100%)	96 (96%)	4 (4%)	31	65
13	YO	100/100 (100%)	96 (96%)	4 (4%)	31	65
14	RP	115/116 (99%)	111 (96%)	4 (4%)	36	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	YP	115/116 (99%)	109 (95%)	6 (5%)	23	55
15	RQ	111/111 (100%)	107 (96%)	4 (4%)	35	67
15	YQ	111/111 (100%)	106 (96%)	5 (4%)	27	60
16	RR	101/101 (100%)	100 (99%)	1 (1%)	76	90
16	YR	101/101 (100%)	99 (98%)	2 (2%)	55	80
17	RS	87/88 (99%)	83 (95%)	4 (5%)	27	59
17	YS	85/88 (97%)	77 (91%)	8 (9%)	8	32
18	RT	115/127 (91%)	106 (92%)	9 (8%)	12	40
18	YT	113/127 (89%)	105 (93%)	8 (7%)	14	44
19	RU	93/94 (99%)	84 (90%)	9 (10%)	8	30
19	YU	93/94 (99%)	85 (91%)	8 (9%)	10	37
20	RV	81/82 (99%)	76 (94%)	5 (6%)	18	49
20	YV	80/82 (98%)	75 (94%)	5 (6%)	18	48
21	RW	90/92 (98%)	85 (94%)	5 (6%)	21	52
21	YW	90/92 (98%)	84 (93%)	6 (7%)	16	46
22	RX	77/78 (99%)	75 (97%)	2 (3%)	46	74
22	YX	77/78 (99%)	77 (100%)	0	100	100
23	RY	86/91 (94%)	80 (93%)	6 (7%)	15	45
23	YY	86/91 (94%)	82 (95%)	4 (5%)	26	59
24	RZ	169/179 (94%)	160 (95%)	9 (5%)	22	54
24	YZ	165/179 (92%)	159 (96%)	6 (4%)	35	67
25	R0	61/67 (91%)	57 (93%)	4 (7%)	16	47
25	Y0	61/67 (91%)	57 (93%)	4 (7%)	16	47
26	R1	79/83 (95%)	76 (96%)	3 (4%)	33	66
26	Y1	81/83 (98%)	77 (95%)	4 (5%)	25	57
27	R2	65/67 (97%)	65 (100%)	0	100	100
27	Y2	66/67 (98%)	63 (96%)	3 (4%)	27	60
28	R3	51/52 (98%)	51 (100%)	0	100	100
28	Y3	50/52 (96%)	48 (96%)	2 (4%)	31	65
29	R4	58/63 (92%)	54 (93%)	4 (7%)	15	45
29	Y4	54/63 (86%)	47 (87%)	7 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	R5	51/52 (98%)	51 (100%)	0	100	100
30	Y5	50/52 (96%)	46 (92%)	4 (8%)	12	40
31	R6	51/52 (98%)	50 (98%)	1 (2%)	55	80
31	Y6	50/52 (96%)	49 (98%)	1 (2%)	55	80
32	R7	41/42 (98%)	40 (98%)	1 (2%)	49	76
32	Y7	41/42 (98%)	39 (95%)	2 (5%)	25	57
33	R8	54/55 (98%)	52 (96%)	2 (4%)	34	66
33	Y8	54/55 (98%)	53 (98%)	1 (2%)	57	81
34	R9	34/34 (100%)	32 (94%)	2 (6%)	19	50
34	Y9	34/34 (100%)	33 (97%)	1 (3%)	42	72
36	QB	191/220 (87%)	181 (95%)	10 (5%)	23	55
36	XB	187/220 (85%)	171 (91%)	16 (9%)	10	37
37	QC	144/188 (77%)	141 (98%)	3 (2%)	53	79
37	XC	140/188 (74%)	134 (96%)	6 (4%)	29	62
38	QD	171/181 (94%)	163 (95%)	8 (5%)	26	59
38	XD	172/181 (95%)	163 (95%)	9 (5%)	23	55
39	QE	114/123 (93%)	111 (97%)	3 (3%)	46	74
39	XE	114/123 (93%)	110 (96%)	4 (4%)	36	68
40	QF	85/90 (94%)	78 (92%)	7 (8%)	11	38
40	XF	85/90 (94%)	79 (93%)	6 (7%)	14	44
41	QG	120/127 (94%)	117 (98%)	3 (2%)	47	75
41	XG	119/127 (94%)	115 (97%)	4 (3%)	37	69
42	QH	116/119 (98%)	112 (97%)	4 (3%)	37	69
42	XH	114/119 (96%)	112 (98%)	2 (2%)	59	82
43	QI	91/99 (92%)	83 (91%)	8 (9%)	10	36
43	XI	88/99 (89%)	83 (94%)	5 (6%)	20	52
44	QJ	68/92 (74%)	66 (97%)	2 (3%)	42	72
44	XJ	68/92 (74%)	68 (100%)	0	100	100
45	QK	83/99 (84%)	81 (98%)	2 (2%)	49	76
45	XK	83/99 (84%)	82 (99%)	1 (1%)	71	88
46	QL	96/108 (89%)	93 (97%)	3 (3%)	40	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	XL	96/108 (89%)	89 (93%)	7 (7%)	14	43
47	QM	90/101 (89%)	89 (99%)	1 (1%)	73	89
47	XM	87/101 (86%)	86 (99%)	1 (1%)	73	89
48	QN	49/50 (98%)	43 (88%)	6 (12%)	5	19
48	XN	49/50 (98%)	49 (100%)	0	100	100
49	QO	78/80 (98%)	76 (97%)	2 (3%)	46	74
49	XO	78/80 (98%)	75 (96%)	3 (4%)	33	66
50	QP	69/74 (93%)	66 (96%)	3 (4%)	29	62
50	XP	68/74 (92%)	62 (91%)	6 (9%)	10	36
51	QQ	94/97 (97%)	93 (99%)	1 (1%)	73	89
51	XQ	94/97 (97%)	90 (96%)	4 (4%)	29	62
52	QR	59/77 (77%)	54 (92%)	5 (8%)	10	37
52	XR	59/77 (77%)	56 (95%)	3 (5%)	24	56
53	QS	68/80 (85%)	65 (96%)	3 (4%)	28	61
53	XS	67/80 (84%)	65 (97%)	2 (3%)	41	71
54	QT	71/82 (87%)	71 (100%)	0	100	100
54	XT	70/82 (85%)	70 (100%)	0	100	100
55	QU	18/22 (82%)	17 (94%)	1 (6%)	21	52
55	XU	18/22 (82%)	18 (100%)	0	100	100
All	All	9971/10712 (93%)	9532 (96%)	439 (4%)	28	61

5 of 439 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
51	XQ	26	GLN
44	QJ	38	ILE
34	R9	35	ARG
20	RV	79	VAL
53	XS	10	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
43	XI	124	GLN

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Mol	Chain	Res	Type
14	RP	27	HIS
36	QB	78	GLN
26	R1	56	GLN
6	RD	96	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QV	76/77 (98%)	17 (22%)	1 (1%)
1	XV	76/77 (98%)	16 (21%)	1 (1%)
2	QX	9/25 (36%)	3 (33%)	0
2	XX	9/25 (36%)	4 (44%)	0
35	QA	1494/1521 (98%)	229 (15%)	14 (0%)
35	XA	1498/1521 (98%)	226 (15%)	18 (1%)
4	RA	2855/2915 (97%)	452 (15%)	28 (0%)
4	YA	2855/2915 (97%)	457 (16%)	26 (0%)
5	RB	119/122 (97%)	9 (7%)	0
5	YB	119/122 (97%)	14 (11%)	0
All	All	9110/9320 (97%)	1427 (15%)	88 (0%)

5 of 1427 RNA backbone outliers are listed below:

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

5 of 88 RNA pucker outliers are listed below:

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PSU	YA	1917	4	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
35	M2G	XA	966	35	20,27,28	1.37	3 (15%)	22,40,43	1.07	3 (13%)
35	5MC	QA	1400	35	18,22,23	0.96	2 (11%)	26,32,35	1.14	2 (7%)
4	4OC	YA	1920	4	19,22,24	0.81	0	26,31,35	0.89	1 (3%)
4	5MU	RA	1915	4,56	19,22,23	1.43	5 (26%)	28,32,35	2.16	8 (28%)
4	OMG	YA	2251	4,56,1	18,26,27	0.97	1 (5%)	19,38,41	1.04	2 (10%)
4	5MC	YA	1942	4	18,22,23	0.95	2 (11%)	26,32,35	1.10	2 (7%)
35	5MC	XA	1407	35	18,22,23	0.95	2 (11%)	26,32,35	1.14	3 (11%)
4	5MU	YA	1915	4	19,22,23	1.48	5 (26%)	28,32,35	2.09	8 (28%)
35	PSU	QA	516	56,35	18,21,22	1.34	2 (11%)	22,30,33	1.86	4 (18%)
4	PSU	YA	2605	4	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
4	2MU	YA	2552	4,56	19,22,24	1.24	2 (10%)	26,31,36	1.81	6 (23%)
35	MA6	XA	1518	35	19,26,27	0.98	1 (5%)	18,38,41	1.71	5 (27%)
4	5MC	RA	1942	4,56	18,22,23	0.96	2 (11%)	26,32,35	1.09	2 (7%)
4	PSU	YA	1911	4	18,21,22	1.36	2 (11%)	22,30,33	1.87	4 (18%)
4	5MU	RA	1939	4	19,22,23	1.39	4 (21%)	28,32,35	2.11	6 (21%)
35	4OC	XA	1402	35	20,23,24	0.75	0	26,32,35	0.97	1 (3%)
4	5MC	RA	1962	4,56	18,22,23	0.94	2 (11%)	26,32,35	1.12	2 (7%)
4	PSU	RA	1917	4	18,21,22	1.37	2 (11%)	22,30,33	1.82	3 (13%)
35	5MC	XA	967	35	18,22,23	0.96	2 (11%)	26,32,35	1.12	2 (7%)
35	5MC	QA	967	35	18,22,23	0.95	2 (11%)	26,32,35	1.10	2 (7%)
4	PSU	RA	2605	4	18,21,22	1.33	2 (11%)	22,30,33	1.88	4 (18%)
4	2MA	YA	2503	4,56	17,25,26	1.00	1 (5%)	17,37,40	0.96	2 (11%)
4	OMG	RA	2251	4,56,1	18,26,27	0.92	1 (5%)	19,38,41	1.11	2 (10%)
35	5MC	QA	1404	35	18,22,23	0.94	1 (5%)	26,32,35	1.07	2 (7%)
35	MA6	QA	1519	35	19,26,27	0.99	1 (5%)	18,38,41	1.64	5 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	MA6	XA	1519	35	19,26,27	0.98	1 (5%)	18,38,41	1.79	5 (27%)
35	2MG	QA	1207	56,35	18,26,27	0.93	1 (5%)	16,38,41	1.37	3 (18%)
35	5MC	XA	1404	35	18,22,23	0.98	2 (11%)	26,32,35	1.12	2 (7%)
4	2MU	RA	2552	4,56	19,22,24	1.23	2 (10%)	26,31,36	1.79	5 (19%)
4	2MA	RA	2503	4,56	17,25,26	1.01	1 (5%)	17,37,40	0.98	2 (11%)
35	PSU	XA	516	35	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
35	5MC	XA	1400	35	18,22,23	0.95	2 (11%)	26,32,35	1.17	3 (11%)
35	5MC	QA	1407	35	18,22,23	0.97	2 (11%)	26,32,35	1.16	3 (11%)
35	2MG	XA	1207	35	18,26,27	0.89	1 (5%)	16,38,41	1.13	3 (18%)
4	PSU	RA	1911	4	18,21,22	1.33	2 (11%)	22,30,33	1.89	4 (18%)
35	7MG	QA	527	56,35	22,26,27	1.31	3 (13%)	29,39,42	2.54	7 (24%)
35	M2G	QA	966	35	20,27,28	1.42	3 (15%)	22,40,43	0.96	2 (9%)
4	4OC	RA	1920	4	19,22,24	0.82	0	26,31,35	0.97	1 (3%)
35	UR3	XA	1498	56,35	19,22,23	1.02	2 (10%)	26,32,35	1.44	1 (3%)
35	UR3	QA	1498	35	19,22,23	0.99	1 (5%)	26,32,35	1.45	1 (3%)
35	4OC	QA	1402	35	20,23,24	0.77	0	26,32,35	0.96	1 (3%)
46	0TD	XL	92	46	7,9,10	1.19	1 (14%)	6,11,13	2.12	3 (50%)
46	0TD	QL	92	46	7,9,10	1.07	0	6,11,13	2.34	3 (50%)
4	5MU	YA	1939	4,56	19,22,23	1.41	6 (31%)	28,32,35	2.19	6 (21%)
35	MA6	QA	1518	35	19,26,27	0.98	1 (5%)	18,38,41	1.69	5 (27%)
4	5MC	YA	1962	4,56	18,22,23	0.99	2 (11%)	26,32,35	1.14	2 (7%)
35	7MG	XA	527	35	22,26,27	1.36	4 (18%)	29,39,42	2.50	7 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	YA	1917	4	-	0/7/25/26	0/2/2/2
35	M2G	XA	966	35	-	0/7/29/30	0/3/3/3
35	5MC	QA	1400	35	-	2/7/25/26	0/2/2/2
4	4OC	YA	1920	4	-	2/9/27/30	0/2/2/2
4	5MU	RA	1915	4,56	-	2/7/25/26	0/2/2/2
4	OMG	YA	2251	4,56,1	-	0/5/27/28	0/3/3/3
4	5MC	YA	1942	4	-	0/7/25/26	0/2/2/2
35	5MC	XA	1407	35	-	0/7/25/26	0/2/2/2

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	7MG	XA	527	35	-	2/7/37/38	0/3/3/3

The worst 5 of 90 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	QA	966	M2G	C2-N3	4.48	1.36	1.30
35	XA	966	M2G	C2-N3	4.27	1.35	1.30
35	QA	516	PSU	C6-C5	3.29	1.39	1.35
4	YA	1911	PSU	C6-C5	3.27	1.39	1.35
4	RA	1917	PSU	C6-C5	3.26	1.39	1.35

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	QA	527	7MG	N9-C4-N3	8.98	138.90	125.47
35	XA	527	7MG	N9-C4-N3	8.73	138.53	125.47
4	YA	1911	PSU	N1-C2-N3	6.07	122.01	115.13
4	RA	1911	PSU	N1-C2-N3	5.97	121.89	115.13
4	RA	2605	PSU	N1-C2-N3	5.90	121.82	115.13

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	YA	1915	5MU	O4'-C1'-N1-C2
4	YA	1915	5MU	O4'-C1'-N1-C6
35	XA	1519	MA6	C5-C6-N6-C9
35	XA	1519	MA6	C5-C6-N6-C10
46	XL	92	0TD	O-C-CA-CB

There are no ring outliers.

19 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	YA	1920	4OC	1	0
4	YA	2251	OMG	1	0
4	YA	1915	5MU	4	0
35	XA	1518	MA6	1	0
4	RA	1942	5MC	1	0
35	XA	1402	4OC	1	0
4	RA	1962	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	QA	967	5MC	1	0
4	YA	2503	2MA	1	0
35	QA	1404	5MC	1	0
35	QA	1519	MA6	2	0
35	QA	1207	2MG	2	0
4	RA	2552	2MU	1	0
35	QA	966	M2G	1	0
4	RA	1920	4OC	1	0
35	QA	1402	4OC	1	0
46	QL	92	0TD	2	0
35	QA	1518	MA6	2	0
4	YA	1962	5MC	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	XD	301	38	-	-	0/6/5/5
58	SF4	QD	302	38	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	QV	77/77 (100%)	0.25	3 (3%) 39 20	57, 94, 173, 210	0
1	XV	77/77 (100%)	0.34	3 (3%) 39 20	49, 84, 141, 212	0
2	QX	10/25 (40%)	1.15	3 (30%) 0 0	69, 105, 168, 212	0
2	XX	10/25 (40%)	1.06	3 (30%) 0 0	52, 112, 150, 183	0
3	QY	357/380 (93%)	2.08	163 (45%) 0 0	77, 135, 202, 220	0
3	XY	357/380 (93%)	2.16	158 (44%) 0 0	73, 132, 203, 228	0
4	RA	2856/2915 (97%)	0.06	136 (4%) 30 14	22, 55, 177, 347	0
4	YA	2856/2915 (97%)	0.04	128 (4%) 33 16	14, 41, 183, 343	0
5	RB	120/122 (98%)	-0.18	0 100 100	56, 91, 116, 152	0
5	YB	120/122 (98%)	-0.27	0 100 100	39, 63, 85, 130	0
6	RD	275/276 (99%)	-0.27	0 100 100	25, 47, 71, 109	0
6	YD	275/276 (99%)	-0.31	1 (0%) 92 84	16, 39, 69, 132	0
7	RE	204/206 (99%)	-0.16	0 100 100	26, 53, 85, 119	0
7	YE	204/206 (99%)	-0.15	0 100 100	19, 46, 86, 135	0
8	RF	203/210 (96%)	-0.13	1 (0%) 91 81	29, 67, 110, 133	0
8	YF	203/210 (96%)	-0.29	1 (0%) 91 81	15, 45, 89, 139	0
9	RG	181/182 (99%)	0.19	6 (3%) 46 24	76, 103, 134, 155	0
9	YG	181/182 (99%)	-0.10	4 (2%) 62 41	55, 78, 121, 184	0
10	RH	174/180 (96%)	0.78	27 (15%) 2 1	74, 111, 147, 158	0
10	YH	173/180 (96%)	-0.11	0 100 100	40, 64, 95, 139	0
11	RI	147/148 (99%)	0.63	15 (10%) 6 2	59, 103, 135, 164	0
11	YI	146/148 (98%)	0.33	5 (3%) 45 24	51, 92, 127, 150	0
12	RN	140/140 (100%)	0.08	4 (2%) 51 28	40, 62, 101, 140	0
12	YN	140/140 (100%)	-0.19	1 (0%) 87 75	27, 47, 87, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	RO	122/122 (100%)	-0.24	0 100 100	33, 52, 78, 113	0
13	YO	122/122 (100%)	-0.23	0 100 100	27, 45, 71, 83	0
14	RP	149/150 (99%)	0.13	3 (2%) 65 44	29, 72, 109, 138	0
14	YP	149/150 (99%)	-0.09	1 (0%) 87 75	18, 52, 84, 115	0
15	RQ	141/141 (100%)	-0.25	0 100 100	43, 67, 88, 112	0
15	YQ	141/141 (100%)	-0.27	0 100 100	30, 48, 74, 124	0
16	RR	118/118 (100%)	-0.22	0 100 100	31, 50, 77, 93	0
16	YR	118/118 (100%)	-0.29	0 100 100	28, 43, 67, 89	0
17	RS	110/112 (98%)	0.20	2 (1%) 68 47	66, 89, 113, 133	0
17	YS	110/112 (98%)	-0.04	0 100 100	47, 62, 89, 106	0
18	RT	131/146 (89%)	-0.21	2 (1%) 73 54	37, 59, 105, 155	0
18	YT	131/146 (89%)	-0.22	0 100 100	36, 53, 98, 122	0
19	RU	116/118 (98%)	-0.18	1 (0%) 84 69	33, 57, 91, 113	0
19	YU	116/118 (98%)	-0.36	0 100 100	23, 37, 67, 104	0
20	RV	101/101 (100%)	-0.18	0 100 100	37, 74, 100, 122	0
20	YV	101/101 (100%)	-0.09	1 (0%) 82 67	21, 50, 88, 109	0
21	RW	112/113 (99%)	-0.17	0 100 100	34, 48, 81, 122	0
21	YW	112/113 (99%)	-0.28	0 100 100	25, 37, 68, 143	0
22	RX	95/96 (98%)	0.04	2 (2%) 63 43	45, 60, 87, 120	0
22	YX	95/96 (98%)	-0.25	0 100 100	28, 42, 80, 115	0
23	RY	107/110 (97%)	0.90	15 (14%) 2 1	57, 83, 131, 176	0
23	YY	107/110 (97%)	0.17	2 (1%) 66 46	38, 64, 107, 150	0
24	RZ	203/206 (98%)	0.62	18 (8%) 9 3	71, 100, 156, 194	0
24	YZ	201/206 (97%)	0.19	15 (7%) 14 5	50, 77, 135, 178	0
25	R0	77/85 (90%)	0.25	2 (2%) 56 33	50, 62, 90, 109	0
25	Y0	77/85 (90%)	-0.03	1 (1%) 77 59	31, 45, 80, 110	0
26	R1	97/98 (98%)	0.05	2 (2%) 63 43	33, 58, 89, 111	0
26	Y1	97/98 (98%)	-0.03	0 100 100	27, 47, 95, 114	0
27	R2	70/72 (97%)	0.05	1 (1%) 75 56	53, 74, 106, 130	0
27	Y2	70/72 (97%)	-0.19	0 100 100	34, 55, 82, 142	0
28	R3	59/60 (98%)	0.47	3 (5%) 28 13	42, 63, 107, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	Y3	59/60 (98%)	-0.03	1 (1%) 70 49	28, 43, 106, 122	0
29	R4	69/71 (97%)	0.81	7 (10%) 7 2	99, 136, 177, 184	0
29	Y4	69/71 (97%)	0.51	8 (11%) 4 2	75, 124, 168, 178	0
30	R5	59/60 (98%)	-0.14	1 (1%) 70 49	29, 51, 94, 160	0
30	Y5	59/60 (98%)	-0.29	0 100 100	18, 42, 91, 141	0
31	R6	53/54 (98%)	2.13	27 (50%) 0 0	82, 102, 143, 150	0
31	Y6	53/54 (98%)	1.51	16 (30%) 0 0	75, 88, 116, 130	0
32	R7	48/49 (97%)	-0.03	1 (2%) 63 43	28, 42, 83, 120	0
32	Y7	48/49 (97%)	-0.12	0 100 100	17, 31, 69, 115	0
33	R8	64/65 (98%)	-0.12	0 100 100	39, 54, 73, 107	0
33	Y8	64/65 (98%)	-0.22	0 100 100	24, 38, 58, 71	0
34	R9	37/37 (100%)	0.84	3 (8%) 12 5	58, 77, 101, 112	0
34	Y9	37/37 (100%)	0.64	1 (2%) 54 31	49, 61, 81, 93	0
35	QA	1488/1521 (97%)	0.05	36 (2%) 59 37	42, 86, 173, 260	0
35	XA	1492/1521 (98%)	0.07	48 (3%) 47 25	32, 84, 168, 253	0
36	QB	231/256 (90%)	0.39	15 (6%) 18 8	85, 122, 153, 178	0
36	XB	231/256 (90%)	0.28	11 (4%) 30 14	80, 110, 143, 161	0
37	QC	206/239 (86%)	0.37	8 (3%) 39 20	88, 115, 144, 168	0
37	XC	206/239 (86%)	0.27	8 (3%) 39 20	80, 104, 134, 167	0
38	QD	208/209 (99%)	-0.04	0 100 100	62, 91, 125, 150	0
38	XD	208/209 (99%)	0.11	1 (0%) 91 81	68, 97, 133, 152	0
39	QE	148/162 (91%)	-0.01	0 100 100	64, 86, 114, 143	0
39	XE	148/162 (91%)	0.10	2 (1%) 75 56	62, 78, 114, 139	0
40	QF	100/101 (99%)	-0.03	2 (2%) 65 44	70, 95, 118, 132	0
40	XF	100/101 (99%)	-0.25	0 100 100	62, 81, 109, 124	0
41	QG	155/156 (99%)	0.55	15 (9%) 7 2	82, 109, 137, 157	0
41	XG	155/156 (99%)	0.45	10 (6%) 18 8	78, 100, 130, 155	0
42	QH	137/138 (99%)	0.21	2 (1%) 73 54	55, 86, 114, 123	0
42	XH	137/138 (99%)	0.10	4 (2%) 51 28	60, 86, 113, 120	0
43	QI	127/128 (99%)	0.97	21 (16%) 1 1	78, 123, 151, 175	0
43	XI	126/128 (98%)	0.44	6 (4%) 30 14	68, 111, 139, 165	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	QJ	97/105 (92%)	1.10	16 (16%) 1 1	90, 121, 149, 161	0
44	XJ	96/105 (91%)	0.85	10 (10%) 6 2	78, 116, 144, 146	0
45	QK	114/129 (88%)	0.37	4 (3%) 44 23	63, 86, 113, 138	0
45	XK	114/129 (88%)	0.15	2 (1%) 68 47	47, 75, 105, 132	0
46	QL	121/132 (91%)	-0.08	1 (0%) 86 72	47, 66, 90, 105	0
46	XL	121/132 (91%)	0.06	2 (1%) 70 49	48, 66, 94, 116	0
47	QM	116/126 (92%)	0.35	7 (6%) 21 10	85, 114, 138, 148	0
47	XM	114/126 (90%)	0.44	7 (6%) 21 9	84, 107, 128, 144	0
48	QN	60/61 (98%)	0.73	6 (10%) 7 2	88, 111, 129, 146	0
48	XN	60/61 (98%)	0.30	1 (1%) 70 49	73, 92, 115, 127	0
49	QO	88/89 (98%)	0.09	1 (1%) 80 64	60, 80, 109, 121	0
49	XO	88/89 (98%)	0.19	2 (2%) 60 39	48, 80, 112, 123	0
50	QP	82/88 (93%)	0.39	3 (3%) 41 21	58, 76, 104, 114	0
50	XP	82/88 (93%)	0.59	6 (7%) 15 6	71, 93, 118, 141	0
51	QQ	99/105 (94%)	0.29	2 (2%) 65 44	53, 78, 114, 138	0
51	XQ	99/105 (94%)	0.05	0 100 100	59, 78, 101, 126	0
52	QR	68/88 (77%)	0.74	9 (13%) 3 1	72, 90, 119, 139	0
52	XR	68/88 (77%)	0.31	1 (1%) 73 54	56, 83, 114, 124	0
53	QS	83/93 (89%)	1.21	20 (24%) 0 0	87, 120, 146, 161	0
53	XS	83/93 (89%)	1.11	18 (21%) 0 0	89, 118, 142, 183	0
54	QT	96/106 (90%)	0.16	1 (1%) 82 67	54, 80, 116, 120	0
54	XT	98/106 (92%)	0.47	5 (5%) 28 13	65, 88, 120, 128	0
55	QU	23/27 (85%)	2.17	14 (60%) 0 0	88, 103, 130, 145	0
55	XU	23/27 (85%)	1.38	6 (26%) 0 0	81, 102, 117, 119	0
All	All	21456/22208 (96%)	0.18	1131 (5%) 26 12	14, 73, 148, 347	0

The worst 5 of 1131 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	XA	88	A	14.3
4	YA	2141	G	11.4
24	YZ	192	ALA	10.3
3	XY	50	PRO	10.2
24	YZ	193	GLU	9.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	5MU	YA	1915	21/22	0.91	0.18	52,76,85,87	0
4	5MU	RA	1915	21/22	0.91	0.13	92,100,114,117	0
46	0TD	XL	92	10/11	0.92	0.20	58,67,84,87	0
35	PSU	XA	516	20/21	0.92	0.19	75,86,95,95	0
4	PSU	YA	1917	20/21	0.93	0.18	51,62,88,91	0
35	PSU	QA	516	20/21	0.93	0.14	71,77,87,88	0
35	M2G	QA	966	25/26	0.93	0.21	71,80,92,93	0
35	4OC	QA	1402	22/23	0.93	0.23	55,67,72,74	0
46	0TD	QL	92	10/11	0.93	0.19	59,72,74,78	0
35	4OC	XA	1402	22/23	0.93	0.23	45,57,67,81	0
4	PSU	RA	1917	20/21	0.93	0.18	53,73,89,103	0
35	5MC	QA	967	21/22	0.94	0.22	71,84,95,99	0
35	2MG	QA	1207	24/25	0.94	0.13	101,124,131,134	0
35	5MC	XA	967	21/22	0.94	0.21	62,75,84,92	0
35	2MG	XA	1207	24/25	0.94	0.17	85,98,106,107	0
35	7MG	QA	527	24/25	0.94	0.21	51,70,76,76	0
35	M2G	XA	966	25/26	0.94	0.19	56,75,94,105	0
4	4OC	RA	1920	21/23	0.95	0.20	55,62,85,94	0
35	MA6	QA	1518	24/25	0.96	0.19	48,58,67,72	0
35	MA6	QA	1519	24/25	0.96	0.25	41,56,68,79	0
35	7MG	XA	527	24/25	0.96	0.20	54,63,74,79	0
4	PSU	RA	1911	20/21	0.96	0.16	55,66,73,74	0
35	5MC	QA	1400	21/22	0.96	0.21	66,75,85,88	0
35	5MC	XA	1400	21/22	0.96	0.18	50,65,74,85	0
35	5MC	QA	1404	21/22	0.96	0.20	55,62,67,73	0
4	4OC	YA	1920	21/23	0.97	0.16	40,47,55,60	0
4	PSU	YA	2605	20/21	0.97	0.22	10,25,42,59	0
4	PSU	YA	1911	20/21	0.97	0.18	45,57,62,63	0
35	5MC	XA	1404	21/22	0.97	0.19	34,45,58,63	0
35	UR3	QA	1498	21/22	0.97	0.18	44,57,69,72	0
35	5MC	XA	1407	21/22	0.97	0.21	46,49,58,59	0
4	5MU	RA	1939	21/22	0.97	0.19	23,37,44,52	0
4	5MC	RA	1942	21/22	0.97	0.20	41,50,62,64	0
4	PSU	RA	2605	20/21	0.97	0.18	19,36,47,48	0
4	2MU	YA	2552	21/23	0.98	0.18	19,28,42,46	0
4	5MU	YA	1939	21/22	0.98	0.18	15,27,36,48	0
4	5MC	YA	1942	21/22	0.98	0.16	25,38,47,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	5MC	YA	1962	21/22	0.98	0.16	25,33,47,55	0
4	OMG	YA	2251	24/25	0.98	0.20	13,25,35,41	0
35	UR3	XA	1498	21/22	0.98	0.16	34,43,57,66	0
35	MA6	XA	1518	24/25	0.98	0.20	31,41,46,52	0
35	MA6	XA	1519	24/25	0.98	0.19	28,45,53,54	0
35	5MC	QA	1407	21/22	0.98	0.16	44,51,62,68	0
4	5MC	RA	1962	21/22	0.98	0.16	39,46,52,62	0
4	OMG	RA	2251	24/25	0.98	0.19	31,38,50,55	0
4	2MU	RA	2552	21/23	0.98	0.17	19,33,40,48	0
4	2MA	YA	2503	23/24	0.98	0.18	8,22,36,38	0
4	2MA	RA	2503	23/24	0.99	0.17	16,24,31,37	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	QA	1647	1/1	-0.54	0.50	134,134,134,134	0
56	MG	QA	1601	1/1	-0.53	0.51	129,129,129,129	0
56	MG	XA	1671	1/1	-0.50	1.23	108,108,108,108	0
56	MG	RA	3727	1/1	-0.47	0.55	108,108,108,108	0
56	MG	RA	3115	1/1	-0.42	1.57	92,92,92,92	0
56	MG	QA	1798	1/1	-0.41	1.41	119,119,119,119	0
56	MG	QA	1799	1/1	-0.39	0.83	83,83,83,83	0
56	MG	RA	3282	1/1	-0.38	2.55	109,109,109,109	0
56	MG	RA	3577	1/1	-0.31	1.19	94,94,94,94	0
56	MG	XF	203	1/1	-0.29	1.43	109,109,109,109	0
56	MG	XA	1673	1/1	-0.25	1.69	103,103,103,103	0
56	MG	YA	3247	1/1	-0.25	0.91	106,106,106,106	0
56	MG	YA	3534	1/1	-0.23	0.55	124,124,124,124	0
56	MG	RA	3828	1/1	-0.22	1.88	94,94,94,94	0
56	MG	QA	1826	1/1	-0.21	0.49	74,74,74,74	0
56	MG	YA	3037	1/1	-0.21	0.91	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	RA	3549	1/1	-0.18	1.04	78,78,78,78	0
56	MG	QA	1839	1/1	-0.16	0.48	93,93,93,93	0
56	MG	RA	3100	1/1	-0.15	1.10	93,93,93,93	0
56	MG	XA	1781	1/1	-0.14	0.82	110,110,110,110	0
56	MG	QA	1612	1/1	-0.14	0.94	97,97,97,97	0
56	MG	YA	3347	1/1	-0.13	0.26	99,99,99,99	0
56	MG	QA	1762	1/1	-0.12	1.14	93,93,93,93	0
56	MG	QA	1686	1/1	-0.12	1.00	103,103,103,103	0
56	MG	YA	3267	1/1	-0.11	1.07	100,100,100,100	0
56	MG	YA	3427	1/1	-0.10	1.13	75,75,75,75	0
56	MG	RA	3746	1/1	-0.10	0.68	112,112,112,112	0
56	MG	RA	3800	1/1	-0.10	0.47	102,102,102,102	0
56	MG	QA	1727	1/1	-0.10	0.74	100,100,100,100	0
56	MG	QA	1691	1/1	-0.08	0.46	104,104,104,104	0
56	MG	YA	3057	1/1	-0.06	0.74	99,99,99,99	0
56	MG	QA	1789	1/1	-0.05	0.38	99,99,99,99	0
56	MG	RA	3644	1/1	-0.05	1.04	84,84,84,84	0
56	MG	QA	1856	1/1	-0.05	1.34	89,89,89,89	0
56	MG	XA	1669	1/1	-0.04	0.96	103,103,103,103	0
56	MG	QA	1681	1/1	-0.04	1.02	85,85,85,85	0
56	MG	QA	1720	1/1	-0.04	0.96	97,97,97,97	0
56	MG	RA	3935	1/1	-0.04	0.53	91,91,91,91	0
56	MG	RA	3825	1/1	-0.03	1.08	98,98,98,98	0
56	MG	QY	401	1/1	-0.02	0.41	111,111,111,111	0
56	MG	YA	3396	1/1	-0.01	0.89	94,94,94,94	0
56	MG	QA	1829	1/1	-0.01	0.95	94,94,94,94	0
56	MG	QA	1754	1/1	0.00	0.78	108,108,108,108	0
56	MG	YA	3086	1/1	0.01	0.93	95,95,95,95	0
56	MG	RA	3782	1/1	0.01	0.59	94,94,94,94	0
56	MG	QA	1735	1/1	0.02	0.69	107,107,107,107	0
56	MG	QA	1760	1/1	0.04	0.99	77,77,77,77	0
56	MG	RA	3994	1/1	0.04	0.90	88,88,88,88	0
56	MG	YA	3166	1/1	0.06	1.13	132,132,132,132	0
56	MG	QA	1757	1/1	0.06	1.01	86,86,86,86	0
56	MG	QA	1769	1/1	0.06	0.56	95,95,95,95	0
56	MG	QA	1871	1/1	0.07	2.54	100,100,100,100	0
56	MG	RA	3005	1/1	0.07	1.07	99,99,99,99	0
56	MG	YA	3246	1/1	0.07	0.51	118,118,118,118	0
56	MG	XA	1651	1/1	0.07	0.56	90,90,90,90	0
56	MG	QA	1693	1/1	0.08	0.40	88,88,88,88	0
56	MG	XA	1654	1/1	0.08	0.95	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YN	201	1/1	0.09	0.84	87,87,87,87	0
56	MG	RA	3942	1/1	0.09	0.90	104,104,104,104	0
56	MG	XA	1692	1/1	0.09	0.81	75,75,75,75	0
56	MG	RV	201	1/1	0.09	0.65	110,110,110,110	0
56	MG	XA	1711	1/1	0.10	0.62	92,92,92,92	0
56	MG	XA	1773	1/1	0.12	0.99	96,96,96,96	0
56	MG	QA	1867	1/1	0.12	1.16	99,99,99,99	0
56	MG	YA	3185	1/1	0.12	0.88	105,105,105,105	0
56	MG	RT	203	1/1	0.12	0.48	88,88,88,88	0
56	MG	XA	1728	1/1	0.12	0.96	101,101,101,101	0
57	ZN	Y4	101	1/1	0.12	0.46	305,305,305,305	0
56	MG	RA	3787	1/1	0.13	1.15	105,105,105,105	0
56	MG	YA	3637	1/1	0.13	1.17	101,101,101,101	0
56	MG	YA	3465	1/1	0.13	0.82	82,82,82,82	0
56	MG	RA	3062	1/1	0.13	0.20	82,82,82,82	0
56	MG	YA	3417	1/1	0.13	0.69	106,106,106,106	0
56	MG	RA	3590	1/1	0.14	0.90	104,104,104,104	0
56	MG	QU	101	1/1	0.14	0.50	81,81,81,81	0
56	MG	RA	3261	1/1	0.14	0.49	82,82,82,82	0
56	MG	QA	1860	1/1	0.14	0.63	100,100,100,100	0
56	MG	RA	3752	1/1	0.14	0.57	102,102,102,102	0
56	MG	RA	3998	1/1	0.14	0.88	87,87,87,87	0
56	MG	RB	226	1/1	0.14	0.71	99,99,99,99	0
56	MG	RA	3429	1/1	0.14	0.21	89,89,89,89	0
56	MG	YA	3415	1/1	0.14	1.04	84,84,84,84	0
56	MG	QA	1791	1/1	0.14	0.85	96,96,96,96	0
56	MG	XA	1718	1/1	0.15	1.31	73,73,73,73	0
56	MG	YA	3056	1/1	0.15	1.13	81,81,81,81	0
56	MG	RA	3322	1/1	0.15	0.89	90,90,90,90	0
56	MG	XA	1634	1/1	0.16	0.48	75,75,75,75	0
56	MG	QY	403	1/1	0.16	0.84	81,81,81,81	0
56	MG	QA	1763	1/1	0.17	1.05	100,100,100,100	0
56	MG	XA	1783	1/1	0.17	1.28	99,99,99,99	0
56	MG	YA	3193	1/1	0.17	0.69	101,101,101,101	0
56	MG	YA	3449	1/1	0.18	0.82	81,81,81,81	0
56	MG	RA	3437	1/1	0.18	0.65	77,77,77,77	0
56	MG	RB	211	1/1	0.19	0.37	95,95,95,95	0
56	MG	QA	1745	1/1	0.19	0.85	98,98,98,98	0
56	MG	XA	1647	1/1	0.19	0.34	92,92,92,92	0
56	MG	RA	3058	1/1	0.19	1.05	88,88,88,88	0
56	MG	RA	3681	1/1	0.19	0.66	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3253	1/1	0.20	0.62	98,98,98,98	0
56	MG	RA	4015	1/1	0.20	0.93	89,89,89,89	0
56	MG	YA	3164	1/1	0.20	0.90	87,87,87,87	0
56	MG	YA	3311	1/1	0.20	1.35	94,94,94,94	0
56	MG	RA	3481	1/1	0.20	0.21	81,81,81,81	0
56	MG	RA	3961	1/1	0.20	1.06	114,114,114,114	0
56	MG	YB	209	1/1	0.20	1.03	102,102,102,102	0
56	MG	YA	3148	1/1	0.21	0.82	92,92,92,92	0
56	MG	YA	3174	1/1	0.21	0.95	95,95,95,95	0
56	MG	QA	1858	1/1	0.21	0.93	115,115,115,115	0
56	MG	QA	1668	1/1	0.21	0.65	102,102,102,102	0
56	MG	YA	3737	1/1	0.21	1.33	107,107,107,107	0
56	MG	QA	1725	1/1	0.21	0.64	90,90,90,90	0
56	MG	QA	1677	1/1	0.22	0.93	94,94,94,94	0
56	MG	QA	1830	1/1	0.22	0.25	85,85,85,85	0
56	MG	RA	3490	1/1	0.23	0.51	86,86,86,86	0
56	MG	XA	1719	1/1	0.23	0.97	95,95,95,95	0
56	MG	RG	201	1/1	0.23	0.52	121,121,121,121	0
56	MG	YA	3722	1/1	0.24	0.51	89,89,89,89	0
56	MG	RA	3733	1/1	0.25	0.97	96,96,96,96	0
56	MG	RA	3198	1/1	0.25	1.25	84,84,84,84	0
56	MG	RA	3279	1/1	0.25	0.58	103,103,103,103	0
56	MG	RA	3525	1/1	0.25	0.89	65,65,65,65	0
56	MG	QA	1878	1/1	0.26	1.22	108,108,108,108	0
56	MG	RA	3669	1/1	0.26	0.63	81,81,81,81	0
56	MG	YA	3565	1/1	0.26	0.82	85,85,85,85	0
56	MG	RA	3603	1/1	0.26	0.49	101,101,101,101	0
56	MG	XA	1668	1/1	0.27	0.71	87,87,87,87	0
56	MG	YB	218	1/1	0.27	0.41	80,80,80,80	0
56	MG	YA	3531	1/1	0.27	0.34	66,66,66,66	0
56	MG	QA	1748	1/1	0.27	0.55	92,92,92,92	0
56	MG	XA	1649	1/1	0.28	0.36	92,92,92,92	0
56	MG	YA	3308	1/1	0.28	0.28	64,64,64,64	0
56	MG	RE	304	1/1	0.28	0.73	75,75,75,75	0
56	MG	YA	3165	1/1	0.28	0.52	73,73,73,73	0
56	MG	RA	3809	1/1	0.28	0.68	76,76,76,76	0
56	MG	RA	3370	1/1	0.28	1.04	88,88,88,88	0
56	MG	QE	202	1/1	0.28	0.55	91,91,91,91	0
56	MG	RA	3688	1/1	0.29	0.33	90,90,90,90	0
56	MG	QA	1819	1/1	0.29	0.58	65,65,65,65	0
56	MG	RB	208	1/1	0.29	0.31	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	RA	3367	1/1	0.29	0.65	74,74,74,74	0
56	MG	RA	3090	1/1	0.29	0.42	93,93,93,93	0
56	MG	RA	3662	1/1	0.29	0.95	89,89,89,89	0
56	MG	QA	1764	1/1	0.29	0.35	101,101,101,101	0
56	MG	RA	3950	1/1	0.29	0.81	87,87,87,87	0
56	MG	RA	3786	1/1	0.29	0.66	87,87,87,87	0
56	MG	YA	3421	1/1	0.29	1.22	75,75,75,75	0
56	MG	QA	1835	1/1	0.30	0.74	89,89,89,89	0
56	MG	QM	201	1/1	0.30	0.64	85,85,85,85	0
56	MG	QA	1736	1/1	0.30	0.83	86,86,86,86	0
56	MG	RA	3197	1/1	0.30	1.25	85,85,85,85	0
56	MG	XA	1652	1/1	0.30	0.51	78,78,78,78	0
56	MG	YA	3069	1/1	0.30	0.81	78,78,78,78	0
56	MG	RA	3824	1/1	0.30	1.41	76,76,76,76	0
56	MG	QD	301	1/1	0.30	1.59	90,90,90,90	0
56	MG	YA	3107	1/1	0.31	0.71	80,80,80,80	0
56	MG	QA	1652	1/1	0.31	0.63	83,83,83,83	0
56	MG	YA	3535	1/1	0.31	0.99	75,75,75,75	0
56	MG	QA	1814	1/1	0.31	0.53	97,97,97,97	0
56	MG	QA	1674	1/1	0.31	0.39	85,85,85,85	0
56	MG	QA	1664	1/1	0.32	0.94	92,92,92,92	0
56	MG	XA	1675	1/1	0.32	0.77	82,82,82,82	0
56	MG	QG	203	1/1	0.32	1.45	100,100,100,100	0
56	MG	QA	1788	1/1	0.32	0.67	81,81,81,81	0
56	MG	QA	1715	1/1	0.32	0.45	77,77,77,77	0
56	MG	YA	3003	1/1	0.33	0.97	106,106,106,106	0
56	MG	RA	3011	1/1	0.33	0.61	84,84,84,84	0
56	MG	YA	3302	1/1	0.33	0.82	72,72,72,72	0
56	MG	RV	204	1/1	0.33	0.48	70,70,70,70	0
56	MG	QA	1768	1/1	0.33	0.29	91,91,91,91	0
56	MG	YA	3462	1/1	0.34	0.78	75,75,75,75	0
56	MG	RA	3636	1/1	0.34	1.26	91,91,91,91	0
56	MG	XA	1682	1/1	0.34	0.74	86,86,86,86	0
56	MG	RA	3039	1/1	0.34	0.57	76,76,76,76	0
56	MG	YT	202	1/1	0.34	0.84	84,84,84,84	0
56	MG	QA	1753	1/1	0.34	0.49	71,71,71,71	0
56	MG	YE	301	1/1	0.34	0.48	95,95,95,95	0
56	MG	RA	3193	1/1	0.35	0.60	94,94,94,94	0
56	MG	RA	3747	1/1	0.35	0.59	96,96,96,96	0
56	MG	QA	1842	1/1	0.35	0.39	84,84,84,84	0
56	MG	RA	3754	1/1	0.35	0.81	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	4054	1/1	0.35	1.00	97,97,97,97	0
56	MG	RA	3740	1/1	0.35	1.03	76,76,76,76	0
56	MG	RA	3954	1/1	0.35	0.70	77,77,77,77	0
56	MG	QA	1787	1/1	0.36	0.75	76,76,76,76	0
56	MG	RA	3271	1/1	0.36	0.45	93,93,93,93	0
56	MG	RA	3277	1/1	0.36	0.69	94,94,94,94	0
56	MG	XA	1637	1/1	0.36	0.69	89,89,89,89	0
56	MG	YF	302	1/1	0.36	0.54	85,85,85,85	0
56	MG	YA	3370	1/1	0.36	0.31	67,67,67,67	0
56	MG	YA	3726	1/1	0.36	0.85	81,81,81,81	0
56	MG	YA	3262	1/1	0.36	0.65	88,88,88,88	0
56	MG	RA	3511	1/1	0.37	1.20	62,62,62,62	0
56	MG	YA	3437	1/1	0.37	0.87	85,85,85,85	0
56	MG	YA	3478	1/1	0.37	0.49	67,67,67,67	0
56	MG	YA	3528	1/1	0.37	0.63	104,104,104,104	0
56	MG	QA	1641	1/1	0.37	0.68	105,105,105,105	0
56	MG	XA	1703	1/1	0.37	0.71	60,60,60,60	0
56	MG	XA	1704	1/1	0.37	0.32	83,83,83,83	0
56	MG	XA	1660	1/1	0.37	0.38	99,99,99,99	0
56	MG	RA	3103	1/1	0.37	0.49	104,104,104,104	0
56	MG	YA	3233	1/1	0.38	0.48	95,95,95,95	0
56	MG	RA	3203	1/1	0.38	0.75	97,97,97,97	0
56	MG	RA	3977	1/1	0.38	0.96	62,62,62,62	0
56	MG	RA	3949	1/1	0.38	0.67	80,80,80,80	0
56	MG	RA	3239	1/1	0.38	0.80	112,112,112,112	0
56	MG	R1	102	1/1	0.38	0.98	71,71,71,71	0
56	MG	RD	313	1/1	0.38	0.78	82,82,82,82	0
56	MG	RA	3790	1/1	0.39	0.48	82,82,82,82	0
56	MG	YA	3578	1/1	0.39	0.94	95,95,95,95	0
56	MG	YA	3094	1/1	0.39	0.40	68,68,68,68	0
56	MG	RA	3672	1/1	0.39	0.70	75,75,75,75	0
56	MG	RA	3985	1/1	0.39	0.67	81,81,81,81	0
56	MG	RA	3512	1/1	0.39	0.90	80,80,80,80	0
56	MG	RA	3620	1/1	0.39	0.59	90,90,90,90	0
56	MG	RA	3699	1/1	0.39	1.15	98,98,98,98	0
56	MG	YA	3099	1/1	0.39	0.63	106,106,106,106	0
56	MG	QA	1813	1/1	0.39	0.81	83,83,83,83	0
56	MG	XA	1608	1/1	0.40	0.49	76,76,76,76	0
56	MG	RA	3086	1/1	0.40	0.76	124,124,124,124	0
56	MG	QA	1866	1/1	0.40	1.86	89,89,89,89	0
56	MG	XA	1604	1/1	0.41	0.70	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	YA	3545	1/1	0.41	0.45	99,99,99,99	0
56	MG	QA	1611	1/1	0.41	0.80	89,89,89,89	0
56	MG	RA	3544	1/1	0.41	0.80	78,78,78,78	0
56	MG	XA	1693	1/1	0.41	0.53	81,81,81,81	0
56	MG	RA	3439	1/1	0.41	0.71	89,89,89,89	0
56	MG	RH	202	1/1	0.41	0.48	96,96,96,96	0
56	MG	RA	3316	1/1	0.41	0.61	84,84,84,84	0
56	MG	YB	206	1/1	0.41	0.61	99,99,99,99	0
56	MG	RA	3849	1/1	0.41	0.67	52,52,52,52	0
56	MG	RZ	301	1/1	0.41	0.34	66,66,66,66	0
56	MG	RA	3882	1/1	0.41	0.75	77,77,77,77	0
56	MG	RA	3694	1/1	0.41	0.52	107,107,107,107	0
56	MG	QN	103	1/1	0.42	0.99	80,80,80,80	0
56	MG	RA	4035	1/1	0.42	0.39	116,116,116,116	0
56	MG	YA	3177	1/1	0.42	0.20	71,71,71,71	0
56	MG	RA	3422	1/1	0.42	0.73	84,84,84,84	0
56	MG	RA	3302	1/1	0.42	0.53	92,92,92,92	0
56	MG	XA	1618	1/1	0.42	0.78	72,72,72,72	0
56	MG	QA	1657	1/1	0.42	0.59	98,98,98,98	0
56	MG	R4	102	1/1	0.42	0.36	88,88,88,88	0
56	MG	RA	3547	1/1	0.42	0.37	74,74,74,74	0
56	MG	RB	229	1/1	0.43	0.50	108,108,108,108	0
56	MG	QA	1873	1/1	0.43	0.63	70,70,70,70	0
56	MG	RA	3798	1/1	0.43	1.30	99,99,99,99	0
56	MG	YA	3501	1/1	0.43	0.67	115,115,115,115	0
56	MG	QA	1756	1/1	0.43	0.57	114,114,114,114	0
56	MG	YA	3344	1/1	0.43	0.28	80,80,80,80	0
56	MG	QA	1738	1/1	0.44	0.60	98,98,98,98	0
56	MG	YA	3214	1/1	0.44	0.73	111,111,111,111	0
56	MG	QA	1680	1/1	0.44	0.38	64,64,64,64	0
56	MG	QA	1642	1/1	0.44	0.65	83,83,83,83	0
56	MG	RA	3179	1/1	0.44	0.93	77,77,77,77	0
56	MG	RA	3399	1/1	0.44	0.73	117,117,117,117	0
56	MG	XA	1661	1/1	0.45	0.34	87,87,87,87	0
56	MG	RA	3142	1/1	0.45	0.43	76,76,76,76	0
56	MG	RE	302	1/1	0.45	0.33	109,109,109,109	0
56	MG	XH	201	1/1	0.45	0.61	78,78,78,78	0
56	MG	RF	310	1/1	0.45	0.70	88,88,88,88	0
56	MG	RA	3556	1/1	0.45	0.71	75,75,75,75	0
56	MG	RA	3840	1/1	0.45	0.55	83,83,83,83	0
56	MG	YA	3658	1/1	0.45	0.29	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	YA	3241	1/1	0.45	0.50	85,85,85,85	0
56	MG	QA	1685	1/1	0.45	0.43	91,91,91,91	0
56	MG	RA	3105	1/1	0.45	0.55	71,71,71,71	0
56	MG	RA	3948	1/1	0.45	0.61	89,89,89,89	0
56	MG	RA	3537	1/1	0.45	0.60	93,93,93,93	0
56	MG	RA	3538	1/1	0.45	0.34	80,80,80,80	0
56	MG	YA	3524	1/1	0.46	0.39	96,96,96,96	0
56	MG	RA	3617	1/1	0.46	0.57	83,83,83,83	0
56	MG	YA	3369	1/1	0.46	0.17	63,63,63,63	0
56	MG	YA	3108	1/1	0.46	0.50	98,98,98,98	0
56	MG	QY	402	1/1	0.46	0.56	111,111,111,111	0
56	MG	QA	1698	1/1	0.46	0.40	100,100,100,100	0
56	MG	R0	104	1/1	0.46	0.45	90,90,90,90	0
56	MG	YA	3461	1/1	0.46	0.93	81,81,81,81	0
56	MG	QD	304	1/1	0.46	0.27	111,111,111,111	0
56	MG	RA	3425	1/1	0.46	0.49	94,94,94,94	0
56	MG	RA	3589	1/1	0.47	0.64	100,100,100,100	0
56	MG	RA	4047	1/1	0.47	0.64	117,117,117,117	0
56	MG	XA	1727	1/1	0.47	0.44	84,84,84,84	0
56	MG	QA	1837	1/1	0.47	0.44	69,69,69,69	0
56	MG	QA	1805	1/1	0.47	0.23	76,76,76,76	0
56	MG	YA	3450	1/1	0.47	0.73	79,79,79,79	0
56	MG	RA	3858	1/1	0.47	0.71	80,80,80,80	0
56	MG	RA	3625	1/1	0.47	0.70	91,91,91,91	0
56	MG	RA	3751	1/1	0.47	0.33	51,51,51,51	0
56	MG	RA	3940	1/1	0.47	0.69	83,83,83,83	0
56	MG	RA	3634	1/1	0.47	0.63	81,81,81,81	0
56	MG	QA	1848	1/1	0.47	0.59	68,68,68,68	0
56	MG	YA	3232	1/1	0.47	0.35	104,104,104,104	0
56	MG	RA	3237	1/1	0.47	0.51	100,100,100,100	0
56	MG	QA	1602	1/1	0.47	0.16	95,95,95,95	0
56	MG	YA	3603	1/1	0.47	0.53	100,100,100,100	0
56	MG	RA	3796	1/1	0.47	1.00	67,67,67,67	0
56	MG	QA	1682	1/1	0.47	0.38	93,93,93,93	0
56	MG	QO	101	1/1	0.47	0.61	79,79,79,79	0
56	MG	YA	3523	1/1	0.47	0.29	56,56,56,56	0
56	MG	RA	3817	1/1	0.47	0.80	76,76,76,76	0
56	MG	RA	3497	1/1	0.48	0.34	82,82,82,82	0
56	MG	XA	1648	1/1	0.48	0.54	74,74,74,74	0
56	MG	XA	1709	1/1	0.48	0.17	72,72,72,72	0
56	MG	RA	3524	1/1	0.48	0.66	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	RA	3375	1/1	0.48	0.70	73,73,73,73	0
56	MG	XA	1672	1/1	0.48	0.58	91,91,91,91	0
56	MG	YA	3459	1/1	0.48	0.38	85,85,85,85	0
56	MG	YA	3511	1/1	0.48	0.61	60,60,60,60	0
56	MG	QA	1630	1/1	0.48	0.64	81,81,81,81	0
56	MG	RA	3875	1/1	0.48	0.62	90,90,90,90	0
56	MG	RA	3312	1/1	0.48	1.05	124,124,124,124	0
56	MG	XA	1725	1/1	0.48	0.71	87,87,87,87	0
56	MG	RA	3457	1/1	0.48	1.14	81,81,81,81	0
56	MG	QA	1861	1/1	0.48	0.95	75,75,75,75	0
56	MG	RA	3351	1/1	0.48	0.67	70,70,70,70	0
56	MG	XA	1723	1/1	0.49	0.28	75,75,75,75	0
56	MG	QA	1728	1/1	0.49	0.31	64,64,64,64	0
56	MG	QA	1823	1/1	0.49	0.63	70,70,70,70	0
56	MG	RA	3285	1/1	0.49	0.65	85,85,85,85	0
56	MG	RA	3126	1/1	0.49	1.11	79,79,79,79	0
56	MG	R0	103	1/1	0.49	1.36	81,81,81,81	0
56	MG	QA	1645	1/1	0.49	0.36	75,75,75,75	0
56	MG	YA	3131	1/1	0.49	0.34	88,88,88,88	0
56	MG	YA	3110	1/1	0.49	0.48	63,63,63,63	0
56	MG	RA	3276	1/1	0.49	0.66	91,91,91,91	0
56	MG	RA	3951	1/1	0.50	0.53	87,87,87,87	0
56	MG	RA	3823	1/1	0.50	0.53	97,97,97,97	0
56	MG	RA	3112	1/1	0.50	0.52	117,117,117,117	0
56	MG	YA	3273	1/1	0.50	0.88	72,72,72,72	0
56	MG	YA	3409	1/1	0.50	0.27	120,120,120,120	0
56	MG	XA	1674	1/1	0.50	0.32	73,73,73,73	0
56	MG	QA	1812	1/1	0.51	1.00	68,68,68,68	0
56	MG	RH	201	1/1	0.51	0.53	88,88,88,88	0
56	MG	RA	3807	1/1	0.51	0.59	70,70,70,70	0
56	MG	YA	3628	1/1	0.51	0.48	105,105,105,105	0
56	MG	RA	3810	1/1	0.51	0.63	75,75,75,75	0
56	MG	RA	3812	1/1	0.51	0.65	106,106,106,106	0
56	MG	QA	1733	1/1	0.51	0.81	60,60,60,60	0
56	MG	RD	310	1/1	0.51	0.40	94,94,94,94	0
56	MG	YA	3466	1/1	0.51	0.56	80,80,80,80	0
56	MG	RA	3580	1/1	0.51	0.66	112,112,112,112	0
56	MG	R3	101	1/1	0.51	0.99	95,95,95,95	0
56	MG	YA	3092	1/1	0.51	0.25	113,113,113,113	0
56	MG	RA	3065	1/1	0.51	0.58	89,89,89,89	0
56	MG	XA	1785	1/1	0.52	0.44	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	QA	1783	1/1	0.52	0.22	77,77,77,77	0
56	MG	XA	1624	1/1	0.52	0.64	76,76,76,76	0
56	MG	RA	3249	1/1	0.52	0.71	94,94,94,94	0
56	MG	YA	3150	1/1	0.52	0.79	84,84,84,84	0
56	MG	XJ	201	1/1	0.52	0.15	97,97,97,97	0
56	MG	XA	1603	1/1	0.52	0.83	76,76,76,76	0
56	MG	QA	1831	1/1	0.52	0.40	93,93,93,93	0
56	MG	XA	1639	1/1	0.52	0.52	98,98,98,98	0
56	MG	YB	201	1/1	0.52	0.52	89,89,89,89	0
56	MG	RA	3283	1/1	0.52	0.61	101,101,101,101	0
56	MG	YA	3236	1/1	0.52	0.34	106,106,106,106	0
56	MG	QA	1697	1/1	0.52	0.31	76,76,76,76	0
56	MG	YA	3467	1/1	0.52	0.97	82,82,82,82	0
56	MG	RA	3871	1/1	0.53	0.49	77,77,77,77	0
56	MG	YA	3676	1/1	0.53	0.89	73,73,73,73	0
56	MG	RA	3963	1/1	0.53	1.90	110,110,110,110	0
56	MG	RA	3311	1/1	0.53	0.41	100,100,100,100	0
56	MG	XA	1621	1/1	0.53	0.63	68,68,68,68	0
56	MG	YT	203	1/1	0.53	0.35	78,78,78,78	0
56	MG	Y1	101	1/1	0.53	1.04	104,104,104,104	0
56	MG	QA	1832	1/1	0.53	0.65	92,92,92,92	0
56	MG	RA	3035	1/1	0.53	0.51	97,97,97,97	0
56	MG	RA	3768	1/1	0.53	0.90	76,76,76,76	0
56	MG	XA	1702	1/1	0.53	0.40	61,61,61,61	0
56	MG	XA	1753	1/1	0.54	0.64	99,99,99,99	0
56	MG	RA	3491	1/1	0.54	0.86	81,81,81,81	0
56	MG	YA	3191	1/1	0.54	0.14	76,76,76,76	0
56	MG	YB	205	1/1	0.54	0.67	89,89,89,89	0
56	MG	XA	1643	1/1	0.54	0.15	80,80,80,80	0
56	MG	RB	215	1/1	0.54	0.32	91,91,91,91	0
56	MG	XA	1662	1/1	0.54	0.24	80,80,80,80	0
56	MG	RA	3976	1/1	0.54	0.72	81,81,81,81	0
56	MG	XE	201	1/1	0.54	0.49	79,79,79,79	0
56	MG	QA	1620	1/1	0.54	0.28	75,75,75,75	0
56	MG	YA	3403	1/1	0.54	0.41	59,59,59,59	0
56	MG	RA	3195	1/1	0.54	0.55	115,115,115,115	0
56	MG	QA	1636	1/1	0.54	0.31	66,66,66,66	0
57	ZN	RY	201	1/1	0.54	0.22	210,210,210,210	0
56	MG	YA	3464	1/1	0.55	0.74	73,73,73,73	0
56	MG	RA	3523	1/1	0.55	0.97	64,64,64,64	0
56	MG	YA	3488	1/1	0.55	0.35	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	4004	1/1	0.55	0.39	93,93,93,93	0
56	MG	QA	1675	1/1	0.55	1.03	94,94,94,94	0
56	MG	YA	3176	1/1	0.55	0.45	102,102,102,102	0
56	MG	QH	201	1/1	0.55	0.46	76,76,76,76	0
56	MG	YA	3211	1/1	0.55	0.55	89,89,89,89	0
56	MG	RB	203	1/1	0.55	0.49	106,106,106,106	0
56	MG	RA	3546	1/1	0.55	0.43	111,111,111,111	0
56	MG	YA	3167	1/1	0.55	0.91	88,88,88,88	0
56	MG	RA	3851	1/1	0.56	0.15	91,91,91,91	0
56	MG	RA	3519	1/1	0.56	0.46	82,82,82,82	0
56	MG	YA	3443	1/1	0.56	0.81	81,81,81,81	0
56	MG	YA	3738	1/1	0.56	0.56	68,68,68,68	0
56	MG	YA	3270	1/1	0.56	0.45	83,83,83,83	0
56	MG	RA	3309	1/1	0.56	0.56	63,63,63,63	0
56	MG	RA	3432	1/1	0.56	0.44	58,58,58,58	0
56	MG	RA	3839	1/1	0.56	0.64	72,72,72,72	0
56	MG	YW	202	1/1	0.56	0.25	55,55,55,55	0
56	MG	XA	1666	1/1	0.56	0.81	63,63,63,63	0
56	MG	RA	3272	1/1	0.57	0.35	83,83,83,83	0
56	MG	RA	3982	1/1	0.57	0.55	83,83,83,83	0
56	MG	RA	3983	1/1	0.57	0.66	84,84,84,84	0
56	MG	RF	302	1/1	0.57	0.77	73,73,73,73	0
56	MG	XA	1664	1/1	0.57	0.32	67,67,67,67	0
56	MG	QA	1792	1/1	0.57	0.61	69,69,69,69	0
56	MG	QA	1794	1/1	0.57	0.48	79,79,79,79	0
56	MG	YA	3667	1/1	0.57	0.67	90,90,90,90	0
56	MG	RN	202	1/1	0.57	1.09	98,98,98,98	0
56	MG	RA	3517	1/1	0.57	0.42	107,107,107,107	0
56	MG	QA	1774	1/1	0.57	0.43	77,77,77,77	0
56	MG	YA	3544	1/1	0.57	0.54	81,81,81,81	0
56	MG	RA	3217	1/1	0.57	0.35	88,88,88,88	0
56	MG	RA	3036	1/1	0.57	0.43	69,69,69,69	0
56	MG	YB	211	1/1	0.57	0.36	70,70,70,70	0
56	MG	YA	3529	1/1	0.57	0.79	73,73,73,73	0
56	MG	RA	3542	1/1	0.57	0.55	76,76,76,76	0
56	MG	YA	3662	1/1	0.57	0.82	91,91,91,91	0
56	MG	R9	101	1/1	0.57	0.39	92,92,92,92	0
56	MG	RA	3463	1/1	0.57	0.51	78,78,78,78	0
56	MG	RA	3162	1/1	0.57	1.08	72,72,72,72	0
56	MG	RB	222	1/1	0.58	0.45	94,94,94,94	0
56	MG	RB	225	1/1	0.58	0.46	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	YA	3085	1/1	0.58	0.28	86,86,86,86	0
56	MG	RA	3867	1/1	0.58	0.15	63,63,63,63	0
56	MG	QA	1780	1/1	0.58	0.24	92,92,92,92	0
56	MG	RA	3364	1/1	0.58	0.39	96,96,96,96	0
56	MG	QA	1793	1/1	0.58	1.27	82,82,82,82	0
56	MG	RA	3967	1/1	0.58	0.60	61,61,61,61	0
56	MG	YE	303	1/1	0.58	0.43	103,103,103,103	0
56	MG	YA	3147	1/1	0.58	0.38	84,84,84,84	0
56	MG	QA	1653	1/1	0.58	0.45	85,85,85,85	0
56	MG	QV	101	1/1	0.58	0.66	118,118,118,118	0
56	MG	RA	3031	1/1	0.58	0.40	75,75,75,75	0
56	MG	RA	3068	1/1	0.59	0.51	79,79,79,79	0
56	MG	RA	3078	1/1	0.59	0.88	70,70,70,70	0
56	MG	YA	3451	1/1	0.59	0.39	64,64,64,64	0
56	MG	YA	3695	1/1	0.59	0.99	76,76,76,76	0
56	MG	RA	3742	1/1	0.59	0.60	81,81,81,81	0
56	MG	YA	3456	1/1	0.59	0.70	68,68,68,68	0
56	MG	YA	3103	1/1	0.59	0.26	63,63,63,63	0
56	MG	QA	1865	1/1	0.59	0.82	75,75,75,75	0
56	MG	QA	1766	1/1	0.59	0.40	71,71,71,71	0
56	MG	RA	3953	1/1	0.59	0.32	86,86,86,86	0
56	MG	QL	203	1/1	0.59	0.21	60,60,60,60	0
56	MG	RA	3958	1/1	0.59	0.53	104,104,104,104	0
56	MG	RA	3252	1/1	0.59	0.63	91,91,91,91	0
56	MG	YA	3184	1/1	0.59	0.43	80,80,80,80	0
56	MG	RA	3134	1/1	0.59	0.56	83,83,83,83	0
56	MG	RA	3675	1/1	0.59	0.35	75,75,75,75	0
56	MG	QA	1847	1/1	0.59	1.11	64,64,64,64	0
56	MG	YA	3061	1/1	0.59	0.60	57,57,57,57	0
56	MG	RA	3066	1/1	0.59	0.58	56,56,56,56	0
56	MG	QA	1661	1/1	0.60	0.63	81,81,81,81	0
56	MG	QA	1749	1/1	0.60	0.98	56,56,56,56	0
56	MG	YA	3379	1/1	0.60	0.35	70,70,70,70	0
56	MG	RA	3916	1/1	0.60	0.74	72,72,72,72	0
56	MG	QA	1836	1/1	0.60	0.41	89,89,89,89	0
56	MG	YA	3431	1/1	0.60	0.62	57,57,57,57	0
56	MG	RA	4008	1/1	0.60	0.34	86,86,86,86	0
56	MG	RA	3654	1/1	0.60	0.44	87,87,87,87	0
56	MG	RA	3818	1/1	0.60	0.68	67,67,67,67	0
56	MG	RA	3564	1/1	0.60	0.60	101,101,101,101	0
56	MG	RA	3051	1/1	0.60	0.62	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	QA	1712	1/1	0.60	0.56	87,87,87,87	0
56	MG	RA	3583	1/1	0.60	0.62	72,72,72,72	0
56	MG	XA	1609	1/1	0.60	1.37	88,88,88,88	0
56	MG	RA	3683	1/1	0.60	0.50	96,96,96,96	0
56	MG	RA	3847	1/1	0.60	0.44	102,102,102,102	0
56	MG	RB	224	1/1	0.60	0.70	78,78,78,78	0
56	MG	YP	201	1/1	0.60	0.57	79,79,79,79	0
56	MG	YA	3718	1/1	0.60	0.37	60,60,60,60	0
56	MG	QA	1785	1/1	0.60	0.52	84,84,84,84	0
56	MG	RA	3722	1/1	0.60	0.38	82,82,82,82	0
56	MG	YA	3119	1/1	0.61	0.57	78,78,78,78	0
56	MG	YA	3203	1/1	0.61	0.53	84,84,84,84	0
56	MG	RA	3057	1/1	0.61	0.54	93,93,93,93	0
56	MG	QA	1862	1/1	0.61	0.52	101,101,101,101	0
56	MG	RA	3061	1/1	0.61	0.22	84,84,84,84	0
56	MG	YA	3446	1/1	0.61	0.66	71,71,71,71	0
56	MG	RA	3202	1/1	0.61	0.59	92,92,92,92	0
56	MG	RA	3691	1/1	0.61	0.47	64,64,64,64	0
56	MG	YA	3419	1/1	0.61	0.49	66,66,66,66	0
56	MG	RA	3695	1/1	0.61	0.37	52,52,52,52	0
56	MG	QA	1854	1/1	0.61	0.36	67,67,67,67	0
56	MG	RB	210	1/1	0.61	0.98	109,109,109,109	0
56	MG	RA	3704	1/1	0.61	0.58	91,91,91,91	0
56	MG	RA	3224	1/1	0.61	0.58	96,96,96,96	0
56	MG	RB	217	1/1	0.61	0.84	94,94,94,94	0
56	MG	RA	3968	1/1	0.61	0.80	66,66,66,66	0
56	MG	RA	3974	1/1	0.61	1.43	70,70,70,70	0
56	MG	QA	1811	1/1	0.61	0.35	83,83,83,83	0
56	MG	RA	3296	1/1	0.61	0.45	102,102,102,102	0
56	MG	RA	3645	1/1	0.61	0.50	84,84,84,84	0
56	MG	YA	3641	1/1	0.61	0.92	86,86,86,86	0
56	MG	RA	3559	1/1	0.62	0.34	97,97,97,97	0
56	MG	YA	3727	1/1	0.62	0.51	59,59,59,59	0
56	MG	RA	4002	1/1	0.62	0.30	83,83,83,83	0
56	MG	RA	3518	1/1	0.62	0.64	82,82,82,82	0
56	MG	Y0	101	1/1	0.62	0.90	65,65,65,65	0
56	MG	RA	3205	1/1	0.62	0.44	76,76,76,76	0
56	MG	RA	3339	1/1	0.62	0.48	68,68,68,68	0
56	MG	RA	4042	1/1	0.62	0.36	80,80,80,80	0
56	MG	RA	3448	1/1	0.62	0.72	71,71,71,71	0
56	MG	RA	3599	1/1	0.62	0.28	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	RR	3204	1/1	0.62	0.51	83,83,83,83	0
56	MG	QA	1734	1/1	0.62	0.68	85,85,85,85	0
56	MG	QA	1637	1/1	0.62	0.80	93,93,93,93	0
56	MG	QA	1718	1/1	0.62	0.79	82,82,82,82	0
56	MG	QA	1796	1/1	0.62	0.44	73,73,73,73	0
56	MG	YA	3473	1/1	0.62	0.55	77,77,77,77	0
56	MG	QA	1743	1/1	0.62	0.35	71,71,71,71	0
56	MG	RA	3725	1/1	0.62	0.51	80,80,80,80	0
56	MG	YA	3060	1/1	0.62	0.42	62,62,62,62	0
56	MG	YG	201	1/1	0.62	1.60	116,116,116,116	0
56	MG	R7	102	1/1	0.62	0.54	72,72,72,72	0
56	MG	RA	3921	1/1	0.62	2.40	88,88,88,88	0
56	MG	RB	228	1/1	0.62	0.53	93,93,93,93	0
56	MG	RA	3649	1/1	0.62	0.38	85,85,85,85	0
56	MG	YB	207	1/1	0.63	0.48	110,110,110,110	0
56	MG	YA	3510	1/1	0.63	0.64	80,80,80,80	0
56	MG	RA	3724	1/1	0.63	0.27	67,67,67,67	0
56	MG	RA	4046	1/1	0.63	0.59	86,86,86,86	0
56	MG	RA	3028	1/1	0.63	0.17	69,69,69,69	0
56	MG	XA	1722	1/1	0.63	0.20	67,67,67,67	0
56	MG	YA	3584	1/1	0.63	0.54	56,56,56,56	0
56	MG	YA	3336	1/1	0.63	0.43	71,71,71,71	0
56	MG	XA	1626	1/1	0.63	0.84	77,77,77,77	0
56	MG	RF	301	1/1	0.63	0.54	101,101,101,101	0
56	MG	RA	3891	1/1	0.63	0.57	59,59,59,59	0
56	MG	YA	3059	1/1	0.63	0.65	79,79,79,79	0
56	MG	YA	3448	1/1	0.63	0.33	81,81,81,81	0
56	MG	RA	3461	1/1	0.63	0.81	76,76,76,76	0
56	MG	RB	223	1/1	0.63	1.00	102,102,102,102	0
56	MG	YA	3497	1/1	0.64	0.44	63,63,63,63	0
56	MG	RA	3553	1/1	0.64	0.88	87,87,87,87	0
56	MG	XA	1697	1/1	0.64	0.85	70,70,70,70	0
56	MG	QA	1747	1/1	0.64	0.49	72,72,72,72	0
56	MG	RD	312	1/1	0.64	0.48	76,76,76,76	0
56	MG	RA	3136	1/1	0.64	0.40	84,84,84,84	0
56	MG	RA	3258	1/1	0.64	0.64	96,96,96,96	0
56	MG	RA	3361	1/1	0.64	0.36	76,76,76,76	0
56	MG	QN	102	1/1	0.64	0.39	68,68,68,68	0
56	MG	RA	3366	1/1	0.64	0.38	72,72,72,72	0
56	MG	RA	3924	1/1	0.64	0.48	65,65,65,65	0
56	MG	YA	3222	1/1	0.64	0.55	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	RA	3171	1/1	0.64	0.54	89,89,89,89	0
56	MG	QA	1696	1/1	0.64	0.36	73,73,73,73	0
56	MG	RN	201	1/1	0.64	0.79	85,85,85,85	0
56	MG	QT	201	1/1	0.64	0.51	65,65,65,65	0
56	MG	YA	3502	1/1	0.64	0.46	79,79,79,79	0
56	MG	RT	201	1/1	0.64	0.95	77,77,77,77	0
56	MG	RA	4052	1/1	0.64	0.69	90,90,90,90	0
56	MG	QA	1821	1/1	0.64	0.91	90,90,90,90	0
56	MG	RA	4058	1/1	0.64	0.52	120,120,120,120	0
56	MG	RA	3630	1/1	0.64	0.64	90,90,90,90	0
56	MG	YA	3406	1/1	0.64	0.45	80,80,80,80	0
56	MG	QA	1824	1/1	0.64	1.31	127,127,127,127	0
56	MG	RA	3637	1/1	0.64	0.65	66,66,66,66	0
56	MG	RA	3834	1/1	0.64	0.43	80,80,80,80	0
56	MG	RA	3962	1/1	0.64	0.86	62,62,62,62	0
56	MG	QA	1853	1/1	0.64	0.62	107,107,107,107	0
56	MG	YA	3208	1/1	0.64	1.18	60,60,60,60	0
56	MG	YA	3414	1/1	0.64	0.71	83,83,83,83	0
56	MG	XA	1616	1/1	0.64	1.62	115,115,115,115	0
56	MG	QA	1732	1/1	0.65	0.42	96,96,96,96	0
56	MG	RA	3801	1/1	0.65	0.20	74,74,74,74	0
56	MG	RA	3969	1/1	0.65	0.46	98,98,98,98	0
56	MG	XA	1716	1/1	0.65	0.32	57,57,57,57	0
56	MG	RA	3646	1/1	0.65	0.69	92,92,92,92	0
56	MG	QA	1660	1/1	0.65	0.19	77,77,77,77	0
56	MG	YA	3111	1/1	0.65	0.60	58,58,58,58	0
56	MG	XA	1623	1/1	0.65	0.80	73,73,73,73	0
56	MG	QA	1666	1/1	0.65	0.23	74,74,74,74	0
56	MG	YA	3418	1/1	0.65	0.81	56,56,56,56	0
56	MG	YA	3504	1/1	0.65	0.28	74,74,74,74	0
56	MG	RA	3256	1/1	0.65	0.40	103,103,103,103	0
56	MG	QA	1801	1/1	0.65	0.32	78,78,78,78	0
56	MG	YA	3083	1/1	0.65	0.43	99,99,99,99	0
56	MG	RA	3781	1/1	0.65	0.42	60,60,60,60	0
56	MG	RA	3459	1/1	0.65	0.54	78,78,78,78	0
56	MG	YA	3100	1/1	0.65	0.29	87,87,87,87	0
56	MG	XT	201	1/1	0.65	0.30	65,65,65,65	0
56	MG	YA	3490	1/1	0.65	0.57	104,104,104,104	0
56	MG	YA	3330	1/1	0.65	0.54	62,62,62,62	0
56	MG	XA	1645	1/1	0.65	0.52	93,93,93,93	0
56	MG	QA	1817	1/1	0.66	0.38	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3314	1/1	0.66	0.66	58,58,58,58	0
56	MG	QA	1609	1/1	0.66	0.59	106,106,106,106	0
56	MG	RA	3446	1/1	0.66	1.21	63,63,63,63	0
56	MG	RA	3263	1/1	0.66	0.23	67,67,67,67	0
56	MG	YA	3171	1/1	0.66	0.38	104,104,104,104	0
56	MG	RR	3203	1/1	0.66	0.30	84,84,84,84	0
56	MG	YA	3206	1/1	0.66	0.46	100,100,100,100	0
56	MG	RA	3048	1/1	0.66	0.35	78,78,78,78	0
56	MG	YA	3228	1/1	0.66	0.33	75,75,75,75	0
56	MG	QA	1843	1/1	0.66	0.30	89,89,89,89	0
56	MG	YA	3053	1/1	0.66	0.54	77,77,77,77	0
56	MG	RB	227	1/1	0.66	0.51	74,74,74,74	0
56	MG	RA	3956	1/1	0.66	0.35	77,77,77,77	0
56	MG	QA	1869	1/1	0.66	0.18	61,61,61,61	0
56	MG	YA	3655	1/1	0.66	0.86	86,86,86,86	0
56	MG	QA	1850	1/1	0.66	0.65	51,51,51,51	0
56	MG	YA	3432	1/1	0.66	0.47	84,84,84,84	0
56	MG	YA	3340	1/1	0.66	0.25	59,59,59,59	0
56	MG	YA	3201	1/1	0.66	0.34	87,87,87,87	0
56	MG	RA	3431	1/1	0.66	0.40	88,88,88,88	0
56	MG	RA	4059	1/1	0.66	0.60	101,101,101,101	0
56	MG	YA	3439	1/1	0.67	0.56	80,80,80,80	0
56	MG	QE	201	1/1	0.67	0.17	84,84,84,84	0
56	MG	RA	3986	1/1	0.67	0.57	79,79,79,79	0
56	MG	XA	1680	1/1	0.67	0.18	77,77,77,77	0
56	MG	XA	1721	1/1	0.67	0.65	86,86,86,86	0
56	MG	RA	3788	1/1	0.67	0.10	75,75,75,75	0
56	MG	QA	1840	1/1	0.67	0.55	89,89,89,89	0
56	MG	RA	3791	1/1	0.67	0.32	64,64,64,64	0
56	MG	RA	3667	1/1	0.67	0.20	60,60,60,60	0
56	MG	YA	3547	1/1	0.67	0.41	80,80,80,80	0
56	MG	RA	3357	1/1	0.67	0.16	61,61,61,61	0
56	MG	R0	102	1/1	0.67	0.21	84,84,84,84	0
56	MG	YA	3400	1/1	0.67	0.62	74,74,74,74	0
56	MG	RA	3631	1/1	0.67	0.41	125,125,125,125	0
56	MG	RA	3488	1/1	0.67	0.33	57,57,57,57	0
56	MG	RA	3684	1/1	0.67	0.52	71,71,71,71	0
56	MG	RA	3686	1/1	0.67	0.38	62,62,62,62	0
56	MG	YA	3714	1/1	0.67	0.37	80,80,80,80	0
56	MG	YA	3026	1/1	0.67	0.24	93,93,93,93	0
56	MG	RA	3541	1/1	0.67	0.93	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	RA	3776	1/1	0.67	0.38	73,73,73,73	0
56	MG	RA	3530	1/1	0.68	0.43	75,75,75,75	0
56	MG	QA	1784	1/1	0.68	0.49	64,64,64,64	0
56	MG	QA	1737	1/1	0.68	0.95	72,72,72,72	0
56	MG	RA	3166	1/1	0.68	1.07	68,68,68,68	0
56	MG	QA	1816	1/1	0.68	0.82	76,76,76,76	0
56	MG	RA	3466	1/1	0.68	0.49	56,56,56,56	0
56	MG	XA	1655	1/1	0.68	0.58	84,84,84,84	0
56	MG	RQ	203	1/1	0.68	0.68	82,82,82,82	0
56	MG	QA	1683	1/1	0.68	0.27	112,112,112,112	0
56	MG	RA	3890	1/1	0.68	0.85	57,57,57,57	0
56	MG	XA	1715	1/1	0.68	0.66	55,55,55,55	0
56	MG	RA	3104	1/1	0.68	0.47	57,57,57,57	0
56	MG	RA	3427	1/1	0.68	0.67	78,78,78,78	0
56	MG	QA	1857	1/1	0.68	0.74	71,71,71,71	0
56	MG	RW	202	1/1	0.68	0.41	89,89,89,89	0
56	MG	RA	3926	1/1	0.68	0.54	83,83,83,83	0
56	MG	QA	1804	1/1	0.68	0.40	71,71,71,71	0
56	MG	RA	3573	1/1	0.68	1.06	91,91,91,91	0
56	MG	RA	3327	1/1	0.68	0.64	62,62,62,62	0
56	MG	R1	101	1/1	0.68	0.64	82,82,82,82	0
56	MG	QD	303	1/1	0.68	0.47	79,79,79,79	0
56	MG	QA	1721	1/1	0.68	0.59	75,75,75,75	0
56	MG	RA	3521	1/1	0.68	0.42	81,81,81,81	0
56	MG	RA	3441	1/1	0.68	0.74	61,61,61,61	0
56	MG	RA	3591	1/1	0.68	0.57	77,77,77,77	0
56	MG	YA	3314	1/1	0.68	0.48	55,55,55,55	0
56	MG	QA	1662	1/1	0.68	0.52	82,82,82,82	0
56	MG	YA	3468	1/1	0.69	0.99	58,58,58,58	0
56	MG	RA	3291	1/1	0.69	0.74	86,86,86,86	0
56	MG	RA	3360	1/1	0.69	0.98	66,66,66,66	0
56	MG	RA	3682	1/1	0.69	0.39	81,81,81,81	0
56	MG	XA	1789	1/1	0.69	0.40	58,58,58,58	0
56	MG	YA	3248	1/1	0.69	0.41	105,105,105,105	0
56	MG	RA	3365	1/1	0.69	0.60	61,61,61,61	0
56	MG	RA	3822	1/1	0.69	0.44	37,37,37,37	0
56	MG	XA	1619	1/1	0.69	0.12	74,74,74,74	0
56	MG	RA	3212	1/1	0.69	0.60	95,95,95,95	0
56	MG	RA	3639	1/1	0.69	1.13	65,65,65,65	0
56	MG	RA	3991	1/1	0.69	0.61	73,73,73,73	0
56	MG	QA	1708	1/1	0.69	0.17	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	QA	1759	1/1	0.69	0.15	78,78,78,78	0
56	MG	RA	3703	1/1	0.69	0.77	71,71,71,71	0
56	MG	RA	4003	1/1	0.69	0.35	51,51,51,51	0
56	MG	QI	201	1/1	0.69	0.55	106,106,106,106	0
56	MG	RA	3846	1/1	0.69	0.72	80,80,80,80	0
56	MG	RA	3402	1/1	0.69	0.84	71,71,71,71	0
56	MG	RA	4018	1/1	0.69	0.67	70,70,70,70	0
56	MG	YA	3117	1/1	0.69	0.17	42,42,42,42	0
56	MG	XA	1610	1/1	0.69	0.39	79,79,79,79	0
56	MG	QA	1644	1/1	0.69	0.51	108,108,108,108	0
56	MG	RA	3340	1/1	0.69	0.52	52,52,52,52	0
56	MG	RA	3868	1/1	0.69	0.46	48,48,48,48	0
56	MG	RA	3710	1/1	0.70	0.89	70,70,70,70	0
56	MG	RA	3596	1/1	0.70	0.42	83,83,83,83	0
56	MG	RB	221	1/1	0.70	0.24	64,64,64,64	0
56	MG	RA	3131	1/1	0.70	0.09	67,67,67,67	0
56	MG	YA	3234	1/1	0.70	0.54	76,76,76,76	0
56	MG	YA	3422	1/1	0.70	0.78	122,122,122,122	0
56	MG	RA	3081	1/1	0.70	0.52	91,91,91,91	0
56	MG	YA	3039	1/1	0.70	0.60	73,73,73,73	0
56	MG	RA	3558	1/1	0.70	0.58	82,82,82,82	0
56	MG	XA	1620	1/1	0.70	0.25	63,63,63,63	0
56	MG	YA	3359	1/1	0.70	0.15	72,72,72,72	0
56	MG	RA	3635	1/1	0.70	0.28	112,112,112,112	0
56	MG	QA	1650	1/1	0.70	0.14	72,72,72,72	0
56	MG	YA	3479	1/1	0.70	0.57	50,50,50,50	0
56	MG	RA	3912	1/1	0.70	0.64	76,76,76,76	0
56	MG	RA	3358	1/1	0.70	0.48	99,99,99,99	0
56	MG	RA	3772	1/1	0.70	0.43	57,57,57,57	0
56	MG	YA	3577	1/1	0.70	0.71	53,53,53,53	0
56	MG	QA	1731	1/1	0.70	0.50	71,71,71,71	0
56	MG	YA	3505	1/1	0.70	1.01	88,88,88,88	0
56	MG	YA	3018	1/1	0.70	0.47	75,75,75,75	0
56	MG	RA	3652	1/1	0.70	0.66	88,88,88,88	0
56	MG	RA	3122	1/1	0.71	0.67	92,92,92,92	0
56	MG	YA	3260	1/1	0.71	0.44	71,71,71,71	0
56	MG	QA	1704	1/1	0.71	0.75	74,74,74,74	0
56	MG	RA	3132	1/1	0.71	0.25	63,63,63,63	0
56	MG	RA	3933	1/1	0.71	0.90	76,76,76,76	0
56	MG	QA	1822	1/1	0.71	0.57	65,65,65,65	0
56	MG	YA	3475	1/1	0.71	0.55	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	RA	3729	1/1	0.71	0.41	59,59,59,59	0
56	MG	RA	4031	1/1	0.71	0.41	102,102,102,102	0
56	MG	XF	202	1/1	0.71	0.45	73,73,73,73	0
56	MG	YG	203	1/1	0.71	0.14	54,54,54,54	0
56	MG	RA	3472	1/1	0.71	0.28	51,51,51,51	0
56	MG	YA	3155	1/1	0.71	0.82	65,65,65,65	0
56	MG	RO	201	1/1	0.71	0.54	93,93,93,93	0
56	MG	QA	1739	1/1	0.71	0.12	87,87,87,87	0
56	MG	RA	3177	1/1	0.71	0.68	72,72,72,72	0
56	MG	YA	3070	1/1	0.71	0.43	62,62,62,62	0
56	MG	YA	3173	1/1	0.71	0.42	85,85,85,85	0
56	MG	RA	4065	1/1	0.71	0.59	86,86,86,86	0
56	MG	RA	3845	1/1	0.71	0.58	94,94,94,94	0
56	MG	QA	1746	1/1	0.71	0.24	65,65,65,65	0
56	MG	YA	3557	1/1	0.71	0.76	67,67,67,67	0
56	MG	QA	1776	1/1	0.71	0.38	80,80,80,80	0
56	MG	RA	3288	1/1	0.71	0.32	95,95,95,95	0
56	MG	RA	3200	1/1	0.71	0.41	99,99,99,99	0
56	MG	RA	3973	1/1	0.71	0.59	84,84,84,84	0
56	MG	YA	3745	1/1	0.71	0.65	67,67,67,67	0
56	MG	RA	3600	1/1	0.71	0.46	87,87,87,87	0
56	MG	QA	1782	1/1	0.71	0.28	69,69,69,69	0
56	MG	QA	1608	1/1	0.71	0.71	110,110,110,110	0
56	MG	QA	1669	1/1	0.71	1.12	71,71,71,71	0
56	MG	YA	3255	1/1	0.71	0.33	88,88,88,88	0
56	MG	QA	1755	1/1	0.71	0.40	69,69,69,69	0
56	MG	RA	3227	1/1	0.71	0.54	93,93,93,93	0
56	MG	RA	3456	1/1	0.72	0.22	58,58,58,58	0
56	MG	RA	3076	1/1	0.72	0.68	83,83,83,83	0
56	MG	QA	1879	1/1	0.72	0.46	78,78,78,78	0
56	MG	XA	1698	1/1	0.72	0.42	66,66,66,66	0
56	MG	QA	1676	1/1	0.72	0.58	88,88,88,88	0
56	MG	RE	305	1/1	0.72	0.32	33,33,33,33	0
56	MG	YA	3500	1/1	0.72	1.02	53,53,53,53	0
56	MG	RA	3187	1/1	0.72	0.52	106,106,106,106	0
56	MG	RA	3741	1/1	0.72	0.22	61,61,61,61	0
56	MG	RF	311	1/1	0.72	0.67	74,74,74,74	0
56	MG	RA	3099	1/1	0.72	0.31	102,102,102,102	0
56	MG	YA	3186	1/1	0.72	0.44	39,39,39,39	0
56	MG	RA	3102	1/1	0.72	0.83	107,107,107,107	0
56	MG	YA	3198	1/1	0.72	0.65	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3836	1/1	0.72	0.41	91,91,91,91	0
56	MG	RA	3199	1/1	0.72	0.26	68,68,68,68	0
56	MG	XA	1708	1/1	0.72	0.39	78,78,78,78	0
56	MG	RA	3759	1/1	0.72	0.29	67,67,67,67	0
56	MG	QA	1624	1/1	0.72	0.57	73,73,73,73	0
56	MG	YA	3715	1/1	0.72	0.76	58,58,58,58	0
56	MG	RB	206	1/1	0.72	0.18	74,74,74,74	0
56	MG	YA	3445	1/1	0.72	0.71	72,72,72,72	0
56	MG	RA	3207	1/1	0.72	0.80	69,69,69,69	0
56	MG	YA	3027	1/1	0.72	0.53	45,45,45,45	0
56	MG	XL	201	1/1	0.72	0.30	85,85,85,85	0
56	MG	QA	1845	1/1	0.72	0.80	77,77,77,77	0
56	MG	XA	1769	1/1	0.72	0.77	64,64,64,64	0
56	MG	RA	3872	1/1	0.72	0.69	78,78,78,78	0
56	MG	YD	301	1/1	0.72	0.72	60,60,60,60	0
56	MG	RA	3532	1/1	0.72	0.13	52,52,52,52	0
56	MG	RA	3067	1/1	0.72	0.40	83,83,83,83	0
56	MG	RA	3245	1/1	0.72	0.41	81,81,81,81	0
56	MG	RA	3987	1/1	0.72	0.72	80,80,80,80	0
56	MG	XA	1605	1/1	0.72	0.50	72,72,72,72	0
57	ZN	YY	201	1/1	0.72	0.18	221,221,221,221	0
56	MG	RA	3251	1/1	0.72	0.49	69,69,69,69	0
56	MG	RD	307	1/1	0.72	0.37	83,83,83,83	0
56	MG	RA	3023	1/1	0.73	0.36	73,73,73,73	0
56	MG	RA	4055	1/1	0.73	0.71	86,86,86,86	0
56	MG	RA	3152	1/1	0.73	0.44	106,106,106,106	0
56	MG	QA	1770	1/1	0.73	0.25	73,73,73,73	0
56	MG	YA	3624	1/1	0.73	0.44	71,71,71,71	0
56	MG	RA	3878	1/1	0.73	0.76	81,81,81,81	0
56	MG	RA	3208	1/1	0.73	0.36	70,70,70,70	0
56	MG	RA	3545	1/1	0.73	0.54	70,70,70,70	0
56	MG	RB	209	1/1	0.73	0.37	92,92,92,92	0
56	MG	RP	202	1/1	0.73	0.21	78,78,78,78	0
56	MG	YA	3052	1/1	0.73	0.32	45,45,45,45	0
56	MG	RA	3903	1/1	0.73	0.29	57,57,57,57	0
56	MG	RA	3275	1/1	0.73	0.45	72,72,72,72	0
56	MG	RA	3331	1/1	0.73	0.79	73,73,73,73	0
56	MG	RA	3755	1/1	0.73	0.60	71,71,71,71	0
56	MG	YA	3312	1/1	0.73	0.44	73,73,73,73	0
56	MG	YA	3269	1/1	0.73	0.57	78,78,78,78	0
56	MG	RA	3040	1/1	0.73	0.50	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3493	1/1	0.73	0.34	74,74,74,74	0
56	MG	RA	3638	1/1	0.73	0.38	85,85,85,85	0
56	MG	YA	3065	1/1	0.73	0.76	88,88,88,88	0
56	MG	RA	3003	1/1	0.73	0.42	73,73,73,73	0
56	MG	RA	3842	1/1	0.73	0.41	72,72,72,72	0
56	MG	YA	3507	1/1	0.73	0.25	44,44,44,44	0
56	MG	RA	3250	1/1	0.73	0.46	69,69,69,69	0
56	MG	XA	1788	1/1	0.73	0.71	62,62,62,62	0
56	MG	RA	3138	1/1	0.73	0.44	53,53,53,53	0
56	MG	RA	3303	1/1	0.73	0.77	79,79,79,79	0
56	MG	RA	3797	1/1	0.73	0.48	84,84,84,84	0
56	MG	RA	3862	1/1	0.73	0.44	79,79,79,79	0
56	MG	RA	3535	1/1	0.73	0.27	57,57,57,57	0
57	ZN	R4	101	1/1	0.73	0.36	269,269,269,269	0
56	MG	QA	1772	1/1	0.74	1.04	79,79,79,79	0
56	MG	YB	204	1/1	0.74	0.42	99,99,99,99	0
56	MG	XA	1700	1/1	0.74	0.44	43,43,43,43	0
56	MG	RA	3663	1/1	0.74	0.51	77,77,77,77	0
56	MG	QA	1851	1/1	0.74	0.42	94,94,94,94	0
56	MG	RA	3515	1/1	0.74	0.58	67,67,67,67	0
56	MG	RA	3426	1/1	0.74	0.49	88,88,88,88	0
56	MG	YA	3080	1/1	0.74	0.38	80,80,80,80	0
56	MG	RA	3259	1/1	0.74	0.28	87,87,87,87	0
56	MG	YA	3265	1/1	0.74	0.45	64,64,64,64	0
56	MG	RA	3595	1/1	0.74	0.41	84,84,84,84	0
56	MG	YA	3694	1/1	0.74	0.49	80,80,80,80	0
56	MG	RA	3436	1/1	0.74	0.98	56,56,56,56	0
56	MG	RA	3863	1/1	0.74	1.34	87,87,87,87	0
56	MG	RA	3264	1/1	0.74	1.24	63,63,63,63	0
56	MG	XA	1705	1/1	0.74	0.27	67,67,67,67	0
56	MG	RA	3607	1/1	0.74	0.35	98,98,98,98	0
56	MG	YA	3237	1/1	0.74	0.68	69,69,69,69	0
56	MG	RA	3150	1/1	0.74	0.17	74,74,74,74	0
56	MG	QA	1726	1/1	0.74	0.25	81,81,81,81	0
56	MG	RA	3452	1/1	0.74	0.29	78,78,78,78	0
56	MG	RA	3540	1/1	0.74	0.27	73,73,73,73	0
56	MG	YA	3491	1/1	0.74	0.70	53,53,53,53	0
56	MG	RA	3896	1/1	0.74	0.81	59,59,59,59	0
56	MG	YA	3550	1/1	0.74	0.87	76,76,76,76	0
56	MG	RA	3993	1/1	0.74	0.49	86,86,86,86	0
56	MG	RA	3225	1/1	0.74	0.43	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3362	1/1	0.74	0.33	93,93,93,93	0
56	MG	QA	1864	1/1	0.74	0.63	90,90,90,90	0
56	MG	RA	3229	1/1	0.74	0.47	82,82,82,82	0
56	MG	YA	3747	1/1	0.74	0.46	108,108,108,108	0
56	MG	QA	1699	1/1	0.74	0.57	65,65,65,65	0
56	MG	YA	3251	1/1	0.74	0.37	100,100,100,100	0
56	MG	QA	1771	1/1	0.74	0.16	57,57,57,57	0
56	MG	YT	201	1/1	0.75	0.43	57,57,57,57	0
56	MG	XA	1740	1/1	0.75	0.31	65,65,65,65	0
56	MG	XA	1748	1/1	0.75	0.49	60,60,60,60	0
56	MG	RA	3567	1/1	0.75	0.27	81,81,81,81	0
56	MG	XA	1713	1/1	0.75	0.26	49,49,49,49	0
56	MG	RA	3317	1/1	0.75	0.34	73,73,73,73	0
56	MG	YA	3095	1/1	0.75	0.17	68,68,68,68	0
56	MG	QA	1758	1/1	0.75	0.51	76,76,76,76	0
56	MG	RA	3909	1/1	0.75	0.80	73,73,73,73	0
56	MG	XA	1770	1/1	0.75	0.36	104,104,104,104	0
56	MG	XA	1632	1/1	0.75	0.88	59,59,59,59	0
56	MG	QR	101	1/1	0.75	0.20	71,71,71,71	0
56	MG	QA	1607	1/1	0.75	0.24	71,71,71,71	0
56	MG	YA	3599	1/1	0.75	0.44	70,70,70,70	0
56	MG	QA	1820	1/1	0.75	0.18	79,79,79,79	0
56	MG	QA	1741	1/1	0.75	0.59	45,45,45,45	0
56	MG	RA	3454	1/1	0.75	0.32	51,51,51,51	0
56	MG	RA	3144	1/1	0.75	0.77	84,84,84,84	0
56	MG	RA	3611	1/1	0.75	0.30	80,80,80,80	0
56	MG	RA	3077	1/1	0.75	0.27	70,70,70,70	0
56	MG	YA	3481	1/1	0.75	0.52	77,77,77,77	0
56	MG	RA	3228	1/1	0.75	0.53	101,101,101,101	0
56	MG	RA	3016	1/1	0.75	0.83	77,77,77,77	0
56	MG	YA	3551	1/1	0.75	0.54	60,60,60,60	0
56	MG	YA	3355	1/1	0.75	0.12	75,75,75,75	0
56	MG	RA	3372	1/1	0.75	0.62	61,61,61,61	0
56	MG	RA	3960	1/1	0.75	0.70	89,89,89,89	0
56	MG	YA	3455	1/1	0.75	0.56	79,79,79,79	0
56	MG	YA	3134	1/1	0.75	0.49	89,89,89,89	0
56	MG	YA	3075	1/1	0.75	0.41	43,43,43,43	0
56	MG	YA	3707	1/1	0.76	0.64	95,95,95,95	0
56	MG	RA	3586	1/1	0.76	0.53	73,73,73,73	0
56	MG	YO	201	1/1	0.76	0.38	78,78,78,78	0
56	MG	RA	3499	1/1	0.76	0.51	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3641	1/1	0.76	0.53	65,65,65,65	0
56	MG	RA	3510	1/1	0.76	0.21	38,38,38,38	0
56	MG	RA	3701	1/1	0.76	0.53	64,64,64,64	0
56	MG	RR	3205	1/1	0.76	0.44	60,60,60,60	0
56	MG	YA	3646	1/1	0.76	0.38	69,69,69,69	0
56	MG	RA	3173	1/1	0.76	0.35	50,50,50,50	0
56	MG	RA	3706	1/1	0.76	0.45	58,58,58,58	0
56	MG	Y8	101	1/1	0.76	0.92	70,70,70,70	0
56	MG	RA	3336	1/1	0.76	0.31	66,66,66,66	0
56	MG	QA	1625	1/1	0.76	0.33	61,61,61,61	0
56	MG	RA	3289	1/1	0.76	0.78	83,83,83,83	0
56	MG	YA	3635	1/1	0.76	0.55	80,80,80,80	0
56	MG	QA	1632	1/1	0.76	0.81	70,70,70,70	0
56	MG	RA	3006	1/1	0.76	0.12	33,33,33,33	0
56	MG	YA	3519	1/1	0.76	0.47	79,79,79,79	0
56	MG	RA	3628	1/1	0.76	0.58	65,65,65,65	0
56	MG	YA	3115	1/1	0.76	0.30	52,52,52,52	0
56	MG	QA	1797	1/1	0.76	0.40	95,95,95,95	0
56	MG	RF	312	1/1	0.76	0.48	62,62,62,62	0
56	MG	QA	1751	1/1	0.76	0.31	83,83,83,83	0
56	MG	RG	204	1/1	0.76	0.20	67,67,67,67	0
56	MG	RA	3995	1/1	0.76	0.38	111,111,111,111	0
56	MG	QA	1640	1/1	0.76	0.70	75,75,75,75	0
56	MG	RA	3226	1/1	0.77	0.95	104,104,104,104	0
56	MG	XA	1790	1/1	0.77	0.24	98,98,98,98	0
56	MG	RA	3730	1/1	0.77	0.22	51,51,51,51	0
56	MG	YD	305	1/1	0.77	0.42	82,82,82,82	0
56	MG	RA	4011	1/1	0.77	0.58	83,83,83,83	0
56	MG	RA	3571	1/1	0.77	0.48	94,94,94,94	0
56	MG	RF	304	1/1	0.77	0.17	63,63,63,63	0
56	MG	YD	307	1/1	0.77	0.71	64,64,64,64	0
56	MG	XX	101	1/1	0.77	0.77	122,122,122,122	0
56	MG	RA	3829	1/1	0.77	1.13	65,65,65,65	0
56	MG	RA	3514	1/1	0.77	0.25	87,87,87,87	0
56	MG	RG	203	1/1	0.77	0.34	79,79,79,79	0
56	MG	RA	3075	1/1	0.77	0.33	56,56,56,56	0
56	MG	XF	204	1/1	0.77	0.68	101,101,101,101	0
56	MG	QA	1807	1/1	0.77	0.33	65,65,65,65	0
56	MG	YA	3139	1/1	0.77	0.50	66,66,66,66	0
56	MG	YA	3129	1/1	0.77	0.36	31,31,31,31	0
56	MG	RN	203	1/1	0.77	0.35	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	RA	3085	1/1	0.77	0.45	76,76,76,76	0
56	MG	YA	3517	1/1	0.77	0.43	92,92,92,92	0
56	MG	YA	3178	1/1	0.77	0.90	62,62,62,62	0
56	MG	YA	3179	1/1	0.77	0.46	69,69,69,69	0
56	MG	YA	3220	1/1	0.77	0.32	87,87,87,87	0
56	MG	RA	3861	1/1	0.77	0.25	43,43,43,43	0
56	MG	YA	3087	1/1	0.77	0.24	64,64,64,64	0
56	MG	YA	3561	1/1	0.77	0.39	45,45,45,45	0
56	MG	YA	3426	1/1	0.77	0.56	50,50,50,50	0
56	MG	YA	3723	1/1	0.77	0.39	67,67,67,67	0
56	MG	RB	216	1/1	0.77	0.31	59,59,59,59	0
56	MG	XA	1686	1/1	0.77	0.28	68,68,68,68	0
56	MG	RA	3042	1/1	0.77	0.32	80,80,80,80	0
56	MG	QH	202	1/1	0.77	0.66	77,77,77,77	0
56	MG	RA	3124	1/1	0.77	0.21	46,46,46,46	0
56	MG	XA	1786	1/1	0.77	0.24	72,72,72,72	0
56	MG	QL	201	1/1	0.77	0.32	66,66,66,66	0
56	MG	YA	3566	1/1	0.77	0.21	60,60,60,60	0
56	MG	RA	3892	1/1	0.77	0.53	55,55,55,55	0
56	MG	RA	3719	1/1	0.77	0.41	55,55,55,55	0
56	MG	R8	101	1/1	0.77	0.75	75,75,75,75	0
56	MG	RA	3368	1/1	0.77	1.39	76,76,76,76	0
56	MG	QA	1700	1/1	0.77	0.47	66,66,66,66	0
56	MG	RD	308	1/1	0.77	0.57	80,80,80,80	0
56	MG	RA	3910	1/1	0.77	0.91	66,66,66,66	0
56	MG	YA	3226	1/1	0.77	0.48	75,75,75,75	0
56	MG	RE	301	1/1	0.78	0.40	81,81,81,81	0
56	MG	XA	1607	1/1	0.78	0.41	47,47,47,47	0
56	MG	RA	3489	1/1	0.78	0.91	50,50,50,50	0
56	MG	XA	1784	1/1	0.78	0.83	72,72,72,72	0
56	MG	QA	1603	1/1	0.78	0.41	105,105,105,105	0
56	MG	QA	1646	1/1	0.78	0.60	46,46,46,46	0
56	MG	RA	4019	1/1	0.78	0.68	87,87,87,87	0
56	MG	YA	3508	1/1	0.78	0.39	102,102,102,102	0
56	MG	YA	3485	1/1	0.78	0.57	77,77,77,77	0
56	MG	RA	3735	1/1	0.78	0.65	66,66,66,66	0
56	MG	RA	3736	1/1	0.78	0.40	74,74,74,74	0
56	MG	QA	1761	1/1	0.78	0.65	72,72,72,72	0
56	MG	RA	3236	1/1	0.78	0.67	69,69,69,69	0
56	MG	RA	4053	1/1	0.78	0.81	74,74,74,74	0
56	MG	RA	3574	1/1	0.78	0.37	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3653	1/1	0.78	0.25	75,75,75,75	0
56	MG	YA	3582	1/1	0.78	0.49	101,101,101,101	0
56	MG	RA	3843	1/1	0.78	0.30	72,72,72,72	0
56	MG	RA	3659	1/1	0.78	0.61	62,62,62,62	0
56	MG	YA	3698	1/1	0.78	0.50	77,77,77,77	0
56	MG	YA	3364	1/1	0.78	0.45	67,67,67,67	0
56	MG	QA	1615	1/1	0.78	0.26	107,107,107,107	0
56	MG	RA	3013	1/1	0.78	0.56	71,71,71,71	0
56	MG	QA	1876	1/1	0.78	0.25	84,84,84,84	0
56	MG	RA	3181	1/1	0.78	0.28	90,90,90,90	0
56	MG	RA	3774	1/1	0.78	0.51	59,59,59,59	0
56	MG	XA	1735	1/1	0.78	0.78	53,53,53,53	0
56	MG	YA	3477	1/1	0.78	0.55	70,70,70,70	0
56	MG	RA	3527	1/1	0.78	0.82	67,67,67,67	0
56	MG	YA	3051	1/1	0.78	0.44	64,64,64,64	0
56	MG	QA	1628	1/1	0.78	0.29	49,49,49,49	0
56	MG	XA	1688	1/1	0.78	0.28	56,56,56,56	0
56	MG	RA	3608	1/1	0.78	0.72	104,104,104,104	0
56	MG	XA	1665	1/1	0.78	0.30	73,73,73,73	0
56	MG	QA	1775	1/1	0.78	0.48	72,72,72,72	0
56	MG	QA	1713	1/1	0.78	0.42	79,79,79,79	0
56	MG	R3	102	1/1	0.78	1.15	80,80,80,80	0
56	MG	QA	1672	1/1	0.78	0.52	45,45,45,45	0
56	MG	YA	3161	1/1	0.78	0.55	76,76,76,76	0
56	MG	XA	1622	1/1	0.78	0.24	42,42,42,42	0
56	MG	RD	309	1/1	0.78	0.30	78,78,78,78	0
56	MG	XR	101	1/1	0.78	0.43	89,89,89,89	0
56	MG	RD	311	1/1	0.78	0.49	70,70,70,70	0
56	MG	RA	3211	1/1	0.78	0.52	88,88,88,88	0
56	MG	YA	3170	1/1	0.78	0.62	56,56,56,56	0
56	MG	RA	3642	1/1	0.79	0.25	70,70,70,70	0
56	MG	QA	1648	1/1	0.79	0.21	67,67,67,67	0
56	MG	YA	3088	1/1	0.79	0.34	42,42,42,42	0
56	MG	XA	1689	1/1	0.79	0.25	64,64,64,64	0
56	MG	YA	3169	1/1	0.79	0.59	91,91,91,91	0
56	MG	YA	3522	1/1	0.79	0.51	65,65,65,65	0
56	MG	RA	3330	1/1	0.79	0.20	41,41,41,41	0
56	MG	RA	3520	1/1	0.79	0.27	34,34,34,34	0
56	MG	XA	1714	1/1	0.79	0.21	58,58,58,58	0
56	MG	XA	1741	1/1	0.79	0.26	67,67,67,67	0
56	MG	RA	3206	1/1	0.79	0.57	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3665	1/1	0.79	0.38	77,77,77,77	0
56	MG	YA	3375	1/1	0.79	0.44	55,55,55,55	0
56	MG	QA	1795	1/1	0.79	0.36	61,61,61,61	0
56	MG	RA	3528	1/1	0.79	0.36	76,76,76,76	0
56	MG	QG	202	1/1	0.79	0.29	92,92,92,92	0
56	MG	RA	4066	1/1	0.79	0.71	78,78,78,78	0
56	MG	RA	3762	1/1	0.79	0.27	76,76,76,76	0
56	MG	YA	3183	1/1	0.79	0.38	47,47,47,47	0
56	MG	RA	3533	1/1	0.79	0.28	49,49,49,49	0
56	MG	QA	1687	1/1	0.79	0.31	97,97,97,97	0
56	MG	QA	1690	1/1	0.79	0.29	72,72,72,72	0
56	MG	RA	3164	1/1	0.79	0.47	87,87,87,87	0
56	MG	QA	1665	1/1	0.79	0.55	102,102,102,102	0
56	MG	RA	3784	1/1	0.79	0.31	94,94,94,94	0
56	MG	YA	3729	1/1	0.79	0.55	61,61,61,61	0
56	MG	RA	3693	1/1	0.79	0.40	67,67,67,67	0
56	MG	YA	3307	1/1	0.79	0.35	73,73,73,73	0
56	MG	RA	3626	1/1	0.79	0.43	68,68,68,68	0
56	MG	QA	1778	1/1	0.79	0.88	61,61,61,61	0
56	MG	RA	3880	1/1	0.79	0.52	54,54,54,54	0
56	MG	YB	208	1/1	0.79	0.31	81,81,81,81	0
56	MG	RA	3988	1/1	0.79	0.68	75,75,75,75	0
56	MG	RA	3293	1/1	0.79	0.21	128,128,128,128	0
56	MG	RA	3992	1/1	0.79	0.17	74,74,74,74	0
56	MG	RD	304	1/1	0.79	2.03	86,86,86,86	0
56	MG	QA	1670	1/1	0.79	0.52	81,81,81,81	0
56	MG	RA	3111	1/1	0.79	0.23	106,106,106,106	0
56	MG	RA	3190	1/1	0.79	0.33	62,62,62,62	0
56	MG	RA	3805	1/1	0.79	0.31	98,98,98,98	0
56	MG	RA	3246	1/1	0.79	0.82	69,69,69,69	0
56	MG	RA	3406	1/1	0.79	0.29	60,60,60,60	0
56	MG	YA	3512	1/1	0.79	0.52	62,62,62,62	0
56	MG	XA	1650	1/1	0.79	0.64	84,84,84,84	0
56	MG	XA	1730	1/1	0.80	0.19	47,47,47,47	0
56	MG	RA	3661	1/1	0.80	0.34	89,89,89,89	0
56	MG	RA	4014	1/1	0.80	0.54	83,83,83,83	0
56	MG	YA	3159	1/1	0.80	0.40	91,91,91,91	0
56	MG	RA	3064	1/1	0.80	0.19	54,54,54,54	0
56	MG	RA	3602	1/1	0.80	0.96	80,80,80,80	0
56	MG	RA	3826	1/1	0.80	0.30	62,62,62,62	0
56	MG	RA	3827	1/1	0.80	0.35	57,57,57,57	0
56	MG	RA	4041	1/1	0.80	1.07	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	QA	1605	1/1	0.80	0.28	67,67,67,67	0
56	MG	RA	3604	1/1	0.80	0.26	91,91,91,91	0
56	MG	RA	3670	1/1	0.80	0.21	80,80,80,80	0
56	MG	YA	3001	1/1	0.80	0.34	90,90,90,90	0
56	MG	QA	1808	1/1	0.80	0.50	54,54,54,54	0
56	MG	RA	3008	1/1	0.80	0.17	46,46,46,46	0
56	MG	RA	3955	1/1	0.80	0.29	74,74,74,74	0
56	MG	RA	3009	1/1	0.80	0.32	53,53,53,53	0
56	MG	RA	3957	1/1	0.80	0.32	66,66,66,66	0
56	MG	RA	3505	1/1	0.80	0.28	64,64,64,64	0
56	MG	YA	3368	1/1	0.80	0.47	62,62,62,62	0
56	MG	QF	201	1/1	0.80	0.28	59,59,59,59	0
56	MG	RA	3771	1/1	0.80	0.34	45,45,45,45	0
56	MG	RA	3687	1/1	0.80	0.30	57,57,57,57	0
56	MG	QG	201	1/1	0.80	0.83	91,91,91,91	0
56	MG	YA	3383	1/1	0.80	0.46	70,70,70,70	0
56	MG	RA	3557	1/1	0.80	0.44	63,63,63,63	0
56	MG	XA	1751	1/1	0.80	0.44	59,59,59,59	0
56	MG	QA	1863	1/1	0.80	0.28	80,80,80,80	0
56	MG	RA	3034	1/1	0.80	0.81	100,100,100,100	0
56	MG	XA	1656	1/1	0.80	0.39	80,80,80,80	0
56	MG	RA	3702	1/1	0.80	1.05	67,67,67,67	0
56	MG	RA	3789	1/1	0.80	0.32	95,95,95,95	0
56	MG	YA	3205	1/1	0.80	0.31	58,58,58,58	0
56	MG	YA	3700	1/1	0.80	0.39	71,71,71,71	0
56	MG	YA	3474	1/1	0.80	0.39	72,72,72,72	0
56	MG	XA	1663	1/1	0.80	0.43	107,107,107,107	0
56	MG	YD	310	1/1	0.80	0.43	64,64,64,64	0
56	MG	RA	3721	1/1	0.80	0.59	73,73,73,73	0
56	MG	RD	301	1/1	0.80	0.57	76,76,76,76	0
56	MG	RA	3290	1/1	0.80	0.37	74,74,74,74	0
56	MG	QA	1656	1/1	0.80	0.21	58,58,58,58	0
56	MG	RA	3240	1/1	0.80	0.44	92,92,92,92	0
56	MG	RA	3531	1/1	0.80	0.25	34,34,34,34	0
56	MG	YA	3633	1/1	0.80	0.72	47,47,47,47	0
56	MG	YE	302	1/1	0.80	0.54	79,79,79,79	0
56	MG	RA	3731	1/1	0.80	0.39	83,83,83,83	0
56	MG	RA	3231	1/1	0.81	0.57	97,97,97,97	0
56	MG	RA	3806	1/1	0.81	0.27	78,78,78,78	0
56	MG	RA	3410	1/1	0.81	0.12	76,76,76,76	0
56	MG	QA	1689	1/1	0.81	0.51	80,80,80,80	0
56	MG	RA	3650	1/1	0.81	0.44	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	4012	1/1	0.81	0.78	89,89,89,89	0
56	MG	YD	302	1/1	0.81	0.38	71,71,71,71	0
56	MG	RA	3922	1/1	0.81	0.47	70,70,70,70	0
56	MG	QA	1802	1/1	0.81	0.67	79,79,79,79	0
56	MG	RA	3732	1/1	0.81	0.15	54,54,54,54	0
56	MG	RA	3819	1/1	0.81	0.23	33,33,33,33	0
56	MG	RA	3934	1/1	0.81	0.17	62,62,62,62	0
56	MG	RA	3088	1/1	0.81	1.59	89,89,89,89	0
56	MG	YA	3428	1/1	0.81	0.36	44,44,44,44	0
56	MG	YA	3025	1/1	0.81	0.08	55,55,55,55	0
56	MG	QA	1695	1/1	0.81	0.49	48,48,48,48	0
56	MG	RA	3433	1/1	0.81	0.42	66,66,66,66	0
56	MG	YA	3249	1/1	0.81	0.57	72,72,72,72	0
56	MG	XA	1787	1/1	0.81	1.44	84,84,84,84	0
56	MG	RA	3598	1/1	0.81	0.38	94,94,94,94	0
56	MG	YA	3089	1/1	0.81	0.39	80,80,80,80	0
56	MG	YA	3552	1/1	0.81	0.74	52,52,52,52	0
56	MG	YA	3553	1/1	0.81	0.50	58,58,58,58	0
56	MG	YE	305	1/1	0.81	0.45	57,57,57,57	0
56	MG	RA	3841	1/1	0.81	0.47	64,64,64,64	0
56	MG	RA	3756	1/1	0.81	0.49	83,83,83,83	0
56	MG	YA	3555	1/1	0.81	0.66	77,77,77,77	0
56	MG	YA	3304	1/1	0.81	0.64	56,56,56,56	0
56	MG	RA	3764	1/1	0.81	0.52	60,60,60,60	0
56	MG	XA	1695	1/1	0.81	0.67	52,52,52,52	0
56	MG	RA	3270	1/1	0.81	0.33	103,103,103,103	0
56	MG	YA	3215	1/1	0.81	0.20	54,54,54,54	0
56	MG	YA	3154	1/1	0.81	0.60	86,86,86,86	0
56	MG	YA	3188	1/1	0.81	0.39	94,94,94,94	0
56	MG	YA	3239	1/1	0.81	0.38	94,94,94,94	0
56	MG	QA	1724	1/1	0.81	0.24	76,76,76,76	0
56	MG	YA	3029	1/1	0.81	0.56	57,57,57,57	0
56	MG	YA	3315	1/1	0.81	0.85	62,62,62,62	0
56	MG	RA	3221	1/1	0.81	0.55	63,63,63,63	0
56	MG	YA	3532	1/1	0.81	0.98	60,60,60,60	0
56	MG	YA	3324	1/1	0.81	0.52	39,39,39,39	0
56	MG	R7	101	1/1	0.81	0.44	66,66,66,66	0
56	MG	YA	3227	1/1	0.81	0.52	64,64,64,64	0
56	MG	RA	3161	1/1	0.81	0.35	72,72,72,72	0
56	MG	RA	3708	1/1	0.81	0.34	54,54,54,54	0
56	MG	RA	3397	1/1	0.81	0.46	65,65,65,65	0
56	MG	RA	3563	1/1	0.81	0.64	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3623	1/1	0.81	0.37	54,54,54,54	0
56	MG	YA	3017	1/1	0.81	0.58	60,60,60,60	0
56	MG	YA	3078	1/1	0.82	0.37	60,60,60,60	0
56	MG	RA	3055	1/1	0.82	0.52	85,85,85,85	0
56	MG	RA	3215	1/1	0.82	0.38	98,98,98,98	0
56	MG	YA	3740	1/1	0.82	0.40	52,52,52,52	0
56	MG	RA	3737	1/1	0.82	0.29	77,77,77,77	0
56	MG	RA	3959	1/1	0.82	0.28	43,43,43,43	0
56	MG	XA	1754	1/1	0.82	0.62	86,86,86,86	0
56	MG	RA	3332	1/1	0.82	0.35	53,53,53,53	0
56	MG	XA	1760	1/1	0.82	0.30	71,71,71,71	0
56	MG	RA	4056	1/1	0.82	0.76	70,70,70,70	0
56	MG	YA	3492	1/1	0.82	0.61	63,63,63,63	0
56	MG	RA	3107	1/1	0.82	0.52	109,109,109,109	0
56	MG	YI	201	1/1	0.82	0.34	110,110,110,110	0
56	MG	RA	3883	1/1	0.82	0.34	93,93,93,93	0
56	MG	RB	202	1/1	0.82	0.15	55,55,55,55	0
56	MG	RA	3690	1/1	0.82	0.98	74,74,74,74	0
56	MG	RA	3278	1/1	0.82	0.68	83,83,83,83	0
56	MG	YA	3190	1/1	0.82	0.12	78,78,78,78	0
56	MG	RA	3186	1/1	0.82	0.35	77,77,77,77	0
56	MG	RA	3758	1/1	0.82	0.17	49,49,49,49	0
56	MG	XA	1630	1/1	0.82	0.34	62,62,62,62	0
56	MG	YA	3263	1/1	0.82	0.58	81,81,81,81	0
56	MG	RA	3643	1/1	0.82	0.81	71,71,71,71	0
56	MG	RA	3455	1/1	0.82	0.43	48,48,48,48	0
56	MG	RU	202	1/1	0.82	0.31	78,78,78,78	0
56	MG	RA	3917	1/1	0.82	0.61	67,67,67,67	0
56	MG	RV	203	1/1	0.82	0.36	55,55,55,55	0
56	MG	YA	3172	1/1	0.82	0.28	69,69,69,69	0
56	MG	YR	201	1/1	0.82	0.36	66,66,66,66	0
56	MG	RA	3923	1/1	0.82	0.31	79,79,79,79	0
56	MG	R0	101	1/1	0.82	0.40	94,94,94,94	0
56	MG	RA	3129	1/1	0.82	0.27	45,45,45,45	0
56	MG	RA	3243	1/1	0.82	0.31	73,73,73,73	0
56	MG	YA	3693	1/1	0.82	0.32	60,60,60,60	0
56	MG	QA	1604	1/1	0.82	0.22	75,75,75,75	0
56	MG	RA	3299	1/1	0.82	0.37	96,96,96,96	0
56	MG	RA	3937	1/1	0.82	0.19	38,38,38,38	0
56	MG	YA	3530	1/1	0.82	0.72	59,59,59,59	0
56	MG	RA	3080	1/1	0.82	0.59	81,81,81,81	0
56	MG	R5	101	1/1	0.82	1.13	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3943	1/1	0.82	0.35	86,86,86,86	0
56	MG	RA	4013	1/1	0.82	0.45	76,76,76,76	0
56	MG	YA	3229	1/1	0.82	0.35	71,71,71,71	0
56	MG	YA	3101	1/1	0.82	0.37	70,70,70,70	0
56	MG	YA	3012	1/1	0.82	0.28	56,56,56,56	0
56	MG	QA	1852	1/1	0.82	0.40	60,60,60,60	0
56	MG	RA	4025	1/1	0.82	0.28	32,32,32,32	0
56	MG	QA	1673	1/1	0.82	0.46	52,52,52,52	0
56	MG	YA	3405	1/1	0.83	0.44	86,86,86,86	0
56	MG	RA	3174	1/1	0.83	0.28	62,62,62,62	0
56	MG	XA	1712	1/1	0.83	0.33	61,61,61,61	0
56	MG	RA	3178	1/1	0.83	0.58	79,79,79,79	0
56	MG	QA	1752	1/1	0.83	0.26	77,77,77,77	0
56	MG	RA	3404	1/1	0.83	0.25	81,81,81,81	0
56	MG	RA	3300	1/1	0.83	1.17	68,68,68,68	0
56	MG	RA	4005	1/1	0.83	0.30	58,58,58,58	0
56	MG	YA	3721	1/1	0.83	0.60	65,65,65,65	0
56	MG	RA	4010	1/1	0.83	0.32	76,76,76,76	0
56	MG	RA	3811	1/1	0.83	0.26	55,55,55,55	0
56	MG	RE	306	1/1	0.83	0.30	59,59,59,59	0
56	MG	RA	3412	1/1	0.83	0.52	71,71,71,71	0
56	MG	RA	3816	1/1	0.83	0.55	102,102,102,102	0
56	MG	RA	3734	1/1	0.83	0.61	70,70,70,70	0
56	MG	RA	3585	1/1	0.83	0.56	59,59,59,59	0
56	MG	RA	4017	1/1	0.83	0.59	90,90,90,90	0
56	MG	RA	3182	1/1	0.83	0.52	85,85,85,85	0
56	MG	RA	3588	1/1	0.83	0.54	63,63,63,63	0
56	MG	RA	3183	1/1	0.83	0.38	81,81,81,81	0
56	MG	RA	3936	1/1	0.83	1.11	74,74,74,74	0
56	MG	YA	3470	1/1	0.83	0.34	59,59,59,59	0
56	MG	RA	4038	1/1	0.83	0.61	66,66,66,66	0
56	MG	RA	3938	1/1	0.83	0.59	100,100,100,100	0
56	MG	YQ	202	1/1	0.83	0.39	59,59,59,59	0
56	MG	YA	3250	1/1	0.83	0.32	45,45,45,45	0
56	MG	YA	3050	1/1	0.83	0.19	85,85,85,85	0
56	MG	RP	201	1/1	0.83	0.73	72,72,72,72	0
56	MG	RA	3748	1/1	0.83	0.22	61,61,61,61	0
56	MG	YA	3664	1/1	0.83	0.46	42,42,42,42	0
56	MG	RA	3832	1/1	0.83	0.35	74,74,74,74	0
56	MG	RA	3319	1/1	0.83	0.76	54,54,54,54	0
56	MG	RA	3434	1/1	0.83	0.35	61,61,61,61	0
56	MG	YA	3597	1/1	0.83	0.81	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	XA	1658	1/1	0.83	0.30	79,79,79,79	0
56	MG	RA	3757	1/1	0.83	0.38	70,70,70,70	0
56	MG	RA	3438	1/1	0.83	0.18	71,71,71,71	0
56	MG	YA	3120	1/1	0.83	0.56	72,72,72,72	0
56	MG	QA	1658	1/1	0.83	0.15	94,94,94,94	0
56	MG	RA	3763	1/1	0.83	0.49	61,61,61,61	0
56	MG	RA	3201	1/1	0.83	0.34	70,70,70,70	0
56	MG	YA	3090	1/1	0.83	0.90	54,54,54,54	0
56	MG	XA	1629	1/1	0.83	0.18	51,51,51,51	0
56	MG	QA	1623	1/1	0.83	0.51	74,74,74,74	0
56	MG	YA	3303	1/1	0.83	0.41	85,85,85,85	0
56	MG	YA	3242	1/1	0.83	0.30	88,88,88,88	0
56	MG	RA	3780	1/1	0.83	0.97	74,74,74,74	0
56	MG	RB	218	1/1	0.83	0.29	79,79,79,79	0
56	MG	QA	1875	1/1	0.83	0.43	75,75,75,75	0
56	MG	YA	3015	1/1	0.83	0.41	23,23,23,23	0
56	MG	YA	3506	1/1	0.83	0.37	53,53,53,53	0
56	MG	YA	3024	1/1	0.83	0.86	59,59,59,59	0
56	MG	YA	3235	1/1	0.83	0.25	91,91,91,91	0
56	MG	XA	1749	1/1	0.83	0.44	82,82,82,82	0
56	MG	RA	3707	1/1	0.83	0.40	69,69,69,69	0
56	MG	RA	3019	1/1	0.83	0.27	113,113,113,113	0
56	MG	QA	1809	1/1	0.83	0.28	67,67,67,67	0
56	MG	YA	3071	1/1	0.83	0.43	77,77,77,77	0
56	MG	YA	3717	1/1	0.83	0.42	45,45,45,45	0
56	MG	QA	1688	1/1	0.84	0.76	62,62,62,62	0
56	MG	YA	3687	1/1	0.84	0.22	75,75,75,75	0
56	MG	YA	3043	1/1	0.84	0.82	62,62,62,62	0
56	MG	RA	3254	1/1	0.84	0.28	92,92,92,92	0
56	MG	YA	3416	1/1	0.84	0.83	39,39,39,39	0
56	MG	YA	3225	1/1	0.84	0.32	74,74,74,74	0
56	MG	RA	3835	1/1	0.84	0.78	56,56,56,56	0
56	MG	RA	3175	1/1	0.84	0.52	70,70,70,70	0
56	MG	YF	301	1/1	0.84	0.21	54,54,54,54	0
56	MG	RA	3074	1/1	0.84	0.28	52,52,52,52	0
56	MG	YA	3197	1/1	0.84	0.34	77,77,77,77	0
56	MG	QL	202	1/1	0.84	0.11	68,68,68,68	0
56	MG	XA	1615	1/1	0.84	0.21	63,63,63,63	0
56	MG	QA	1849	1/1	0.84	0.73	81,81,81,81	0
56	MG	RA	3743	1/1	0.84	0.32	35,35,35,35	0
56	MG	XA	1696	1/1	0.84	0.14	67,67,67,67	0
56	MG	YA	3516	1/1	0.84	0.66	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YB	203	1/1	0.84	0.14	72,72,72,72	0
56	MG	YA	3567	1/1	0.84	0.23	42,42,42,42	0
56	MG	YA	3570	1/1	0.84	0.57	59,59,59,59	0
56	MG	RA	3648	1/1	0.84	0.49	82,82,82,82	0
56	MG	RA	3196	1/1	0.84	0.96	104,104,104,104	0
56	MG	QA	1711	1/1	0.84	0.28	63,63,63,63	0
56	MG	RA	3091	1/1	0.84	1.47	104,104,104,104	0
56	MG	YA	3442	1/1	0.84	0.50	53,53,53,53	0
56	MG	YA	3649	1/1	0.84	0.38	60,60,60,60	0
56	MG	RA	3656	1/1	0.84	0.60	44,44,44,44	0
56	MG	RA	4006	1/1	0.84	0.79	81,81,81,81	0
56	MG	YA	3292	1/1	0.84	0.77	81,81,81,81	0
56	MG	XA	1764	1/1	0.84	0.56	52,52,52,52	0
56	MG	QA	1610	1/1	0.84	0.34	105,105,105,105	0
56	MG	XA	1706	1/1	0.84	0.26	67,67,67,67	0
56	MG	YA	3719	1/1	0.84	0.43	79,79,79,79	0
56	MG	QA	1815	1/1	0.84	0.36	65,65,65,65	0
56	MG	RA	3775	1/1	0.84	0.44	56,56,56,56	0
56	MG	XA	1772	1/1	0.84	0.42	51,51,51,51	0
56	MG	RA	3114	1/1	0.84	0.32	91,91,91,91	0
56	MG	RA	3449	1/1	0.84	0.24	45,45,45,45	0
56	MG	RA	4021	1/1	0.84	0.29	56,56,56,56	0
56	MG	XA	1625	1/1	0.84	0.76	74,74,74,74	0
56	MG	RA	3116	1/1	0.84	0.71	104,104,104,104	0
56	MG	XA	1779	1/1	0.84	0.86	60,60,60,60	0
56	MG	XA	1710	1/1	0.84	0.37	66,66,66,66	0
56	MG	RA	3578	1/1	0.84	0.53	60,60,60,60	0
56	MG	RA	3685	1/1	0.84	0.47	97,97,97,97	0
56	MG	RA	3222	1/1	0.84	0.11	72,72,72,72	0
56	MG	YA	3293	1/1	0.84	1.25	70,70,70,70	0
56	MG	RA	3795	1/1	0.84	0.54	75,75,75,75	0
56	MG	QA	1874	1/1	0.84	0.39	74,74,74,74	0
56	MG	YB	215	1/1	0.84	0.23	92,92,92,92	0
56	MG	YA	3158	1/1	0.84	0.71	49,49,49,49	0
56	MG	RA	3329	1/1	0.84	0.29	86,86,86,86	0
56	MG	QA	1678	1/1	0.84	0.24	80,80,80,80	0
56	MG	YA	3180	1/1	0.84	0.45	43,43,43,43	0
56	MG	RA	4063	1/1	0.84	1.40	68,68,68,68	0
56	MG	RA	3592	1/1	0.84	0.60	56,56,56,56	0
56	MG	QA	1635	1/1	0.84	0.18	58,58,58,58	0
56	MG	YA	3146	1/1	0.84	0.13	60,60,60,60	0
56	MG	RA	3337	1/1	0.84	0.49	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	RA	3053	1/1	0.84	0.43	89,89,89,89	0
56	MG	YA	3130	1/1	0.84	0.62	65,65,65,65	0
56	MG	RA	3346	1/1	0.84	0.87	72,72,72,72	0
56	MG	Y5	101	1/1	0.84	0.32	63,63,63,63	0
56	MG	RA	3157	1/1	0.84	0.23	72,72,72,72	0
56	MG	YA	3679	1/1	0.84	0.48	36,36,36,36	0
56	MG	YA	3730	1/1	0.84	0.48	87,87,87,87	0
56	MG	RA	3247	1/1	0.84	0.61	88,88,88,88	0
56	MG	RA	3163	1/1	0.84	0.94	93,93,93,93	0
56	MG	RA	3618	1/1	0.84	0.35	48,48,48,48	0
56	MG	YA	3259	1/1	0.85	0.36	66,66,66,66	0
56	MG	RA	3154	1/1	0.85	0.12	88,88,88,88	0
56	MG	XA	1731	1/1	0.85	0.27	65,65,65,65	0
56	MG	RA	3158	1/1	0.85	0.36	67,67,67,67	0
56	MG	RA	3159	1/1	0.85	0.41	107,107,107,107	0
56	MG	RA	3234	1/1	0.85	0.37	64,64,64,64	0
56	MG	YA	3020	1/1	0.85	0.27	80,80,80,80	0
56	MG	YA	3716	1/1	0.85	0.42	65,65,65,65	0
56	MG	QA	1639	1/1	0.85	0.20	79,79,79,79	0
56	MG	YA	3209	1/1	0.85	0.45	48,48,48,48	0
56	MG	YA	3084	1/1	0.85	0.39	66,66,66,66	0
56	MG	YA	3243	1/1	0.85	0.34	67,67,67,67	0
56	MG	YA	3469	1/1	0.85	0.35	88,88,88,88	0
56	MG	RA	3671	1/1	0.85	0.31	71,71,71,71	0
56	MG	RA	3767	1/1	0.85	0.38	37,37,37,37	0
56	MG	QA	1684	1/1	0.85	0.52	97,97,97,97	0
56	MG	YB	213	1/1	0.85	0.41	57,57,57,57	0
56	MG	RA	3176	1/1	0.85	0.71	96,96,96,96	0
56	MG	YA	3447	1/1	0.85	0.63	68,68,68,68	0
56	MG	YB	217	1/1	0.85	0.34	77,77,77,77	0
56	MG	XA	1762	1/1	0.85	0.27	48,48,48,48	0
56	MG	RA	3018	1/1	0.85	0.30	89,89,89,89	0
56	MG	YA	3266	1/1	0.85	0.82	70,70,70,70	0
56	MG	QA	1651	1/1	0.85	0.65	89,89,89,89	0
56	MG	RA	3024	1/1	0.85	0.41	74,74,74,74	0
56	MG	RF	308	1/1	0.85	0.51	74,74,74,74	0
56	MG	YA	3725	1/1	0.85	0.41	68,68,68,68	0
56	MG	RA	3029	1/1	0.85	0.74	66,66,66,66	0
56	MG	RA	3692	1/1	0.85	0.72	87,87,87,87	0
56	MG	RA	3268	1/1	0.85	0.41	95,95,95,95	0
56	MG	QA	1744	1/1	0.85	0.69	65,65,65,65	0
56	MG	RA	3109	1/1	0.85	0.55	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3696	1/1	0.85	1.18	74,74,74,74	0
56	MG	RA	3919	1/1	0.85	0.60	47,47,47,47	0
56	MG	YA	3058	1/1	0.85	0.21	75,75,75,75	0
56	MG	YA	3230	1/1	0.85	0.61	57,57,57,57	0
56	MG	RA	4026	1/1	0.85	0.47	71,71,71,71	0
56	MG	YA	3476	1/1	0.85	0.57	52,52,52,52	0
56	MG	RA	3377	1/1	0.85	0.49	42,42,42,42	0
56	MG	RA	3392	1/1	0.85	0.28	28,28,28,28	0
56	MG	RA	4040	1/1	0.85	0.53	69,69,69,69	0
56	MG	RA	3927	1/1	0.85	0.42	81,81,81,81	0
56	MG	RA	3802	1/1	0.85	1.15	89,89,89,89	0
56	MG	RA	3522	1/1	0.85	0.31	55,55,55,55	0
56	MG	XA	1601	1/1	0.85	0.25	75,75,75,75	0
56	MG	RA	4049	1/1	0.85	0.44	92,92,92,92	0
56	MG	YA	3187	1/1	0.85	0.25	40,40,40,40	0
56	MG	RA	3401	1/1	0.85	0.18	44,44,44,44	0
56	MG	RA	3713	1/1	0.85	0.47	47,47,47,47	0
56	MG	YA	3219	1/1	0.85	0.47	60,60,60,60	0
56	MG	RA	3281	1/1	0.85	1.19	85,85,85,85	0
56	MG	QA	1614	1/1	0.85	0.20	48,48,48,48	0
56	MG	YA	3128	1/1	0.85	0.21	26,26,26,26	0
56	MG	RA	4060	1/1	0.85	0.58	82,82,82,82	0
56	MG	RA	3632	1/1	0.85	0.52	55,55,55,55	0
56	MG	QA	1705	1/1	0.85	0.28	37,37,37,37	0
56	MG	RA	3130	1/1	0.85	0.07	69,69,69,69	0
56	MG	YA	3221	1/1	0.85	0.35	77,77,77,77	0
56	MG	QA	1709	1/1	0.85	0.49	53,53,53,53	0
56	MG	QA	1621	1/1	0.85	0.39	71,71,71,71	0
56	MG	YA	3140	1/1	0.85	0.62	65,65,65,65	0
56	MG	YE	307	1/1	0.85	0.24	64,64,64,64	0
56	MG	RA	3297	1/1	0.85	0.15	39,39,39,39	0
56	MG	RA	3140	1/1	0.85	0.81	93,93,93,93	0
56	MG	RB	212	1/1	0.85	0.17	74,74,74,74	0
56	MG	YA	3034	1/1	0.85	0.30	68,68,68,68	0
56	MG	YA	3463	1/1	0.85	0.24	47,47,47,47	0
56	MG	RA	3146	1/1	0.85	0.23	37,37,37,37	0
56	MG	YA	3710	1/1	0.85	0.62	61,61,61,61	0
56	MG	RA	3552	1/1	0.85	0.16	97,97,97,97	0
56	MG	XA	1724	1/1	0.86	0.39	65,65,65,65	0
56	MG	RA	3001	1/1	0.86	0.34	68,68,68,68	0
56	MG	YA	3105	1/1	0.86	0.39	37,37,37,37	0
56	MG	RA	3997	1/1	0.86	0.28	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3627	1/1	0.86	0.66	76,76,76,76	0
56	MG	YA	3200	1/1	0.86	0.39	70,70,70,70	0
56	MG	RA	3629	1/1	0.86	0.46	60,60,60,60	0
56	MG	RA	3898	1/1	0.86	0.33	48,48,48,48	0
56	MG	QA	1767	1/1	0.86	0.23	90,90,90,90	0
56	MG	QA	1633	1/1	0.86	0.19	95,95,95,95	0
56	MG	YA	3713	1/1	0.86	0.74	67,67,67,67	0
56	MG	XE	202	1/1	0.86	0.08	67,67,67,67	0
56	MG	RA	3913	1/1	0.86	0.45	43,43,43,43	0
56	MG	RA	3716	1/1	0.86	0.23	52,52,52,52	0
56	MG	YA	3638	1/1	0.86	0.34	65,65,65,65	0
56	MG	YA	3454	1/1	0.86	1.16	52,52,52,52	0
56	MG	YA	3040	1/1	0.86	0.20	66,66,66,66	0
56	MG	YA	3153	1/1	0.86	0.20	37,37,37,37	0
56	MG	YA	3032	1/1	0.86	0.28	80,80,80,80	0
56	MG	RA	3450	1/1	0.86	1.29	53,53,53,53	0
56	MG	RA	3925	1/1	0.86	0.31	83,83,83,83	0
56	MG	RA	3253	1/1	0.86	0.31	66,66,66,66	0
56	MG	YA	3223	1/1	0.86	0.49	91,91,91,91	0
56	MG	QA	1779	1/1	0.86	0.22	80,80,80,80	0
56	MG	RG	202	1/1	0.86	0.08	85,85,85,85	0
56	MG	RA	4034	1/1	0.86	0.74	73,73,73,73	0
56	MG	QA	1825	1/1	0.86	0.40	74,74,74,74	0
56	MG	YA	3295	1/1	0.86	0.32	44,44,44,44	0
56	MG	RA	3033	1/1	0.86	0.27	91,91,91,91	0
56	MG	YA	3301	1/1	0.86	0.23	42,42,42,42	0
56	MG	QB	301	1/1	0.86	0.13	91,91,91,91	0
56	MG	RA	3265	1/1	0.86	0.10	111,111,111,111	0
56	MG	YA	3028	1/1	0.86	0.33	51,51,51,51	0
56	MG	RA	4048	1/1	0.86	0.58	81,81,81,81	0
56	MG	XA	1707	1/1	0.86	0.55	58,58,58,58	0
56	MG	RA	3363	1/1	0.86	0.54	50,50,50,50	0
56	MG	XA	1758	1/1	0.86	0.56	60,60,60,60	0
56	MG	XA	1627	1/1	0.86	0.50	62,62,62,62	0
56	MG	YA	3674	1/1	0.86	0.65	74,74,74,74	0
56	MG	RA	3582	1/1	0.86	0.83	72,72,72,72	0
56	MG	RA	3749	1/1	0.86	0.31	63,63,63,63	0
56	MG	QA	1606	1/1	0.86	0.48	93,93,93,93	0
56	MG	RA	3498	1/1	0.86	0.49	58,58,58,58	0
56	MG	YA	3168	1/1	0.86	0.38	88,88,88,88	0
56	MG	RA	3054	1/1	0.86	0.35	78,78,78,78	0
56	MG	YA	3098	1/1	0.86	0.14	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	RA	3373	1/1	0.86	0.55	44,44,44,44	0
56	MG	YA	3210	1/1	0.86	0.31	65,65,65,65	0
56	MG	YA	3692	1/1	0.86	0.33	39,39,39,39	0
56	MG	QA	1702	1/1	0.86	0.36	64,64,64,64	0
56	MG	YA	3732	1/1	0.86	1.09	73,73,73,73	0
56	MG	XA	1777	1/1	0.86	0.63	98,98,98,98	0
56	MG	YA	3264	1/1	0.86	0.57	88,88,88,88	0
56	MG	RA	3853	1/1	0.86	1.17	64,64,64,64	0
56	MG	XA	1677	1/1	0.86	0.28	71,71,71,71	0
56	MG	YA	3627	1/1	0.86	0.46	38,38,38,38	0
56	MG	YA	3104	1/1	0.86	0.55	85,85,85,85	0
56	MG	YA	3632	1/1	0.86	0.35	62,62,62,62	0
56	MG	YA	3160	1/1	0.86	0.48	67,67,67,67	0
56	MG	QQ	201	1/1	0.86	0.21	71,71,71,71	0
56	MG	RA	3777	1/1	0.86	0.45	93,93,93,93	0
56	MG	RA	3609	1/1	0.86	0.27	71,71,71,71	0
56	MG	YA	3748	1/1	0.86	0.49	95,95,95,95	0
56	MG	QA	1626	1/1	0.86	0.10	78,78,78,78	0
56	MG	RA	3233	1/1	0.86	0.30	72,72,72,72	0
56	MG	RA	3561	1/1	0.87	0.36	42,42,42,42	0
56	MG	YA	3272	1/1	0.87	0.42	39,39,39,39	0
56	MG	RA	3844	1/1	0.87	0.43	113,113,113,113	0
56	MG	XA	1768	1/1	0.87	0.24	45,45,45,45	0
56	MG	RA	3657	1/1	0.87	0.59	65,65,65,65	0
56	MG	RA	3980	1/1	0.87	0.35	49,49,49,49	0
56	MG	RA	3120	1/1	0.87	0.26	63,63,63,63	0
56	MG	RA	3260	1/1	0.87	1.03	71,71,71,71	0
56	MG	RA	3121	1/1	0.87	0.53	83,83,83,83	0
56	MG	YA	3106	1/1	0.87	0.10	30,30,30,30	0
56	MG	QA	1810	1/1	0.87	0.43	69,69,69,69	0
56	MG	RA	3859	1/1	0.87	0.75	72,72,72,72	0
56	MG	YA	3281	1/1	0.87	0.96	60,60,60,60	0
56	MG	RA	3486	1/1	0.87	0.41	78,78,78,78	0
56	MG	RA	3266	1/1	0.87	0.41	74,74,74,74	0
56	MG	YA	3365	1/1	0.87	0.44	48,48,48,48	0
56	MG	YA	3036	1/1	0.87	0.34	55,55,55,55	0
56	MG	RA	3996	1/1	0.87	0.90	73,73,73,73	0
56	MG	RA	3766	1/1	0.87	0.56	29,29,29,29	0
56	MG	RA	3674	1/1	0.87	0.61	77,77,77,77	0
56	MG	YA	3081	1/1	0.87	0.50	71,71,71,71	0
56	MG	YA	3323	1/1	0.87	0.35	37,37,37,37	0
56	MG	RA	3274	1/1	0.87	0.34	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	RA	3133	1/1	0.87	0.30	79,79,79,79	0
56	MG	YA	3526	1/1	0.87	0.45	43,43,43,43	0
56	MG	XA	1681	1/1	0.87	0.31	106,106,106,106	0
56	MG	RF	305	1/1	0.87	0.88	69,69,69,69	0
56	MG	YA	3755	1/1	0.87	0.62	80,80,80,80	0
56	MG	RA	3374	1/1	0.87	0.75	92,92,92,92	0
56	MG	RA	3139	1/1	0.87	0.29	72,72,72,72	0
56	MG	RA	3689	1/1	0.87	0.86	70,70,70,70	0
56	MG	YA	3181	1/1	0.87	0.30	66,66,66,66	0
56	MG	RA	3907	1/1	0.87	0.59	78,78,78,78	0
56	MG	XA	1687	1/1	0.87	0.70	101,101,101,101	0
56	MG	YA	3046	1/1	0.87	0.41	75,75,75,75	0
56	MG	YA	3254	1/1	0.87	0.35	67,67,67,67	0
56	MG	RA	3149	1/1	0.87	0.28	39,39,39,39	0
56	MG	RA	3605	1/1	0.87	0.33	70,70,70,70	0
56	MG	YA	3424	1/1	0.87	0.18	27,27,27,27	0
56	MG	QA	1870	1/1	0.87	0.65	47,47,47,47	0
56	MG	XA	1653	1/1	0.87	0.33	79,79,79,79	0
56	MG	RA	3610	1/1	0.87	0.25	67,67,67,67	0
56	MG	RA	3156	1/1	0.87	0.28	117,117,117,117	0
56	MG	QA	1872	1/1	0.87	0.23	85,85,85,85	0
56	MG	RR	3202	1/1	0.87	0.38	69,69,69,69	0
56	MG	YA	3453	1/1	0.87	0.25	35,35,35,35	0
56	MG	QA	1629	1/1	0.87	0.32	51,51,51,51	0
56	MG	RA	3803	1/1	0.87	0.14	64,64,64,64	0
56	MG	YA	3661	1/1	0.87	0.63	63,63,63,63	0
56	MG	RT	202	1/1	0.87	0.31	65,65,65,65	0
56	MG	YA	3127	1/1	0.87	0.30	50,50,50,50	0
56	MG	RA	3428	1/1	0.87	0.31	60,60,60,60	0
56	MG	RA	3715	1/1	0.87	0.43	76,76,76,76	0
56	MG	XA	1657	1/1	0.87	0.45	65,65,65,65	0
56	MG	YA	3397	1/1	0.87	0.66	68,68,68,68	0
56	MG	RW	201	1/1	0.87	0.31	64,64,64,64	0
56	MG	YA	3586	1/1	0.87	0.85	48,48,48,48	0
56	MG	RA	3095	1/1	0.87	0.57	88,88,88,88	0
56	MG	RA	3723	1/1	0.87	0.24	68,68,68,68	0
56	MG	RA	3539	1/1	0.87	0.56	39,39,39,39	0
56	MG	YA	3257	1/1	0.87	0.21	84,84,84,84	0
56	MG	YA	3055	1/1	0.87	0.33	45,45,45,45	0
56	MG	RA	3030	1/1	0.87	0.72	113,113,113,113	0
56	MG	QA	1723	1/1	0.87	0.20	50,50,50,50	0
56	MG	RA	3032	1/1	0.87	0.15	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	RA	3248	1/1	0.87	0.33	56,56,56,56	0
56	MG	RA	3328	1/1	0.87	0.23	34,34,34,34	0
56	MG	RA	3447	1/1	0.87	0.31	57,57,57,57	0
56	MG	RA	3550	1/1	0.87	0.37	70,70,70,70	0
56	MG	YA	3546	1/1	0.87	0.56	47,47,47,47	0
56	MG	YA	3351	1/1	0.87	0.53	51,51,51,51	0
56	MG	RA	3554	1/1	0.87	0.54	55,55,55,55	0
56	MG	YV	201	1/1	0.87	0.29	44,44,44,44	0
56	MG	QA	1803	1/1	0.87	0.54	49,49,49,49	0
56	MG	YW	201	1/1	0.87	0.64	75,75,75,75	0
56	MG	YA	3688	1/1	0.87	0.59	62,62,62,62	0
56	MG	YA	3192	1/1	0.88	0.21	71,71,71,71	0
56	MG	RA	3038	1/1	0.88	0.20	63,63,63,63	0
56	MG	RA	3371	1/1	0.88	0.59	75,75,75,75	0
56	MG	XA	1775	1/1	0.88	0.86	72,72,72,72	0
56	MG	YA	3372	1/1	0.88	0.30	49,49,49,49	0
56	MG	YA	3182	1/1	0.88	0.26	68,68,68,68	0
56	MG	YA	3377	1/1	0.88	0.86	52,52,52,52	0
56	MG	YA	3378	1/1	0.88	0.27	53,53,53,53	0
56	MG	RA	3869	1/1	0.88	1.08	77,77,77,77	0
56	MG	RA	3383	1/1	0.88	0.56	40,40,40,40	0
56	MG	XA	1636	1/1	0.88	0.08	60,60,60,60	0
56	MG	RA	3396	1/1	0.88	0.50	58,58,58,58	0
56	MG	YA	3194	1/1	0.88	0.31	70,70,70,70	0
56	MG	XA	1720	1/1	0.88	1.10	63,63,63,63	0
56	MG	YA	3433	1/1	0.88	0.30	19,19,19,19	0
56	MG	YA	3196	1/1	0.88	0.37	109,109,109,109	0
56	MG	RA	3884	1/1	0.88	0.34	71,71,71,71	0
56	MG	XA	1644	1/1	0.88	0.36	61,61,61,61	0
56	MG	RA	3405	1/1	0.88	0.58	32,32,32,32	0
56	MG	RA	3697	1/1	0.88	0.35	55,55,55,55	0
56	MG	XA	1683	1/1	0.88	0.84	69,69,69,69	0
56	MG	YA	3393	1/1	0.88	0.22	66,66,66,66	0
56	MG	YA	3114	1/1	0.88	0.29	90,90,90,90	0
56	MG	XF	201	1/1	0.88	0.22	39,39,39,39	0
56	MG	YA	3653	1/1	0.88	0.57	55,55,55,55	0
56	MG	RA	3705	1/1	0.88	0.58	50,50,50,50	0
56	MG	XA	1729	1/1	0.88	0.25	58,58,58,58	0
56	MG	YA	3252	1/1	0.88	0.53	70,70,70,70	0
56	MG	RA	3799	1/1	0.88	0.46	54,54,54,54	0
56	MG	RA	3534	1/1	0.88	0.26	44,44,44,44	0
56	MG	YA	3217	1/1	0.88	0.22	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3536	1/1	0.88	0.40	64,64,64,64	0
56	MG	RA	4022	1/1	0.88	0.39	73,73,73,73	0
56	MG	RA	4024	1/1	0.88	0.51	59,59,59,59	0
56	MG	QA	1694	1/1	0.88	0.36	97,97,97,97	0
56	MG	QA	1750	1/1	0.88	0.35	67,67,67,67	0
56	MG	RA	4029	1/1	0.88	0.71	91,91,91,91	0
56	MG	RA	3718	1/1	0.88	0.15	62,62,62,62	0
56	MG	YA	3659	1/1	0.88	0.45	29,29,29,29	0
56	MG	QA	1855	1/1	0.88	0.32	56,56,56,56	0
56	MG	YA	3031	1/1	0.88	0.43	46,46,46,46	0
56	MG	RA	3084	1/1	0.88	0.46	79,79,79,79	0
56	MG	RQ	202	1/1	0.88	0.38	51,51,51,51	0
56	MG	YA	3116	1/1	0.88	0.23	58,58,58,58	0
56	MG	RQ	204	1/1	0.88	0.37	72,72,72,72	0
56	MG	RA	3814	1/1	0.88	0.78	63,63,63,63	0
56	MG	XA	1747	1/1	0.88	0.52	59,59,59,59	0
56	MG	RA	3169	1/1	0.88	0.18	82,82,82,82	0
56	MG	RA	3440	1/1	0.88	0.50	57,57,57,57	0
56	MG	RA	3170	1/1	0.88	0.24	66,66,66,66	0
56	MG	RA	3087	1/1	0.88	0.60	99,99,99,99	0
56	MG	YA	3520	1/1	0.88	0.62	68,68,68,68	0
56	MG	QA	1806	1/1	0.88	0.18	73,73,73,73	0
56	MG	YA	3256	1/1	0.88	0.39	43,43,43,43	0
56	MG	QA	1701	1/1	0.88	0.83	50,50,50,50	0
56	MG	XA	1750	1/1	0.88	0.32	87,87,87,87	0
56	MG	QA	1654	1/1	0.88	0.38	64,64,64,64	0
56	MG	YA	3035	1/1	0.88	0.28	73,73,73,73	0
56	MG	RA	4061	1/1	0.88	0.46	96,96,96,96	0
56	MG	YA	3093	1/1	0.88	0.24	18,18,18,18	0
56	MG	RA	4064	1/1	0.88	1.05	64,64,64,64	0
56	MG	RA	3350	1/1	0.88	0.12	65,65,65,65	0
56	MG	YA	3525	1/1	0.88	0.56	86,86,86,86	0
56	MG	YA	3204	1/1	0.88	0.15	42,42,42,42	0
56	MG	RA	3570	1/1	0.88	0.13	35,35,35,35	0
56	MG	R1	103	1/1	0.88	0.32	55,55,55,55	0
56	MG	RA	3027	1/1	0.88	0.50	103,103,103,103	0
56	MG	RB	207	1/1	0.88	0.16	82,82,82,82	0
56	MG	YA	3261	1/1	0.88	0.25	55,55,55,55	0
56	MG	YA	3588	1/1	0.88	0.22	76,76,76,76	0
56	MG	R5	104	1/1	0.88	0.58	67,67,67,67	0
56	MG	RA	3477	1/1	0.88	0.41	46,46,46,46	0
56	MG	YA	3133	1/1	0.88	0.52	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3163	1/1	0.88	0.20	52,52,52,52	0
56	MG	YA	3367	1/1	0.88	0.17	56,56,56,56	0
56	MG	RA	3972	1/1	0.88	0.44	81,81,81,81	0
56	MG	YA	3102	1/1	0.88	0.55	60,60,60,60	0
56	MG	YA	3309	1/1	0.88	0.40	37,37,37,37	0
56	MG	QA	1619	1/1	0.88	0.25	75,75,75,75	0
56	MG	RA	3462	1/1	0.89	0.47	52,52,52,52	0
56	MG	XA	1778	1/1	0.89	0.73	60,60,60,60	0
56	MG	YA	3708	1/1	0.89	0.67	37,37,37,37	0
56	MG	RA	3804	1/1	0.89	0.56	78,78,78,78	0
56	MG	YA	3594	1/1	0.89	0.34	35,35,35,35	0
56	MG	RA	3021	1/1	0.89	0.73	101,101,101,101	0
56	MG	YA	3657	1/1	0.89	0.64	34,34,34,34	0
56	MG	RA	3647	1/1	0.89	0.31	88,88,88,88	0
56	MG	RA	3218	1/1	0.89	0.51	65,65,65,65	0
56	MG	RA	3280	1/1	0.89	0.23	78,78,78,78	0
56	MG	RA	3219	1/1	0.89	0.20	66,66,66,66	0
56	MG	RA	3651	1/1	0.89	0.22	41,41,41,41	0
56	MG	YA	3238	1/1	0.89	0.31	91,91,91,91	0
56	MG	RA	3931	1/1	0.89	0.27	73,73,73,73	0
56	MG	YA	3757	1/1	0.89	0.49	70,70,70,70	0
56	MG	RF	307	1/1	0.89	0.32	65,65,65,65	0
56	MG	YA	3064	1/1	0.89	0.44	55,55,55,55	0
56	MG	RA	3160	1/1	0.89	0.95	83,83,83,83	0
56	MG	YG	202	1/1	0.89	0.19	78,78,78,78	0
56	MG	YB	202	1/1	0.89	0.17	56,56,56,56	0
56	MG	YA	3118	1/1	0.89	0.39	91,91,91,91	0
56	MG	QA	1844	1/1	0.89	0.17	80,80,80,80	0
56	MG	RA	3101	1/1	0.89	0.35	68,68,68,68	0
56	MG	RA	3232	1/1	0.89	0.78	57,57,57,57	0
56	MG	RA	3167	1/1	0.89	0.13	69,69,69,69	0
56	MG	XA	1732	1/1	0.89	0.70	44,44,44,44	0
56	MG	XA	1734	1/1	0.89	0.17	78,78,78,78	0
56	MG	YA	3423	1/1	0.89	0.66	59,59,59,59	0
56	MG	RA	3593	1/1	0.89	0.59	66,66,66,66	0
56	MG	QV	102	1/1	0.89	0.41	45,45,45,45	0
56	MG	RA	3421	1/1	0.89	0.33	42,42,42,42	0
56	MG	RA	3679	1/1	0.89	0.91	54,54,54,54	0
56	MG	YA	3509	1/1	0.89	0.28	71,71,71,71	0
56	MG	YA	3373	1/1	0.89	0.39	41,41,41,41	0
56	MG	YA	3629	1/1	0.89	0.39	44,44,44,44	0
56	MG	RR	3201	1/1	0.89	0.57	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	YA	3072	1/1	0.89	0.40	99,99,99,99	0
56	MG	RA	3760	1/1	0.89	0.16	74,74,74,74	0
56	MG	YA	3123	1/1	0.89	0.13	86,86,86,86	0
56	MG	YA	3429	1/1	0.89	0.31	67,67,67,67	0
56	MG	XA	1628	1/1	0.89	0.25	56,56,56,56	0
56	MG	YA	3541	1/1	0.89	0.43	20,20,20,20	0
56	MG	YA	3074	1/1	0.89	0.31	63,63,63,63	0
56	MG	RU	201	1/1	0.89	0.42	70,70,70,70	0
56	MG	YA	3068	1/1	0.89	0.35	65,65,65,65	0
56	MG	YA	3645	1/1	0.89	0.66	67,67,67,67	0
56	MG	RA	3059	1/1	0.89	0.14	76,76,76,76	0
56	MG	RA	3612	1/1	0.89	0.81	64,64,64,64	0
56	MG	XA	1763	1/1	0.89	0.60	49,49,49,49	0
56	MG	YA	3733	1/1	0.89	0.22	62,62,62,62	0
56	MG	YA	3735	1/1	0.89	0.61	71,71,71,71	0
56	MG	Y7	101	1/1	0.89	0.57	75,75,75,75	0
56	MG	RA	3444	1/1	0.89	1.03	83,83,83,83	0
56	MG	RB	213	1/1	0.89	0.63	58,58,58,58	0
56	MG	RA	3700	1/1	0.89	0.24	53,53,53,53	0
56	MG	YA	3258	1/1	0.89	0.40	68,68,68,68	0
56	MG	QA	1742	1/1	0.89	0.78	58,58,58,58	0
56	MG	YA	3389	1/1	0.89	0.31	50,50,50,50	0
56	MG	RA	3069	1/1	0.89	0.31	55,55,55,55	0
56	MG	RA	3354	1/1	0.89	0.18	61,61,61,61	0
56	MG	QA	1655	1/1	0.89	0.40	64,64,64,64	0
56	MG	YA	3062	1/1	0.89	0.24	57,57,57,57	0
56	MG	RA	3794	1/1	0.89	0.75	86,86,86,86	0
56	MG	RA	3269	1/1	0.89	0.28	74,74,74,74	0
56	MG	RA	3709	1/1	0.89	0.20	75,75,75,75	0
56	MG	RA	4001	1/1	0.89	0.35	58,58,58,58	0
56	MG	XA	1646	1/1	0.89	0.58	63,63,63,63	0
56	MG	YA	3742	1/1	0.89	0.41	36,36,36,36	0
56	MG	RD	303	1/1	0.89	0.28	41,41,41,41	0
56	MG	RA	3015	1/1	0.89	0.30	72,72,72,72	0
56	MG	RA	3273	1/1	0.89	0.58	76,76,76,76	0
56	MG	RA	3244	1/1	0.90	0.08	71,71,71,71	0
56	MG	YA	3585	1/1	0.90	0.44	75,75,75,75	0
56	MG	YA	3350	1/1	0.90	0.26	23,23,23,23	0
56	MG	YA	3749	1/1	0.90	0.30	54,54,54,54	0
56	MG	RA	3037	1/1	0.90	0.38	88,88,88,88	0
56	MG	XA	1684	1/1	0.90	0.51	40,40,40,40	0
56	MG	YA	3097	1/1	0.90	0.55	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3498	1/1	0.90	0.44	64,64,64,64	0
56	MG	QA	1846	1/1	0.90	0.60	47,47,47,47	0
56	MG	YA	3759	1/1	0.90	0.58	64,64,64,64	0
56	MG	YA	3548	1/1	0.90	0.59	32,32,32,32	0
56	MG	YA	3499	1/1	0.90	0.47	38,38,38,38	0
56	MG	RA	4016	1/1	0.90	0.35	68,68,68,68	0
56	MG	RA	3633	1/1	0.90	0.38	74,74,74,74	0
56	MG	YA	3077	1/1	0.90	0.25	35,35,35,35	0
56	MG	YA	3611	1/1	0.90	0.27	31,31,31,31	0
56	MG	YA	3357	1/1	0.90	0.33	39,39,39,39	0
56	MG	YA	3671	1/1	0.90	0.48	37,37,37,37	0
56	MG	XA	1733	1/1	0.90	0.28	72,72,72,72	0
56	MG	RA	3343	1/1	0.90	0.16	68,68,68,68	0
56	MG	YA	3434	1/1	0.90	0.37	55,55,55,55	0
56	MG	RA	3551	1/1	0.90	0.31	72,72,72,72	0
56	MG	RA	3349	1/1	0.90	0.31	40,40,40,40	0
56	MG	YA	3435	1/1	0.90	0.51	36,36,36,36	0
56	MG	RA	3728	1/1	0.90	0.35	74,74,74,74	0
56	MG	RA	4037	1/1	0.90	0.47	69,69,69,69	0
56	MG	RA	3453	1/1	0.90	0.25	64,64,64,64	0
56	MG	RA	3555	1/1	0.90	1.20	68,68,68,68	0
56	MG	QQ	202	1/1	0.90	0.16	68,68,68,68	0
56	MG	QA	1765	1/1	0.90	0.19	83,83,83,83	0
56	MG	XA	1736	1/1	0.90	0.30	58,58,58,58	0
56	MG	XA	1738	1/1	0.90	0.65	58,58,58,58	0
56	MG	YA	3218	1/1	0.90	0.37	89,89,89,89	0
56	MG	YA	3683	1/1	0.90	0.58	39,39,39,39	0
56	MG	RQ	201	1/1	0.90	0.21	47,47,47,47	0
56	MG	YA	3402	1/1	0.90	0.54	32,32,32,32	0
56	MG	RA	3739	1/1	0.90	0.32	78,78,78,78	0
56	MG	YB	214	1/1	0.90	0.17	45,45,45,45	0
56	MG	YA	3376	1/1	0.90	0.17	58,58,58,58	0
56	MG	QA	1773	1/1	0.90	0.31	71,71,71,71	0
56	MG	RA	3151	1/1	0.90	0.62	59,59,59,59	0
56	MG	RA	3479	1/1	0.90	0.34	19,19,19,19	0
56	MG	RA	3575	1/1	0.90	0.42	62,62,62,62	0
56	MG	YA	3224	1/1	0.90	0.10	66,66,66,66	0
56	MG	RA	4062	1/1	0.90	0.40	78,78,78,78	0
56	MG	QA	1643	1/1	0.90	0.69	86,86,86,86	0
56	MG	RA	3155	1/1	0.90	0.47	78,78,78,78	0
56	MG	YA	3162	1/1	0.90	0.16	27,27,27,27	0
56	MG	RA	3082	1/1	0.90	0.97	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3425	1/1	0.90	0.29	49,49,49,49	0
56	MG	RA	3284	1/1	0.90	0.35	97,97,97,97	0
56	MG	RA	3017	1/1	0.90	0.58	68,68,68,68	0
56	MG	RA	3376	1/1	0.90	0.20	52,52,52,52	0
56	MG	RX	101	1/1	0.90	0.36	51,51,51,51	0
56	MG	YA	3573	1/1	0.90	0.67	38,38,38,38	0
56	MG	XA	1635	1/1	0.90	0.21	29,29,29,29	0
56	MG	XA	1759	1/1	0.90	0.32	56,56,56,56	0
56	MG	YD	303	1/1	0.90	0.74	44,44,44,44	0
56	MG	RA	3855	1/1	0.90	0.87	62,62,62,62	0
56	MG	XA	1761	1/1	0.90	0.22	38,38,38,38	0
56	MG	QA	1877	1/1	0.90	0.38	94,94,94,94	0
56	MG	YA	3275	1/1	0.90	0.53	53,53,53,53	0
56	MG	QA	1786	1/1	0.90	0.31	54,54,54,54	0
56	MG	XA	1638	1/1	0.90	0.07	118,118,118,118	0
56	MG	RA	3301	1/1	0.90	0.85	66,66,66,66	0
56	MG	YA	3536	1/1	0.90	0.25	42,42,42,42	0
56	MG	YA	3411	1/1	0.90	0.27	83,83,83,83	0
56	MG	RA	3304	1/1	0.90	0.19	39,39,39,39	0
56	MG	RA	3305	1/1	0.90	0.85	98,98,98,98	0
56	MG	RA	3779	1/1	0.90	0.24	86,86,86,86	0
56	MG	RA	3308	1/1	0.90	0.50	64,64,64,64	0
56	MG	R9	103	1/1	0.90	0.24	67,67,67,67	0
56	MG	RA	3424	1/1	0.90	0.36	80,80,80,80	0
56	MG	YA	3175	1/1	0.90	0.50	123,123,123,123	0
56	MG	RA	3529	1/1	0.90	0.26	77,77,77,77	0
56	MG	RA	3785	1/1	0.90	0.44	56,56,56,56	0
56	MG	YA	3705	1/1	0.91	0.44	32,32,32,32	0
56	MG	YA	3392	1/1	0.91	0.59	54,54,54,54	0
56	MG	RA	3837	1/1	0.91	0.24	59,59,59,59	0
56	MG	YA	3458	1/1	0.91	0.32	46,46,46,46	0
56	MG	RA	3007	1/1	0.91	0.24	61,61,61,61	0
56	MG	XA	1782	1/1	0.91	0.21	46,46,46,46	0
56	MG	YQ	201	1/1	0.91	0.27	33,33,33,33	0
56	MG	RA	3744	1/1	0.91	0.44	41,41,41,41	0
56	MG	YA	3436	1/1	0.91	0.41	51,51,51,51	0
56	MG	YA	3240	1/1	0.91	0.72	70,70,70,70	0
56	MG	XA	1726	1/1	0.91	0.23	74,74,74,74	0
56	MG	RA	3565	1/1	0.91	0.33	44,44,44,44	0
56	MG	RA	3658	1/1	0.91	0.70	95,95,95,95	0
56	MG	RA	3458	1/1	0.91	0.21	74,74,74,74	0
56	MG	RA	3660	1/1	0.91	0.24	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3569	1/1	0.91	0.47	64,64,64,64	0
56	MG	RA	3096	1/1	0.91	0.18	48,48,48,48	0
56	MG	YA	3574	1/1	0.91	0.47	30,30,30,30	0
56	MG	RA	3572	1/1	0.91	0.39	83,83,83,83	0
56	MG	RA	3353	1/1	0.91	0.52	35,35,35,35	0
56	MG	RA	3668	1/1	0.91	0.34	49,49,49,49	0
56	MG	YA	3482	1/1	0.91	0.41	65,65,65,65	0
56	MG	QA	1692	1/1	0.91	0.39	52,52,52,52	0
56	MG	YA	3294	1/1	0.91	0.38	52,52,52,52	0
56	MG	YA	3157	1/1	0.91	0.43	44,44,44,44	0
56	MG	YA	3537	1/1	0.91	0.40	57,57,57,57	0
56	MG	RA	3185	1/1	0.91	0.46	94,94,94,94	0
56	MG	RA	4007	1/1	0.91	0.67	49,49,49,49	0
56	MG	RF	306	1/1	0.91	0.69	79,79,79,79	0
56	MG	XA	1641	1/1	0.91	0.38	61,61,61,61	0
56	MG	RA	3584	1/1	0.91	0.13	45,45,45,45	0
56	MG	YA	3538	1/1	0.91	0.40	44,44,44,44	0
56	MG	YA	3231	1/1	0.91	0.31	59,59,59,59	0
56	MG	XA	1690	1/1	0.91	0.30	53,53,53,53	0
56	MG	RA	3889	1/1	0.91	0.59	48,48,48,48	0
56	MG	XA	1691	1/1	0.91	0.47	60,60,60,60	0
56	MG	YA	3513	1/1	0.91	0.29	80,80,80,80	0
56	MG	YA	3514	1/1	0.91	0.41	62,62,62,62	0
56	MG	YA	3019	1/1	0.91	0.37	81,81,81,81	0
56	MG	RA	3117	1/1	0.91	0.27	64,64,64,64	0
56	MG	RA	3900	1/1	0.91	0.28	30,30,30,30	0
56	MG	XA	1742	1/1	0.91	0.41	52,52,52,52	0
56	MG	QA	1818	1/1	0.91	0.25	63,63,63,63	0
56	MG	XA	1744	1/1	0.91	0.64	59,59,59,59	0
56	MG	YA	3598	1/1	0.91	0.51	49,49,49,49	0
56	MG	YA	3212	1/1	0.91	0.50	62,62,62,62	0
56	MG	YA	3600	1/1	0.91	0.44	51,51,51,51	0
56	MG	YA	3030	1/1	0.91	0.27	39,39,39,39	0
56	MG	QA	1659	1/1	0.91	1.39	84,84,84,84	0
56	MG	RA	3209	1/1	0.91	1.06	100,100,100,100	0
56	MG	RA	3920	1/1	0.91	0.54	41,41,41,41	0
56	MG	YD	304	1/1	0.91	0.32	49,49,49,49	0
56	MG	YA	3609	1/1	0.91	0.28	51,51,51,51	0
56	MG	RA	3214	1/1	0.91	0.45	59,59,59,59	0
56	MG	RA	3052	1/1	0.91	0.23	85,85,85,85	0
56	MG	YA	3013	1/1	0.91	0.19	23,23,23,23	0
56	MG	YA	3613	1/1	0.91	0.70	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	RA	3295	1/1	0.91	0.15	73,73,73,73	0
56	MG	YA	3622	1/1	0.91	0.55	49,49,49,49	0
56	MG	RA	3416	1/1	0.91	0.20	60,60,60,60	0
56	MG	RA	3621	1/1	0.91	0.38	61,61,61,61	0
56	MG	XA	1613	1/1	0.91	0.14	51,51,51,51	0
56	MG	QA	1833	1/1	0.91	0.58	51,51,51,51	0
56	MG	RA	4057	1/1	0.91	0.68	77,77,77,77	0
56	MG	RA	3223	1/1	0.91	0.64	63,63,63,63	0
56	MG	RA	3808	1/1	0.91	0.38	56,56,56,56	0
56	MG	RA	3939	1/1	0.91	0.28	58,58,58,58	0
56	MG	RA	3143	1/1	0.91	0.17	72,72,72,72	0
56	MG	QA	1834	1/1	0.91	0.38	43,43,43,43	0
56	MG	YA	3021	1/1	0.91	0.39	69,69,69,69	0
56	MG	YA	3135	1/1	0.91	1.18	89,89,89,89	0
56	MG	YE	304	1/1	0.91	0.31	51,51,51,51	0
56	MG	RA	3815	1/1	0.91	0.31	68,68,68,68	0
56	MG	QA	1838	1/1	0.91	0.28	85,85,85,85	0
56	MG	QA	1730	1/1	0.91	0.33	49,49,49,49	0
56	MG	YA	3096	1/1	0.91	0.20	26,26,26,26	0
56	MG	RA	3726	1/1	0.91	0.17	53,53,53,53	0
56	MG	QA	1618	1/1	0.91	0.23	96,96,96,96	0
56	MG	YA	3286	1/1	0.91	0.10	35,35,35,35	0
56	MG	YA	3313	1/1	0.91	0.86	46,46,46,46	0
56	MG	YA	3697	1/1	0.91	0.67	38,38,38,38	0
56	MG	YA	3527	1/1	0.91	0.39	50,50,50,50	0
56	MG	YA	3699	1/1	0.91	0.78	66,66,66,66	0
56	MG	RB	214	1/1	0.91	0.51	44,44,44,44	0
56	MG	RA	3241	1/1	0.91	0.32	108,108,108,108	0
56	MG	QA	1679	1/1	0.91	0.21	64,64,64,64	0
56	MG	YA	3008	1/1	0.91	0.21	47,47,47,47	0
56	MG	YA	3758	1/1	0.91	0.54	76,76,76,76	0
56	MG	RA	3083	1/1	0.92	0.35	80,80,80,80	0
56	MG	YA	3202	1/1	0.92	0.28	38,38,38,38	0
56	MG	RA	3012	1/1	0.92	0.19	53,53,53,53	0
56	MG	XA	1739	1/1	0.92	0.52	61,61,61,61	0
56	MG	YA	3654	1/1	0.92	0.81	54,54,54,54	0
56	MG	YA	3063	1/1	0.92	0.25	35,35,35,35	0
56	MG	RA	3089	1/1	0.92	0.07	67,67,67,67	0
56	MG	QA	1649	1/1	0.92	0.19	50,50,50,50	0
56	MG	YA	3412	1/1	0.92	0.57	72,72,72,72	0
56	MG	RA	3242	1/1	0.92	0.32	54,54,54,54	0
56	MG	RA	3966	1/1	0.92	0.74	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3044	1/1	0.92	0.20	35,35,35,35	0
56	MG	XA	1699	1/1	0.92	0.43	44,44,44,44	0
56	MG	RA	3548	1/1	0.92	0.46	38,38,38,38	0
56	MG	QA	1703	1/1	0.92	0.29	60,60,60,60	0
56	MG	XA	1602	1/1	0.92	0.29	86,86,86,86	0
56	MG	YA	3720	1/1	0.92	0.49	83,83,83,83	0
56	MG	YA	3142	1/1	0.92	0.24	58,58,58,58	0
56	MG	RA	3445	1/1	0.92	0.29	58,58,58,58	0
56	MG	YA	3361	1/1	0.92	0.16	65,65,65,65	0
56	MG	RA	3981	1/1	0.92	0.09	69,69,69,69	0
56	MG	YA	3387	1/1	0.92	0.40	37,37,37,37	0
56	MG	YA	3495	1/1	0.92	0.57	63,63,63,63	0
56	MG	YA	3296	1/1	0.92	0.60	32,32,32,32	0
56	MG	YA	3300	1/1	0.92	0.27	40,40,40,40	0
56	MG	YA	3420	1/1	0.92	0.49	39,39,39,39	0
56	MG	YA	3620	1/1	0.92	0.27	34,34,34,34	0
56	MG	RA	3750	1/1	0.92	0.96	66,66,66,66	0
56	MG	RA	3562	1/1	0.92	0.19	59,59,59,59	0
56	MG	QA	1663	1/1	0.92	0.21	73,73,73,73	0
56	MG	RA	3188	1/1	0.92	0.77	115,115,115,115	0
56	MG	YA	3366	1/1	0.92	0.75	59,59,59,59	0
56	MG	RA	3566	1/1	0.92	0.26	57,57,57,57	0
56	MG	RA	3191	1/1	0.92	0.16	69,69,69,69	0
56	MG	RA	3865	1/1	0.92	0.50	51,51,51,51	0
56	MG	RA	4000	1/1	0.92	0.26	30,30,30,30	0
56	MG	RA	3866	1/1	0.92	0.11	76,76,76,76	0
56	MG	RA	3262	1/1	0.92	0.59	80,80,80,80	0
56	MG	RA	3192	1/1	0.92	0.73	92,92,92,92	0
56	MG	RF	309	1/1	0.92	0.15	68,68,68,68	0
56	MG	RA	3666	1/1	0.92	0.99	69,69,69,69	0
56	MG	RA	3356	1/1	0.92	0.10	23,23,23,23	0
56	MG	YA	3682	1/1	0.92	0.35	37,37,37,37	0
56	MG	RA	3874	1/1	0.92	0.41	25,25,25,25	0
56	MG	YA	3244	1/1	0.92	0.66	39,39,39,39	0
56	MG	RA	3464	1/1	0.92	0.29	71,71,71,71	0
56	MG	QA	1777	1/1	0.92	0.18	81,81,81,81	0
56	MG	RA	3881	1/1	0.92	1.26	68,68,68,68	0
56	MG	RA	3468	1/1	0.92	0.19	40,40,40,40	0
56	MG	YA	3736	1/1	0.92	0.16	39,39,39,39	0
56	MG	RA	3046	1/1	0.92	0.66	68,68,68,68	0
56	MG	RA	3886	1/1	0.92	0.61	52,52,52,52	0
56	MG	RA	3677	1/1	0.92	1.13	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	RA	3678	1/1	0.92	0.28	31,31,31,31	0
56	MG	RA	3581	1/1	0.92	0.28	75,75,75,75	0
56	MG	RA	3680	1/1	0.92	0.56	46,46,46,46	0
56	MG	YA	3471	1/1	0.92	0.66	58,58,58,58	0
56	MG	RA	3050	1/1	0.92	0.42	88,88,88,88	0
56	MG	YA	3503	1/1	0.92	0.20	18,18,18,18	0
56	MG	XA	1717	1/1	0.92	0.50	59,59,59,59	0
56	MG	YA	3689	1/1	0.92	0.46	67,67,67,67	0
56	MG	QA	1622	1/1	0.92	0.30	62,62,62,62	0
56	MG	YA	3278	1/1	0.92	0.26	38,38,38,38	0
56	MG	YA	3399	1/1	0.92	0.65	36,36,36,36	0
56	MG	YA	3279	1/1	0.92	0.15	61,61,61,61	0
56	MG	RA	3914	1/1	0.92	0.53	56,56,56,56	0
56	MG	RA	4039	1/1	0.92	1.36	73,73,73,73	0
56	MG	YA	3280	1/1	0.92	0.34	14,14,14,14	0
56	MG	RA	3500	1/1	0.92	0.52	25,25,25,25	0
56	MG	QA	1627	1/1	0.92	0.09	42,42,42,42	0
56	MG	YA	3576	1/1	0.92	0.36	37,37,37,37	0
56	MG	RA	3213	1/1	0.92	0.33	105,105,105,105	0
56	MG	YA	3751	1/1	0.92	0.28	39,39,39,39	0
56	MG	RA	3381	1/1	0.92	0.29	39,39,39,39	0
56	MG	RA	4051	1/1	0.92	0.28	63,63,63,63	0
56	MG	YA	3636	1/1	0.92	0.28	45,45,45,45	0
56	MG	RA	3388	1/1	0.92	0.56	49,49,49,49	0
56	MG	YA	3245	1/1	0.92	0.57	107,107,107,107	0
56	MG	RA	3286	1/1	0.92	0.47	118,118,118,118	0
56	MG	RA	3930	1/1	0.92	0.43	54,54,54,54	0
56	MG	YA	3121	1/1	0.92	0.74	47,47,47,47	0
56	MG	QA	1634	1/1	0.92	0.19	44,44,44,44	0
56	MG	RA	3220	1/1	0.92	0.39	75,75,75,75	0
56	MG	YA	3703	1/1	0.92	0.41	35,35,35,35	0
56	MG	YA	3639	1/1	0.92	0.69	74,74,74,74	0
56	MG	YA	3580	1/1	0.92	0.47	27,27,27,27	0
56	MG	RA	3526	1/1	0.92	0.63	51,51,51,51	0
56	MG	YA	3288	1/1	0.92	0.49	53,53,53,53	0
56	MG	RA	3619	1/1	0.92	0.50	27,27,27,27	0
56	MG	YA	3709	1/1	0.92	0.92	58,58,58,58	0
56	MG	RA	3411	1/1	0.92	0.35	31,31,31,31	0
56	MG	RA	3298	1/1	0.92	0.30	24,24,24,24	0
56	MG	YA	3408	1/1	0.92	0.37	17,17,17,17	0
56	MG	YA	3711	1/1	0.92	0.72	47,47,47,47	0
56	MG	YA	3540	1/1	0.92	0.47	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3952	1/1	0.92	0.25	49,49,49,49	0
56	MG	YA	3650	1/1	0.92	0.65	48,48,48,48	0
57	ZN	R6	101	1/1	0.92	0.16	160,160,160,160	0
56	MG	RA	3118	1/1	0.93	0.47	76,76,76,76	0
56	MG	YA	3049	1/1	0.93	0.32	78,78,78,78	0
56	MG	RA	3184	1/1	0.93	0.56	60,60,60,60	0
56	MG	RA	3414	1/1	0.93	0.36	34,34,34,34	0
56	MG	YA	3562	1/1	0.93	0.35	70,70,70,70	0
56	MG	RA	3928	1/1	0.93	0.39	59,59,59,59	0
56	MG	RA	3929	1/1	0.93	0.23	65,65,65,65	0
56	MG	YA	3007	1/1	0.93	0.25	63,63,63,63	0
56	MG	RA	3123	1/1	0.93	0.25	30,30,30,30	0
56	MG	YA	3199	1/1	0.93	0.67	102,102,102,102	0
56	MG	QA	1616	1/1	0.93	0.19	92,92,92,92	0
56	MG	RA	3128	1/1	0.93	0.37	48,48,48,48	0
56	MG	RA	3323	1/1	0.93	0.28	38,38,38,38	0
56	MG	RA	3010	1/1	0.93	0.28	50,50,50,50	0
56	MG	YA	3122	1/1	0.93	0.53	60,60,60,60	0
56	MG	XA	1617	1/1	0.93	0.30	44,44,44,44	0
56	MG	RA	3257	1/1	0.93	0.55	100,100,100,100	0
56	MG	RA	3941	1/1	0.93	0.15	69,69,69,69	0
56	MG	YA	3356	1/1	0.93	0.39	50,50,50,50	0
56	MG	RA	3071	1/1	0.93	0.62	63,63,63,63	0
56	MG	RA	3073	1/1	0.93	0.34	64,64,64,64	0
56	MG	YA	3665	1/1	0.93	0.39	31,31,31,31	0
56	MG	QA	1790	1/1	0.93	0.91	56,56,56,56	0
56	MG	YA	3189	1/1	0.93	0.28	96,96,96,96	0
56	MG	RA	4043	1/1	0.93	0.62	86,86,86,86	0
56	MG	RA	3342	1/1	0.93	0.49	60,60,60,60	0
56	MG	YA	3384	1/1	0.93	0.57	38,38,38,38	0
56	MG	YA	3082	1/1	0.93	0.25	78,78,78,78	0
56	MG	RA	3204	1/1	0.93	0.76	59,59,59,59	0
56	MG	RA	3769	1/1	0.93	0.41	46,46,46,46	0
56	MG	YA	3360	1/1	0.93	0.76	53,53,53,53	0
56	MG	YA	3678	1/1	0.93	0.58	50,50,50,50	0
56	MG	RA	3352	1/1	0.93	0.58	65,65,65,65	0
56	MG	RA	3145	1/1	0.93	0.18	43,43,43,43	0
56	MG	YA	3268	1/1	0.93	0.43	73,73,73,73	0
56	MG	RA	3148	1/1	0.93	0.34	66,66,66,66	0
56	MG	RA	3026	1/1	0.93	0.67	72,72,72,72	0
56	MG	YA	3216	1/1	0.93	0.39	25,25,25,25	0
56	MG	YA	3634	1/1	0.93	0.82	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3126	1/1	0.93	0.18	91,91,91,91	0
56	MG	XA	1667	1/1	0.93	0.36	77,77,77,77	0
56	MG	RA	3970	1/1	0.93	0.38	31,31,31,31	0
56	MG	RA	3216	1/1	0.93	0.30	77,77,77,77	0
56	MG	QA	1716	1/1	0.93	0.14	81,81,81,81	0
56	MG	YA	3521	1/1	0.93	0.43	95,95,95,95	0
56	MG	RA	3975	1/1	0.93	0.26	63,63,63,63	0
56	MG	YA	3137	1/1	0.93	0.35	40,40,40,40	0
56	MG	RB	204	1/1	0.93	0.19	71,71,71,71	0
56	MG	RV	202	1/1	0.93	0.30	55,55,55,55	0
56	MG	YA	3398	1/1	0.93	0.24	25,25,25,25	0
56	MG	RA	3093	1/1	0.93	0.12	72,72,72,72	0
56	MG	YA	3549	1/1	0.93	0.32	34,34,34,34	0
56	MG	RA	3640	1/1	0.93	0.16	48,48,48,48	0
56	MG	YA	3593	1/1	0.93	0.53	28,28,28,28	0
56	MG	XK	201	1/1	0.93	0.07	53,53,53,53	0
56	MG	RA	3717	1/1	0.93	0.48	38,38,38,38	0
56	MG	YA	3644	1/1	0.93	0.70	57,57,57,57	0
56	MG	YA	3109	1/1	0.93	0.43	35,35,35,35	0
56	MG	YA	3335	1/1	0.93	0.17	30,30,30,30	0
56	MG	XA	1678	1/1	0.93	0.62	81,81,81,81	0
56	MG	YA	3648	1/1	0.93	0.29	40,40,40,40	0
56	MG	RA	3294	1/1	0.93	0.33	61,61,61,61	0
56	MG	YA	3067	1/1	0.93	1.05	53,53,53,53	0
56	MG	YD	309	1/1	0.93	0.35	14,14,14,14	0
56	MG	RA	3492	1/1	0.93	0.43	68,68,68,68	0
56	MG	RA	3493	1/1	0.93	0.46	60,60,60,60	0
56	MG	R5	103	1/1	0.93	0.81	59,59,59,59	0
56	MG	RA	3108	1/1	0.93	0.53	69,69,69,69	0
56	MG	YA	3337	1/1	0.93	0.31	35,35,35,35	0
56	MG	RA	3576	1/1	0.93	0.43	43,43,43,43	0
56	MG	YA	3704	1/1	0.93	0.45	29,29,29,29	0
56	MG	YA	3207	1/1	0.93	0.38	70,70,70,70	0
56	MG	YA	3079	1/1	0.93	0.30	91,91,91,91	0
56	MG	XA	1771	1/1	0.93	0.57	62,62,62,62	0
56	MG	RA	3002	1/1	0.93	0.30	70,70,70,70	0
56	MG	RD	305	1/1	0.93	0.45	86,86,86,86	0
56	MG	RA	3180	1/1	0.93	0.34	75,75,75,75	0
56	MG	YA	3607	1/1	0.93	0.61	53,53,53,53	0
56	MG	YA	3672	1/1	0.94	0.72	26,26,26,26	0
56	MG	QA	1859	1/1	0.94	0.35	50,50,50,50	0
56	MG	YB	212	1/1	0.94	0.53	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3168	1/1	0.94	0.21	71,71,71,71	0
56	MG	RB	220	1/1	0.94	0.53	47,47,47,47	0
56	MG	YA	3341	1/1	0.94	0.52	42,42,42,42	0
56	MG	RA	3326	1/1	0.94	0.20	20,20,20,20	0
56	MG	YA	3066	1/1	0.94	0.30	50,50,50,50	0
56	MG	YA	3136	1/1	0.94	0.48	59,59,59,59	0
56	MG	XA	1606	1/1	0.94	0.13	95,95,95,95	0
56	MG	RA	3856	1/1	0.94	0.32	33,33,33,33	0
56	MG	XA	1776	1/1	0.94	0.59	61,61,61,61	0
56	MG	YA	3348	1/1	0.94	0.34	17,17,17,17	0
56	MG	RA	3860	1/1	0.94	0.50	25,25,25,25	0
56	MG	YA	3487	1/1	0.94	0.76	46,46,46,46	0
56	MG	RA	3984	1/1	0.94	0.40	41,41,41,41	0
56	MG	YB	219	1/1	0.94	0.43	31,31,31,31	0
56	MG	YA	3349	1/1	0.94	0.38	49,49,49,49	0
56	MG	RD	306	1/1	0.94	0.19	33,33,33,33	0
56	MG	YA	3684	1/1	0.94	0.60	39,39,39,39	0
56	MG	YA	3542	1/1	0.94	0.30	21,21,21,21	0
56	MG	RA	3341	1/1	0.94	0.53	30,30,30,30	0
56	MG	YA	3543	1/1	0.94	0.54	36,36,36,36	0
56	MG	YA	3731	1/1	0.94	0.31	32,32,32,32	0
56	MG	YA	3054	1/1	0.94	0.11	27,27,27,27	0
56	MG	YA	3691	1/1	0.94	0.30	38,38,38,38	0
56	MG	YA	3298	1/1	0.94	0.58	19,19,19,19	0
56	MG	YA	3352	1/1	0.94	0.48	11,11,11,11	0
56	MG	YA	3354	1/1	0.94	0.48	47,47,47,47	0
56	MG	RA	3113	1/1	0.94	0.59	65,65,65,65	0
56	MG	XA	1676	1/1	0.94	0.31	42,42,42,42	0
56	MG	YA	3138	1/1	0.94	0.24	61,61,61,61	0
56	MG	YA	3316	1/1	0.94	0.49	53,53,53,53	0
56	MG	RA	3676	1/1	0.94	0.43	86,86,86,86	0
56	MG	YA	3042	1/1	0.94	0.20	61,61,61,61	0
56	MG	RA	3267	1/1	0.94	0.27	47,47,47,47	0
56	MG	RA	3043	1/1	0.94	0.15	38,38,38,38	0
56	MG	RA	3044	1/1	0.94	0.36	29,29,29,29	0
56	MG	RA	3045	1/1	0.94	0.68	71,71,71,71	0
56	MG	YA	3744	1/1	0.94	0.38	33,33,33,33	0
56	MG	RA	3897	1/1	0.94	0.40	61,61,61,61	0
56	MG	YA	3124	1/1	0.94	0.59	54,54,54,54	0
56	MG	RA	3049	1/1	0.94	0.12	48,48,48,48	0
56	MG	YA	3746	1/1	0.94	0.20	35,35,35,35	0
56	MG	RA	3905	1/1	0.94	0.44	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3326	1/1	0.94	0.49	27,27,27,27	0
56	MG	YA	3701	1/1	0.94	0.61	60,60,60,60	0
56	MG	RA	3494	1/1	0.94	0.93	55,55,55,55	0
56	MG	YA	3702	1/1	0.94	0.17	30,30,30,30	0
56	MG	RA	3594	1/1	0.94	0.21	67,67,67,67	0
56	MG	RA	4023	1/1	0.94	0.21	49,49,49,49	0
56	MG	YA	3271	1/1	0.94	0.37	70,70,70,70	0
56	MG	YA	3753	1/1	0.94	0.49	54,54,54,54	0
56	MG	YA	3394	1/1	0.94	0.48	19,19,19,19	0
56	MG	QA	1714	1/1	0.94	0.30	42,42,42,42	0
56	MG	RA	3135	1/1	0.94	0.38	77,77,77,77	0
56	MG	RA	3601	1/1	0.94	0.79	87,87,87,87	0
56	MG	YA	3756	1/1	0.94	0.61	80,80,80,80	0
56	MG	RA	3380	1/1	0.94	0.48	43,43,43,43	0
56	MG	YA	3331	1/1	0.94	0.42	9,9,9,9	0
56	MG	YA	3558	1/1	0.94	0.30	25,25,25,25	0
56	MG	RA	3606	1/1	0.94	0.78	53,53,53,53	0
56	MG	RA	3385	1/1	0.94	0.54	27,27,27,27	0
56	MG	RA	3387	1/1	0.94	0.67	50,50,50,50	0
56	MG	RA	3063	1/1	0.94	0.31	41,41,41,41	0
56	MG	RA	4045	1/1	0.94	0.73	71,71,71,71	0
56	MG	RA	3287	1/1	0.94	0.16	83,83,83,83	0
56	MG	YA	3290	1/1	0.94	0.45	47,47,47,47	0
56	MG	RU	203	1/1	0.94	0.75	64,64,64,64	0
56	MG	RA	3932	1/1	0.94	0.68	61,61,61,61	0
56	MG	YA	3760	1/1	0.94	0.50	85,85,85,85	0
56	MG	YA	3291	1/1	0.94	0.49	24,24,24,24	0
56	MG	YA	3617	1/1	0.94	0.30	17,17,17,17	0
56	MG	RA	3712	1/1	0.94	0.65	53,53,53,53	0
56	MG	YA	3563	1/1	0.94	0.78	76,76,76,76	0
56	MG	RA	3403	1/1	0.94	0.37	25,25,25,25	0
56	MG	YA	3621	1/1	0.94	0.35	49,49,49,49	0
56	MG	XA	1757	1/1	0.94	0.28	30,30,30,30	0
56	MG	RA	3072	1/1	0.94	0.95	93,93,93,93	0
56	MG	RA	3408	1/1	0.94	0.33	24,24,24,24	0
56	MG	QA	1667	1/1	0.94	0.23	67,67,67,67	0
56	MG	QA	1729	1/1	0.94	0.40	50,50,50,50	0
56	MG	RA	3153	1/1	0.94	0.12	35,35,35,35	0
56	MG	XA	1701	1/1	0.94	0.46	51,51,51,51	0
56	MG	YA	3023	1/1	0.94	0.14	16,16,16,16	0
56	MG	RA	3420	1/1	0.94	0.16	19,19,19,19	0
56	MG	YA	3452	1/1	0.94	0.21	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	RB	201	1/1	0.94	0.19	72,72,72,72	0
56	MG	QA	1671	1/1	0.94	0.17	64,64,64,64	0
56	MG	YA	3666	1/1	0.94	0.48	36,36,36,36	0
56	MG	QA	1617	1/1	0.94	0.37	61,61,61,61	0
56	MG	YA	3002	1/1	0.94	0.23	64,64,64,64	0
56	MG	YA	3625	1/1	0.94	0.32	19,19,19,19	0
56	MG	RA	3310	1/1	0.94	0.63	96,96,96,96	0
56	MG	RA	3235	1/1	0.94	0.31	70,70,70,70	0
56	MG	YB	210	1/1	0.94	0.42	57,57,57,57	0
56	MG	RA	3313	1/1	0.94	0.42	21,21,21,21	0
56	MG	Y8	102	1/1	0.94	0.51	41,41,41,41	0
56	MG	RA	3964	1/1	0.94	0.11	44,44,44,44	0
56	MG	RA	3738	1/1	0.94	0.42	53,53,53,53	0
56	MG	YA	3345	1/1	0.95	0.45	39,39,39,39	0
56	MG	YA	3149	1/1	0.95	0.41	56,56,56,56	0
56	MG	RD	302	1/1	0.95	0.67	53,53,53,53	0
56	MG	YA	3690	1/1	0.95	0.33	31,31,31,31	0
56	MG	RA	3899	1/1	0.95	0.34	66,66,66,66	0
56	MG	RA	3451	1/1	0.95	0.47	27,27,27,27	0
56	MG	RA	3902	1/1	0.95	0.27	49,49,49,49	0
56	MG	RA	3110	1/1	0.95	0.22	70,70,70,70	0
56	MG	YA	3005	1/1	0.95	0.34	63,63,63,63	0
56	MG	YA	3583	1/1	0.95	0.52	29,29,29,29	0
56	MG	RA	3714	1/1	0.95	0.40	36,36,36,36	0
56	MG	YA	3091	1/1	0.95	0.14	36,36,36,36	0
56	MG	YA	3047	1/1	0.95	0.11	44,44,44,44	0
56	MG	YA	3643	1/1	0.95	0.65	36,36,36,36	0
56	MG	RA	3238	1/1	0.95	0.38	106,106,106,106	0
56	MG	RA	3056	1/1	0.95	0.57	70,70,70,70	0
56	MG	RA	3460	1/1	0.95	0.89	51,51,51,51	0
56	MG	RA	3918	1/1	0.95	0.55	71,71,71,71	0
56	MG	YA	3010	1/1	0.95	0.25	41,41,41,41	0
56	MG	YA	3156	1/1	0.95	0.39	40,40,40,40	0
56	MG	RA	3119	1/1	0.95	0.46	74,74,74,74	0
56	MG	RF	303	1/1	0.95	0.50	80,80,80,80	0
56	MG	RA	3379	1/1	0.95	0.48	44,44,44,44	0
56	MG	YA	3591	1/1	0.95	0.46	42,42,42,42	0
56	MG	RA	3813	1/1	0.95	0.37	23,23,23,23	0
56	MG	YA	3386	1/1	0.95	0.57	23,23,23,23	0
56	MG	RA	3470	1/1	0.95	0.41	34,34,34,34	0
56	MG	YA	3041	1/1	0.95	0.07	35,35,35,35	0
56	MG	RA	3475	1/1	0.95	0.59	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3388	1/1	0.95	0.28	33,33,33,33	0
56	MG	RA	3386	1/1	0.95	0.41	26,26,26,26	0
56	MG	RA	3480	1/1	0.95	0.49	42,42,42,42	0
56	MG	RA	4033	1/1	0.95	0.28	17,17,17,17	0
56	MG	RA	3307	1/1	0.95	0.45	76,76,76,76	0
56	MG	QA	1707	1/1	0.95	0.32	28,28,28,28	0
56	MG	YA	3317	1/1	0.95	0.20	24,24,24,24	0
56	MG	RA	3395	1/1	0.95	0.10	22,22,22,22	0
56	MG	YA	3484	1/1	0.95	0.35	21,21,21,21	0
56	MG	YA	3076	1/1	0.95	0.31	4,4,4,4	0
56	MG	YA	3752	1/1	0.95	0.12	52,52,52,52	0
56	MG	XA	1765	1/1	0.95	0.59	49,49,49,49	0
56	MG	YA	3706	1/1	0.95	0.29	79,79,79,79	0
56	MG	QA	1868	1/1	0.95	0.71	58,58,58,58	0
56	MG	RA	3664	1/1	0.95	0.25	48,48,48,48	0
56	MG	YF	303	1/1	0.95	0.25	85,85,85,85	0
56	MG	YA	3011	1/1	0.95	0.23	40,40,40,40	0
56	MG	XA	1670	1/1	0.95	0.32	80,80,80,80	0
56	MG	RA	3407	1/1	0.95	0.52	34,34,34,34	0
56	MG	RA	3507	1/1	0.95	0.19	109,109,109,109	0
56	MG	RA	3509	1/1	0.95	1.08	69,69,69,69	0
56	MG	RA	3137	1/1	0.95	0.82	97,97,97,97	0
56	MG	RA	3753	1/1	0.95	0.53	48,48,48,48	0
56	MG	RA	3409	1/1	0.95	0.33	33,33,33,33	0
56	MG	YA	3274	1/1	0.95	0.42	48,48,48,48	0
56	MG	YA	3608	1/1	0.95	0.67	44,44,44,44	0
56	MG	YA	3660	1/1	0.95	0.26	34,34,34,34	0
56	MG	YA	3033	1/1	0.95	0.12	13,13,13,13	0
56	MG	RA	3854	1/1	0.95	0.28	47,47,47,47	0
56	MG	RA	3415	1/1	0.95	0.56	42,42,42,42	0
56	MG	YA	3457	1/1	0.95	0.13	33,33,33,33	0
56	MG	RA	3597	1/1	0.95	0.26	19,19,19,19	0
56	MG	YA	3144	1/1	0.95	0.37	57,57,57,57	0
56	MG	YA	3332	1/1	0.95	0.33	28,28,28,28	0
56	MG	XA	1780	1/1	0.95	0.66	40,40,40,40	0
56	MG	YA	3460	1/1	0.95	0.23	28,28,28,28	0
56	MG	XA	1679	1/1	0.95	0.42	52,52,52,52	0
56	MG	YA	3333	1/1	0.95	0.67	26,26,26,26	0
56	MG	YA	3430	1/1	0.95	0.21	20,20,20,20	0
56	MG	YA	3038	1/1	0.95	0.28	48,48,48,48	0
56	MG	YA	3132	1/1	0.95	0.58	86,86,86,86	0
56	MG	YA	3568	1/1	0.95	0.26	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3347	1/1	0.95	0.49	23,23,23,23	0
56	MG	XA	1685	1/1	0.95	0.29	65,65,65,65	0
56	MG	RA	3978	1/1	0.95	0.56	55,55,55,55	0
56	MG	RA	3778	1/1	0.95	0.72	41,41,41,41	0
56	MG	YA	3569	1/1	0.95	0.41	32,32,32,32	0
56	MG	YA	3045	1/1	0.95	0.48	27,27,27,27	0
56	MG	RA	3097	1/1	0.95	0.48	93,93,93,93	0
56	MG	RA	3616	1/1	0.95	0.37	33,33,33,33	0
56	MG	RA	3098	1/1	0.95	0.20	12,12,12,12	0
56	MG	XA	1642	1/1	0.95	0.25	55,55,55,55	0
56	MG	RA	3041	1/1	0.95	0.05	44,44,44,44	0
56	MG	YA	3339	1/1	0.95	0.52	15,15,15,15	0
56	MG	RA	3989	1/1	0.95	0.34	39,39,39,39	0
56	MG	YA	3305	1/1	0.95	0.14	19,19,19,19	0
56	MG	YA	3283	1/1	0.95	0.27	36,36,36,36	0
56	MG	YA	3728	1/1	0.95	0.25	8,8,8,8	0
56	MG	YA	3285	1/1	0.95	0.57	25,25,25,25	0
56	MG	RA	3895	1/1	0.95	0.73	54,54,54,54	0
56	MG	YA	3342	1/1	0.96	0.31	20,20,20,20	0
56	MG	RA	3673	1/1	0.96	0.44	45,45,45,45	0
56	MG	YA	3343	1/1	0.96	0.41	21,21,21,21	0
56	MG	RA	3587	1/1	0.96	0.89	53,53,53,53	0
56	MG	RA	3864	1/1	0.96	0.81	76,76,76,76	0
56	MG	RA	3004	1/1	0.96	0.10	29,29,29,29	0
56	MG	RA	3189	1/1	0.96	0.25	39,39,39,39	0
56	MG	RA	3979	1/1	0.96	0.20	37,37,37,37	0
56	MG	XA	1756	1/1	0.96	0.31	27,27,27,27	0
56	MG	RA	3325	1/1	0.96	0.33	42,42,42,42	0
56	MG	YA	3486	1/1	0.96	0.57	30,30,30,30	0
56	MG	YA	3647	1/1	0.96	0.52	27,27,27,27	0
56	MG	YA	3321	1/1	0.96	0.45	29,29,29,29	0
56	MG	RA	3194	1/1	0.96	0.27	67,67,67,67	0
56	MG	RA	3773	1/1	0.96	0.24	25,25,25,25	0
56	MG	RA	3876	1/1	0.96	0.72	54,54,54,54	0
56	MG	YA	3438	1/1	0.96	0.34	45,45,45,45	0
56	MG	YA	3289	1/1	0.96	0.25	38,38,38,38	0
56	MG	YA	3696	1/1	0.96	0.40	17,17,17,17	0
56	MG	RA	3417	1/1	0.96	0.12	42,42,42,42	0
56	MG	RA	3419	1/1	0.96	0.47	17,17,17,17	0
56	MG	RA	3334	1/1	0.96	0.38	46,46,46,46	0
56	MG	RA	3335	1/1	0.96	0.30	46,46,46,46	0
56	MG	RA	3887	1/1	0.96	0.38	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	YA	3616	1/1	0.96	0.66	53,53,53,53	0
56	MG	YA	3276	1/1	0.96	0.64	67,67,67,67	0
56	MG	RA	3999	1/1	0.96	0.24	21,21,21,21	0
56	MG	RA	3338	1/1	0.96	0.69	38,38,38,38	0
56	MG	RA	3014	1/1	0.96	0.23	38,38,38,38	0
56	MG	RA	3894	1/1	0.96	0.50	23,23,23,23	0
56	MG	YB	216	1/1	0.96	0.42	45,45,45,45	0
56	MG	XA	1767	1/1	0.96	0.46	37,37,37,37	0
56	MG	YA	3619	1/1	0.96	0.21	38,38,38,38	0
56	MG	RA	3698	1/1	0.96	0.14	73,73,73,73	0
56	MG	YA	3325	1/1	0.96	0.34	20,20,20,20	0
56	MG	RA	3345	1/1	0.96	0.48	20,20,20,20	0
56	MG	RA	3793	1/1	0.96	0.42	38,38,38,38	0
56	MG	RA	3141	1/1	0.96	0.59	93,93,93,93	0
56	MG	RA	3614	1/1	0.96	0.44	32,32,32,32	0
56	MG	YA	3444	1/1	0.96	0.44	27,27,27,27	0
56	MG	RA	3348	1/1	0.96	0.40	34,34,34,34	0
56	MG	YA	3277	1/1	0.96	0.50	17,17,17,17	0
56	MG	RA	3911	1/1	0.96	0.33	46,46,46,46	0
56	MG	YA	3006	1/1	0.96	0.14	18,18,18,18	0
56	MG	YA	3579	1/1	0.96	0.61	36,36,36,36	0
56	MG	XA	1774	1/1	0.96	0.39	59,59,59,59	0
56	MG	RA	4020	1/1	0.96	0.88	88,88,88,88	0
56	MG	QA	1717	1/1	0.96	0.56	29,29,29,29	0
56	MG	YA	3213	1/1	0.96	0.31	67,67,67,67	0
56	MG	RA	3711	1/1	0.96	0.59	80,80,80,80	0
56	MG	QA	1719	1/1	0.96	0.51	32,32,32,32	0
56	MG	YA	3141	1/1	0.96	0.21	23,23,23,23	0
56	MG	YA	3353	1/1	0.96	0.31	14,14,14,14	0
56	MG	QA	1722	1/1	0.96	0.75	61,61,61,61	0
56	MG	RA	4030	1/1	0.96	0.85	71,71,71,71	0
56	MG	RA	3543	1/1	0.96	0.31	26,26,26,26	0
56	MG	YA	3125	1/1	0.96	0.37	58,58,58,58	0
56	MG	RA	3092	1/1	0.96	0.64	79,79,79,79	0
56	MG	YA	3630	1/1	0.96	0.53	32,32,32,32	0
56	MG	YA	3004	1/1	0.96	0.14	43,43,43,43	0
56	MG	YA	3195	1/1	0.96	0.27	33,33,33,33	0
56	MG	YA	3712	1/1	0.96	0.56	51,51,51,51	0
56	MG	YA	3381	1/1	0.96	0.38	11,11,11,11	0
56	MG	YA	3299	1/1	0.96	0.55	10,10,10,10	0
56	MG	RA	3369	1/1	0.96	0.62	47,47,47,47	0
56	MG	QA	1781	1/1	0.96	0.43	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	XA	1612	1/1	0.96	0.09	41,41,41,41	0
56	MG	YE	306	1/1	0.96	0.42	13,13,13,13	0
56	MG	XA	1614	1/1	0.96	0.25	60,60,60,60	0
56	MG	YA	3677	1/1	0.96	0.78	42,42,42,42	0
56	MG	YA	3145	1/1	0.96	0.52	59,59,59,59	0
56	MG	RA	3106	1/1	0.96	0.26	102,102,102,102	0
56	MG	RA	3560	1/1	0.96	0.64	23,23,23,23	0
56	MG	QA	1841	1/1	0.96	0.35	28,28,28,28	0
56	MG	RA	3830	1/1	0.96	0.19	66,66,66,66	0
56	MG	RA	3047	1/1	0.96	0.11	12,12,12,12	0
56	MG	RA	3944	1/1	0.96	0.20	22,22,22,22	0
56	MG	RA	3946	1/1	0.96	0.17	18,18,18,18	0
56	MG	RA	3172	1/1	0.96	0.50	80,80,80,80	0
56	MG	RA	3471	1/1	0.96	0.42	42,42,42,42	0
56	MG	XA	1659	1/1	0.96	0.14	75,75,75,75	0
56	MG	YA	3559	1/1	0.96	0.42	54,54,54,54	0
56	MG	RA	3476	1/1	0.96	0.46	30,30,30,30	0
56	MG	QA	1638	1/1	0.96	0.17	41,41,41,41	0
56	MG	XA	1743	1/1	0.96	0.79	44,44,44,44	0
56	MG	YA	3681	1/1	0.96	0.79	38,38,38,38	0
56	MG	RA	3745	1/1	0.96	0.31	21,21,21,21	0
56	MG	XA	1745	1/1	0.96	0.49	44,44,44,44	0
56	MG	RA	3482	1/1	0.96	0.52	21,21,21,21	0
56	MG	RA	3483	1/1	0.96	0.47	21,21,21,21	0
56	MG	RA	3485	1/1	0.96	0.78	65,65,65,65	0
56	MG	XA	1746	1/1	0.96	0.47	35,35,35,35	0
56	MG	RA	3487	1/1	0.96	0.20	17,17,17,17	0
56	MG	RA	3852	1/1	0.96	0.38	47,47,47,47	0
56	MG	YA	3287	1/1	0.96	0.44	35,35,35,35	0
56	MG	RA	3965	1/1	0.96	0.13	45,45,45,45	0
56	MG	YA	3413	1/1	0.96	0.41	36,36,36,36	0
56	MG	YA	3640	1/1	0.96	0.59	40,40,40,40	0
57	ZN	QN	101	1/1	0.96	0.13	105,105,105,105	0
56	MG	YA	3073	1/1	0.96	0.55	67,67,67,67	0
56	MG	YA	3564	1/1	0.96	0.13	42,42,42,42	0
56	MG	RA	3060	1/1	0.96	0.16	21,21,21,21	0
56	MG	RA	3971	1/1	0.97	0.40	19,19,19,19	0
56	MG	YA	3754	1/1	0.97	0.32	26,26,26,26	0
56	MG	QA	1613	1/1	0.97	0.09	97,97,97,97	0
56	MG	RA	3870	1/1	0.97	0.45	24,24,24,24	0
56	MG	XA	1766	1/1	0.97	0.75	52,52,52,52	0
56	MG	YA	3322	1/1	0.97	0.31	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	QA	1827	1/1	0.97	0.19	52,52,52,52	0
56	MG	QA	1828	1/1	0.97	0.26	41,41,41,41	0
56	MG	YA	3390	1/1	0.97	0.58	33,33,33,33	0
56	MG	YA	3554	1/1	0.97	0.23	44,44,44,44	0
56	MG	RA	3879	1/1	0.97	0.37	29,29,29,29	0
56	MG	RA	3783	1/1	0.97	0.44	42,42,42,42	0
56	MG	YA	3675	1/1	0.97	0.32	29,29,29,29	0
56	MG	RA	3359	1/1	0.97	0.34	32,32,32,32	0
56	MG	RA	3443	1/1	0.97	0.59	20,20,20,20	0
56	MG	RA	3165	1/1	0.97	0.48	99,99,99,99	0
56	MG	RA	3885	1/1	0.97	0.51	66,66,66,66	0
56	MG	YA	3587	1/1	0.97	0.30	31,31,31,31	0
56	MG	YA	3282	1/1	0.97	0.37	10,10,10,10	0
56	MG	RA	3990	1/1	0.97	0.34	109,109,109,109	0
56	MG	RA	3888	1/1	0.97	0.49	24,24,24,24	0
56	MG	YA	3556	1/1	0.97	0.33	41,41,41,41	0
56	MG	RA	3292	1/1	0.97	0.10	83,83,83,83	0
56	MG	YA	3310	1/1	0.97	0.52	38,38,38,38	0
56	MG	YA	3374	1/1	0.97	0.58	34,34,34,34	0
56	MG	YA	3596	1/1	0.97	0.43	39,39,39,39	0
56	MG	YA	3112	1/1	0.97	0.23	9,9,9,9	0
56	MG	YA	3533	1/1	0.97	0.25	48,48,48,48	0
56	MG	YA	3685	1/1	0.97	0.48	19,19,19,19	0
56	MG	YA	3724	1/1	0.97	0.62	51,51,51,51	0
56	MG	YA	3642	1/1	0.97	0.73	58,58,58,58	0
56	MG	YA	3483	1/1	0.97	0.36	26,26,26,26	0
56	MG	RE	303	1/1	0.97	0.35	15,15,15,15	0
56	MG	QA	1631	1/1	0.97	0.09	34,34,34,34	0
56	MG	YX	101	1/1	0.97	0.32	31,31,31,31	0
56	MG	YA	3284	1/1	0.97	0.24	8,8,8,8	0
56	MG	RA	3906	1/1	0.97	0.31	20,20,20,20	0
56	MG	YA	3601	1/1	0.97	0.63	29,29,29,29	0
56	MG	RA	3908	1/1	0.97	0.42	22,22,22,22	0
56	MG	RA	4009	1/1	0.97	0.60	70,70,70,70	0
56	MG	RA	3306	1/1	0.97	0.97	66,66,66,66	0
56	MG	RA	3720	1/1	0.97	0.45	33,33,33,33	0
56	MG	YA	3328	1/1	0.97	0.35	15,15,15,15	0
56	MG	QA	1740	1/1	0.97	0.35	55,55,55,55	0
56	MG	XA	1737	1/1	0.97	0.46	47,47,47,47	0
56	MG	YA	3440	1/1	0.97	0.27	29,29,29,29	0
56	MG	RA	3915	1/1	0.97	0.31	41,41,41,41	0
56	MG	RA	3469	1/1	0.97	0.68	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3329	1/1	0.97	0.35	19,19,19,19	0
56	MG	YA	3539	1/1	0.97	0.32	18,18,18,18	0
56	MG	XA	1694	1/1	0.97	0.36	30,30,30,30	0
56	MG	RA	3389	1/1	0.97	0.39	23,23,23,23	0
56	MG	YA	3151	1/1	0.97	0.14	8,8,8,8	0
56	MG	RA	3315	1/1	0.97	0.32	29,29,29,29	0
56	MG	RA	3478	1/1	0.97	0.39	34,34,34,34	0
56	MG	RA	3821	1/1	0.97	0.49	29,29,29,29	0
56	MG	QA	1800	1/1	0.97	0.22	41,41,41,41	0
56	MG	RA	4027	1/1	0.97	0.38	39,39,39,39	0
56	MG	RA	4028	1/1	0.97	0.30	78,78,78,78	0
56	MG	YA	3734	1/1	0.97	0.50	41,41,41,41	0
56	MG	RA	3398	1/1	0.97	0.47	20,20,20,20	0
56	MG	RA	3568	1/1	0.97	0.36	27,27,27,27	0
56	MG	RA	4032	1/1	0.97	0.45	76,76,76,76	0
56	MG	RA	3655	1/1	0.97	0.30	25,25,25,25	0
56	MG	YA	3401	1/1	0.97	0.53	19,19,19,19	0
56	MG	RA	3255	1/1	0.97	0.57	100,100,100,100	0
56	MG	RA	4036	1/1	0.97	0.76	85,85,85,85	0
56	MG	RA	3070	1/1	0.97	0.59	78,78,78,78	0
56	MG	RA	3324	1/1	0.97	0.38	14,14,14,14	0
56	MG	YA	3152	1/1	0.97	0.26	50,50,50,50	0
56	MG	YA	3572	1/1	0.97	0.26	28,28,28,28	0
56	MG	YA	3382	1/1	0.97	0.26	29,29,29,29	0
56	MG	YA	3739	1/1	0.97	0.47	79,79,79,79	0
56	MG	YA	3022	1/1	0.97	0.38	62,62,62,62	0
56	MG	RA	4044	1/1	0.97	0.52	95,95,95,95	0
56	MG	RA	3838	1/1	0.97	0.55	17,17,17,17	0
56	MG	YA	3741	1/1	0.97	0.30	57,57,57,57	0
56	MG	YA	3009	1/1	0.97	0.14	37,37,37,37	0
56	MG	XA	1611	1/1	0.97	0.46	73,73,73,73	0
56	MG	RA	3079	1/1	0.97	0.38	64,64,64,64	0
56	MG	RA	4050	1/1	0.97	0.47	59,59,59,59	0
56	MG	RA	3413	1/1	0.97	0.41	34,34,34,34	0
56	MG	YA	3743	1/1	0.97	0.42	43,43,43,43	0
56	MG	RA	3947	1/1	0.97	0.21	20,20,20,20	0
56	MG	XA	1755	1/1	0.97	0.61	43,43,43,43	0
56	MG	RA	3502	1/1	0.97	0.31	20,20,20,20	0
56	MG	RA	3504	1/1	0.97	0.37	38,38,38,38	0
56	MG	RA	3848	1/1	0.97	0.72	50,50,50,50	0
56	MG	YA	3496	1/1	0.97	0.45	18,18,18,18	0
56	MG	RA	3850	1/1	0.97	0.31	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3506	1/1	0.97	0.23	26,26,26,26	0
56	MG	QA	1706	1/1	0.97	0.48	35,35,35,35	0
56	MG	RA	3418	1/1	0.97	0.71	36,36,36,36	0
56	MG	RA	3025	1/1	0.97	0.14	23,23,23,23	0
56	MG	YA	3407	1/1	0.97	0.49	18,18,18,18	0
56	MG	YA	3334	1/1	0.97	0.53	14,14,14,14	0
56	MG	RA	3857	1/1	0.97	0.35	35,35,35,35	0
56	MG	YA	3297	1/1	0.97	0.51	19,19,19,19	0
56	MG	YA	3581	1/1	0.97	0.59	24,24,24,24	0
56	MG	RA	3516	1/1	0.97	0.45	13,13,13,13	0
56	MG	RA	3344	1/1	0.97	0.39	51,51,51,51	0
56	MG	YA	3410	1/1	0.97	0.33	31,31,31,31	0
56	MG	RA	3770	1/1	0.97	0.37	22,22,22,22	0
57	ZN	Y9	101	1/1	0.97	0.10	107,107,107,107	0
56	MG	YA	3048	1/1	0.97	0.30	57,57,57,57	0
56	MG	YA	3668	1/1	0.97	0.43	28,28,28,28	0
56	MG	YA	3670	1/1	0.97	0.36	12,12,12,12	0
56	MG	RA	3430	1/1	0.97	0.27	9,9,9,9	0
56	MG	XA	1752	1/1	0.98	0.19	51,51,51,51	0
56	MG	YA	3652	1/1	0.98	0.49	24,24,24,24	0
56	MG	YA	3489	1/1	0.98	0.38	15,15,15,15	0
56	MG	RA	3765	1/1	0.98	0.61	40,40,40,40	0
56	MG	RA	3613	1/1	0.98	0.42	35,35,35,35	0
56	MG	YA	3592	1/1	0.98	0.42	28,28,28,28	0
56	MG	RA	3615	1/1	0.98	0.61	34,34,34,34	0
56	MG	YA	3571	1/1	0.98	0.50	23,23,23,23	0
56	MG	RA	3474	1/1	0.98	0.28	45,45,45,45	0
56	MG	YA	3626	1/1	0.98	0.30	25,25,25,25	0
56	MG	YA	3391	1/1	0.98	0.47	18,18,18,18	0
56	MG	RA	3210	1/1	0.98	0.33	67,67,67,67	0
56	MG	YA	3595	1/1	0.98	0.53	12,12,12,12	0
56	MG	RA	3623	1/1	0.98	0.55	34,34,34,34	0
56	MG	RA	3624	1/1	0.98	0.24	38,38,38,38	0
56	MG	QA	1710	1/1	0.98	0.31	28,28,28,28	0
56	MG	RA	3355	1/1	0.98	0.59	24,24,24,24	0
56	MG	YA	3014	1/1	0.98	0.26	39,39,39,39	0
56	MG	RA	3125	1/1	0.98	0.20	36,36,36,36	0
56	MG	YA	3327	1/1	0.98	0.50	7,7,7,7	0
56	MG	RA	3484	1/1	0.98	0.48	30,30,30,30	0
56	MG	RA	3127	1/1	0.98	0.43	52,52,52,52	0
56	MG	YA	3631	1/1	0.98	0.14	55,55,55,55	0
56	MG	YA	3663	1/1	0.98	0.75	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3575	1/1	0.98	0.54	30,30,30,30	0
56	MG	YA	3404	1/1	0.98	0.55	13,13,13,13	0
56	MG	YA	3494	1/1	0.98	0.21	36,36,36,36	0
56	MG	YA	3480	1/1	0.98	0.42	17,17,17,17	0
56	MG	YA	3560	1/1	0.98	0.24	6,6,6,6	0
56	MG	YA	3669	1/1	0.98	0.39	15,15,15,15	0
56	MG	RA	3792	1/1	0.98	0.43	35,35,35,35	0
56	MG	RA	3873	1/1	0.98	0.48	31,31,31,31	0
56	MG	YA	3604	1/1	0.98	0.43	11,11,11,11	0
56	MG	RA	3495	1/1	0.98	0.51	43,43,43,43	0
56	MG	RA	3496	1/1	0.98	0.45	16,16,16,16	0
56	MG	RA	3877	1/1	0.98	0.39	23,23,23,23	0
56	MG	RA	3318	1/1	0.98	0.33	19,19,19,19	0
56	MG	RA	3094	1/1	0.98	0.84	71,71,71,71	0
56	MG	RA	3320	1/1	0.98	0.38	14,14,14,14	0
56	MG	RA	3321	1/1	0.98	0.28	19,19,19,19	0
56	MG	RA	3501	1/1	0.98	0.68	22,22,22,22	0
56	MG	YA	3606	1/1	0.98	0.66	25,25,25,25	0
56	MG	RA	3503	1/1	0.98	0.28	21,21,21,21	0
56	MG	YA	3338	1/1	0.98	0.44	16,16,16,16	0
56	MG	RA	3435	1/1	0.98	0.61	23,23,23,23	0
56	MG	YA	3318	1/1	0.98	0.43	26,26,26,26	0
56	MG	RA	3230	1/1	0.98	0.52	81,81,81,81	0
56	MG	RA	3508	1/1	0.98	0.50	42,42,42,42	0
56	MG	RA	3579	1/1	0.98	0.32	24,24,24,24	0
56	MG	YA	3346	1/1	0.98	0.55	16,16,16,16	0
56	MG	RA	3378	1/1	0.98	0.43	25,25,25,25	0
56	MG	RA	3893	1/1	0.98	0.66	34,34,34,34	0
56	MG	YA	3320	1/1	0.98	0.37	26,26,26,26	0
56	MG	YA	3472	1/1	0.98	0.45	23,23,23,23	0
56	MG	RA	3513	1/1	0.98	0.12	14,14,14,14	0
56	MG	YA	3380	1/1	0.98	0.39	7,7,7,7	0
56	MG	RA	3382	1/1	0.98	0.33	20,20,20,20	0
56	MG	YA	3518	1/1	0.98	0.37	16,16,16,16	0
56	MG	RB	205	1/1	0.98	0.21	47,47,47,47	0
56	MG	RA	3384	1/1	0.98	0.63	21,21,21,21	0
56	MG	RA	3901	1/1	0.98	0.40	16,16,16,16	0
56	MG	RA	3022	1/1	0.98	0.70	76,76,76,76	0
56	MG	RA	3147	1/1	0.98	0.21	39,39,39,39	0
56	MG	RA	3904	1/1	0.98	0.30	24,24,24,24	0
56	MG	RA	3820	1/1	0.98	0.26	28,28,28,28	0
56	MG	RA	3333	1/1	0.98	0.38	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3680	1/1	0.98	0.77	50,50,50,50	0
56	MG	YA	3618	1/1	0.98	0.34	24,24,24,24	0
56	MG	RA	3390	1/1	0.98	0.32	27,27,27,27	0
56	MG	RA	3391	1/1	0.98	0.49	17,17,17,17	0
56	MG	YA	3143	1/1	0.98	0.11	56,56,56,56	0
56	MG	RA	3393	1/1	0.98	0.48	14,14,14,14	0
56	MG	RB	219	1/1	0.98	0.14	57,57,57,57	0
56	MG	RA	3394	1/1	0.98	0.47	31,31,31,31	0
56	MG	XA	1633	1/1	0.98	0.34	51,51,51,51	0
56	MG	YA	3441	1/1	0.98	0.46	34,34,34,34	0
56	MG	RA	3831	1/1	0.98	0.32	65,65,65,65	0
56	MG	YD	306	1/1	0.98	0.41	53,53,53,53	0
56	MG	RA	3833	1/1	0.98	0.42	29,29,29,29	0
56	MG	YA	3589	1/1	0.98	0.45	31,31,31,31	0
56	MG	YD	308	1/1	0.98	0.27	71,71,71,71	0
56	MG	RA	3400	1/1	0.98	0.48	21,21,21,21	0
57	ZN	Y5	102	1/1	0.98	0.05	119,119,119,119	0
57	ZN	Y6	101	1/1	0.98	0.18	169,169,169,169	0
56	MG	YA	3590	1/1	0.98	0.73	41,41,41,41	0
57	ZN	XN	101	1/1	0.98	0.10	94,94,94,94	0
56	MG	YA	3651	1/1	0.98	0.59	15,15,15,15	0
56	MG	RA	3465	1/1	0.98	0.39	27,27,27,27	0
56	MG	XA	1640	1/1	0.98	0.15	66,66,66,66	0
56	MG	RA	3467	1/1	0.98	0.40	21,21,21,21	0
56	MG	RA	3761	1/1	0.99	0.47	22,22,22,22	0
56	MG	YA	3358	1/1	0.99	0.63	18,18,18,18	0
56	MG	YA	3614	1/1	0.99	0.45	26,26,26,26	0
56	MG	YA	3686	1/1	0.99	0.37	15,15,15,15	0
56	MG	YA	3615	1/1	0.99	0.54	11,11,11,11	0
56	MG	RA	3473	1/1	0.99	0.39	26,26,26,26	0
56	MG	RA	3423	1/1	0.99	0.42	21,21,21,21	0
56	MG	XA	1631	1/1	0.99	0.40	60,60,60,60	0
56	MG	YA	3306	1/1	0.99	0.18	9,9,9,9	0
56	MG	YA	3319	1/1	0.99	0.46	20,20,20,20	0
56	MG	YA	3750	1/1	0.99	0.44	22,22,22,22	0
56	MG	YA	3016	1/1	0.99	0.17	29,29,29,29	0
56	MG	YA	3602	1/1	0.99	0.43	16,16,16,16	0
56	MG	YA	3385	1/1	0.99	0.36	23,23,23,23	0
56	MG	YA	3673	1/1	0.99	0.24	13,13,13,13	0
56	MG	YA	3515	1/1	0.99	0.42	12,12,12,12	0
56	MG	RA	3945	1/1	0.99	0.49	25,25,25,25	0
56	MG	YA	3656	1/1	0.99	0.31	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3605	1/1	0.99	0.33	19,19,19,19	0
56	MG	RA	3020	1/1	0.99	0.45	89,89,89,89	0
56	MG	YA	3395	1/1	0.99	0.43	17,17,17,17	0
56	MG	YA	3362	1/1	0.99	0.52	18,18,18,18	0
56	MG	YA	3363	1/1	0.99	0.60	11,11,11,11	0
56	MG	YA	3371	1/1	0.99	0.46	14,14,14,14	0
56	MG	YA	3610	1/1	0.99	0.43	20,20,20,20	0
56	MG	RA	3622	1/1	0.99	0.35	20,20,20,20	0
56	MG	YA	3113	1/1	0.99	0.21	104,104,104,104	0
56	MG	RA	3442	1/1	0.99	0.62	18,18,18,18	0
57	ZN	R5	102	1/1	0.99	0.03	119,119,119,119	0
56	MG	YA	3612	1/1	0.99	0.24	23,23,23,23	0
57	ZN	R9	102	1/1	0.99	0.05	92,92,92,92	0
58	SF4	XD	301	8/8	0.99	0.14	58,74,100,102	0
58	SF4	QD	302	8/8	0.99	0.15	51,57,76,106	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.