



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 10:31 am BST

PDB ID : 5CZP
Title : 70S termination complex containing E. coli RF2
Authors : Hoffer, E.D.; Dunham, C.M.
Deposited on : 2015-07-31
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

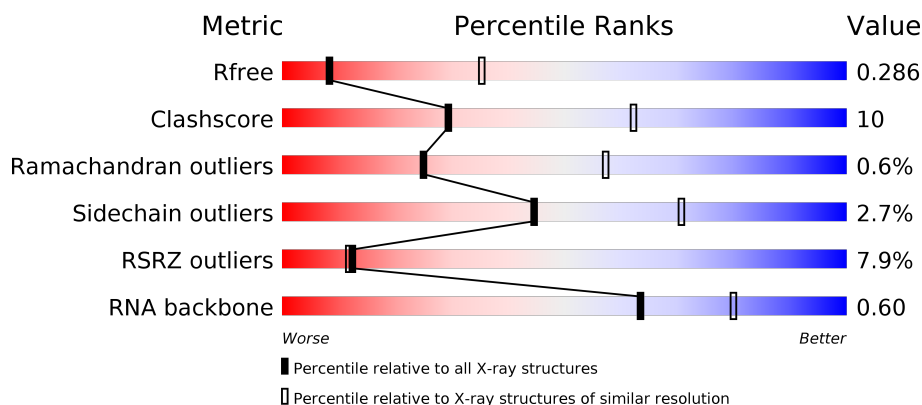
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	RA	2915	<div> <div>4%</div> <div>61%</div> <div>31%</div> <div>5%</div> <div>•</div> </div>
1	YA	2915	<div> <div>4%</div> <div>62%</div> <div>31%</div> <div>5%</div> <div>•</div> </div>
2	RB	122	<div> <div>2%</div> <div>78%</div> <div>19%</div> <div>••</div> </div>
2	YB	122	<div> <div>2%</div> <div>66%</div> <div>30%</div> <div>••</div> </div>

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Mol	Chain	Length	Quality of chain
3	RD	276	
3	YD	276	
4	RE	206	
4	YE	206	
5	RF	210	
5	YF	210	
6	RG	182	
6	YG	182	
7	RH	180	
7	YH	180	
8	RI	148	
8	YI	148	
9	RN	140	
9	YN	140	
10	RO	122	
10	YO	122	
11	RP	150	
11	YP	150	
12	RQ	141	
12	YQ	141	
13	RR	118	
13	YR	118	
14	RS	112	
14	YS	112	
15	RT	146	

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Mol	Chain	Length	Quality of chain
15	YT	146	
16	RU	118	
16	YU	118	
17	RV	101	
17	YV	101	
18	RW	113	
18	YW	113	
19	RX	96	
19	YX	96	
20	RY	110	
20	YY	110	
21	RZ	206	
21	YZ	206	
22	R0	85	
22	Y0	85	
23	R1	98	
23	Y1	98	
24	R2	72	
24	Y2	72	
25	R3	60	
25	Y3	60	
26	R4	71	
26	Y4	71	
27	R5	60	
27	Y5	60	

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Mol	Chain	Length	Quality of chain
28	R6	54	
28	Y6	54	
29	R7	49	
29	Y7	49	
30	R8	65	
30	Y8	65	
31	R9	37	
31	Y9	37	
32	QA	1521	
32	XA	1521	
33	QB	256	
33	XB	256	
34	QC	239	
34	XC	239	
35	QD	209	
35	XD	209	
36	QE	162	
36	XE	162	
37	QF	101	
37	XF	101	
38	QG	156	
38	XG	156	
39	QH	138	
39	XH	138	
40	QI	128	

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Mol	Chain	Length	Quality of chain
40	XI	128	
41	QJ	105	
41	XJ	105	
42	QK	129	
42	XK	129	
43	QL	132	
43	XL	132	
44	QM	126	
44	XM	126	
45	QN	61	
45	XN	61	
46	QO	89	
46	XO	89	
47	QP	88	
47	XP	88	
48	QQ	105	
48	XQ	105	
49	QR	88	
49	XR	88	
50	QS	93	
50	XS	93	
51	QT	106	
51	XT	106	
52	QU	27	
52	XU	27	

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Mol	Chain	Length	Quality of chain
53	QV	77	
53	XV	77	
54	QY	380	
54	XY	380	
55	QX	25	
55	XX	25	

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	1603	-	-	-	X
56	MG	QA	1604	-	-	-	X
56	MG	QA	1611	-	-	-	X
56	MG	QA	1612	-	-	-	X
56	MG	QA	1614	-	-	-	X
56	MG	QA	1622	-	-	-	X
56	MG	QA	1624	-	-	-	X
56	MG	QA	1625	-	-	-	X
56	MG	QA	1630	-	-	-	X
56	MG	QA	1632	-	-	-	X
56	MG	QA	1636	-	-	-	X
56	MG	QA	1637	-	-	-	X
56	MG	QA	1640	-	-	-	X
56	MG	QA	1642	-	-	-	X
56	MG	QA	1643	-	-	-	X
56	MG	QA	1646	-	-	-	X
56	MG	QA	1651	-	-	-	X
56	MG	QA	1653	-	-	-	X
56	MG	QA	1654	-	-	-	X
56	MG	QA	1657	-	-	-	X
56	MG	QA	1661	-	-	-	X
56	MG	QA	1664	-	-	-	X
56	MG	QA	1666	-	-	-	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	1673	-	-	-	X
56	MG	QA	1676	-	-	-	X
56	MG	QA	1677	-	-	-	X
56	MG	QA	1679	-	-	-	X
56	MG	QA	1680	-	-	-	X
56	MG	QA	1681	-	-	-	X
56	MG	QA	1682	-	-	-	X
56	MG	QA	1684	-	-	-	X
56	MG	QA	1686	-	-	-	X
56	MG	QA	1687	-	-	-	X
56	MG	QA	1688	-	-	-	X
56	MG	QA	1691	-	-	-	X
56	MG	QA	1694	-	-	-	X
56	MG	QA	1696	-	-	-	X
56	MG	QA	1697	-	-	-	X
56	MG	QA	1698	-	-	-	X
56	MG	QA	1700	-	-	-	X
56	MG	QA	1701	-	-	-	X
56	MG	QA	1702	-	-	-	X
56	MG	QA	1703	-	-	-	X
56	MG	QA	1704	-	-	-	X
56	MG	QA	1705	-	-	-	X
56	MG	QA	1710	-	-	-	X
56	MG	QA	1712	-	-	-	X
56	MG	QA	1713	-	-	-	X
56	MG	QA	1714	-	-	-	X
56	MG	QA	1719	-	-	-	X
56	MG	QA	1720	-	-	-	X
56	MG	QA	1722	-	-	-	X
56	MG	QA	1723	-	-	-	X
56	MG	QA	1724	-	-	-	X
56	MG	QA	1727	-	-	-	X
56	MG	QA	1729	-	-	-	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	1739	-	-	-	X
56	MG	QA	1740	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	QA	1741	-	-	-	X
56	MG	QA	1745	-	-	-	X
56	MG	QA	1746	-	-	-	X
56	MG	QA	1747	-	-	-	X
56	MG	QA	1748	-	-	-	X
56	MG	QA	1749	-	-	-	X
56	MG	QA	1751	-	-	-	X
56	MG	QA	1753	-	-	-	X
56	MG	QA	1755	-	-	-	X
56	MG	QA	1756	-	-	-	X
56	MG	QA	1757	-	-	-	X
56	MG	QA	1759	-	-	-	X
56	MG	QA	1760	-	-	-	X
56	MG	QA	1762	-	-	-	X
56	MG	QA	1764	-	-	-	X
56	MG	QA	1765	-	-	-	X
56	MG	QA	1768	-	-	-	X
56	MG	QA	1769	-	-	-	X
56	MG	QA	1771	-	-	-	X
56	MG	QA	1774	-	-	-	X
56	MG	QA	1775	-	-	-	X
56	MG	QA	1778	-	-	-	X
56	MG	QA	1780	-	-	-	X
56	MG	QA	1786	-	-	-	X
56	MG	QA	1787	-	-	-	X
56	MG	QA	1790	-	-	-	X
56	MG	QA	1793	-	-	-	X
56	MG	QA	1794	-	-	-	X
56	MG	QA	1795	-	-	-	X
56	MG	QA	1796	-	-	-	X
56	MG	QA	1799	-	-	-	X
56	MG	QA	1800	-	-	-	X
56	MG	QA	1805	-	-	-	X
56	MG	QA	1806	-	-	-	X
56	MG	QA	1807	-	-	-	X
56	MG	QA	1809	-	-	-	X
56	MG	QA	1814	-	-	-	X
56	MG	QA	1816	-	-	-	X
56	MG	QA	1817	-	-	-	X
56	MG	QA	1818	-	-	-	X
56	MG	QA	1819	-	-	-	X
56	MG	QA	1820	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	QA	1821	-	-	-	X
56	MG	QA	1823	-	-	-	X
56	MG	QA	1824	-	-	-	X
56	MG	QA	1825	-	-	-	X
56	MG	QA	1828	-	-	-	X
56	MG	QA	1831	-	-	-	X
56	MG	QA	1832	-	-	-	X
56	MG	QA	1834	-	-	-	X
56	MG	QA	1835	-	-	-	X
56	MG	QA	1836	-	-	-	X
56	MG	QA	1837	-	-	-	X
56	MG	QA	1838	-	-	-	X
56	MG	QA	1839	-	-	-	X
56	MG	QA	1840	-	-	-	X
56	MG	QA	1842	-	-	-	X
56	MG	QA	1847	-	-	-	X
56	MG	QA	1848	-	-	-	X
56	MG	QA	1849	-	-	-	X
56	MG	QA	1851	-	-	-	X
56	MG	QA	1852	-	-	-	X
56	MG	QA	1853	-	-	-	X
56	MG	QA	1854	-	-	-	X
56	MG	QA	1855	-	-	-	X
56	MG	QA	1856	-	-	-	X
56	MG	QA	1858	-	-	-	X
56	MG	QA	1859	-	-	-	X
56	MG	QA	1860	-	-	-	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	1868	-	-	-	X
56	MG	QA	1869	-	-	-	X
56	MG	QA	1870	-	-	-	X
56	MG	QA	1872	-	-	-	X
56	MG	QA	1873	-	-	-	X
56	MG	QA	1877	-	-	-	X
56	MG	QA	1879	-	-	-	X
56	MG	QD	301	-	-	-	X
56	MG	QD	303	-	-	-	X
56	MG	QD	304	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	QE	202	-	-	-	X
56	MG	QG	201	-	-	-	X
56	MG	QG	202	-	-	-	X
56	MG	QG	203	-	-	-	X
56	MG	QH	201	-	-	-	X
56	MG	QH	202	-	-	-	X
56	MG	QI	201	-	-	-	X
56	MG	QL	202	-	-	-	X
56	MG	QN	102	-	-	-	X
56	MG	QN	103	-	-	-	X
56	MG	QR	101	-	-	-	X
56	MG	QT	201	-	-	-	X
56	MG	QV	103	-	-	-	X
56	MG	QV	104	-	-	-	X
56	MG	QY	401	-	-	-	X
56	MG	QY	402	-	-	-	X
56	MG	R0	102	-	-	-	X
56	MG	R0	103	-	-	-	X
56	MG	R0	104	-	-	-	X
56	MG	R1	101	-	-	-	X
56	MG	R1	102	-	-	-	X
56	MG	R1	103	-	-	-	X
56	MG	R1	104	-	-	-	X
56	MG	R3	101	-	-	-	X
56	MG	R3	102	-	-	-	X
56	MG	R4	102	-	-	-	X
56	MG	R5	101	-	-	-	X
56	MG	R5	102	-	-	-	X
56	MG	R5	104	-	-	-	X
56	MG	R5	105	-	-	-	X
56	MG	R7	101	-	-	-	X
56	MG	R7	102	-	-	-	X
56	MG	R8	101	-	-	-	X
56	MG	R9	101	-	-	-	X
56	MG	R9	103	-	-	-	X
56	MG	RA	3001	-	-	-	X
56	MG	RA	3003	-	-	-	X
56	MG	RA	3005	-	-	-	X
56	MG	RA	3011	-	-	-	X
56	MG	RA	3012	-	-	-	X
56	MG	RA	3013	-	-	-	X
56	MG	RA	3016	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3022	-	-	-	X
56	MG	RA	3024	-	-	-	X
56	MG	RA	3027	-	-	-	X
56	MG	RA	3029	-	-	-	X
56	MG	RA	3031	-	-	-	X
56	MG	RA	3033	-	-	-	X
56	MG	RA	3036	-	-	-	X
56	MG	RA	3037	-	-	-	X
56	MG	RA	3039	-	-	-	X
56	MG	RA	3040	-	-	-	X
56	MG	RA	3042	-	-	-	X
56	MG	RA	3045	-	-	-	X
56	MG	RA	3050	-	-	-	X
56	MG	RA	3052	-	-	-	X
56	MG	RA	3053	-	-	-	X
56	MG	RA	3054	-	-	-	X
56	MG	RA	3057	-	-	-	X
56	MG	RA	3058	-	-	-	X
56	MG	RA	3065	-	-	-	X
56	MG	RA	3066	-	-	-	X
56	MG	RA	3067	-	-	-	X
56	MG	RA	3074	-	-	-	X
56	MG	RA	3076	-	-	-	X
56	MG	RA	3077	-	-	-	X
56	MG	RA	3079	-	-	-	X
56	MG	RA	3081	-	-	-	X
56	MG	RA	3085	-	-	-	X
56	MG	RA	3086	-	-	-	X
56	MG	RA	3087	-	-	-	X
56	MG	RA	3090	-	-	-	X
56	MG	RA	3091	-	-	-	X
56	MG	RA	3097	-	-	-	X
56	MG	RA	3098	-	-	-	X
56	MG	RA	3099	-	-	-	X
56	MG	RA	3100	-	-	-	X
56	MG	RA	3101	-	-	-	X
56	MG	RA	3102	-	-	-	X
56	MG	RA	3103	-	-	-	X
56	MG	RA	3105	-	-	-	X
56	MG	RA	3106	-	-	-	X
56	MG	RA	3108	-	-	-	X
56	MG	RA	3109	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3111	-	-	-	X
56	MG	RA	3112	-	-	-	X
56	MG	RA	3113	-	-	-	X
56	MG	RA	3114	-	-	-	X
56	MG	RA	3115	-	-	-	X
56	MG	RA	3116	-	-	-	X
56	MG	RA	3117	-	-	-	X
56	MG	RA	3120	-	-	-	X
56	MG	RA	3121	-	-	-	X
56	MG	RA	3122	-	-	-	X
56	MG	RA	3124	-	-	-	X
56	MG	RA	3126	-	-	-	X
56	MG	RA	3133	-	-	-	X
56	MG	RA	3134	-	-	-	X
56	MG	RA	3137	-	-	-	X
56	MG	RA	3138	-	-	-	X
56	MG	RA	3141	-	-	-	X
56	MG	RA	3142	-	-	-	X
56	MG	RA	3144	-	-	-	X
56	MG	RA	3145	-	-	-	X
56	MG	RA	3148	-	-	-	X
56	MG	RA	3149	-	-	-	X
56	MG	RA	3155	-	-	-	X
56	MG	RA	3156	-	-	-	X
56	MG	RA	3159	-	-	-	X
56	MG	RA	3164	-	-	-	X
56	MG	RA	3165	-	-	-	X
56	MG	RA	3166	-	-	-	X
56	MG	RA	3171	-	-	-	X
56	MG	RA	3172	-	-	-	X
56	MG	RA	3173	-	-	-	X
56	MG	RA	3174	-	-	-	X
56	MG	RA	3176	-	-	-	X
56	MG	RA	3177	-	-	-	X
56	MG	RA	3179	-	-	-	X
56	MG	RA	3180	-	-	-	X
56	MG	RA	3181	-	-	-	X
56	MG	RA	3182	-	-	-	X
56	MG	RA	3183	-	-	-	X
56	MG	RA	3187	-	-	-	X
56	MG	RA	3188	-	-	-	X
56	MG	RA	3189	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3193	-	-	-	X
56	MG	RA	3194	-	-	-	X
56	MG	RA	3196	-	-	-	X
56	MG	RA	3197	-	-	-	X
56	MG	RA	3198	-	-	-	X
56	MG	RA	3199	-	-	-	X
56	MG	RA	3203	-	-	-	X
56	MG	RA	3204	-	-	-	X
56	MG	RA	3205	-	-	-	X
56	MG	RA	3207	-	-	-	X
56	MG	RA	3208	-	-	-	X
56	MG	RA	3210	-	-	-	X
56	MG	RA	3213	-	-	-	X
56	MG	RA	3215	-	-	-	X
56	MG	RA	3216	-	-	-	X
56	MG	RA	3218	-	-	-	X
56	MG	RA	3219	-	-	-	X
56	MG	RA	3222	-	-	-	X
56	MG	RA	3224	-	-	-	X
56	MG	RA	3225	-	-	-	X
56	MG	RA	3227	-	-	-	X
56	MG	RA	3228	-	-	-	X
56	MG	RA	3229	-	-	-	X
56	MG	RA	3234	-	-	-	X
56	MG	RA	3235	-	-	-	X
56	MG	RA	3236	-	-	-	X
56	MG	RA	3237	-	-	-	X
56	MG	RA	3238	-	-	-	X
56	MG	RA	3239	-	-	-	X
56	MG	RA	3241	-	-	-	X
56	MG	RA	3242	-	-	-	X
56	MG	RA	3244	-	-	-	X
56	MG	RA	3246	-	-	-	X
56	MG	RA	3247	-	-	-	X
56	MG	RA	3248	-	-	-	X
56	MG	RA	3250	-	-	-	X
56	MG	RA	3251	-	-	-	X
56	MG	RA	3253	-	-	-	X
56	MG	RA	3254	-	-	-	X
56	MG	RA	3255	-	-	-	X
56	MG	RA	3257	-	-	-	X
56	MG	RA	3259	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3261	-	-	-	X
56	MG	RA	3267	-	-	-	X
56	MG	RA	3272	-	-	-	X
56	MG	RA	3273	-	-	-	X
56	MG	RA	3275	-	-	-	X
56	MG	RA	3276	-	-	-	X
56	MG	RA	3278	-	-	-	X
56	MG	RA	3279	-	-	-	X
56	MG	RA	3280	-	-	-	X
56	MG	RA	3282	-	-	-	X
56	MG	RA	3284	-	-	-	X
56	MG	RA	3286	-	-	-	X
56	MG	RA	3288	-	-	-	X
56	MG	RA	3290	-	-	-	X
56	MG	RA	3292	-	-	-	X
56	MG	RA	3294	-	-	-	X
56	MG	RA	3295	-	-	-	X
56	MG	RA	3296	-	-	-	X
56	MG	RA	3299	-	-	-	X
56	MG	RA	3300	-	-	-	X
56	MG	RA	3301	-	-	-	X
56	MG	RA	3303	-	-	-	X
56	MG	RA	3306	-	-	-	X
56	MG	RA	3307	-	-	-	X
56	MG	RA	3309	-	-	-	X
56	MG	RA	3310	-	-	-	X
56	MG	RA	3311	-	-	-	X
56	MG	RA	3314	-	-	-	X
56	MG	RA	3316	-	-	-	X
56	MG	RA	3317	-	-	-	X
56	MG	RA	3322	-	-	-	X
56	MG	RA	3323	-	-	-	X
56	MG	RA	3327	-	-	-	X
56	MG	RA	3332	-	-	-	X
56	MG	RA	3336	-	-	-	X
56	MG	RA	3337	-	-	-	X
56	MG	RA	3338	-	-	-	X
56	MG	RA	3339	-	-	-	X
56	MG	RA	3340	-	-	-	X
56	MG	RA	3341	-	-	-	X
56	MG	RA	3342	-	-	-	X
56	MG	RA	3352	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3353	-	-	-	X
56	MG	RA	3354	-	-	-	X
56	MG	RA	3359	-	-	-	X
56	MG	RA	3361	-	-	-	X
56	MG	RA	3362	-	-	-	X
56	MG	RA	3364	-	-	-	X
56	MG	RA	3365	-	-	-	X
56	MG	RA	3366	-	-	-	X
56	MG	RA	3367	-	-	-	X
56	MG	RA	3368	-	-	-	X
56	MG	RA	3369	-	-	-	X
56	MG	RA	3370	-	-	-	X
56	MG	RA	3371	-	-	-	X
56	MG	RA	3373	-	-	-	X
56	MG	RA	3374	-	-	-	X
56	MG	RA	3375	-	-	-	X
56	MG	RA	3376	-	-	-	X
56	MG	RA	3379	-	-	-	X
56	MG	RA	3388	-	-	-	X
56	MG	RA	3397	-	-	-	X
56	MG	RA	3398	-	-	-	X
56	MG	RA	3400	-	-	-	X
56	MG	RA	3401	-	-	-	X
56	MG	RA	3407	-	-	-	X
56	MG	RA	3411	-	-	-	X
56	MG	RA	3413	-	-	-	X
56	MG	RA	3422	-	-	-	X
56	MG	RA	3423	-	-	-	X
56	MG	RA	3425	-	-	-	X
56	MG	RA	3427	-	-	-	X
56	MG	RA	3428	-	-	-	X
56	MG	RA	3432	-	-	-	X
56	MG	RA	3433	-	-	-	X
56	MG	RA	3434	-	-	-	X
56	MG	RA	3435	-	-	-	X
56	MG	RA	3436	-	-	-	X
56	MG	RA	3437	-	-	-	X
56	MG	RA	3438	-	-	-	X
56	MG	RA	3440	-	-	-	X
56	MG	RA	3441	-	-	-	X
56	MG	RA	3442	-	-	-	X
56	MG	RA	3445	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3446	-	-	-	X
56	MG	RA	3447	-	-	-	X
56	MG	RA	3448	-	-	-	X
56	MG	RA	3449	-	-	-	X
56	MG	RA	3451	-	-	-	X
56	MG	RA	3454	-	-	-	X
56	MG	RA	3456	-	-	-	X
56	MG	RA	3458	-	-	-	X
56	MG	RA	3461	-	-	-	X
56	MG	RA	3462	-	-	-	X
56	MG	RA	3465	-	-	-	X
56	MG	RA	3467	-	-	-	X
56	MG	RA	3478	-	-	-	X
56	MG	RA	3481	-	-	-	X
56	MG	RA	3486	-	-	-	X
56	MG	RA	3487	-	-	-	X
56	MG	RA	3492	-	-	-	X
56	MG	RA	3494	-	-	-	X
56	MG	RA	3495	-	-	-	X
56	MG	RA	3498	-	-	-	X
56	MG	RA	3499	-	-	-	X
56	MG	RA	3500	-	-	-	X
56	MG	RA	3512	-	-	-	X
56	MG	RA	3513	-	-	-	X
56	MG	RA	3518	-	-	-	X
56	MG	RA	3519	-	-	-	X
56	MG	RA	3520	-	-	-	X
56	MG	RA	3521	-	-	-	X
56	MG	RA	3523	-	-	-	X
56	MG	RA	3524	-	-	-	X
56	MG	RA	3525	-	-	-	X
56	MG	RA	3526	-	-	-	X
56	MG	RA	3527	-	-	-	X
56	MG	RA	3528	-	-	-	X
56	MG	RA	3529	-	-	-	X
56	MG	RA	3531	-	-	-	X
56	MG	RA	3535	-	-	-	X
56	MG	RA	3536	-	-	-	X
56	MG	RA	3537	-	-	-	X
56	MG	RA	3538	-	-	-	X
56	MG	RA	3540	-	-	-	X
56	MG	RA	3542	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3543	-	-	-	X
56	MG	RA	3546	-	-	-	X
56	MG	RA	3547	-	-	-	X
56	MG	RA	3548	-	-	-	X
56	MG	RA	3550	-	-	-	X
56	MG	RA	3551	-	-	-	X
56	MG	RA	3552	-	-	-	X
56	MG	RA	3554	-	-	-	X
56	MG	RA	3555	-	-	-	X
56	MG	RA	3556	-	-	-	X
56	MG	RA	3557	-	-	-	X
56	MG	RA	3559	-	-	-	X
56	MG	RA	3560	-	-	-	X
56	MG	RA	3562	-	-	-	X
56	MG	RA	3564	-	-	-	X
56	MG	RA	3565	-	-	-	X
56	MG	RA	3566	-	-	-	X
56	MG	RA	3567	-	-	-	X
56	MG	RA	3568	-	-	-	X
56	MG	RA	3570	-	-	-	X
56	MG	RA	3572	-	-	-	X
56	MG	RA	3573	-	-	-	X
56	MG	RA	3576	-	-	-	X
56	MG	RA	3578	-	-	-	X
56	MG	RA	3579	-	-	-	X
56	MG	RA	3581	-	-	-	X
56	MG	RA	3582	-	-	-	X
56	MG	RA	3583	-	-	-	X
56	MG	RA	3584	-	-	-	X
56	MG	RA	3586	-	-	-	X
56	MG	RA	3587	-	-	-	X
56	MG	RA	3588	-	-	-	X
56	MG	RA	3590	-	-	-	X
56	MG	RA	3592	-	-	-	X
56	MG	RA	3595	-	-	-	X
56	MG	RA	3597	-	-	-	X
56	MG	RA	3599	-	-	-	X
56	MG	RA	3600	-	-	-	X
56	MG	RA	3601	-	-	-	X
56	MG	RA	3602	-	-	-	X
56	MG	RA	3603	-	-	-	X
56	MG	RA	3604	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3606	-	-	-	X
56	MG	RA	3608	-	-	-	X
56	MG	RA	3609	-	-	-	X
56	MG	RA	3611	-	-	-	X
56	MG	RA	3613	-	-	-	X
56	MG	RA	3615	-	-	-	X
56	MG	RA	3618	-	-	-	X
56	MG	RA	3621	-	-	-	X
56	MG	RA	3622	-	-	-	X
56	MG	RA	3626	-	-	-	X
56	MG	RA	3628	-	-	-	X
56	MG	RA	3629	-	-	-	X
56	MG	RA	3630	-	-	-	X
56	MG	RA	3631	-	-	-	X
56	MG	RA	3632	-	-	-	X
56	MG	RA	3633	-	-	-	X
56	MG	RA	3634	-	-	-	X
56	MG	RA	3635	-	-	-	X
56	MG	RA	3637	-	-	-	X
56	MG	RA	3639	-	-	-	X
56	MG	RA	3640	-	-	-	X
56	MG	RA	3642	-	-	-	X
56	MG	RA	3643	-	-	-	X
56	MG	RA	3644	-	-	-	X
56	MG	RA	3645	-	-	-	X
56	MG	RA	3647	-	-	-	X
56	MG	RA	3649	-	-	-	X
56	MG	RA	3653	-	-	-	X
56	MG	RA	3658	-	-	-	X
56	MG	RA	3660	-	-	-	X
56	MG	RA	3662	-	-	-	X
56	MG	RA	3663	-	-	-	X
56	MG	RA	3666	-	-	-	X
56	MG	RA	3668	-	-	-	X
56	MG	RA	3669	-	-	-	X
56	MG	RA	3670	-	-	-	X
56	MG	RA	3672	-	-	-	X
56	MG	RA	3675	-	-	-	X
56	MG	RA	3677	-	-	-	X
56	MG	RA	3681	-	-	-	X
56	MG	RA	3682	-	-	-	X
56	MG	RA	3684	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3685	-	-	-	X
56	MG	RA	3686	-	-	-	X
56	MG	RA	3688	-	-	-	X
56	MG	RA	3690	-	-	-	X
56	MG	RA	3691	-	-	-	X
56	MG	RA	3693	-	-	-	X
56	MG	RA	3694	-	-	-	X
56	MG	RA	3695	-	-	-	X
56	MG	RA	3696	-	-	-	X
56	MG	RA	3697	-	-	-	X
56	MG	RA	3698	-	-	-	X
56	MG	RA	3699	-	-	-	X
56	MG	RA	3700	-	-	-	X
56	MG	RA	3701	-	-	-	X
56	MG	RA	3703	-	-	-	X
56	MG	RA	3704	-	-	-	X
56	MG	RA	3705	-	-	-	X
56	MG	RA	3707	-	-	-	X
56	MG	RA	3708	-	-	-	X
56	MG	RA	3709	-	-	-	X
56	MG	RA	3710	-	-	-	X
56	MG	RA	3711	-	-	-	X
56	MG	RA	3712	-	-	-	X
56	MG	RA	3713	-	-	-	X
56	MG	RA	3721	-	-	-	X
56	MG	RA	3725	-	-	-	X
56	MG	RA	3727	-	-	-	X
56	MG	RA	3728	-	-	-	X
56	MG	RA	3729	-	-	-	X
56	MG	RA	3730	-	-	-	X
56	MG	RA	3732	-	-	-	X
56	MG	RA	3734	-	-	-	X
56	MG	RA	3735	-	-	-	X
56	MG	RA	3736	-	-	-	X
56	MG	RA	3737	-	-	-	X
56	MG	RA	3738	-	-	-	X
56	MG	RA	3741	-	-	-	X
56	MG	RA	3743	-	-	-	X
56	MG	RA	3745	-	-	-	X
56	MG	RA	3747	-	-	-	X
56	MG	RA	3748	-	-	-	X
56	MG	RA	3750	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3751	-	-	-	X
56	MG	RA	3752	-	-	-	X
56	MG	RA	3753	-	-	-	X
56	MG	RA	3755	-	-	-	X
56	MG	RA	3756	-	-	-	X
56	MG	RA	3758	-	-	-	X
56	MG	RA	3760	-	-	-	X
56	MG	RA	3764	-	-	-	X
56	MG	RA	3767	-	-	-	X
56	MG	RA	3769	-	-	-	X
56	MG	RA	3772	-	-	-	X
56	MG	RA	3775	-	-	-	X
56	MG	RA	3776	-	-	-	X
56	MG	RA	3778	-	-	-	X
56	MG	RA	3780	-	-	-	X
56	MG	RA	3781	-	-	-	X
56	MG	RA	3782	-	-	-	X
56	MG	RA	3783	-	-	-	X
56	MG	RA	3787	-	-	-	X
56	MG	RA	3788	-	-	-	X
56	MG	RA	3790	-	-	-	X
56	MG	RA	3791	-	-	-	X
56	MG	RA	3796	-	-	-	X
56	MG	RA	3797	-	-	-	X
56	MG	RA	3798	-	-	-	X
56	MG	RA	3799	-	-	-	X
56	MG	RA	3802	-	-	-	X
56	MG	RA	3803	-	-	-	X
56	MG	RA	3804	-	-	-	X
56	MG	RA	3805	-	-	-	X
56	MG	RA	3806	-	-	-	X
56	MG	RA	3807	-	-	-	X
56	MG	RA	3808	-	-	-	X
56	MG	RA	3809	-	-	-	X
56	MG	RA	3810	-	-	-	X
56	MG	RA	3811	-	-	-	X
56	MG	RA	3813	-	-	-	X
56	MG	RA	3817	-	-	-	X
56	MG	RA	3818	-	-	-	X
56	MG	RA	3819	-	-	-	X
56	MG	RA	3823	-	-	-	X
56	MG	RA	3824	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3825	-	-	-	X
56	MG	RA	3827	-	-	-	X
56	MG	RA	3828	-	-	-	X
56	MG	RA	3829	-	-	-	X
56	MG	RA	3830	-	-	-	X
56	MG	RA	3833	-	-	-	X
56	MG	RA	3835	-	-	-	X
56	MG	RA	3836	-	-	-	X
56	MG	RA	3837	-	-	-	X
56	MG	RA	3838	-	-	-	X
56	MG	RA	3840	-	-	-	X
56	MG	RA	3841	-	-	-	X
56	MG	RA	3843	-	-	-	X
56	MG	RA	3844	-	-	-	X
56	MG	RA	3845	-	-	-	X
56	MG	RA	3846	-	-	-	X
56	MG	RA	3847	-	-	-	X
56	MG	RA	3848	-	-	-	X
56	MG	RA	3849	-	-	-	X
56	MG	RA	3850	-	-	-	X
56	MG	RA	3854	-	-	-	X
56	MG	RA	3859	-	-	-	X
56	MG	RA	3860	-	-	-	X
56	MG	RA	3864	-	-	-	X
56	MG	RA	3869	-	-	-	X
56	MG	RA	3872	-	-	-	X
56	MG	RA	3873	-	-	-	X
56	MG	RA	3876	-	-	-	X
56	MG	RA	3879	-	-	-	X
56	MG	RA	3882	-	-	-	X
56	MG	RA	3883	-	-	-	X
56	MG	RA	3885	-	-	-	X
56	MG	RA	3886	-	-	-	X
56	MG	RA	3887	-	-	-	X
56	MG	RA	3888	-	-	-	X
56	MG	RA	3890	-	-	-	X
56	MG	RA	3892	-	-	-	X
56	MG	RA	3896	-	-	-	X
56	MG	RA	3897	-	-	-	X
56	MG	RA	3898	-	-	-	X
56	MG	RA	3899	-	-	-	X
56	MG	RA	3900	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3904	-	-	-	X
56	MG	RA	3908	-	-	-	X
56	MG	RA	3910	-	-	-	X
56	MG	RA	3913	-	-	-	X
56	MG	RA	3915	-	-	-	X
56	MG	RA	3917	-	-	-	X
56	MG	RA	3918	-	-	-	X
56	MG	RA	3919	-	-	-	X
56	MG	RA	3920	-	-	-	X
56	MG	RA	3922	-	-	-	X
56	MG	RA	3924	-	-	-	X
56	MG	RA	3926	-	-	-	X
56	MG	RA	3927	-	-	-	X
56	MG	RA	3931	-	-	-	X
56	MG	RA	3932	-	-	-	X
56	MG	RA	3933	-	-	-	X
56	MG	RA	3935	-	-	-	X
56	MG	RA	3937	-	-	-	X
56	MG	RA	3939	-	-	-	X
56	MG	RA	3940	-	-	-	X
56	MG	RA	3941	-	-	-	X
56	MG	RA	3942	-	-	-	X
56	MG	RA	3943	-	-	-	X
56	MG	RA	3944	-	-	-	X
56	MG	RA	3948	-	-	-	X
56	MG	RA	3949	-	-	-	X
56	MG	RA	3950	-	-	-	X
56	MG	RA	3951	-	-	-	X
56	MG	RA	3952	-	-	-	X
56	MG	RA	3955	-	-	-	X
56	MG	RA	3957	-	-	-	X
56	MG	RA	3958	-	-	-	X
56	MG	RA	3959	-	-	-	X
56	MG	RA	3960	-	-	-	X
56	MG	RA	3961	-	-	-	X
56	MG	RA	3962	-	-	-	X
56	MG	RA	3963	-	-	-	X
56	MG	RA	3964	-	-	-	X
56	MG	RA	3967	-	-	-	X
56	MG	RA	3968	-	-	-	X
56	MG	RA	3969	-	-	-	X
56	MG	RA	3970	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3977	-	-	-	X
56	MG	RA	3978	-	-	-	X
56	MG	RA	3979	-	-	-	X
56	MG	RA	3984	-	-	-	X
56	MG	RA	3988	-	-	-	X
56	MG	RA	3989	-	-	-	X
56	MG	RA	3990	-	-	-	X
56	MG	RA	3991	-	-	-	X
56	MG	RA	3993	-	-	-	X
56	MG	RA	3995	-	-	-	X
56	MG	RA	3996	-	-	-	X
56	MG	RA	3997	-	-	-	X
56	MG	RA	3999	-	-	-	X
56	MG	RA	4000	-	-	-	X
56	MG	RA	4003	-	-	-	X
56	MG	RA	4007	-	-	-	X
56	MG	RA	4008	-	-	-	X
56	MG	RA	4009	-	-	-	X
56	MG	RA	4010	-	-	-	X
56	MG	RA	4012	-	-	-	X
56	MG	RA	4013	-	-	-	X
56	MG	RA	4015	-	-	-	X
56	MG	RA	4016	-	-	-	X
56	MG	RA	4019	-	-	-	X
56	MG	RA	4020	-	-	-	X
56	MG	RA	4021	-	-	-	X
56	MG	RA	4024	-	-	-	X
56	MG	RA	4025	-	-	-	X
56	MG	RA	4028	-	-	-	X
56	MG	RA	4031	-	-	-	X
56	MG	RA	4032	-	-	-	X
56	MG	RA	4035	-	-	-	X
56	MG	RA	4037	-	-	-	X
56	MG	RA	4042	-	-	-	X
56	MG	RA	4043	-	-	-	X
56	MG	RA	4044	-	-	-	X
56	MG	RA	4046	-	-	-	X
56	MG	RA	4047	-	-	-	X
56	MG	RA	4048	-	-	-	X
56	MG	RA	4053	-	-	-	X
56	MG	RA	4054	-	-	-	X
56	MG	RA	4055	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	4057	-	-	-	X
56	MG	RA	4058	-	-	-	X
56	MG	RA	4061	-	-	-	X
56	MG	RA	4062	-	-	-	X
56	MG	RA	4063	-	-	-	X
56	MG	RA	4065	-	-	-	X
56	MG	RA	4068	-	-	-	X
56	MG	RA	4069	-	-	-	X
56	MG	RB	201	-	-	-	X
56	MG	RB	203	-	-	-	X
56	MG	RB	211	-	-	-	X
56	MG	RB	212	-	-	-	X
56	MG	RB	214	-	-	-	X
56	MG	RB	217	-	-	-	X
56	MG	RB	218	-	-	-	X
56	MG	RB	222	-	-	-	X
56	MG	RB	223	-	-	-	X
56	MG	RB	224	-	-	-	X
56	MG	RB	228	-	-	-	X
56	MG	RD	303	-	-	-	X
56	MG	RD	304	-	-	-	X
56	MG	RD	308	-	-	-	X
56	MG	RD	309	-	-	-	X
56	MG	RD	310	-	-	-	X
56	MG	RD	311	-	-	-	X
56	MG	RD	312	-	-	-	X
56	MG	RD	313	-	-	-	X
56	MG	RD	314	-	-	-	X
56	MG	RE	302	-	-	-	X
56	MG	RE	305	-	-	-	X
56	MG	RE	306	-	-	-	X
56	MG	RE	307	-	-	-	X
56	MG	RF	301	-	-	-	X
56	MG	RF	302	-	-	-	X
56	MG	RF	303	-	-	-	X
56	MG	RF	305	-	-	-	X
56	MG	RF	306	-	-	-	X
56	MG	RF	308	-	-	-	X
56	MG	RF	309	-	-	-	X
56	MG	RF	310	-	-	-	X
56	MG	RF	311	-	-	-	X
56	MG	RG	203	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RH	201	-	-	-	X
56	MG	RN	201	-	-	-	X
56	MG	RN	202	-	-	-	X
56	MG	RN	203	-	-	-	X
56	MG	RP	201	-	-	-	X
56	MG	RP	202	-	-	-	X
56	MG	RQ	202	-	-	-	X
56	MG	RQ	203	-	-	-	X
56	MG	RQ	204	-	-	-	X
56	MG	RR	201	-	-	-	X
56	MG	RR	202	-	-	-	X
56	MG	RR	203	-	-	-	X
56	MG	RR	204	-	-	-	X
56	MG	RT	202	-	-	-	X
56	MG	RT	203	-	-	-	X
56	MG	RU	202	-	-	-	X
56	MG	RV	202	-	-	-	X
56	MG	RV	203	-	-	-	X
56	MG	RW	201	-	-	-	X
56	MG	RW	202	-	-	-	X
56	MG	RZ	301	-	-	-	X
56	MG	XA	1601	-	-	-	X
56	MG	XA	1602	-	-	-	X
56	MG	XA	1604	-	-	-	X
56	MG	XA	1605	-	-	-	X
56	MG	XA	1608	-	-	-	X
56	MG	XA	1610	-	-	-	X
56	MG	XA	1611	-	-	-	X
56	MG	XA	1612	-	-	-	X
56	MG	XA	1616	-	-	-	X
56	MG	XA	1617	-	-	-	X
56	MG	XA	1619	-	-	-	X
56	MG	XA	1622	-	-	-	X
56	MG	XA	1623	-	-	-	X
56	MG	XA	1624	-	-	-	X
56	MG	XA	1625	-	-	-	X
56	MG	XA	1626	-	-	-	X
56	MG	XA	1627	-	-	-	X
56	MG	XA	1629	-	-	-	X
56	MG	XA	1631	-	-	-	X
56	MG	XA	1633	-	-	-	X
56	MG	XA	1638	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	XA	1640	-	-	-	X
56	MG	XA	1646	-	-	-	X
56	MG	XA	1649	-	-	-	X
56	MG	XA	1651	-	-	-	X
56	MG	XA	1652	-	-	-	X
56	MG	XA	1653	-	-	-	X
56	MG	XA	1655	-	-	-	X
56	MG	XA	1656	-	-	-	X
56	MG	XA	1657	-	-	-	X
56	MG	XA	1658	-	-	-	X
56	MG	XA	1661	-	-	-	X
56	MG	XA	1664	-	-	-	X
56	MG	XA	1667	-	-	-	X
56	MG	XA	1669	-	-	-	X
56	MG	XA	1672	-	-	-	X
56	MG	XA	1673	-	-	-	X
56	MG	XA	1674	-	-	-	X
56	MG	XA	1675	-	-	-	X
56	MG	XA	1676	-	-	-	X
56	MG	XA	1680	-	-	-	X
56	MG	XA	1682	-	-	-	X
56	MG	XA	1683	-	-	-	X
56	MG	XA	1684	-	-	-	X
56	MG	XA	1685	-	-	-	X
56	MG	XA	1686	-	-	-	X
56	MG	XA	1690	-	-	-	X
56	MG	XA	1693	-	-	-	X
56	MG	XA	1696	-	-	-	X
56	MG	XA	1698	-	-	-	X
56	MG	XA	1699	-	-	-	X
56	MG	XA	1701	-	-	-	X
56	MG	XA	1702	-	-	-	X
56	MG	XA	1703	-	-	-	X
56	MG	XA	1704	-	-	-	X
56	MG	XA	1711	-	-	-	X
56	MG	XA	1712	-	-	-	X
56	MG	XA	1714	-	-	-	X
56	MG	XA	1715	-	-	-	X
56	MG	XA	1716	-	-	-	X
56	MG	XA	1719	-	-	-	X
56	MG	XA	1720	-	-	-	X
56	MG	XA	1721	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	XA	1722	-	-	-	X
56	MG	XA	1725	-	-	-	X
56	MG	XA	1726	-	-	-	X
56	MG	XA	1728	-	-	-	X
56	MG	XA	1729	-	-	-	X
56	MG	XA	1730	-	-	-	X
56	MG	XA	1733	-	-	-	X
56	MG	XA	1740	-	-	-	X
56	MG	XA	1742	-	-	-	X
56	MG	XA	1743	-	-	-	X
56	MG	XA	1745	-	-	-	X
56	MG	XA	1748	-	-	-	X
56	MG	XA	1749	-	-	-	X
56	MG	XA	1750	-	-	-	X
56	MG	XA	1754	-	-	-	X
56	MG	XA	1755	-	-	-	X
56	MG	XA	1756	-	-	-	X
56	MG	XA	1765	-	-	-	X
56	MG	XA	1766	-	-	-	X
56	MG	XA	1767	-	-	-	X
56	MG	XA	1773	-	-	-	X
56	MG	XA	1775	-	-	-	X
56	MG	XA	1778	-	-	-	X
56	MG	XA	1779	-	-	-	X
56	MG	XA	1780	-	-	-	X
56	MG	XA	1782	-	-	-	X
56	MG	XA	1783	-	-	-	X
56	MG	XA	1786	-	-	-	X
56	MG	XA	1787	-	-	-	X
56	MG	XA	1788	-	-	-	X
56	MG	XA	1790	-	-	-	X
56	MG	XA	1792	-	-	-	X
56	MG	XA	1793	-	-	-	X
56	MG	XE	201	-	-	-	X
56	MG	XF	202	-	-	-	X
56	MG	XF	203	-	-	-	X
56	MG	XH	201	-	-	-	X
56	MG	XL	201	-	-	-	X
56	MG	XT	201	-	-	-	X
56	MG	XV	103	-	-	-	X
56	MG	XY	401	-	-	-	X
56	MG	Y0	101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	Y5	101	-	-	-	X
56	MG	Y6	102	-	-	-	X
56	MG	Y8	101	-	-	-	X
56	MG	Y8	102	-	-	-	X
56	MG	YA	3001	-	-	-	X
56	MG	YA	3005	-	-	-	X
56	MG	YA	3006	-	-	-	X
56	MG	YA	3008	-	-	-	X
56	MG	YA	3011	-	-	-	X
56	MG	YA	3013	-	-	-	X
56	MG	YA	3015	-	-	-	X
56	MG	YA	3016	-	-	-	X
56	MG	YA	3017	-	-	-	X
56	MG	YA	3018	-	-	-	X
56	MG	YA	3019	-	-	-	X
56	MG	YA	3022	-	-	-	X
56	MG	YA	3025	-	-	-	X
56	MG	YA	3026	-	-	-	X
56	MG	YA	3027	-	-	-	X
56	MG	YA	3028	-	-	-	X
56	MG	YA	3030	-	-	-	X
56	MG	YA	3032	-	-	-	X
56	MG	YA	3033	-	-	-	X
56	MG	YA	3035	-	-	-	X
56	MG	YA	3040	-	-	-	X
56	MG	YA	3041	-	-	-	X
56	MG	YA	3043	-	-	-	X
56	MG	YA	3047	-	-	-	X
56	MG	YA	3049	-	-	-	X
56	MG	YA	3050	-	-	-	X
56	MG	YA	3051	-	-	-	X
56	MG	YA	3056	-	-	-	X
56	MG	YA	3057	-	-	-	X
56	MG	YA	3058	-	-	-	X
56	MG	YA	3059	-	-	-	X
56	MG	YA	3061	-	-	-	X
56	MG	YA	3062	-	-	-	X
56	MG	YA	3063	-	-	-	X
56	MG	YA	3064	-	-	-	X
56	MG	YA	3069	-	-	-	X
56	MG	YA	3070	-	-	-	X
56	MG	YA	3074	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3075	-	-	-	X
56	MG	YA	3076	-	-	-	X
56	MG	YA	3078	-	-	-	X
56	MG	YA	3079	-	-	-	X
56	MG	YA	3082	-	-	-	X
56	MG	YA	3084	-	-	-	X
56	MG	YA	3086	-	-	-	X
56	MG	YA	3091	-	-	-	X
56	MG	YA	3092	-	-	-	X
56	MG	YA	3095	-	-	-	X
56	MG	YA	3102	-	-	-	X
56	MG	YA	3105	-	-	-	X
56	MG	YA	3106	-	-	-	X
56	MG	YA	3108	-	-	-	X
56	MG	YA	3109	-	-	-	X
56	MG	YA	3112	-	-	-	X
56	MG	YA	3113	-	-	-	X
56	MG	YA	3114	-	-	-	X
56	MG	YA	3116	-	-	-	X
56	MG	YA	3117	-	-	-	X
56	MG	YA	3118	-	-	-	X
56	MG	YA	3119	-	-	-	X
56	MG	YA	3120	-	-	-	X
56	MG	YA	3122	-	-	-	X
56	MG	YA	3123	-	-	-	X
56	MG	YA	3128	-	-	-	X
56	MG	YA	3129	-	-	-	X
56	MG	YA	3130	-	-	-	X
56	MG	YA	3131	-	-	-	X
56	MG	YA	3134	-	-	-	X
56	MG	YA	3137	-	-	-	X
56	MG	YA	3141	-	-	-	X
56	MG	YA	3143	-	-	-	X
56	MG	YA	3146	-	-	-	X
56	MG	YA	3147	-	-	-	X
56	MG	YA	3152	-	-	-	X
56	MG	YA	3153	-	-	-	X
56	MG	YA	3154	-	-	-	X
56	MG	YA	3156	-	-	-	X
56	MG	YA	3157	-	-	-	X
56	MG	YA	3161	-	-	-	X
56	MG	YA	3162	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3163	-	-	-	X
56	MG	YA	3164	-	-	-	X
56	MG	YA	3166	-	-	-	X
56	MG	YA	3167	-	-	-	X
56	MG	YA	3168	-	-	-	X
56	MG	YA	3170	-	-	-	X
56	MG	YA	3171	-	-	-	X
56	MG	YA	3173	-	-	-	X
56	MG	YA	3175	-	-	-	X
56	MG	YA	3177	-	-	-	X
56	MG	YA	3178	-	-	-	X
56	MG	YA	3179	-	-	-	X
56	MG	YA	3181	-	-	-	X
56	MG	YA	3182	-	-	-	X
56	MG	YA	3183	-	-	-	X
56	MG	YA	3185	-	-	-	X
56	MG	YA	3186	-	-	-	X
56	MG	YA	3190	-	-	-	X
56	MG	YA	3191	-	-	-	X
56	MG	YA	3192	-	-	-	X
56	MG	YA	3193	-	-	-	X
56	MG	YA	3194	-	-	-	X
56	MG	YA	3196	-	-	-	X
56	MG	YA	3197	-	-	-	X
56	MG	YA	3200	-	-	-	X
56	MG	YA	3202	-	-	-	X
56	MG	YA	3203	-	-	-	X
56	MG	YA	3205	-	-	-	X
56	MG	YA	3206	-	-	-	X
56	MG	YA	3208	-	-	-	X
56	MG	YA	3209	-	-	-	X
56	MG	YA	3211	-	-	-	X
56	MG	YA	3216	-	-	-	X
56	MG	YA	3218	-	-	-	X
56	MG	YA	3219	-	-	-	X
56	MG	YA	3220	-	-	-	X
56	MG	YA	3222	-	-	-	X
56	MG	YA	3223	-	-	-	X
56	MG	YA	3225	-	-	-	X
56	MG	YA	3226	-	-	-	X
56	MG	YA	3227	-	-	-	X
56	MG	YA	3228	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3230	-	-	-	X
56	MG	YA	3231	-	-	-	X
56	MG	YA	3233	-	-	-	X
56	MG	YA	3235	-	-	-	X
56	MG	YA	3236	-	-	-	X
56	MG	YA	3238	-	-	-	X
56	MG	YA	3239	-	-	-	X
56	MG	YA	3240	-	-	-	X
56	MG	YA	3242	-	-	-	X
56	MG	YA	3243	-	-	-	X
56	MG	YA	3244	-	-	-	X
56	MG	YA	3245	-	-	-	X
56	MG	YA	3246	-	-	-	X
56	MG	YA	3247	-	-	-	X
56	MG	YA	3248	-	-	-	X
56	MG	YA	3249	-	-	-	X
56	MG	YA	3251	-	-	-	X
56	MG	YA	3255	-	-	-	X
56	MG	YA	3257	-	-	-	X
56	MG	YA	3258	-	-	-	X
56	MG	YA	3259	-	-	-	X
56	MG	YA	3261	-	-	-	X
56	MG	YA	3262	-	-	-	X
56	MG	YA	3263	-	-	-	X
56	MG	YA	3265	-	-	-	X
56	MG	YA	3267	-	-	-	X
56	MG	YA	3269	-	-	-	X
56	MG	YA	3270	-	-	-	X
56	MG	YA	3278	-	-	-	X
56	MG	YA	3284	-	-	-	X
56	MG	YA	3289	-	-	-	X
56	MG	YA	3290	-	-	-	X
56	MG	YA	3291	-	-	-	X
56	MG	YA	3292	-	-	-	X
56	MG	YA	3293	-	-	-	X
56	MG	YA	3299	-	-	-	X
56	MG	YA	3300	-	-	-	X
56	MG	YA	3301	-	-	-	X
56	MG	YA	3306	-	-	-	X
56	MG	YA	3307	-	-	-	X
56	MG	YA	3308	-	-	-	X
56	MG	YA	3309	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3310	-	-	-	X
56	MG	YA	3311	-	-	-	X
56	MG	YA	3312	-	-	-	X
56	MG	YA	3313	-	-	-	X
56	MG	YA	3314	-	-	-	X
56	MG	YA	3317	-	-	-	X
56	MG	YA	3320	-	-	-	X
56	MG	YA	3323	-	-	-	X
56	MG	YA	3327	-	-	-	X
56	MG	YA	3333	-	-	-	X
56	MG	YA	3336	-	-	-	X
56	MG	YA	3338	-	-	-	X
56	MG	YA	3346	-	-	-	X
56	MG	YA	3348	-	-	-	X
56	MG	YA	3349	-	-	-	X
56	MG	YA	3350	-	-	-	X
56	MG	YA	3351	-	-	-	X
56	MG	YA	3353	-	-	-	X
56	MG	YA	3354	-	-	-	X
56	MG	YA	3357	-	-	-	X
56	MG	YA	3358	-	-	-	X
56	MG	YA	3361	-	-	-	X
56	MG	YA	3374	-	-	-	X
56	MG	YA	3376	-	-	-	X
56	MG	YA	3381	-	-	-	X
56	MG	YA	3385	-	-	-	X
56	MG	YA	3387	-	-	-	X
56	MG	YA	3389	-	-	-	X
56	MG	YA	3393	-	-	-	X
56	MG	YA	3394	-	-	-	X
56	MG	YA	3396	-	-	-	X
56	MG	YA	3397	-	-	-	X
56	MG	YA	3399	-	-	-	X
56	MG	YA	3406	-	-	-	X
56	MG	YA	3408	-	-	-	X
56	MG	YA	3409	-	-	-	X
56	MG	YA	3411	-	-	-	X
56	MG	YA	3412	-	-	-	X
56	MG	YA	3413	-	-	-	X
56	MG	YA	3414	-	-	-	X
56	MG	YA	3416	-	-	-	X
56	MG	YA	3418	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3421	-	-	-	X
56	MG	YA	3425	-	-	-	X
56	MG	YA	3427	-	-	-	X
56	MG	YA	3428	-	-	-	X
56	MG	YA	3431	-	-	-	X
56	MG	YA	3433	-	-	-	X
56	MG	YA	3435	-	-	-	X
56	MG	YA	3437	-	-	-	X
56	MG	YA	3438	-	-	-	X
56	MG	YA	3439	-	-	-	X
56	MG	YA	3441	-	-	-	X
56	MG	YA	3442	-	-	-	X
56	MG	YA	3445	-	-	-	X
56	MG	YA	3446	-	-	-	X
56	MG	YA	3447	-	-	-	X
56	MG	YA	3450	-	-	-	X
56	MG	YA	3451	-	-	-	X
56	MG	YA	3452	-	-	-	X
56	MG	YA	3455	-	-	-	X
56	MG	YA	3456	-	-	-	X
56	MG	YA	3457	-	-	-	X
56	MG	YA	3458	-	-	-	X
56	MG	YA	3461	-	-	-	X
56	MG	YA	3462	-	-	-	X
56	MG	YA	3463	-	-	-	X
56	MG	YA	3464	-	-	-	X
56	MG	YA	3465	-	-	-	X
56	MG	YA	3466	-	-	-	X
56	MG	YA	3467	-	-	-	X
56	MG	YA	3469	-	-	-	X
56	MG	YA	3470	-	-	-	X
56	MG	YA	3471	-	-	-	X
56	MG	YA	3472	-	-	-	X
56	MG	YA	3473	-	-	-	X
56	MG	YA	3474	-	-	-	X
56	MG	YA	3475	-	-	-	X
56	MG	YA	3477	-	-	-	X
56	MG	YA	3478	-	-	-	X
56	MG	YA	3481	-	-	-	X
56	MG	YA	3483	-	-	-	X
56	MG	YA	3484	-	-	-	X
56	MG	YA	3486	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3488	-	-	-	X
56	MG	YA	3493	-	-	-	X
56	MG	YA	3495	-	-	-	X
56	MG	YA	3496	-	-	-	X
56	MG	YA	3497	-	-	-	X
56	MG	YA	3499	-	-	-	X
56	MG	YA	3501	-	-	-	X
56	MG	YA	3504	-	-	-	X
56	MG	YA	3505	-	-	-	X
56	MG	YA	3506	-	-	-	X
56	MG	YA	3507	-	-	-	X
56	MG	YA	3509	-	-	-	X
56	MG	YA	3513	-	-	-	X
56	MG	YA	3515	-	-	-	X
56	MG	YA	3516	-	-	-	X
56	MG	YA	3518	-	-	-	X
56	MG	YA	3521	-	-	-	X
56	MG	YA	3522	-	-	-	X
56	MG	YA	3523	-	-	-	X
56	MG	YA	3524	-	-	-	X
56	MG	YA	3525	-	-	-	X
56	MG	YA	3528	-	-	-	X
56	MG	YA	3529	-	-	-	X
56	MG	YA	3530	-	-	-	X
56	MG	YA	3531	-	-	-	X
56	MG	YA	3541	-	-	-	X
56	MG	YA	3542	-	-	-	X
56	MG	YA	3544	-	-	-	X
56	MG	YA	3547	-	-	-	X
56	MG	YA	3548	-	-	-	X
56	MG	YA	3549	-	-	-	X
56	MG	YA	3551	-	-	-	X
56	MG	YA	3552	-	-	-	X
56	MG	YA	3553	-	-	-	X
56	MG	YA	3556	-	-	-	X
56	MG	YA	3557	-	-	-	X
56	MG	YA	3558	-	-	-	X
56	MG	YA	3561	-	-	-	X
56	MG	YA	3562	-	-	-	X
56	MG	YA	3566	-	-	-	X
56	MG	YA	3569	-	-	-	X
56	MG	YA	3574	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3580	-	-	-	X
56	MG	YA	3581	-	-	-	X
56	MG	YA	3582	-	-	-	X
56	MG	YA	3583	-	-	-	X
56	MG	YA	3586	-	-	-	X
56	MG	YA	3594	-	-	-	X
56	MG	YA	3595	-	-	-	X
56	MG	YA	3596	-	-	-	X
56	MG	YA	3599	-	-	-	X
56	MG	YA	3603	-	-	-	X
56	MG	YA	3604	-	-	-	X
56	MG	YA	3618	-	-	-	X
56	MG	YA	3619	-	-	-	X
56	MG	YA	3624	-	-	-	X
56	MG	YA	3625	-	-	-	X
56	MG	YA	3629	-	-	-	X
56	MG	YA	3631	-	-	-	X
56	MG	YA	3633	-	-	-	X
56	MG	YA	3635	-	-	-	X
56	MG	YA	3636	-	-	-	X
56	MG	YA	3637	-	-	-	X
56	MG	YA	3638	-	-	-	X
56	MG	YA	3640	-	-	-	X
56	MG	YA	3642	-	-	-	X
56	MG	YA	3644	-	-	-	X
56	MG	YA	3647	-	-	-	X
56	MG	YA	3649	-	-	-	X
56	MG	YA	3650	-	-	-	X
56	MG	YA	3651	-	-	-	X
56	MG	YA	3658	-	-	-	X
56	MG	YA	3659	-	-	-	X
56	MG	YA	3660	-	-	-	X
56	MG	YA	3662	-	-	-	X
56	MG	YA	3663	-	-	-	X
56	MG	YA	3666	-	-	-	X
56	MG	YA	3670	-	-	-	X
56	MG	YA	3672	-	-	-	X
56	MG	YA	3675	-	-	-	X
56	MG	YA	3678	-	-	-	X
56	MG	YA	3685	-	-	-	X
56	MG	YA	3687	-	-	-	X
56	MG	YA	3688	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3690	-	-	-	X
56	MG	YA	3691	-	-	-	X
56	MG	YA	3692	-	-	-	X
56	MG	YA	3693	-	-	-	X
56	MG	YA	3694	-	-	-	X
56	MG	YA	3695	-	-	-	X
56	MG	YA	3696	-	-	-	X
56	MG	YA	3697	-	-	-	X
56	MG	YA	3698	-	-	-	X
56	MG	YA	3699	-	-	-	X
56	MG	YA	3705	-	-	-	X
56	MG	YA	3706	-	-	-	X
56	MG	YA	3707	-	-	-	X
56	MG	YA	3708	-	-	-	X
56	MG	YA	3709	-	-	-	X
56	MG	YA	3710	-	-	-	X
56	MG	YA	3712	-	-	-	X
56	MG	YA	3713	-	-	-	X
56	MG	YA	3714	-	-	-	X
56	MG	YA	3715	-	-	-	X
56	MG	YA	3716	-	-	-	X
56	MG	YA	3717	-	-	-	X
56	MG	YA	3718	-	-	-	X
56	MG	YA	3720	-	-	-	X
56	MG	YA	3721	-	-	-	X
56	MG	YA	3722	-	-	-	X
56	MG	YA	3723	-	-	-	X
56	MG	YA	3724	-	-	-	X
56	MG	YA	3728	-	-	-	X
56	MG	YA	3731	-	-	-	X
56	MG	YA	3734	-	-	-	X
56	MG	YA	3735	-	-	-	X
56	MG	YA	3736	-	-	-	X
56	MG	YA	3739	-	-	-	X
56	MG	YA	3741	-	-	-	X
56	MG	YA	3747	-	-	-	X
56	MG	YA	3749	-	-	-	X
56	MG	YA	3751	-	-	-	X
56	MG	YA	3752	-	-	-	X
56	MG	YA	3756	-	-	-	X
56	MG	YB	201	-	-	-	X
56	MG	YB	204	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YB	205	-	-	-	X
56	MG	YB	206	-	-	-	X
56	MG	YB	208	-	-	-	X
56	MG	YB	209	-	-	-	X
56	MG	YB	210	-	-	-	X
56	MG	YB	212	-	-	-	X
56	MG	YB	213	-	-	-	X
56	MG	YD	301	-	-	-	X
56	MG	YD	302	-	-	-	X
56	MG	YD	303	-	-	-	X
56	MG	YD	305	-	-	-	X
56	MG	YD	307	-	-	-	X
56	MG	YD	309	-	-	-	X
56	MG	YE	301	-	-	-	X
56	MG	YE	302	-	-	-	X
56	MG	YE	303	-	-	-	X
56	MG	YE	305	-	-	-	X
56	MG	YE	306	-	-	-	X
56	MG	YF	301	-	-	-	X
56	MG	YG	201	-	-	-	X
56	MG	YN	201	-	-	-	X
56	MG	YO	201	-	-	-	X
56	MG	YQ	202	-	-	-	X
56	MG	YR	201	-	-	-	X
56	MG	YT	201	-	-	-	X
56	MG	YT	202	-	-	-	X
56	MG	YT	203	-	-	-	X
56	MG	YV	201	-	-	-	X
56	MG	YW	201	-	-	-	X
56	MG	YW	202	-	-	-	X
56	MG	YX	101	-	-	-	X
57	ZN	R4	101	-	-	-	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 296497 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	YI	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			
8	RI	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

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

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

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

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

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

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y4	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R4	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

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

- Molecule 28 is a protein called 50S ribosomal protein L33.

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

- Molecule 29 is a protein called 50S ribosomal protein L34.

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

- Molecule 30 is a protein called 50S ribosomal protein L35.

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

- Molecule 31 is a protein called 50S ribosomal protein L36.

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

- Molecule 32 is a RNA chain called 16S rRNA.

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

- Molecule 33 is a protein called 30S ribosomal protein S2.

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

- Molecule 34 is a protein called 30S ribosomal protein S3.

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

- Molecule 35 is a protein called 30S ribosomal protein S4.

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

- Molecule 36 is a protein called 30S ribosomal protein S5.

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

- Molecule 37 is a protein called 30S ribosomal protein S6.

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

- Molecule 38 is a protein called 30S ribosomal protein S7.

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

- Molecule 39 is a protein called 30S ribosomal protein S8.

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

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	XI	126	Total	C	N	O	0	0	0
			966	613	186	167			
40	QI	127	Total	C	N	O	0	0	0
			986	625	193	168			

- Molecule 41 is a protein called 30S ribosomal protein S10.

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

- Molecule 42 is a protein called 30S ribosomal protein S11.

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

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

- Molecule 43 is a protein called 30S ribosomal protein S12.

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

- Molecule 44 is a protein called 30S ribosomal protein S13.

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

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 46 is a protein called 30S ribosomal protein S15.

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

- Molecule 47 is a protein called 30S ribosomal protein S16.

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

- Molecule 48 is a protein called 30S ribosomal protein S17.

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

- Molecule 49 is a protein called 30S ribosomal protein S18.

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

- Molecule 50 is a protein called 30S ribosomal protein S19.

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

- Molecule 51 is a protein called 30S ribosomal protein S20.

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

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

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

- Molecule 53 is a RNA chain called P-site tRNA fMet.

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

- Molecule 54 is a protein called Peptide chain release factor 2.

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

There are 32 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
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
QY	298	VAL	LEU	conflict	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
XY	298	VAL	LEU	conflict	UNP P07012

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	XX	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			
55	QX	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	280	Total	Mg	0	0
			280	280		
56	YV	1	Total	Mg	0	0
			1	1		
56	RP	2	Total	Mg	0	0
			2	2		
56	R7	2	Total	Mg	0	0
			2	2		
56	YA	756	Total	Mg	0	0
			756	756		
56	Y5	1	Total	Mg	0	0
			1	1		
56	YR	1	Total	Mg	0	0
			1	1		
56	RT	3	Total	Mg	0	0
			3	3		
56	QD	4	Total	Mg	0	0
			4	4		
56	RN	3	Total	Mg	0	0
			3	3		
56	XE	2	Total	Mg	0	0
			2	2		
56	RG	4	Total	Mg	0	0
			4	4		
56	Y1	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	YD	9	Total 9	Mg 9	0	0
56	QV	4	Total 4	Mg 4	0	0
56	RX	1	Total 1	Mg 1	0	0
56	Y8	2	Total 2	Mg 2	0	0
56	YO	2	Total 2	Mg 2	0	0
56	XA	193	Total 193	Mg 193	0	0
56	QI	1	Total 1	Mg 1	0	0
56	RQ	4	Total 4	Mg 4	0	0
56	R0	4	Total 4	Mg 4	0	0
56	XT	1	Total 1	Mg 1	0	0
56	QR	1	Total 1	Mg 1	0	0
56	QL	2	Total 2	Mg 2	0	0
56	RU	3	Total 3	Mg 3	0	0
56	QG	3	Total 3	Mg 3	0	0
56	RO	1	Total 1	Mg 1	0	0
56	XJ	1	Total 1	Mg 1	0	0
56	QO	1	Total 1	Mg 1	0	0
56	Y0	1	Total 1	Mg 1	0	0
56	YG	3	Total 3	Mg 3	0	0
56	XY	1	Total 1	Mg 1	0	0
56	YQ	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	YN	1	Total 1	Mg 1	0	0
56	XF	3	Total 3	Mg 3	0	0
56	YX	1	Total 1	Mg 1	0	0
56	RR	4	Total 4	Mg 4	0	0
56	RD	14	Total 14	Mg 14	0	0
56	R1	4	Total 4	Mg 4	0	0
56	Y7	1	Total 1	Mg 1	0	0
56	YT	3	Total 3	Mg 3	0	0
56	RV	4	Total 4	Mg 4	0	0
56	QF	1	Total 1	Mg 1	0	0
56	RH	2	Total 2	Mg 2	0	0
56	XK	1	Total 1	Mg 1	0	0
56	QH	2	Total 2	Mg 2	0	0
56	QQ	2	Total 2	Mg 2	0	0
56	RA	1069	Total 1069	Mg 1069	0	0
56	R4	1	Total 1	Mg 1	0	0
56	YF	3	Total 3	Mg 3	0	0
56	YP	1	Total 1	Mg 1	0	0
56	RZ	1	Total 1	Mg 1	0	0
56	QB	1	Total 1	Mg 1	0	0
56	QM	1	Total 1	Mg 1	0	0

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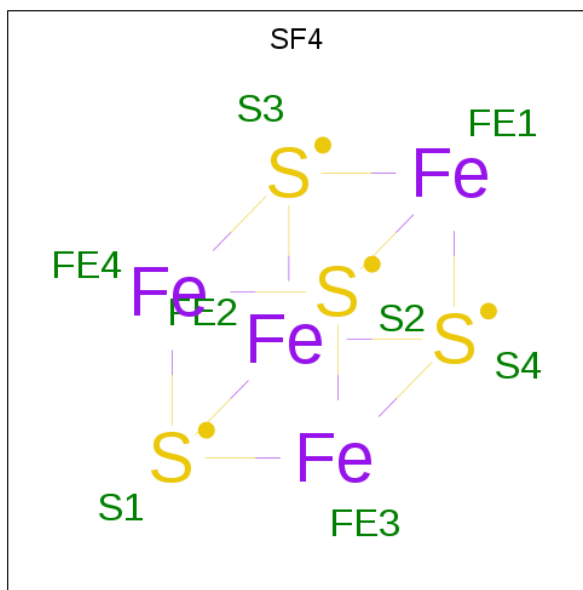
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	R9	2	Total	Mg	0	0
			2	2		
56	RE	7	Total	Mg	0	0
			7	7		
56	XL	1	Total	Mg	0	0
			1	1		
56	YB	19	Total	Mg	0	0
			19	19		
56	QT	1	Total	Mg	0	0
			1	1		
56	QN	2	Total	Mg	0	0
			2	2		
56	Y6	1	Total	Mg	0	0
			1	1		
56	YW	2	Total	Mg	0	0
			2	2		
56	RW	2	Total	Mg	0	0
			2	2		
56	QY	2	Total	Mg	0	0
			2	2		
56	XH	1	Total	Mg	0	0
			1	1		
56	XV	3	Total	Mg	0	0
			3	3		
56	RB	28	Total	Mg	0	0
			28	28		
56	YI	1	Total	Mg	0	0
			1	1		
56	QE	2	Total	Mg	0	0
			2	2		
56	R5	4	Total	Mg	0	0
			4	4		
56	R8	1	Total	Mg	0	0
			1	1		
56	RF	11	Total	Mg	0	0
			11	11		
56	R3	2	Total	Mg	0	0
			2	2		
56	YE	7	Total	Mg	0	0
			7	7		

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

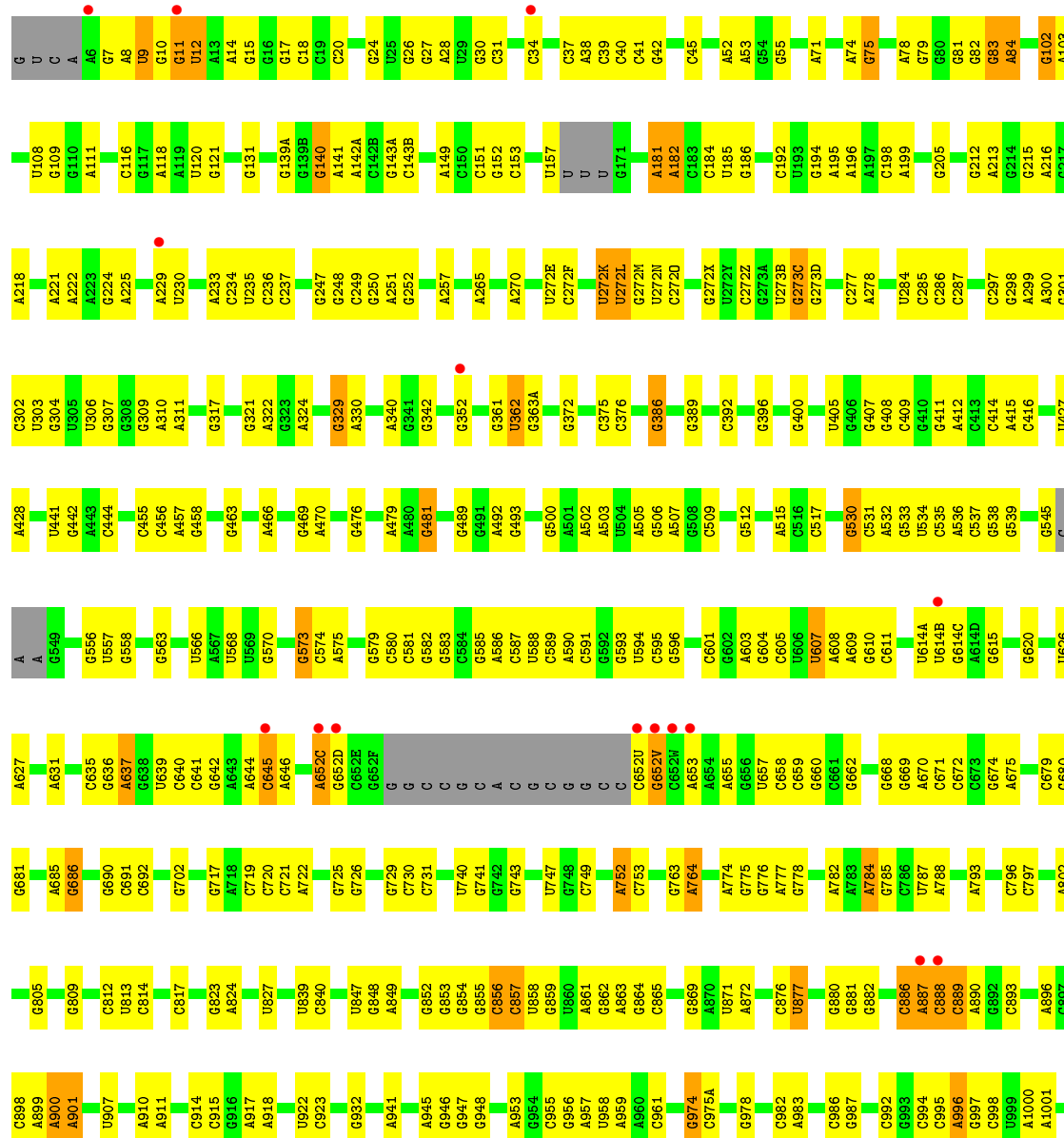
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	Y9	1	Total Zn 1 1	0	0
57	QN	1	Total Zn 1 1	0	0
57	Y6	1	Total Zn 1 1	0	0
57	XN	1	Total Zn 1 1	0	0
57	R9	1	Total Zn 1 1	0	0
57	Y4	1	Total Zn 1 1	0	0
57	R6	1	Total Zn 1 1	0	0
57	Y5	1	Total Zn 1 1	0	0
57	R5	1	Total Zn 1 1	0	0
57	YY	1	Total Zn 1 1	0	0
57	R4	1	Total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

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

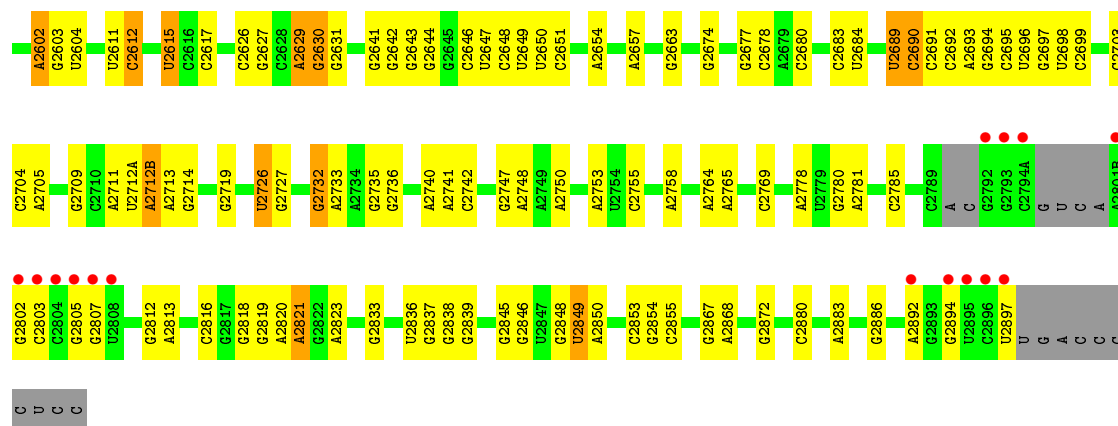


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	XD	1	Total 8	Fe 4	S 4	0	0
58	QD	1	Total 8	Fe 4	S 4	0	0

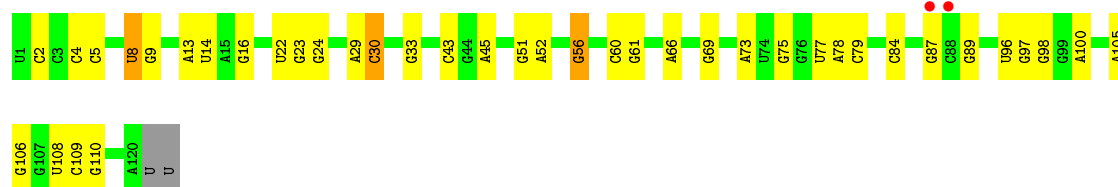




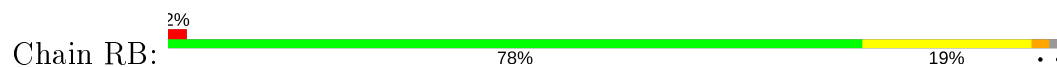
G2489	G2375	U2262	G2159	G2002	A1853	A1741	C1582	C1445B	G1310	G1171	U1078	G1005
G2490	A2376	A2266	G2160	G2010	A1854	G1747B	A1583	C1446	U1313	G	C1079	G1006
U2491	A2267	A2267	G2161	G2100	U1864	G1747B	C1584	C1447	U1314	A	U1080	U1012
G2383	G2268	A2268	C2162	G2101	U1865	U1756	A1586	G1448	U1315	U	U1081	C1013
C2385	A2269	A2269	C2163	U2102	G1865	U1757	C1587	G1449	U1316	G	U1082	
			G2165	C2103	A1876	U1758	C1588	G1450A	A1317	A	U1083	
			G2166	G2104	A1877	G1758	C1589	U1453		G1178	A1084	G1017
			U2167	C2020	A1878		A1596	G1455			A1085	C1018
			G2168	G2106	G1878	A1762	A1608	G1459	A1322		A1086	U1019
			A2169	C2107	A1889	G1764	A1609	A1460	U1323		G1087	A1020
			A2170	G2108	A1899	G1764	A1610		U1340		A1088	A1021
			A2171	C2024	G1899	A1773	A1614	C1467	U1341		G1089	G1024
			U2172	G2025	A1900	C1774	A1614	A1471	U1341		G1090	G1025
			A2173	C2026	G1906				U1352		C1092	U1026
			C2174	A2030	G1906	U1779	U1629	A1471	U1353		C1093	A1028
			C2175	G2032	C1914	A1780	U1630	C1474	A1353		U1094	A1029
			A2176	A2033	U1915	G1781	C1631A	G1475	G1355		A1095	
			C2177	G2033	A1916	C1782	C1636	C1476			A1096	U1033
			C2178	C2043	A1916	A1783	C1637		A1359		U1097	
			U2180	U2047	G1929	A1784	C1638		A1210		U1101	G1034
			G2182	G2048	G1930	A1786	C1638	G1482	U1211		C1102	U1035
			C2183		G1935	A1791	C1640	C1493	G1212		A1103	G1036
				A2081	A1936			U1497	A1220		C1104	C1041
			G2186	G2081	A1937	U1794	G1647	A1507	G1223		G1106	
			G2187	C2055	A1938	C1795	C1648	C1508	G1226		A1045	G1046
			U2188	G2056	U1939	U1796	C1656	A1509A	A1384		G1109	G1047
			G2190	A2059	G1942	C1797	C1657	A1509B	G1236		A1110	A1048
			C2191	G2060	G1945	U1798	C1658		G1250		A1111	C1049
			G2192	G2061	U1946	G1799	C1659	U1514	C1251		G1112	A1050
			A2198	C2062	C1947	A1801	A1669	G1515	C1252		G1113	
			G2206	C2063	G1948	A1802			G1388		G1114	C1052
			G2207	G2064	G1949	A1803	G1674	G1529	A1253		G1125	
			A2208	C2065	G1950	G1804		C1530	G1256		A1054	A1054
			U2218	C2066	U1951	U1805	C1531	C1531	A1395		G1055	
			G2223	G2069	A1952	G1811	C1532	C1532	U1396		U1130	G1056
			G2224	G2070	U1955	A1812	G1686	U	U1263		G1131	A1057
			A2225	G2071	G1963	A1812	G1687	A	G1264		A1132	G1058
			G2233	G2072	G1964	A1815	U1688	C1536	A1265		U1133	G1059
			G2234	G2073	G1967	A1816	A1689		G1266		G1135	U1060
			G2238	C2074	U1967	G1817	G1686	A1542	G1271		G1136	U
			G2239	U2074	U1963	A1824	A1700	C1543	A1272		G1139	G1062
			U2243	U2075	G1964	G1824	A1701	C1546	U1273		C1140	C1064
			U2244	A2077	G1967	G1827	U1709		G1418		U1141	U1065
			G2246	G2078	A1970	G1828	A1568		A1278		U1142A	U1066
			G2247	C2080	A1971	A1829	A1566		G1279		A1142B	A1067
			A2248	C2081	A1972	C1710	A1567		U1292		A1143	G1068
			G2249	A2082	U1991	C1712	A1569		C1293		G1144	A1069
			C2248	U2086	G1992	G1719	U1720		G1296		C1153	G1071
			U2249	G2087	U1993	G1721	U1722		U1300		G1154	A1072
			G2250	C2088	G1997	A1847	A1578		A1301		G1164	G1074
				U2096	A2001	A1848	A1579		A1302		U1165	C1075
							U1739		G1444		C1166	C1076
							G1740		A1445A		U1167	A1077



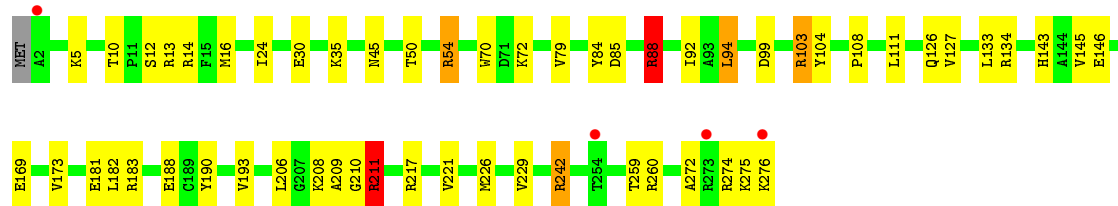
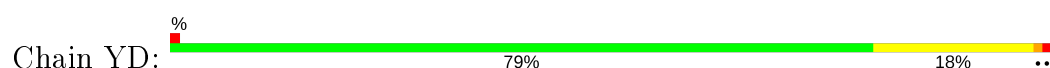
- Molecule 2: 5S rRNA



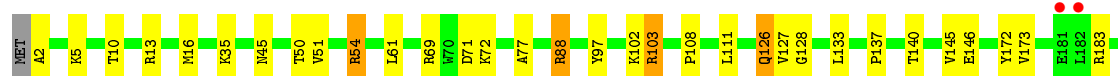
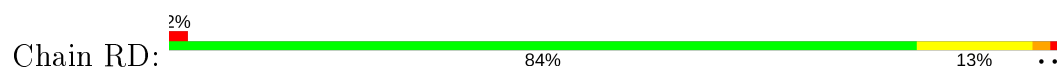
- Molecule 2: 5S rRNA

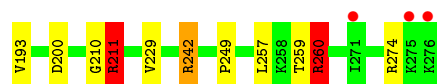


- Molecule 3: 50S ribosomal protein L2

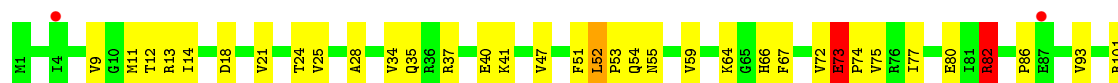
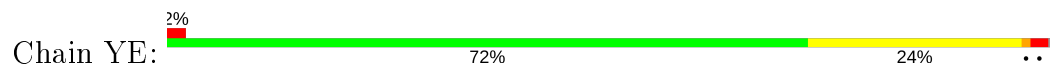


- Molecule 3: 50S ribosomal protein L2

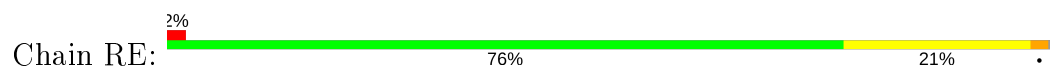




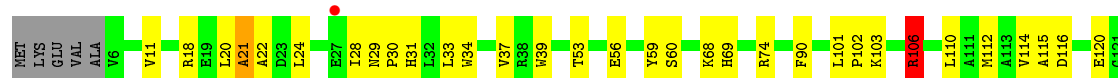
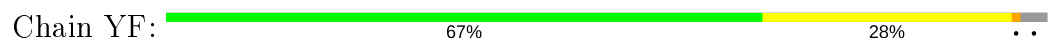
- Molecule 4: 50S ribosomal protein L3



- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4

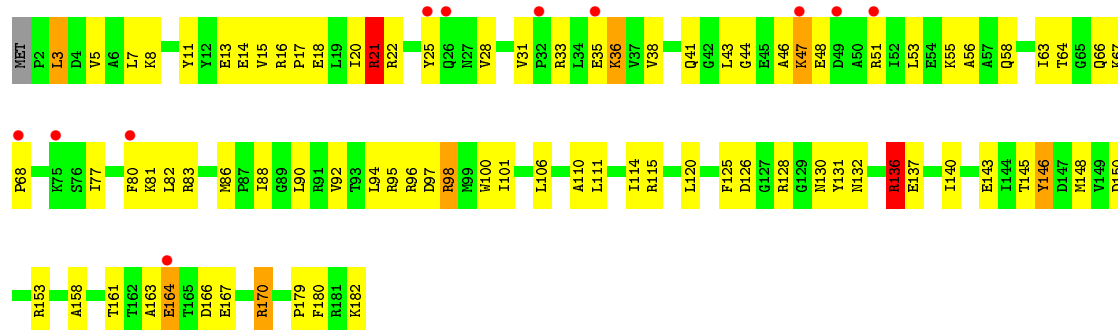


- Molecule 5: 50S ribosomal protein L4

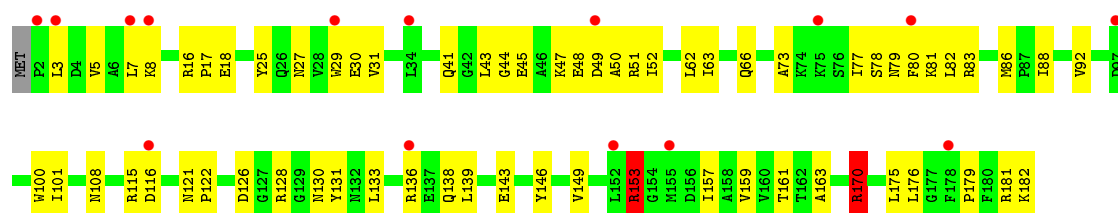


- Molecule 6: 50S ribosomal protein L5

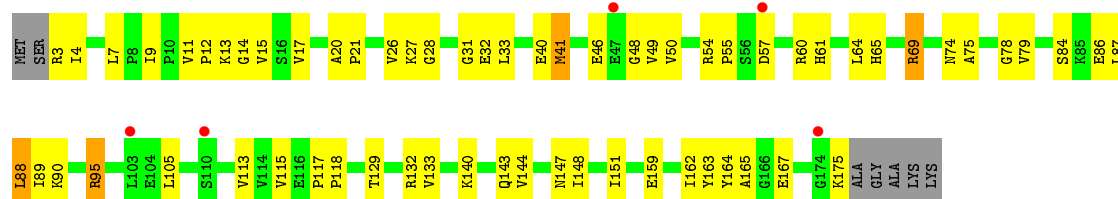




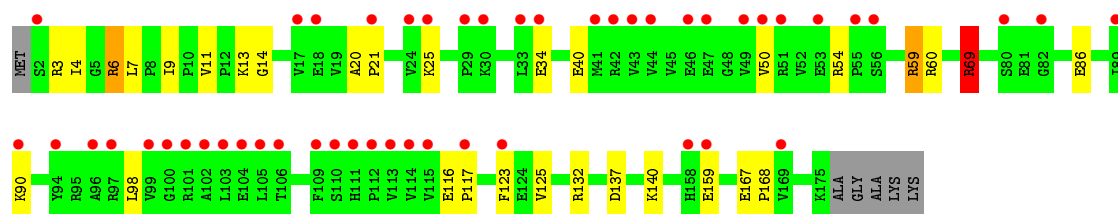
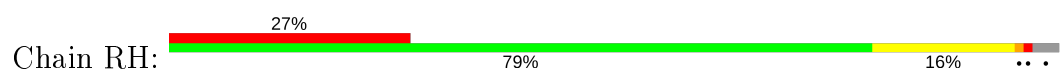
• Molecule 6: 50S ribosomal protein L5



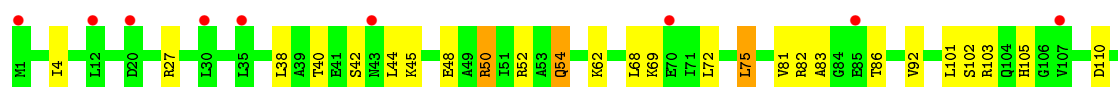
• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6

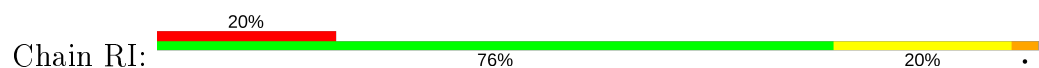


• Molecule 8: 50S ribosomal protein L9

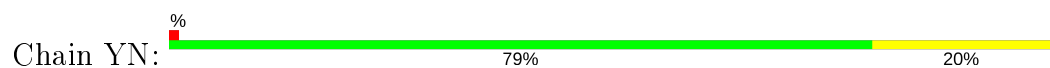




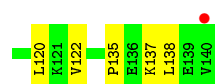
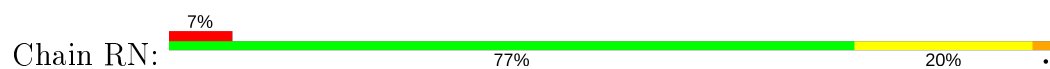
- Molecule 8: 50S ribosomal protein L9



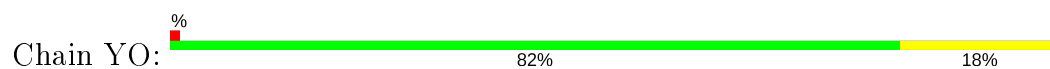
- Molecule 9: 50S ribosomal protein L13



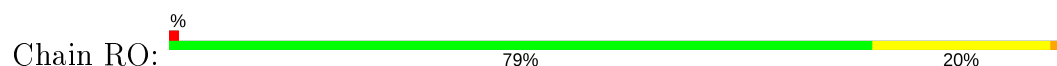
- Molecule 9: 50S ribosomal protein L13



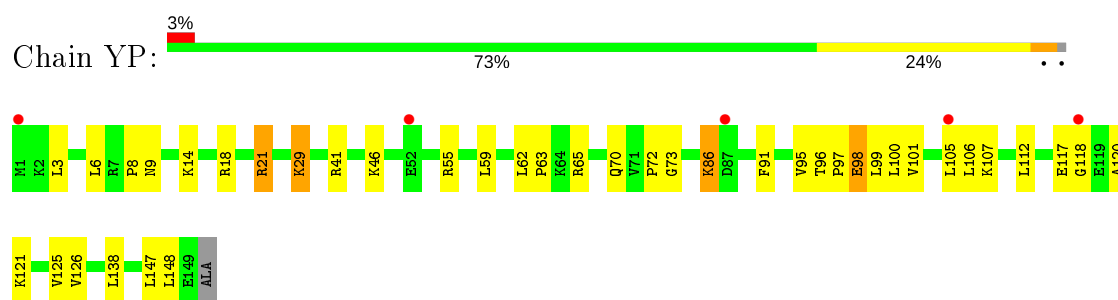
- Molecule 10: 50S ribosomal protein L14



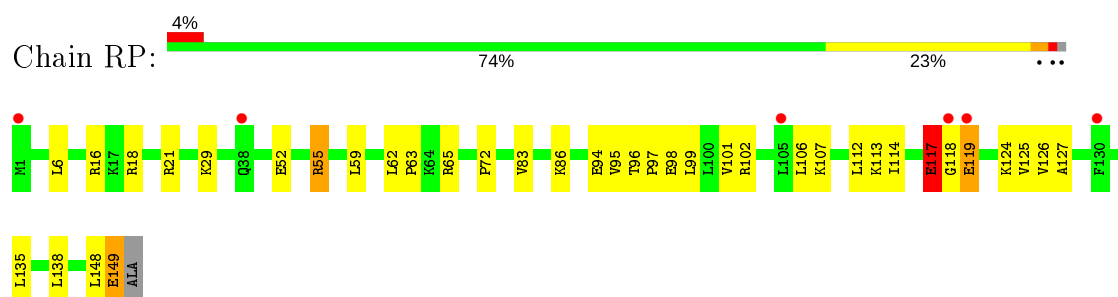
- Molecule 10: 50S ribosomal protein L14



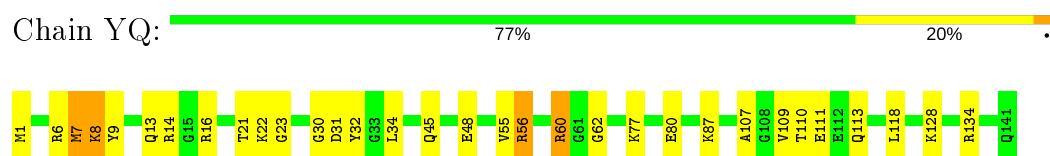
- Molecule 11: 50S ribosomal protein L15



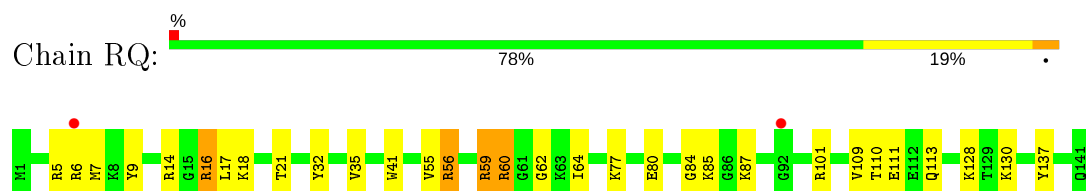
- Molecule 11: 50S ribosomal protein L15



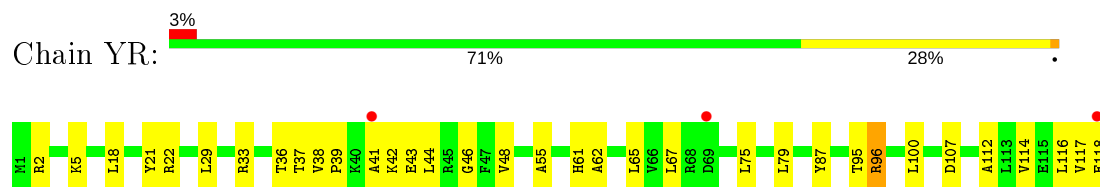
- Molecule 12: 50S ribosomal protein L16



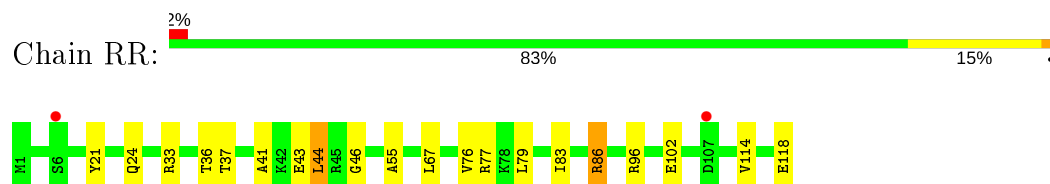
- Molecule 12: 50S ribosomal protein L16



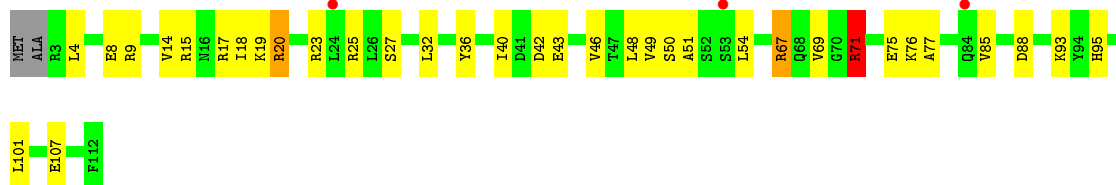
- Molecule 13: 50S ribosomal protein L17



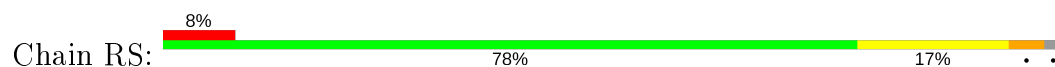
- Molecule 13: 50S ribosomal protein L17



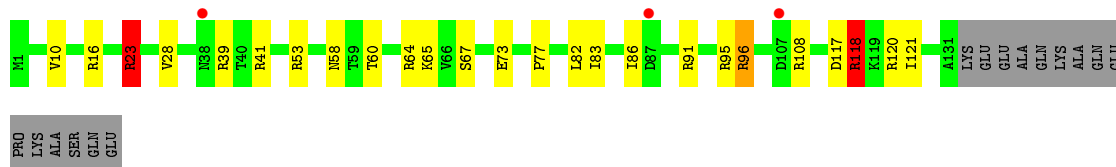
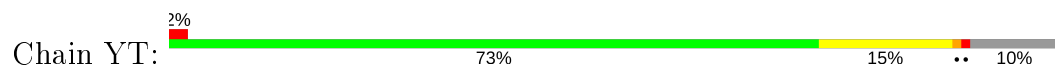
- Molecule 14: 50S ribosomal protein L18



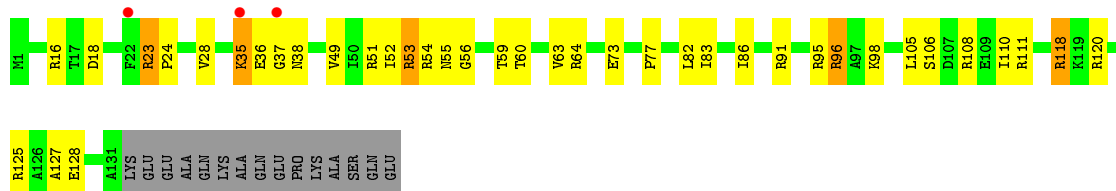
- Molecule 14: 50S ribosomal protein L18



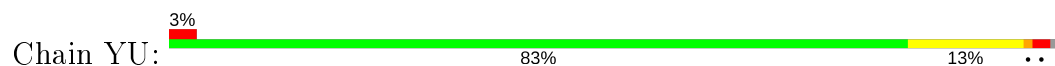
- Molecule 15: 50S ribosomal protein L19



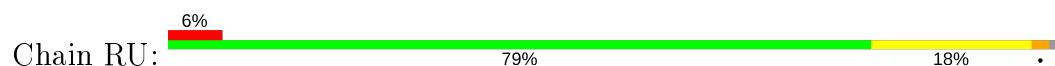
- Molecule 15: 50S ribosomal protein L19

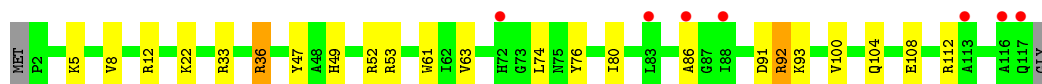


- Molecule 16: 50S ribosomal protein L20

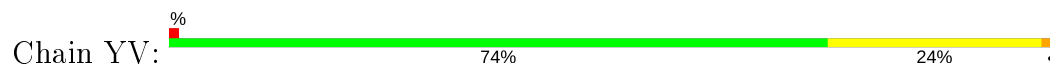


- Molecule 16: 50S ribosomal protein L20

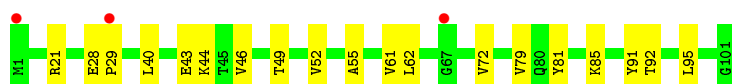
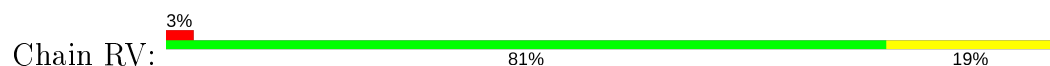




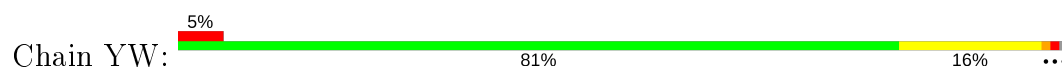
- Molecule 17: 50S ribosomal protein L21



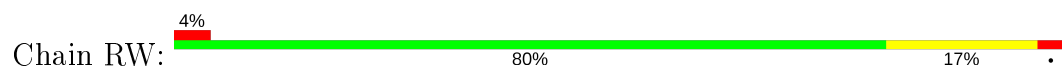
- Molecule 17: 50S ribosomal protein L21



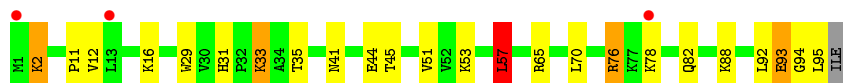
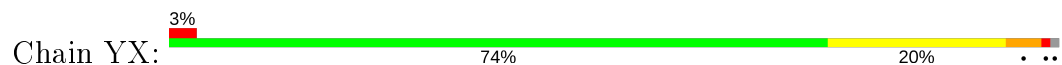
- Molecule 18: 50S ribosomal protein L22



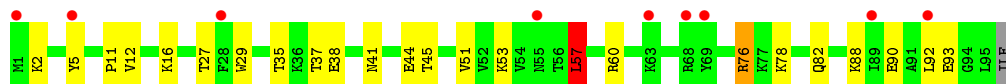
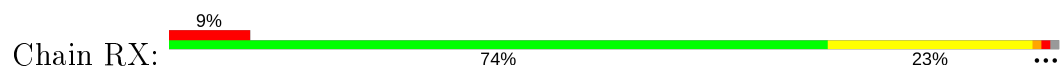
- Molecule 18: 50S ribosomal protein L22



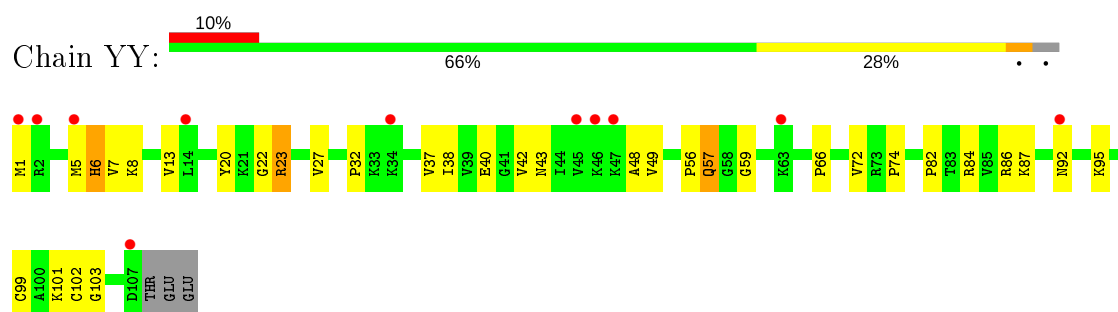
- Molecule 19: 50S ribosomal protein L23



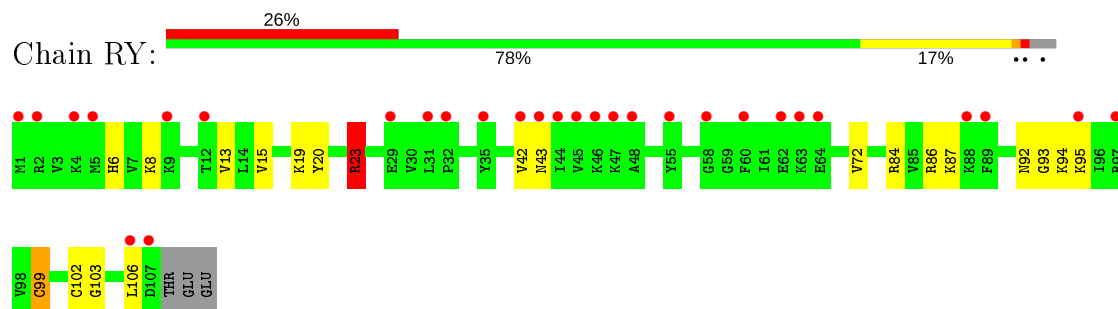
- Molecule 19: 50S ribosomal protein L23



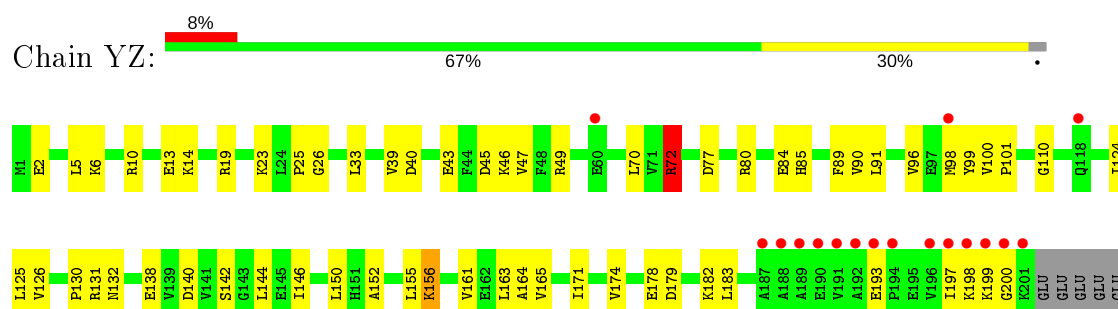
- Molecule 20: 50S ribosomal protein L24



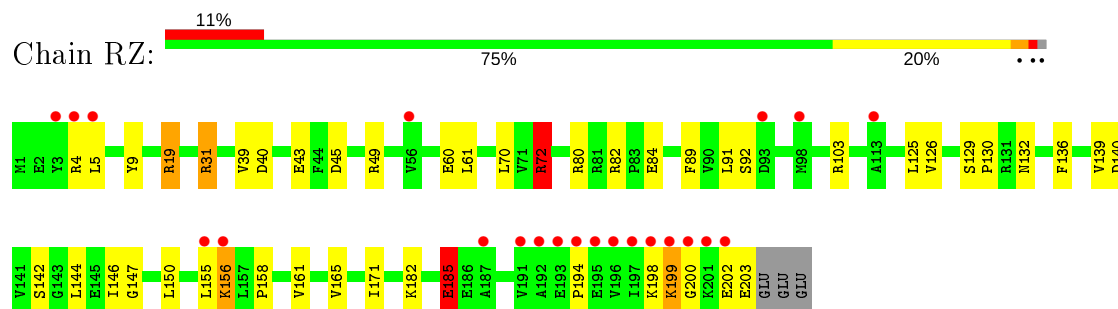
- Molecule 20: 50S ribosomal protein L24



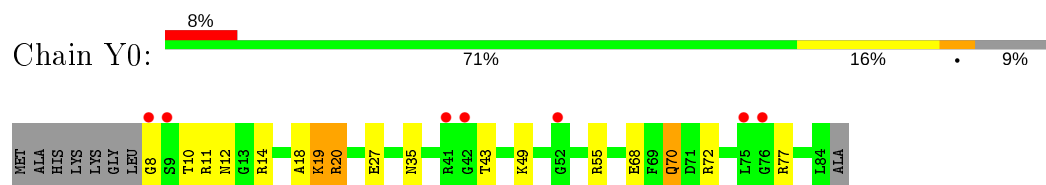
- Molecule 21: 50S ribosomal protein L25



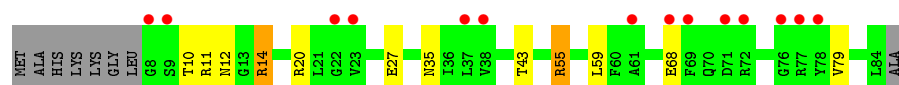
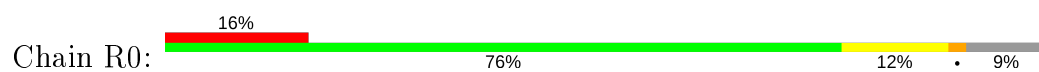
- Molecule 21: 50S ribosomal protein L25



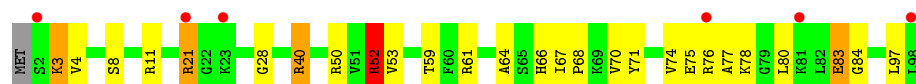
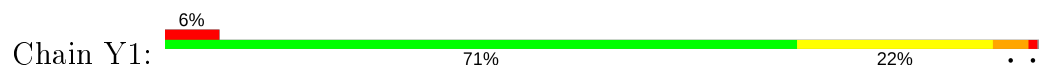
- Molecule 22: 50S ribosomal protein L27



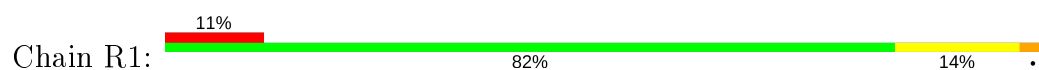
- Molecule 22: 50S ribosomal protein L27



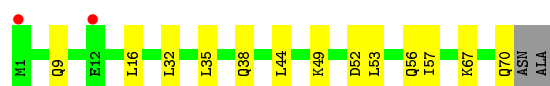
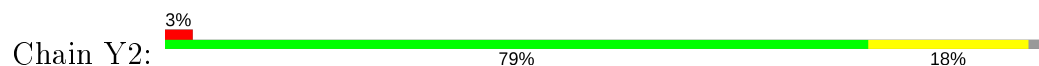
- Molecule 23: 50S ribosomal protein L28



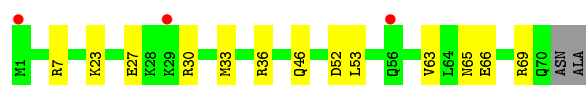
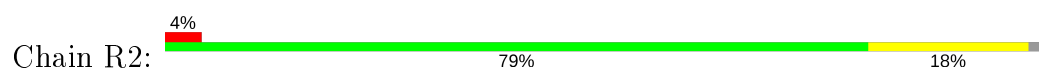
- Molecule 23: 50S ribosomal protein L28



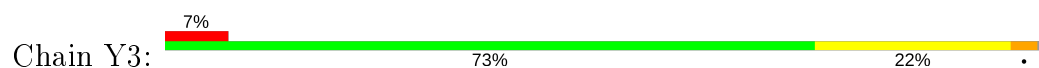
- Molecule 24: 50S ribosomal protein L29



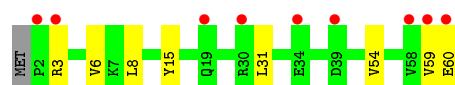
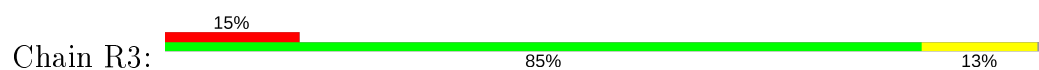
- Molecule 24: 50S ribosomal protein L29



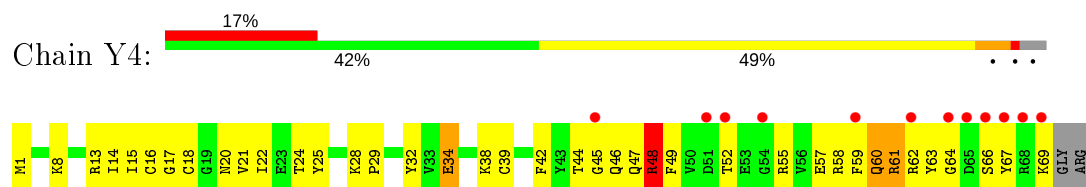
- Molecule 25: 50S ribosomal protein L30



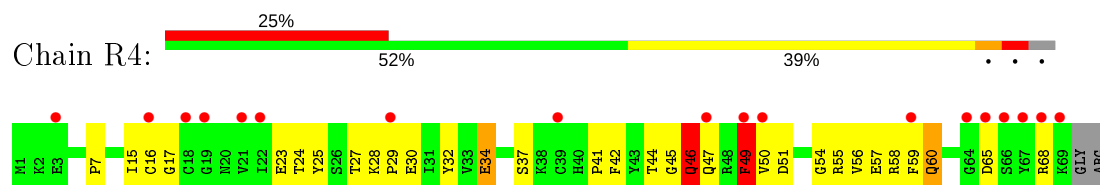
- Molecule 25: 50S ribosomal protein L30



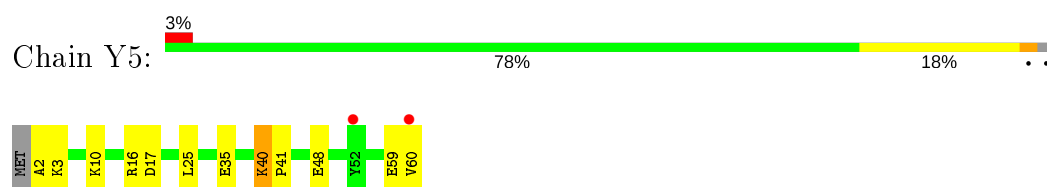
• Molecule 26: 50S ribosomal protein L31



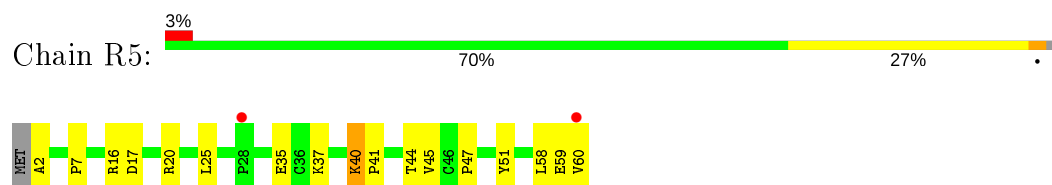
• Molecule 26: 50S ribosomal protein L31



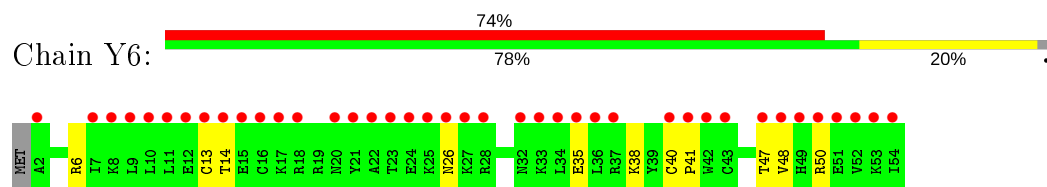
• Molecule 27: 50S ribosomal protein L32



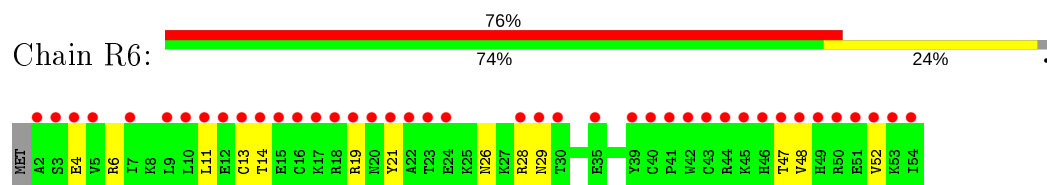
• Molecule 27: 50S ribosomal protein L32



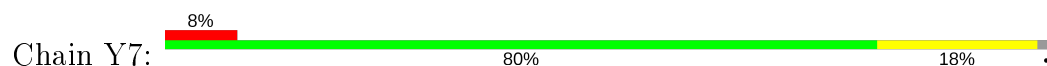
• Molecule 28: 50S ribosomal protein L33



• Molecule 28: 50S ribosomal protein L33

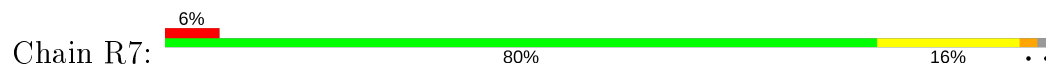


• Molecule 29: 50S ribosomal protein L34





- Molecule 29: 50S ribosomal protein L34



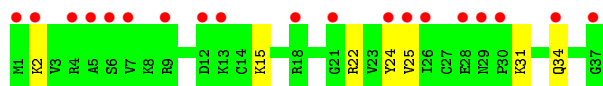
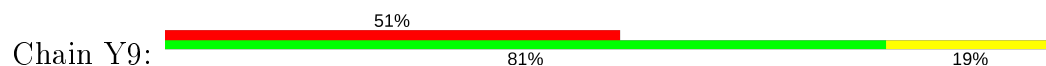
- Molecule 30: 50S ribosomal protein L35



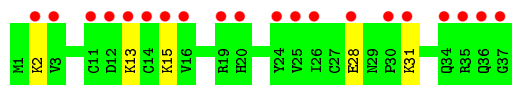
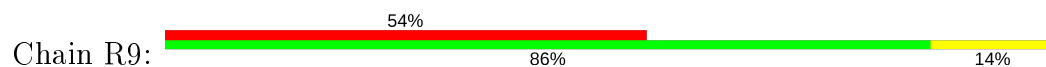
- Molecule 30: 50S ribosomal protein L35



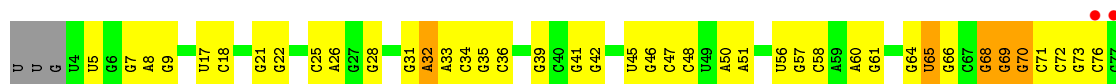
- Molecule 31: 50S ribosomal protein L36

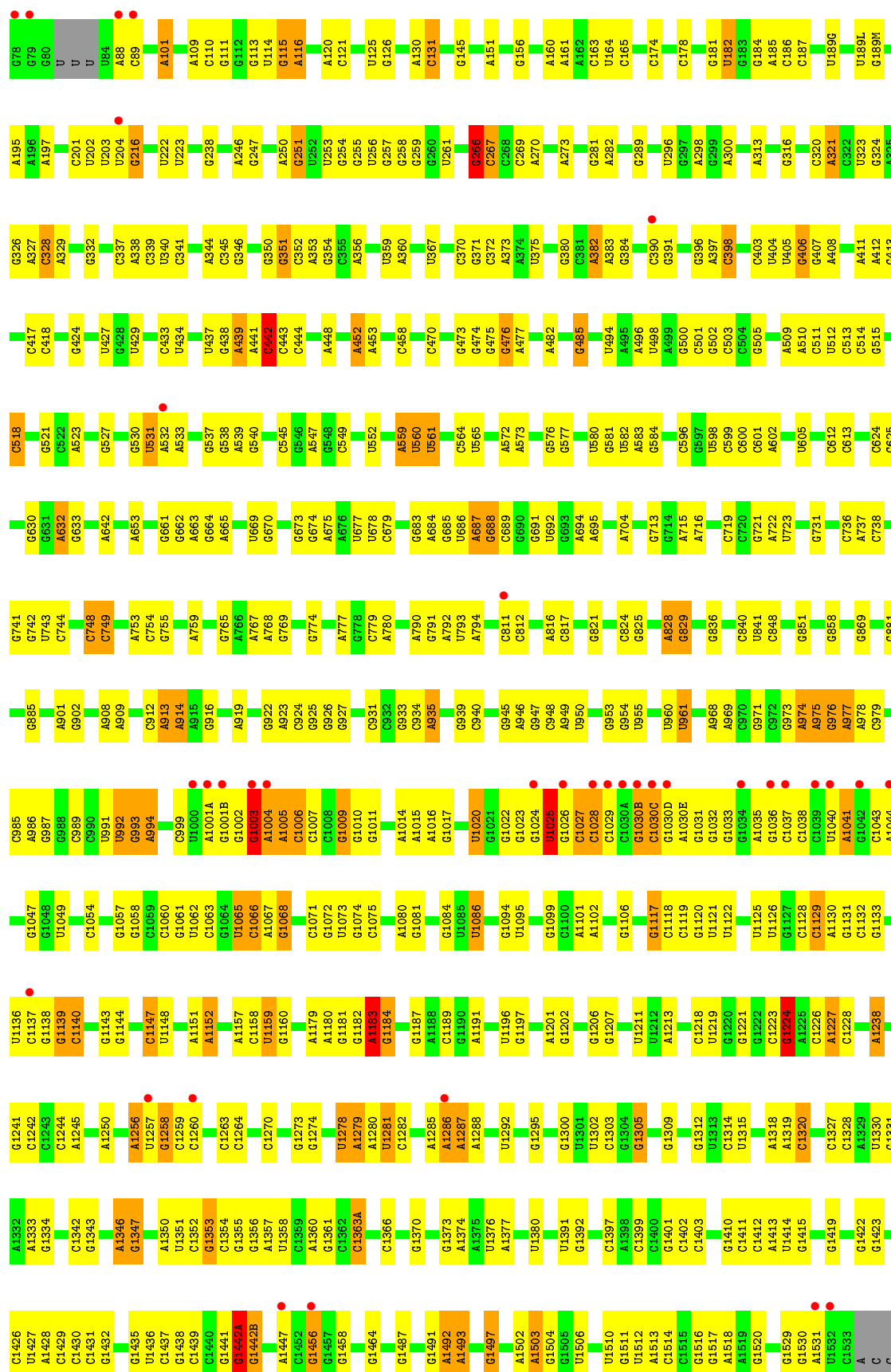


- Molecule 31: 50S ribosomal protein L36



- Molecule 32: 16S rRNA

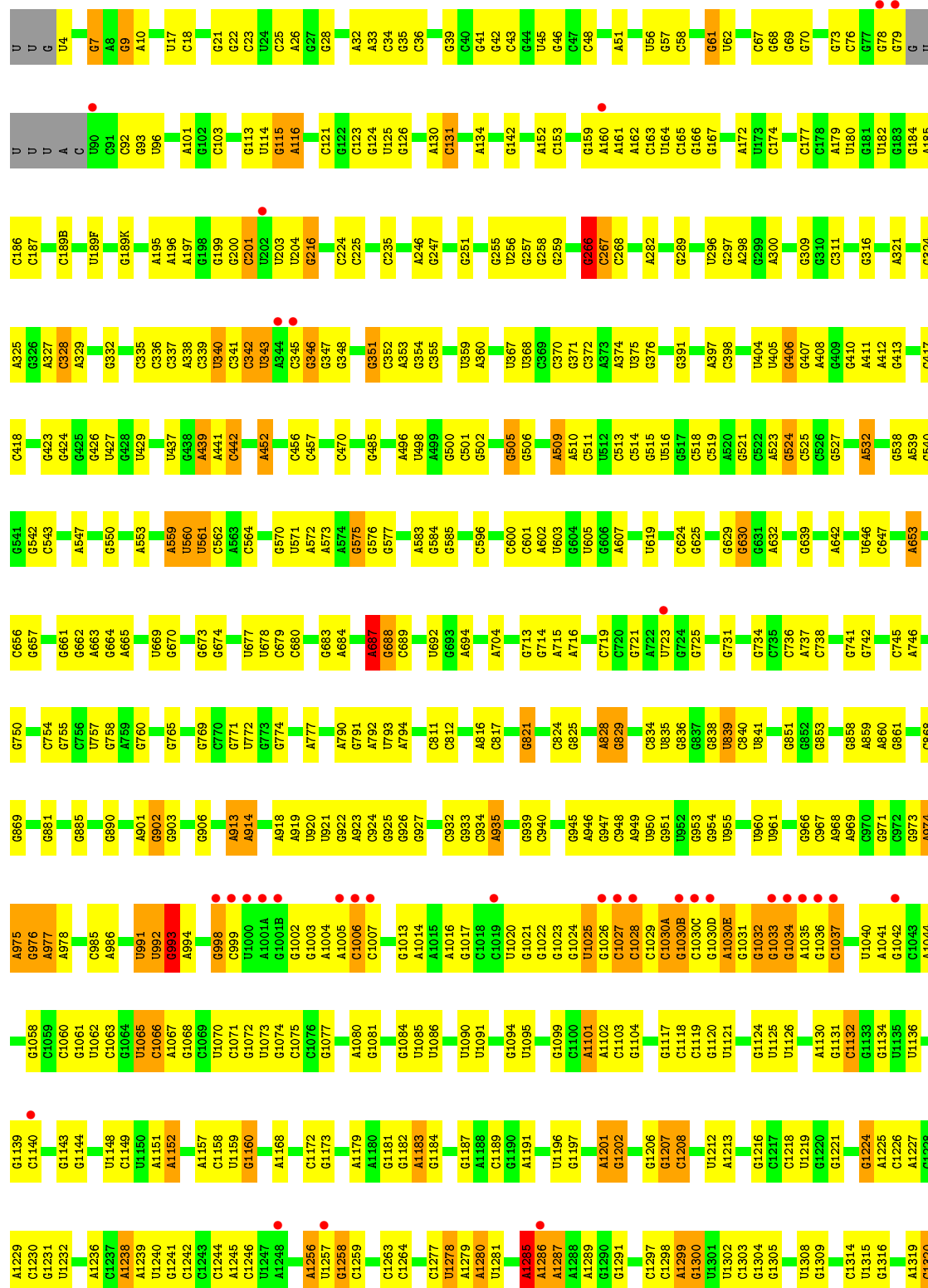


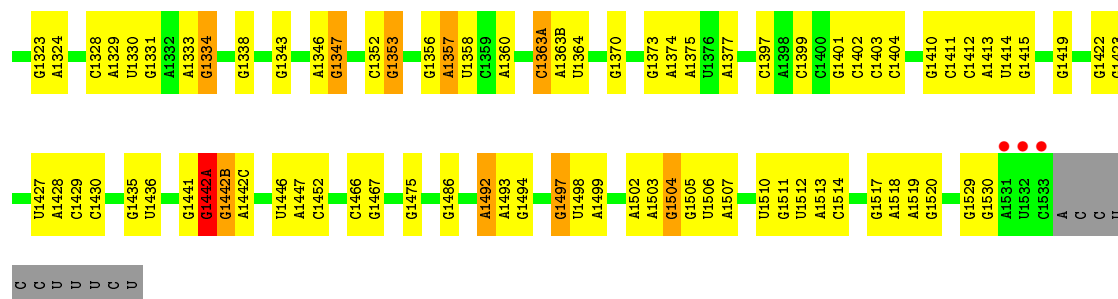


U C C U U C D

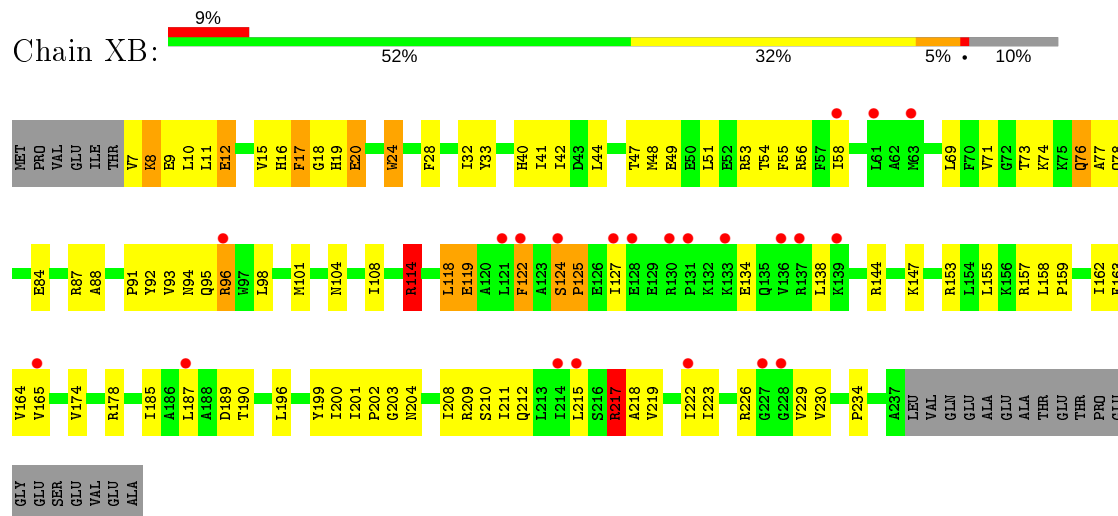
● Molecule 32: 16S rRNA

Chain QA: 29% 58% 35% 6%

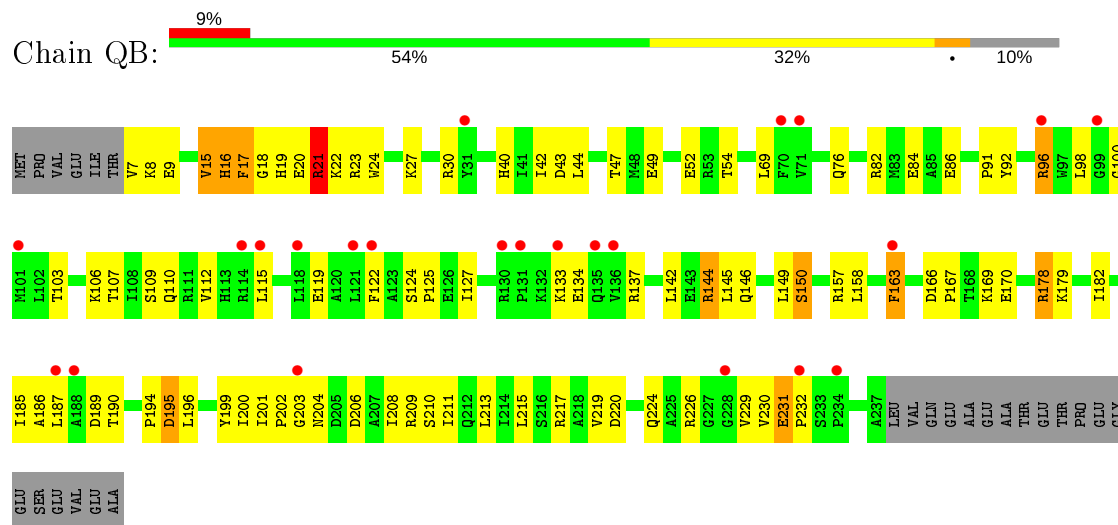




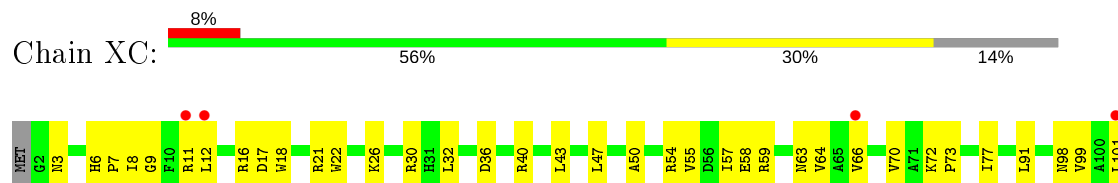
• Molecule 33: 30S ribosomal protein S2

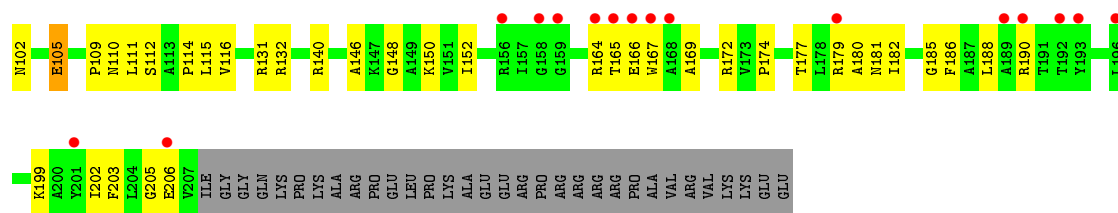


• Molecule 33: 30S ribosomal protein S2

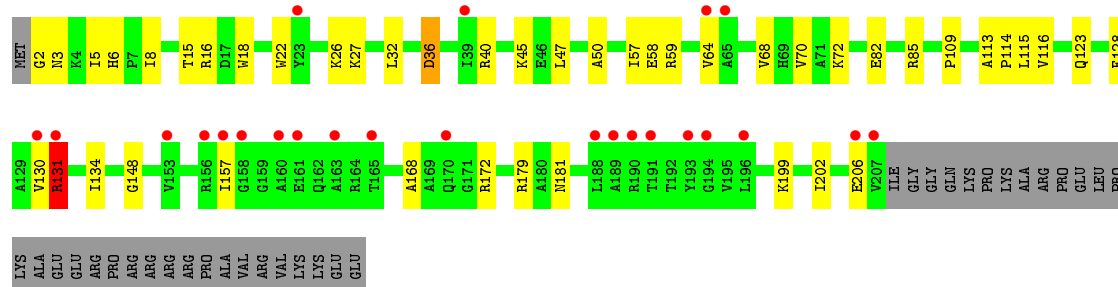


• Molecule 34: 30S ribosomal protein S3

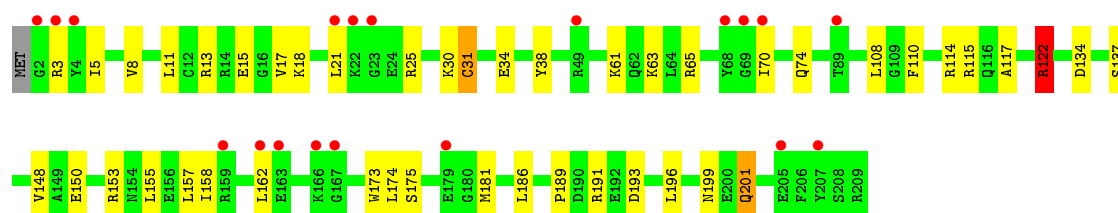
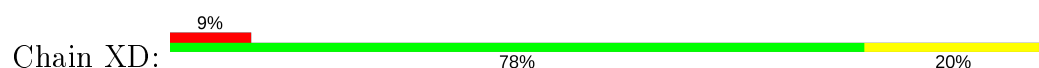




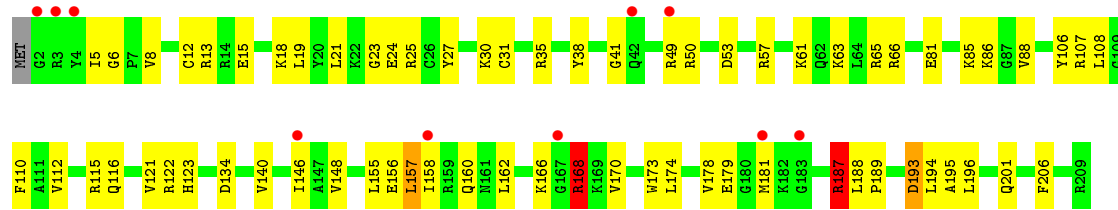
• Molecule 34: 30S ribosomal protein S3



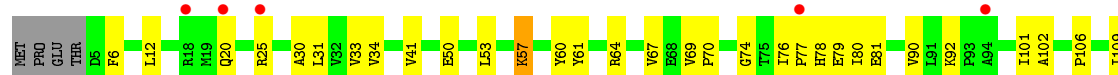
• Molecule 35: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S4

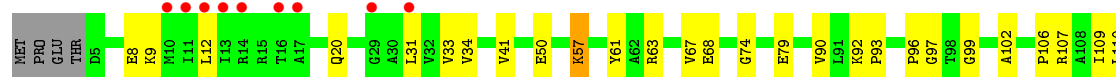


• Molecule 36: 30S ribosomal protein S5

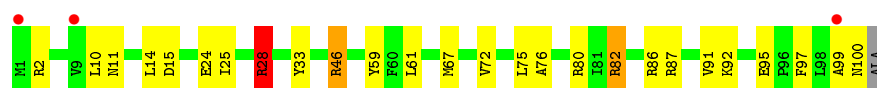
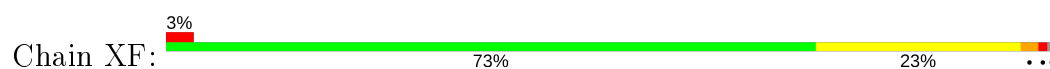




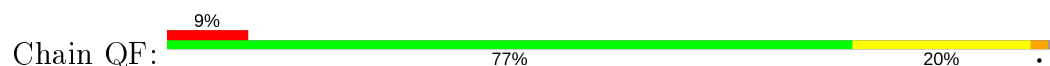
- Molecule 36: 30S ribosomal protein S5



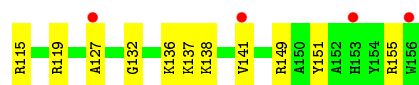
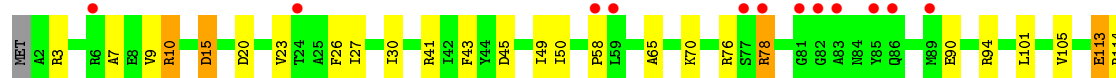
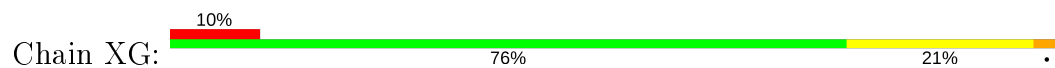
- Molecule 37: 30S ribosomal protein S6



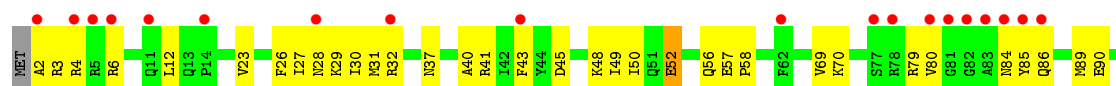
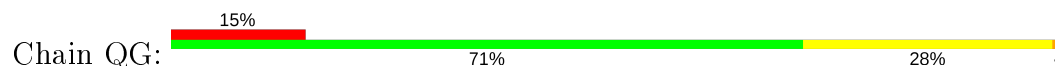
- Molecule 37: 30S ribosomal protein S6

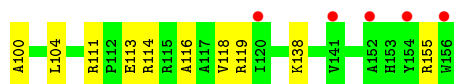


- Molecule 38: 30S ribosomal protein S7

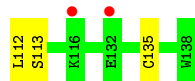
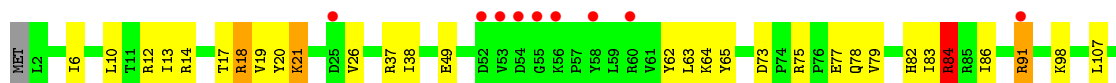
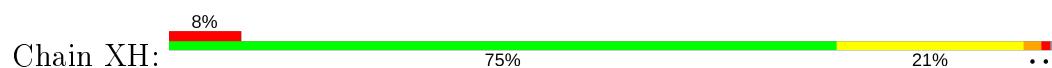


- Molecule 38: 30S ribosomal protein S7

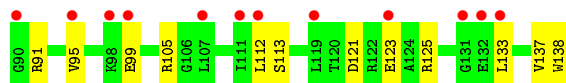




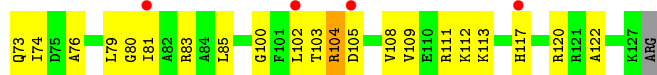
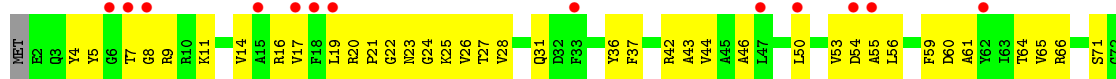
- Molecule 39: 30S ribosomal protein S8



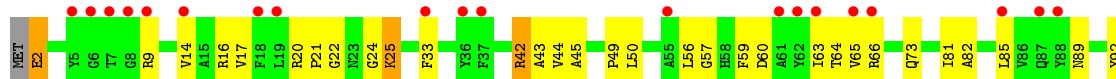
- Molecule 39: 30S ribosomal protein S8



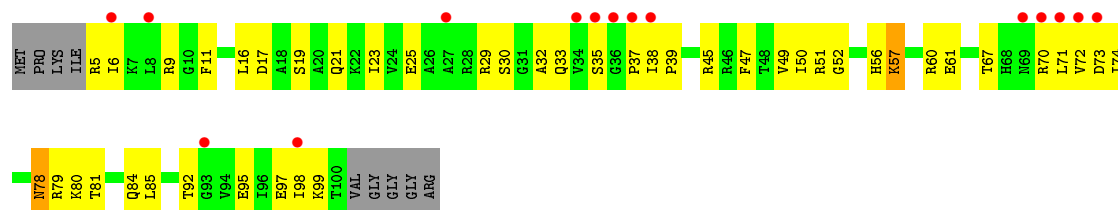
- Molecule 40: 30S ribosomal protein S9



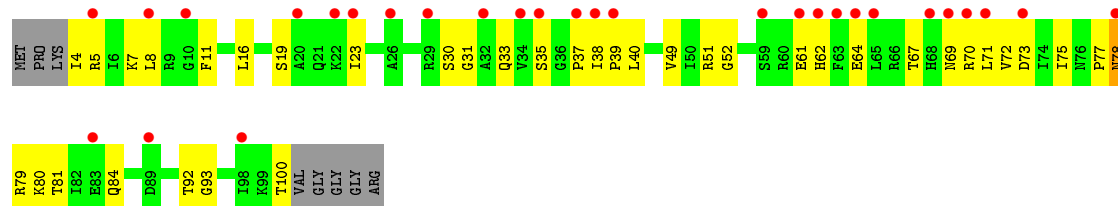
- Molecule 40: 30S ribosomal protein S9



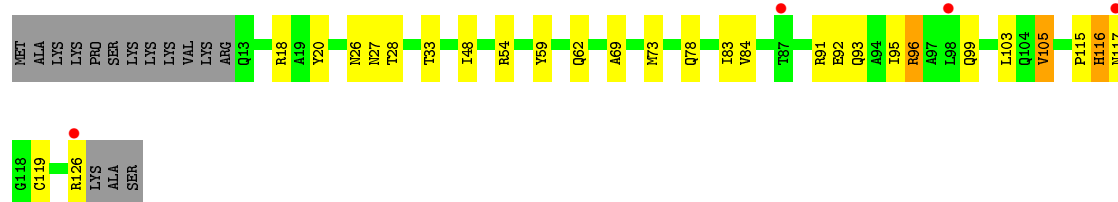
- Molecule 41: 30S ribosomal protein S10



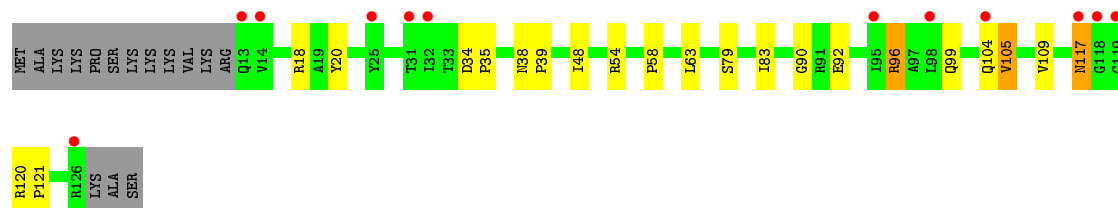
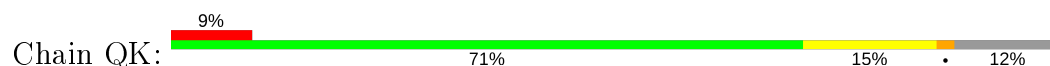
- Molecule 41: 30S ribosomal protein S10



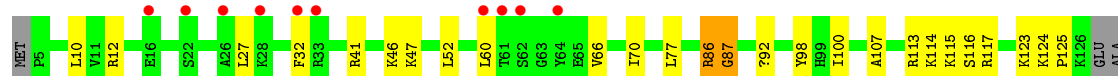
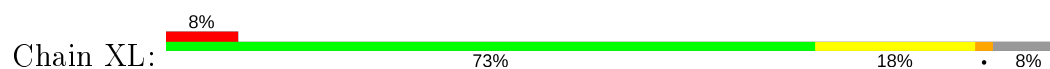
- Molecule 42: 30S ribosomal protein S11



- Molecule 42: 30S ribosomal protein S11




- Molecule 43: 30S ribosomal protein S12



ALA
LYS
THR
ALA
ALA
LYS
LYS

- Molecule 43: 30S ribosomal protein S12

Chain QL: 

MET P6 R12 R15 V24 L27 K28 R29 A30 F31 F32 R33 R41 K47 S50 L60 T61 S62 G63 Y64 E65 V66 I70 P71 V83 Q92 R97 Y98 H99 I100 V101 R102 K114 K115 K126 GLU ALA ALA LYS THR ALA LYS LYS

- Molecule 44: 30S ribosomal protein S13

Chain XM: 

MET ALA R3 G6 V7 E8 P10 K13 R14 V15 D16 V17 A18 L19 T20 Y23 G24 I25 G26 K27 E32 A33 L34 E35 G38 P41 R44 V54 E55 L56 R57 Y59 M62 T63 E67 V74 N77 I78 K79 R80 L81 I84 G85 C86 Y87

R88 G89 L90 R91 H92 R93 R94 G95 R96 P97 R98 R99 R102 R103 R104 A107 R108 T109 R110 K111 K115 T116 VAL ALA GLY LYS LYS ALA PRO ARG LYS

- Molecule 44: 30S ribosomal protein S13

Chain QM: 

MET A2 R3 T4 A5 R11 R12 R13 R14 R15 L19 G24 A28 E32 A33 L34 E35 R36 R40 P41 A42 T43 R44 V45 L48 V54 R55 L56 R57 E61 M62 T63 W64 K65 L66 E67 G68 I78 L81 I84 G85 C86 Y87 R88 R92 G95

L96 P97 V98 R99 G100 Q101 R102 T103 R110 R113 T116 V117 ALA GLY LYS LYS ALA ALA PRO ARG LYS

- Molecule 45: 30S ribosomal protein S14 type Z

Chain XN: 


MET A2 R3 K4 I7 R12 V18 T22 R23 C27 G28 R29 A30 R31 R32 S32 Y33 Y34 R35 F36 F37 G38 L39 C40 R41 R45 H49 R50 G51 Q52 L53 P54 R57 K58 R61

- Molecule 45: 30S ribosomal protein S14 type Z

Chain QN: 

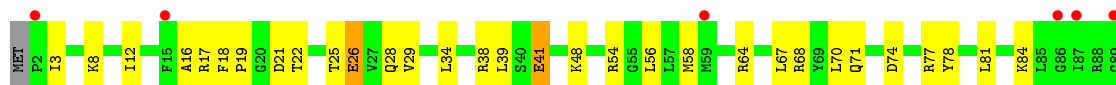
MET A2 R3 K4 L6 I7 E8 R9 A10 K17 V18 T22 R23 C24 V25 R26 C27 G28 R29 S32 Y33 Y34 R35 F36 F37 G38 L39 C40 R41 A48 H49 L53 P54 R57 K58 A59 S60 R61

- Molecule 46: 30S ribosomal protein S15

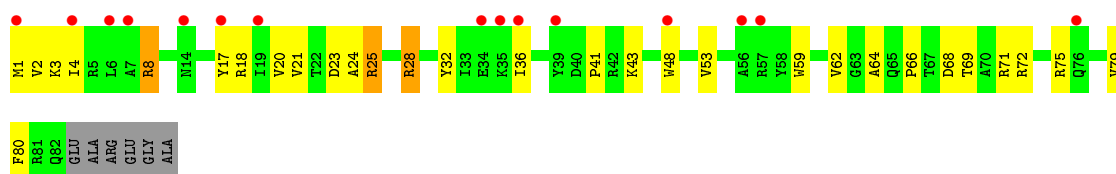
Chain XO: 



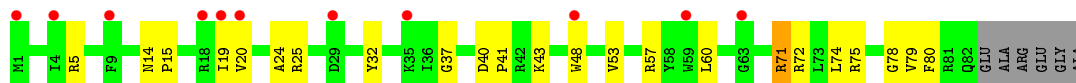
- Molecule 46: 30S ribosomal protein S15



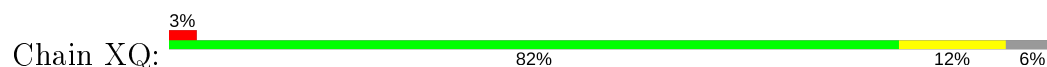
- Molecule 47: 30S ribosomal protein S16



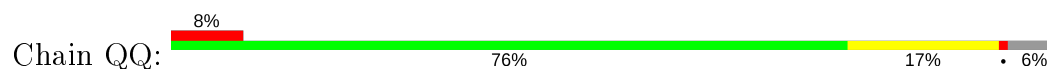
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17

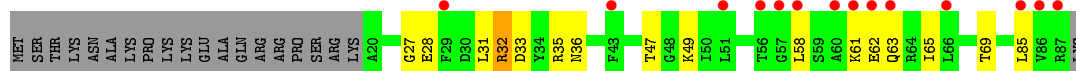


- Molecule 49: 30S ribosomal protein S18

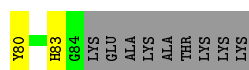
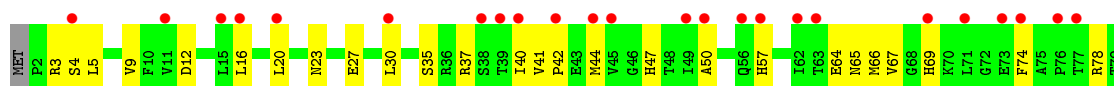




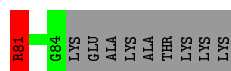
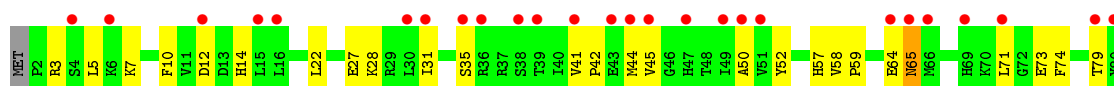
- Molecule 49: 30S ribosomal protein S18



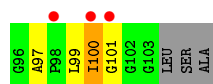
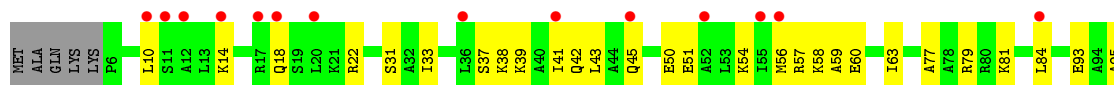
- Molecule 50: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S19

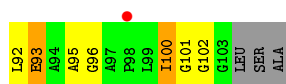


- Molecule 51: 30S ribosomal protein S20

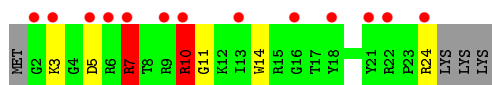


- Molecule 51: 30S ribosomal protein S20

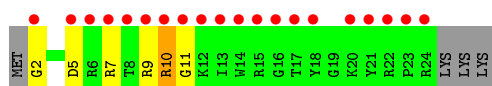
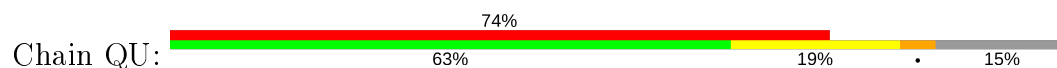




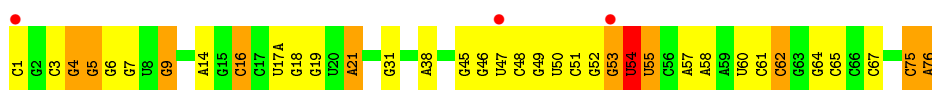
- Molecule 52: 30S ribosomal protein Thx



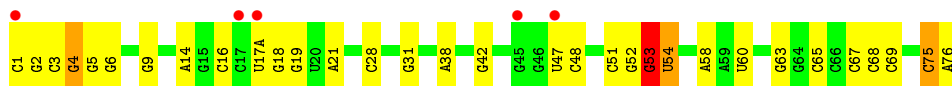
- Molecule 52: 30S ribosomal protein Thx



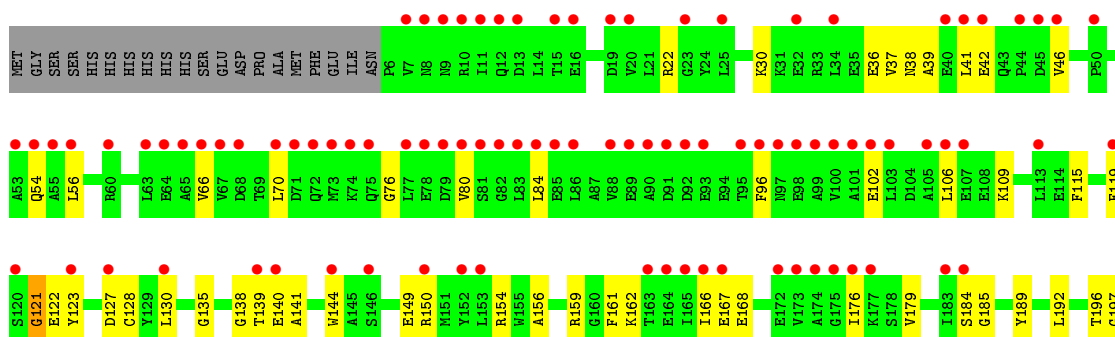
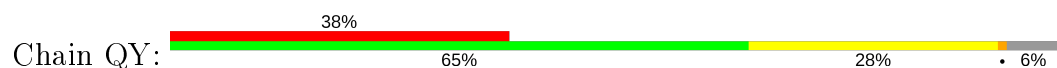
- Molecule 53: P-site tRNA fMet

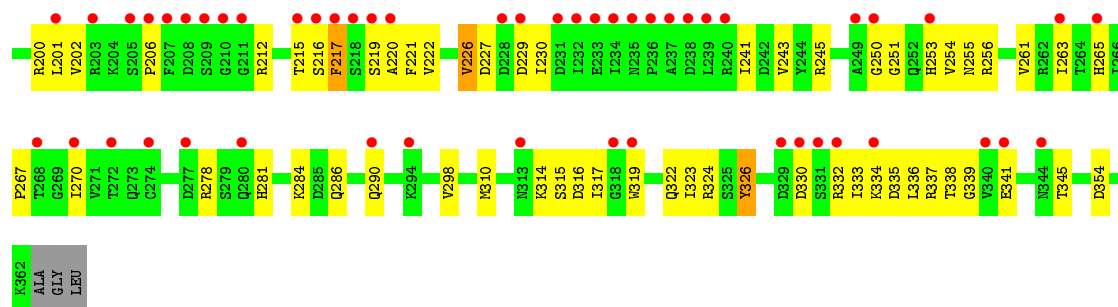


- Molecule 53: P-site tRNA fMet



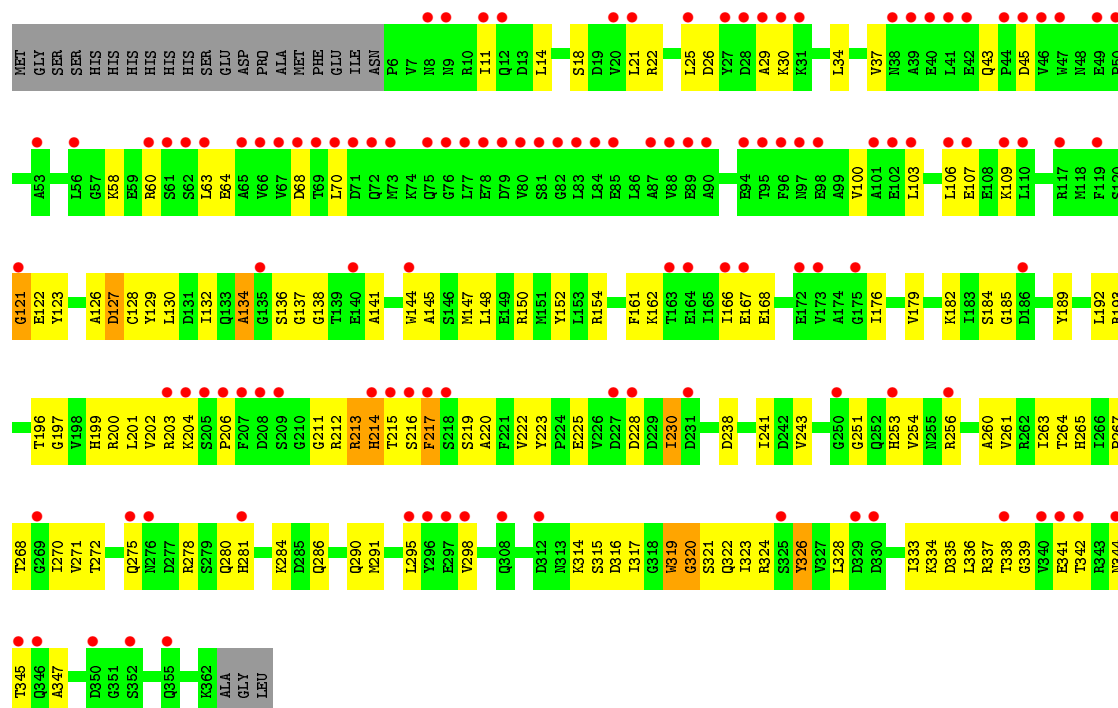
- Molecule 54: Peptide chain release factor 2





• Molecule 54: Peptide chain release factor 2

Chain XY: 32% 59% 32% 6%



• Molecule 55: mRNA

Chain XX: 20% 76%



• Molecule 55: mRNA

Chain QX: 20% 76%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.89Å 450.12Å 620.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 3.30 49.92 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.92-3.30) 98.9 (49.92-3.30)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.267 , 0.286 0.267 , 0.286	Depositor DCC
R_{free} test set	40129 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	99.5	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	296497	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	RA	0.25	0/68901	0.81	30/107544 (0.0%)
1	YA	0.27	0/68901	0.81	39/107544 (0.0%)
2	RB	0.22	0/2876	0.78	0/4486
2	YB	0.23	0/2878	0.79	0/4490
3	RD	0.71	8/2181 (0.4%)	0.69	1/2940 (0.0%)
3	YD	0.75	13/2186 (0.6%)	0.66	0/2944
4	RE	1.10	19/1592 (1.2%)	0.65	0/2149
4	YE	1.36	19/1592 (1.2%)	0.69	3/2149 (0.1%)
5	RF	0.59	2/1619 (0.1%)	0.68	2/2193 (0.1%)
5	YF	0.50	2/1615 (0.1%)	0.62	0/2188
6	RG	0.69	9/1451 (0.6%)	0.59	0/1961
6	YG	0.71	9/1449 (0.6%)	0.56	0/1957
7	RH	0.77	8/1356 (0.6%)	0.56	0/1834
7	YH	0.62	6/1350 (0.4%)	0.59	1/1826 (0.1%)
8	RI	0.84	7/1109 (0.6%)	0.60	0/1512
8	YI	0.55	3/1091 (0.3%)	0.63	2/1490 (0.1%)
9	RN	0.76	6/1148 (0.5%)	0.67	1/1547 (0.1%)
9	YN	0.81	7/1144 (0.6%)	0.57	0/1543
10	RO	0.63	4/943 (0.4%)	0.67	1/1269 (0.1%)
10	YO	0.61	4/943 (0.4%)	0.62	1/1269 (0.1%)
11	RP	0.89	8/1152 (0.7%)	0.71	0/1533
11	YP	0.64	6/1152 (0.5%)	0.61	1/1533 (0.1%)
12	RQ	0.91	12/1143 (1.0%)	0.67	0/1527
12	YQ	0.81	9/1143 (0.8%)	0.60	0/1527
13	RR	0.97	8/982 (0.8%)	0.72	2/1312 (0.2%)
13	YR	0.81	7/982 (0.7%)	0.66	0/1312
14	RS	0.74	4/887 (0.5%)	0.61	0/1180
14	YS	0.87	9/880 (1.0%)	0.63	0/1172
15	RT	0.87	12/1105 (1.1%)	0.66	0/1477
15	YT	0.83	10/1097 (0.9%)	0.63	0/1468
16	RU	0.87	7/977 (0.7%)	0.67	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	YU	0.98	11/977 (1.1%)	0.66	2/1301 (0.2%)
17	RV	0.71	2/786 (0.3%)	0.62	0/1053
17	YV	0.63	0/782	0.63	0/1049
18	RW	0.89	9/897 (1.0%)	0.67	2/1205 (0.2%)
18	YW	0.71	6/897 (0.7%)	0.60	0/1205
19	RX	0.76	4/764 (0.5%)	0.65	1/1025 (0.1%)
19	YX	0.70	3/764 (0.4%)	0.65	1/1025 (0.1%)
20	RY	0.78	4/823 (0.5%)	0.66	0/1099
20	YY	0.49	0/823	0.59	0/1100
21	RZ	0.70	9/1620 (0.6%)	0.58	1/2200 (0.0%)
21	YZ	1.52	14/1590 (0.9%)	0.59	0/2162
22	R0	0.69	2/616 (0.3%)	0.68	1/821 (0.1%)
22	Y0	0.53	2/616 (0.3%)	0.55	0/821
23	R1	0.76	3/761 (0.4%)	0.61	0/1013
23	Y1	0.81	5/766 (0.7%)	0.62	0/1018
24	R2	0.40	0/590	0.55	0/781
24	Y2	0.44	0/594	0.51	0/785
25	R3	0.49	0/474	0.62	0/635
25	Y3	0.66	3/469 (0.6%)	0.62	0/630
26	R4	0.98	5/559 (0.9%)	0.74	0/754
26	Y4	1.29	10/549 (1.8%)	0.71	0/741
27	R5	0.65	2/473 (0.4%)	0.69	0/639
27	Y5	0.77	4/469 (0.9%)	0.58	0/635
28	R6	0.80	1/460 (0.2%)	0.59	0/613
28	Y6	0.56	0/456	0.54	0/608
29	R7	0.67	0/426	0.77	2/561 (0.4%)
29	Y7	0.69	2/426 (0.5%)	0.67	0/561
30	R8	0.83	4/525 (0.8%)	0.65	1/691 (0.1%)
30	Y8	0.82	4/525 (0.8%)	0.64	0/691
31	R9	0.44	0/310	0.58	0/407
31	Y9	0.37	0/310	0.54	0/407
32	QA	0.23	0/35795	0.79	14/55864 (0.0%)
32	XA	0.24	0/35890	0.80	20/56012 (0.0%)
33	QB	0.76	15/1876 (0.8%)	0.63	2/2533 (0.1%)
33	XB	1.13	25/1860 (1.3%)	0.62	0/2518
34	QC	0.51	3/1582 (0.2%)	0.54	0/2137
34	XC	0.60	4/1566 (0.3%)	0.55	0/2119
35	QD	0.63	7/1695 (0.4%)	0.58	0/2274
35	XD	0.58	8/1698 (0.5%)	0.53	0/2277
36	QE	0.62	3/1149 (0.3%)	0.58	0/1548
36	XE	0.77	6/1149 (0.5%)	0.56	0/1548
37	QF	0.63	4/827 (0.5%)	0.58	0/1120
37	XF	0.91	10/829 (1.2%)	0.57	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	QG	0.75	6/1254 (0.5%)	0.50	0/1683
38	XG	1.05	17/1248 (1.4%)	0.57	0/1676
39	QH	0.69	5/1118 (0.4%)	0.55	0/1506
39	XH	0.60	3/1108 (0.3%)	0.57	1/1494 (0.1%)
40	QI	0.82	8/1005 (0.8%)	0.58	0/1351
40	XI	0.49	0/985	0.58	1/1329 (0.1%)
41	QJ	0.52	2/732 (0.3%)	0.58	0/993
41	XJ	0.39	0/723	0.56	0/984
42	QK	0.76	6/849 (0.7%)	0.58	1/1150 (0.1%)
42	XK	0.65	4/848 (0.5%)	0.59	0/1149
43	QL	0.63	2/937 (0.2%)	0.57	1/1260 (0.1%)
43	XL	0.44	0/937	0.62	1/1260 (0.1%)
44	QM	0.69	5/924 (0.5%)	0.59	0/1242
44	XM	0.67	4/905 (0.4%)	0.60	0/1217
45	QN	0.76	4/501 (0.8%)	0.49	0/664
45	XN	1.04	9/501 (1.8%)	0.59	0/664
46	QO	0.81	7/739 (0.9%)	0.56	0/985
46	XO	0.78	7/739 (0.9%)	0.56	0/985
47	QP	0.57	2/697 (0.3%)	0.62	0/939
47	XP	0.94	7/693 (1.0%)	0.59	0/935
48	QQ	0.61	4/836 (0.5%)	0.56	0/1117
48	XQ	0.77	8/836 (1.0%)	0.58	1/1117 (0.1%)
49	QR	0.78	4/560 (0.7%)	0.64	0/746
49	XR	0.56	2/560 (0.4%)	0.57	0/746
50	QS	0.66	4/663 (0.6%)	0.59	0/895
50	XS	0.45	0/660	0.56	0/893
51	QT	0.61	2/734 (0.3%)	0.58	0/969
51	XT	0.53	2/736 (0.3%)	0.51	0/976
52	QU	1.23	7/203 (3.4%)	0.50	0/266
52	XU	1.42	8/203 (3.9%)	0.59	0/266
53	QV	0.36	1/1836 (0.1%)	0.86	9/2859 (0.3%)
53	XV	0.35	1/1836 (0.1%)	0.79	2/2859 (0.1%)
54	QY	0.38	0/2862	0.60	0/3854
54	XY	0.38	1/2862 (0.0%)	0.59	0/3854
55	QX	0.22	0/144	0.72	0/222
55	XX	0.19	0/144	0.70	0/222
All	All	0.47	554/317956 (0.2%)	0.75	148/474813 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	RS	0	1
19	RX	0	1
19	YX	0	1
33	QB	0	1
43	XL	0	1
54	XY	0	1
All	All	0	6

The worst 5 of 554 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	YZ	72	ARG	NE-CZ	-30.04	0.94	1.33
21	YZ	72	ARG	CZ-NH1	-26.71	0.98	1.33
21	YZ	72	ARG	CZ-NH2	-26.64	0.98	1.33
21	YZ	72	ARG	CD-NE	-22.76	1.07	1.46
4	YE	144	ARG	NE-CZ	-22.31	1.04	1.33

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	1064	C	N1-C2-O2	9.58	124.65	118.90
1	RA	1064	C	N1-C2-O2	8.93	124.26	118.90
19	YX	57	LEU	CA-CB-CG	7.78	133.19	115.30
21	RZ	31	ARG	NE-CZ-NH1	-7.56	116.52	120.30
32	QA	639	G	N3-C4-N9	-7.37	121.58	126.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	QB	231	GLU	Peptide
14	RS	58	LEU	Peptide
19	RX	93	GLU	Peptide
43	XL	86	ARG	Peptide
19	YX	93	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	RA	61758	0	31146	667	0
1	YA	61758	0	31149	669	1
2	RB	2572	0	1305	12	0
2	YB	2573	0	1306	22	0
3	RD	2131	0	2207	48	0
3	YD	2136	0	2218	49	0
4	RE	1559	0	1618	36	0
4	YE	1559	0	1618	58	0
5	RF	1584	0	1625	43	0
5	YF	1580	0	1619	67	0
6	RG	1426	0	1445	61	0
6	YG	1424	0	1441	99	0
7	RH	1330	0	1407	26	0
7	YH	1324	0	1402	56	6
8	RI	1094	0	1127	33	0
8	YI	1076	0	1094	47	0
9	RN	1121	0	1195	27	0
9	YN	1117	0	1184	27	0
10	RO	933	0	996	25	0
10	YO	933	0	996	18	0
11	RP	1135	0	1212	39	0
11	YP	1135	0	1212	42	0
12	RQ	1122	0	1179	26	0
12	YQ	1122	0	1179	27	0
13	RR	968	0	1033	15	0
13	YR	968	0	1033	34	0
14	RS	877	0	938	15	0
14	YS	870	0	923	21	0
15	RT	1091	0	1151	38	0
15	YT	1083	0	1136	32	0
16	RU	959	0	1019	16	0
16	YU	959	0	1019	11	0
17	RV	775	0	841	22	0
17	YV	771	0	830	17	5
18	RW	886	0	940	18	1
18	YW	886	0	940	23	0
19	RX	750	0	814	26	0
19	YX	750	0	814	16	0
20	RY	810	0	892	16	0
20	YY	810	0	887	22	7
21	RZ	1587	0	1598	44	0
21	YZ	1557	0	1564	52	0
22	R0	608	0	622	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	Y0	608	0	622	16	0
23	R1	754	0	823	12	0
23	Y1	759	0	837	24	0
24	R2	588	0	643	16	1
24	Y2	592	0	654	7	0
25	R3	469	0	518	8	0
25	Y3	464	0	514	16	0
26	R4	546	0	522	55	0
26	Y4	536	0	514	58	0
27	R5	459	0	476	18	0
27	Y5	455	0	465	10	5
28	R6	453	0	473	9	0
28	Y6	449	0	469	6	0
29	R7	418	0	467	13	0
29	Y7	418	0	467	5	0
30	R8	517	0	582	24	0
30	Y8	517	0	582	20	0
31	R9	307	0	335	6	0
31	Y9	307	0	335	5	0
32	QA	32246	0	16293	408	0
32	XA	32331	0	16339	421	0
33	QB	1842	0	1862	86	0
33	XB	1825	0	1828	88	0
34	QC	1558	0	1557	44	0
34	XC	1542	0	1517	56	0
35	QD	1665	0	1687	71	0
35	XD	1668	0	1703	38	0
36	QE	1133	0	1191	47	0
36	XE	1133	0	1191	31	0
37	QF	814	0	808	18	0
37	XF	816	0	808	24	0
38	QG	1235	0	1249	37	0
38	XG	1229	0	1238	25	0
39	QH	1098	0	1143	42	0
39	XH	1088	0	1126	22	0
40	QI	986	0	990	44	0
40	XI	966	0	953	46	0
41	QJ	719	0	672	33	0
41	XJ	710	0	661	41	0
42	QK	834	0	838	16	0
42	XK	833	0	836	24	0
43	QL	932	0	981	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	XL	932	0	981	22	0
44	QM	914	0	954	53	0
44	XM	895	0	920	50	0
45	QN	492	0	529	20	0
45	XN	492	0	529	23	0
46	QO	728	0	760	27	0
46	XO	728	0	760	6	0
47	QP	681	0	697	20	0
47	XP	677	0	686	28	0
48	QQ	823	0	891	15	0
48	XQ	823	0	891	10	0
49	QR	555	0	618	16	0
49	XR	555	0	618	26	0
50	QS	648	0	658	29	0
50	XS	645	0	635	43	0
51	QT	732	0	809	34	0
51	XT	733	0	795	31	0
52	QU	199	0	208	3	0
52	XU	199	0	208	5	0
53	QV	1644	0	836	30	0
53	XV	1644	0	836	22	0
54	QY	2833	0	2729	96	0
54	XY	2833	0	2728	124	0
55	QX	129	0	64	1	0
55	XX	129	0	65	1	0
56	QA	280	0	0	0	0
56	QB	1	0	0	0	0
56	QD	4	0	0	0	0
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	2	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	QV	4	0	0	0	0
56	QY	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	R0	4	0	0	0	0
56	R1	4	0	0	0	0
56	R3	2	0	0	0	0
56	R4	1	0	0	0	0
56	R5	4	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	1069	0	0	0	0
56	RB	28	0	0	0	0
56	RD	14	0	0	0	0
56	RE	7	0	0	0	0
56	RF	11	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	4	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	193	0	0	0	0
56	XE	2	0	0	0	0
56	XF	3	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	XT	1	0	0	0	0
56	XV	3	0	0	0	0
56	XY	1	0	0	0	0
56	Y0	1	0	0	0	0
56	Y1	2	0	0	0	0
56	Y5	1	0	0	0	0
56	Y6	1	0	0	0	0
56	Y7	1	0	0	0	0
56	Y8	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	YA	756	0	0	0	0
56	YB	19	0	0	0	0
56	YD	9	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	2	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
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
All	All	296497	0	200048	4678	13

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 10.

The worst 5 of 4678 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)
33:XB:114:ARG:NH1	33:XB:118:LEU:HG	1.41	1.36
42:QK:48:ILE:HD12	42:QK:63:LEU:CB	1.60	1.29
7:YH:7:LEU:O	7:YH:69:ARG:NH1	1.63	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:QK:48:ILE:CD1	42:QK:63:LEU:HB2	1.66	1.25
26:Y4:59:PHE:CE1	50:XS:64:GLU:HB2	1.73	1.23

The worst 5 of 13 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:YH:46:GLU:OE1	20:YY:22:GLY:C[4_445]	0.78	1.42
7:YH:46:GLU:OE1	20:YY:22:GLY:O[4_445]	1.12	1.08
7:YH:46:GLU:OE1	20:YY:23:ARG:N[4_445]	1.56	0.64
17:YV:49:THR:O	27:Y5:60:VAL:O[4_445]	1.77	0.43
17:YV:53:GLU:OE2	27:Y5:59:GLU:CA[4_445]	1.88	0.32

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	RD	273/276 (99%)	262 (96%)	11 (4%)	0	100	100
3	YD	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
4	RE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	61
4	YE	202/206 (98%)	196 (97%)	6 (3%)	0	100	100
5	RF	201/210 (96%)	197 (98%)	4 (2%)	0	100	100
5	YF	201/210 (96%)	196 (98%)	3 (2%)	2 (1%)	15	46
6	RG	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	25	57
6	YG	179/182 (98%)	170 (95%)	8 (4%)	1 (1%)	25	57
7	RH	172/180 (96%)	167 (97%)	5 (3%)	0	100	100
7	YH	171/180 (95%)	165 (96%)	6 (4%)	0	100	100
8	RI	145/148 (98%)	133 (92%)	11 (8%)	1 (1%)	22	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	YI	144/148 (97%)	135 (94%)	9 (6%)	0	100	100
9	RN	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
9	YN	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
10	RO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	YO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
11	RP	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
11	YP	147/150 (98%)	141 (96%)	5 (3%)	1 (1%)	22	54
12	RQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
12	YQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
13	RR	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	YR	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
14	RS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	17	48
14	YS	108/112 (96%)	105 (97%)	3 (3%)	0	100	100
15	RT	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
15	YT	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
16	RU	114/118 (97%)	114 (100%)	0	0	100	100
16	YU	114/118 (97%)	114 (100%)	0	0	100	100
17	RV	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
17	YV	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
18	RW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	YW	110/113 (97%)	110 (100%)	0	0	100	100
19	RX	93/96 (97%)	92 (99%)	1 (1%)	0	100	100
19	YX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
20	RY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
20	YY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
21	RZ	201/206 (98%)	196 (98%)	5 (2%)	0	100	100
21	YZ	199/206 (97%)	194 (98%)	5 (2%)	0	100	100
22	R0	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
22	Y0	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
23	R1	95/98 (97%)	94 (99%)	0	1 (1%)	14	45
23	Y1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	R2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	Y2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	R4	67/71 (94%)	55 (82%)	6 (9%)	6 (9%)	1	4
26	Y4	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	2	15
27	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	Y5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	R7	46/49 (94%)	46 (100%)	0	0	100	100
29	Y7	46/49 (94%)	46 (100%)	0	0	100	100
30	R8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	Y8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	R9	35/37 (95%)	35 (100%)	0	0	100	100
31	Y9	35/37 (95%)	35 (100%)	0	0	100	100
33	QB	229/256 (90%)	202 (88%)	20 (9%)	7 (3%)	4	23
33	XB	229/256 (90%)	205 (90%)	19 (8%)	5 (2%)	6	30
34	QC	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
34	XC	204/239 (85%)	187 (92%)	17 (8%)	0	100	100
35	QD	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
35	XD	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
36	QE	146/162 (90%)	144 (99%)	2 (1%)	0	100	100
36	XE	146/162 (90%)	145 (99%)	1 (1%)	0	100	100
37	QF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	XF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	QG	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
38	XG	153/156 (98%)	148 (97%)	4 (3%)	1 (1%)	22	54
39	QH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
39	XH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
40	QI	125/128 (98%)	115 (92%)	9 (7%)	1 (1%)	19	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	XI	124/128 (97%)	113 (91%)	8 (6%)	3 (2%)	6	28
41	QJ	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	3	17
41	XJ	94/105 (90%)	85 (90%)	7 (7%)	2 (2%)	7	31
42	QK	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	8	35
42	XK	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	17	48
43	QL	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
43	XL	119/132 (90%)	116 (98%)	3 (2%)	0	100	100
44	QM	114/126 (90%)	105 (92%)	7 (6%)	2 (2%)	8	35
44	XM	112/126 (89%)	105 (94%)	6 (5%)	1 (1%)	17	48
45	QN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	XN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
46	QO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	XO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
47	QP	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
47	XP	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
48	QQ	97/105 (92%)	94 (97%)	2 (2%)	1 (1%)	15	46
48	XQ	97/105 (92%)	95 (98%)	2 (2%)	0	100	100
49	QR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
49	XR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	QS	81/93 (87%)	78 (96%)	3 (4%)	0	100	100
50	XS	81/93 (87%)	79 (98%)	2 (2%)	0	100	100
51	QT	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	7	31
51	XT	96/106 (91%)	88 (92%)	6 (6%)	2 (2%)	7	31
52	QU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	XU	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	14
54	QY	354/380 (93%)	309 (87%)	37 (10%)	8 (2%)	6	29
54	XY	354/380 (93%)	309 (87%)	36 (10%)	9 (2%)	5	27
All	All	12148/12888 (94%)	11573 (95%)	504 (4%)	71 (1%)	25	57

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	Y1	3	LYS

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Mol	Chain	Res	Type
33	XB	17	PHE
33	XB	20	GLU
33	XB	124	SER
40	XI	44	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	RD	214/218 (98%)	209 (98%)	5 (2%)	50	73
3	YD	215/218 (99%)	209 (97%)	6 (3%)	43	70
4	RE	164/166 (99%)	163 (99%)	1 (1%)	86	91
4	YE	164/166 (99%)	159 (97%)	5 (3%)	41	68
5	RF	160/166 (96%)	152 (95%)	8 (5%)	24	55
5	YF	159/166 (96%)	154 (97%)	5 (3%)	40	67
6	RG	144/156 (92%)	139 (96%)	5 (4%)	36	64
6	YG	142/156 (91%)	133 (94%)	9 (6%)	18	47
7	RH	144/148 (97%)	142 (99%)	2 (1%)	67	82
7	YH	143/148 (97%)	140 (98%)	3 (2%)	53	75
8	RI	111/124 (90%)	105 (95%)	6 (5%)	22	53
8	YI	108/124 (87%)	108 (100%)	0	100	100
9	RN	119/119 (100%)	115 (97%)	4 (3%)	37	65
9	YN	118/119 (99%)	115 (98%)	3 (2%)	47	72
10	RO	100/100 (100%)	100 (100%)	0	100	100
10	YO	100/100 (100%)	100 (100%)	0	100	100
11	RP	115/116 (99%)	112 (97%)	3 (3%)	46	71
11	YP	115/116 (99%)	113 (98%)	2 (2%)	60	78
12	RQ	111/111 (100%)	107 (96%)	4 (4%)	35	63
12	YQ	111/111 (100%)	106 (96%)	5 (4%)	27	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	RR	101/101 (100%)	99 (98%)	2 (2%)	55	76
13	YR	101/101 (100%)	101 (100%)	0	100	100
14	RS	87/88 (99%)	84 (97%)	3 (3%)	37	65
14	YS	85/88 (97%)	82 (96%)	3 (4%)	36	64
15	RT	115/127 (91%)	110 (96%)	5 (4%)	29	59
15	YT	113/127 (89%)	110 (97%)	3 (3%)	44	71
16	RU	93/94 (99%)	90 (97%)	3 (3%)	39	67
16	YU	93/94 (99%)	89 (96%)	4 (4%)	29	59
17	RV	81/82 (99%)	80 (99%)	1 (1%)	71	83
17	YV	80/82 (98%)	78 (98%)	2 (2%)	47	72
18	RW	90/92 (98%)	86 (96%)	4 (4%)	28	59
18	YW	90/92 (98%)	88 (98%)	2 (2%)	52	74
19	RX	77/78 (99%)	76 (99%)	1 (1%)	69	82
19	YX	77/78 (99%)	74 (96%)	3 (4%)	32	62
20	RY	86/91 (94%)	83 (96%)	3 (4%)	36	64
20	YY	86/91 (94%)	82 (95%)	4 (5%)	26	57
21	RZ	169/179 (94%)	165 (98%)	4 (2%)	49	73
21	YZ	165/179 (92%)	159 (96%)	6 (4%)	35	63
22	R0	61/67 (91%)	59 (97%)	2 (3%)	38	66
22	Y0	61/67 (91%)	56 (92%)	5 (8%)	11	36
23	R1	79/83 (95%)	77 (98%)	2 (2%)	47	72
23	Y1	81/83 (98%)	79 (98%)	2 (2%)	47	72
24	R2	65/67 (97%)	63 (97%)	2 (3%)	40	67
24	Y2	66/67 (98%)	64 (97%)	2 (3%)	41	68
25	R3	51/52 (98%)	51 (100%)	0	100	100
25	Y3	50/52 (96%)	47 (94%)	3 (6%)	19	49
26	R4	58/63 (92%)	55 (95%)	3 (5%)	23	54
26	Y4	54/63 (86%)	47 (87%)	7 (13%)	4	17
27	R5	51/52 (98%)	50 (98%)	1 (2%)	55	76
27	Y5	50/52 (96%)	49 (98%)	1 (2%)	55	76
28	R6	51/52 (98%)	50 (98%)	1 (2%)	55	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	Y6	50/52 (96%)	50 (100%)	0	100	100
29	R7	41/42 (98%)	41 (100%)	0	100	100
29	Y7	41/42 (98%)	41 (100%)	0	100	100
30	R8	54/55 (98%)	52 (96%)	2 (4%)	34	63
30	Y8	54/55 (98%)	52 (96%)	2 (4%)	34	63
31	R9	34/34 (100%)	34 (100%)	0	100	100
31	Y9	34/34 (100%)	34 (100%)	0	100	100
33	QB	191/220 (87%)	182 (95%)	9 (5%)	26	57
33	XB	187/220 (85%)	176 (94%)	11 (6%)	19	49
34	QC	144/188 (77%)	141 (98%)	3 (2%)	53	75
34	XC	140/188 (74%)	135 (96%)	5 (4%)	35	63
35	QD	171/181 (94%)	166 (97%)	5 (3%)	42	69
35	XD	172/181 (95%)	168 (98%)	4 (2%)	50	73
36	QE	114/123 (93%)	112 (98%)	2 (2%)	59	78
36	XE	114/123 (93%)	113 (99%)	1 (1%)	78	87
37	QF	85/90 (94%)	83 (98%)	2 (2%)	49	73
37	XF	85/90 (94%)	83 (98%)	2 (2%)	49	73
38	QG	120/127 (94%)	117 (98%)	3 (2%)	47	72
38	XG	119/127 (94%)	116 (98%)	3 (2%)	47	72
39	QH	116/119 (98%)	114 (98%)	2 (2%)	60	78
39	XH	114/119 (96%)	109 (96%)	5 (4%)	28	59
40	QI	91/99 (92%)	85 (93%)	6 (7%)	16	46
40	XI	88/99 (89%)	86 (98%)	2 (2%)	50	73
41	QJ	68/92 (74%)	67 (98%)	1 (2%)	65	81
41	XJ	68/92 (74%)	67 (98%)	1 (2%)	65	81
42	QK	83/99 (84%)	82 (99%)	1 (1%)	71	83
42	XK	83/99 (84%)	81 (98%)	2 (2%)	49	73
43	QL	96/108 (89%)	95 (99%)	1 (1%)	76	86
43	XL	96/108 (89%)	95 (99%)	1 (1%)	76	86
44	QM	90/101 (89%)	86 (96%)	4 (4%)	28	59
44	XM	87/101 (86%)	85 (98%)	2 (2%)	50	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	QN	49/50 (98%)	46 (94%)	3 (6%)	18	48
45	XN	49/50 (98%)	48 (98%)	1 (2%)	55	76
46	QO	78/80 (98%)	76 (97%)	2 (3%)	46	71
46	XO	78/80 (98%)	75 (96%)	3 (4%)	33	62
47	QP	69/74 (93%)	69 (100%)	0	100	100
47	XP	68/74 (92%)	66 (97%)	2 (3%)	42	69
48	QQ	94/97 (97%)	93 (99%)	1 (1%)	73	85
48	XQ	94/97 (97%)	94 (100%)	0	100	100
49	QR	59/77 (77%)	58 (98%)	1 (2%)	60	78
49	XR	59/77 (77%)	58 (98%)	1 (2%)	60	78
50	QS	68/80 (85%)	65 (96%)	3 (4%)	28	59
50	XS	67/80 (84%)	67 (100%)	0	100	100
51	QT	71/82 (87%)	70 (99%)	1 (1%)	67	82
51	XT	70/82 (85%)	70 (100%)	0	100	100
52	QU	18/22 (82%)	17 (94%)	1 (6%)	21	52
52	XU	18/22 (82%)	16 (89%)	2 (11%)	6	23
54	QY	303/323 (94%)	301 (99%)	2 (1%)	84	90
54	XY	303/323 (94%)	301 (99%)	2 (1%)	84	90
All	All	9969/10710 (93%)	9702 (97%)	267 (3%)	44	71

5 of 267 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	XJ	57	LYS
35	QD	168	ARG
21	RZ	72	ARG
44	XM	94	ARG
33	QB	21	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
50	QS	57	HIS
50	QS	65	ASN
54	XY	54	GLN

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Mol	Chain	Res	Type
38	QG	56	GLN
54	QY	308	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	RA	2855/2915 (97%)	427 (14%)	21 (0%)
1	YA	2855/2915 (97%)	430 (15%)	24 (0%)
2	RB	119/122 (97%)	10 (8%)	0
2	YB	119/122 (97%)	12 (10%)	0
32	QA	1494/1521 (98%)	220 (14%)	14 (0%)
32	XA	1498/1521 (98%)	232 (15%)	18 (1%)
53	QV	76/77 (98%)	19 (25%)	1 (1%)
53	XV	76/77 (98%)	18 (23%)	1 (1%)
55	QX	5/25 (20%)	1 (20%)	0
55	XX	5/25 (20%)	1 (20%)	0
All	All	9102/9320 (97%)	1370 (15%)	79 (0%)

5 of 1370 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	YA	10	G
1	YA	11	G
1	YA	12	U
1	YA	15	G
1	YA	34	C

5 of 79 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	XA	991	U
32	QA	509	A
1	RA	2171	A
32	XA	992	U
32	XA	1256	A

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

50 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$
32	UR3	XA	1498	32,56	14,22,23	0.79	1 (7%)	15,32,35	0.68	0
1	5MC	RA	1942	1	15,22,23	1.29	1 (6%)	19,32,35	1.30	3 (15%)
1	5MC	YA	1942	1	15,22,23	1.27	1 (6%)	19,32,35	1.35	2 (10%)
43	0TD	XL	92	43	4,9,10	3.20	1 (25%)	3,11,13	2.56	1 (33%)
32	2MG	QA	1207	32	19,26,27	1.27	2 (10%)	21,38,41	2.28	7 (33%)
1	5MU	YA	1915	1	15,22,23	0.99	1 (6%)	16,32,35	2.03	1 (6%)
32	5MC	XA	1407	32	15,22,23	1.27	1 (6%)	19,32,35	1.40	2 (10%)
1	PSU	RA	1917	1	17,21,22	1.54	2 (11%)	20,30,33	3.18	6 (30%)
32	MA6	QA	1519	32	19,26,27	1.02	1 (5%)	18,38,41	1.67	5 (27%)
1	2MU	RA	2552	1,56	14,22,24	0.89	0	14,31,36	0.73	0
1	4OC	YA	1920	1	15,22,24	0.70	0	17,31,35	1.45	2 (11%)
32	5MC	XA	1400	32	15,22,23	1.33	1 (6%)	19,32,35	1.31	3 (15%)
54	MEQ	XY	252	54	8,9,10	0.86	0	5,10,12	0.65	0
32	PSU	XA	516	32	17,21,22	1.49	3 (17%)	20,30,33	3.05	6 (30%)
32	M2G	XA	966	32	20,27,28	1.42	3 (15%)	22,40,43	2.17	5 (22%)
1	PSU	YA	1911	1	17,21,22	1.55	3 (17%)	20,30,33	3.11	6 (30%)
1	5MU	YA	1939	1,56	15,22,23	1.07	2 (13%)	16,32,35	1.84	2 (12%)
1	2MA	RA	2503	1,56	17,25,26	1.40	2 (11%)	19,37,40	2.12	3 (15%)
32	5MC	XA	1404	32	15,22,23	1.28	1 (6%)	19,32,35	1.38	3 (15%)
1	2MU	YA	2552	1,56	14,22,24	0.90	0	14,31,36	0.72	1 (7%)
1	4OC	RA	1920	1	15,22,24	0.59	0	17,31,35	1.39	2 (11%)
43	0TD	QL	92	43	4,9,10	4.45	3 (75%)	3,11,13	5.66	2 (66%)
32	MA6	QA	1518	32	19,26,27	0.98	1 (5%)	18,38,41	1.70	5 (27%)
32	5MC	QA	967	32	15,22,23	1.34	1 (6%)	19,32,35	1.27	3 (15%)
54	MEQ	QY	252	54	8,9,10	0.88	0	5,10,12	0.64	0
32	4OC	XA	1402	32	16,23,24	0.63	0	17,32,35	1.25	1 (5%)
32	PSU	QA	516	32,56	17,21,22	1.53	3 (17%)	20,30,33	3.01	6 (30%)
1	5MC	YA	1962	1,56	15,22,23	1.29	1 (6%)	19,32,35	1.33	3 (15%)
32	4OC	QA	1402	32	16,23,24	0.61	0	17,32,35	1.16	1 (5%)
1	PSU	RA	1911	1	17,21,22	1.57	3 (17%)	20,30,33	3.08	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	QA	1404	32	15,22,23	1.32	1 (6%)	19,32,35	1.34	3 (15%)
32	2MG	XA	1207	32	19,26,27	1.27	2 (10%)	21,38,41	2.24	7 (33%)
1	2MA	YA	2503	1,56	17,25,26	1.41	2 (11%)	19,37,40	2.17	3 (15%)
1	PSU	YA	2605	1	17,21,22	1.61	3 (17%)	20,30,33	3.19	6 (30%)
32	7MG	XA	527	32,56	22,26,27	1.75	4 (18%)	28,39,42	2.77	9 (32%)
32	M2G	QA	966	32	20,27,28	1.38	3 (15%)	22,40,43	2.13	5 (22%)
32	MA6	XA	1519	32	19,26,27	0.98	1 (5%)	18,38,41	1.85	6 (33%)
1	5MU	RA	1939	1	15,22,23	1.03	1 (6%)	16,32,35	1.85	2 (12%)
1	PSU	RA	2605	1	17,21,22	1.62	2 (11%)	20,30,33	3.12	6 (30%)
32	MA6	XA	1518	32	19,26,27	0.98	1 (5%)	18,38,41	1.78	6 (33%)
32	5MC	QA	1400	32	15,22,23	1.31	1 (6%)	19,32,35	1.35	3 (15%)
32	UR3	QA	1498	32	14,22,23	0.75	0	15,32,35	0.64	0
32	5MC	QA	1407	32	15,22,23	1.32	1 (6%)	19,32,35	1.36	3 (15%)
1	5MC	RA	1962	1,56	15,22,23	1.31	1 (6%)	19,32,35	1.34	3 (15%)
32	5MC	XA	967	32	15,22,23	1.36	1 (6%)	19,32,35	1.32	3 (15%)
1	5MU	RA	1915	1,56	15,22,23	1.04	1 (6%)	16,32,35	2.00	1 (6%)
32	7MG	QA	527	32,56	22,26,27	1.77	4 (18%)	28,39,42	2.80	9 (32%)
1	OMG	YA	2251	1,56,53	18,26,27	1.22	2 (11%)	20,38,41	2.11	6 (30%)
1	PSU	YA	1917	1	17,21,22	1.54	2 (11%)	20,30,33	3.15	6 (30%)
1	OMG	RA	2251	1,56,53	18,26,27	1.21	2 (11%)	20,38,41	2.14	6 (30%)

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
32	UR3	XA	1498	32,56	-	0/5/25/26	0/2/2/2
1	5MC	RA	1942	1	-	0/5/25/26	0/2/2/2
1	5MC	YA	1942	1	-	0/5/25/26	0/2/2/2
43	0TD	XL	92	43	-	3/3/12/14	-
32	2MG	QA	1207	32	-	0/5/27/28	0/3/3/3
1	5MU	YA	1915	1	-	2/5/25/26	0/2/2/2
32	5MC	XA	1407	32	-	0/5/25/26	0/2/2/2
1	PSU	RA	1917	1	-	0/7/25/26	0/2/2/2
32	MA6	QA	1519	32	-	3/7/29/30	0/3/3/3
1	2MU	RA	2552	1,56	-	0/7/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4OC	YA	1920	1	-	0/7/27/30	0/2/2/2
32	5MC	XA	1400	32	-	2/5/25/26	0/2/2/2
54	MEQ	XY	252	54	-	2/8/9/11	-
32	PSU	XA	516	32	-	0/7/25/26	0/2/2/2
32	M2G	XA	966	32	-	0/7/29/30	0/3/3/3
1	PSU	YA	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	YA	1939	1,56	-	0/5/25/26	0/2/2/2
1	2MA	RA	2503	1,56	-	1/3/25/26	0/3/3/3
32	5MC	XA	1404	32	-	0/5/25/26	0/2/2/2
1	2MU	YA	2552	1,56	-	0/7/27/28	0/2/2/2
1	4OC	RA	1920	1	-	1/7/27/30	0/2/2/2
43	0TD	QL	92	43	-	1/3/12/14	-
32	MA6	QA	1518	32	-	2/7/29/30	0/3/3/3
32	5MC	QA	967	32	-	0/5/25/26	0/2/2/2
54	MEQ	QY	252	54	-	4/8/9/11	-
32	4OC	XA	1402	32	-	4/9/29/30	0/2/2/2
32	PSU	QA	516	32,56	-	0/7/25/26	0/2/2/2
1	5MC	YA	1962	1,56	-	2/5/25/26	0/2/2/2
32	4OC	QA	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	RA	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	QA	1404	32	-	1/5/25/26	0/2/2/2
32	2MG	XA	1207	32	-	0/5/27/28	0/3/3/3
1	2MA	YA	2503	1,56	-	1/3/25/26	0/3/3/3
1	PSU	YA	2605	1	-	0/7/25/26	0/2/2/2
32	7MG	XA	527	32,56	-	3/7/37/38	0/3/3/3
32	M2G	QA	966	32	-	0/7/29/30	0/3/3/3
32	MA6	XA	1519	32	-	3/7/29/30	0/3/3/3
1	5MU	RA	1939	1	-	0/5/25/26	0/2/2/2
1	PSU	RA	2605	1	-	0/7/25/26	0/2/2/2
32	MA6	XA	1518	32	-	1/7/29/30	0/3/3/3
32	5MC	QA	1400	32	-	2/5/25/26	0/2/2/2
32	UR3	QA	1498	32	-	0/5/25/26	0/2/2/2
32	5MC	QA	1407	32	-	0/5/25/26	0/2/2/2
1	5MC	RA	1962	1,56	-	2/5/25/26	0/2/2/2
32	5MC	XA	967	32	-	0/5/25/26	0/2/2/2
1	5MU	RA	1915	1,56	-	1/5/25/26	0/2/2/2
32	7MG	QA	527	32,56	-	3/7/37/38	0/3/3/3
1	OMG	YA	2251	1,56,53	-	0/5/27/28	0/3/3/3
1	PSU	YA	1917	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	RA	2251	1,56,53	-	0/5/27/28	0/3/3/3

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	QL	92	0TD	CB-SB	-7.92	1.64	1.84
43	XL	92	0TD	CB-SB	-6.04	1.69	1.84
32	XA	967	5MC	C5-C4	4.94	1.49	1.41
32	QA	527	7MG	C6-C5	4.89	1.48	1.41
32	QA	967	5MC	C5-C4	4.86	1.48	1.41

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	QA	527	7MG	N3-C4-N9	9.32	138.88	126.91
32	XA	527	7MG	N3-C4-N9	9.25	138.79	126.91
1	YA	2605	PSU	N1-C2-N3	-8.64	121.56	128.43
1	RA	1917	PSU	N1-C2-N3	-8.55	121.63	128.43
32	XA	516	PSU	N1-C2-N3	-8.52	121.66	128.43

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	XL	92	0TD	O-C-CA-CB
43	XL	92	0TD	CG-CB-SB-CSB
1	YA	1915	5MU	C2'-C1'-N1-C6
1	YA	1915	5MU	O4'-C1'-N1-C6
32	QA	1519	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

22 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	RA	1942	5MC	1	0
43	XL	92	0TD	1	0
32	QA	1207	2MG	2	0
32	QA	1519	MA6	1	0
1	YA	1920	4OC	2	0
1	YA	1939	5MU	1	0
1	RA	2503	2MA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	QL	92	0TD	1	0
32	QA	1518	MA6	1	0
32	QA	967	5MC	1	0
32	XA	1402	4OC	1	0
32	QA	516	PSU	1	0
1	YA	1962	5MC	1	0
32	QA	1402	4OC	1	0
32	XA	1207	2MG	1	0
1	YA	2503	2MA	2	0
32	QA	966	M2G	1	0
1	RA	1939	5MU	1	0
32	XA	1518	MA6	1	0
32	QA	1498	UR3	1	0
1	RA	1962	5MC	1	0
1	YA	2251	OMG	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2534 ligands modelled in this entry, 2532 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	QD	302	35	0,12,12	0.00	-	-		
58	SF4	XD	301	35	0,12,12	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	QD	302	35	-	-	0/6/5/5
58	SF4	XD	301	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	RA	2856/2915 (97%)	0.33	131 (4%) 32 30	76, 86, 96, 102	0
1	YA	2856/2915 (97%)	0.44	116 (4%) 37 35	71, 83, 96, 100	0
2	RB	120/122 (98%)	-0.10	2 (1%) 70 68	84, 90, 93, 96	0
2	YB	120/122 (98%)	-0.16	2 (1%) 70 68	80, 87, 91, 94	0
3	RD	275/276 (99%)	0.47	5 (1%) 68 67	77, 85, 89, 96	0
3	YD	275/276 (99%)	0.50	4 (1%) 73 72	76, 83, 89, 90	0
4	RE	204/206 (99%)	0.49	5 (2%) 57 54	78, 86, 91, 93	0
4	YE	204/206 (99%)	0.54	4 (1%) 65 64	77, 86, 90, 94	0
5	RF	203/210 (96%)	0.32	1 (0%) 91 91	81, 87, 92, 95	0
5	YF	203/210 (96%)	0.34	1 (0%) 91 91	76, 85, 91, 94	0
6	RG	181/182 (99%)	0.48	15 (8%) 11 11	87, 91, 94, 97	0
6	YG	181/182 (99%)	0.31	11 (6%) 21 20	85, 89, 93, 95	0
7	RH	174/180 (96%)	1.30	49 (28%) 0 0	86, 92, 95, 97	0
7	YH	173/180 (96%)	0.32	5 (2%) 51 50	82, 88, 92, 95	0
8	RI	147/148 (99%)	0.91	30 (20%) 1 1	85, 91, 94, 97	0
8	YI	146/148 (98%)	0.53	11 (7%) 14 13	84, 90, 94, 96	0
9	RN	140/140 (100%)	0.64	10 (7%) 16 16	83, 88, 92, 96	0
9	YN	140/140 (100%)	0.52	1 (0%) 87 88	80, 86, 91, 94	0
10	RO	122/122 (100%)	0.44	1 (0%) 86 86	79, 85, 90, 91	0
10	YO	122/122 (100%)	0.42	1 (0%) 86 86	78, 85, 89, 92	0
11	RP	149/150 (99%)	0.77	6 (4%) 38 36	78, 88, 92, 95	0
11	YP	149/150 (99%)	0.62	5 (3%) 45 43	77, 85, 90, 94	0
12	RQ	141/141 (100%)	0.26	2 (1%) 75 75	82, 87, 91, 93	0
12	YQ	141/141 (100%)	0.36	0 100 100	77, 85, 89, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	RR	118/118 (100%)	0.47	2 (1%) 70 68	81, 86, 89, 91	0
13	YR	118/118 (100%)	0.52	3 (2%) 57 54	80, 85, 89, 92	0
14	RS	110/112 (98%)	0.56	9 (8%) 11 11	84, 89, 93, 95	0
14	YS	110/112 (98%)	0.46	3 (2%) 54 52	82, 88, 91, 94	0
15	RT	131/146 (89%)	0.29	3 (2%) 60 59	82, 87, 91, 95	0
15	YT	131/146 (89%)	0.34	3 (2%) 60 59	82, 86, 92, 95	0
16	RU	116/118 (98%)	0.44	7 (6%) 21 21	82, 87, 92, 93	0
16	YU	116/118 (98%)	0.45	3 (2%) 56 53	78, 84, 90, 91	0
17	RV	101/101 (100%)	0.21	3 (2%) 50 49	81, 89, 92, 95	0
17	YV	101/101 (100%)	0.50	1 (0%) 82 82	80, 86, 91, 93	0
18	RW	112/113 (99%)	0.62	4 (3%) 42 40	80, 85, 90, 95	0
18	YW	112/113 (99%)	0.59	6 (5%) 25 24	78, 84, 90, 95	0
19	RX	95/96 (98%)	0.70	9 (9%) 8 8	83, 87, 90, 93	0
19	YX	95/96 (98%)	0.44	3 (3%) 47 46	79, 84, 89, 94	0
20	RY	107/110 (97%)	1.50	29 (27%) 0 0	85, 90, 93, 100	0
20	YY	107/110 (97%)	0.73	11 (10%) 6 6	82, 88, 92, 98	0
21	RZ	203/206 (98%)	0.92	22 (10%) 5 5	87, 90, 94, 99	0
21	YZ	201/206 (97%)	0.50	17 (8%) 10 10	83, 89, 94, 96	0
22	R0	77/85 (90%)	1.16	14 (18%) 1 1	83, 87, 90, 95	0
22	Y0	77/85 (90%)	0.72	7 (9%) 9 9	80, 85, 90, 95	0
23	R1	97/98 (98%)	0.78	11 (11%) 5 5	82, 86, 92, 94	0
23	Y1	97/98 (98%)	0.81	6 (6%) 20 20	78, 85, 91, 94	0
24	R2	70/72 (97%)	0.38	3 (4%) 35 34	83, 89, 92, 94	0
24	Y2	70/72 (97%)	0.40	2 (2%) 51 50	79, 86, 90, 97	0
25	R3	59/60 (98%)	1.12	9 (15%) 2 2	82, 88, 93, 98	0
25	Y3	59/60 (98%)	0.87	4 (6%) 17 17	79, 85, 91, 95	0
26	R4	69/71 (97%)	1.28	18 (26%) 0 0	89, 93, 96, 97	0
26	Y4	69/71 (97%)	0.69	12 (17%) 1 1	87, 92, 96, 97	0
27	R5	59/60 (98%)	0.41	2 (3%) 45 43	78, 86, 92, 95	0
27	Y5	59/60 (98%)	0.38	2 (3%) 45 43	78, 85, 92, 97	0
28	R6	53/54 (98%)	3.34	41 (77%) 0 0	89, 93, 96, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	Y6	53/54 (98%)	3.02	40 (75%) 0 0	88, 92, 95, 97	0
29	R7	48/49 (97%)	0.74	3 (6%) 20 20	79, 84, 91, 93	0
29	Y7	48/49 (97%)	1.05	4 (8%) 11 11	76, 81, 88, 93	0
30	R8	64/65 (98%)	0.78	2 (3%) 49 48	81, 86, 90, 91	0
30	Y8	64/65 (98%)	0.64	0 100 100	76, 83, 89, 90	0
31	R9	37/37 (100%)	2.39	20 (54%) 0 0	88, 90, 94, 97	0
31	Y9	37/37 (100%)	2.13	19 (51%) 0 0	84, 89, 91, 91	0
32	QA	1488/1521 (97%)	0.10	36 (2%) 59 56	83, 90, 96, 103	0
32	XA	1492/1521 (98%)	0.10	38 (2%) 57 54	78, 90, 96, 101	0
33	QB	231/256 (90%)	0.61	23 (9%) 7 7	88, 92, 95, 97	0
33	XB	231/256 (90%)	0.46	22 (9%) 8 8	87, 91, 95, 98	0
34	QC	206/239 (86%)	0.58	24 (11%) 4 4	88, 91, 94, 96	0
34	XC	206/239 (86%)	0.58	20 (9%) 7 8	87, 90, 93, 96	0
35	QD	208/209 (99%)	0.34	10 (4%) 30 28	85, 89, 93, 97	0
35	XD	208/209 (99%)	0.52	19 (9%) 9 9	85, 90, 94, 97	0
36	QE	148/162 (91%)	0.38	9 (6%) 21 20	85, 90, 93, 95	0
36	XE	148/162 (91%)	0.52	9 (6%) 21 20	85, 88, 92, 94	0
37	QF	100/101 (99%)	0.31	9 (9%) 9 9	87, 90, 93, 95	0
37	XF	100/101 (99%)	0.15	3 (3%) 50 49	83, 89, 93, 95	0
38	QG	155/156 (99%)	0.90	24 (15%) 2 2	88, 91, 94, 96	0
38	XG	155/156 (99%)	0.66	16 (10%) 6 6	87, 91, 95, 96	0
39	QH	137/138 (99%)	0.63	14 (10%) 6 6	86, 89, 92, 94	0
39	XH	137/138 (99%)	0.62	11 (8%) 12 11	82, 89, 92, 94	0
40	QI	127/128 (99%)	1.33	30 (23%) 0 1	86, 92, 95, 96	0
40	XI	126/128 (98%)	0.89	17 (13%) 3 3	85, 92, 95, 98	0
41	QJ	97/105 (92%)	1.33	29 (29%) 0 0	86, 92, 95, 97	0
41	XJ	96/105 (91%)	0.96	15 (15%) 2 2	87, 91, 94, 96	0
42	QK	114/129 (88%)	0.75	12 (10%) 6 6	86, 90, 93, 94	0
42	XK	114/129 (88%)	0.51	4 (3%) 44 42	82, 88, 92, 95	0
43	QL	121/132 (91%)	0.51	6 (4%) 28 27	81, 87, 90, 92	0
43	XL	121/132 (91%)	0.66	10 (8%) 11 11	83, 87, 91, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	QM	116/126 (92%)	0.76	19 (16%) 1 2	88, 92, 95, 97	0
44	XM	114/126 (90%)	0.96	22 (19%) 1 1	87, 91, 94, 95	0
45	QN	60/61 (98%)	1.47	14 (23%) 0 1	87, 91, 94, 95	0
45	XN	60/61 (98%)	0.52	3 (5%) 28 27	88, 90, 93, 95	0
46	QO	88/89 (98%)	0.50	6 (6%) 17 17	86, 89, 93, 94	0
46	XO	88/89 (98%)	0.59	6 (6%) 17 17	84, 89, 92, 94	0
47	QP	82/88 (93%)	1.02	11 (13%) 3 3	84, 89, 91, 93	0
47	XP	82/88 (93%)	0.95	15 (18%) 1 1	86, 90, 92, 95	0
48	QQ	99/105 (94%)	0.69	8 (8%) 12 11	85, 89, 93, 95	0
48	XQ	99/105 (94%)	0.43	3 (3%) 50 49	85, 88, 91, 93	0
49	QR	68/88 (77%)	1.22	14 (20%) 1 1	87, 90, 94, 96	0
49	XR	68/88 (77%)	0.66	3 (4%) 34 33	83, 89, 92, 93	0
50	QS	83/93 (89%)	1.55	26 (31%) 0 0	88, 92, 95, 97	0
50	XS	83/93 (89%)	1.50	24 (28%) 0 0	89, 92, 94, 96	0
51	QT	96/106 (90%)	0.65	6 (6%) 20 20	84, 89, 91, 93	0
51	XT	98/106 (92%)	1.18	17 (17%) 1 1	86, 90, 93, 94	0
52	QU	23/27 (85%)	3.04	20 (86%) 0 0	88, 92, 94, 95	0
52	XU	23/27 (85%)	2.18	13 (56%) 0 0	89, 91, 93, 93	0
53	QV	77/77 (100%)	0.22	3 (3%) 39 37	85, 91, 96, 98	0
53	XV	77/77 (100%)	0.41	5 (6%) 18 18	83, 90, 96, 100	0
54	QY	356/380 (93%)	1.86	144 (40%) 0 0	86, 92, 96, 99	0
54	XY	356/380 (93%)	1.63	120 (33%) 0 0	84, 91, 96, 99	0
55	QX	6/25 (24%)	0.63	0 100 100	87, 90, 91, 92	0
55	XX	6/25 (24%)	0.63	0 100 100	85, 88, 91, 91	0
All	All	21446/22208 (96%)	0.54	1687 (7%) 12 12	71, 88, 95, 103	0

The worst 5 of 1687 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
28	R6	20	ASN	11.5
21	YZ	192	ALA	10.7
20	YY	1	MET	9.1
31	R9	37	GLY	8.8
20	RY	1	MET	8.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	5MU	YA	1915	21/22	0.86	0.21	85,89,92,95	0
32	4OC	XA	1402	22/23	0.89	0.28	83,85,87,89	0
32	4OC	QA	1402	22/23	0.89	0.23	84,87,89,90	0
32	PSU	QA	516	20/21	0.90	0.15	87,89,91,91	0
32	2MG	XA	1207	24/25	0.90	0.22	88,90,95,97	0
32	UR3	QA	1498	21/22	0.90	0.26	80,84,87,92	0
1	5MU	RA	1915	21/22	0.90	0.13	84,89,93,97	0
32	PSU	XA	516	20/21	0.91	0.16	89,90,93,94	0
1	PSU	RA	1917	20/21	0.92	0.16	84,87,91,91	0
32	2MG	QA	1207	24/25	0.92	0.18	89,91,96,97	0
32	M2G	XA	966	25/26	0.92	0.19	83,87,94,94	0
1	5MC	YA	1942	21/22	0.93	0.23	76,81,87,88	0
1	5MC	RA	1942	21/22	0.93	0.23	81,85,88,90	0
1	2MU	YA	2552	21/23	0.93	0.29	74,78,86,87	0
1	4OC	RA	1920	21/23	0.93	0.20	83,85,89,92	0
32	7MG	XA	527	24/25	0.93	0.24	83,86,87,88	0
32	M2G	QA	966	25/26	0.93	0.18	85,87,91,93	0
1	PSU	RA	2605	20/21	0.93	0.26	72,79,84,84	0
1	PSU	YA	1917	20/21	0.93	0.18	81,86,88,89	0
32	MA6	QA	1518	24/25	0.93	0.27	82,86,88,89	0
32	5MC	XA	967	21/22	0.93	0.25	87,88,89,89	0
54	MEQ	QY	252	10/11	0.93	0.32	85,87,90,90	0
32	7MG	QA	527	24/25	0.93	0.21	85,87,87,88	0
1	PSU	YA	2605	20/21	0.94	0.28	69,77,81,83	0
32	5MC	QA	967	21/22	0.94	0.20	83,87,90,93	0
32	MA6	QA	1519	24/25	0.94	0.28	82,85,85,87	0
1	4OC	YA	1920	21/23	0.94	0.23	81,83,85,87	0
54	MEQ	XY	252	10/11	0.94	0.34	86,87,91,91	0
32	5MC	QA	1400	21/22	0.94	0.24	85,89,90,90	0
43	0TD	QL	92	10/11	0.94	0.20	87,90,94,95	0
1	5MC	RA	1962	21/22	0.94	0.18	76,84,87,87	0
32	5MC	QA	1404	21/22	0.94	0.20	83,86,88,88	0
32	5MC	XA	1407	21/22	0.94	0.22	81,84,89,91	0
1	2MA	YA	2503	23/24	0.94	0.29	72,78,79,81	0
1	PSU	RA	1911	20/21	0.95	0.14	82,85,88,89	0
1	PSU	YA	1911	20/21	0.95	0.18	79,85,88,90	0
1	5MU	YA	1939	21/22	0.95	0.27	72,77,82,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	2MA	RA	2503	23/24	0.95	0.25	75,81,83,84	0
1	2MU	RA	2552	21/23	0.95	0.27	75,82,84,87	0
43	0TD	XL	92	10/11	0.95	0.26	85,89,93,95	0
32	5MC	XA	1400	21/22	0.95	0.21	78,85,86,88	0
1	5MU	RA	1939	21/22	0.95	0.23	76,82,84,85	0
1	OMG	RA	2251	24/25	0.95	0.27	80,83,85,85	0
32	5MC	QA	1407	21/22	0.96	0.16	80,83,85,86	0
32	5MC	XA	1404	21/22	0.96	0.18	79,84,85,87	0
1	5MC	YA	1962	21/22	0.96	0.19	73,81,85,85	0
32	UR3	XA	1498	21/22	0.96	0.22	74,83,87,88	0
32	MA6	XA	1518	24/25	0.96	0.29	70,82,82,83	0
32	MA6	XA	1519	24/25	0.96	0.27	76,83,84,86	0
1	OMG	YA	2251	24/25	0.97	0.28	72,78,83,84	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3670	1/1	-0.72	1.67	103,103,103,103	0
56	MG	YG	201	1/1	-0.60	2.02	103,103,103,103	0
56	MG	YA	3208	1/1	-0.55	1.37	102,102,102,102	0
56	MG	QA	1769	1/1	-0.54	1.08	99,99,99,99	0
56	MG	YA	3267	1/1	-0.52	1.71	102,102,102,102	0
56	MG	QA	1722	1/1	-0.51	0.98	93,93,93,93	0
56	MG	RH	201	1/1	-0.49	0.82	89,89,89,89	0
56	MG	QA	1855	1/1	-0.48	0.74	106,106,106,106	0
56	MG	QA	1733	1/1	-0.46	0.77	94,94,94,94	0
56	MG	XA	1617	1/1	-0.45	1.65	100,100,100,100	0
56	MG	RF	309	1/1	-0.42	0.85	103,103,103,103	0
56	MG	RA	3171	1/1	-0.40	0.92	92,92,92,92	0
56	MG	YA	3433	1/1	-0.37	0.75	97,97,97,97	0
56	MG	RA	3548	1/1	-0.37	0.94	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3512	1/1	-0.35	0.94	94,94,94,94	0
56	MG	RA	3783	1/1	-0.35	0.71	96,96,96,96	0
56	MG	YA	3509	1/1	-0.35	0.79	97,97,97,97	0
56	MG	QA	1873	1/1	-0.34	1.73	91,91,91,91	0
56	MG	XA	1728	1/1	-0.32	0.41	84,84,84,84	0
56	MG	RA	3371	1/1	-0.32	1.54	97,97,97,97	0
56	MG	YA	3695	1/1	-0.31	1.26	88,88,88,88	0
56	MG	RT	203	1/1	-0.29	2.38	100,100,100,100	0
56	MG	RA	4069	1/1	-0.29	1.53	86,86,86,86	0
56	MG	RA	3482	1/1	-0.27	0.33	100,100,100,100	0
56	MG	YA	3035	1/1	-0.27	1.00	93,93,93,93	0
56	MG	RA	3748	1/1	-0.26	0.49	86,86,86,86	0
56	MG	R4	102	1/1	-0.26	0.52	97,97,97,97	0
56	MG	RN	202	1/1	-0.26	2.07	102,102,102,102	0
56	MG	RA	3959	1/1	-0.25	0.92	97,97,97,97	0
56	MG	YA	3163	1/1	-0.24	2.14	99,99,99,99	0
56	MG	YA	3078	1/1	-0.24	0.65	97,97,97,97	0
56	MG	RF	301	1/1	-0.24	0.83	99,99,99,99	0
56	MG	QA	1664	1/1	-0.24	1.43	91,91,91,91	0
56	MG	RA	3737	1/1	-0.23	1.18	84,84,84,84	0
56	MG	R5	105	1/1	-0.23	1.69	95,95,95,95	0
56	MG	RP	202	1/1	-0.23	0.48	98,98,98,98	0
56	MG	RB	203	1/1	-0.22	0.93	102,102,102,102	0
56	MG	RA	3067	1/1	-0.21	1.48	100,100,100,100	0
56	MG	RB	227	1/1	-0.20	0.37	88,88,88,88	0
56	MG	YA	3461	1/1	-0.19	0.91	87,87,87,87	0
56	MG	QA	1795	1/1	-0.18	1.25	97,97,97,97	0
56	MG	XA	1674	1/1	-0.17	1.35	94,94,94,94	0
56	MG	QA	1834	1/1	-0.17	0.93	97,97,97,97	0
56	MG	RA	3440	1/1	-0.17	1.19	89,89,89,89	0
56	MG	XA	1662	1/1	-0.17	0.37	97,97,97,97	0
56	MG	QG	203	1/1	-0.15	1.48	97,97,97,97	0
56	MG	XA	1754	1/1	-0.15	1.24	88,88,88,88	0
56	MG	YA	3530	1/1	-0.14	0.59	102,102,102,102	0
56	MG	R5	102	1/1	-0.14	0.54	97,97,97,97	0
56	MG	RA	3498	1/1	-0.14	0.57	83,83,83,83	0
56	MG	QA	1771	1/1	-0.14	1.08	93,93,93,93	0
56	MG	QA	1700	1/1	-0.13	1.00	94,94,94,94	0
56	MG	YB	205	1/1	-0.13	0.92	93,93,93,93	0
56	MG	XE	201	1/1	-0.13	0.99	93,93,93,93	0
56	MG	YA	3599	1/1	-0.13	0.96	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	QA	1748	1/1	-0.13	1.49	98,98,98,98	0
56	MG	RA	3629	1/1	-0.13	0.85	88,88,88,88	0
56	MG	YA	3308	1/1	-0.13	1.09	92,92,92,92	0
56	MG	RA	3352	1/1	-0.12	0.80	97,97,97,97	0
56	MG	YA	3289	1/1	-0.11	1.36	92,92,92,92	0
56	MG	QY	402	1/1	-0.11	1.11	92,92,92,92	0
56	MG	QA	1736	1/1	-0.11	1.42	82,82,82,82	0
56	MG	YF	301	1/1	-0.11	0.45	94,94,94,94	0
56	MG	YA	3484	1/1	-0.11	0.63	99,99,99,99	0
56	MG	XA	1712	1/1	-0.11	0.71	96,96,96,96	0
56	MG	RA	4011	1/1	-0.10	0.38	102,102,102,102	0
56	MG	XH	201	1/1	-0.10	0.60	99,99,99,99	0
56	MG	YA	3161	1/1	-0.10	1.02	91,91,91,91	0
56	MG	QA	1757	1/1	-0.10	0.58	102,102,102,102	0
56	MG	YA	3086	1/1	-0.10	0.76	92,92,92,92	0
56	MG	QA	1852	1/1	-0.10	1.03	84,84,84,84	0
56	MG	QA	1816	1/1	-0.09	0.57	98,98,98,98	0
56	MG	XA	1698	1/1	-0.09	1.09	87,87,87,87	0
56	MG	RA	3039	1/1	-0.09	1.10	97,97,97,97	0
56	MG	RA	3547	1/1	-0.09	0.61	99,99,99,99	0
56	MG	YA	3147	1/1	-0.08	1.01	86,86,86,86	0
56	MG	Y0	101	1/1	-0.08	1.09	78,78,78,78	0
56	MG	RA	3885	1/1	-0.08	0.46	98,98,98,98	0
56	MG	QA	1879	1/1	-0.07	1.41	105,105,105,105	0
56	MG	R3	101	1/1	-0.07	1.30	87,87,87,87	0
56	MG	RA	3033	1/1	-0.07	0.48	100,100,100,100	0
56	MG	XA	1672	1/1	-0.06	1.00	95,95,95,95	0
56	MG	RA	3531	1/1	-0.06	0.58	90,90,90,90	0
56	MG	YA	3059	1/1	-0.06	1.01	86,86,86,86	0
56	MG	RA	3042	1/1	-0.06	0.74	92,92,92,92	0
56	MG	RA	3829	1/1	-0.05	1.55	96,96,96,96	0
56	MG	RA	3054	1/1	-0.05	0.86	94,94,94,94	0
56	MG	XA	1623	1/1	-0.04	0.50	83,83,83,83	0
56	MG	YA	3306	1/1	-0.04	0.99	87,87,87,87	0
56	MG	YA	3458	1/1	-0.04	1.00	88,88,88,88	0
56	MG	RA	3537	1/1	-0.04	1.02	84,84,84,84	0
56	MG	RA	3677	1/1	-0.04	1.12	86,86,86,86	0
56	MG	QA	1745	1/1	-0.03	0.89	82,82,82,82	0
56	MG	QA	1668	1/1	-0.02	0.85	92,92,92,92	0
56	MG	XY	401	1/1	-0.02	1.97	97,97,97,97	0
56	MG	QA	1705	1/1	-0.02	1.00	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3486	1/1	-0.02	1.11	105,105,105,105	0
56	MG	RA	3653	1/1	-0.02	1.12	100,100,100,100	0
56	MG	RA	3968	1/1	-0.01	0.98	84,84,84,84	0
56	MG	RA	3368	1/1	-0.01	0.68	90,90,90,90	0
56	MG	YA	3175	1/1	-0.01	1.24	101,101,101,101	0
56	MG	RR	202	1/1	-0.01	0.59	87,87,87,87	0
56	MG	YA	3222	1/1	0.00	0.74	88,88,88,88	0
56	MG	RA	3196	1/1	0.00	0.51	114,114,114,114	0
56	MG	QN	102	1/1	0.00	0.88	90,90,90,90	0
56	MG	RA	3578	1/1	-0.00	0.88	90,90,90,90	0
56	MG	YA	3356	1/1	0.00	0.28	85,85,85,85	0
56	MG	QA	1818	1/1	-0.00	0.58	93,93,93,93	0
56	MG	RA	3797	1/1	0.01	0.44	109,109,109,109	0
56	MG	YA	3205	1/1	0.01	2.40	86,86,86,86	0
56	MG	RA	3036	1/1	0.01	0.85	94,94,94,94	0
56	MG	YA	3112	1/1	0.02	0.72	85,85,85,85	0
56	MG	RA	3716	1/1	0.02	0.37	91,91,91,91	0
56	MG	YA	3525	1/1	0.02	1.07	88,88,88,88	0
56	MG	RA	3467	1/1	0.02	0.66	89,89,89,89	0
56	MG	YA	3327	1/1	0.02	1.00	85,85,85,85	0
56	MG	R3	102	1/1	0.02	0.87	102,102,102,102	0
56	MG	QA	1869	1/1	0.02	1.38	105,105,105,105	0
56	MG	RA	3213	1/1	0.03	0.73	112,112,112,112	0
56	MG	YA	3084	1/1	0.03	1.21	101,101,101,101	0
56	MG	YA	3471	1/1	0.03	0.98	99,99,99,99	0
56	MG	RA	3848	1/1	0.03	1.02	91,91,91,91	0
56	MG	YA	3033	1/1	0.03	0.52	99,99,99,99	0
56	MG	RA	3886	1/1	0.03	0.56	97,97,97,97	0
56	MG	YA	3211	1/1	0.04	1.03	98,98,98,98	0
56	MG	QA	1713	1/1	0.04	0.72	95,95,95,95	0
56	MG	YA	3164	1/1	0.04	1.21	98,98,98,98	0
56	MG	RA	3513	1/1	0.04	1.32	87,87,87,87	0
56	MG	RA	3628	1/1	0.04	1.21	89,89,89,89	0
56	MG	RA	3172	1/1	0.04	0.72	105,105,105,105	0
56	MG	YA	3506	1/1	0.06	1.07	95,95,95,95	0
56	MG	YA	3070	1/1	0.06	0.72	99,99,99,99	0
56	MG	RA	3525	1/1	0.06	0.98	92,92,92,92	0
56	MG	RA	3690	1/1	0.06	0.84	90,90,90,90	0
56	MG	YA	3050	1/1	0.06	0.68	92,92,92,92	0
56	MG	QA	1819	1/1	0.06	0.82	83,83,83,83	0
56	MG	QA	1738	1/1	0.06	0.77	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3170	1/1	0.06	0.52	92,92,92,92	0
56	MG	RA	3316	1/1	0.06	0.81	93,93,93,93	0
56	MG	RA	3218	1/1	0.07	0.47	88,88,88,88	0
56	MG	YI	201	1/1	0.07	0.37	94,94,94,94	0
56	MG	YA	3309	1/1	0.07	1.03	90,90,90,90	0
56	MG	RA	3400	1/1	0.07	0.80	101,101,101,101	0
56	MG	YA	3041	1/1	0.07	0.90	96,96,96,96	0
56	MG	RA	3179	1/1	0.08	0.99	105,105,105,105	0
56	MG	RA	3244	1/1	0.08	1.24	98,98,98,98	0
56	MG	RA	3526	1/1	0.08	0.84	89,89,89,89	0
56	MG	XA	1652	1/1	0.08	0.68	92,92,92,92	0
56	MG	QG	201	1/1	0.08	0.87	101,101,101,101	0
56	MG	RA	3425	1/1	0.08	1.09	91,91,91,91	0
56	MG	XA	1697	1/1	0.08	0.20	87,87,87,87	0
56	MG	XA	1749	1/1	0.09	1.01	98,98,98,98	0
56	MG	YA	3186	1/1	0.09	0.40	106,106,106,106	0
56	MG	RA	4058	1/1	0.09	0.92	96,96,96,96	0
56	MG	RD	308	1/1	0.09	0.61	83,83,83,83	0
56	MG	RA	3448	1/1	0.09	1.18	87,87,87,87	0
56	MG	QA	1847	1/1	0.09	1.27	94,94,94,94	0
56	MG	RA	3819	1/1	0.09	0.92	90,90,90,90	0
56	MG	RR	203	1/1	0.09	0.47	81,81,81,81	0
56	MG	YA	3152	1/1	0.10	1.07	83,83,83,83	0
56	MG	YA	3167	1/1	0.10	1.02	87,87,87,87	0
56	MG	RA	3927	1/1	0.10	0.96	91,91,91,91	0
56	MG	QA	1682	1/1	0.10	0.53	87,87,87,87	0
56	MG	RA	3600	1/1	0.11	0.93	94,94,94,94	0
56	MG	RA	3879	1/1	0.11	0.96	93,93,93,93	0
56	MG	XA	1601	1/1	0.11	0.89	93,93,93,93	0
56	MG	YA	3435	1/1	0.11	1.10	87,87,87,87	0
56	MG	RA	3066	1/1	0.11	0.78	104,104,104,104	0
56	MG	QL	202	1/1	0.12	0.46	82,82,82,82	0
56	MG	YA	3457	1/1	0.12	0.64	87,87,87,87	0
56	MG	YA	3518	1/1	0.12	0.89	70,70,70,70	0
56	MG	YA	3723	1/1	0.12	1.35	89,89,89,89	0
56	MG	YA	3177	1/1	0.12	0.61	95,95,95,95	0
56	MG	R9	101	1/1	0.12	0.47	100,100,100,100	0
56	MG	YA	3504	1/1	0.12	0.54	93,93,93,93	0
56	MG	YA	3233	1/1	0.12	0.44	96,96,96,96	0
56	MG	RA	3138	1/1	0.12	0.51	79,79,79,79	0
56	MG	RA	3872	1/1	0.12	0.59	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	QH	201	1/1	0.13	0.50	87,87,87,87	0
56	MG	YA	3714	1/1	0.13	0.63	85,85,85,85	0
56	MG	RA	3435	1/1	0.13	0.68	75,75,75,75	0
56	MG	QA	1862	1/1	0.13	0.67	82,82,82,82	0
56	MG	YA	3230	1/1	0.13	0.50	92,92,92,92	0
56	MG	YB	206	1/1	0.13	0.85	89,89,89,89	0
56	MG	QA	1860	1/1	0.13	0.83	92,92,92,92	0
56	MG	YA	3312	1/1	0.14	1.26	80,80,80,80	0
56	MG	RA	3296	1/1	0.14	0.70	91,91,91,91	0
56	MG	YA	3524	1/1	0.14	0.83	85,85,85,85	0
56	MG	YA	3367	1/1	0.14	0.27	76,76,76,76	0
56	MG	YA	3493	1/1	0.14	0.84	86,86,86,86	0
56	MG	RA	3225	1/1	0.14	0.97	111,111,111,111	0
56	MG	RA	3728	1/1	0.14	0.76	99,99,99,99	0
56	MG	RA	3828	1/1	0.14	0.49	84,84,84,84	0
56	MG	RA	3609	1/1	0.14	1.12	90,90,90,90	0
56	MG	YA	3549	1/1	0.15	0.71	90,90,90,90	0
56	MG	RA	3106	1/1	0.15	0.56	107,107,107,107	0
56	MG	RA	3365	1/1	0.15	0.61	88,88,88,88	0
56	MG	RA	3778	1/1	0.15	0.48	105,105,105,105	0
56	MG	YA	3463	1/1	0.15	0.91	86,86,86,86	0
56	MG	RA	3198	1/1	0.15	3.00	98,98,98,98	0
56	MG	RA	3027	1/1	0.15	0.84	112,112,112,112	0
56	MG	RA	4057	1/1	0.15	1.27	97,97,97,97	0
56	MG	QA	1636	1/1	0.16	0.55	90,90,90,90	0
56	MG	RA	3134	1/1	0.16	0.99	96,96,96,96	0
56	MG	RA	3618	1/1	0.16	0.82	88,88,88,88	0
56	MG	RA	3181	1/1	0.16	0.82	86,86,86,86	0
56	MG	RA	3787	1/1	0.16	0.79	88,88,88,88	0
56	MG	RA	3438	1/1	0.16	0.82	91,91,91,91	0
56	MG	YA	3425	1/1	0.16	0.55	88,88,88,88	0
56	MG	YA	3603	1/1	0.17	1.23	82,82,82,82	0
56	MG	QA	1697	1/1	0.17	0.69	88,88,88,88	0
56	MG	QA	1832	1/1	0.17	0.40	84,84,84,84	0
56	MG	XA	1620	1/1	0.17	0.17	93,93,93,93	0
56	MG	RA	3309	1/1	0.17	0.90	93,93,93,93	0
56	MG	XA	1669	1/1	0.17	0.62	106,106,106,106	0
56	MG	RA	3804	1/1	0.17	0.51	92,92,92,92	0
56	MG	RA	4065	1/1	0.17	1.01	91,91,91,91	0
56	MG	RA	3008	1/1	0.17	0.22	83,83,83,83	0
56	MG	YA	3244	1/1	0.17	1.19	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RF	311	1/1	0.17	0.68	94,94,94,94	0
56	MG	RA	3251	1/1	0.17	0.88	82,82,82,82	0
56	MG	RA	4054	1/1	0.17	1.94	91,91,91,91	0
56	MG	YA	3017	1/1	0.18	0.63	91,91,91,91	0
56	MG	RA	3999	1/1	0.18	0.42	98,98,98,98	0
56	MG	RT	202	1/1	0.18	0.81	87,87,87,87	0
56	MG	RA	3876	1/1	0.18	0.90	92,92,92,92	0
56	MG	RA	3684	1/1	0.18	0.52	93,93,93,93	0
56	MG	RA	3247	1/1	0.18	0.86	89,89,89,89	0
56	MG	RA	3952	1/1	0.18	0.52	96,96,96,96	0
56	MG	RA	3603	1/1	0.18	1.54	90,90,90,90	0
56	MG	QA	1694	1/1	0.18	0.77	91,91,91,91	0
56	MG	RA	3960	1/1	0.18	0.72	92,92,92,92	0
56	MG	RA	3427	1/1	0.18	0.46	90,90,90,90	0
56	MG	YA	3469	1/1	0.19	0.63	91,91,91,91	0
56	MG	YA	3403	1/1	0.19	0.35	81,81,81,81	0
56	MG	YA	3452	1/1	0.19	0.88	84,84,84,84	0
56	MG	QA	1640	1/1	0.20	0.71	99,99,99,99	0
56	MG	YA	3507	1/1	0.20	0.79	80,80,80,80	0
56	MG	XF	203	1/1	0.20	2.52	103,103,103,103	0
56	MG	YQ	202	1/1	0.20	0.70	89,89,89,89	0
56	MG	RA	3841	1/1	0.20	0.95	91,91,91,91	0
56	MG	YA	3427	1/1	0.20	0.58	88,88,88,88	0
56	MG	RA	3227	1/1	0.20	1.13	103,103,103,103	0
56	MG	RA	3495	1/1	0.20	0.84	83,83,83,83	0
56	MG	QA	1728	1/1	0.20	0.35	80,80,80,80	0
56	MG	RA	3693	1/1	0.20	0.99	102,102,102,102	0
56	MG	RA	3925	1/1	0.20	0.33	95,95,95,95	0
56	MG	YA	3094	1/1	0.21	0.25	77,77,77,77	0
56	MG	YA	3311	1/1	0.21	0.86	73,73,73,73	0
56	MG	RA	3840	1/1	0.21	1.95	97,97,97,97	0
56	MG	RA	3808	1/1	0.21	0.76	85,85,85,85	0
56	MG	XA	1729	1/1	0.21	0.74	83,83,83,83	0
56	MG	RA	3606	1/1	0.21	0.64	87,87,87,87	0
56	MG	XA	1605	1/1	0.21	1.09	96,96,96,96	0
56	MG	RA	4019	1/1	0.21	1.37	103,103,103,103	0
56	MG	QA	1858	1/1	0.21	0.82	86,86,86,86	0
56	MG	QA	1853	1/1	0.21	0.76	89,89,89,89	0
56	MG	R8	101	1/1	0.21	0.88	90,90,90,90	0
56	MG	RA	3499	1/1	0.22	1.29	80,80,80,80	0
56	MG	YA	3394	1/1	0.22	0.93	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3904	1/1	0.22	0.65	80,80,80,80	0
56	MG	YA	3344	1/1	0.22	0.20	90,90,90,90	0
56	MG	YA	3694	1/1	0.22	0.88	82,82,82,82	0
56	MG	YA	3027	1/1	0.22	0.91	83,83,83,83	0
56	MG	RA	3398	1/1	0.23	0.73	80,80,80,80	0
56	MG	QA	1831	1/1	0.23	0.82	99,99,99,99	0
56	MG	YA	3633	1/1	0.23	1.20	95,95,95,95	0
56	MG	XA	1715	1/1	0.23	0.96	94,94,94,94	0
56	MG	RA	3197	1/1	0.23	0.56	100,100,100,100	0
56	MG	QA	1854	1/1	0.23	0.97	94,94,94,94	0
56	MG	RA	3825	1/1	0.23	0.83	85,85,85,85	0
56	MG	QA	1799	1/1	0.23	0.66	99,99,99,99	0
56	MG	RA	3941	1/1	0.23	0.77	87,87,87,87	0
56	MG	RA	3250	1/1	0.23	0.93	84,84,84,84	0
56	MG	YA	3185	1/1	0.23	0.68	99,99,99,99	0
56	MG	RA	3798	1/1	0.23	0.74	93,93,93,93	0
56	MG	RA	3205	1/1	0.24	1.13	87,87,87,87	0
56	MG	QA	1808	1/1	0.24	0.38	74,74,74,74	0
56	MG	RA	3115	1/1	0.24	0.41	78,78,78,78	0
56	MG	QA	1611	1/1	0.24	1.18	80,80,80,80	0
56	MG	RA	3995	1/1	0.24	0.46	91,91,91,91	0
56	MG	XA	1657	1/1	0.24	0.97	91,91,91,91	0
56	MG	RB	211	1/1	0.24	0.45	89,89,89,89	0
56	MG	RA	3648	1/1	0.24	0.29	97,97,97,97	0
56	MG	QA	1768	1/1	0.24	0.54	89,89,89,89	0
56	MG	YA	3218	1/1	0.24	0.56	82,82,82,82	0
56	MG	RA	3824	1/1	0.24	0.61	92,92,92,92	0
56	MG	RD	310	1/1	0.24	0.91	86,86,86,86	0
56	MG	RA	3079	1/1	0.24	0.80	111,111,111,111	0
56	MG	RA	3428	1/1	0.24	0.82	92,92,92,92	0
56	MG	YA	3505	1/1	0.24	0.75	88,88,88,88	0
56	MG	QA	1838	1/1	0.24	0.52	87,87,87,87	0
56	MG	YA	3710	1/1	0.25	1.18	80,80,80,80	0
56	MG	QA	1840	1/1	0.25	0.60	88,88,88,88	0
56	MG	YA	3297	1/1	0.25	0.35	70,70,70,70	0
56	MG	XA	1602	1/1	0.25	1.04	88,88,88,88	0
56	MG	YA	3173	1/1	0.25	0.58	99,99,99,99	0
56	MG	RA	3076	1/1	0.25	1.20	96,96,96,96	0
56	MG	QA	1642	1/1	0.25	1.32	101,101,101,101	0
56	MG	YA	3291	1/1	0.25	0.84	88,88,88,88	0
56	MG	RA	3833	1/1	0.25	0.53	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3962	1/1	0.25	1.22	95,95,95,95	0
56	MG	YA	3541	1/1	0.25	0.43	94,94,94,94	0
56	MG	XA	1691	1/1	0.25	0.40	84,84,84,84	0
56	MG	R7	101	1/1	0.25	0.54	88,88,88,88	0
56	MG	XA	1638	1/1	0.25	0.83	98,98,98,98	0
56	MG	QA	1704	1/1	0.25	0.77	89,89,89,89	0
56	MG	YA	3739	1/1	0.25	0.77	75,75,75,75	0
56	MG	YA	3408	1/1	0.25	0.81	90,90,90,90	0
56	MG	RG	204	1/1	0.25	0.18	84,84,84,84	0
56	MG	YA	3025	1/1	0.25	0.88	74,74,74,74	0
56	MG	YA	3531	1/1	0.25	1.32	80,80,80,80	0
56	MG	RA	3700	1/1	0.26	0.89	104,104,104,104	0
56	MG	YA	3474	1/1	0.26	0.44	78,78,78,78	0
56	MG	YA	3030	1/1	0.26	0.59	88,88,88,88	0
56	MG	YA	3090	1/1	0.26	0.32	100,100,100,100	0
56	MG	YE	303	1/1	0.26	0.44	93,93,93,93	0
56	MG	YA	3421	1/1	0.26	0.55	82,82,82,82	0
56	MG	YA	3561	1/1	0.26	1.18	89,89,89,89	0
56	MG	RG	203	1/1	0.26	0.81	83,83,83,83	0
56	MG	YA	3258	1/1	0.26	0.72	86,86,86,86	0
56	MG	YA	3320	1/1	0.26	1.08	87,87,87,87	0
56	MG	RA	3111	1/1	0.27	0.43	100,100,100,100	0
56	MG	YA	3227	1/1	0.27	1.12	87,87,87,87	0
56	MG	YA	3109	1/1	0.27	0.62	85,85,85,85	0
56	MG	YA	3055	1/1	0.27	0.36	88,88,88,88	0
56	MG	YA	3447	1/1	0.27	0.56	80,80,80,80	0
56	MG	QA	1807	1/1	0.27	0.55	95,95,95,95	0
56	MG	RA	3568	1/1	0.27	0.54	89,89,89,89	0
56	MG	YA	3397	1/1	0.27	0.65	75,75,75,75	0
56	MG	RA	4053	1/1	0.27	1.72	103,103,103,103	0
56	MG	QA	1681	1/1	0.27	1.11	92,92,92,92	0
56	MG	RA	3813	1/1	0.28	1.07	107,107,107,107	0
56	MG	RA	3099	1/1	0.28	0.66	94,94,94,94	0
56	MG	XA	1624	1/1	0.28	0.89	85,85,85,85	0
56	MG	YA	3168	1/1	0.28	0.90	100,100,100,100	0
56	MG	YA	3722	1/1	0.28	0.89	93,93,93,93	0
56	MG	RA	3434	1/1	0.28	0.60	85,85,85,85	0
56	MG	RA	3458	1/1	0.28	0.90	84,84,84,84	0
56	MG	RA	3174	1/1	0.28	1.01	85,85,85,85	0
56	MG	QA	1793	1/1	0.28	0.79	93,93,93,93	0
56	MG	YA	3075	1/1	0.29	1.80	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3432	1/1	0.29	0.74	77,77,77,77	0
56	MG	RQ	203	1/1	0.29	0.84	96,96,96,96	0
56	MG	YA	3352	1/1	0.29	0.13	88,88,88,88	0
56	MG	RA	3899	1/1	0.29	0.87	93,93,93,93	0
56	MG	QA	1794	1/1	0.29	0.79	72,72,72,72	0
56	MG	YA	3250	1/1	0.29	0.37	103,103,103,103	0
56	MG	YA	3108	1/1	0.29	0.62	90,90,90,90	0
56	MG	YA	3064	1/1	0.29	0.52	86,86,86,86	0
56	MG	QA	1637	1/1	0.29	0.84	85,85,85,85	0
56	MG	RA	3090	1/1	0.29	0.71	84,84,84,84	0
56	MG	QA	1877	1/1	0.30	0.69	92,92,92,92	0
56	MG	RA	3085	1/1	0.30	0.86	91,91,91,91	0
56	MG	RA	3806	1/1	0.30	0.73	90,90,90,90	0
56	MG	RA	3703	1/1	0.30	0.49	95,95,95,95	0
56	MG	RA	3682	1/1	0.30	0.44	104,104,104,104	0
56	MG	XA	1690	1/1	0.30	0.78	94,94,94,94	0
56	MG	RU	202	1/1	0.30	0.67	94,94,94,94	0
56	MG	RA	3963	1/1	0.30	0.71	88,88,88,88	0
56	MG	RA	3709	1/1	0.30	0.57	91,91,91,91	0
56	MG	RA	3764	1/1	0.30	0.47	77,77,77,77	0
56	MG	RB	208	1/1	0.30	0.34	95,95,95,95	0
56	MG	YA	3462	1/1	0.31	0.86	97,97,97,97	0
56	MG	QY	401	1/1	0.31	0.68	90,90,90,90	0
56	MG	YA	3188	1/1	0.31	0.28	92,92,92,92	0
56	MG	XA	1651	1/1	0.31	1.55	96,96,96,96	0
56	MG	RA	3192	1/1	0.31	0.37	83,83,83,83	0
56	MG	RA	3951	1/1	0.31	0.76	85,85,85,85	0
56	MG	YA	3716	1/1	0.31	0.90	87,87,87,87	0
56	MG	R1	102	1/1	0.31	0.92	83,83,83,83	0
56	MG	RA	4010	1/1	0.31	1.60	79,79,79,79	0
56	MG	YA	3551	1/1	0.31	0.50	73,73,73,73	0
56	MG	QA	1647	1/1	0.31	0.25	101,101,101,101	0
56	MG	RA	3957	1/1	0.31	0.51	79,79,79,79	0
56	MG	RA	3676	1/1	0.32	0.29	84,84,84,84	0
56	MG	RA	3649	1/1	0.32	0.47	94,94,94,94	0
56	MG	XA	1686	1/1	0.32	0.64	96,96,96,96	0
56	MG	RA	3827	1/1	0.32	0.69	81,81,81,81	0
56	MG	YA	3574	1/1	0.32	0.82	86,86,86,86	0
56	MG	RA	3631	1/1	0.32	1.07	94,94,94,94	0
56	MG	YA	3497	1/1	0.32	0.58	95,95,95,95	0
56	MG	RA	3433	1/1	0.32	0.91	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	R0	102	1/1	0.32	0.57	88,88,88,88	0
56	MG	RA	3522	1/1	0.32	0.35	84,84,84,84	0
56	MG	RA	3137	1/1	0.32	1.17	102,102,102,102	0
56	MG	RA	3156	1/1	0.32	0.59	105,105,105,105	0
56	MG	YA	3414	1/1	0.33	0.71	92,92,92,92	0
56	MG	RA	3564	1/1	0.33	0.76	91,91,91,91	0
56	MG	QA	1780	1/1	0.33	1.33	80,80,80,80	0
56	MG	YA	3663	1/1	0.33	1.32	98,98,98,98	0
56	MG	YA	3581	1/1	0.33	0.59	80,80,80,80	0
56	MG	QD	301	1/1	0.33	1.27	94,94,94,94	0
56	MG	RA	3164	1/1	0.33	0.80	100,100,100,100	0
56	MG	QA	1764	1/1	0.33	1.27	83,83,83,83	0
56	MG	RB	204	1/1	0.34	0.26	85,85,85,85	0
56	MG	QA	1698	1/1	0.34	0.73	97,97,97,97	0
56	MG	RA	3686	1/1	0.34	0.73	97,97,97,97	0
56	MG	QA	1842	1/1	0.34	0.78	95,95,95,95	0
56	MG	XA	1775	1/1	0.34	0.72	98,98,98,98	0
56	MG	RA	3559	1/1	0.34	0.72	84,84,84,84	0
56	MG	RA	3918	1/1	0.34	0.94	93,93,93,93	0
56	MG	RA	3150	1/1	0.34	0.27	84,84,84,84	0
56	MG	RA	3246	1/1	0.34	0.75	84,84,84,84	0
56	MG	YA	3752	1/1	0.34	1.10	100,100,100,100	0
56	MG	YA	3496	1/1	0.34	1.39	85,85,85,85	0
56	MG	QA	1867	1/1	0.34	0.74	96,96,96,96	0
56	MG	RA	3058	1/1	0.34	0.77	89,89,89,89	0
56	MG	QA	1696	1/1	0.34	0.82	71,71,71,71	0
56	MG	YA	3719	1/1	0.34	0.25	89,89,89,89	0
56	MG	YA	3032	1/1	0.35	0.72	93,93,93,93	0
56	MG	YA	3556	1/1	0.35	0.55	73,73,73,73	0
56	MG	RA	3943	1/1	0.35	0.63	91,91,91,91	0
56	MG	RA	3123	1/1	0.35	0.37	80,80,80,80	0
56	MG	RA	3278	1/1	0.35	0.97	89,89,89,89	0
56	MG	RA	3437	1/1	0.35	1.16	77,77,77,77	0
56	MG	RA	3040	1/1	0.35	0.72	97,97,97,97	0
56	MG	YA	3201	1/1	0.35	0.29	90,90,90,90	0
56	MG	RA	3057	1/1	0.36	0.58	96,96,96,96	0
56	MG	RA	3176	1/1	0.36	1.01	102,102,102,102	0
56	MG	RR	201	1/1	0.36	0.77	98,98,98,98	0
56	MG	QA	1751	1/1	0.36	1.17	78,78,78,78	0
56	MG	RA	3760	1/1	0.36	0.80	98,98,98,98	0
56	MG	RA	3572	1/1	0.36	0.57	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	4003	1/1	0.36	0.81	92,92,92,92	0
56	MG	XA	1701	1/1	0.36	0.45	74,74,74,74	0
56	MG	RA	3775	1/1	0.36	1.34	94,94,94,94	0
56	MG	RA	3727	1/1	0.36	0.54	78,78,78,78	0
56	MG	RA	4031	1/1	0.36	0.50	108,108,108,108	0
56	MG	YA	3219	1/1	0.37	0.60	95,95,95,95	0
56	MG	RV	201	1/1	0.37	0.30	100,100,100,100	0
56	MG	YA	3411	1/1	0.37	0.64	90,90,90,90	0
56	MG	QA	1680	1/1	0.37	0.52	84,84,84,84	0
56	MG	YA	3299	1/1	0.37	0.49	64,64,64,64	0
56	MG	RA	3105	1/1	0.37	1.09	92,92,92,92	0
56	MG	QA	1859	1/1	0.37	0.81	85,85,85,85	0
56	MG	RA	3546	1/1	0.37	0.57	95,95,95,95	0
56	MG	RA	3528	1/1	0.37	1.11	81,81,81,81	0
56	MG	QA	1778	1/1	0.37	0.67	88,88,88,88	0
56	MG	XA	1788	1/1	0.37	0.67	95,95,95,95	0
56	MG	YA	3562	1/1	0.37	0.52	82,82,82,82	0
56	MG	QA	1735	1/1	0.37	0.59	93,93,93,93	0
56	MG	RA	3487	1/1	0.37	0.74	83,83,83,83	0
56	MG	RA	3397	1/1	0.37	0.69	76,76,76,76	0
56	MG	RA	3219	1/1	0.37	1.34	88,88,88,88	0
56	MG	QA	1685	1/1	0.38	0.31	89,89,89,89	0
56	MG	RA	3791	1/1	0.38	0.46	84,84,84,84	0
56	MG	RA	4047	1/1	0.38	0.70	97,97,97,97	0
56	MG	YA	3193	1/1	0.38	0.47	85,85,85,85	0
56	MG	QA	1630	1/1	0.38	1.45	79,79,79,79	0
56	MG	YA	3705	1/1	0.38	1.20	78,78,78,78	0
56	MG	RA	3590	1/1	0.38	0.72	100,100,100,100	0
56	MG	RA	3131	1/1	0.38	0.14	88,88,88,88	0
56	MG	RA	3536	1/1	0.38	0.66	86,86,86,86	0
56	MG	RA	3303	1/1	0.38	0.56	92,92,92,92	0
56	MG	YA	3157	1/1	0.38	0.79	66,66,66,66	0
56	MG	YN	201	1/1	0.38	1.55	90,90,90,90	0
56	MG	RB	217	1/1	0.38	0.47	87,87,87,87	0
56	MG	RV	202	1/1	0.38	0.47	86,86,86,86	0
56	MG	YA	3756	1/1	0.39	0.71	96,96,96,96	0
56	MG	R5	104	1/1	0.39	1.32	97,97,97,97	0
56	MG	RA	3997	1/1	0.39	0.52	106,106,106,106	0
56	MG	RA	3582	1/1	0.39	0.78	87,87,87,87	0
56	MG	XA	1710	1/1	0.39	0.33	78,78,78,78	0
56	MG	RA	3047	1/1	0.39	0.34	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3083	1/1	0.39	0.32	90,90,90,90	0
56	MG	RA	3193	1/1	0.39	0.69	103,103,103,103	0
56	MG	RA	3426	1/1	0.39	0.32	79,79,79,79	0
56	MG	QI	201	1/1	0.39	1.11	100,100,100,100	0
56	MG	RB	209	1/1	0.39	0.29	76,76,76,76	0
56	MG	YA	3001	1/1	0.39	0.75	96,96,96,96	0
56	MG	RA	3747	1/1	0.39	1.51	93,93,93,93	0
56	MG	QA	1821	1/1	0.39	0.79	89,89,89,89	0
56	MG	RA	3741	1/1	0.39	0.81	92,92,92,92	0
56	MG	RA	3955	1/1	0.39	0.89	90,90,90,90	0
56	MG	RA	3142	1/1	0.39	0.49	85,85,85,85	0
56	MG	RA	3900	1/1	0.39	0.59	92,92,92,92	0
56	MG	XA	1782	1/1	0.39	1.40	79,79,79,79	0
56	MG	RA	3636	1/1	0.39	0.19	94,94,94,94	0
56	MG	QA	1753	1/1	0.39	0.61	87,87,87,87	0
56	MG	RA	3312	1/1	0.39	0.34	96,96,96,96	0
56	MG	RF	302	1/1	0.39	0.75	80,80,80,80	0
56	MG	RA	3964	1/1	0.40	2.02	104,104,104,104	0
56	MG	YA	3198	1/1	0.40	0.35	88,88,88,88	0
56	MG	YA	3057	1/1	0.40	0.69	90,90,90,90	0
56	MG	XJ	201	1/1	0.40	0.38	97,97,97,97	0
56	MG	RA	3869	1/1	0.40	0.92	88,88,88,88	0
56	MG	RA	3738	1/1	0.40	0.62	93,93,93,93	0
56	MG	YA	3341	1/1	0.40	0.38	91,91,91,91	0
56	MG	XA	1685	1/1	0.40	0.77	62,62,62,62	0
56	MG	YA	3247	1/1	0.40	0.74	80,80,80,80	0
56	MG	RF	303	1/1	0.40	1.36	98,98,98,98	0
56	MG	RA	3011	1/1	0.40	0.69	93,93,93,93	0
56	MG	YA	3228	1/1	0.40	1.00	73,73,73,73	0
56	MG	RA	3273	1/1	0.40	1.24	99,99,99,99	0
56	MG	YA	3231	1/1	0.40	0.85	93,93,93,93	0
56	MG	YA	3548	1/1	0.40	0.86	66,66,66,66	0
56	MG	YA	3058	1/1	0.40	1.07	93,93,93,93	0
56	MG	RD	314	1/1	0.40	0.79	80,80,80,80	0
56	MG	RA	3705	1/1	0.40	0.59	89,89,89,89	0
56	MG	YA	3473	1/1	0.40	0.44	82,82,82,82	0
56	MG	RB	224	1/1	0.41	0.86	86,86,86,86	0
56	MG	RE	305	1/1	0.41	0.56	92,92,92,92	0
56	MG	RA	3050	1/1	0.41	0.77	89,89,89,89	0
56	MG	RA	3586	1/1	0.41	0.67	76,76,76,76	0
56	MG	RA	3662	1/1	0.41	0.55	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3464	1/1	0.41	1.57	79,79,79,79	0
56	MG	QA	1635	1/1	0.41	0.19	77,77,77,77	0
56	MG	RA	3322	1/1	0.41	0.79	93,93,93,93	0
56	MG	RA	3604	1/1	0.41	0.77	107,107,107,107	0
56	MG	RA	3535	1/1	0.41	0.57	97,97,97,97	0
56	MG	RA	3109	1/1	0.41	0.72	97,97,97,97	0
56	MG	QA	1765	1/1	0.41	0.92	80,80,80,80	0
56	MG	QA	1866	1/1	0.41	0.77	90,90,90,90	0
56	MG	YA	3396	1/1	0.42	0.89	67,67,67,67	0
56	MG	YA	3270	1/1	0.42	0.89	79,79,79,79	0
56	MG	RA	3939	1/1	0.42	2.08	95,95,95,95	0
56	MG	XA	1683	1/1	0.42	0.56	76,76,76,76	0
56	MG	YA	3547	1/1	0.42	0.64	88,88,88,88	0
56	MG	YA	3724	1/1	0.42	0.53	71,71,71,71	0
56	MG	XA	1658	1/1	0.42	0.67	86,86,86,86	0
56	MG	R1	101	1/1	0.42	0.65	89,89,89,89	0
56	MG	YA	3125	1/1	0.42	0.34	81,81,81,81	0
56	MG	RA	3228	1/1	0.42	0.57	104,104,104,104	0
56	MG	YA	3446	1/1	0.42	0.64	89,89,89,89	0
56	MG	RE	306	1/1	0.42	0.41	63,63,63,63	0
56	MG	RA	3524	1/1	0.42	0.69	85,85,85,85	0
56	MG	XA	1711	1/1	0.42	0.69	94,94,94,94	0
56	MG	YA	3409	1/1	0.43	1.29	95,95,95,95	0
56	MG	RA	3189	1/1	0.43	1.91	109,109,109,109	0
56	MG	YA	3113	1/1	0.43	0.63	79,79,79,79	0
56	MG	RA	3081	1/1	0.43	0.53	92,92,92,92	0
56	MG	QA	1690	1/1	0.43	0.32	68,68,68,68	0
56	MG	RA	3843	1/1	0.43	0.67	88,88,88,88	0
56	MG	RA	3658	1/1	0.43	0.45	90,90,90,90	0
56	MG	YA	3629	1/1	0.43	0.81	80,80,80,80	0
56	MG	RA	3013	1/1	0.43	0.68	83,83,83,83	0
56	MG	RA	3122	1/1	0.43	1.93	102,102,102,102	0
56	MG	XA	1676	1/1	0.43	0.83	98,98,98,98	0
56	MG	YB	218	1/1	0.43	0.31	85,85,85,85	0
56	MG	YA	3192	1/1	0.43	0.44	74,74,74,74	0
56	MG	RA	3238	1/1	0.43	0.46	109,109,109,109	0
56	MG	RA	3663	1/1	0.43	1.20	103,103,103,103	0
56	MG	RA	3224	1/1	0.44	0.72	93,93,93,93	0
56	MG	RA	3184	1/1	0.44	0.32	92,92,92,92	0
56	MG	RA	3850	1/1	0.44	0.56	72,72,72,72	0
56	MG	RA	3563	1/1	0.44	0.36	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	QA	1702	1/1	0.44	0.91	86,86,86,86	0
56	MG	RA	3373	1/1	0.44	0.77	82,82,82,82	0
56	MG	RA	3729	1/1	0.44	0.69	82,82,82,82	0
56	MG	QA	1612	1/1	0.44	0.56	89,89,89,89	0
56	MG	YA	3465	1/1	0.44	0.58	85,85,85,85	0
56	MG	RA	3734	1/1	0.44	0.59	85,85,85,85	0
56	MG	YB	201	1/1	0.44	0.64	103,103,103,103	0
56	MG	YA	3249	1/1	0.44	0.70	94,94,94,94	0
56	MG	RA	3527	1/1	0.44	1.06	73,73,73,73	0
56	MG	RA	3687	1/1	0.44	0.37	86,86,86,86	0
56	MG	YB	216	1/1	0.44	0.39	66,66,66,66	0
56	MG	RA	3445	1/1	0.45	0.95	81,81,81,81	0
56	MG	RA	3367	1/1	0.45	0.54	80,80,80,80	0
56	MG	QA	1828	1/1	0.45	0.55	86,86,86,86	0
56	MG	XA	1745	1/1	0.45	0.91	71,71,71,71	0
56	MG	RA	3977	1/1	0.45	0.43	89,89,89,89	0
56	MG	RA	3694	1/1	0.45	0.50	93,93,93,93	0
56	MG	QA	1759	1/1	0.45	0.76	77,77,77,77	0
56	MG	RA	3958	1/1	0.45	0.48	80,80,80,80	0
56	MG	YO	201	1/1	0.45	0.65	86,86,86,86	0
56	MG	RA	3994	1/1	0.45	0.17	91,91,91,91	0
56	MG	RE	303	1/1	0.45	0.39	102,102,102,102	0
56	MG	RF	308	1/1	0.45	0.79	92,92,92,92	0
56	MG	RW	201	1/1	0.45	0.54	83,83,83,83	0
56	MG	YA	3361	1/1	0.45	0.63	88,88,88,88	0
56	MG	RN	201	1/1	0.45	1.15	91,91,91,91	0
56	MG	R0	103	1/1	0.45	0.82	70,70,70,70	0
56	MG	RA	3301	1/1	0.45	1.67	93,93,93,93	0
56	MG	RA	3453	1/1	0.46	0.30	82,82,82,82	0
56	MG	XA	1726	1/1	0.46	0.53	96,96,96,96	0
56	MG	YA	3016	1/1	0.46	0.63	89,89,89,89	0
56	MG	YA	3390	1/1	0.46	0.33	88,88,88,88	0
56	MG	RA	4061	1/1	0.46	0.66	105,105,105,105	0
56	MG	RA	3551	1/1	0.46	0.46	79,79,79,79	0
56	MG	QA	1679	1/1	0.46	0.80	87,87,87,87	0
56	MG	RA	3375	1/1	0.46	0.53	98,98,98,98	0
56	MG	YA	3269	1/1	0.46	0.54	75,75,75,75	0
56	MG	RA	3975	1/1	0.46	0.34	98,98,98,98	0
56	MG	RA	3215	1/1	0.46	0.75	90,90,90,90	0
56	MG	QA	1686	1/1	0.46	0.72	89,89,89,89	0
56	MG	RA	3769	1/1	0.46	0.51	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3399	1/1	0.46	0.80	76,76,76,76	0
56	MG	RA	3844	1/1	0.46	0.47	100,100,100,100	0
56	MG	XA	1619	1/1	0.46	0.82	76,76,76,76	0
56	MG	YA	3696	1/1	0.46	0.82	91,91,91,91	0
56	MG	QA	1646	1/1	0.46	0.74	71,71,71,71	0
56	MG	QA	1841	1/1	0.46	0.37	94,94,94,94	0
56	MG	RA	3236	1/1	0.46	1.07	97,97,97,97	0
56	MG	RQ	201	1/1	0.46	0.39	87,87,87,87	0
56	MG	RA	3492	1/1	0.46	0.57	78,78,78,78	0
56	MG	RA	3758	1/1	0.46	0.69	93,93,93,93	0
56	MG	RE	302	1/1	0.46	0.95	97,97,97,97	0
56	MG	YA	3428	1/1	0.47	0.56	104,104,104,104	0
56	MG	YA	3456	1/1	0.47	0.77	84,84,84,84	0
56	MG	RA	3148	1/1	0.47	0.47	81,81,81,81	0
56	MG	RA	3120	1/1	0.47	0.55	83,83,83,83	0
56	MG	R7	102	1/1	0.47	0.66	75,75,75,75	0
56	MG	RA	3993	1/1	0.47	0.84	85,85,85,85	0
56	MG	YA	3654	1/1	0.47	0.38	91,91,91,91	0
56	MG	RE	307	1/1	0.47	0.59	86,86,86,86	0
56	MG	RA	3203	1/1	0.47	0.99	98,98,98,98	0
56	MG	YA	3628	1/1	0.47	0.34	87,87,87,87	0
56	MG	R1	104	1/1	0.47	0.68	88,88,88,88	0
56	MG	YT	202	1/1	0.47	0.89	80,80,80,80	0
56	MG	QA	1628	1/1	0.47	0.38	77,77,77,77	0
56	MG	RA	3767	1/1	0.47	0.91	63,63,63,63	0
56	MG	QA	1604	1/1	0.47	0.65	96,96,96,96	0
56	MG	RA	3446	1/1	0.47	1.01	77,77,77,77	0
56	MG	RA	3456	1/1	0.47	0.45	71,71,71,71	0
56	MG	RA	3053	1/1	0.47	0.54	98,98,98,98	0
56	MG	RA	3592	1/1	0.47	0.67	93,93,93,93	0
56	MG	XV	102	1/1	0.47	0.13	84,84,84,84	0
56	MG	RA	3924	1/1	0.47	0.66	89,89,89,89	0
56	MG	YV	201	1/1	0.47	0.54	84,84,84,84	0
56	MG	QE	201	1/1	0.47	0.33	95,95,95,95	0
56	MG	RA	3242	1/1	0.47	0.43	99,99,99,99	0
56	MG	QA	1724	1/1	0.47	1.90	85,85,85,85	0
56	MG	RA	3552	1/1	0.47	0.73	93,93,93,93	0
56	MG	YA	3635	1/1	0.47	0.84	83,83,83,83	0
56	MG	XA	1720	1/1	0.47	0.65	96,96,96,96	0
56	MG	RA	3113	1/1	0.47	1.02	90,90,90,90	0
56	MG	YB	209	1/1	0.47	0.53	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3225	1/1	0.48	0.96	96,96,96,96	0
56	MG	YA	3450	1/1	0.48	0.94	79,79,79,79	0
56	MG	YA	3190	1/1	0.48	0.69	92,92,92,92	0
56	MG	RA	3332	1/1	0.48	0.52	93,93,93,93	0
56	MG	YA	3381	1/1	0.48	0.67	70,70,70,70	0
56	MG	RA	4000	1/1	0.48	0.64	95,95,95,95	0
56	MG	RP	201	1/1	0.48	1.11	86,86,86,86	0
56	MG	RA	3187	1/1	0.48	0.57	90,90,90,90	0
56	MG	RA	3560	1/1	0.48	0.56	97,97,97,97	0
56	MG	YA	3529	1/1	0.48	0.61	72,72,72,72	0
56	MG	RD	304	1/1	0.48	0.52	75,75,75,75	0
56	MG	RA	3486	1/1	0.48	0.78	83,83,83,83	0
56	MG	XA	1723	1/1	0.48	0.28	91,91,91,91	0
56	MG	RA	3295	1/1	0.48	0.44	92,92,92,92	0
56	MG	QA	1837	1/1	0.48	0.75	87,87,87,87	0
56	MG	YA	3099	1/1	0.49	0.38	82,82,82,82	0
56	MG	YA	3096	1/1	0.49	0.19	87,87,87,87	0
56	MG	RA	3751	1/1	0.49	1.29	83,83,83,83	0
56	MG	RA	3337	1/1	0.49	0.69	92,92,92,92	0
56	MG	YA	3313	1/1	0.49	0.67	89,89,89,89	0
56	MG	RA	3177	1/1	0.49	0.53	83,83,83,83	0
56	MG	YA	3292	1/1	0.49	0.50	74,74,74,74	0
56	MG	RA	3996	1/1	0.49	0.58	89,89,89,89	0
56	MG	RA	3557	1/1	0.49	0.41	94,94,94,94	0
56	MG	RA	3112	1/1	0.49	0.76	96,96,96,96	0
56	MG	QA	1660	1/1	0.49	0.16	81,81,81,81	0
56	MG	RA	3630	1/1	0.49	0.58	68,68,68,68	0
56	MG	RA	3565	1/1	0.49	0.55	103,103,103,103	0
56	MG	RA	3237	1/1	0.49	0.96	96,96,96,96	0
56	MG	RA	3159	1/1	0.49	0.68	94,94,94,94	0
56	MG	RA	3538	1/1	0.49	0.89	95,95,95,95	0
56	MG	YO	202	1/1	0.49	0.20	81,81,81,81	0
56	MG	XA	1648	1/1	0.49	0.29	89,89,89,89	0
56	MG	RA	3642	1/1	0.49	0.55	92,92,92,92	0
56	MG	RA	3978	1/1	0.49	0.85	75,75,75,75	0
56	MG	XA	1656	1/1	0.49	0.55	85,85,85,85	0
56	MG	XA	1783	1/1	0.50	0.47	97,97,97,97	0
56	MG	QA	1755	1/1	0.50	0.88	81,81,81,81	0
56	MG	YA	3006	1/1	0.50	0.62	82,82,82,82	0
56	MG	XT	201	1/1	0.50	0.66	93,93,93,93	0
56	MG	RA	3723	1/1	0.50	0.38	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3611	1/1	0.50	0.50	95,95,95,95	0
56	MG	RA	3644	1/1	0.50	0.57	91,91,91,91	0
56	MG	RA	3991	1/1	0.50	0.63	75,75,75,75	0
56	MG	RA	3753	1/1	0.50	0.70	92,92,92,92	0
56	MG	YA	3043	1/1	0.50	0.58	63,63,63,63	0
56	MG	YA	3013	1/1	0.50	0.55	72,72,72,72	0
56	MG	RA	3003	1/1	0.50	0.56	91,91,91,91	0
56	MG	YA	3713	1/1	0.50	0.63	83,83,83,83	0
56	MG	RB	226	1/1	0.50	0.40	98,98,98,98	0
56	MG	RV	204	1/1	0.50	0.34	79,79,79,79	0
56	MG	YA	3685	1/1	0.50	0.60	87,87,87,87	0
56	MG	YE	305	1/1	0.50	0.41	82,82,82,82	0
56	MG	YA	3216	1/1	0.50	0.47	80,80,80,80	0
56	MG	QA	1734	1/1	0.50	0.76	84,84,84,84	0
56	MG	YB	211	1/1	0.51	0.30	80,80,80,80	0
56	MG	RA	3447	1/1	0.51	0.61	78,78,78,78	0
56	MG	QA	1849	1/1	0.51	1.44	76,76,76,76	0
56	MG	YA	3649	1/1	0.51	0.82	79,79,79,79	0
56	MG	YA	3079	1/1	0.51	0.67	97,97,97,97	0
56	MG	XA	1780	1/1	0.51	1.11	74,74,74,74	0
56	MG	XA	1702	1/1	0.51	0.54	75,75,75,75	0
56	MG	RA	3859	1/1	0.51	1.25	89,89,89,89	0
56	MG	YA	3179	1/1	0.51	0.59	102,102,102,102	0
56	MG	RA	3864	1/1	0.51	0.82	93,93,93,93	0
56	MG	YA	3276	1/1	0.51	0.31	77,77,77,77	0
56	MG	RA	3689	1/1	0.51	0.22	85,85,85,85	0
56	MG	RA	3032	1/1	0.51	0.29	92,92,92,92	0
56	MG	XA	1687	1/1	0.52	0.34	90,90,90,90	0
56	MG	QA	1784	1/1	0.52	0.36	96,96,96,96	0
56	MG	RA	3888	1/1	0.52	0.73	89,89,89,89	0
56	MG	YD	309	1/1	0.52	0.69	62,62,62,62	0
56	MG	QH	202	1/1	0.52	0.47	91,91,91,91	0
56	MG	RA	3529	1/1	0.52	0.54	90,90,90,90	0
56	MG	YA	3202	1/1	0.52	0.42	82,82,82,82	0
56	MG	YA	3171	1/1	0.52	0.55	90,90,90,90	0
56	MG	RA	3772	1/1	0.52	0.56	69,69,69,69	0
56	MG	RA	3883	1/1	0.52	0.87	88,88,88,88	0
56	MG	QA	1848	1/1	0.52	0.80	81,81,81,81	0
56	MG	QA	1823	1/1	0.52	0.66	94,94,94,94	0
56	MG	RA	3637	1/1	0.52	0.73	85,85,85,85	0
56	MG	YA	3393	1/1	0.52	0.60	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	QA	1868	1/1	0.52	1.40	82,82,82,82	0
56	MG	RA	3887	1/1	0.52	0.57	91,91,91,91	0
56	MG	XA	1743	1/1	0.52	0.53	89,89,89,89	0
56	MG	YQ	201	1/1	0.52	0.34	69,69,69,69	0
56	MG	RA	3655	1/1	0.52	0.27	94,94,94,94	0
56	MG	YA	3508	1/1	0.52	0.40	83,83,83,83	0
56	MG	YA	3534	1/1	0.53	0.34	85,85,85,85	0
56	MG	YA	3209	1/1	0.53	0.84	85,85,85,85	0
56	MG	YA	3183	1/1	0.53	0.66	88,88,88,88	0
56	MG	RA	3310	1/1	0.53	0.56	93,93,93,93	0
56	MG	RA	3520	1/1	0.53	0.53	91,91,91,91	0
56	MG	RA	3229	1/1	0.53	0.82	104,104,104,104	0
56	MG	RA	3439	1/1	0.53	0.24	84,84,84,84	0
56	MG	QA	1674	1/1	0.53	0.36	94,94,94,94	0
56	MG	QA	1835	1/1	0.53	0.52	72,72,72,72	0
56	MG	XA	1610	1/1	0.53	1.05	88,88,88,88	0
56	MG	RA	3849	1/1	0.53	0.88	85,85,85,85	0
56	MG	QM	201	1/1	0.53	0.29	91,91,91,91	0
56	MG	RA	3735	1/1	0.53	0.59	77,77,77,77	0
56	MG	RA	3837	1/1	0.53	0.63	90,90,90,90	0
56	MG	YA	3620	1/1	0.53	0.34	75,75,75,75	0
56	MG	YE	301	1/1	0.53	0.50	66,66,66,66	0
56	MG	YA	3245	1/1	0.53	0.41	88,88,88,88	0
56	MG	YA	3333	1/1	0.53	0.45	85,85,85,85	0
56	MG	YA	3119	1/1	0.53	0.74	68,68,68,68	0
56	MG	XA	1793	1/1	0.54	0.59	94,94,94,94	0
56	MG	YA	3143	1/1	0.54	0.45	106,106,106,106	0
56	MG	QD	303	1/1	0.54	0.55	94,94,94,94	0
56	MG	YA	3137	1/1	0.54	0.59	81,81,81,81	0
56	MG	YA	3720	1/1	0.54	0.44	75,75,75,75	0
56	MG	RA	3917	1/1	0.54	0.48	92,92,92,92	0
56	MG	XA	1625	1/1	0.54	0.77	90,90,90,90	0
56	MG	RA	3362	1/1	0.54	0.60	91,91,91,91	0
56	MG	XF	201	1/1	0.54	0.29	68,68,68,68	0
56	MG	RA	3423	1/1	0.54	0.59	92,92,92,92	0
56	MG	RA	3441	1/1	0.54	0.77	67,67,67,67	0
56	MG	YA	3521	1/1	0.54	0.53	97,97,97,97	0
56	MG	RA	3450	1/1	0.54	0.28	79,79,79,79	0
56	MG	YA	3558	1/1	0.54	0.70	87,87,87,87	0
56	MG	YA	3501	1/1	0.54	1.04	74,74,74,74	0
56	MG	QA	1676	1/1	0.54	0.88	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RB	215	1/1	0.54	0.18	81,81,81,81	0
56	MG	RA	3374	1/1	0.54	0.75	72,72,72,72	0
56	MG	YA	3196	1/1	0.54	0.71	91,91,91,91	0
56	MG	XA	1637	1/1	0.54	0.19	86,86,86,86	0
56	MG	XA	1792	1/1	0.54	0.59	95,95,95,95	0
56	MG	QA	1730	1/1	0.54	0.32	73,73,73,73	0
56	MG	RR	204	1/1	0.54	0.51	75,75,75,75	0
56	MG	YA	3242	1/1	0.55	0.86	107,107,107,107	0
56	MG	QD	305	1/1	0.55	0.32	99,99,99,99	0
56	MG	RD	312	1/1	0.55	0.51	90,90,90,90	0
56	MG	YA	3102	1/1	0.55	1.80	101,101,101,101	0
56	MG	QA	1833	1/1	0.55	0.38	106,106,106,106	0
56	MG	YA	3265	1/1	0.55	0.53	77,77,77,77	0
56	MG	RA	3518	1/1	0.55	0.57	96,96,96,96	0
56	MG	XA	1699	1/1	0.55	0.55	82,82,82,82	0
56	MG	RA	3300	1/1	0.55	0.65	100,100,100,100	0
56	MG	QA	1719	1/1	0.55	1.13	73,73,73,73	0
56	MG	XA	1766	1/1	0.55	1.07	88,88,88,88	0
56	MG	YA	3721	1/1	0.55	0.69	74,74,74,74	0
56	MG	RA	3567	1/1	0.55	0.44	90,90,90,90	0
56	MG	RA	4028	1/1	0.55	1.02	108,108,108,108	0
56	MG	RA	3809	1/1	0.55	0.55	89,89,89,89	0
56	MG	QL	201	1/1	0.55	0.19	87,87,87,87	0
56	MG	RA	3103	1/1	0.55	0.48	101,101,101,101	0
56	MG	YA	3642	1/1	0.55	0.74	69,69,69,69	0
56	MG	QA	1786	1/1	0.55	0.58	80,80,80,80	0
56	MG	XA	1786	1/1	0.55	0.69	89,89,89,89	0
56	MG	XA	1748	1/1	0.55	0.72	79,79,79,79	0
56	MG	YA	3040	1/1	0.55	0.49	88,88,88,88	0
56	MG	YA	3735	1/1	0.56	0.60	85,85,85,85	0
56	MG	YA	3455	1/1	0.56	0.45	86,86,86,86	0
56	MG	RA	3640	1/1	0.56	0.49	84,84,84,84	0
56	MG	Y6	102	1/1	0.56	0.48	102,102,102,102	0
56	MG	RA	3280	1/1	0.56	0.83	95,95,95,95	0
56	MG	QA	1703	1/1	0.56	0.41	63,63,63,63	0
57	ZN	Y4	101	1/1	0.56	0.40	176,176,176,176	0
56	MG	RA	3288	1/1	0.56	0.54	96,96,96,96	0
56	MG	RA	3940	1/1	0.56	0.79	90,90,90,90	0
56	MG	YA	3365	1/1	0.56	0.38	86,86,86,86	0
56	MG	XA	1646	1/1	0.56	0.58	104,104,104,104	0
56	MG	QA	1677	1/1	0.56	0.49	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3862	1/1	0.56	0.38	75,75,75,75	0
56	MG	RA	4024	1/1	0.56	1.49	98,98,98,98	0
56	MG	YA	3248	1/1	0.56	0.55	88,88,88,88	0
57	ZN	YY	201	1/1	0.56	0.23	167,167,167,167	0
56	MG	RA	3597	1/1	0.56	0.74	89,89,89,89	0
56	MG	YA	3092	1/1	0.56	0.42	85,85,85,85	0
56	MG	RZ	301	1/1	0.56	0.72	87,87,87,87	0
56	MG	RA	4042	1/1	0.56	0.56	81,81,81,81	0
56	MG	YA	3672	1/1	0.56	0.67	76,76,76,76	0
56	MG	RA	3613	1/1	0.56	1.03	75,75,75,75	0
56	MG	RD	311	1/1	0.56	0.86	101,101,101,101	0
56	MG	XA	1675	1/1	0.56	0.44	90,90,90,90	0
56	MG	YA	3712	1/1	0.56	0.77	80,80,80,80	0
56	MG	QA	1782	1/1	0.56	0.27	98,98,98,98	0
56	MG	XA	1722	1/1	0.56	0.67	88,88,88,88	0
56	MG	RA	3061	1/1	0.56	0.25	89,89,89,89	0
56	MG	YA	3489	1/1	0.57	0.40	77,77,77,77	0
56	MG	YA	3203	1/1	0.57	0.63	93,93,93,93	0
56	MG	XA	1742	1/1	0.57	0.42	78,78,78,78	0
56	MG	RA	3812	1/1	0.57	0.38	76,76,76,76	0
56	MG	QA	1643	1/1	0.57	0.70	86,86,86,86	0
56	MG	RA	3154	1/1	0.57	0.33	85,85,85,85	0
56	MG	RA	3944	1/1	0.57	0.61	97,97,97,97	0
56	MG	RA	3711	1/1	0.57	0.89	88,88,88,88	0
56	MG	RA	3259	1/1	0.57	0.75	86,86,86,86	0
56	MG	YA	3026	1/1	0.57	0.54	84,84,84,84	0
56	MG	XA	1704	1/1	0.57	0.51	90,90,90,90	0
56	MG	RA	3146	1/1	0.57	0.36	68,68,68,68	0
56	MG	RA	3873	1/1	0.57	0.40	77,77,77,77	0
56	MG	QA	1803	1/1	0.57	0.37	81,81,81,81	0
56	MG	YA	3019	1/1	0.57	0.57	102,102,102,102	0
56	MG	XA	1616	1/1	0.57	0.43	81,81,81,81	0
56	MG	RA	3253	1/1	0.57	0.52	81,81,81,81	0
56	MG	RA	3585	1/1	0.57	0.21	77,77,77,77	0
56	MG	QA	1809	1/1	0.57	0.47	86,86,86,86	0
56	MG	RA	3100	1/1	0.57	0.53	102,102,102,102	0
56	MG	QA	1615	1/1	0.57	0.34	93,93,93,93	0
56	MG	YB	203	1/1	0.57	0.25	72,72,72,72	0
56	MG	RA	3817	1/1	0.57	0.80	92,92,92,92	0
56	MG	RA	3969	1/1	0.57	0.52	97,97,97,97	0
56	MG	RA	4062	1/1	0.57	1.40	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3235	1/1	0.57	0.55	93,93,93,93	0
56	MG	XA	1682	1/1	0.57	0.71	83,83,83,83	0
56	MG	RA	3845	1/1	0.57	0.73	97,97,97,97	0
56	MG	YA	3544	1/1	0.58	0.47	63,63,63,63	0
56	MG	RA	3035	1/1	0.58	0.35	95,95,95,95	0
56	MG	RA	3988	1/1	0.58	0.72	86,86,86,86	0
56	MG	QA	1774	1/1	0.58	1.11	84,84,84,84	0
56	MG	YA	3569	1/1	0.58	0.97	67,67,67,67	0
56	MG	QA	1749	1/1	0.58	0.50	83,83,83,83	0
56	MG	QA	1747	1/1	0.58	1.23	81,81,81,81	0
56	MG	QA	1741	1/1	0.58	0.60	97,97,97,97	0
56	MG	QA	1729	1/1	0.58	0.68	87,87,87,87	0
56	MG	QA	1661	1/1	0.58	0.90	85,85,85,85	0
56	MG	YD	305	1/1	0.58	0.70	92,92,92,92	0
56	MG	RA	3180	1/1	0.58	1.08	80,80,80,80	0
56	MG	YA	3692	1/1	0.58	0.53	84,84,84,84	0
56	MG	YA	3105	1/1	0.58	0.60	81,81,81,81	0
56	MG	RA	3742	1/1	0.58	0.35	88,88,88,88	0
56	MG	YA	3281	1/1	0.58	0.33	62,62,62,62	0
56	MG	RA	4068	1/1	0.58	0.58	91,91,91,91	0
56	MG	RA	3194	1/1	0.58	0.68	99,99,99,99	0
56	MG	QE	202	1/1	0.58	0.71	88,88,88,88	0
56	MG	RA	3696	1/1	0.58	0.92	82,82,82,82	0
56	MG	YA	3178	1/1	0.59	0.60	78,78,78,78	0
56	MG	RA	3550	1/1	0.59	0.48	88,88,88,88	0
56	MG	YA	3182	1/1	0.59	0.63	103,103,103,103	0
56	MG	RA	4008	1/1	0.59	0.48	92,92,92,92	0
56	MG	QA	1787	1/1	0.59	0.40	89,89,89,89	0
56	MG	RA	3007	1/1	0.59	0.39	75,75,75,75	0
56	MG	QA	1654	1/1	0.59	0.43	77,77,77,77	0
56	MG	YA	3741	1/1	0.59	0.60	96,96,96,96	0
56	MG	RA	3254	1/1	0.59	0.44	105,105,105,105	0
56	MG	QA	1871	1/1	0.59	0.12	77,77,77,77	0
56	MG	RA	3807	1/1	0.59	0.60	91,91,91,91	0
56	MG	YW	201	1/1	0.59	0.94	98,98,98,98	0
56	MG	XA	1633	1/1	0.59	0.79	66,66,66,66	0
56	MG	RA	3208	1/1	0.59	0.69	89,89,89,89	0
56	MG	QA	1845	1/1	0.59	0.12	79,79,79,79	0
56	MG	RA	3124	1/1	0.59	0.47	73,73,73,73	0
56	MG	XA	1673	1/1	0.59	0.46	89,89,89,89	0
56	MG	QG	202	1/1	0.59	0.70	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3146	1/1	0.59	0.50	83,83,83,83	0
56	MG	RA	3695	1/1	0.59	0.83	107,107,107,107	0
56	MG	XA	1787	1/1	0.59	0.65	78,78,78,78	0
56	MG	XV	103	1/1	0.59	0.58	84,84,84,84	0
56	MG	RB	212	1/1	0.59	0.67	85,85,85,85	0
56	MG	YA	3332	1/1	0.59	0.28	62,62,62,62	0
56	MG	YA	3472	1/1	0.59	0.65	82,82,82,82	0
56	MG	YA	3226	1/1	0.59	0.56	87,87,87,87	0
56	MG	RA	3286	1/1	0.59	0.80	100,100,100,100	0
56	MG	RA	3279	1/1	0.59	0.71	98,98,98,98	0
56	MG	Y5	101	1/1	0.59	0.57	91,91,91,91	0
56	MG	QA	1673	1/1	0.59	0.71	75,75,75,75	0
56	MG	QA	1801	1/1	0.59	0.33	76,76,76,76	0
56	MG	YA	3131	1/1	0.60	1.25	105,105,105,105	0
56	MG	RA	3016	1/1	0.60	0.86	109,109,109,109	0
56	MG	RA	3583	1/1	0.60	0.95	79,79,79,79	0
56	MG	RA	3166	1/1	0.60	0.81	83,83,83,83	0
56	MG	RA	3462	1/1	0.60	0.75	86,86,86,86	0
56	MG	YA	3477	1/1	0.60	0.59	77,77,77,77	0
56	MG	YA	3624	1/1	0.60	0.45	92,92,92,92	0
56	MG	RA	3634	1/1	0.60	0.61	79,79,79,79	0
56	MG	YA	3513	1/1	0.60	0.85	81,81,81,81	0
56	MG	YA	3441	1/1	0.60	0.58	80,80,80,80	0
56	MG	QA	1762	1/1	0.60	0.70	80,80,80,80	0
56	MG	YA	3106	1/1	0.60	0.44	92,92,92,92	0
56	MG	YA	3439	1/1	0.60	0.90	88,88,88,88	0
56	MG	RA	3685	1/1	0.60	0.57	80,80,80,80	0
56	MG	YA	3223	1/1	0.60	0.44	65,65,65,65	0
56	MG	XA	1755	1/1	0.60	0.74	87,87,87,87	0
56	MG	QA	1701	1/1	0.60	0.50	77,77,77,77	0
56	MG	QB	301	1/1	0.60	0.35	81,81,81,81	0
56	MG	YA	3495	1/1	0.60	0.69	77,77,77,77	0
56	MG	RA	3935	1/1	0.60	0.60	90,90,90,90	0
56	MG	YA	3658	1/1	0.60	0.70	87,87,87,87	0
56	MG	QR	101	1/1	0.60	0.41	93,93,93,93	0
56	MG	YA	3278	1/1	0.60	0.96	72,72,72,72	0
56	MG	RA	3183	1/1	0.61	0.50	97,97,97,97	0
56	MG	RA	3340	1/1	0.61	0.56	82,82,82,82	0
56	MG	XA	1655	1/1	0.61	0.49	82,82,82,82	0
56	MG	QA	1739	1/1	0.61	0.56	80,80,80,80	0
56	MG	RA	3001	1/1	0.61	0.47	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3542	1/1	0.61	0.81	71,71,71,71	0
56	MG	RA	3835	1/1	0.61	0.54	89,89,89,89	0
56	MG	RA	3800	1/1	0.61	0.40	93,93,93,93	0
56	MG	RB	214	1/1	0.61	0.64	67,67,67,67	0
56	MG	RA	3576	1/1	0.61	0.51	92,92,92,92	0
56	MG	RA	3086	1/1	0.61	1.22	111,111,111,111	0
56	MG	RA	3672	1/1	0.61	0.47	89,89,89,89	0
56	MG	RA	3417	1/1	0.61	0.29	89,89,89,89	0
56	MG	RA	3562	1/1	0.61	0.69	82,82,82,82	0
56	MG	RA	3543	1/1	0.61	0.41	83,83,83,83	0
56	MG	YA	3114	1/1	0.61	0.75	90,90,90,90	0
56	MG	RA	3790	1/1	0.61	0.58	102,102,102,102	0
56	MG	RA	3555	1/1	0.61	0.52	80,80,80,80	0
56	MG	RA	3402	1/1	0.61	0.33	80,80,80,80	0
56	MG	YA	3697	1/1	0.61	0.41	78,78,78,78	0
56	MG	RB	225	1/1	0.61	0.34	80,80,80,80	0
56	MG	RB	222	1/1	0.62	0.48	79,79,79,79	0
56	MG	XA	1649	1/1	0.62	0.46	94,94,94,94	0
56	MG	RA	3098	1/1	0.62	0.54	68,68,68,68	0
56	MG	XA	1790	1/1	0.62	0.84	87,87,87,87	0
56	MG	RA	3984	1/1	0.62	0.57	87,87,87,87	0
56	MG	YA	3638	1/1	0.62	0.85	64,64,64,64	0
56	MG	QA	1669	1/1	0.62	0.79	81,81,81,81	0
56	MG	RA	3961	1/1	0.62	0.48	87,87,87,87	0
56	MG	YA	3338	1/1	0.62	1.03	85,85,85,85	0
56	MG	RA	3077	1/1	0.62	0.53	80,80,80,80	0
56	MG	QA	1806	1/1	0.62	0.55	79,79,79,79	0
56	MG	YF	302	1/1	0.62	0.24	75,75,75,75	0
56	MG	XA	1713	1/1	0.62	0.34	74,74,74,74	0
56	MG	RA	3336	1/1	0.62	0.47	86,86,86,86	0
56	MG	YA	3444	1/1	0.62	0.35	97,97,97,97	0
56	MG	XA	1650	1/1	0.62	0.30	87,87,87,87	0
56	MG	QA	1825	1/1	0.62	0.59	86,86,86,86	0
56	MG	RA	3854	1/1	0.62	1.73	87,87,87,87	0
56	MG	YA	3181	1/1	0.62	0.54	93,93,93,93	0
56	MG	XF	202	1/1	0.62	0.64	96,96,96,96	0
56	MG	YA	3240	1/1	0.62	0.47	93,93,93,93	0
56	MG	RB	223	1/1	0.62	1.09	96,96,96,96	0
56	MG	XA	1608	1/1	0.62	0.70	76,76,76,76	0
56	MG	YA	3101	1/1	0.62	0.38	92,92,92,92	0
56	MG	RA	3776	1/1	0.62	0.68	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3687	1/1	0.62	0.72	62,62,62,62	0
56	MG	RA	3608	1/1	0.62	0.61	83,83,83,83	0
56	MG	YA	3515	1/1	0.62	1.05	69,69,69,69	0
56	MG	QA	1737	1/1	0.62	0.47	88,88,88,88	0
56	MG	RA	3149	1/1	0.62	0.59	73,73,73,73	0
56	MG	YA	3717	1/1	0.62	0.72	100,100,100,100	0
56	MG	RA	3919	1/1	0.62	0.85	83,83,83,83	0
56	MG	YP	201	1/1	0.63	0.29	89,89,89,89	0
56	MG	XA	1716	1/1	0.63	0.56	79,79,79,79	0
56	MG	YA	3123	1/1	0.63	0.70	105,105,105,105	0
56	MG	XA	1714	1/1	0.63	0.42	76,76,76,76	0
56	MG	QA	1714	1/1	0.63	0.57	82,82,82,82	0
56	MG	RA	3116	1/1	0.63	1.15	104,104,104,104	0
56	MG	YA	3283	1/1	0.63	0.14	74,74,74,74	0
56	MG	YA	3310	1/1	0.63	2.02	80,80,80,80	0
56	MG	QA	1817	1/1	0.63	0.47	85,85,85,85	0
56	MG	RA	3584	1/1	0.63	0.57	76,76,76,76	0
56	MG	YA	3503	1/1	0.63	0.28	67,67,67,67	0
56	MG	XA	1631	1/1	0.63	0.47	88,88,88,88	0
56	MG	XA	1765	1/1	0.63	1.09	77,77,77,77	0
56	MG	YA	3022	1/1	0.63	1.79	91,91,91,91	0
56	MG	YA	3640	1/1	0.63	1.02	70,70,70,70	0
56	MG	RA	3581	1/1	0.63	0.68	97,97,97,97	0
56	MG	RA	3743	1/1	0.63	0.80	89,89,89,89	0
56	MG	YA	3305	1/1	0.63	0.25	69,69,69,69	0
56	MG	YD	301	1/1	0.63	0.43	66,66,66,66	0
56	MG	RA	4038	1/1	0.63	0.23	75,75,75,75	0
56	MG	RA	3612	1/1	0.63	0.20	80,80,80,80	0
56	MG	RA	3407	1/1	0.63	0.60	95,95,95,95	0
56	MG	RA	3323	1/1	0.63	0.44	69,69,69,69	0
56	MG	XA	1767	1/1	0.63	0.81	78,78,78,78	0
56	MG	RA	3782	1/1	0.63	0.90	99,99,99,99	0
56	MG	YA	3451	1/1	0.63	0.64	94,94,94,94	0
56	MG	RW	202	1/1	0.63	0.47	99,99,99,99	0
56	MG	YA	3586	1/1	0.63	1.12	76,76,76,76	0
56	MG	XA	1653	1/1	0.63	0.58	89,89,89,89	0
56	MG	YA	3596	1/1	0.63	0.57	66,66,66,66	0
56	MG	YA	3670	1/1	0.64	0.55	85,85,85,85	0
56	MG	YA	3619	1/1	0.64	0.60	65,65,65,65	0
56	MG	RA	3866	1/1	0.64	0.38	76,76,76,76	0
56	MG	YA	3364	1/1	0.64	0.23	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3074	1/1	0.64	0.65	68,68,68,68	0
56	MG	RA	3990	1/1	0.64	0.73	68,68,68,68	0
56	MG	RA	3248	1/1	0.64	0.58	89,89,89,89	0
56	MG	RA	3688	1/1	0.64	0.71	79,79,79,79	0
56	MG	RA	3763	1/1	0.64	0.27	77,77,77,77	0
56	MG	RA	3635	1/1	0.64	0.40	96,96,96,96	0
56	MG	YA	3749	1/1	0.64	0.98	90,90,90,90	0
56	MG	RA	4043	1/1	0.64	1.09	92,92,92,92	0
56	MG	RA	3788	1/1	0.64	0.55	90,90,90,90	0
56	MG	QA	1652	1/1	0.64	0.26	83,83,83,83	0
56	MG	RA	3647	1/1	0.64	1.10	102,102,102,102	0
56	MG	YA	3236	1/1	0.64	0.48	80,80,80,80	0
56	MG	RA	3781	1/1	0.64	0.71	90,90,90,90	0
56	MG	RA	3031	1/1	0.64	0.49	96,96,96,96	0
56	MG	RA	3169	1/1	0.64	0.23	90,90,90,90	0
56	MG	QA	1621	1/1	0.64	0.28	85,85,85,85	0
56	MG	YA	3498	1/1	0.64	0.21	89,89,89,89	0
56	MG	QA	1880	1/1	0.64	0.39	102,102,102,102	0
56	MG	RA	3802	1/1	0.64	0.48	85,85,85,85	0
56	MG	RA	3926	1/1	0.64	0.46	78,78,78,78	0
56	MG	RA	3892	1/1	0.64	0.49	78,78,78,78	0
56	MG	RA	3922	1/1	0.64	0.63	80,80,80,80	0
56	MG	YA	3736	1/1	0.64	0.76	115,115,115,115	0
56	MG	YA	3130	1/1	0.64	0.86	90,90,90,90	0
56	MG	XA	1612	1/1	0.64	0.51	84,84,84,84	0
56	MG	RA	3141	1/1	0.65	1.21	92,92,92,92	0
56	MG	YE	306	1/1	0.65	0.81	62,62,62,62	0
56	MG	RA	3298	1/1	0.65	0.16	79,79,79,79	0
56	MG	RA	3489	1/1	0.65	0.37	67,67,67,67	0
56	MG	RA	3422	1/1	0.65	0.55	73,73,73,73	0
56	MG	YA	3412	1/1	0.65	0.43	90,90,90,90	0
56	MG	YA	3637	1/1	0.65	0.55	85,85,85,85	0
56	MG	RA	3173	1/1	0.65	0.54	90,90,90,90	0
56	MG	YG	203	1/1	0.65	0.15	91,91,91,91	0
56	MG	QA	1666	1/1	0.65	0.42	96,96,96,96	0
56	MG	RA	3579	1/1	0.65	0.62	63,63,63,63	0
56	MG	QA	1601	1/1	0.65	0.39	101,101,101,101	0
56	MG	QA	1727	1/1	0.65	0.47	86,86,86,86	0
56	MG	RA	3633	1/1	0.65	0.45	93,93,93,93	0
56	MG	RA	3666	1/1	0.65	0.56	80,80,80,80	0
56	MG	RA	3359	1/1	0.65	0.58	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3264	1/1	0.65	0.34	93,93,93,93	0
56	MG	QA	1760	1/1	0.65	0.58	97,97,97,97	0
56	MG	RA	3540	1/1	0.65	0.53	68,68,68,68	0
56	MG	RA	3846	1/1	0.65	0.53	98,98,98,98	0
56	MG	RA	3275	1/1	0.65	0.56	110,110,110,110	0
56	MG	RA	3796	1/1	0.65	0.57	90,90,90,90	0
56	MG	QA	1846	1/1	0.65	0.28	92,92,92,92	0
56	MG	YA	3300	1/1	0.65	0.47	91,91,91,91	0
56	MG	RA	3074	1/1	0.65	0.45	69,69,69,69	0
56	MG	RA	3595	1/1	0.65	0.55	91,91,91,91	0
56	MG	QA	1856	1/1	0.65	0.57	94,94,94,94	0
56	MG	RA	3126	1/1	0.65	0.92	89,89,89,89	0
56	MG	YA	3481	1/1	0.65	0.60	79,79,79,79	0
56	MG	RA	3717	1/1	0.65	0.40	65,65,65,65	0
56	MG	RA	3632	1/1	0.65	0.90	88,88,88,88	0
56	MG	RA	3818	1/1	0.65	0.96	92,92,92,92	0
56	MG	RA	3639	1/1	0.65	0.57	82,82,82,82	0
56	MG	YW	202	1/1	0.65	0.41	81,81,81,81	0
56	MG	RA	3601	1/1	0.65	0.49	83,83,83,83	0
56	MG	YA	3354	1/1	0.65	0.52	84,84,84,84	0
56	MG	RA	3673	1/1	0.65	0.38	86,86,86,86	0
56	MG	RA	3299	1/1	0.66	0.45	68,68,68,68	0
56	MG	RA	3721	1/1	0.66	0.86	67,67,67,67	0
56	MG	RF	310	1/1	0.66	0.68	78,78,78,78	0
56	MG	RA	3626	1/1	0.66	0.50	72,72,72,72	0
56	MG	RA	3621	1/1	0.66	0.54	95,95,95,95	0
56	MG	YB	210	1/1	0.66	0.81	88,88,88,88	0
56	MG	RA	3342	1/1	0.66	0.44	79,79,79,79	0
56	MG	RA	3810	1/1	0.66	0.79	79,79,79,79	0
56	MG	YA	3200	1/1	0.66	0.47	77,77,77,77	0
56	MG	RA	3712	1/1	0.66	0.79	83,83,83,83	0
56	MG	YA	3413	1/1	0.66	0.80	85,85,85,85	0
56	MG	YA	3445	1/1	0.66	0.59	94,94,94,94	0
56	MG	YA	3061	1/1	0.66	0.48	65,65,65,65	0
56	MG	RA	3121	1/1	0.66	0.95	100,100,100,100	0
56	MG	RA	3459	1/1	0.66	0.38	88,88,88,88	0
56	MG	QA	1632	1/1	0.66	0.52	91,91,91,91	0
56	MG	RA	3155	1/1	0.66	0.55	95,95,95,95	0
56	MG	XA	1667	1/1	0.66	1.24	83,83,83,83	0
56	MG	RA	3065	1/1	0.66	0.44	92,92,92,92	0
57	ZN	R4	101	1/1	0.66	0.51	177,177,177,177	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3970	1/1	0.66	0.56	96,96,96,96	0
56	MG	RA	3284	1/1	0.66	0.69	87,87,87,87	0
56	MG	RA	3847	1/1	0.66	0.62	103,103,103,103	0
56	MG	YA	3523	1/1	0.66	0.69	72,72,72,72	0
56	MG	RA	4029	1/1	0.66	0.36	62,62,62,62	0
56	MG	YA	3255	1/1	0.66	0.46	81,81,81,81	0
56	MG	RA	3430	1/1	0.66	0.31	93,93,93,93	0
56	MG	RA	3780	1/1	0.66	0.48	89,89,89,89	0
56	MG	YA	3082	1/1	0.66	1.11	108,108,108,108	0
56	MG	RA	3005	1/1	0.66	0.74	91,91,91,91	0
56	MG	QA	1723	1/1	0.66	0.68	86,86,86,86	0
56	MG	RA	3199	1/1	0.66	0.64	81,81,81,81	0
56	MG	YA	3314	1/1	0.66	0.60	69,69,69,69	0
56	MG	RA	3938	1/1	0.66	0.39	78,78,78,78	0
56	MG	YA	3206	1/1	0.67	0.56	73,73,73,73	0
56	MG	QA	1820	1/1	0.67	0.41	76,76,76,76	0
56	MG	RA	3145	1/1	0.67	0.45	71,71,71,71	0
56	MG	RA	3707	1/1	0.67	0.46	73,73,73,73	0
56	MG	YA	3076	1/1	0.67	0.52	92,92,92,92	0
56	MG	YA	3470	1/1	0.67	0.51	74,74,74,74	0
56	MG	YA	3204	1/1	0.67	0.39	89,89,89,89	0
56	MG	YA	3194	1/1	0.67	0.53	89,89,89,89	0
56	MG	RA	3936	1/1	0.67	0.36	82,82,82,82	0
56	MG	YA	3018	1/1	0.67	0.41	97,97,97,97	0
56	MG	RF	306	1/1	0.67	1.38	106,106,106,106	0
56	MG	QA	1805	1/1	0.67	0.94	76,76,76,76	0
56	MG	RA	3660	1/1	0.67	0.82	77,77,77,77	0
56	MG	RB	218	1/1	0.67	0.49	86,86,86,86	0
56	MG	YA	3631	1/1	0.67	0.45	76,76,76,76	0
56	MG	YA	3049	1/1	0.67	0.49	85,85,85,85	0
56	MG	RA	3204	1/1	0.67	0.61	103,103,103,103	0
56	MG	RA	3317	1/1	0.67	0.46	82,82,82,82	0
56	MG	YA	3688	1/1	0.67	0.41	72,72,72,72	0
56	MG	RA	3097	1/1	0.67	1.29	90,90,90,90	0
56	MG	YA	3062	1/1	0.67	0.40	84,84,84,84	0
56	MG	XA	1664	1/1	0.67	0.51	102,102,102,102	0
56	MG	QA	1874	1/1	0.67	0.23	93,93,93,93	0
56	MG	YA	3376	1/1	0.67	0.41	84,84,84,84	0
56	MG	YA	3660	1/1	0.67	0.61	69,69,69,69	0
56	MG	YA	3650	1/1	0.67	0.90	76,76,76,76	0
56	MG	RA	3596	1/1	0.67	0.38	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3533	1/1	0.67	0.35	89,89,89,89	0
56	MG	YA	3527	1/1	0.67	0.38	74,74,74,74	0
56	MG	RA	3910	1/1	0.67	0.50	83,83,83,83	0
56	MG	QA	1670	1/1	0.67	0.42	84,84,84,84	0
56	MG	QA	1872	1/1	0.67	0.85	70,70,70,70	0
56	MG	RA	4032	1/1	0.67	0.86	89,89,89,89	0
56	MG	RA	3521	1/1	0.68	0.47	69,69,69,69	0
56	MG	RA	3369	1/1	0.68	1.87	79,79,79,79	0
56	MG	YA	3195	1/1	0.68	0.31	89,89,89,89	0
56	MG	YA	3252	1/1	0.68	0.24	96,96,96,96	0
56	MG	RA	3062	1/1	0.68	0.13	84,84,84,84	0
56	MG	RA	3044	1/1	0.68	0.39	82,82,82,82	0
56	MG	QA	1800	1/1	0.68	0.55	85,85,85,85	0
56	MG	RA	4046	1/1	0.68	0.54	91,91,91,91	0
56	MG	QA	1746	1/1	0.68	0.42	80,80,80,80	0
56	MG	RA	3836	1/1	0.68	0.51	73,73,73,73	0
56	MG	YA	3389	1/1	0.68	0.62	71,71,71,71	0
56	MG	QA	1606	1/1	0.68	0.20	88,88,88,88	0
56	MG	RA	3306	1/1	0.68	1.04	97,97,97,97	0
56	MG	Y1	102	1/1	0.68	0.35	87,87,87,87	0
56	MG	YA	3718	1/1	0.68	0.42	94,94,94,94	0
56	MG	RA	3675	1/1	0.68	0.60	84,84,84,84	0
56	MG	RA	3587	1/1	0.68	0.48	78,78,78,78	0
56	MG	QA	1865	1/1	0.68	0.80	98,98,98,98	0
56	MG	RA	3037	1/1	0.68	0.48	100,100,100,100	0
56	MG	QD	304	1/1	0.68	0.51	97,97,97,97	0
56	MG	RA	4025	1/1	0.68	0.82	97,97,97,97	0
56	MG	RA	3376	1/1	0.68	0.78	78,78,78,78	0
56	MG	RA	4050	1/1	0.68	0.38	98,98,98,98	0
56	MG	RA	3942	1/1	0.68	0.43	95,95,95,95	0
56	MG	RA	3725	1/1	0.68	0.45	86,86,86,86	0
56	MG	YA	3141	1/1	0.68	0.44	79,79,79,79	0
56	MG	YA	3307	1/1	0.68	0.71	71,71,71,71	0
56	MG	RA	3566	1/1	0.68	0.56	67,67,67,67	0
56	MG	RA	3272	1/1	0.68	0.65	90,90,90,90	0
56	MG	RA	3290	1/1	0.69	1.48	99,99,99,99	0
56	MG	RA	3691	1/1	0.69	1.05	93,93,93,93	0
56	MG	YA	3007	1/1	0.69	0.35	69,69,69,69	0
56	MG	YA	3351	1/1	0.69	0.55	68,68,68,68	0
56	MG	QA	1710	1/1	0.69	0.64	74,74,74,74	0
56	MG	YA	3097	1/1	0.69	0.39	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3350	1/1	0.69	0.26	74,74,74,74	0
56	MG	RA	3915	1/1	0.69	0.74	73,73,73,73	0
56	MG	RA	3683	1/1	0.69	0.32	85,85,85,85	0
56	MG	RA	3101	1/1	0.69	0.82	95,95,95,95	0
56	MG	RA	3556	1/1	0.69	1.66	83,83,83,83	0
56	MG	YA	3093	1/1	0.69	0.37	86,86,86,86	0
56	MG	YA	3460	1/1	0.69	0.38	85,85,85,85	0
56	MG	YA	3008	1/1	0.69	0.65	66,66,66,66	0
56	MG	RA	3234	1/1	0.69	0.51	101,101,101,101	0
56	MG	YA	3709	1/1	0.69	0.43	71,71,71,71	0
56	MG	RB	205	1/1	0.69	0.21	92,92,92,92	0
56	MG	RA	3732	1/1	0.69	0.78	85,85,85,85	0
56	MG	XA	1703	1/1	0.69	0.47	82,82,82,82	0
56	MG	RA	3920	1/1	0.69	0.47	80,80,80,80	0
56	MG	XA	1621	1/1	0.69	0.13	83,83,83,83	0
56	MG	RA	3029	1/1	0.69	1.46	104,104,104,104	0
56	MG	XA	1629	1/1	0.69	0.41	68,68,68,68	0
56	MG	RA	3328	1/1	0.69	0.29	73,73,73,73	0
56	MG	YA	3336	1/1	0.69	0.75	62,62,62,62	0
56	MG	YA	3691	1/1	0.69	0.50	82,82,82,82	0
56	MG	QV	104	1/1	0.69	0.60	79,79,79,79	0
56	MG	RA	3358	1/1	0.70	0.26	81,81,81,81	0
56	MG	RA	3043	1/1	0.70	0.22	67,67,67,67	0
56	MG	RA	3599	1/1	0.70	0.62	99,99,99,99	0
56	MG	RA	3898	1/1	0.70	0.44	85,85,85,85	0
56	MG	QA	1651	1/1	0.70	0.46	90,90,90,90	0
56	MG	YA	3644	1/1	0.70	0.50	75,75,75,75	0
56	MG	YA	3051	1/1	0.70	0.42	82,82,82,82	0
56	MG	XL	201	1/1	0.70	0.40	82,82,82,82	0
56	MG	RA	4009	1/1	0.70	0.53	84,84,84,84	0
56	MG	QA	1720	1/1	0.70	0.87	85,85,85,85	0
56	MG	YA	3442	1/1	0.70	0.56	90,90,90,90	0
56	MG	RA	3091	1/1	0.70	1.16	102,102,102,102	0
56	MG	YA	3728	1/1	0.70	0.50	89,89,89,89	0
56	MG	RA	3949	1/1	0.70	0.78	95,95,95,95	0
56	MG	RA	3519	1/1	0.70	0.95	86,86,86,86	0
56	MG	QA	1625	1/1	0.70	0.53	88,88,88,88	0
56	MG	RA	3645	1/1	0.70	0.74	85,85,85,85	0
56	MG	YA	3132	1/1	0.70	0.38	93,93,93,93	0
56	MG	QA	1706	1/1	0.70	0.34	76,76,76,76	0
56	MG	XA	1731	1/1	0.70	0.24	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3457	1/1	0.70	0.17	89,89,89,89	0
56	MG	RA	3756	1/1	0.70	0.53	73,73,73,73	0
56	MG	YA	3301	1/1	0.70	0.83	74,74,74,74	0
56	MG	RA	3704	1/1	0.70	0.56	82,82,82,82	0
56	MG	RA	3553	1/1	0.70	0.23	100,100,100,100	0
56	MG	YA	3651	1/1	0.70	0.64	78,78,78,78	0
56	MG	RA	3276	1/1	0.70	0.76	95,95,95,95	0
56	MG	QV	101	1/1	0.70	0.17	86,86,86,86	0
56	MG	RA	3789	1/1	0.70	0.23	80,80,80,80	0
56	MG	R9	103	1/1	0.70	0.47	93,93,93,93	0
56	MG	YA	3129	1/1	0.70	0.47	77,77,77,77	0
56	MG	YA	3024	1/1	0.70	0.24	91,91,91,91	0
56	MG	RA	3052	1/1	0.70	0.45	95,95,95,95	0
56	MG	YA	3734	1/1	0.70	0.42	83,83,83,83	0
56	MG	RA	3931	1/1	0.70	0.47	78,78,78,78	0
56	MG	RA	3989	1/1	0.70	0.73	84,84,84,84	0
56	MG	RV	203	1/1	0.70	0.76	83,83,83,83	0
56	MG	RA	3464	1/1	0.70	0.40	90,90,90,90	0
56	MG	RA	3698	1/1	0.70	0.53	87,87,87,87	0
56	MG	YA	3128	1/1	0.70	0.57	82,82,82,82	0
56	MG	YA	3580	1/1	0.70	0.51	70,70,70,70	0
56	MG	RA	4048	1/1	0.70	1.12	103,103,103,103	0
56	MG	YA	3257	1/1	0.71	0.48	89,89,89,89	0
56	MG	RA	4007	1/1	0.71	0.44	76,76,76,76	0
56	MG	YA	3373	1/1	0.71	0.19	71,71,71,71	0
56	MG	YA	3180	1/1	0.71	0.27	73,73,73,73	0
56	MG	RA	3305	1/1	0.71	0.29	73,73,73,73	0
56	MG	RA	3573	1/1	0.71	0.53	88,88,88,88	0
56	MG	RA	3114	1/1	0.71	0.52	95,95,95,95	0
56	MG	QA	1814	1/1	0.71	0.89	89,89,89,89	0
56	MG	XA	1604	1/1	0.71	1.06	98,98,98,98	0
56	MG	YA	3047	1/1	0.71	0.41	86,86,86,86	0
56	MG	YA	3302	1/1	0.71	0.27	89,89,89,89	0
56	MG	RA	3897	1/1	0.71	0.60	72,72,72,72	0
56	MG	RH	202	1/1	0.71	0.22	95,95,95,95	0
56	MG	RA	3024	1/1	0.71	0.69	105,105,105,105	0
56	MG	YA	3293	1/1	0.71	1.28	65,65,65,65	0
56	MG	YA	3699	1/1	0.71	0.49	77,77,77,77	0
56	MG	RA	3860	1/1	0.71	1.49	85,85,85,85	0
56	MG	RA	3736	1/1	0.71	0.70	85,85,85,85	0
56	MG	YA	3251	1/1	0.71	0.49	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3823	1/1	0.71	0.55	73,73,73,73	0
56	MG	RB	207	1/1	0.71	0.23	93,93,93,93	0
56	MG	RA	3950	1/1	0.71	1.05	86,86,86,86	0
56	MG	R1	103	1/1	0.71	0.68	76,76,76,76	0
56	MG	YA	3467	1/1	0.71	0.79	76,76,76,76	0
56	MG	RA	3451	1/1	0.71	1.35	74,74,74,74	0
56	MG	RA	3913	1/1	0.71	0.73	94,94,94,94	0
56	MG	XA	1750	1/1	0.71	0.91	85,85,85,85	0
56	MG	RA	3311	1/1	0.71	0.50	83,83,83,83	0
56	MG	RA	3132	1/1	0.71	0.39	95,95,95,95	0
56	MG	YA	3104	1/1	0.71	0.28	69,69,69,69	0
56	MG	RA	4020	1/1	0.71	0.45	91,91,91,91	0
56	MG	XA	1779	1/1	0.71	0.43	92,92,92,92	0
56	MG	YA	3031	1/1	0.71	0.32	63,63,63,63	0
56	MG	RA	3364	1/1	0.71	0.95	74,74,74,74	0
56	MG	RA	4013	1/1	0.71	0.40	77,77,77,77	0
56	MG	RA	3108	1/1	0.71	0.86	89,89,89,89	0
56	MG	RA	3752	1/1	0.71	0.58	85,85,85,85	0
56	MG	RA	3805	1/1	0.71	0.61	97,97,97,97	0
56	MG	XE	202	1/1	0.71	0.14	94,94,94,94	0
56	MG	QA	1773	1/1	0.71	0.27	78,78,78,78	0
56	MG	RA	3170	1/1	0.71	0.38	86,86,86,86	0
56	MG	QA	1775	1/1	0.71	0.43	91,91,91,91	0
56	MG	XA	1705	1/1	0.71	0.26	84,84,84,84	0
56	MG	QA	1712	1/1	0.71	0.48	75,75,75,75	0
56	MG	RA	3506	1/1	0.71	0.34	70,70,70,70	0
56	MG	RA	3681	1/1	0.71	0.88	72,72,72,72	0
56	MG	RA	3314	1/1	0.71	0.55	77,77,77,77	0
56	MG	XA	1622	1/1	0.71	0.60	78,78,78,78	0
56	MG	YA	3153	1/1	0.72	0.51	68,68,68,68	0
56	MG	RA	3697	1/1	0.72	2.06	101,101,101,101	0
56	MG	RA	3627	1/1	0.72	0.37	81,81,81,81	0
56	MG	XA	1684	1/1	0.72	1.05	70,70,70,70	0
56	MG	QA	1732	1/1	0.72	0.57	72,72,72,72	0
56	MG	RA	3708	1/1	0.72	0.98	77,77,77,77	0
56	MG	RA	3327	1/1	0.72	0.56	69,69,69,69	0
56	MG	RA	4012	1/1	0.72	2.55	103,103,103,103	0
56	MG	QA	1672	1/1	0.72	0.55	85,85,85,85	0
56	MG	QA	1687	1/1	0.72	0.63	94,94,94,94	0
56	MG	YA	3418	1/1	0.72	0.69	90,90,90,90	0
56	MG	YA	3134	1/1	0.72	0.62	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3473	1/1	0.72	0.25	80,80,80,80	0
56	MG	RA	3182	1/1	0.72	0.99	97,97,97,97	0
56	MG	XA	1661	1/1	0.72	0.55	95,95,95,95	0
56	MG	QV	103	1/1	0.72	0.48	86,86,86,86	0
56	MG	RA	3749	1/1	0.72	0.20	70,70,70,70	0
56	MG	QA	1609	1/1	0.72	0.20	95,95,95,95	0
56	MG	QA	1772	1/1	0.72	0.37	96,96,96,96	0
56	MG	RA	3750	1/1	0.72	0.61	83,83,83,83	0
56	MG	YA	3475	1/1	0.72	0.56	65,65,65,65	0
56	MG	YA	3166	1/1	0.72	0.96	109,109,109,109	0
56	MG	RA	3025	1/1	0.72	0.21	69,69,69,69	0
56	MG	RA	3948	1/1	0.72	0.59	64,64,64,64	0
56	MG	YA	3406	1/1	0.72	0.43	95,95,95,95	0
56	MG	YA	3120	1/1	0.72	0.60	86,86,86,86	0
56	MG	RA	3209	1/1	0.72	0.38	88,88,88,88	0
56	MG	QA	1756	1/1	0.72	0.75	80,80,80,80	0
56	MG	RQ	204	1/1	0.72	0.65	89,89,89,89	0
56	MG	RD	303	1/1	0.72	1.20	88,88,88,88	0
56	MG	RA	3449	1/1	0.72	0.50	83,83,83,83	0
56	MG	YA	3466	1/1	0.72	0.56	79,79,79,79	0
56	MG	RA	3353	1/1	0.72	0.65	84,84,84,84	0
56	MG	RA	3045	1/1	0.72	0.88	86,86,86,86	0
56	MG	RA	3022	1/1	0.72	0.86	98,98,98,98	0
56	MG	RA	3826	1/1	0.72	0.30	95,95,95,95	0
56	MG	RA	3757	1/1	0.72	0.33	98,98,98,98	0
56	MG	XA	1665	1/1	0.72	0.28	72,72,72,72	0
56	MG	RA	4016	1/1	0.72	0.45	87,87,87,87	0
56	MG	YA	3448	1/1	0.72	0.17	80,80,80,80	0
56	MG	QA	1864	1/1	0.72	0.41	97,97,97,97	0
56	MG	YB	208	1/1	0.72	0.47	93,93,93,93	0
56	MG	YA	3116	1/1	0.72	0.67	95,95,95,95	0
56	MG	RA	3048	1/1	0.72	0.25	88,88,88,88	0
56	MG	RA	3207	1/1	0.72	0.62	96,96,96,96	0
56	MG	RA	3401	1/1	0.73	0.70	62,62,62,62	0
56	MG	RA	3294	1/1	0.73	0.49	108,108,108,108	0
56	MG	RA	3405	1/1	0.73	0.20	85,85,85,85	0
56	MG	YD	307	1/1	0.73	0.52	79,79,79,79	0
56	MG	YA	3483	1/1	0.73	0.62	88,88,88,88	0
56	MG	YA	3519	1/1	0.73	0.36	72,72,72,72	0
56	MG	YA	3005	1/1	0.73	0.42	85,85,85,85	0
56	MG	RA	3239	1/1	0.73	0.64	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YE	302	1/1	0.73	0.69	95,95,95,95	0
56	MG	RA	3200	1/1	0.73	0.39	85,85,85,85	0
56	MG	YA	3438	1/1	0.73	0.55	80,80,80,80	0
56	MG	YA	3304	1/1	0.73	0.34	82,82,82,82	0
56	MG	RA	3245	1/1	0.73	0.11	86,86,86,86	0
56	MG	YA	3478	1/1	0.73	0.57	62,62,62,62	0
56	MG	RA	3012	1/1	0.73	0.51	84,84,84,84	0
56	MG	QA	1875	1/1	0.73	0.32	78,78,78,78	0
56	MG	RA	3523	1/1	0.73	0.44	94,94,94,94	0
56	MG	RA	3388	1/1	0.73	0.76	96,96,96,96	0
56	MG	RA	3291	1/1	0.73	0.38	81,81,81,81	0
56	MG	YA	3063	1/1	0.73	0.66	92,92,92,92	0
56	MG	YA	3197	1/1	0.73	0.45	93,93,93,93	0
56	MG	RA	3838	1/1	0.73	0.54	77,77,77,77	0
56	MG	RA	3349	1/1	0.73	0.39	68,68,68,68	0
56	MG	RA	3465	1/1	0.73	0.46	69,69,69,69	0
56	MG	RA	3481	1/1	0.73	0.67	71,71,71,71	0
56	MG	Y1	101	1/1	0.73	0.31	62,62,62,62	0
56	MG	YA	3290	1/1	0.73	0.88	91,91,91,91	0
56	MG	YT	203	1/1	0.73	0.55	91,91,91,91	0
56	MG	XA	1663	1/1	0.73	0.23	83,83,83,83	0
56	MG	YA	3115	1/1	0.73	0.17	77,77,77,77	0
56	MG	XA	1756	1/1	0.73	1.16	81,81,81,81	0
56	MG	YA	3015	1/1	0.73	0.80	89,89,89,89	0
56	MG	RA	3803	1/1	0.73	1.18	101,101,101,101	0
56	MG	RA	3494	1/1	0.73	0.47	81,81,81,81	0
56	MG	RA	3354	1/1	0.73	0.67	70,70,70,70	0
56	MG	YA	3156	1/1	0.73	0.47	103,103,103,103	0
56	MG	RA	4037	1/1	0.74	0.69	95,95,95,95	0
56	MG	YA	3707	1/1	0.74	0.56	82,82,82,82	0
56	MG	QA	1758	1/1	0.74	0.35	93,93,93,93	0
56	MG	YA	3346	1/1	0.74	0.52	79,79,79,79	0
56	MG	YA	3683	1/1	0.74	0.27	82,82,82,82	0
56	MG	YA	3706	1/1	0.74	0.89	75,75,75,75	0
56	MG	QA	1603	1/1	0.74	0.46	86,86,86,86	0
56	MG	RA	3602	1/1	0.74	1.58	97,97,97,97	0
56	MG	RA	3167	1/1	0.74	0.26	84,84,84,84	0
56	MG	YA	3516	1/1	0.74	1.25	85,85,85,85	0
56	MG	YA	3520	1/1	0.74	0.22	100,100,100,100	0
56	MG	XA	1636	1/1	0.74	0.22	68,68,68,68	0
56	MG	RA	4001	1/1	0.74	0.34	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3442	1/1	0.74	0.89	82,82,82,82	0
56	MG	YA	3563	1/1	0.74	0.27	72,72,72,72	0
56	MG	YA	3487	1/1	0.74	0.36	84,84,84,84	0
56	MG	XA	1693	1/1	0.74	0.54	95,95,95,95	0
56	MG	RA	3713	1/1	0.74	1.83	89,89,89,89	0
56	MG	RA	3216	1/1	0.74	0.74	104,104,104,104	0
56	MG	YA	3647	1/1	0.74	1.16	62,62,62,62	0
56	MG	XA	1640	1/1	0.74	0.47	92,92,92,92	0
56	MG	QA	1656	1/1	0.74	0.25	78,78,78,78	0
56	MG	RA	3413	1/1	0.74	0.53	83,83,83,83	0
56	MG	XA	1659	1/1	0.74	0.21	88,88,88,88	0
56	MG	YA	3557	1/1	0.74	0.59	66,66,66,66	0
56	MG	YA	3238	1/1	0.74	0.45	100,100,100,100	0
56	MG	YA	3349	1/1	0.74	0.57	62,62,62,62	0
56	MG	YA	3263	1/1	0.74	0.52	70,70,70,70	0
56	MG	RA	3541	1/1	0.74	0.40	87,87,87,87	0
56	MG	YA	3690	1/1	0.74	0.47	78,78,78,78	0
56	MG	XA	1627	1/1	0.74	0.97	80,80,80,80	0
56	MG	RA	3745	1/1	0.74	0.61	73,73,73,73	0
56	MG	RA	3411	1/1	0.74	0.52	93,93,93,93	0
56	MG	RA	3558	1/1	0.74	0.36	76,76,76,76	0
56	MG	RB	228	1/1	0.74	0.71	92,92,92,92	0
56	MG	YA	3708	1/1	0.74	1.08	66,66,66,66	0
56	MG	YA	3747	1/1	0.74	1.25	98,98,98,98	0
56	MG	QN	103	1/1	0.75	1.01	81,81,81,81	0
56	MG	XK	201	1/1	0.75	0.18	87,87,87,87	0
56	MG	RN	203	1/1	0.75	0.96	90,90,90,90	0
56	MG	QA	1684	1/1	0.75	1.17	97,97,97,97	0
56	MG	XA	1611	1/1	0.75	0.65	81,81,81,81	0
56	MG	YA	3028	1/1	0.75	0.41	85,85,85,85	0
56	MG	YA	3386	1/1	0.75	0.40	82,82,82,82	0
56	MG	YA	3437	1/1	0.75	0.51	62,62,62,62	0
56	MG	XA	1778	1/1	0.75	0.85	70,70,70,70	0
56	MG	RA	3133	1/1	0.75	0.57	85,85,85,85	0
56	MG	XA	1730	1/1	0.75	0.46	88,88,88,88	0
56	MG	RA	3816	1/1	0.75	0.29	79,79,79,79	0
56	MG	RA	3379	1/1	0.75	0.52	62,62,62,62	0
56	MG	YA	3220	1/1	0.75	0.55	105,105,105,105	0
56	MG	YA	3261	1/1	0.75	0.58	85,85,85,85	0
56	MG	YB	212	1/1	0.75	0.55	79,79,79,79	0
56	MG	RA	3669	1/1	0.75	0.55	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3799	1/1	0.75	1.02	82,82,82,82	0
56	MG	RA	3710	1/1	0.75	0.41	98,98,98,98	0
56	MG	RA	3646	1/1	0.75	0.35	92,92,92,92	0
56	MG	RA	3830	1/1	0.75	1.56	78,78,78,78	0
56	MG	YA	3582	1/1	0.75	1.24	74,74,74,74	0
56	MG	RA	4044	1/1	0.75	1.12	106,106,106,106	0
56	MG	RA	3615	1/1	0.75	0.51	62,62,62,62	0
56	MG	QA	1839	1/1	0.75	0.57	79,79,79,79	0
56	MG	YA	3416	1/1	0.75	0.46	75,75,75,75	0
56	MG	YA	3259	1/1	0.75	0.78	98,98,98,98	0
56	MG	YA	3323	1/1	0.75	0.64	62,62,62,62	0
56	MG	XA	1740	1/1	0.75	0.59	70,70,70,70	0
56	MG	RD	313	1/1	0.75	0.86	84,84,84,84	0
56	MG	XA	1696	1/1	0.75	0.90	67,67,67,67	0
56	MG	YA	3693	1/1	0.75	0.64	70,70,70,70	0
56	MG	RA	3281	1/1	0.75	0.24	90,90,90,90	0
56	MG	RA	3701	1/1	0.75	0.42	64,64,64,64	0
56	MG	RA	3852	1/1	0.75	0.20	90,90,90,90	0
56	MG	YA	3678	1/1	0.76	0.51	62,62,62,62	0
56	MG	YA	3751	1/1	0.76	0.71	102,102,102,102	0
56	MG	RA	4063	1/1	0.76	1.57	100,100,100,100	0
56	MG	YB	213	1/1	0.76	0.53	81,81,81,81	0
56	MG	RA	3661	1/1	0.76	0.34	73,73,73,73	0
56	MG	QA	1657	1/1	0.76	0.43	101,101,101,101	0
56	MG	RB	206	1/1	0.76	0.15	80,80,80,80	0
56	MG	RA	3339	1/1	0.76	0.74	86,86,86,86	0
56	MG	YA	3358	1/1	0.76	0.84	90,90,90,90	0
56	MG	RA	3514	1/1	0.76	0.34	63,63,63,63	0
56	MG	RA	3699	1/1	0.76	0.51	107,107,107,107	0
56	MG	RA	3366	1/1	0.76	0.42	71,71,71,71	0
56	MG	YA	3625	1/1	0.76	0.53	86,86,86,86	0
56	MG	RU	201	1/1	0.76	0.34	85,85,85,85	0
56	MG	YB	215	1/1	0.76	0.22	79,79,79,79	0
56	MG	RA	3933	1/1	0.76	0.60	84,84,84,84	0
56	MG	QA	1653	1/1	0.76	0.55	84,84,84,84	0
56	MG	RA	3307	1/1	0.76	1.83	99,99,99,99	0
56	MG	RA	3341	1/1	0.76	0.82	73,73,73,73	0
56	MG	YA	3091	1/1	0.76	0.48	76,76,76,76	0
56	MG	RA	3801	1/1	0.76	0.32	92,92,92,92	0
56	MG	RA	3370	1/1	0.76	0.75	78,78,78,78	0
56	MG	RA	3262	1/1	0.76	0.18	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3246	1/1	0.76	0.57	81,81,81,81	0
56	MG	R0	104	1/1	0.76	0.49	86,86,86,86	0
56	MG	YA	3566	1/1	0.76	0.42	73,73,73,73	0
56	MG	XA	1725	1/1	0.76	0.50	85,85,85,85	0
56	MG	YA	3659	1/1	0.76	1.06	65,65,65,65	0
56	MG	YA	3011	1/1	0.76	0.42	70,70,70,70	0
56	MG	XA	1773	1/1	0.76	0.90	79,79,79,79	0
56	MG	RA	3261	1/1	0.76	1.22	87,87,87,87	0
56	MG	RA	3087	1/1	0.76	1.00	113,113,113,113	0
56	MG	YA	3056	1/1	0.76	0.46	86,86,86,86	0
56	MG	RA	3117	1/1	0.76	0.66	96,96,96,96	0
56	MG	RA	3932	1/1	0.76	0.77	88,88,88,88	0
56	MG	XA	1694	1/1	0.76	0.37	77,77,77,77	0
56	MG	YA	3698	1/1	0.76	0.81	76,76,76,76	0
56	MG	YA	3243	1/1	0.76	1.33	90,90,90,90	0
56	MG	RA	3908	1/1	0.76	0.74	92,92,92,92	0
56	MG	RA	3454	1/1	0.76	0.41	87,87,87,87	0
56	MG	QA	1811	1/1	0.76	0.23	78,78,78,78	0
56	MG	YA	3374	1/1	0.76	0.98	75,75,75,75	0
56	MG	RA	3222	1/1	0.76	0.64	88,88,88,88	0
56	MG	XA	1626	1/1	0.76	0.66	78,78,78,78	0
56	MG	RA	3730	1/1	0.76	0.69	89,89,89,89	0
56	MG	QA	1691	1/1	0.76	0.41	96,96,96,96	0
56	MG	YA	3553	1/1	0.77	0.71	73,73,73,73	0
56	MG	RA	3491	1/1	0.77	0.29	85,85,85,85	0
56	MG	RA	3967	1/1	0.77	0.47	97,97,97,97	0
56	MG	RA	3255	1/1	0.77	0.57	97,97,97,97	0
56	MG	RA	3679	1/1	0.77	0.40	72,72,72,72	0
56	MG	RA	3937	1/1	0.77	0.82	80,80,80,80	0
56	MG	RA	3890	1/1	0.77	0.99	77,77,77,77	0
56	MG	RA	3396	1/1	0.77	0.25	67,67,67,67	0
56	MG	YA	3317	1/1	0.77	0.69	69,69,69,69	0
56	MG	RA	3882	1/1	0.77	1.20	87,87,87,87	0
56	MG	YE	304	1/1	0.77	0.29	71,71,71,71	0
56	MG	RA	3191	1/1	0.77	0.28	90,90,90,90	0
56	MG	RA	3144	1/1	0.77	0.69	86,86,86,86	0
56	MG	YA	3069	1/1	0.77	0.58	98,98,98,98	0
56	MG	R5	101	1/1	0.77	1.50	105,105,105,105	0
56	MG	YA	3488	1/1	0.77	0.46	77,77,77,77	0
56	MG	YA	3594	1/1	0.77	0.71	70,70,70,70	0
56	MG	YA	3666	1/1	0.77	0.45	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3067	1/1	0.77	0.31	76,76,76,76	0
56	MG	QA	1789	1/1	0.77	0.37	85,85,85,85	0
56	MG	QA	1790	1/1	0.77	0.40	81,81,81,81	0
56	MG	YA	3348	1/1	0.77	0.59	88,88,88,88	0
56	MG	RA	4035	1/1	0.77	1.19	90,90,90,90	0
56	MG	RA	3210	1/1	0.77	2.13	110,110,110,110	0
56	MG	XA	1733	1/1	0.77	0.98	69,69,69,69	0
56	MG	YA	3595	1/1	0.77	0.48	83,83,83,83	0
56	MG	RA	3478	1/1	0.77	0.67	78,78,78,78	0
56	MG	QT	201	1/1	0.77	0.53	77,77,77,77	0
56	MG	RA	3515	1/1	0.77	0.38	90,90,90,90	0
56	MG	YA	3191	1/1	0.77	0.47	86,86,86,86	0
56	MG	Y8	101	1/1	0.77	0.79	72,72,72,72	0
56	MG	RA	3641	1/1	0.77	0.33	79,79,79,79	0
56	MG	RA	4021	1/1	0.77	0.64	78,78,78,78	0
56	MG	RA	3202	1/1	0.77	0.40	87,87,87,87	0
56	MG	YA	3604	1/1	0.77	0.85	66,66,66,66	0
56	MG	XA	1719	1/1	0.77	0.45	78,78,78,78	0
56	MG	QA	1688	1/1	0.77	1.09	81,81,81,81	0
56	MG	YB	204	1/1	0.77	0.52	95,95,95,95	0
56	MG	RA	3267	1/1	0.77	0.71	85,85,85,85	0
56	MG	YA	3095	1/1	0.77	0.54	64,64,64,64	0
56	MG	QA	1812	1/1	0.77	0.37	69,69,69,69	0
56	MG	YA	3162	1/1	0.77	0.50	96,96,96,96	0
56	MG	QA	1683	1/1	0.77	0.27	95,95,95,95	0
56	MG	YA	3284	1/1	0.77	0.51	63,63,63,63	0
56	MG	YA	3431	1/1	0.78	0.97	84,84,84,84	0
56	MG	RQ	202	1/1	0.78	0.70	73,73,73,73	0
56	MG	RA	3257	1/1	0.78	0.52	100,100,100,100	0
56	MG	YR	201	1/1	0.78	0.46	82,82,82,82	0
56	MG	QA	1824	1/1	0.78	0.57	69,69,69,69	0
56	MG	YA	3499	1/1	0.78	0.42	65,65,65,65	0
56	MG	YA	3645	1/1	0.78	0.39	88,88,88,88	0
56	MG	QA	1740	1/1	0.78	0.64	69,69,69,69	0
56	MG	YA	3098	1/1	0.78	0.36	95,95,95,95	0
56	MG	YA	3160	1/1	0.78	0.30	88,88,88,88	0
56	MG	RA	3461	1/1	0.78	1.47	84,84,84,84	0
56	MG	RA	3335	1/1	0.78	0.33	75,75,75,75	0
56	MG	RA	3811	1/1	0.78	0.89	85,85,85,85	0
56	MG	YA	3172	1/1	0.78	0.28	101,101,101,101	0
56	MG	RA	3542	1/1	0.78	0.72	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	QA	1639	1/1	0.78	0.18	93,93,93,93	0
56	MG	XA	1735	1/1	0.78	0.24	83,83,83,83	0
56	MG	QA	1851	1/1	0.78	0.66	78,78,78,78	0
56	MG	RA	3554	1/1	0.78	0.56	74,74,74,74	0
56	MG	QA	1796	1/1	0.78	0.54	90,90,90,90	0
56	MG	YA	3554	1/1	0.78	0.32	79,79,79,79	0
56	MG	YA	3715	1/1	0.78	0.43	83,83,83,83	0
56	MG	XA	1609	1/1	0.78	0.26	87,87,87,87	0
56	MG	YD	303	1/1	0.78	1.07	84,84,84,84	0
56	MG	YA	3423	1/1	0.78	0.35	83,83,83,83	0
56	MG	RB	201	1/1	0.78	0.77	104,104,104,104	0
56	MG	RA	3643	1/1	0.78	0.49	88,88,88,88	0
56	MG	RA	3500	1/1	0.78	0.64	94,94,94,94	0
56	MG	YT	201	1/1	0.78	0.73	85,85,85,85	0
56	MG	RA	3075	1/1	0.78	0.24	76,76,76,76	0
56	MG	XA	1628	1/1	0.78	0.27	79,79,79,79	0
56	MG	RA	3622	1/1	0.78	0.43	87,87,87,87	0
56	MG	YA	3357	1/1	0.78	1.26	78,78,78,78	0
56	MG	YA	3689	1/1	0.78	0.32	78,78,78,78	0
56	MG	QA	1836	1/1	0.78	0.42	77,77,77,77	0
56	MG	YA	3387	1/1	0.78	0.71	62,62,62,62	0
56	MG	QQ	201	1/1	0.79	0.24	91,91,91,91	0
56	MG	RA	3129	1/1	0.79	0.38	91,91,91,91	0
56	MG	RA	3588	1/1	0.79	1.02	76,76,76,76	0
56	MG	YA	3454	1/1	0.79	0.35	94,94,94,94	0
56	MG	YA	3118	1/1	0.79	0.44	74,74,74,74	0
56	MG	QA	1870	1/1	0.79	0.90	81,81,81,81	0
56	MG	YA	3117	1/1	0.79	0.45	87,87,87,87	0
56	MG	RA	3241	1/1	0.79	0.62	91,91,91,91	0
56	MG	RA	3361	1/1	0.79	0.49	82,82,82,82	0
56	MG	RA	3755	1/1	0.79	1.16	100,100,100,100	0
56	MG	QA	1622	1/1	0.79	0.48	89,89,89,89	0
56	MG	XV	101	1/1	0.79	0.11	87,87,87,87	0
56	MG	YA	3662	1/1	0.79	0.51	68,68,68,68	0
56	MG	XA	1681	1/1	0.79	0.17	100,100,100,100	0
56	MG	YA	3262	1/1	0.79	0.56	88,88,88,88	0
56	MG	QA	1614	1/1	0.79	0.80	85,85,85,85	0
56	MG	YA	3552	1/1	0.79	0.68	65,65,65,65	0
56	MG	YA	3675	1/1	0.79	0.64	68,68,68,68	0
56	MG	RA	3282	1/1	0.79	0.99	102,102,102,102	0
56	MG	YA	3298	1/1	0.79	0.25	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3528	1/1	0.79	1.35	72,72,72,72	0
56	MG	QA	1623	1/1	0.79	0.33	86,86,86,86	0
56	MG	RD	309	1/1	0.79	0.64	100,100,100,100	0
56	MG	RA	4055	1/1	0.79	0.60	95,95,95,95	0
56	MG	XA	1680	1/1	0.79	0.76	80,80,80,80	0
56	MG	XA	1707	1/1	0.79	0.27	80,80,80,80	0
56	MG	YA	3048	1/1	0.79	0.32	98,98,98,98	0
56	MG	RA	3570	1/1	0.79	0.56	71,71,71,71	0
56	MG	RA	3505	1/1	0.79	0.31	68,68,68,68	0
56	MG	YA	3154	1/1	0.79	0.52	81,81,81,81	0
56	MG	RA	3429	1/1	0.79	0.25	98,98,98,98	0
56	MG	Y8	102	1/1	0.79	0.61	68,68,68,68	0
56	MG	RA	3338	1/1	0.79	0.74	62,62,62,62	0
56	MG	RA	3589	1/1	0.79	0.35	94,94,94,94	0
56	MG	YA	3385	1/1	0.79	0.49	69,69,69,69	0
56	MG	YA	3636	1/1	0.79	0.93	72,72,72,72	0
56	MG	RA	3188	1/1	0.79	0.56	104,104,104,104	0
56	MG	QA	1608	1/1	0.79	0.33	107,107,107,107	0
56	MG	RA	3165	1/1	0.79	1.06	103,103,103,103	0
56	MG	YA	3122	1/1	0.79	0.55	82,82,82,82	0
56	MG	RA	3651	1/1	0.79	0.40	80,80,80,80	0
56	MG	YA	3618	1/1	0.79	0.80	82,82,82,82	0
56	MG	RA	3532	1/1	0.79	0.27	63,63,63,63	0
56	MG	QA	1658	1/1	0.79	0.30	88,88,88,88	0
56	MG	XA	1734	1/1	0.79	0.35	89,89,89,89	0
56	MG	YA	3522	1/1	0.79	0.60	75,75,75,75	0
56	MG	RA	3023	1/1	0.79	0.36	78,78,78,78	0
56	MG	RA	3292	1/1	0.79	0.66	93,93,93,93	0
56	MG	YA	3169	1/1	0.80	0.40	85,85,85,85	0
56	MG	YA	3500	1/1	0.80	1.04	84,84,84,84	0
56	MG	RA	3068	1/1	0.80	0.48	91,91,91,91	0
56	MG	YA	3295	1/1	0.80	1.09	62,62,62,62	0
56	MG	YA	3353	1/1	0.80	0.54	68,68,68,68	0
56	MG	YA	3583	1/1	0.80	0.52	74,74,74,74	0
56	MG	RA	3777	1/1	0.80	0.34	84,84,84,84	0
56	MG	YA	3235	1/1	0.80	0.45	93,93,93,93	0
56	MG	RA	3436	1/1	0.80	1.11	63,63,63,63	0
56	MG	RA	3794	1/1	0.80	0.36	72,72,72,72	0
56	MG	YA	3174	1/1	0.80	0.21	78,78,78,78	0
56	MG	QA	1645	1/1	0.80	0.25	76,76,76,76	0
57	ZN	R6	101	1/1	0.80	0.32	159,159,159,159	0
56	MG	RA	3965	1/1	0.80	0.18	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3350	1/1	0.80	0.58	76,76,76,76	0
56	MG	RA	3168	1/1	0.80	0.51	91,91,91,91	0
56	MG	YF	303	1/1	0.80	0.96	108,108,108,108	0
56	MG	RA	3605	1/1	0.80	0.57	90,90,90,90	0
56	MG	RA	3896	1/1	0.80	1.21	72,72,72,72	0
56	MG	YA	3731	1/1	0.80	1.43	78,78,78,78	0
56	MG	YX	101	1/1	0.80	0.41	69,69,69,69	0
56	MG	RA	3118	1/1	0.80	0.72	96,96,96,96	0
56	MG	RA	3343	1/1	0.80	0.29	80,80,80,80	0
56	MG	XA	1763	1/1	0.80	0.42	70,70,70,70	0
56	MG	RA	3266	1/1	0.80	0.13	106,106,106,106	0
56	MG	RA	3954	1/1	0.80	0.26	82,82,82,82	0
56	MG	RA	3983	1/1	0.80	0.38	91,91,91,91	0
56	MG	YA	3600	1/1	0.80	0.68	65,65,65,65	0
56	MG	RA	3102	1/1	0.80	0.84	88,88,88,88	0
56	MG	YA	3239	1/1	0.80	0.53	98,98,98,98	0
56	MG	RA	3668	1/1	0.80	0.47	80,80,80,80	0
56	MG	YA	3060	1/1	0.80	0.34	68,68,68,68	0
56	MG	RA	3795	1/1	0.80	0.60	75,75,75,75	0
56	MG	RA	4066	1/1	0.80	0.77	86,86,86,86	0
56	MG	YA	3543	1/1	0.80	0.35	80,80,80,80	0
56	MG	YA	3110	1/1	0.80	0.44	62,62,62,62	0
56	MG	RA	4015	1/1	0.80	0.71	93,93,93,93	0
56	MG	RA	3041	1/1	0.80	0.20	70,70,70,70	0
56	MG	QA	1626	1/1	0.80	0.33	87,87,87,87	0
56	MG	YD	302	1/1	0.80	0.85	81,81,81,81	0
56	MG	YA	3334	1/1	0.80	0.57	66,66,66,66	0
56	MG	RA	3624	1/1	0.80	0.81	75,75,75,75	0
56	MG	XA	1771	1/1	0.80	0.95	72,72,72,72	0
56	MG	QA	1662	1/1	0.80	0.32	90,90,90,90	0
56	MG	XA	1721	1/1	0.80	1.29	78,78,78,78	0
56	MG	QA	1624	1/1	0.80	0.51	74,74,74,74	0
56	MG	RF	305	1/1	0.80	0.94	101,101,101,101	0
56	MG	XA	1670	1/1	0.80	0.34	89,89,89,89	0
56	MG	RA	3021	1/1	0.80	0.95	103,103,103,103	0
56	MG	QA	1709	1/1	0.80	0.22	90,90,90,90	0
56	MG	RA	3979	1/1	0.80	0.78	70,70,70,70	0
56	MG	RA	3274	1/1	0.80	0.37	88,88,88,88	0
56	MG	RA	4017	1/1	0.80	0.97	92,92,92,92	0
56	MG	YA	3432	1/1	0.80	0.36	76,76,76,76	0
56	MG	RA	3722	1/1	0.80	0.42	83,83,83,83	0
56	MG	RA	3157	1/1	0.80	0.25	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	QA	1791	1/1	0.80	0.27	89,89,89,89	0
56	MG	RA	3614	1/1	0.81	0.37	68,68,68,68	0
56	MG	RD	306	1/1	0.81	0.52	84,84,84,84	0
56	MG	YA	3429	1/1	0.81	0.41	73,73,73,73	0
56	MG	RA	3152	1/1	0.81	0.26	93,93,93,93	0
56	MG	QA	1605	1/1	0.81	0.17	90,90,90,90	0
56	MG	RD	307	1/1	0.81	0.26	72,72,72,72	0
56	MG	RA	3178	1/1	0.81	0.44	107,107,107,107	0
56	MG	QA	1678	1/1	0.81	0.33	93,93,93,93	0
56	MG	RA	4064	1/1	0.81	1.12	84,84,84,84	0
56	MG	XA	1614	1/1	0.81	0.19	77,77,77,77	0
56	MG	RA	3377	1/1	0.81	0.32	69,69,69,69	0
56	MG	QA	1675	1/1	0.81	0.51	91,91,91,91	0
56	MG	RA	3051	1/1	0.81	0.75	97,97,97,97	0
56	MG	RA	3893	1/1	0.81	0.59	76,76,76,76	0
56	MG	YA	3704	1/1	0.81	0.37	66,66,66,66	0
56	MG	YA	3610	1/1	0.81	0.55	64,64,64,64	0
56	MG	RA	3477	1/1	0.81	0.50	63,63,63,63	0
56	MG	XA	1706	1/1	0.81	0.14	78,78,78,78	0
56	MG	RA	3409	1/1	0.81	0.45	65,65,65,65	0
56	MG	YA	3657	1/1	0.81	0.67	81,81,81,81	0
56	MG	YA	3107	1/1	0.81	0.42	74,74,74,74	0
56	MG	RA	3415	1/1	0.81	0.42	62,62,62,62	0
56	MG	XA	1607	1/1	0.81	0.28	95,95,95,95	0
56	MG	QA	1810	1/1	0.81	0.67	81,81,81,81	0
56	MG	YA	3148	1/1	0.81	0.33	63,63,63,63	0
56	MG	RA	3856	1/1	0.81	0.55	77,77,77,77	0
56	MG	YA	3286	1/1	0.81	0.28	80,80,80,80	0
56	MG	RA	3160	1/1	0.81	0.94	102,102,102,102	0
56	MG	YA	3632	1/1	0.81	0.56	67,67,67,67	0
56	MG	RA	3151	1/1	0.81	0.52	84,84,84,84	0
56	MG	XA	1635	1/1	0.81	0.32	70,70,70,70	0
56	MG	RA	4034	1/1	0.81	0.97	88,88,88,88	0
56	MG	YA	3042	1/1	0.81	0.24	76,76,76,76	0
56	MG	YA	3189	1/1	0.81	0.32	83,83,83,83	0
56	MG	XA	1724	1/1	0.81	0.35	75,75,75,75	0
56	MG	RD	301	1/1	0.81	1.08	93,93,93,93	0
56	MG	RA	3139	1/1	0.81	0.45	89,89,89,89	0
56	MG	RA	3929	1/1	0.81	0.43	85,85,85,85	0
56	MG	XA	1603	1/1	0.81	0.33	83,83,83,83	0
56	MG	RB	216	1/1	0.81	0.55	88,88,88,88	0
56	MG	RA	3249	1/1	0.81	0.46	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3738	1/1	0.81	0.92	99,99,99,99	0
56	MG	YA	3229	1/1	0.81	0.30	83,83,83,83	0
56	MG	XA	1606	1/1	0.81	0.33	90,90,90,90	0
56	MG	QA	1857	1/1	0.81	0.34	83,83,83,83	0
56	MG	QA	1776	1/1	0.81	0.42	83,83,83,83	0
56	MG	QA	1827	1/1	0.81	0.40	74,74,74,74	0
56	MG	XA	1654	1/1	0.81	0.29	87,87,87,87	0
56	MG	YA	3592	1/1	0.81	0.32	78,78,78,78	0
56	MG	YA	3673	1/1	0.81	1.15	66,66,66,66	0
56	MG	QA	1752	1/1	0.81	0.37	94,94,94,94	0
56	MG	RA	3226	1/1	0.82	0.81	113,113,113,113	0
56	MG	QA	1843	1/1	0.82	0.50	68,68,68,68	0
56	MG	RA	3265	1/1	0.82	0.77	94,94,94,94	0
56	MG	RA	4005	1/1	0.82	0.22	80,80,80,80	0
56	MG	RA	3263	1/1	0.82	0.64	93,93,93,93	0
56	MG	QA	1617	1/1	0.82	0.34	98,98,98,98	0
56	MG	RA	3289	1/1	0.82	0.40	99,99,99,99	0
56	MG	RA	3088	1/1	0.82	1.03	98,98,98,98	0
56	MG	RA	3726	1/1	0.82	0.51	74,74,74,74	0
56	MG	QA	1797	1/1	0.82	0.51	75,75,75,75	0
56	MG	RA	3692	1/1	0.82	0.59	84,84,84,84	0
56	MG	YA	3053	1/1	0.82	0.23	62,62,62,62	0
56	MG	YA	3273	1/1	0.82	0.36	84,84,84,84	0
56	MG	YA	3422	1/1	0.82	0.32	90,90,90,90	0
56	MG	RA	3680	1/1	0.82	1.04	69,69,69,69	0
56	MG	YA	3745	1/1	0.82	0.95	104,104,104,104	0
56	MG	YB	214	1/1	0.82	0.25	78,78,78,78	0
56	MG	YA	3089	1/1	0.82	0.29	80,80,80,80	0
56	MG	QO	101	1/1	0.82	0.29	86,86,86,86	0
56	MG	YA	3135	1/1	0.82	0.40	63,63,63,63	0
56	MG	RX	101	1/1	0.82	0.41	78,78,78,78	0
56	MG	QA	1655	1/1	0.82	0.31	93,93,93,93	0
56	MG	YA	3753	1/1	0.82	1.12	81,81,81,81	0
56	MG	YA	3593	1/1	0.82	0.61	87,87,87,87	0
56	MG	YA	3068	1/1	0.82	0.40	79,79,79,79	0
56	MG	RA	3894	1/1	0.82	0.79	69,69,69,69	0
56	MG	QA	1633	1/1	0.82	0.15	84,84,84,84	0
56	MG	RA	3509	1/1	0.82	0.45	81,81,81,81	0
56	MG	RA	3652	1/1	0.82	0.16	81,81,81,81	0
56	MG	RA	3304	1/1	0.82	0.68	76,76,76,76	0
56	MG	RA	3610	1/1	0.82	0.50	91,91,91,91	0
56	MG	YA	3643	1/1	0.82	0.30	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3653	1/1	0.82	0.83	64,64,64,64	0
56	MG	YA	3602	1/1	0.82	1.45	75,75,75,75	0
56	MG	RA	3868	1/1	0.82	0.14	83,83,83,83	0
56	MG	RA	3909	1/1	0.82	0.67	62,62,62,62	0
56	MG	QA	1644	1/1	0.82	0.39	95,95,95,95	0
56	MG	RA	3986	1/1	0.82	0.56	79,79,79,79	0
56	MG	YA	3158	1/1	0.82	0.43	84,84,84,84	0
56	MG	YA	3085	1/1	0.82	0.18	85,85,85,85	0
56	MG	RA	3744	1/1	0.82	0.58	73,73,73,73	0
56	MG	XA	1692	1/1	0.82	0.55	69,69,69,69	0
56	MG	YA	3054	1/1	0.82	0.46	102,102,102,102	0
56	MG	QA	1844	1/1	0.82	0.33	100,100,100,100	0
56	MG	RA	3015	1/1	0.82	0.54	84,84,84,84	0
56	MG	RG	201	1/1	0.82	0.33	89,89,89,89	0
56	MG	YA	3623	1/1	0.82	0.55	65,65,65,65	0
56	MG	RA	3096	1/1	0.82	0.29	83,83,83,83	0
56	MG	RA	3378	1/1	0.82	0.54	66,66,66,66	0
56	MG	RT	201	1/1	0.82	1.45	78,78,78,78	0
56	MG	YA	3010	1/1	0.82	0.43	84,84,84,84	0
56	MG	RA	3575	1/1	0.82	0.43	70,70,70,70	0
56	MG	RA	3678	1/1	0.82	0.88	78,78,78,78	0
56	MG	RA	3221	1/1	0.82	1.14	92,92,92,92	0
56	MG	YA	3176	1/1	0.82	0.34	78,78,78,78	0
57	ZN	Y6	101	1/1	0.82	0.37	156,156,156,156	0
56	MG	RF	307	1/1	0.82	0.65	74,74,74,74	0
56	MG	YA	3587	1/1	0.82	0.39	68,68,68,68	0
56	MG	QA	1708	1/1	0.82	0.44	69,69,69,69	0
56	MG	YA	3655	1/1	0.82	0.53	62,62,62,62	0
56	MG	YA	3380	1/1	0.82	0.47	83,83,83,83	0
56	MG	RA	3240	1/1	0.82	0.52	106,106,106,106	0
56	MG	YA	3012	1/1	0.82	0.26	70,70,70,70	0
56	MG	RA	3947	1/1	0.83	0.40	63,63,63,63	0
56	MG	RA	4022	1/1	0.83	0.47	77,77,77,77	0
56	MG	RA	3657	1/1	0.83	1.07	70,70,70,70	0
56	MG	YA	3540	1/1	0.83	0.59	82,82,82,82	0
56	MG	RB	221	1/1	0.83	0.23	84,84,84,84	0
56	MG	RA	3974	1/1	0.83	0.31	88,88,88,88	0
56	MG	QA	1695	1/1	0.83	0.46	93,93,93,93	0
56	MG	QA	1767	1/1	0.83	0.38	88,88,88,88	0
56	MG	XA	1785	1/1	0.83	0.89	82,82,82,82	0
56	MG	RA	3765	1/1	0.83	0.28	91,91,91,91	0
56	MG	RA	3297	1/1	0.83	0.33	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3976	1/1	0.83	0.34	76,76,76,76	0
56	MG	RA	3143	1/1	0.83	0.27	77,77,77,77	0
56	MG	YA	3732	1/1	0.83	0.26	86,86,86,86	0
56	MG	XA	1639	1/1	0.83	0.21	86,86,86,86	0
56	MG	RA	3768	1/1	0.83	0.53	74,74,74,74	0
56	MG	RA	3761	1/1	0.83	0.26	70,70,70,70	0
56	MG	RA	3625	1/1	0.83	0.30	73,73,73,73	0
56	MG	RA	3381	1/1	0.83	0.41	64,64,64,64	0
56	MG	RB	213	1/1	0.83	0.81	71,71,71,71	0
56	MG	YA	3701	1/1	0.83	0.61	62,62,62,62	0
56	MG	RA	3945	1/1	0.83	0.21	63,63,63,63	0
56	MG	QA	1659	1/1	0.83	0.97	92,92,92,92	0
56	MG	XA	1789	1/1	0.83	0.69	81,81,81,81	0
56	MG	YA	3073	1/1	0.83	0.31	86,86,86,86	0
56	MG	YA	3613	1/1	0.83	0.41	75,75,75,75	0
56	MG	RA	4052	1/1	0.83	1.02	90,90,90,90	0
56	MG	RA	3463	1/1	0.83	0.54	69,69,69,69	0
56	MG	QA	1742	1/1	0.83	0.18	92,92,92,92	0
56	MG	YA	3510	1/1	0.83	0.46	77,77,77,77	0
56	MG	QA	1692	1/1	0.83	0.56	98,98,98,98	0
56	MG	RA	3153	1/1	0.83	0.48	90,90,90,90	0
56	MG	YA	3402	1/1	0.83	0.27	86,86,86,86	0
56	MG	YA	3686	1/1	0.83	0.46	77,77,77,77	0
56	MG	YA	3555	1/1	0.83	0.40	64,64,64,64	0
56	MG	RA	3002	1/1	0.83	0.34	67,67,67,67	0
56	MG	RA	3330	1/1	0.83	0.41	68,68,68,68	0
56	MG	RA	3403	1/1	0.83	1.01	87,87,87,87	0
56	MG	YA	3526	1/1	0.83	0.68	65,65,65,65	0
56	MG	RA	3718	1/1	0.83	0.84	65,65,65,65	0
56	MG	YA	3366	1/1	0.83	0.12	95,95,95,95	0
56	MG	YA	3316	1/1	0.83	0.62	62,62,62,62	0
56	MG	YA	3646	1/1	0.83	0.43	68,68,68,68	0
56	MG	RA	3853	1/1	0.83	0.55	90,90,90,90	0
56	MG	YA	3617	1/1	0.83	0.51	74,74,74,74	0
56	MG	RA	3571	1/1	0.83	0.17	74,74,74,74	0
56	MG	RA	3056	1/1	0.83	0.83	87,87,87,87	0
56	MG	RD	305	1/1	0.83	0.84	102,102,102,102	0
56	MG	RD	302	1/1	0.83	0.82	71,71,71,71	0
56	MG	RA	3256	1/1	0.84	0.88	96,96,96,96	0
56	MG	RA	3479	1/1	0.84	0.39	80,80,80,80	0
56	MG	YB	217	1/1	0.84	0.34	84,84,84,84	0
56	MG	YA	3648	1/1	0.84	0.63	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3544	1/1	0.84	0.39	65,65,65,65	0
56	MG	RA	3110	1/1	0.84	0.77	94,94,94,94	0
56	MG	RA	3201	1/1	0.84	0.54	96,96,96,96	0
56	MG	QA	1815	1/1	0.84	0.32	87,87,87,87	0
56	MG	RA	3069	1/1	0.84	0.37	70,70,70,70	0
56	MG	RA	3674	1/1	0.84	0.84	70,70,70,70	0
56	MG	QA	1610	1/1	0.84	0.27	93,93,93,93	0
56	MG	YA	3088	1/1	0.84	0.97	90,90,90,90	0
56	MG	XA	1744	1/1	0.84	0.90	63,63,63,63	0
56	MG	XA	1709	1/1	0.84	0.26	88,88,88,88	0
56	MG	QA	1725	1/1	0.84	0.40	76,76,76,76	0
56	MG	XA	1781	1/1	0.84	1.36	79,79,79,79	0
56	MG	RA	3720	1/1	0.84	0.45	73,73,73,73	0
56	MG	YA	3140	1/1	0.84	0.36	79,79,79,79	0
56	MG	YA	3081	1/1	0.84	0.41	81,81,81,81	0
56	MG	QA	1726	1/1	0.84	0.53	88,88,88,88	0
56	MG	QA	1763	1/1	0.84	0.36	84,84,84,84	0
56	MG	R0	101	1/1	0.84	0.73	77,77,77,77	0
57	ZN	RY	201	1/1	0.84	0.24	158,158,158,158	0
56	MG	QA	1813	1/1	0.84	0.46	90,90,90,90	0
56	MG	QQ	202	1/1	0.84	0.24	92,92,92,92	0
56	MG	RA	3574	1/1	0.84	1.32	90,90,90,90	0
56	MG	RA	3082	1/1	0.84	0.95	100,100,100,100	0
56	MG	YA	3740	1/1	0.84	0.86	96,96,96,96	0
56	MG	YA	3372	1/1	0.84	0.46	69,69,69,69	0
56	MG	QA	1863	1/1	0.84	0.51	81,81,81,81	0
56	MG	RA	3206	1/1	0.84	0.31	86,86,86,86	0
56	MG	RA	3650	1/1	0.84	0.29	76,76,76,76	0
56	MG	YA	3362	1/1	0.84	0.64	70,70,70,70	0
56	MG	RA	3285	1/1	0.84	0.69	108,108,108,108	0
56	MG	YA	3217	1/1	0.84	0.34	98,98,98,98	0
56	MG	YA	3045	1/1	0.84	0.26	64,64,64,64	0
56	MG	RA	4060	1/1	0.84	1.10	109,109,109,109	0
56	MG	YA	3616	1/1	0.84	0.34	65,65,65,65	0
56	MG	RA	3431	1/1	0.84	0.48	63,63,63,63	0
56	MG	YA	3605	1/1	0.84	0.33	84,84,84,84	0
56	MG	RA	3793	1/1	0.84	0.57	71,71,71,71	0
56	MG	QA	1627	1/1	0.84	0.10	79,79,79,79	0
56	MG	RA	3070	1/1	0.84	0.76	85,85,85,85	0
56	MG	YA	3436	1/1	0.84	0.50	65,65,65,65	0
56	MG	YA	3077	1/1	0.84	0.81	107,107,107,107	0
56	MG	QA	1699	1/1	0.84	0.20	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3711	1/1	0.84	0.30	83,83,83,83	0
56	MG	RA	3714	1/1	0.84	0.57	63,63,63,63	0
56	MG	YA	3371	1/1	0.84	1.01	68,68,68,68	0
56	MG	QA	1750	1/1	0.84	0.24	69,69,69,69	0
56	MG	RA	3258	1/1	0.84	0.49	102,102,102,102	0
56	MG	XA	1717	1/1	0.84	0.38	82,82,82,82	0
56	MG	RA	3659	1/1	0.84	0.75	95,95,95,95	0
56	MG	YA	3370	1/1	0.84	0.41	66,66,66,66	0
56	MG	YA	3237	1/1	0.84	0.91	95,95,95,95	0
56	MG	YA	3634	1/1	0.84	0.40	86,86,86,86	0
56	MG	RA	3545	1/1	0.84	0.35	85,85,85,85	0
56	MG	RA	3018	1/1	0.84	0.47	95,95,95,95	0
56	MG	YA	3417	1/1	0.84	0.67	69,69,69,69	0
56	MG	YA	3641	1/1	0.84	0.94	83,83,83,83	0
56	MG	QA	1629	1/1	0.84	0.89	83,83,83,83	0
56	MG	XA	1738	1/1	0.84	0.61	64,64,64,64	0
56	MG	RA	3483	1/1	0.84	0.66	62,62,62,62	0
56	MG	RA	3140	1/1	0.84	1.04	97,97,97,97	0
56	MG	QA	1716	1/1	0.84	0.55	75,75,75,75	0
56	MG	YA	3502	1/1	0.84	0.29	71,71,71,71	0
56	MG	XA	1688	1/1	0.84	0.43	97,97,97,97	0
56	MG	YA	3480	1/1	0.84	0.47	62,62,62,62	0
56	MG	RA	3857	1/1	0.85	0.69	76,76,76,76	0
56	MG	RA	3455	1/1	0.85	0.22	81,81,81,81	0
56	MG	QA	1718	1/1	0.85	0.33	94,94,94,94	0
56	MG	RA	3815	1/1	0.85	1.16	99,99,99,99	0
56	MG	RA	3346	1/1	0.85	0.62	83,83,83,83	0
56	MG	RA	3293	1/1	0.85	0.25	87,87,87,87	0
56	MG	YA	3725	1/1	0.85	0.35	62,62,62,62	0
56	MG	YA	3584	1/1	0.85	0.45	77,77,77,77	0
56	MG	RA	3049	1/1	0.85	0.17	80,80,80,80	0
56	MG	YA	3573	1/1	0.85	0.82	64,64,64,64	0
56	MG	YA	3426	1/1	0.85	0.32	72,72,72,72	0
56	MG	YA	3159	1/1	0.85	0.14	76,76,76,76	0
56	MG	YA	3511	1/1	0.85	0.56	62,62,62,62	0
56	MG	RA	3059	1/1	0.85	0.16	84,84,84,84	0
56	MG	YA	3742	1/1	0.85	0.27	85,85,85,85	0
56	MG	YA	3020	1/1	0.85	0.58	96,96,96,96	0
56	MG	YA	3546	1/1	0.85	0.77	75,75,75,75	0
56	MG	RA	3004	1/1	0.85	0.17	63,63,63,63	0
56	MG	RA	3386	1/1	0.85	0.71	76,76,76,76	0
56	MG	RA	3130	1/1	0.85	0.17	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3664	1/1	0.85	0.37	91,91,91,91	0
56	MG	RA	3243	1/1	0.85	0.84	103,103,103,103	0
56	MG	RA	3324	1/1	0.85	0.65	62,62,62,62	0
56	MG	RA	3475	1/1	0.85	0.30	82,82,82,82	0
56	MG	YA	3369	1/1	0.85	0.32	72,72,72,72	0
56	MG	YA	3459	1/1	0.85	0.29	63,63,63,63	0
56	MG	RA	3786	1/1	0.85	0.69	89,89,89,89	0
56	MG	RA	3163	1/1	0.85	1.46	88,88,88,88	0
56	MG	YA	3375	1/1	0.85	0.33	80,80,80,80	0
56	MG	QA	1861	1/1	0.85	0.38	72,72,72,72	0
56	MG	RA	3019	1/1	0.85	0.40	108,108,108,108	0
56	MG	YA	3165	1/1	0.85	0.46	100,100,100,100	0
56	MG	YA	3139	1/1	0.85	0.30	63,63,63,63	0
56	MG	RA	3230	1/1	0.85	0.57	106,106,106,106	0
56	MG	XA	1708	1/1	0.85	0.82	75,75,75,75	0
56	MG	RA	3820	1/1	0.85	0.42	76,76,76,76	0
56	MG	RA	4030	1/1	0.85	1.21	103,103,103,103	0
56	MG	RA	3517	1/1	0.85	0.94	62,62,62,62	0
56	MG	RA	3466	1/1	0.85	0.70	62,62,62,62	0
56	MG	RA	3078	1/1	0.85	0.84	90,90,90,90	0
56	MG	YA	3210	1/1	0.85	0.39	70,70,70,70	0
56	MG	YA	3275	1/1	0.85	0.51	89,89,89,89	0
56	MG	RA	3534	1/1	0.85	0.38	75,75,75,75	0
56	MG	XA	1762	1/1	0.85	0.29	70,70,70,70	0
56	MG	YA	3576	1/1	0.85	0.76	74,74,74,74	0
56	MG	YG	202	1/1	0.86	0.20	92,92,92,92	0
56	MG	YA	3415	1/1	0.86	0.78	68,68,68,68	0
56	MG	RA	4006	1/1	0.86	0.30	74,74,74,74	0
56	MG	RA	3831	1/1	0.86	0.23	90,90,90,90	0
56	MG	QA	1829	1/1	0.86	0.32	81,81,81,81	0
56	MG	RA	3269	1/1	0.86	0.32	90,90,90,90	0
56	MG	QA	1711	1/1	0.86	0.50	78,78,78,78	0
56	MG	RG	202	1/1	0.86	0.07	86,86,86,86	0
56	MG	YA	3253	1/1	0.86	0.62	87,87,87,87	0
56	MG	RA	3072	1/1	0.86	1.19	110,110,110,110	0
56	MG	RA	3271	1/1	0.86	0.37	97,97,97,97	0
56	MG	YA	3684	1/1	0.86	0.52	63,63,63,63	0
56	MG	YA	3347	1/1	0.86	0.23	79,79,79,79	0
56	MG	YA	3468	1/1	0.86	0.59	62,62,62,62	0
56	MG	XA	1678	1/1	0.86	0.30	72,72,72,72	0
56	MG	QA	1602	1/1	0.86	0.18	88,88,88,88	0
56	MG	QA	1770	1/1	0.86	0.15	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3363	1/1	0.86	0.60	75,75,75,75	0
56	MG	YA	3034	1/1	0.86	0.28	74,74,74,74	0
56	MG	RA	3671	1/1	0.86	0.12	79,79,79,79	0
56	MG	RA	3987	1/1	0.86	0.80	79,79,79,79	0
56	MG	QA	1665	1/1	0.86	0.29	95,95,95,95	0
56	MG	RA	3863	1/1	0.86	0.29	86,86,86,86	0
56	MG	YA	3021	1/1	0.86	0.20	66,66,66,66	0
56	MG	RA	3665	1/1	0.86	0.28	62,62,62,62	0
56	MG	YA	3550	1/1	0.86	0.39	80,80,80,80	0
56	MG	YA	3221	1/1	0.86	0.17	80,80,80,80	0
56	MG	XA	1727	1/1	0.86	0.23	79,79,79,79	0
56	MG	YA	3145	1/1	0.86	0.25	88,88,88,88	0
56	MG	YA	3627	1/1	0.86	0.32	82,82,82,82	0
56	MG	RA	3186	1/1	0.86	0.94	98,98,98,98	0
56	MG	RA	3092	1/1	0.86	0.39	91,91,91,91	0
56	MG	RA	3928	1/1	0.86	0.43	90,90,90,90	0
56	MG	YA	3342	1/1	0.86	0.67	62,62,62,62	0
56	MG	RA	3064	1/1	0.86	0.27	81,81,81,81	0
56	MG	YA	3533	1/1	0.86	0.44	76,76,76,76	0
56	MG	RA	3329	1/1	0.86	0.30	94,94,94,94	0
56	MG	RA	3094	1/1	0.86	1.24	85,85,85,85	0
56	MG	XA	1739	1/1	0.86	0.73	82,82,82,82	0
56	MG	QA	1648	1/1	0.86	0.17	87,87,87,87	0
56	MG	YA	3150	1/1	0.86	0.41	79,79,79,79	0
56	MG	QA	1804	1/1	0.86	0.40	85,85,85,85	0
56	MG	XA	1618	1/1	0.86	0.30	81,81,81,81	0
56	MG	QA	1743	1/1	0.86	0.27	71,71,71,71	0
56	MG	YA	3703	1/1	0.86	0.44	90,90,90,90	0
56	MG	RA	3308	1/1	0.86	0.83	94,94,94,94	0
56	MG	YA	3215	1/1	0.86	0.32	86,86,86,86	0
56	MG	RA	3881	1/1	0.86	0.28	80,80,80,80	0
56	MG	RA	3593	1/1	0.86	1.03	84,84,84,84	0
56	MG	QA	1693	1/1	0.86	0.60	87,87,87,87	0
56	MG	RA	3724	1/1	0.86	0.25	82,82,82,82	0
56	MG	RA	3867	1/1	0.87	0.15	81,81,81,81	0
56	MG	QA	1631	1/1	0.87	0.17	73,73,73,73	0
56	MG	RA	4041	1/1	0.87	0.77	109,109,109,109	0
56	MG	RA	3185	1/1	0.87	0.73	85,85,85,85	0
56	MG	RA	3539	1/1	0.87	0.45	98,98,98,98	0
56	MG	XA	1741	1/1	0.87	0.34	78,78,78,78	0
56	MG	XA	1751	1/1	0.87	0.23	87,87,87,87	0
56	MG	QA	1663	1/1	0.87	0.23	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3328	1/1	0.87	0.59	62,62,62,62	0
56	MG	RA	3842	1/1	0.87	0.68	75,75,75,75	0
56	MG	RA	3891	1/1	0.87	0.91	69,69,69,69	0
56	MG	YA	3545	1/1	0.87	0.56	82,82,82,82	0
56	MG	QA	1822	1/1	0.87	0.33	97,97,97,97	0
56	MG	YA	3743	1/1	0.87	0.42	63,63,63,63	0
56	MG	RA	3460	1/1	0.87	0.48	79,79,79,79	0
56	MG	YA	3443	1/1	0.87	0.27	83,83,83,83	0
56	MG	RA	3667	1/1	0.87	0.62	88,88,88,88	0
56	MG	YA	3036	1/1	0.87	0.34	76,76,76,76	0
56	MG	RA	3363	1/1	0.87	0.16	91,91,91,91	0
56	MG	XA	1666	1/1	0.87	0.32	92,92,92,92	0
56	MG	YA	3039	1/1	0.87	0.19	67,67,67,67	0
56	MG	RA	3392	1/1	0.87	0.80	62,62,62,62	0
56	MG	YA	3419	1/1	0.87	0.74	77,77,77,77	0
56	MG	YA	3453	1/1	0.87	0.17	79,79,79,79	0
56	MG	RA	3231	1/1	0.87	0.82	89,89,89,89	0
56	MG	RA	3877	1/1	0.87	0.88	74,74,74,74	0
56	MG	RA	3834	1/1	0.87	0.91	63,63,63,63	0
56	MG	YA	3589	1/1	0.87	0.40	62,62,62,62	0
56	MG	YA	3029	1/1	0.87	0.62	62,62,62,62	0
56	MG	RA	3490	1/1	0.87	0.52	67,67,67,67	0
56	MG	XA	1752	1/1	0.87	0.59	81,81,81,81	0
56	MG	YA	3405	1/1	0.87	0.52	71,71,71,71	0
56	MG	YA	3046	1/1	0.87	0.32	82,82,82,82	0
56	MG	YA	3232	1/1	0.87	0.25	84,84,84,84	0
56	MG	RA	3638	1/1	0.87	0.89	85,85,85,85	0
56	MG	RA	4004	1/1	0.87	0.34	64,64,64,64	0
56	MG	RA	3792	1/1	0.87	0.47	87,87,87,87	0
56	MG	RA	3884	1/1	0.87	0.29	96,96,96,96	0
56	MG	RA	3089	1/1	0.87	0.14	91,91,91,91	0
56	MG	RA	3028	1/1	0.87	0.15	84,84,84,84	0
56	MG	RA	3083	1/1	0.87	0.69	95,95,95,95	0
56	MG	QA	1731	1/1	0.87	0.63	76,76,76,76	0
56	MG	RA	3875	1/1	0.87	0.65	62,62,62,62	0
56	MG	YA	3296	1/1	0.87	0.63	62,62,62,62	0
56	MG	RA	3095	1/1	0.87	0.49	92,92,92,92	0
56	MG	XA	1746	1/1	0.87	0.62	62,62,62,62	0
56	MG	YA	3384	1/1	0.87	0.59	64,64,64,64	0
56	MG	RA	3034	1/1	0.87	0.70	97,97,97,97	0
56	MG	RA	4014	1/1	0.87	0.31	79,79,79,79	0
56	MG	RA	4040	1/1	0.87	0.57	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3511	1/1	0.87	0.16	71,71,71,71	0
56	MG	RA	3020	1/1	0.87	0.72	95,95,95,95	0
56	MG	YA	3449	1/1	0.87	0.46	66,66,66,66	0
56	MG	YA	3578	1/1	0.87	0.62	101,101,101,101	0
56	MG	YA	3044	1/1	0.87	0.30	68,68,68,68	0
56	MG	RF	304	1/1	0.88	0.40	74,74,74,74	0
56	MG	XA	1760	1/1	0.88	0.49	67,67,67,67	0
56	MG	YA	3331	1/1	0.88	0.73	62,62,62,62	0
56	MG	YA	3321	1/1	0.88	0.51	62,62,62,62	0
56	MG	RB	210	1/1	0.88	0.75	96,96,96,96	0
56	MG	YA	3335	1/1	0.88	0.67	62,62,62,62	0
56	MG	QA	1783	1/1	0.88	0.51	63,63,63,63	0
56	MG	RA	3212	1/1	0.88	0.58	80,80,80,80	0
56	MG	YA	3241	1/1	0.88	0.65	91,91,91,91	0
56	MG	YA	3754	1/1	0.88	0.41	84,84,84,84	0
56	MG	YA	3491	1/1	0.88	0.54	91,91,91,91	0
56	MG	RA	3501	1/1	0.88	0.84	63,63,63,63	0
56	MG	XA	1644	1/1	0.88	0.13	94,94,94,94	0
56	MG	XA	1718	1/1	0.88	0.59	78,78,78,78	0
56	MG	RA	3973	1/1	0.88	0.84	99,99,99,99	0
56	MG	QA	1792	1/1	0.88	0.83	84,84,84,84	0
56	MG	YA	3609	1/1	0.88	0.58	75,75,75,75	0
56	MG	QA	1826	1/1	0.88	0.98	110,110,110,110	0
56	MG	YA	3572	1/1	0.88	0.43	72,72,72,72	0
56	MG	XA	1642	1/1	0.88	0.61	84,84,84,84	0
56	MG	YA	3622	1/1	0.88	0.37	66,66,66,66	0
56	MG	XA	1736	1/1	0.88	0.87	70,70,70,70	0
56	MG	RA	3071	1/1	0.88	0.80	86,86,86,86	0
56	MG	RA	3992	1/1	0.88	0.51	101,101,101,101	0
56	MG	YA	3559	1/1	0.88	0.33	80,80,80,80	0
56	MG	RA	3591	1/1	0.88	0.69	92,92,92,92	0
56	MG	XA	1770	1/1	0.88	0.52	87,87,87,87	0
56	MG	RA	3283	1/1	0.88	0.56	88,88,88,88	0
56	MG	YA	3260	1/1	0.88	0.56	95,95,95,95	0
56	MG	RA	3334	1/1	0.88	0.43	82,82,82,82	0
56	MG	YA	3126	1/1	0.88	0.19	65,65,65,65	0
56	MG	YB	219	1/1	0.88	0.47	63,63,63,63	0
56	MG	YA	3750	1/1	0.88	0.99	92,92,92,92	0
56	MG	RA	3889	1/1	0.88	0.66	62,62,62,62	0
56	MG	RA	3966	1/1	0.88	0.20	71,71,71,71	0
56	MG	RA	3476	1/1	0.88	0.72	78,78,78,78	0
56	MG	QA	1876	1/1	0.88	0.29	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3214	1/1	0.88	0.42	76,76,76,76	0
56	MG	QA	1607	1/1	0.88	0.28	91,91,91,91	0
56	MG	YA	3254	1/1	0.88	0.40	87,87,87,87	0
56	MG	QA	1781	1/1	0.88	0.28	95,95,95,95	0
56	MG	QA	1777	1/1	0.88	0.52	83,83,83,83	0
56	MG	QA	1850	1/1	0.88	0.37	78,78,78,78	0
56	MG	YA	3142	1/1	0.88	0.63	76,76,76,76	0
56	MG	QA	1707	1/1	0.88	0.50	66,66,66,66	0
56	MG	RA	3719	1/1	0.88	0.30	79,79,79,79	0
56	MG	RA	3754	1/1	0.88	0.82	62,62,62,62	0
56	MG	YA	3560	1/1	0.88	0.27	64,64,64,64	0
56	MG	QA	1618	1/1	0.88	0.21	101,101,101,101	0
56	MG	QA	1634	1/1	0.88	0.28	68,68,68,68	0
56	MG	RA	4033	1/1	0.88	0.69	96,96,96,96	0
56	MG	RO	201	1/1	0.89	0.26	72,72,72,72	0
56	MG	YA	3368	1/1	0.89	0.63	62,62,62,62	0
56	MG	RA	3616	1/1	0.89	0.86	62,62,62,62	0
56	MG	RA	3785	1/1	0.89	0.22	83,83,83,83	0
56	MG	RA	3158	1/1	0.89	0.18	81,81,81,81	0
56	MG	YA	3652	1/1	0.89	0.49	79,79,79,79	0
56	MG	RA	3998	1/1	0.89	0.46	84,84,84,84	0
56	MG	YA	3597	1/1	0.89	0.94	71,71,71,71	0
56	MG	RA	3923	1/1	0.89	0.30	74,74,74,74	0
56	MG	RA	3030	1/1	0.89	0.74	94,94,94,94	0
56	MG	YA	3378	1/1	0.89	0.65	62,62,62,62	0
56	MG	RA	3382	1/1	0.89	0.52	76,76,76,76	0
56	MG	YA	3256	1/1	0.89	0.21	85,85,85,85	0
56	MG	YA	3072	1/1	0.89	0.52	100,100,100,100	0
56	MG	YA	3322	1/1	0.89	0.41	64,64,64,64	0
56	MG	YA	3420	1/1	0.89	0.30	68,68,68,68	0
56	MG	QA	1616	1/1	0.89	0.30	101,101,101,101	0
56	MG	YA	3400	1/1	0.89	0.40	75,75,75,75	0
56	MG	RA	4026	1/1	0.89	0.69	105,105,105,105	0
56	MG	RA	3345	1/1	0.89	0.66	62,62,62,62	0
56	MG	YA	3639	1/1	0.89	0.77	65,65,65,65	0
56	MG	YA	3677	1/1	0.89	1.45	79,79,79,79	0
56	MG	RA	3264	1/1	0.89	0.38	84,84,84,84	0
56	MG	YA	3138	1/1	0.89	0.27	72,72,72,72	0
56	MG	RA	3746	1/1	0.89	0.47	62,62,62,62	0
56	MG	XA	1759	1/1	0.89	0.46	68,68,68,68	0
56	MG	YA	3630	1/1	0.89	0.87	66,66,66,66	0
56	MG	YA	3037	1/1	0.89	0.29	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3674	1/1	0.89	0.70	77,77,77,77	0
56	MG	RA	3211	1/1	0.89	0.29	78,78,78,78	0
56	MG	RA	3277	1/1	0.89	0.34	85,85,85,85	0
56	MG	RA	3985	1/1	0.89	0.53	70,70,70,70	0
56	MG	YA	3679	1/1	0.89	0.59	65,65,65,65	0
56	MG	RA	3912	1/1	0.89	0.27	78,78,78,78	0
57	ZN	R5	103	1/1	0.89	0.04	135,135,135,135	0
56	MG	QA	1766	1/1	0.89	0.10	96,96,96,96	0
56	MG	QA	1798	1/1	0.89	0.20	89,89,89,89	0
56	MG	RA	3055	1/1	0.89	0.94	112,112,112,112	0
56	MG	RA	3128	1/1	0.89	0.41	85,85,85,85	0
56	MG	YA	3669	1/1	0.89	0.37	65,65,65,65	0
56	MG	YA	3681	1/1	0.89	0.62	62,62,62,62	0
56	MG	RA	4027	1/1	0.89	0.60	88,88,88,88	0
56	MG	RU	203	1/1	0.89	0.40	81,81,81,81	0
56	MG	XA	1630	1/1	0.89	0.20	64,64,64,64	0
57	ZN	Y5	102	1/1	0.89	0.06	144,144,144,144	0
56	MG	XA	1641	1/1	0.90	0.24	77,77,77,77	0
56	MG	XA	1791	1/1	0.90	0.11	74,74,74,74	0
56	MG	RA	3485	1/1	0.90	0.56	70,70,70,70	0
56	MG	RA	3410	1/1	0.90	0.69	70,70,70,70	0
56	MG	Y7	101	1/1	0.90	0.93	99,99,99,99	0
56	MG	YE	307	1/1	0.90	0.35	85,85,85,85	0
56	MG	RA	4036	1/1	0.90	1.05	99,99,99,99	0
56	MG	QF	201	1/1	0.90	0.45	75,75,75,75	0
56	MG	RA	3865	1/1	0.90	0.33	93,93,93,93	0
56	MG	YA	3682	1/1	0.90	0.41	62,62,62,62	0
56	MG	YA	3144	1/1	0.90	0.10	82,82,82,82	0
56	MG	YA	3532	1/1	0.90	0.47	84,84,84,84	0
56	MG	YA	3590	1/1	0.90	0.38	65,65,65,65	0
56	MG	RA	3759	1/1	0.90	0.23	73,73,73,73	0
56	MG	YA	3424	1/1	0.90	0.46	70,70,70,70	0
56	MG	RA	3739	1/1	0.90	0.40	69,69,69,69	0
56	MG	YA	3388	1/1	0.90	0.54	62,62,62,62	0
56	MG	YA	3746	1/1	0.90	0.42	85,85,85,85	0
56	MG	YA	3517	1/1	0.90	0.51	97,97,97,97	0
56	MG	QA	1620	1/1	0.90	0.20	69,69,69,69	0
56	MG	XA	1764	1/1	0.90	0.23	73,73,73,73	0
56	MG	YA	3588	1/1	0.90	0.42	64,64,64,64	0
56	MG	YA	3288	1/1	0.90	0.65	62,62,62,62	0
56	MG	QA	1754	1/1	0.90	0.28	85,85,85,85	0
56	MG	RA	3333	1/1	0.90	0.46	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3383	1/1	0.90	0.35	63,63,63,63	0
56	MG	RA	3389	1/1	0.90	0.82	69,69,69,69	0
56	MG	YA	3744	1/1	0.90	0.85	98,98,98,98	0
56	MG	YA	3100	1/1	0.90	0.32	78,78,78,78	0
56	MG	YA	3608	1/1	0.90	0.30	66,66,66,66	0
56	MG	XA	1660	1/1	0.90	0.23	91,91,91,91	0
56	MG	YA	3395	1/1	0.90	0.29	63,63,63,63	0
56	MG	RA	3084	1/1	0.90	0.26	76,76,76,76	0
56	MG	YA	3280	1/1	0.90	0.33	64,64,64,64	0
56	MG	RA	3902	1/1	0.90	0.58	62,62,62,62	0
56	MG	RA	3412	1/1	0.90	0.46	62,62,62,62	0
56	MG	RA	3946	1/1	0.90	0.86	67,67,67,67	0
56	MG	RA	3619	1/1	0.90	0.43	67,67,67,67	0
56	MG	YA	3155	1/1	0.90	0.65	85,85,85,85	0
56	MG	YA	3272	1/1	0.90	0.76	77,77,77,77	0
56	MG	XA	1615	1/1	0.90	0.19	89,89,89,89	0
56	MG	RA	3444	1/1	0.90	1.29	62,62,62,62	0
56	MG	YA	3271	1/1	0.90	0.89	67,67,67,67	0
56	MG	YA	3680	1/1	0.90	0.79	62,62,62,62	0
56	MG	RB	220	1/1	0.90	0.71	75,75,75,75	0
56	MG	YA	3303	1/1	0.90	0.36	62,62,62,62	0
56	MG	RA	3980	1/1	0.90	0.36	77,77,77,77	0
56	MG	QV	102	1/1	0.90	0.22	94,94,94,94	0
56	MG	RA	3421	1/1	0.90	0.51	62,62,62,62	0
56	MG	QA	1715	1/1	0.90	0.52	71,71,71,71	0
56	MG	RA	3319	1/1	0.90	0.80	69,69,69,69	0
56	MG	RA	3232	1/1	0.90	0.82	100,100,100,100	0
56	MG	YA	3512	1/1	0.90	0.26	74,74,74,74	0
56	MG	XA	1677	1/1	0.90	0.33	63,63,63,63	0
56	MG	RA	3038	1/1	0.90	0.15	86,86,86,86	0
56	MG	YA	3103	1/1	0.90	0.32	67,67,67,67	0
56	MG	YA	3661	1/1	0.91	0.62	73,73,73,73	0
56	MG	RA	3380	1/1	0.91	0.68	64,64,64,64	0
56	MG	RA	4039	1/1	0.91	0.23	92,92,92,92	0
56	MG	RA	3161	1/1	0.91	0.27	83,83,83,83	0
56	MG	QA	1619	1/1	0.91	0.37	95,95,95,95	0
56	MG	RA	3480	1/1	0.91	0.50	62,62,62,62	0
56	MG	RA	3740	1/1	0.91	0.47	85,85,85,85	0
56	MG	RA	3488	1/1	0.91	0.19	67,67,67,67	0
56	MG	RA	3561	1/1	0.91	1.17	62,62,62,62	0
56	MG	YA	3667	1/1	0.91	0.66	65,65,65,65	0
56	MG	QA	1667	1/1	0.91	0.20	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3190	1/1	0.91	0.31	69,69,69,69	0
56	MG	YA	3407	1/1	0.91	0.33	62,62,62,62	0
56	MG	RA	3510	1/1	0.91	0.98	71,71,71,71	0
56	MG	RA	3982	1/1	0.91	0.14	79,79,79,79	0
56	MG	YA	3184	1/1	0.91	0.15	78,78,78,78	0
56	MG	YA	3266	1/1	0.91	0.37	91,91,91,91	0
56	MG	YA	3004	1/1	0.91	0.23	63,63,63,63	0
56	MG	YA	3485	1/1	0.91	0.56	62,62,62,62	0
56	MG	QA	1689	1/1	0.91	0.49	81,81,81,81	0
56	MG	RA	3287	1/1	0.91	0.59	102,102,102,102	0
56	MG	RA	3384	1/1	0.91	0.62	67,67,67,67	0
56	MG	XA	1776	1/1	0.91	0.32	80,80,80,80	0
56	MG	YA	3282	1/1	0.91	0.64	62,62,62,62	0
56	MG	RA	3901	1/1	0.91	0.24	71,71,71,71	0
56	MG	YA	3330	1/1	0.91	1.11	62,62,62,62	0
56	MG	RA	4059	1/1	0.91	0.83	98,98,98,98	0
56	MG	RA	3107	1/1	0.91	0.96	90,90,90,90	0
56	MG	YA	3579	1/1	0.91	0.69	62,62,62,62	0
56	MG	YA	3268	1/1	0.91	0.63	83,83,83,83	0
56	MG	RE	301	1/1	0.91	0.58	107,107,107,107	0
56	MG	RA	3313	1/1	0.91	0.72	63,63,63,63	0
56	MG	RA	3493	1/1	0.91	0.59	70,70,70,70	0
56	MG	RA	3832	1/1	0.91	0.33	84,84,84,84	0
56	MG	XA	1758	1/1	0.91	0.42	68,68,68,68	0
56	MG	RA	3063	1/1	0.91	0.31	83,83,83,83	0
56	MG	RA	3654	1/1	0.91	0.20	71,71,71,71	0
56	MG	YA	3539	1/1	0.91	0.75	72,72,72,72	0
56	MG	RA	3399	1/1	0.91	0.53	62,62,62,62	0
56	MG	RA	3706	1/1	0.91	0.47	78,78,78,78	0
56	MG	RA	3733	1/1	0.91	0.27	79,79,79,79	0
56	MG	YA	3565	1/1	0.91	0.39	64,64,64,64	0
56	MG	RA	3302	1/1	0.91	0.77	91,91,91,91	0
56	MG	XA	1679	1/1	0.91	0.68	102,102,102,102	0
56	MG	QA	1802	1/1	0.91	0.24	82,82,82,82	0
56	MG	YA	3733	1/1	0.91	0.82	89,89,89,89	0
56	MG	XA	1777	1/1	0.91	0.46	74,74,74,74	0
56	MG	RA	3468	1/1	0.91	0.46	63,63,63,63	0
56	MG	RA	3372	1/1	0.91	0.23	87,87,87,87	0
56	MG	RA	3010	1/1	0.91	0.50	79,79,79,79	0
56	MG	XA	1772	1/1	0.91	0.34	76,76,76,76	0
56	MG	RA	3914	1/1	0.91	0.56	70,70,70,70	0
56	MG	YA	3514	1/1	0.91	0.62	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3615	1/1	0.91	0.26	65,65,65,65	0
56	MG	RA	3406	1/1	0.91	0.75	68,68,68,68	0
56	MG	YA	3149	1/1	0.91	0.86	95,95,95,95	0
56	MG	RA	3119	1/1	0.92	1.26	94,94,94,94	0
56	MG	YA	3337	1/1	0.92	0.26	76,76,76,76	0
56	MG	YA	3277	1/1	0.92	0.51	62,62,62,62	0
56	MG	XA	1737	1/1	0.92	0.29	78,78,78,78	0
56	MG	YB	202	1/1	0.92	0.14	72,72,72,72	0
56	MG	RA	4002	1/1	0.92	0.42	74,74,74,74	0
56	MG	YA	3023	1/1	0.92	0.17	80,80,80,80	0
56	MG	RA	3315	1/1	0.92	0.31	82,82,82,82	0
56	MG	RA	3080	1/1	0.92	0.83	98,98,98,98	0
56	MG	YA	3748	1/1	0.92	0.63	93,93,93,93	0
56	MG	RA	3895	1/1	0.92	0.83	63,63,63,63	0
56	MG	YA	3440	1/1	0.92	0.55	64,64,64,64	0
56	MG	YA	3080	1/1	0.92	0.33	84,84,84,84	0
56	MG	RA	3217	1/1	0.92	0.53	97,97,97,97	0
56	MG	QA	1878	1/1	0.92	0.20	98,98,98,98	0
56	MG	XA	1613	1/1	0.92	0.09	73,73,73,73	0
56	MG	YA	3324	1/1	0.92	1.09	62,62,62,62	0
56	MG	YA	3730	1/1	0.92	0.27	80,80,80,80	0
56	MG	RA	3953	1/1	0.92	0.33	81,81,81,81	0
56	MG	QA	1761	1/1	0.92	0.14	88,88,88,88	0
56	MG	YA	3570	1/1	0.92	0.76	62,62,62,62	0
56	MG	YA	3151	1/1	0.92	0.23	87,87,87,87	0
56	MG	RA	3162	1/1	0.92	0.70	83,83,83,83	0
56	MG	YA	3585	1/1	0.92	0.64	64,64,64,64	0
56	MG	RA	4051	1/1	0.92	0.71	105,105,105,105	0
56	MG	RA	3607	1/1	0.92	0.92	91,91,91,91	0
56	MG	XA	1668	1/1	0.92	0.53	92,92,92,92	0
56	MG	QA	1721	1/1	0.92	0.69	62,62,62,62	0
56	MG	RA	3073	1/1	0.92	0.66	96,96,96,96	0
56	MG	YA	3355	1/1	0.92	0.96	62,62,62,62	0
56	MG	RA	3502	1/1	0.92	1.11	64,64,64,64	0
56	MG	RA	3404	1/1	0.92	0.49	71,71,71,71	0
56	MG	RA	3580	1/1	0.92	0.41	64,64,64,64	0
56	MG	YA	3066	1/1	0.92	0.61	78,78,78,78	0
56	MG	QA	1613	1/1	0.92	0.15	98,98,98,98	0
56	MG	YA	3234	1/1	0.92	0.35	92,92,92,92	0
56	MG	RA	3419	1/1	0.92	0.78	62,62,62,62	0
56	MG	YA	3591	1/1	0.92	0.79	62,62,62,62	0
56	MG	RA	3360	1/1	0.92	0.54	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	4023	1/1	0.92	0.66	101,101,101,101	0
56	MG	YA	3535	1/1	0.92	0.28	69,69,69,69	0
56	MG	RA	4018	1/1	0.92	0.38	106,106,106,106	0
56	MG	YA	3359	1/1	0.92	1.02	62,62,62,62	0
56	MG	RA	3507	1/1	0.92	0.33	75,75,75,75	0
56	MG	QA	1717	1/1	0.92	0.17	92,92,92,92	0
56	MG	XA	1671	1/1	0.92	0.25	84,84,84,84	0
56	MG	RA	3870	1/1	0.92	1.63	86,86,86,86	0
56	MG	YA	3538	1/1	0.92	0.44	64,64,64,64	0
56	MG	YA	3111	1/1	0.92	0.26	88,88,88,88	0
56	MG	RA	3233	1/1	0.92	0.80	96,96,96,96	0
56	MG	RA	3320	1/1	0.92	0.57	62,62,62,62	0
56	MG	YA	3598	1/1	0.92	0.53	62,62,62,62	0
56	MG	YA	3133	1/1	0.92	1.09	87,87,87,87	0
56	MG	RA	3331	1/1	0.92	0.93	75,75,75,75	0
56	MG	RA	3874	1/1	0.92	0.51	63,63,63,63	0
56	MG	YA	3038	1/1	0.92	0.48	77,77,77,77	0
56	MG	YA	3391	1/1	0.93	0.79	62,62,62,62	0
56	MG	RA	3135	1/1	0.93	0.38	91,91,91,91	0
56	MG	RA	3906	1/1	0.93	0.43	62,62,62,62	0
56	MG	YA	3404	1/1	0.93	0.60	62,62,62,62	0
56	MG	RB	202	1/1	0.93	0.26	80,80,80,80	0
56	MG	YA	3575	1/1	0.93	0.75	67,67,67,67	0
56	MG	RA	3351	1/1	0.93	0.19	89,89,89,89	0
56	MG	RA	3223	1/1	0.93	0.06	77,77,77,77	0
56	MG	RA	3260	1/1	0.93	0.16	99,99,99,99	0
56	MG	YA	3568	1/1	0.93	0.45	63,63,63,63	0
56	MG	YA	3224	1/1	0.93	0.35	71,71,71,71	0
56	MG	YA	3285	1/1	0.93	0.33	76,76,76,76	0
56	MG	YA	3668	1/1	0.93	0.74	62,62,62,62	0
56	MG	QA	1744	1/1	0.93	0.37	77,77,77,77	0
56	MG	RA	3390	1/1	0.93	0.42	65,65,65,65	0
56	MG	YA	3287	1/1	0.93	0.52	78,78,78,78	0
56	MG	RA	3814	1/1	0.93	0.49	73,73,73,73	0
56	MG	RA	3871	1/1	0.93	0.66	62,62,62,62	0
56	MG	RA	3127	1/1	0.93	0.50	81,81,81,81	0
56	MG	RA	3766	1/1	0.93	1.11	71,71,71,71	0
56	MG	RA	3416	1/1	0.93	0.36	75,75,75,75	0
56	MG	YD	306	1/1	0.93	0.50	81,81,81,81	0
56	MG	RA	3484	1/1	0.93	0.84	62,62,62,62	0
56	MG	YA	3340	1/1	0.93	0.56	62,62,62,62	0
56	MG	YA	3212	1/1	0.93	0.24	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3729	1/1	0.93	0.50	69,69,69,69	0
56	MG	RA	4049	1/1	0.93	0.94	99,99,99,99	0
56	MG	YA	3009	1/1	0.93	0.22	70,70,70,70	0
56	MG	RA	3577	1/1	0.93	0.32	69,69,69,69	0
56	MG	RA	3911	1/1	0.93	0.44	71,71,71,71	0
56	MG	YA	3127	1/1	0.93	0.36	70,70,70,70	0
56	MG	XA	1784	1/1	0.93	0.34	80,80,80,80	0
56	MG	YA	3410	1/1	0.93	0.59	68,68,68,68	0
56	MG	RA	3530	1/1	0.93	0.30	62,62,62,62	0
56	MG	YA	3329	1/1	0.93	0.46	62,62,62,62	0
56	MG	RA	3921	1/1	0.93	0.88	63,63,63,63	0
56	MG	RA	3175	1/1	0.93	0.69	78,78,78,78	0
56	MG	RA	3497	1/1	0.93	0.70	62,62,62,62	0
56	MG	RA	3420	1/1	0.93	0.63	62,62,62,62	0
56	MG	YA	3274	1/1	0.93	0.85	62,62,62,62	0
56	MG	RA	3916	1/1	0.93	0.32	71,71,71,71	0
56	MG	YA	3476	1/1	0.93	0.93	62,62,62,62	0
56	MG	RA	3452	1/1	0.93	0.60	62,62,62,62	0
56	MG	YA	3398	1/1	0.93	0.84	63,63,63,63	0
56	MG	RA	3093	1/1	0.93	0.18	97,97,97,97	0
56	MG	RA	3508	1/1	0.93	0.19	89,89,89,89	0
56	MG	RA	3930	1/1	0.93	0.28	73,73,73,73	0
56	MG	RA	3617	1/1	0.93	0.52	62,62,62,62	0
56	MG	RA	4045	1/1	0.93	0.72	101,101,101,101	0
56	MG	RA	3325	1/1	0.93	0.33	77,77,77,77	0
56	MG	RB	219	1/1	0.93	0.21	73,73,73,73	0
56	MG	QA	1788	1/1	0.93	0.59	93,93,93,93	0
56	MG	YA	3002	1/1	0.93	0.19	75,75,75,75	0
56	MG	RA	3623	1/1	0.93	0.69	65,65,65,65	0
56	MG	RA	3934	1/1	0.93	0.53	81,81,81,81	0
56	MG	RA	3026	1/1	0.93	1.22	100,100,100,100	0
56	MG	QA	1649	1/1	0.93	0.27	73,73,73,73	0
56	MG	RA	3318	1/1	0.93	0.72	71,71,71,71	0
56	MG	YA	3339	1/1	0.93	0.36	62,62,62,62	0
56	MG	RE	304	1/1	0.93	0.76	62,62,62,62	0
56	MG	YA	3199	1/1	0.93	0.34	71,71,71,71	0
56	MG	YA	3279	1/1	0.93	0.81	62,62,62,62	0
56	MG	YA	3434	1/1	0.93	0.45	72,72,72,72	0
56	MG	YA	3003	1/1	0.93	0.67	70,70,70,70	0
56	MG	YA	3626	1/1	0.93	0.70	62,62,62,62	0
56	MG	RA	3393	1/1	0.94	0.35	64,64,64,64	0
56	MG	YA	3727	1/1	0.94	0.36	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YB	207	1/1	0.94	0.35	97,97,97,97	0
56	MG	XA	1732	1/1	0.94	0.53	87,87,87,87	0
56	MG	RA	3702	1/1	0.94	0.20	83,83,83,83	0
56	MG	YA	3479	1/1	0.94	0.48	62,62,62,62	0
56	MG	YA	3614	1/1	0.94	0.53	68,68,68,68	0
56	MG	YA	3430	1/1	0.94	0.27	80,80,80,80	0
56	MG	YA	3124	1/1	0.94	0.17	93,93,93,93	0
57	ZN	R9	102	1/1	0.94	0.10	125,125,125,125	0
56	MG	YA	3571	1/1	0.94	0.69	64,64,64,64	0
56	MG	YA	3136	1/1	0.94	0.33	65,65,65,65	0
56	MG	XA	1695	1/1	0.94	0.54	73,73,73,73	0
56	MG	QA	1638	1/1	0.94	0.25	75,75,75,75	0
56	MG	RA	3046	1/1	0.94	0.80	99,99,99,99	0
56	MG	YA	3065	1/1	0.94	0.85	86,86,86,86	0
56	MG	QA	1785	1/1	0.94	0.15	95,95,95,95	0
56	MG	YA	3567	1/1	0.94	0.65	62,62,62,62	0
56	MG	RA	3504	1/1	0.94	0.40	62,62,62,62	0
56	MG	RA	3971	1/1	0.94	0.47	63,63,63,63	0
56	MG	YA	3343	1/1	0.94	0.83	62,62,62,62	0
56	MG	YA	3537	1/1	0.94	0.50	62,62,62,62	0
56	MG	YA	3392	1/1	0.94	0.65	62,62,62,62	0
56	MG	YA	3360	1/1	0.94	1.11	62,62,62,62	0
56	MG	RA	3549	1/1	0.94	0.44	76,76,76,76	0
56	MG	RA	3326	1/1	0.94	0.29	63,63,63,63	0
56	MG	RA	3839	1/1	0.94	0.86	62,62,62,62	0
56	MG	RA	3443	1/1	0.94	0.99	62,62,62,62	0
56	MG	RA	3503	1/1	0.94	0.47	65,65,65,65	0
56	MG	RA	3414	1/1	0.94	0.42	62,62,62,62	0
56	MG	YA	3494	1/1	0.94	0.41	64,64,64,64	0
56	MG	RA	3104	1/1	0.94	0.33	77,77,77,77	0
56	MG	YA	3052	1/1	0.94	0.10	80,80,80,80	0
56	MG	RA	3878	1/1	0.94	0.37	62,62,62,62	0
56	MG	RA	3347	1/1	0.94	0.74	62,62,62,62	0
56	MG	YA	3377	1/1	0.94	0.52	62,62,62,62	0
56	MG	RA	3779	1/1	0.94	1.31	71,71,71,71	0
56	MG	YA	3213	1/1	0.94	0.52	63,63,63,63	0
56	MG	YA	3121	1/1	0.94	0.09	77,77,77,77	0
56	MG	RA	3516	1/1	0.94	0.48	84,84,84,84	0
56	MG	QA	1641	1/1	0.94	0.31	95,95,95,95	0
56	MG	XA	1774	1/1	0.94	0.66	80,80,80,80	0
56	MG	YA	3577	1/1	0.94	0.65	62,62,62,62	0
56	MG	RA	3598	1/1	0.94	0.37	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3379	1/1	0.94	0.27	73,73,73,73	0
56	MG	YA	3383	1/1	0.94	0.61	63,63,63,63	0
56	MG	XA	1643	1/1	0.94	0.31	81,81,81,81	0
56	MG	RA	4056	1/1	0.94	0.79	112,112,112,112	0
56	MG	YA	3482	1/1	0.94	0.85	62,62,62,62	0
56	MG	YA	3401	1/1	0.94	0.69	62,62,62,62	0
56	MG	XA	1747	1/1	0.94	0.67	63,63,63,63	0
57	ZN	Y9	101	1/1	0.94	0.06	116,116,116,116	0
56	MG	XA	1753	1/1	0.94	0.25	81,81,81,81	0
56	MG	YA	3536	1/1	0.94	0.47	63,63,63,63	0
56	MG	XA	1689	1/1	0.94	0.44	75,75,75,75	0
56	MG	RA	3125	1/1	0.94	0.52	93,93,93,93	0
56	MG	YA	3014	1/1	0.95	0.19	82,82,82,82	0
56	MG	RA	3195	1/1	0.95	0.61	97,97,97,97	0
56	MG	RA	3395	1/1	0.95	0.60	62,62,62,62	0
56	MG	YA	3319	1/1	0.95	0.62	62,62,62,62	0
56	MG	RA	3348	1/1	0.95	0.59	74,74,74,74	0
56	MG	YA	3318	1/1	0.95	0.48	62,62,62,62	0
56	MG	YA	3345	1/1	0.95	0.35	62,62,62,62	0
56	MG	RA	3469	1/1	0.95	0.39	68,68,68,68	0
56	MG	YA	3326	1/1	0.95	0.46	65,65,65,65	0
56	MG	RA	3594	1/1	0.95	0.51	80,80,80,80	0
56	MG	RA	3903	1/1	0.95	0.46	79,79,79,79	0
56	MG	YA	3656	1/1	0.95	0.43	78,78,78,78	0
56	MG	YA	3612	1/1	0.95	0.59	64,64,64,64	0
56	MG	YD	308	1/1	0.95	0.60	97,97,97,97	0
56	MG	RA	3784	1/1	0.95	0.24	88,88,88,88	0
56	MG	XA	1757	1/1	0.95	0.61	76,76,76,76	0
56	MG	YA	3702	1/1	0.95	0.44	66,66,66,66	0
56	MG	RA	3822	1/1	0.95	0.55	73,73,73,73	0
56	MG	RA	3474	1/1	0.95	0.38	70,70,70,70	0
56	MG	RA	3861	1/1	0.95	0.92	62,62,62,62	0
56	MG	YA	3187	1/1	0.95	0.07	89,89,89,89	0
56	MG	RA	3956	1/1	0.95	0.29	80,80,80,80	0
56	MG	XA	1761	1/1	0.95	0.66	80,80,80,80	0
56	MG	RA	3014	1/1	0.95	0.31	68,68,68,68	0
56	MG	YA	3207	1/1	0.95	0.29	87,87,87,87	0
56	MG	YA	3676	1/1	0.95	0.94	63,63,63,63	0
56	MG	RA	3470	1/1	0.95	0.80	62,62,62,62	0
56	MG	QA	1830	1/1	0.95	0.37	69,69,69,69	0
56	MG	RA	3569	1/1	0.95	0.45	62,62,62,62	0
56	MG	RA	3496	1/1	0.95	0.69	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3726	1/1	0.95	0.74	85,85,85,85	0
56	MG	RA	3220	1/1	0.95	0.29	82,82,82,82	0
56	MG	RA	3972	1/1	0.95	0.74	62,62,62,62	0
56	MG	YA	3490	1/1	0.95	0.23	67,67,67,67	0
56	MG	YA	3611	1/1	0.95	1.04	62,62,62,62	0
56	MG	RA	3252	1/1	0.95	0.68	89,89,89,89	0
56	MG	RA	3357	1/1	0.95	0.21	62,62,62,62	0
56	MG	RA	3214	1/1	0.95	0.32	86,86,86,86	0
56	MG	RA	3006	1/1	0.95	0.35	73,73,73,73	0
56	MG	RA	3770	1/1	0.95	0.44	66,66,66,66	0
56	MG	XA	1647	1/1	0.96	0.89	70,70,70,70	0
56	MG	RA	3715	1/1	0.96	0.46	65,65,65,65	0
56	MG	RA	3858	1/1	0.96	0.54	70,70,70,70	0
56	MG	RA	3981	1/1	0.96	0.23	78,78,78,78	0
56	MG	YA	3294	1/1	0.96	0.69	62,62,62,62	0
57	ZN	QN	101	1/1	0.96	0.12	110,110,110,110	0
56	MG	YA	3737	1/1	0.96	0.61	63,63,63,63	0
56	MG	YA	3665	1/1	0.96	0.49	63,63,63,63	0
56	MG	YA	3755	1/1	0.96	0.36	74,74,74,74	0
56	MG	RA	3471	1/1	0.96	0.64	74,74,74,74	0
56	MG	YA	3606	1/1	0.96	0.50	62,62,62,62	0
56	MG	RA	3472	1/1	0.96	0.49	78,78,78,78	0
56	MG	RA	3009	1/1	0.96	0.20	73,73,73,73	0
56	MG	RA	3060	1/1	0.96	0.22	83,83,83,83	0
56	MG	RA	3907	1/1	0.96	0.45	70,70,70,70	0
56	MG	RA	3387	1/1	0.96	0.48	75,75,75,75	0
56	MG	RA	3418	1/1	0.96	0.16	64,64,64,64	0
56	MG	RA	3017	1/1	0.96	0.90	82,82,82,82	0
56	MG	YA	3564	1/1	0.96	0.29	63,63,63,63	0
56	MG	RA	3656	1/1	0.96	0.35	74,74,74,74	0
56	MG	YA	3325	1/1	0.96	0.51	62,62,62,62	0
56	MG	RA	3268	1/1	0.96	0.32	79,79,79,79	0
56	MG	QA	1650	1/1	0.96	0.09	93,93,93,93	0
56	MG	RA	3855	1/1	0.96	0.33	71,71,71,71	0
56	MG	RA	3821	1/1	0.96	0.34	76,76,76,76	0
56	MG	XA	1768	1/1	0.96	0.89	62,62,62,62	0
56	MG	RA	3408	1/1	0.96	0.76	62,62,62,62	0
56	MG	YA	3700	1/1	0.96	0.43	64,64,64,64	0
56	MG	RA	3851	1/1	0.96	0.39	73,73,73,73	0
56	MG	RA	3731	1/1	0.97	0.31	74,74,74,74	0
56	MG	XA	1769	1/1	0.97	0.57	77,77,77,77	0
56	MG	YA	3607	1/1	0.97	0.34	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3394	1/1	0.97	0.91	62,62,62,62	0
56	MG	XA	1632	1/1	0.97	0.58	84,84,84,84	0
56	MG	RA	3385	1/1	0.97	1.01	62,62,62,62	0
56	MG	YA	3382	1/1	0.97	0.63	62,62,62,62	0
56	MG	YA	3492	1/1	0.97	0.81	62,62,62,62	0
56	MG	RA	3344	1/1	0.97	0.25	67,67,67,67	0
56	MG	YD	304	1/1	0.97	0.55	104,104,104,104	0
56	MG	QA	1671	1/1	0.97	0.37	85,85,85,85	0
56	MG	RA	3773	1/1	0.97	0.76	70,70,70,70	0
56	MG	RA	3321	1/1	0.97	0.50	63,63,63,63	0
56	MG	YA	3671	1/1	0.97	0.52	62,62,62,62	0
56	MG	RA	3136	1/1	0.97	0.47	94,94,94,94	0
56	MG	XA	1645	1/1	0.97	0.64	82,82,82,82	0
56	MG	YA	3621	1/1	0.97	0.53	62,62,62,62	0
56	MG	RA	3620	1/1	0.97	0.80	81,81,81,81	0
56	MG	XA	1700	1/1	0.97	0.55	65,65,65,65	0
56	MG	YA	3315	1/1	0.97	0.41	64,64,64,64	0
56	MG	RA	3356	1/1	0.97	0.82	78,78,78,78	0
56	MG	RA	3355	1/1	0.97	0.07	88,88,88,88	0
56	MG	RA	3270	1/1	0.97	0.57	95,95,95,95	0
56	MG	YA	3664	1/1	0.98	0.65	72,72,72,72	0
58	SF4	XD	301	8/8	0.98	0.15	65,79,98,112	0
56	MG	RA	3880	1/1	0.98	0.63	62,62,62,62	0
56	MG	XA	1634	1/1	0.98	0.48	69,69,69,69	0
56	MG	RA	3762	1/1	0.98	0.59	65,65,65,65	0
56	MG	RA	4067	1/1	0.98	0.41	72,72,72,72	0
57	ZN	XN	101	1/1	0.98	0.13	91,91,91,91	0
56	MG	YA	3087	1/1	0.98	0.36	100,100,100,100	0
56	MG	RA	3905	1/1	0.98	0.63	63,63,63,63	0
56	MG	RA	3391	1/1	0.98	0.42	74,74,74,74	0
56	MG	RA	3424	1/1	0.98	0.54	62,62,62,62	0
56	MG	RA	3774	1/1	0.98	0.32	64,64,64,64	0
56	MG	YA	3601	1/1	0.98	0.36	62,62,62,62	0
56	MG	YA	3071	1/1	0.99	0.45	90,90,90,90	0
56	MG	RA	3771	1/1	0.99	0.61	72,72,72,72	0
56	MG	RA	3147	1/1	0.99	0.17	84,84,84,84	0
56	MG	QA	1779	1/1	0.99	0.07	91,91,91,91	0
58	SF4	QD	302	8/8	0.99	0.17	71,79,94,101	0

6.5 Other polymers ⓘ

There are no such residues in this entry.