



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 3, 2026 – 07:20 AM EDT

PDB ID : 5J30 / pdb_00005j30
Title : Thermus thermophilus 70S termination complex containing E. coli RF1
Authors : Hoffer, E.D.; Dunham, C.M.
Deposited on : 2016-03-30
Resolution : 3.20 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 types of validation reports are described at

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

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

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

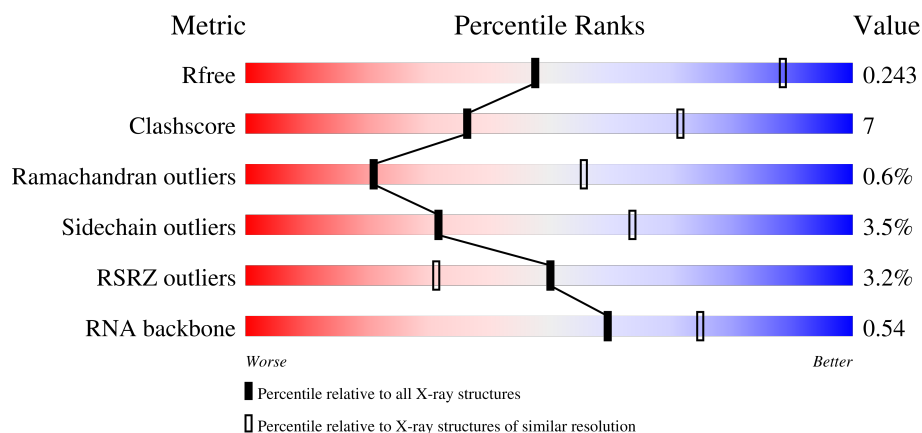
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	64% 28% 6% •
1	YA	2915	64% 28% 7% •
2	RB	122	81% 16% • •
2	YB	122	68% 26% • •

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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	QX	25	
54	XX	25	
55	QY	360	
55	XY	360	

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	1641	-	-	-	X
56	MG	QA	1660	-	-	-	X
56	MG	QA	1670	-	-	-	X
56	MG	QA	1716	-	-	-	X
56	MG	QA	1721	-	-	-	X
56	MG	QA	1775	-	-	-	X
56	MG	QA	1778	-	-	-	X
56	MG	QA	1820	-	-	-	X
56	MG	QA	1821	-	-	-	X
56	MG	QA	1840	-	-	-	X
56	MG	QA	1850	-	-	-	X
56	MG	R0	103	-	-	-	X
56	MG	R1	101	-	-	-	X
56	MG	RA	3018	-	-	-	X
56	MG	RA	3030	-	-	-	X
56	MG	RA	3049	-	-	-	X
56	MG	RA	3051	-	-	-	X
56	MG	RA	3053	-	-	-	X
56	MG	RA	3077	-	-	-	X
56	MG	RA	3099	-	-	-	X
56	MG	RA	3101	-	-	-	X
56	MG	RA	3109	-	-	-	X
56	MG	RA	3113	-	-	-	X
56	MG	RA	3120	-	-	-	X
56	MG	RA	3162	-	-	-	X
56	MG	RA	3172	-	-	-	X
56	MG	RA	3174	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3175	-	-	-	X
56	MG	RA	3179	-	-	-	X
56	MG	RA	3180	-	-	-	X
56	MG	RA	3184	-	-	-	X
56	MG	RA	3190	-	-	-	X
56	MG	RA	3192	-	-	-	X
56	MG	RA	3223	-	-	-	X
56	MG	RA	3227	-	-	-	X
56	MG	RA	3235	-	-	-	X
56	MG	RA	3239	-	-	-	X
56	MG	RA	3241	-	-	-	X
56	MG	RA	3247	-	-	-	X
56	MG	RA	3254	-	-	-	X
56	MG	RA	3267	-	-	-	X
56	MG	RA	3281	-	-	-	X
56	MG	RA	3298	-	-	-	X
56	MG	RA	3306	-	-	-	X
56	MG	RA	3364	-	-	-	X
56	MG	RA	3366	-	-	-	X
56	MG	RA	3370	-	-	-	X
56	MG	RA	3379	-	-	-	X
56	MG	RA	3393	-	-	-	X
56	MG	RA	3417	-	-	-	X
56	MG	RA	3423	-	-	-	X
56	MG	RA	3440	-	-	-	X
56	MG	RA	3471	-	-	-	X
56	MG	RA	3482	-	-	-	X
56	MG	RA	3512	-	-	-	X
56	MG	RA	3522	-	-	-	X
56	MG	RA	3531	-	-	-	X
56	MG	RA	3539	-	-	-	X
56	MG	RA	3552	-	-	-	X
56	MG	RA	3566	-	-	-	X
56	MG	RA	3579	-	-	-	X
56	MG	RA	3590	-	-	-	X
56	MG	RA	3594	-	-	-	X
56	MG	RA	3596	-	-	-	X
56	MG	RA	3623	-	-	-	X
56	MG	RA	3628	-	-	-	X
56	MG	RA	3636	-	-	-	X
56	MG	RA	3637	-	-	-	X
56	MG	RA	3682	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3696	-	-	-	X
56	MG	RA	3698	-	-	-	X
56	MG	RA	3699	-	-	-	X
56	MG	RA	3752	-	-	-	X
56	MG	RA	3764	-	-	-	X
56	MG	RA	3767	-	-	-	X
56	MG	RA	3772	-	-	-	X
56	MG	RA	3817	-	-	-	X
56	MG	RA	3883	-	-	-	X
56	MG	RA	3894	-	-	-	X
56	MG	RA	3899	-	-	-	X
56	MG	RA	3900	-	-	-	X
56	MG	RA	3927	-	-	-	X
56	MG	RA	3932	-	-	-	X
56	MG	RA	3943	-	-	-	X
56	MG	RA	3967	-	-	-	X
56	MG	RA	3972	-	-	-	X
56	MG	RA	3973	-	-	-	X
56	MG	RA	3974	-	-	-	X
56	MG	RA	3986	-	-	-	X
56	MG	RA	3999	-	-	-	X
56	MG	RA	4037	-	-	-	X
56	MG	RB	212	-	-	-	X
56	MG	RE	302	-	-	-	X
56	MG	RE	304	-	-	-	X
56	MG	RF	301	-	-	-	X
56	MG	RF	303	-	-	-	X
56	MG	RF	308	-	-	-	X
56	MG	RN	201	-	-	-	X
56	MG	XA	1610	-	-	-	X
56	MG	XA	1625	-	-	-	X
56	MG	XA	1684	-	-	-	X
56	MG	XA	1688	-	-	-	X
56	MG	XA	1742	-	-	-	X
56	MG	XA	1746	-	-	-	X
56	MG	XA	1764	-	-	-	X
56	MG	XA	1765	-	-	-	X
56	MG	XA	1769	-	-	-	X
56	MG	XA	1773	-	-	-	X
56	MG	XA	1775	-	-	-	X
56	MG	XA	1779	-	-	-	X
56	MG	Y7	102	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3019	-	-	-	X
56	MG	YA	3022	-	-	-	X
56	MG	YA	3024	-	-	-	X
56	MG	YA	3030	-	-	-	X
56	MG	YA	3033	-	-	-	X
56	MG	YA	3083	-	-	-	X
56	MG	YA	3105	-	-	-	X
56	MG	YA	3146	-	-	-	X
56	MG	YA	3164	-	-	-	X
56	MG	YA	3184	-	-	-	X
56	MG	YA	3223	-	-	-	X
56	MG	YA	3234	-	-	-	X
56	MG	YA	3246	-	-	-	X
56	MG	YA	3247	-	-	-	X
56	MG	YA	3250	-	-	-	X
56	MG	YA	3257	-	-	-	X
56	MG	YA	3260	-	-	-	X
56	MG	YA	3281	-	-	-	X
56	MG	YA	3300	-	-	-	X
56	MG	YA	3302	-	-	-	X
56	MG	YA	3357	-	-	-	X
56	MG	YA	3390	-	-	-	X
56	MG	YA	3400	-	-	-	X
56	MG	YA	3419	-	-	-	X
56	MG	YA	3433	-	-	-	X
56	MG	YA	3443	-	-	-	X
56	MG	YA	3452	-	-	-	X
56	MG	YA	3454	-	-	-	X
56	MG	YA	3455	-	-	-	X
56	MG	YA	3456	-	-	-	X
56	MG	YA	3476	-	-	-	X
56	MG	YA	3504	-	-	-	X
56	MG	YA	3509	-	-	-	X
56	MG	YA	3512	-	-	-	X
56	MG	YA	3534	-	-	-	X
56	MG	YA	3545	-	-	-	X
56	MG	YA	3547	-	-	-	X
56	MG	YA	3583	-	-	-	X
56	MG	YA	3587	-	-	-	X
56	MG	YA	3621	-	-	-	X
56	MG	YA	3673	-	-	-	X
56	MG	YA	3679	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3682	-	-	-	X
56	MG	YA	3698	-	-	-	X
56	MG	YA	3704	-	-	-	X
56	MG	YA	3711	-	-	-	X
56	MG	YB	206	-	-	-	X
56	MG	YD	305	-	-	-	X
56	MG	YE	301	-	-	-	X
56	MG	YE	303	-	-	-	X

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 294739 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	RA	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			
1	YA	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	RB	120	Total	C	N	O	P	0	0	0
			2572	1145	476	832	119			
2	YB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	RE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	YE	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	RF	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	YF	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	RO	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	YO	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	RP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
11	YP	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	RQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	YQ	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	RR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	YR	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	RS	110	Total	C	N	O	0	0	0
			877	553	175	149			
14	YS	110	Total	C	N	O	0	0	0
			870	549	173	148			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	RU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	YU	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	RV	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
17	YV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	RW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
18	YW	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	RX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	YX	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	RY	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
20	YY	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	RZ	189	Total	C	N	O	S	0	0	0
			1485	946	265	272	2			
21	YZ	189	Total	C	N	O	S	0	0	0
			1469	938	259	270	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	R0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	Y0	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	R1	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			
23	Y1	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	R7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	Y7	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	R8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
30	Y8	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	R9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	Y9	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	QA	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	XA	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	QE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
36	XE	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	QF	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
37	XF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	QL	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
43	XL	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	QM	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	XM	114	Total	C	N	O	S	0	0	0
			895	550	186	157	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	QN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
45	XN	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	QO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
46	XO	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	QP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
47	XP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	QQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	XQ	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	QR	68	Total	C	N	O		0	0	0
			555	355	108	92				
49	XR	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	QS	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
50	XS	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	QX	10	Total	C	N	O	P	0	0	0
			215	97	42	66	10			
54	XX	9	Total	C	N	O	P	0	0	0
			193	87	37	60	9			

- Molecule 55 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	QY	258	Total	C	N	O	S	0	0	0
			2014	1235	382	389	8			
55	XY	259	Total	C	N	O	S	0	0	0
			2023	1240	384	391	8			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	RA	1039	Total	Mg	0	0
			1039	1039		
56	RB	27	Total	Mg	0	0
			27	27		
56	RD	15	Total	Mg	0	0
			15	15		
56	RE	8	Total	Mg	0	0
			8	8		
56	RF	12	Total	Mg	0	0
			12	12		
56	RG	4	Total	Mg	0	0
			4	4		
56	RH	1	Total	Mg	0	0
			1	1		
56	RN	2	Total	Mg	0	0
			2	2		
56	RO	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	RP	1	Total 1	Mg 1	0	0
56	RQ	6	Total 6	Mg 6	0	0
56	RR	3	Total 3	Mg 3	0	0
56	RT	2	Total 2	Mg 2	0	0
56	RU	2	Total 2	Mg 2	0	0
56	RV	4	Total 4	Mg 4	0	0
56	RW	2	Total 2	Mg 2	0	0
56	RX	1	Total 1	Mg 1	0	0
56	RY	1	Total 1	Mg 1	0	0
56	RZ	1	Total 1	Mg 1	0	0
56	R0	4	Total 4	Mg 4	0	0
56	R1	4	Total 4	Mg 4	0	0
56	R3	2	Total 2	Mg 2	0	0
56	R5	3	Total 3	Mg 3	0	0
56	R7	2	Total 2	Mg 2	0	0
56	R8	1	Total 1	Mg 1	0	0
56	QA	256	Total 256	Mg 256	0	0
56	QB	1	Total 1	Mg 1	0	0
56	QD	3	Total 3	Mg 3	0	0
56	QE	2	Total 2	Mg 2	0	0
56	QF	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QG	2	Total 2	Mg 2	0	0
56	QH	1	Total 1	Mg 1	0	0
56	QI	1	Total 1	Mg 1	0	0
56	QL	2	Total 2	Mg 2	0	0
56	QM	1	Total 1	Mg 1	0	0
56	QN	2	Total 2	Mg 2	0	0
56	QO	1	Total 1	Mg 1	0	0
56	QQ	1	Total 1	Mg 1	0	0
56	QR	1	Total 1	Mg 1	0	0
56	QT	2	Total 2	Mg 2	0	0
56	QV	6	Total 6	Mg 6	0	0
56	YA	744	Total 744	Mg 744	0	0
56	YB	18	Total 18	Mg 18	0	0
56	YD	9	Total 9	Mg 9	0	0
56	YE	5	Total 5	Mg 5	0	0
56	YF	3	Total 3	Mg 3	0	0
56	YG	2	Total 2	Mg 2	0	0
56	YI	1	Total 1	Mg 1	0	0
56	YN	1	Total 1	Mg 1	0	0
56	YO	2	Total 2	Mg 2	0	0
56	YP	1	Total 1	Mg 1	0	0

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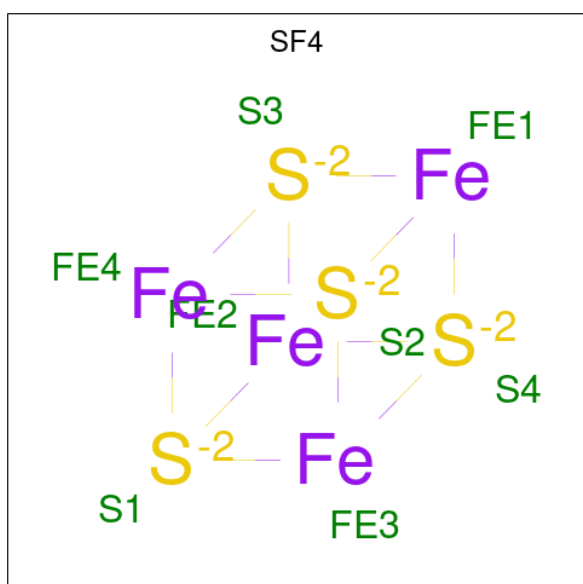
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	YQ	2	Total 2	Mg 2	0	0
56	YR	1	Total 1	Mg 1	0	0
56	YT	4	Total 4	Mg 4	0	0
56	YV	1	Total 1	Mg 1	0	0
56	YW	2	Total 2	Mg 2	0	0
56	YX	1	Total 1	Mg 1	0	0
56	Y0	1	Total 1	Mg 1	0	0
56	Y1	1	Total 1	Mg 1	0	0
56	Y5	1	Total 1	Mg 1	0	0
56	Y7	2	Total 2	Mg 2	0	0
56	Y8	2	Total 2	Mg 2	0	0
56	XA	183	Total 183	Mg 183	0	0
56	XE	1	Total 1	Mg 1	0	0
56	XF	2	Total 2	Mg 2	0	0
56	XJ	1	Total 1	Mg 1	0	0
56	XK	1	Total 1	Mg 1	0	0
56	XL	1	Total 1	Mg 1	0	0
56	XR	1	Total 1	Mg 1	0	0
56	XT	1	Total 1	Mg 1	0	0
56	XV	4	Total 4	Mg 4	0	0
56	XX	1	Total 1	Mg 1	0	0

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

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

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

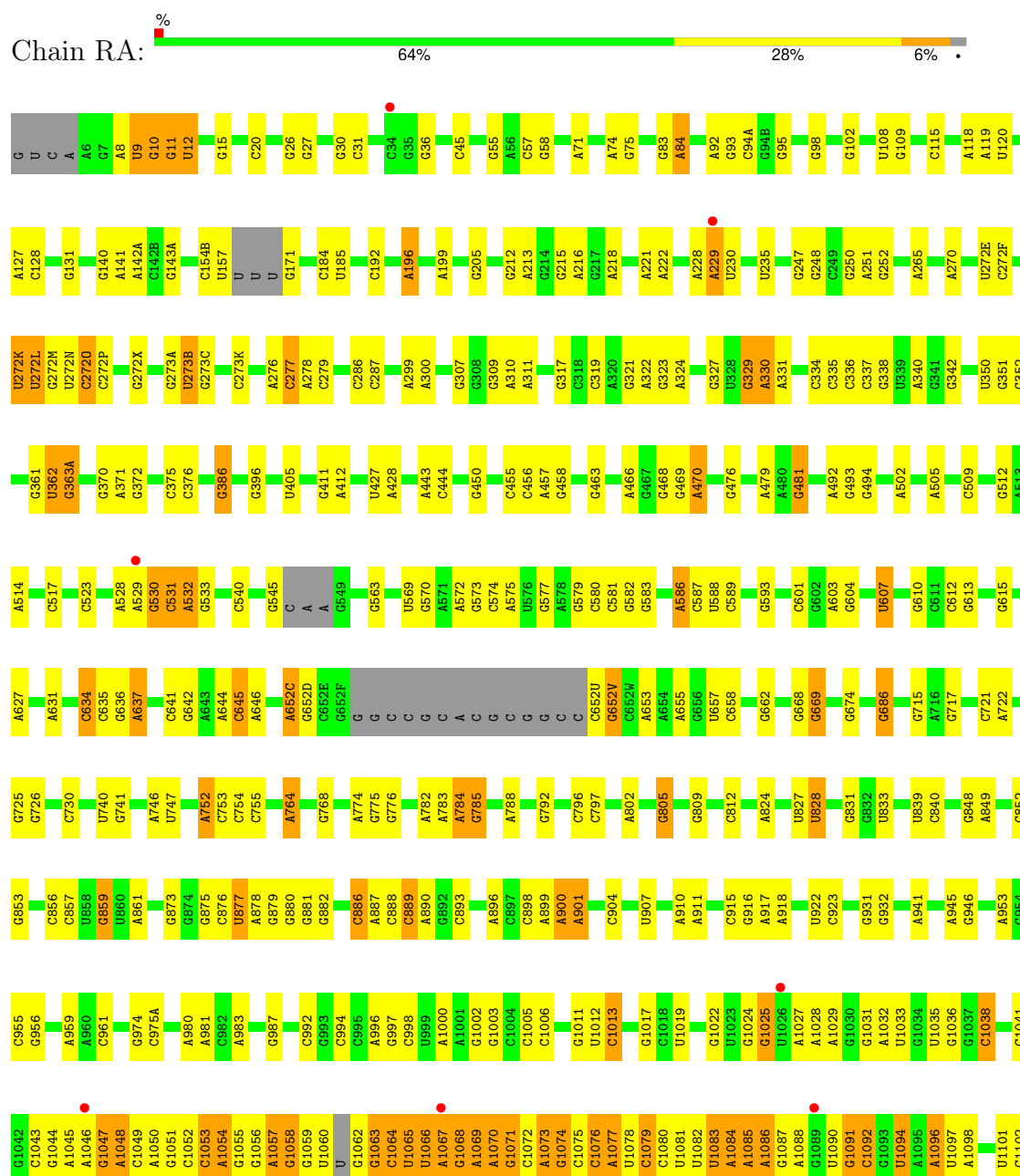


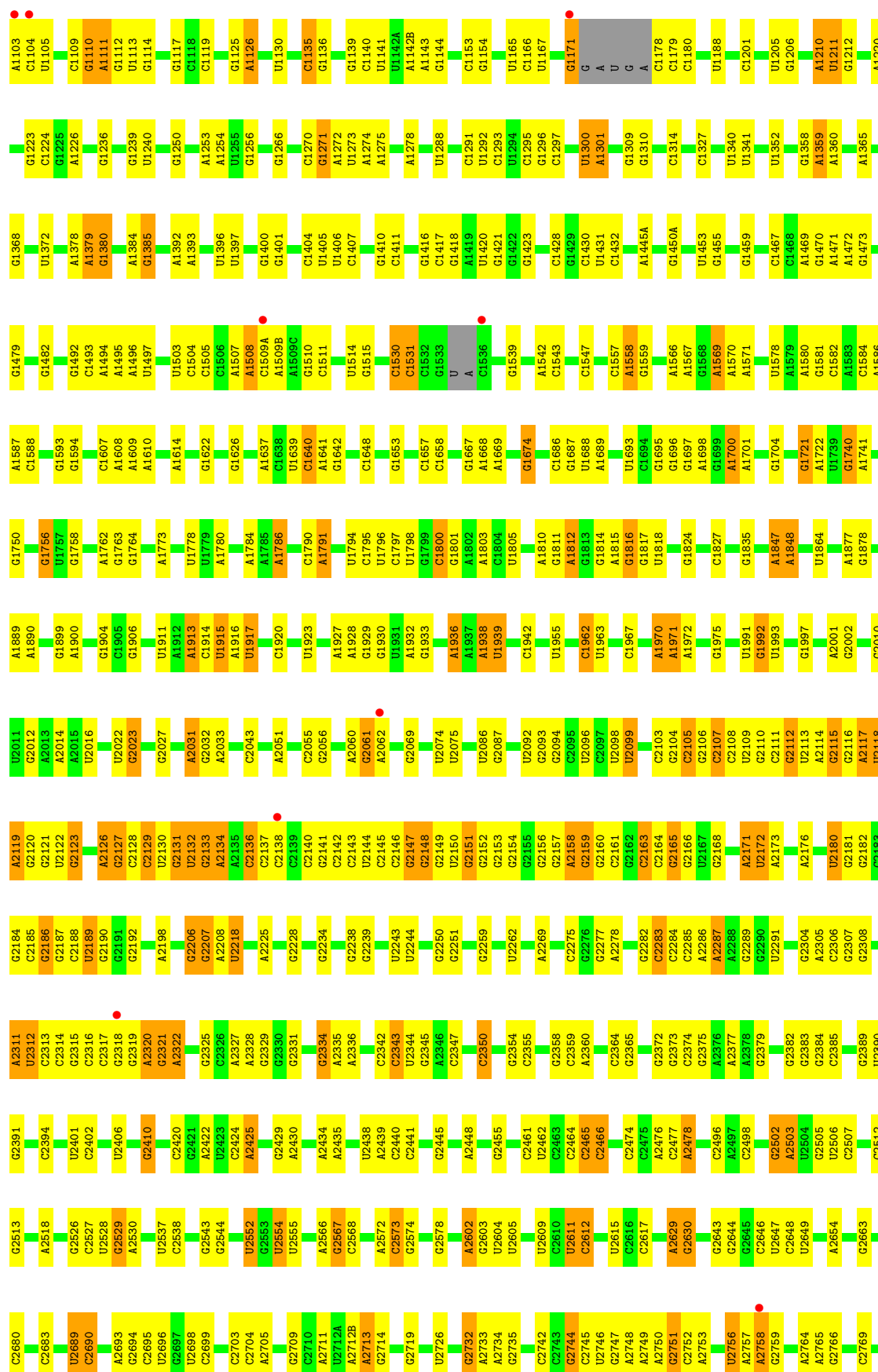
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	QD	1	Total 8	Fe 4	S 4	0	0
58	XD	1	Total 8	Fe 4	S 4	0	0

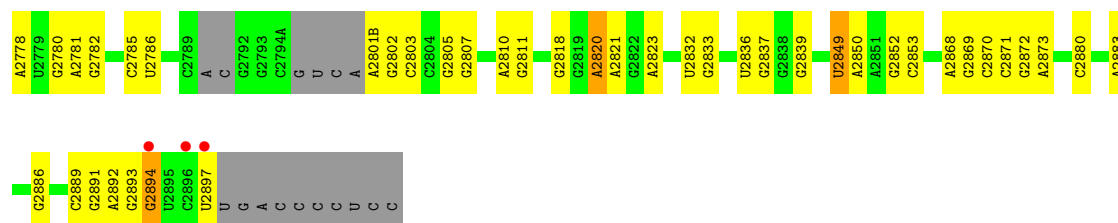
3 Residue-property plots

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

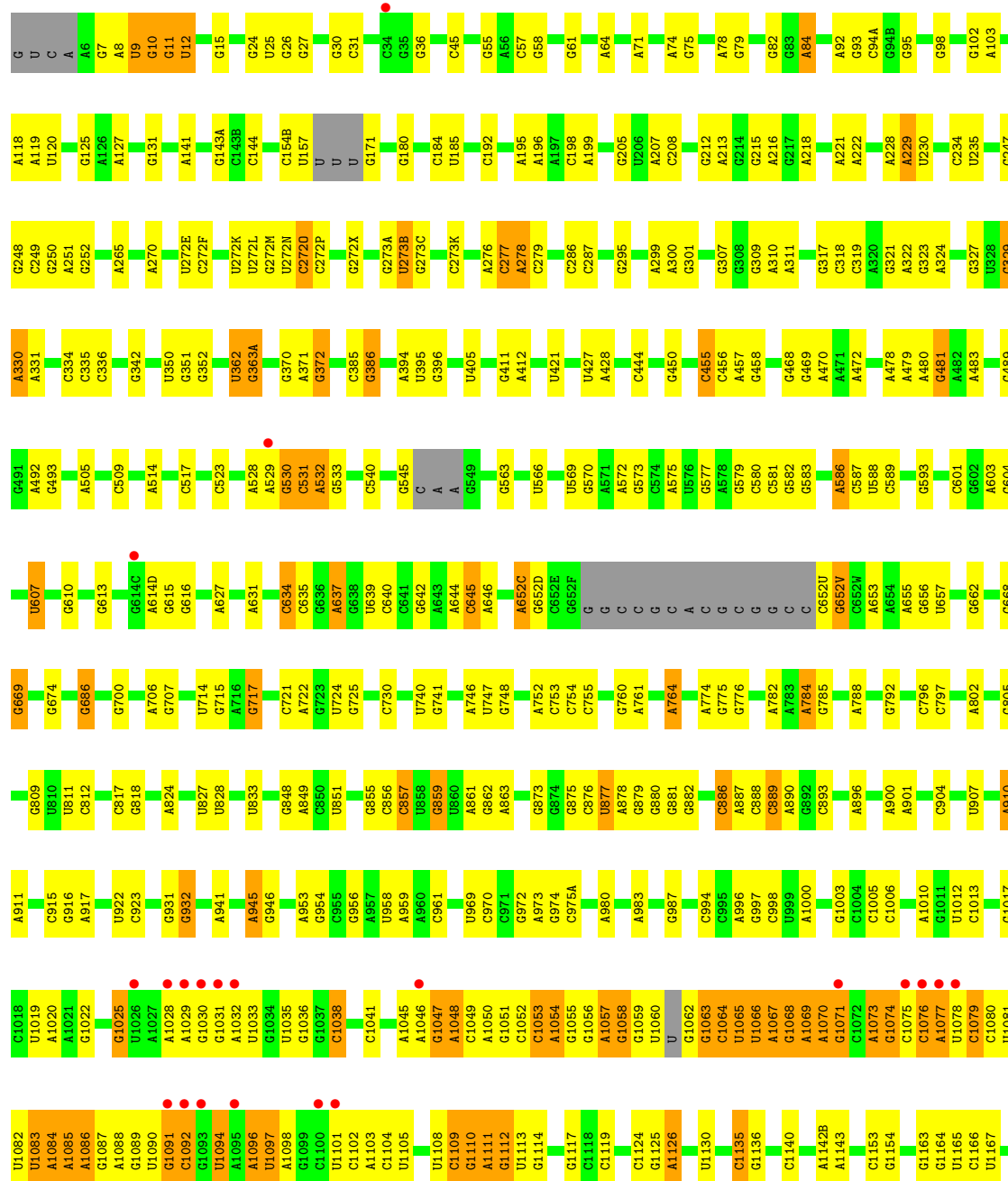
• Molecule 1: 23S rRNA







• Molecule 1: 23S rRNA



C2742	C2743	C2744	C2474	C2364	G2279	G2182	U2099	U1963	A1810	C1683	A1542	U1431	G1303	G1171
G2745	G2746	G2747	G2475	G2365	G2282	G2183	C2103	C1987	G1811	C1684	C1543	A1445A	G1310	G
G2748	G2749	G2750	G2476	G2366	G2283	G2184	G2104	A1970	G1812	U1688	C1547	A1449	G1314	A
G2751	G2752	G2753	G2477	G2367	G2284	G2185	C2105	A1971	G1813	U1693	C1557	G1450A	G1315	G
G2754	G2755	G2756	G2478	G2368	G2285	G2186	G2106	A1972	G1814	G1695	A1558	C1178	G1316	A
G2757	G2758	G2759	G2479	G2369	G2286	G2187	G2107	A1973	G1815	G1696	A1560	C1179	G1317	C
G2760	G2761	G2762	G2480	G2370	G2287	G2188	G2108	G1975	G1816	A1700	G1566	C1181	G1341	C
G2763	G2764	G2765	G2481	G2371	G2288	G2189	G2109	U1991	G1822	A1701	A1567	G1184	U1352	G
G2766	G2767	G2768	G2482	G2372	G2289	G2190	G2110	U1992	G1823	U1709	A1569	G1187	G1358	C
G2769	G2770	G2771	G2483	G2373	G2290	G2191	G2111	U1993	G1824	C1710	A1571	G1188	U1188	C
G2772	G2773	G2774	G2484	G2374	G2291	G2192	G2112	U1994	G1825	G1721	A1577	U1205	G1364	C
G2775	G2776	G2777	G2485	G2375	G2292	G2193	G2113	U1995	G1826	G1722	U1578	U1206	G1365	C
G2778	G2779	G2780	G2486	G2376	G2293	G2194	G2114	U1996	G1827	G1723	G1482	G1212	G1368	C
G2781	G2782	G2783	G2487	G2377	G2294	G2195	G2115	U1997	G1828	G1724	G1483	A1220	A1220	C
G2784	G2785	G2786	G2488	G2378	G2295	G2196	G2116	U1998	G1829	G1725	G1484	G1236	G1371	C
G2787	G2788	G2789	G2489	G2379	G2296	G2197	G2117	U1999	G1830	G1726	A1586	G1239	G1372	C
G2790	G2791	G2792	G2490	G2380	G2297	G2198	G2118	U2000	G1831	G1727	A1587	U1240	G1373	C
G2793	G2794	G2795	G2491	G2381	G2298	G2199	G2119	U2001	G1832	G1728	A1588	G1250	G1380	C
G2796	G2797	G2798	G2492	G2382	G2299	G2200	G2120	U2002	G1833	G1729	A1589	G1251	G1381	C
G2799	G2800	G2801	G2493	G2383	G2300	G2201	G2121	U2003	G1834	G1730	A1590	G1252	G1382	C
G2802	G2803	G2804	G2494	G2384	G2301	G2202	G2122	U2004	G1835	G1731	A1591	G1253	G1383	C
G2805	G2806	G2807	G2495	G2385	G2302	G2203	G2123	U2005	G1836	G1732	A1592	G1254	G1384	C
G2808	G2809	G2810	G2496	G2386	G2303	G2204	G2124	U2006	G1837	G1733	A1593	G1255	G1385	C
G2811	G2812	G2813	G2497	G2387	G2304	G2205	G2125	U2007	G1838	G1734	A1594	G1256	G1386	C
G2814	G2815	G2816	G2498	G2388	G2305	G2206	G2126	U2008	G1839	G1735	A1595	G1257	G1387	C
G2817	G2818	G2819	G2499	G2389	G2306	G2207	G2127	U2009	G1840	G1736	A1596	G1258	G1388	C
G2820	G2821	G2822	G2500	G2390	G2307	G2208	G2128	U2010	G1841	G1737	A1597	G1259	G1389	C
G2823	G2824	G2825	G2501	G2391	G2308	G2209	G2129	U2011	G1842	G1738	A1598	G1260	G1390	C
G2826	G2827	G2828	G2502	G2392	G2309	G2210	G2130	U2012	G1843	G1739	A1599	G1261	G1391	C
G2829	G2830	G2831	G2503	G2393	G2310	G2211	G2131	U2013	G1844	G1740	A1600	G1262	G1392	C
G2832	G2833	G2834	G2504	G2394	G2311	G2212	G2132	U2014	G1845	G1741	A1601	G1263	G1393	C
G2835	G2836	G2837	G2505	G2395	G2312	G2213	G2133	U2015	G1846	G1742	A1602	G1264	G1394	C
G2838	G2839	G2840	G2506	G2396	G2313	G2214	G2134	U2016	G1847	G1743	A1603	G1265	G1395	C
G2841	G2842	G2843	G2507	G2397	G2314	G2215	G2135	U2017	G1848	G1744	A1604	G1266	G1396	C
G2844	G2845	G2846	G2508	G2398	G2315	G2216	G2136	U2018	G1849	G1745	A1605	G1267	G1397	C
G2847	G2848	G2849	G2509	G2399	G2316	G2217	G2137	U2019	G1850	G1746	A1606	G1268	G1398	C
G2850	G2851	G2852	G2510	G2400	G2317	G2218	G2138	U2020	G1851	G1747	A1607	G1269	G1399	C
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G														



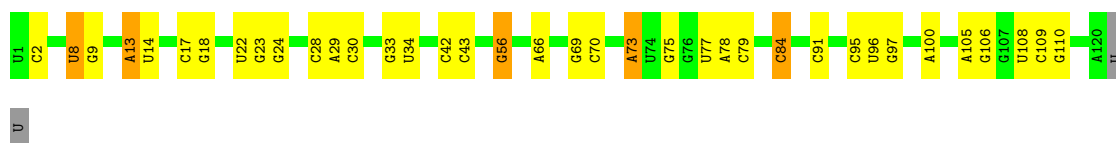
• Molecule 2: 5S rRNA

Chain RB: 81% 16% . .



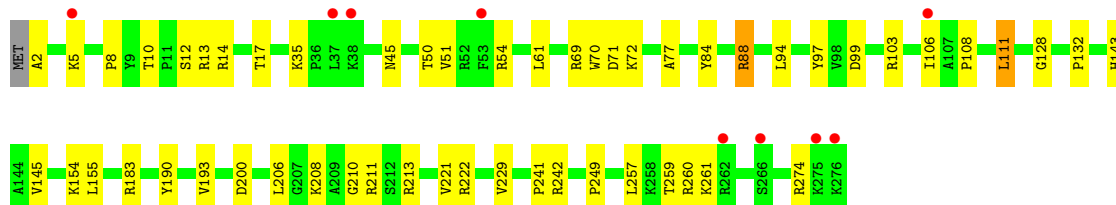
• Molecule 2: 5S rRNA

Chain YB: 68% 26% . .



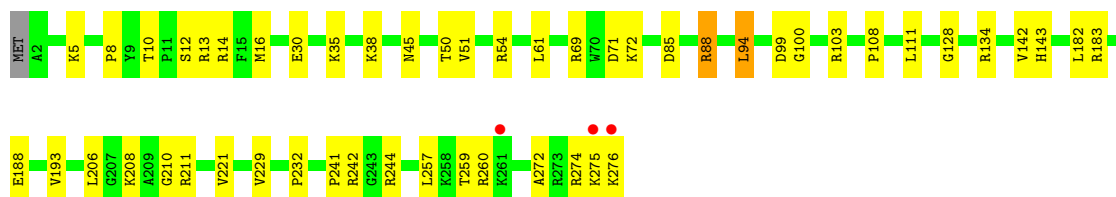
• Molecule 3: 50S ribosomal protein L2

Chain RD: 3% 80% 19% .



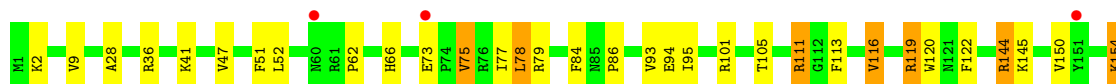
• Molecule 3: 50S ribosomal protein L2

Chain YD: 81% 18% .



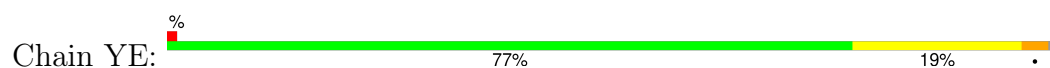
• Molecule 4: 50S ribosomal protein L3

Chain RE: 2% 80% 15% . .

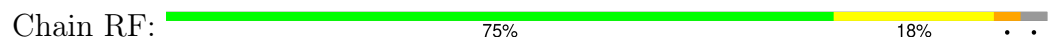




- Molecule 4: 50S ribosomal protein L3



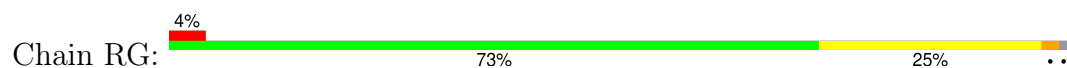
- Molecule 5: 50S ribosomal protein L4



- Molecule 5: 50S ribosomal protein L4

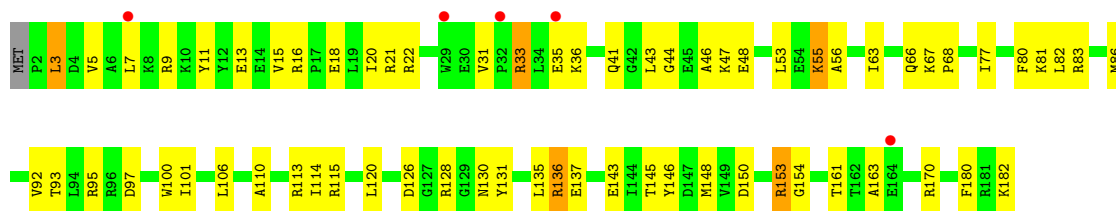


- Molecule 6: 50S ribosomal protein L5

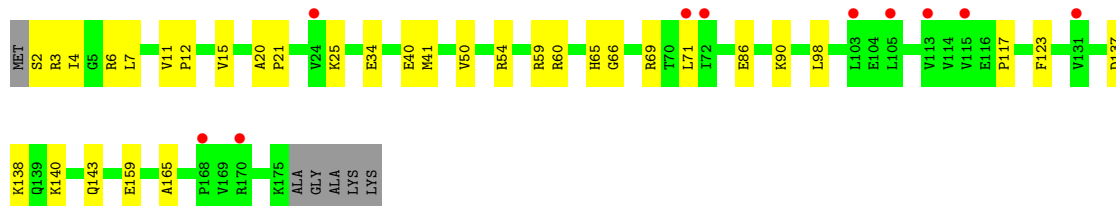
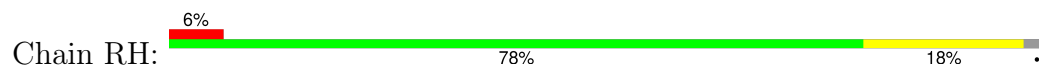


- Molecule 6: 50S ribosomal protein L5

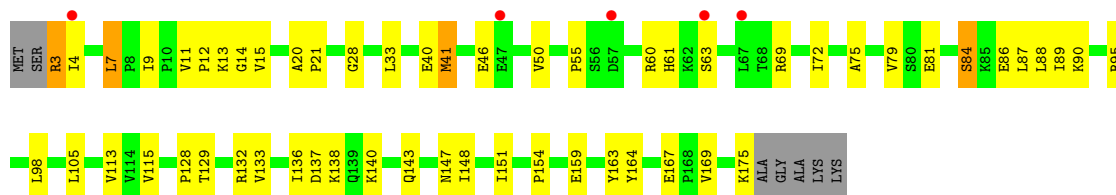




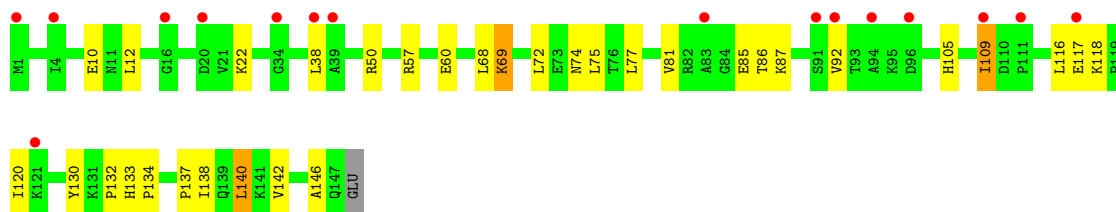
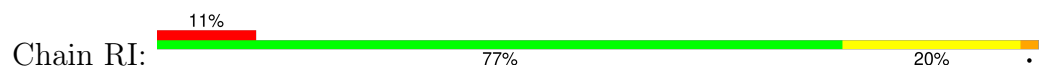
• Molecule 7: 50S ribosomal protein L6



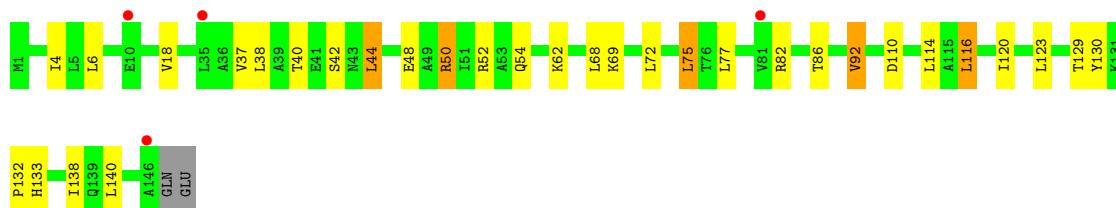
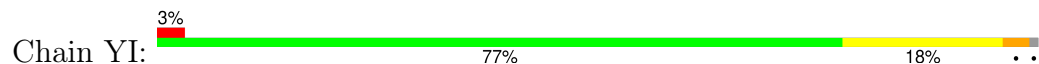
• Molecule 7: 50S ribosomal protein L6



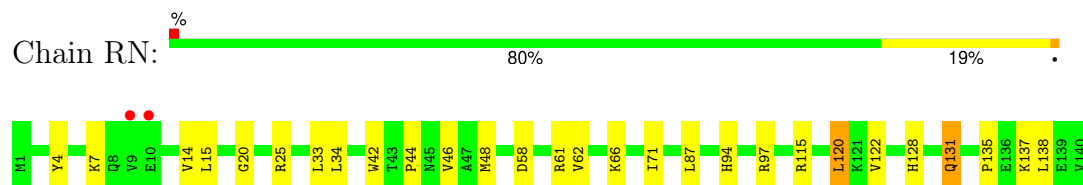
• Molecule 8: 50S ribosomal protein L9



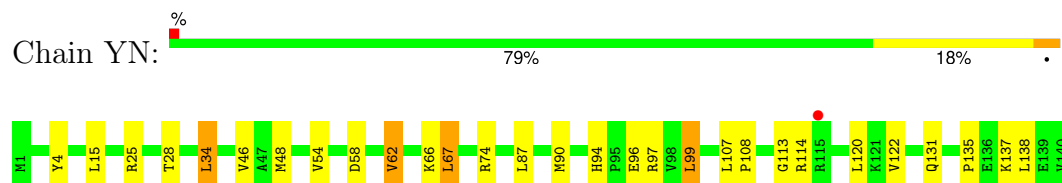
• Molecule 8: 50S ribosomal protein L9



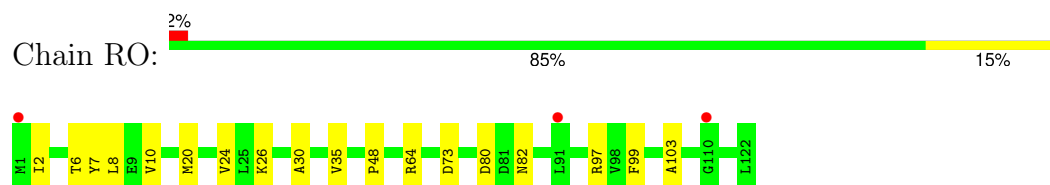
- Molecule 9: 50S ribosomal protein L13



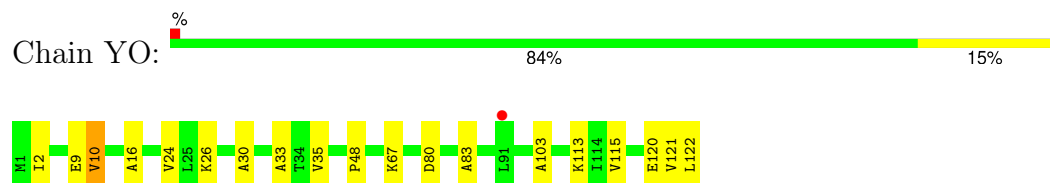
- Molecule 9: 50S ribosomal protein L13



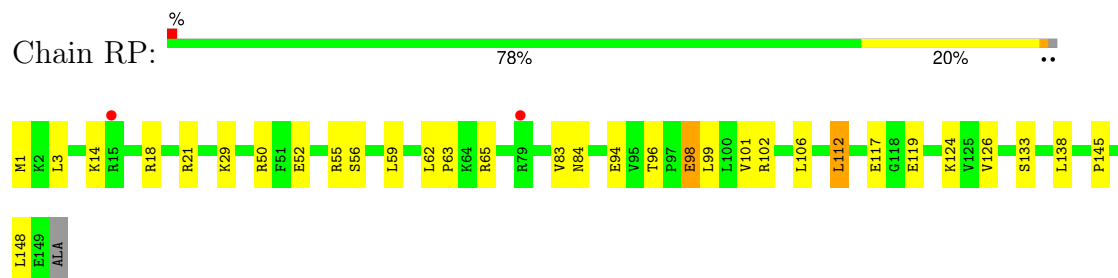
- Molecule 10: 50S ribosomal protein L14



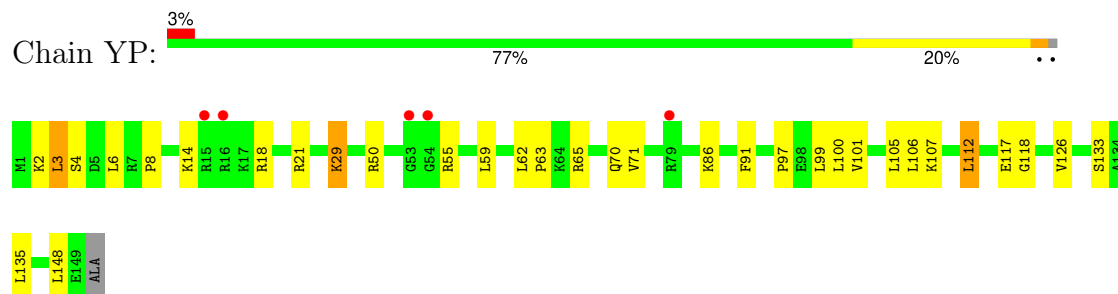
- Molecule 10: 50S ribosomal protein L14



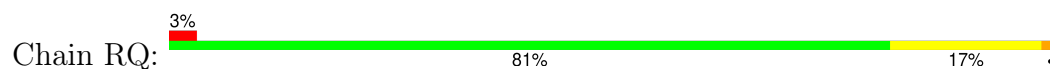
- Molecule 11: 50S ribosomal protein L15



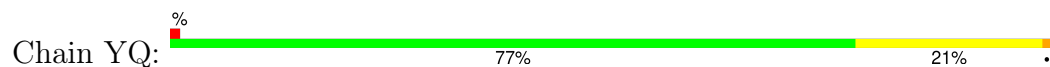
- Molecule 11: 50S ribosomal protein L15



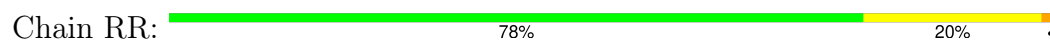
● Molecule 12: 50S ribosomal protein L16



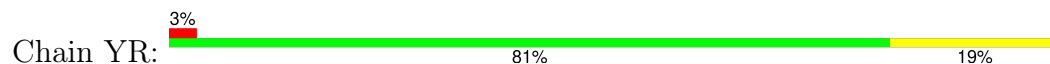
● Molecule 12: 50S ribosomal protein L16



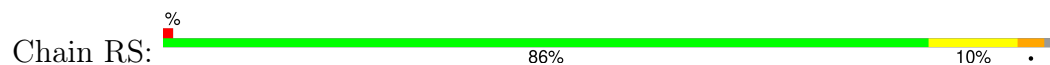
● Molecule 13: 50S ribosomal protein L17



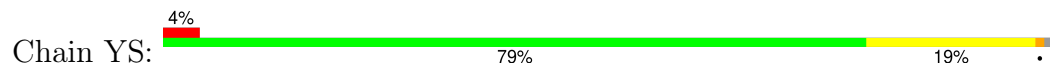
● Molecule 13: 50S ribosomal protein L17



● Molecule 14: 50S ribosomal protein L18

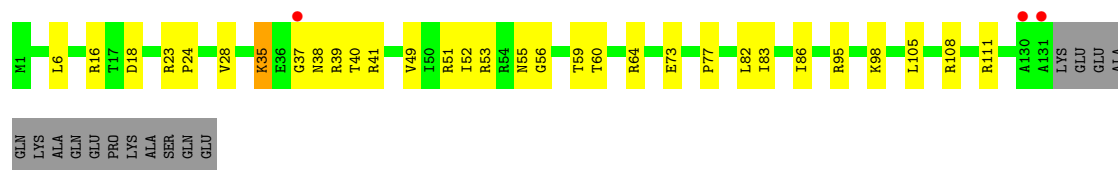


● Molecule 14: 50S ribosomal protein L18

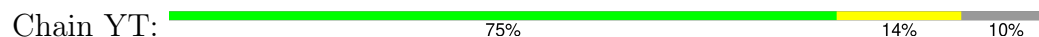


● Molecule 15: 50S ribosomal protein L19

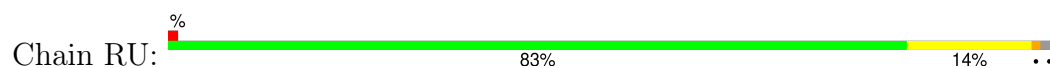




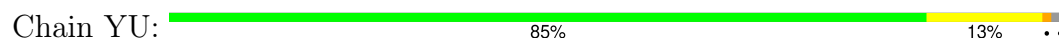
- Molecule 15: 50S ribosomal protein L19



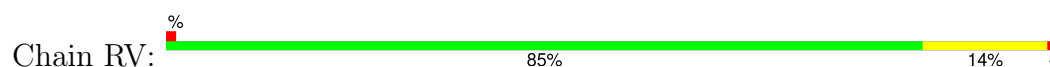
- Molecule 16: 50S ribosomal protein L20



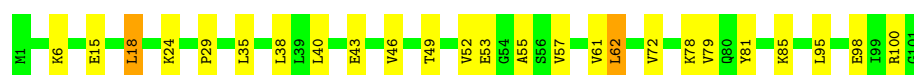
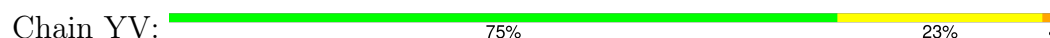
- Molecule 16: 50S ribosomal protein L20



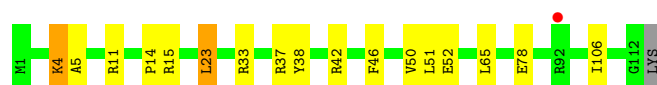
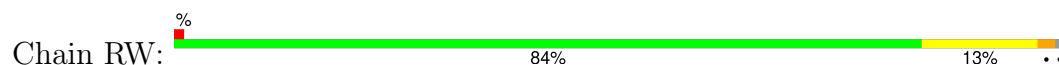
- Molecule 17: 50S ribosomal protein L21



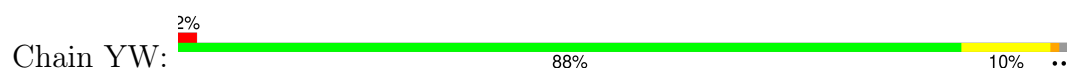
- Molecule 17: 50S ribosomal protein L21



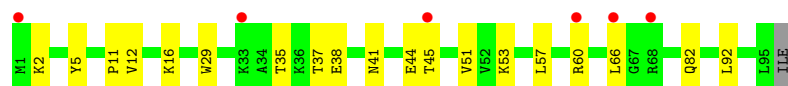
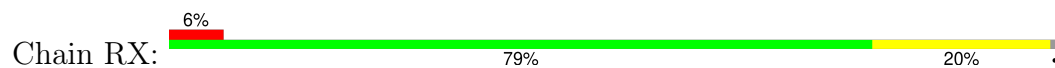
- Molecule 18: 50S ribosomal protein L22



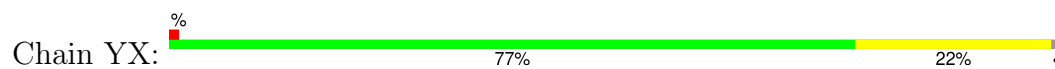
- Molecule 18: 50S ribosomal protein L22



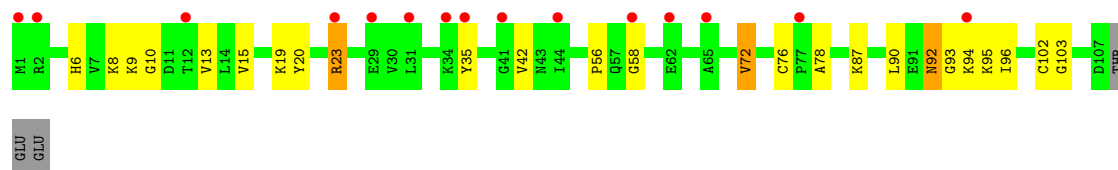
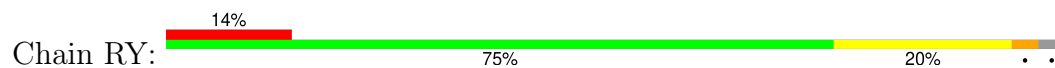
- Molecule 19: 50S ribosomal protein L23



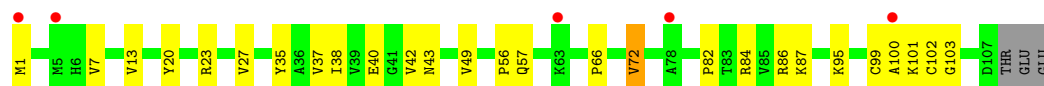
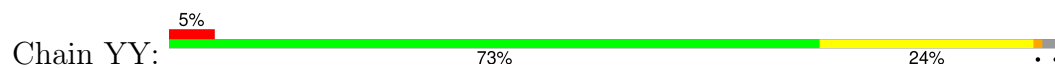
- Molecule 19: 50S ribosomal protein L23



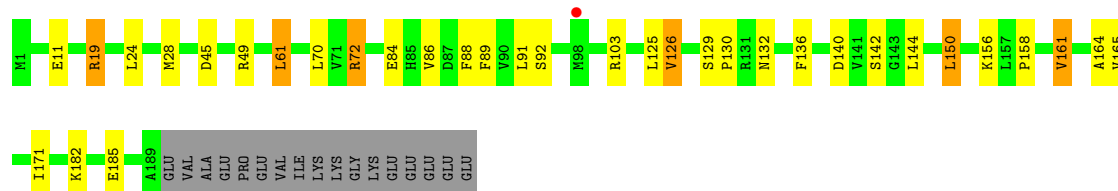
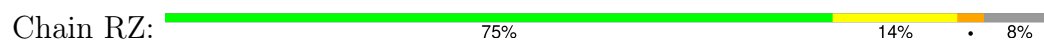
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25

Chain YZ:  74% 16% 8%



- Molecule 22: 50S ribosomal protein L27

Chain R0:  76% 12% 9%



- Molecule 22: 50S ribosomal protein L27

Chain Y0:  73% 18% 9%



- Molecule 23: 50S ribosomal protein L28

Chain R1:  85% 12% 3%



- Molecule 23: 50S ribosomal protein L28

Chain Y1:  73% 22% 5%



- Molecule 24: 50S ribosomal protein L29

Chain R2:  86% 10% 4%

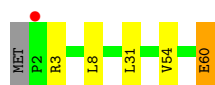
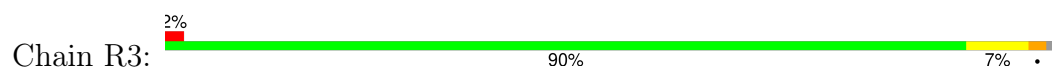


- Molecule 24: 50S ribosomal protein L29

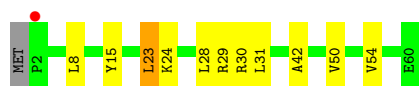
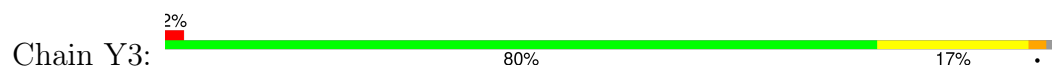
Chain Y2:  78% 17% 5%



- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



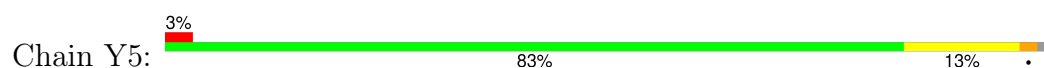
- Molecule 26: 50S ribosomal protein L31



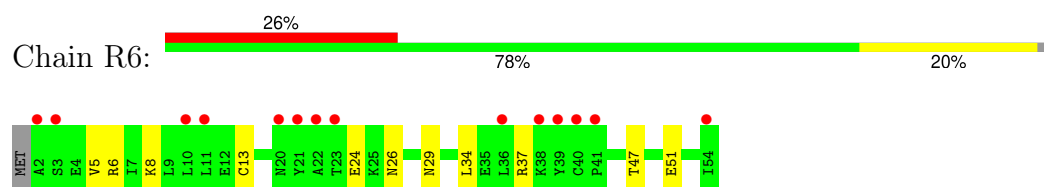
- Molecule 27: 50S ribosomal protein L32



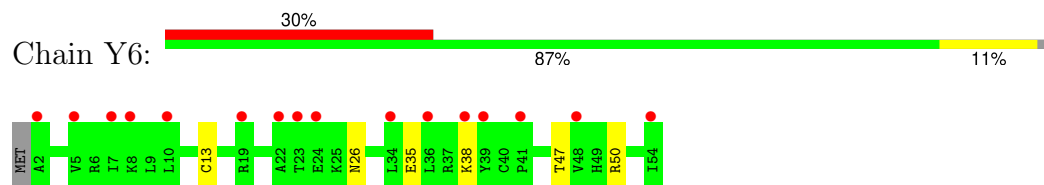
- Molecule 27: 50S ribosomal protein L32



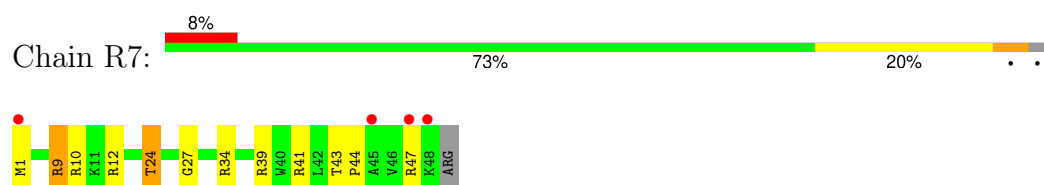
- Molecule 28: 50S ribosomal protein L33



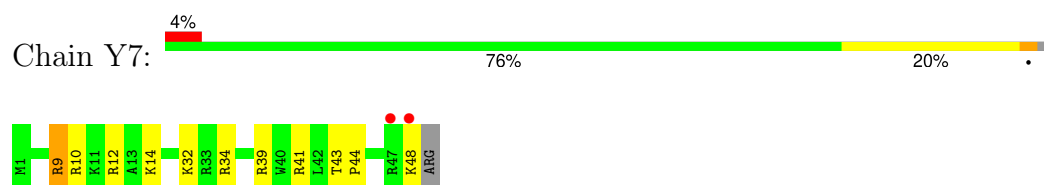
- Molecule 28: 50S ribosomal protein L33



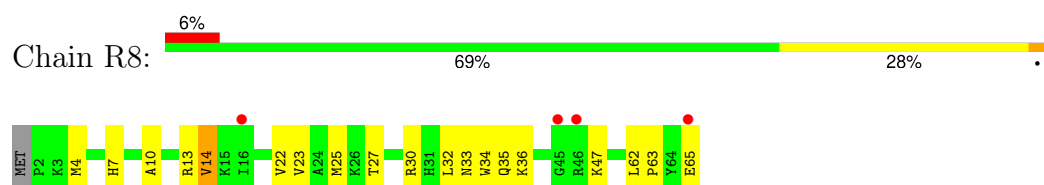
- Molecule 29: 50S ribosomal protein L34



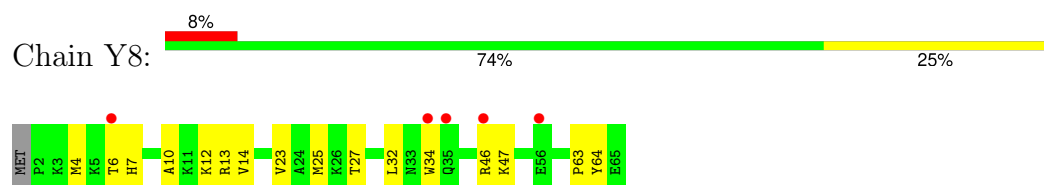
- Molecule 29: 50S ribosomal protein L34



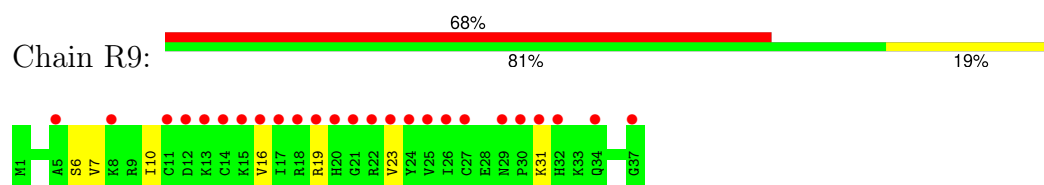
- Molecule 30: 50S ribosomal protein L35



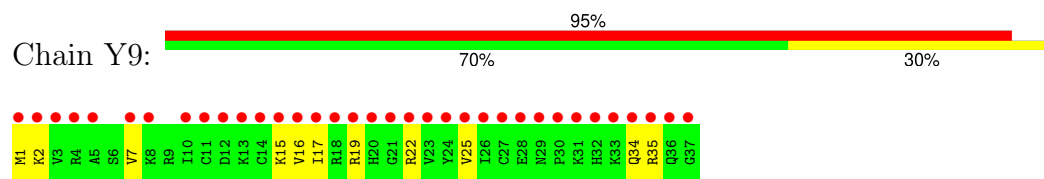
- Molecule 30: 50S ribosomal protein L35



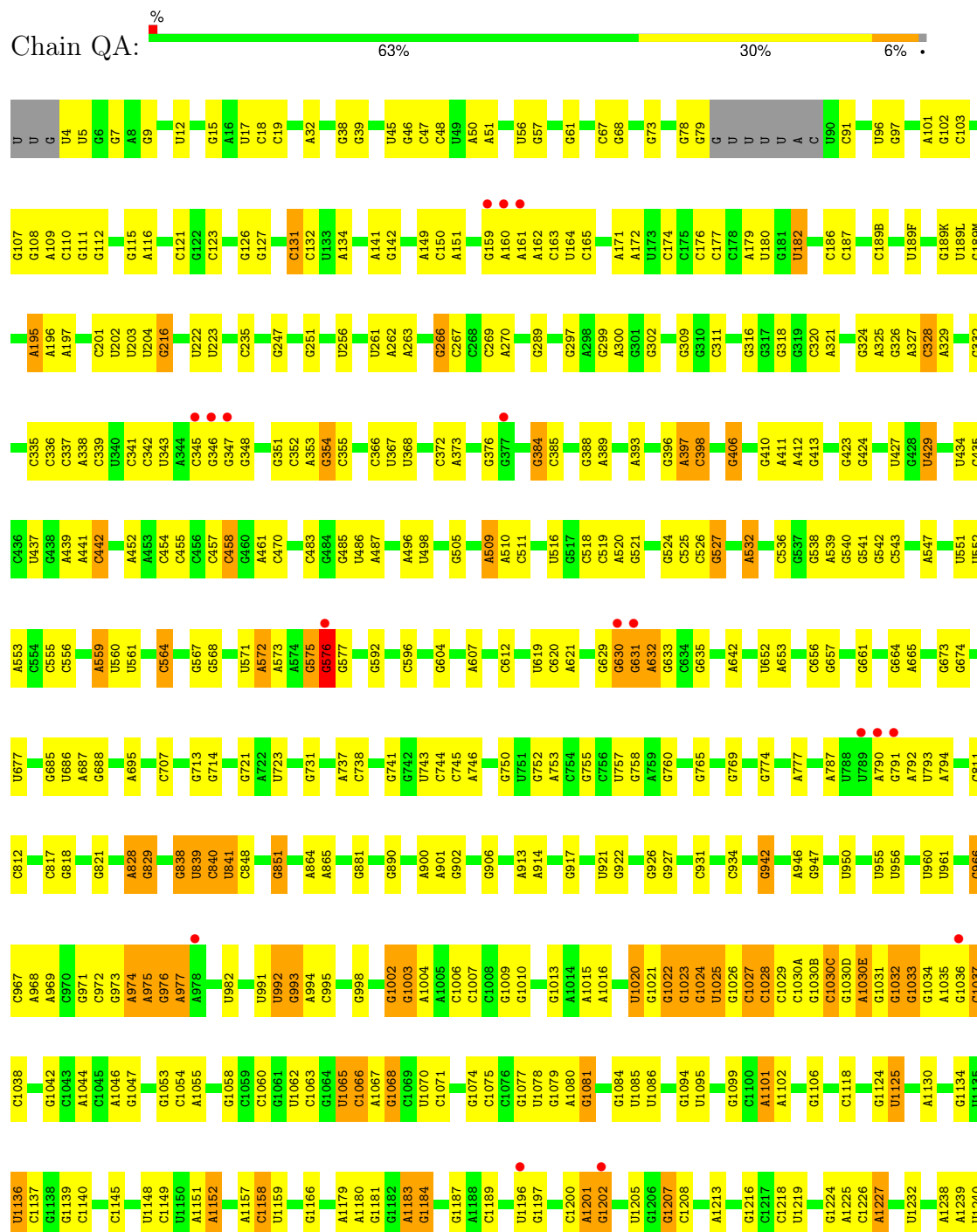
- Molecule 31: 50S ribosomal protein L36

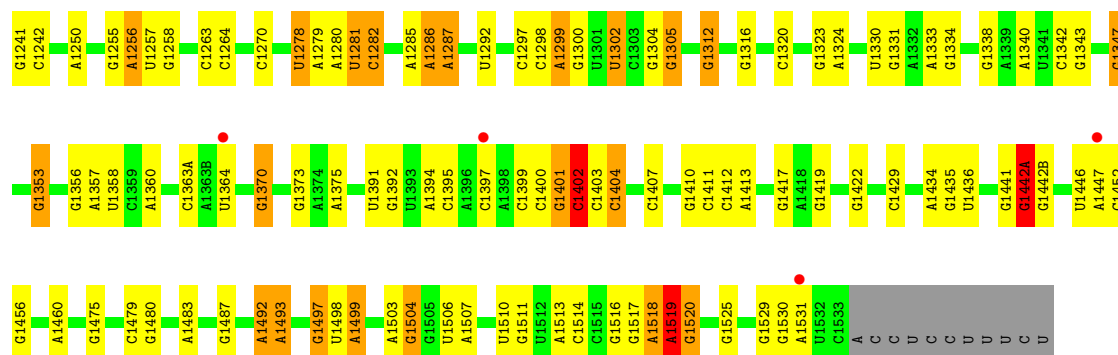


• Molecule 31: 50S ribosomal protein L36

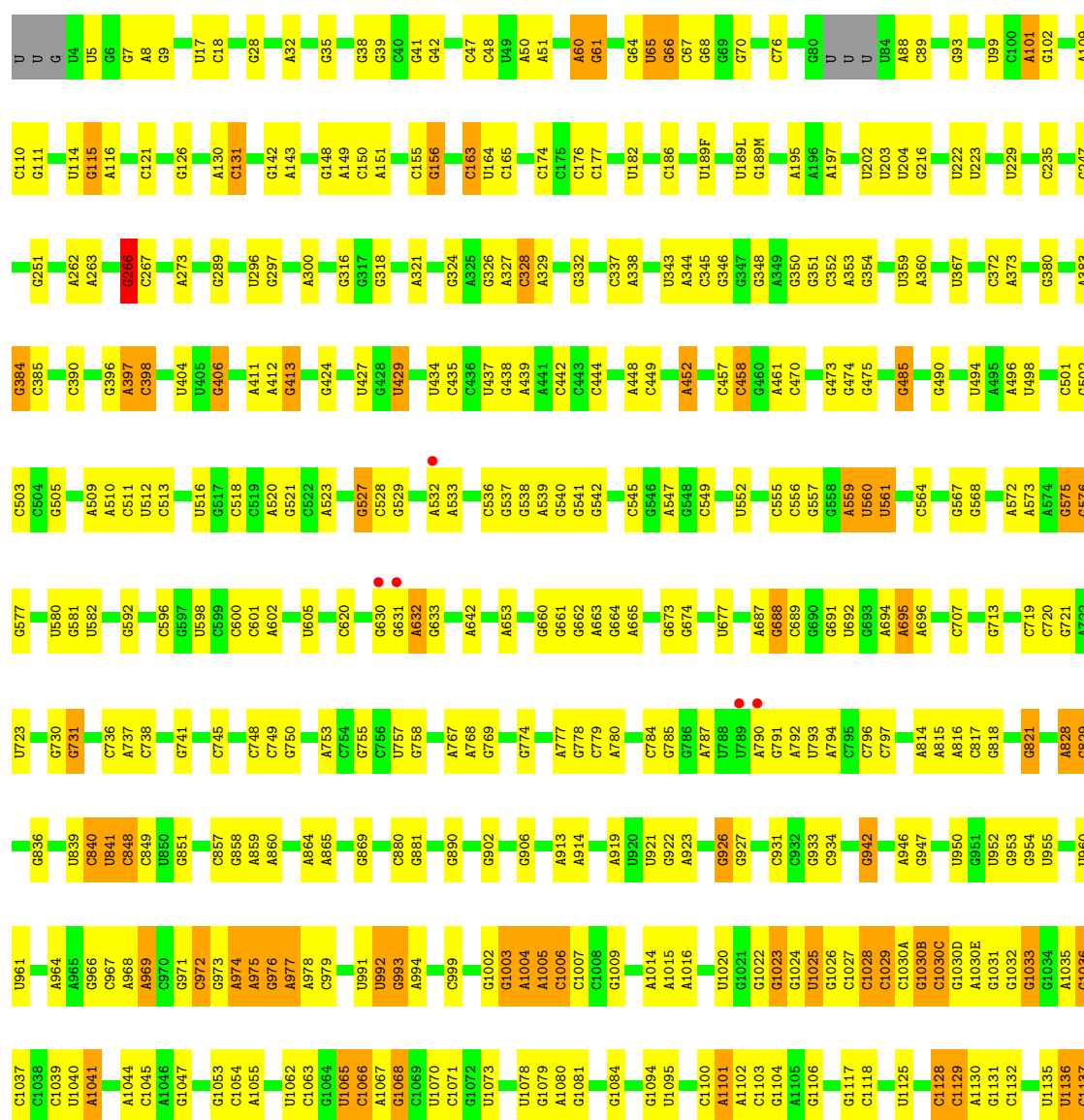


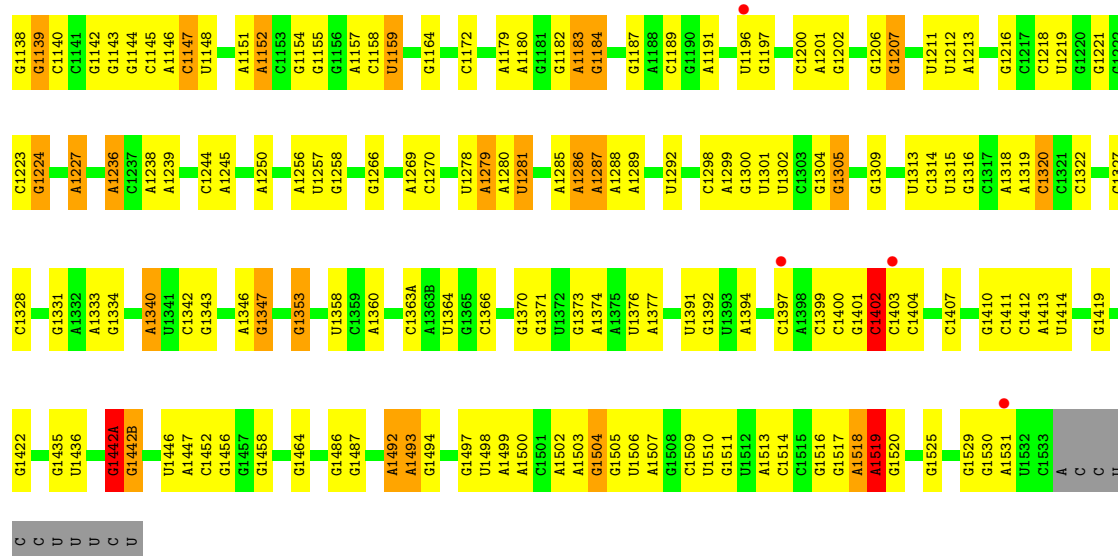
• Molecule 32: 16S rRNA



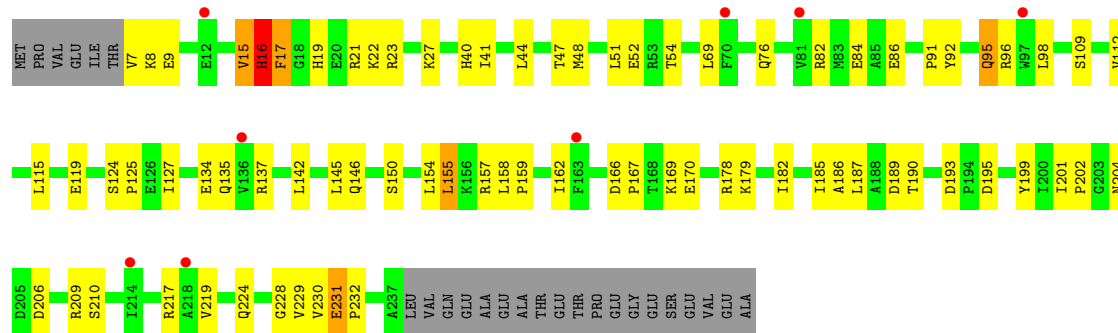


• Molecule 32: 16S rRNA

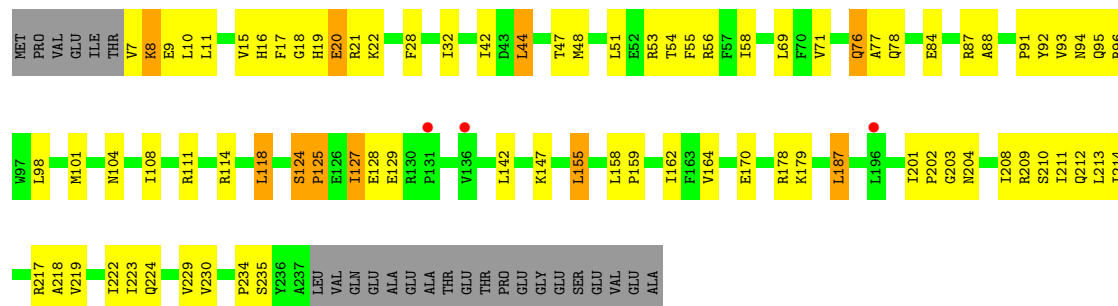




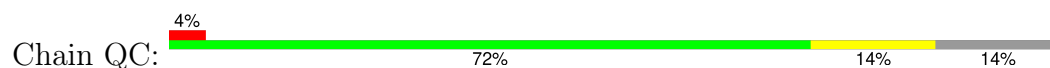
• Molecule 33: 30S ribosomal protein S2

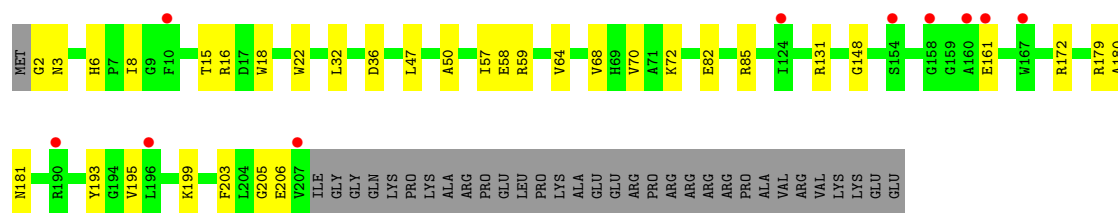


• Molecule 33: 30S ribosomal protein S2

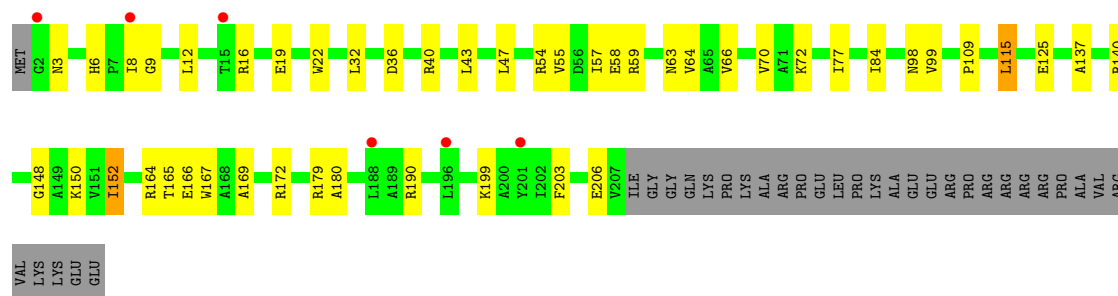


• Molecule 34: 30S ribosomal protein S3

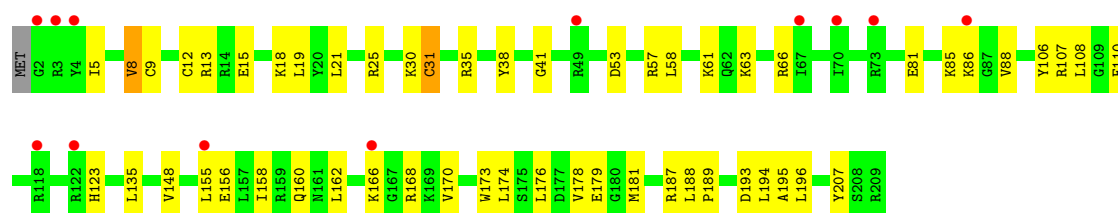
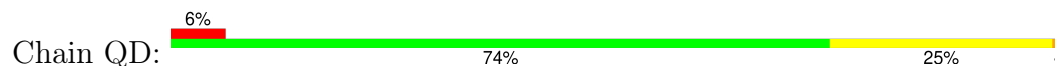




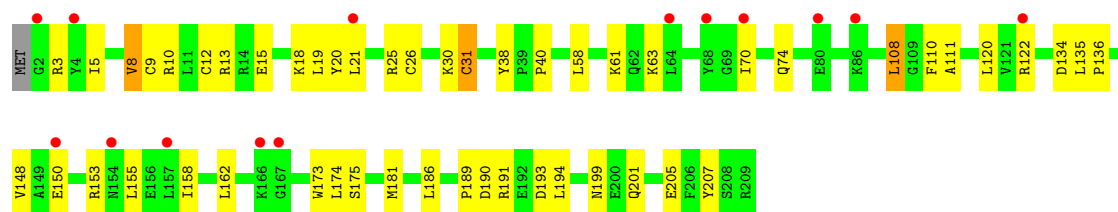
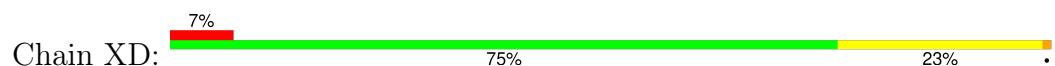
• Molecule 34: 30S ribosomal protein S3



• Molecule 35: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S4

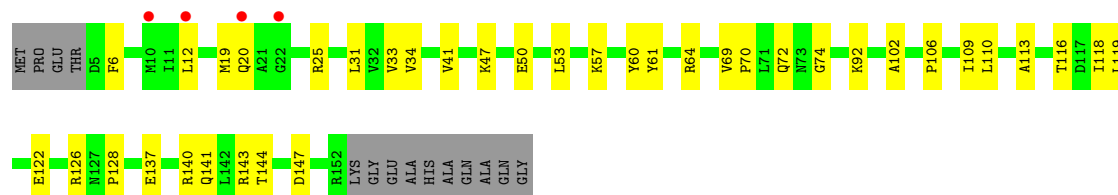


• Molecule 36: 30S ribosomal protein S5

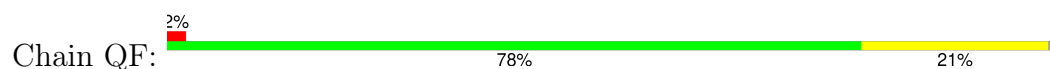




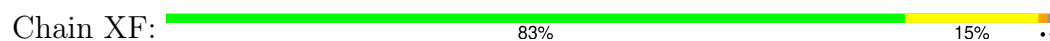
- Molecule 36: 30S ribosomal protein S5



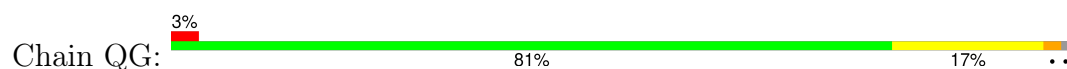
- Molecule 37: 30S ribosomal protein S6



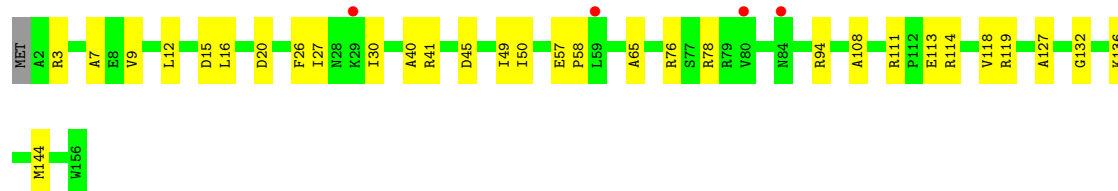
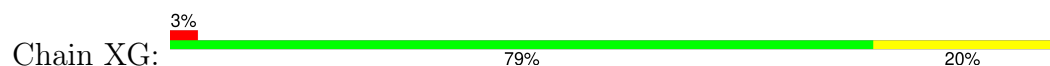
- Molecule 37: 30S ribosomal protein S6



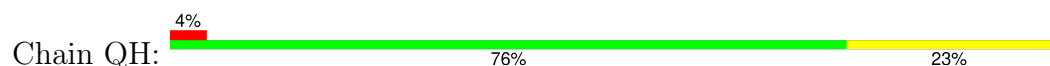
- Molecule 38: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S7

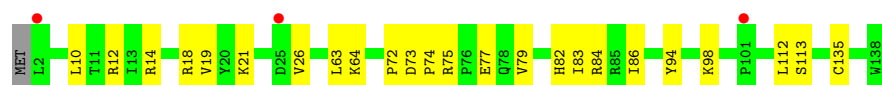
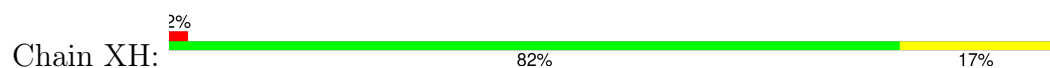


- Molecule 39: 30S ribosomal protein S8

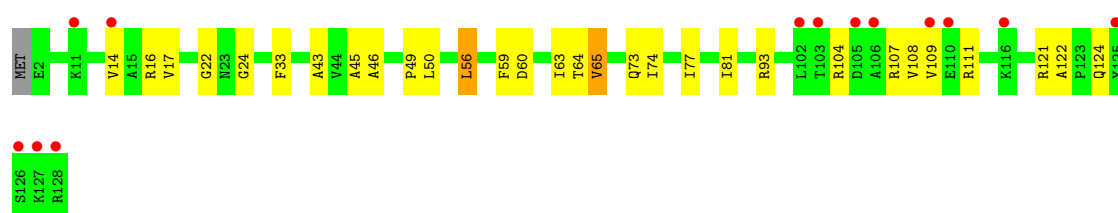
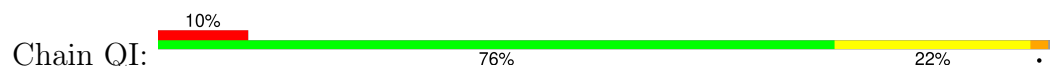




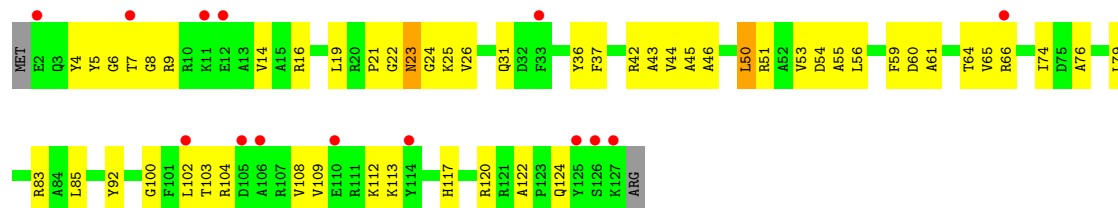
- Molecule 39: 30S ribosomal protein S8



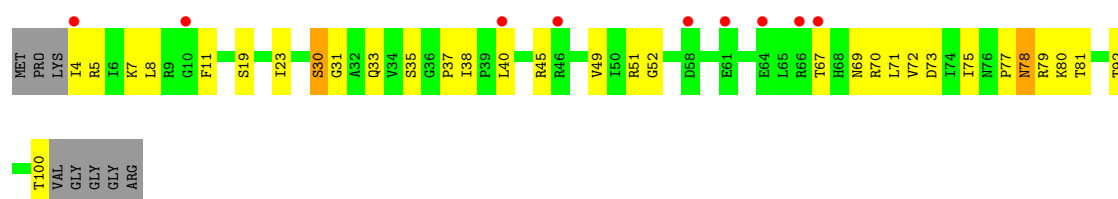
- Molecule 40: 30S ribosomal protein S9



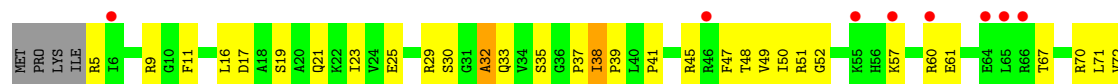
- Molecule 40: 30S ribosomal protein S9



- Molecule 41: 30S ribosomal protein S10

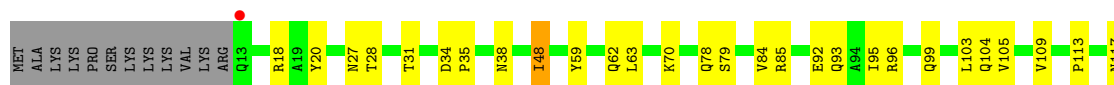


- Molecule 41: 30S ribosomal protein S10

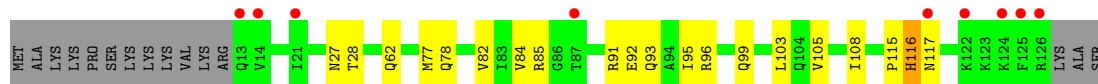
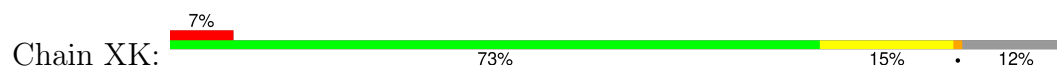




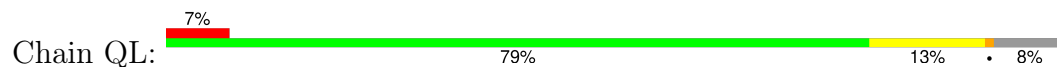
- Molecule 42: 30S ribosomal protein S11



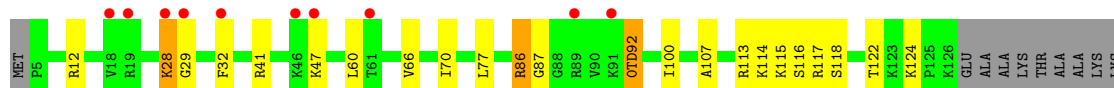
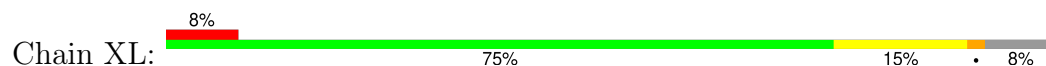
- Molecule 42: 30S ribosomal protein S11



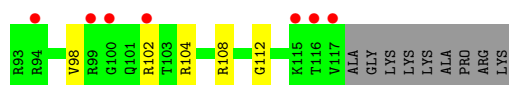
- Molecule 43: 30S ribosomal protein S12



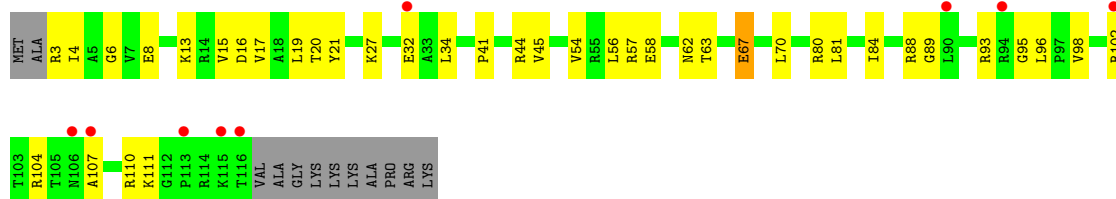
- Molecule 43: 30S ribosomal protein S12



- Molecule 44: 30S ribosomal protein S13



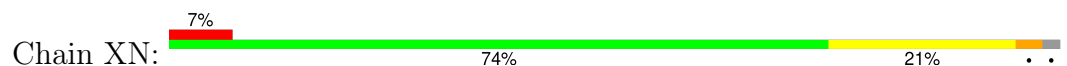
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



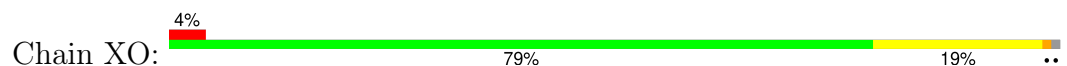
- Molecule 45: 30S ribosomal protein S14 type Z



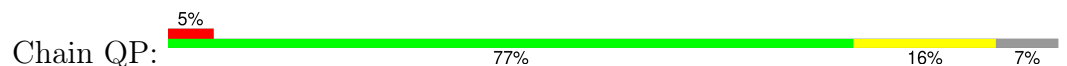
- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15

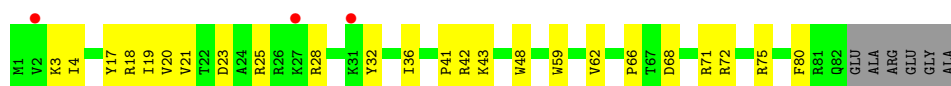


- Molecule 47: 30S ribosomal protein S16

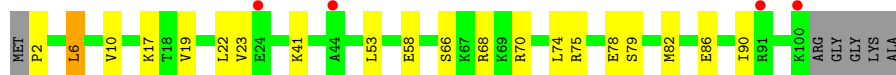
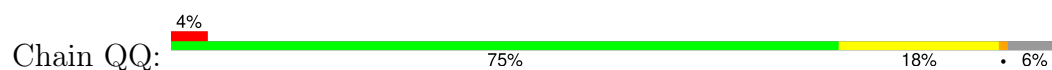


- Molecule 47: 30S ribosomal protein S16

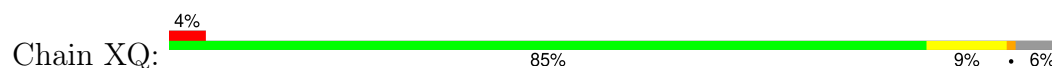




- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18



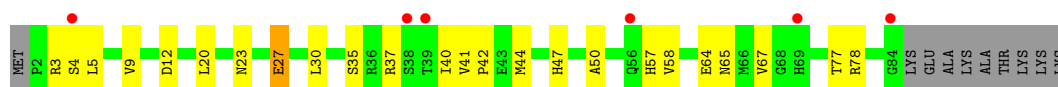
- Molecule 49: 30S ribosomal protein S18



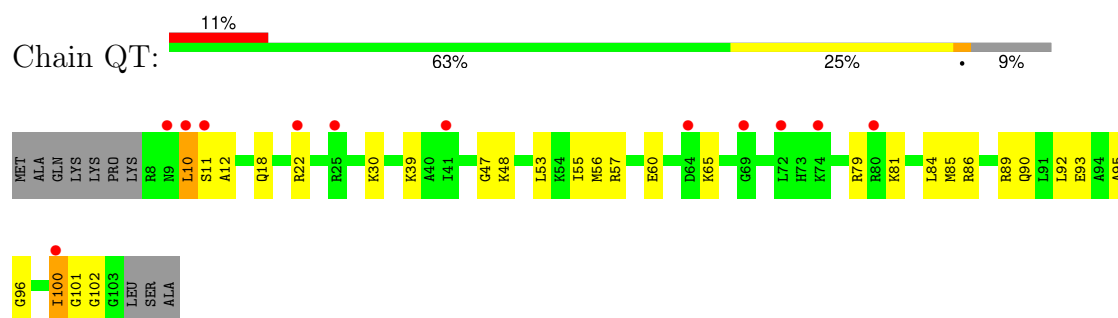
- Molecule 50: 30S ribosomal protein S19



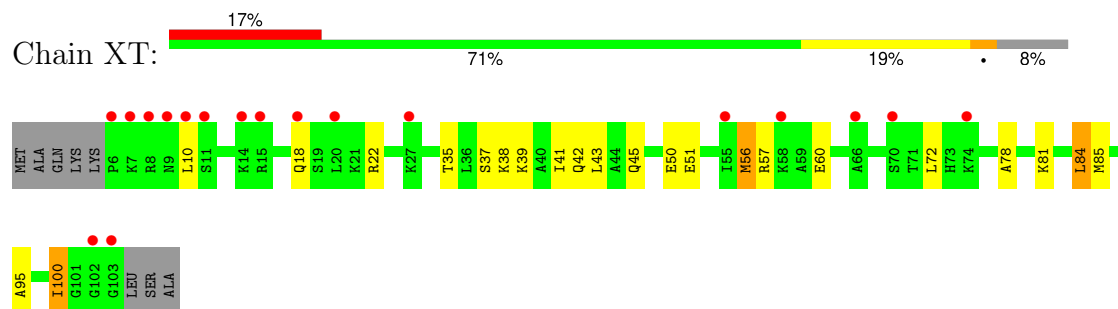
- Molecule 50: 30S ribosomal protein S19



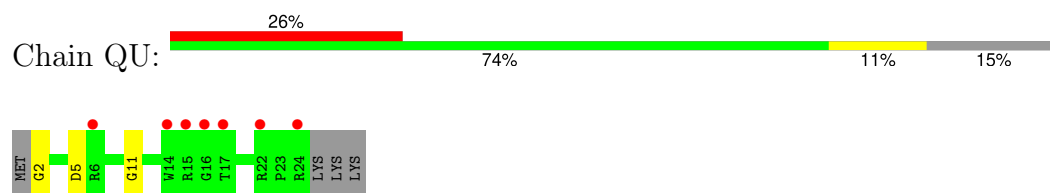
- Molecule 51: 30S ribosomal protein S20



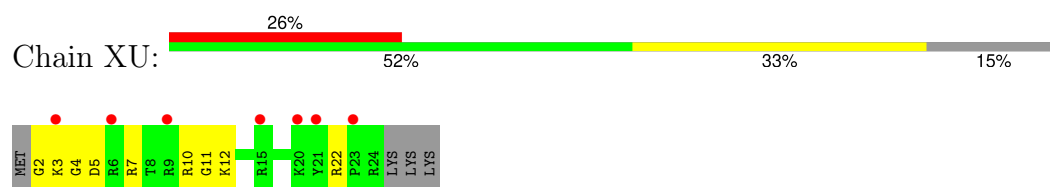
- Molecule 51: 30S ribosomal protein S20



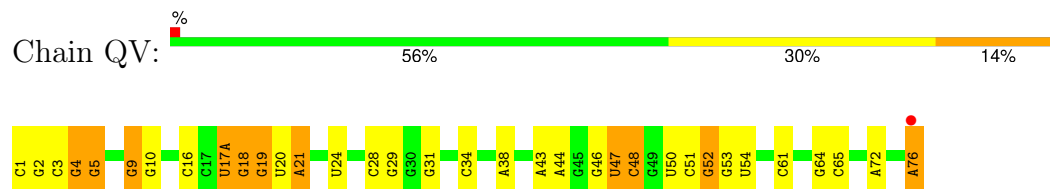
- Molecule 52: 30S ribosomal protein Thx



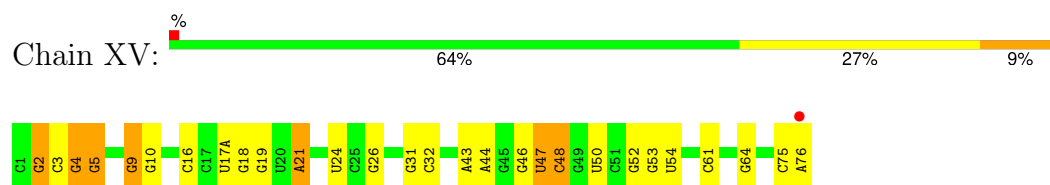
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: P-site tRNA fMet



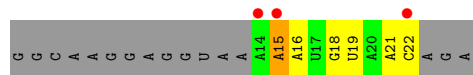
- Molecule 53: P-site tRNA fMet



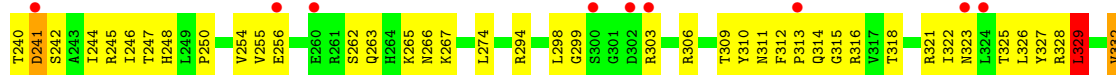
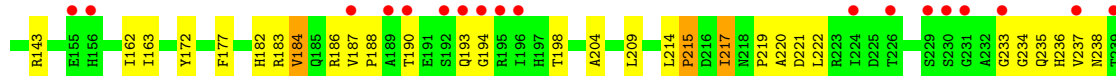
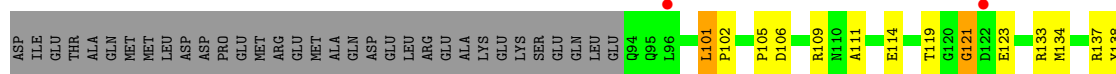
- Molecule 54: messenger RNA



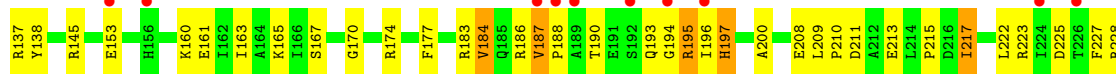
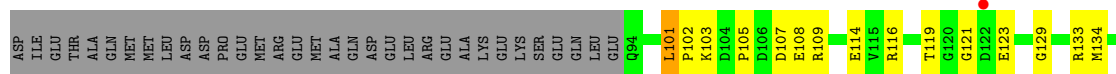
- Molecule 54: messenger RNA

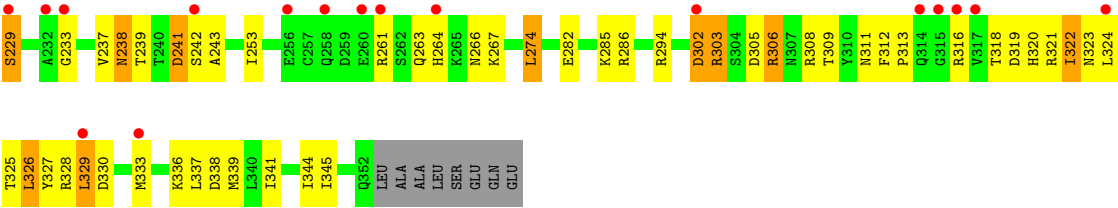


- Molecule 55: Peptide chain release factor 1



- Molecule 55: Peptide chain release factor 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.03Å 449.71Å 620.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 3.20 49.81 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.81-3.20) 99.9 (49.81-3.20)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.214 , 0.244 0.213 , 0.243	Depositor DCC
R_{free} test set	44469 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	93.8	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 80.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	294739	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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: ZN, 7MG, 5MU, UR3, MA6, 4OC, MEQ, M2G, SF4, 2MU, OMG, 0TD, 2MG, MG, 2MA, PSU, 5MC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	RA	0.15	0/68901	0.37	2/107544 (0.0%)
1	YA	0.16	0/68901	0.38	0/107544
2	RB	0.14	0/2876	0.34	0/4486
2	YB	0.16	0/2878	0.36	0/4490
3	RD	0.20	0/2181	0.49	0/2940
3	YD	0.20	0/2186	0.51	0/2944
4	RE	0.19	0/1592	0.46	0/2149
4	YE	0.22	0/1592	0.53	2/2149 (0.1%)
5	RF	0.17	0/1619	0.47	0/2193
5	YF	0.22	0/1615	0.52	0/2188
6	RG	0.18	0/1451	0.49	0/1961
6	YG	0.19	0/1449	0.50	0/1957
7	RH	0.18	0/1356	0.42	0/1834
7	YH	0.20	0/1350	0.50	0/1826
8	RI	0.18	0/1109	0.47	0/1512
8	YI	0.17	0/1091	0.44	0/1490
9	RN	0.18	0/1148	0.45	0/1547
9	YN	0.18	0/1144	0.45	0/1543
10	RO	0.19	0/943	0.46	0/1269
10	YO	0.19	0/943	0.48	0/1269
11	RP	0.20	0/1152	0.50	0/1533
11	YP	0.19	0/1152	0.49	0/1533
12	RQ	0.21	0/1143	0.46	0/1527
12	YQ	0.20	0/1143	0.45	0/1527
13	RR	0.19	0/982	0.48	0/1312
13	YR	0.20	0/982	0.47	0/1312
14	RS	0.17	0/887	0.48	0/1180
14	YS	0.21	0/880	0.51	0/1172
15	RT	0.20	0/1105	0.54	0/1477
15	YT	0.20	0/1097	0.48	0/1468
16	RU	0.18	0/977	0.41	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	YU	0.20	0/977	0.44	0/1301
17	RV	0.20	0/786	0.44	0/1053
17	YV	0.22	0/782	0.50	0/1049
18	RW	0.18	0/897	0.43	0/1205
18	YW	0.18	0/897	0.41	0/1205
19	RX	0.20	0/764	0.47	0/1025
19	YX	0.20	0/764	0.46	0/1025
20	RY	0.21	0/823	0.59	1/1099 (0.1%)
20	YY	0.25	0/823	0.51	0/1100
21	RZ	0.19	0/1517	0.45	0/2062
21	YZ	0.18	0/1501	0.46	0/2043
22	R0	0.19	0/616	0.42	0/821
22	Y0	0.18	0/616	0.48	0/821
23	R1	0.16	0/761	0.42	0/1013
23	Y1	0.18	0/766	0.46	0/1018
24	R2	0.42	2/590 (0.3%)	0.54	0/781
24	Y2	0.17	0/594	0.43	0/785
25	R3	0.18	0/474	0.46	0/635
25	Y3	0.20	0/469	0.48	0/630
26	R4	0.30	0/559	0.79	1/754 (0.1%)
26	Y4	0.27	0/549	0.76	3/741 (0.4%)
27	R5	0.23	0/473	0.44	0/639
27	Y5	0.24	0/469	0.45	0/635
28	R6	0.21	0/460	0.44	0/613
28	Y6	0.15	0/456	0.40	0/608
29	R7	0.20	0/426	0.49	0/561
29	Y7	0.20	0/426	0.46	0/561
30	R8	0.20	0/525	0.42	0/691
30	Y8	0.19	0/525	0.44	0/691
31	R9	0.17	0/310	0.40	0/407
31	Y9	0.20	0/310	0.44	0/407
32	QA	0.15	0/35795	0.38	3/55864 (0.0%)
32	XA	0.15	0/35890	0.37	2/56012 (0.0%)
33	QB	0.21	0/1876	0.56	0/2533
33	XB	0.22	0/1860	0.57	0/2518
34	QC	0.18	0/1582	0.48	0/2137
34	XC	0.20	0/1566	0.47	0/2119
35	QD	0.19	0/1695	0.47	0/2274
35	XD	0.17	0/1698	0.46	0/2277
36	QE	0.20	0/1149	0.46	0/1548
36	XE	0.19	0/1149	0.46	0/1548
37	QF	0.16	0/827	0.43	0/1120
37	XF	0.17	0/829	0.44	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	QG	0.16	0/1254	0.41	0/1683
38	XG	0.17	0/1248	0.43	0/1676
39	QH	0.16	0/1118	0.43	0/1506
39	XH	0.17	0/1108	0.42	0/1494
40	QI	0.19	0/1005	0.53	0/1351
40	XI	0.18	0/985	0.51	0/1329
41	QJ	0.20	0/732	0.51	0/993
41	XJ	0.19	0/723	0.55	1/984 (0.1%)
42	QK	0.16	0/849	0.42	0/1150
42	XK	0.19	0/848	0.51	1/1149 (0.1%)
43	QL	0.19	0/937	0.41	0/1260
43	XL	0.22	0/937	0.56	1/1260 (0.1%)
44	QM	0.18	0/924	0.51	0/1242
44	XM	0.17	0/905	0.53	0/1217
45	QN	0.17	0/501	0.42	0/664
45	XN	0.19	0/501	0.46	0/664
46	QO	0.18	0/739	0.46	0/985
46	XO	0.17	0/739	0.45	0/985
47	QP	0.17	0/697	0.49	0/939
47	XP	0.20	0/693	0.46	0/935
48	QQ	0.16	0/836	0.45	0/1117
48	XQ	0.16	0/836	0.44	0/1117
49	QR	0.15	0/560	0.48	0/746
49	XR	0.18	0/560	0.44	0/746
50	QS	0.20	0/663	0.56	0/895
50	XS	0.20	0/660	0.49	0/893
51	QT	0.20	0/734	0.51	0/969
51	XT	0.20	0/736	0.41	0/976
52	QU	0.19	0/203	0.51	0/266
52	XU	0.21	0/203	0.54	0/266
53	QV	0.13	0/1836	0.32	0/2859
53	XV	0.14	0/1836	0.35	0/2859
54	QX	0.17	0/241	0.45	0/373
54	XX	0.17	0/216	0.50	0/334
55	QY	0.25	0/2035	0.47	0/2742
55	XY	0.22	0/2044	0.42	0/2754
All	All	0.17	2/316288 (0.0%)	0.40	17/472607 (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
26	R4	0	1
33	QB	0	1
43	XL	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R2	48	HIS	ND1-CE1	7.54	1.40	1.32
24	R2	48	HIS	CE1-NE2	-5.43	1.27	1.32

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	QA	576	G	OP1-P-O3'	-9.14	80.59	108.00
1	RA	2602	A	OP2-P-O3'	-9.13	80.60	108.00
32	QA	576	G	OP2-P-O3'	-8.56	82.31	108.00
20	RY	92	ASN	N-CA-C	7.89	120.87	111.33
41	XJ	32	ALA	N-CA-C	-6.60	100.69	110.46

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	QB	231	GLU	Peptide
26	R4	67	TYR	Peptide
14	RS	58	LEU	Peptide
43	XL	86	ARG	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	31145	577	0
1	YA	61758	0	31148	608	1
2	RB	2572	0	1305	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	YB	2573	0	1306	23	0
3	RD	2131	0	2207	47	0
3	YD	2136	0	2218	40	0
4	RE	1559	0	1618	27	0
4	YE	1559	0	1618	29	0
5	RF	1584	0	1625	34	0
5	YF	1580	0	1619	44	0
6	RG	1426	0	1445	36	0
6	YG	1424	0	1441	46	0
7	RH	1330	0	1407	26	0
7	YH	1324	0	1402	37	0
8	RI	1094	0	1127	23	0
8	YI	1076	0	1094	21	0
9	RN	1121	0	1195	14	0
9	YN	1117	0	1184	22	0
10	RO	933	0	996	11	0
10	YO	933	0	996	10	0
11	RP	1135	0	1212	26	0
11	YP	1135	0	1212	32	0
12	RQ	1122	0	1179	22	0
12	YQ	1122	0	1179	22	0
13	RR	968	0	1033	17	0
13	YR	968	0	1033	12	0
14	RS	877	0	938	9	0
14	YS	870	0	923	15	0
15	RT	1091	0	1151	22	0
15	YT	1083	0	1136	19	0
16	RU	959	0	1019	13	0
16	YU	959	0	1019	13	0
17	RV	775	0	841	10	0
17	YV	771	0	830	15	0
18	RW	886	0	940	12	0
18	YW	886	0	940	9	0
19	RX	750	0	814	17	0
19	YX	750	0	814	12	0
20	RY	810	0	892	16	0
20	YY	810	0	888	18	0
21	RZ	1485	0	1493	20	0
21	YZ	1469	0	1467	26	0
22	R0	608	0	622	10	0
22	Y0	608	0	622	14	0
23	R1	754	0	823	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	Y1	759	0	837	21	0
24	R2	588	0	643	5	1
24	Y2	592	0	654	8	0
25	R3	469	0	518	4	0
25	Y3	464	0	514	8	0
26	R4	546	0	522	28	0
26	Y4	536	0	514	33	0
27	R5	459	0	476	11	0
27	Y5	455	0	465	7	0
28	R6	453	0	473	15	0
28	Y6	449	0	469	4	0
29	R7	418	0	467	12	0
29	Y7	418	0	467	8	0
30	R8	517	0	582	22	0
30	Y8	517	0	582	19	0
31	R9	307	0	335	9	0
31	Y9	307	0	335	15	0
32	QA	32246	0	16294	318	0
32	XA	32331	0	16338	348	0
33	QB	1842	0	1862	55	0
33	XB	1825	0	1828	59	0
34	QC	1558	0	1557	30	0
34	XC	1542	0	1517	38	0
35	QD	1665	0	1688	45	0
35	XD	1668	0	1704	39	0
36	QE	1133	0	1191	33	0
36	XE	1133	0	1191	24	0
37	QF	814	0	808	16	0
37	XF	816	0	808	12	0
38	QG	1235	0	1249	22	0
38	XG	1229	0	1238	16	0
39	QH	1098	0	1143	27	0
39	XH	1088	0	1126	14	0
40	QI	986	0	990	28	0
40	XI	966	0	953	37	0
41	QJ	719	0	672	22	0
41	XJ	710	0	661	30	0
42	QK	834	0	838	16	0
42	XK	833	0	836	13	0
43	QL	932	0	980	14	0
43	XL	932	0	981	20	0
44	QM	914	0	954	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	XM	895	0	920	25	0
45	QN	492	0	529	19	0
45	XN	492	0	529	19	0
46	QO	728	0	760	19	0
46	XO	728	0	760	12	0
47	QP	681	0	697	11	0
47	XP	677	0	686	19	0
48	QQ	823	0	891	13	0
48	XQ	823	0	891	7	0
49	QR	555	0	618	11	0
49	XR	555	0	618	14	0
50	QS	648	0	658	16	0
50	XS	645	0	635	27	0
51	QT	732	0	809	18	0
51	XT	733	0	795	17	0
52	QU	199	0	208	2	0
52	XU	199	0	208	7	0
53	QV	1644	0	835	23	0
53	XV	1644	0	836	15	0
54	QX	215	0	109	1	0
54	XX	193	0	97	4	0
55	QY	2014	0	1981	64	0
55	XY	2023	0	1988	79	0
56	QA	256	0	0	0	0
56	QB	1	0	0	0	0
56	QD	3	0	0	0	0
56	QE	2	0	0	0	0
56	QF	1	0	0	0	0
56	QG	2	0	0	0	0
56	QH	1	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	1	0	0	0	0
56	QR	1	0	0	0	0
56	QT	2	0	0	0	0
56	QV	6	0	0	0	0
56	R0	4	0	0	0	0
56	R1	4	0	0	0	0
56	R3	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	R5	3	0	0	0	0
56	R7	2	0	0	0	0
56	R8	1	0	0	0	0
56	RA	1039	0	0	0	0
56	RB	27	0	0	0	0
56	RD	15	0	0	0	0
56	RE	8	0	0	0	0
56	RF	12	0	0	0	0
56	RG	4	0	0	0	0
56	RH	1	0	0	0	0
56	RN	2	0	0	0	0
56	RO	1	0	0	0	0
56	RP	1	0	0	0	0
56	RQ	6	0	0	0	0
56	RR	3	0	0	0	0
56	RT	2	0	0	0	0
56	RU	2	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	RY	1	0	0	0	0
56	RZ	1	0	0	0	0
56	XA	183	0	0	0	0
56	XE	1	0	0	0	0
56	XF	2	0	0	0	0
56	XJ	1	0	0	0	0
56	XK	1	0	0	0	0
56	XL	1	0	0	0	0
56	XR	1	0	0	0	0
56	XT	1	0	0	0	0
56	XV	4	0	0	0	0
56	XX	1	0	0	0	0
56	Y0	1	0	0	0	0
56	Y1	1	0	0	0	0
56	Y5	1	0	0	0	0
56	Y7	2	0	0	0	0
56	Y8	2	0	0	0	0
56	YA	744	0	0	0	0
56	YB	18	0	0	0	0
56	YD	9	0	0	0	0
56	YE	5	0	0	0	0
56	YF	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	YG	2	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	4	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	294739	0	198434	3449	1

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 7.

The worst 5 of 3449 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:2552:2MU:C4	1:YA:2552:2MU:C5	1.80	1.59
1:RA:2552:2MU:C5	1:RA:2552:2MU:C4	1.80	1.58
32:XA:1003:G:H2'	32:XA:1004:A:H4'	1.32	1.08
1:YA:1029:A:N6	1:YA:1125:G:O2'	1.87	1.06
26:Y4:59:PHE:HA	26:Y4:61:ARG:N	1.76	1.00

All (1) 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)
24:R2:46:GLN:OE1	1:YA:277:C:O2'[3_555]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	RD	273/276 (99%)	261 (96%)	12 (4%)	0	100	100
3	YD	273/276 (99%)	262 (96%)	11 (4%)	0	100	100
4	RE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	24	59
4	YE	202/206 (98%)	195 (96%)	7 (4%)	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%)	12	45
6	RG	179/182 (98%)	166 (93%)	12 (7%)	1 (1%)	21	56
6	YG	179/182 (98%)	170 (95%)	8 (4%)	1 (1%)	21	56
7	RH	172/180 (96%)	167 (97%)	5 (3%)	0	100	100
7	YH	171/180 (95%)	164 (96%)	7 (4%)	0	100	100
8	RI	145/148 (98%)	135 (93%)	10 (7%)	0	100	100
8	YI	144/148 (97%)	137 (95%)	7 (5%)	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%)	114 (95%)	6 (5%)	0	100	100
11	RP	147/150 (98%)	142 (97%)	4 (3%)	1 (1%)	18	52
11	YP	147/150 (98%)	142 (97%)	4 (3%)	1 (1%)	18	52
12	RQ	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
12	YQ	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
13	RR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	YR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
14	RS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	14	47
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%)	113 (99%)	1 (1%)	0	100	100
16	YU	114/118 (97%)	114 (100%)	0	0	100	100
17	RV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12	45
17	YV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12	45
18	RW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	YW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	RX	93/96 (97%)	92 (99%)	1 (1%)	0	100	100
19	YX	93/96 (97%)	92 (99%)	1 (1%)	0	100	100
20	RY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
20	YY	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
21	RZ	187/206 (91%)	182 (97%)	5 (3%)	0	100	100
21	YZ	187/206 (91%)	181 (97%)	6 (3%)	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%)	11	43
23	Y1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	43
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%)	56 (84%)	7 (10%)	4 (6%)	1	10
26	Y4	67/71 (94%)	55 (82%)	9 (13%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	62 (100%)	0	0	100	100
30	Y8	62/65 (95%)	62 (100%)	0	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%)	201 (88%)	24 (10%)	4 (2%)	7	35
33	XB	229/256 (90%)	205 (90%)	19 (8%)	5 (2%)	5	29
34	QC	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
34	XC	204/239 (85%)	189 (93%)	15 (7%)	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%)	144 (99%)	2 (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%)	151 (99%)	2 (1%)	0	100	100
38	XG	153/156 (98%)	149 (97%)	3 (2%)	1 (1%)	18	52
39	QH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
39	XH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
40	QI	125/128 (98%)	116 (93%)	9 (7%)	0	100	100
40	XI	124/128 (97%)	113 (91%)	9 (7%)	2 (2%)	7	36
41	QJ	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	2	16
41	XJ	94/105 (90%)	84 (89%)	8 (8%)	2 (2%)	5	31
42	QK	112/129 (87%)	105 (94%)	6 (5%)	1 (1%)	14	47
42	XK	112/129 (87%)	106 (95%)	6 (5%)	0	100	100
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%)	6	34
44	XM	112/126 (89%)	105 (94%)	6 (5%)	1 (1%)	14	47
45	QN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	XN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
46	QO	86/89 (97%)	83 (96%)	3 (4%)	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%)	77 (96%)	3 (4%)	0	100	100
48	QQ	97/105 (92%)	94 (97%)	2 (2%)	1 (1%)	12	45
48	XQ	97/105 (92%)	95 (98%)	2 (2%)	0	100	100
49	QR	66/88 (75%)	66 (100%)	0	0	100	100
49	XR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	QS	81/93 (87%)	78 (96%)	2 (2%)	1 (1%)	10	42
50	XS	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
51	QT	94/106 (89%)	88 (94%)	5 (5%)	1 (1%)	11	43
51	XT	96/106 (91%)	89 (93%)	5 (5%)	2 (2%)	5	31
52	QU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	XU	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	14
55	QY	255/360 (71%)	224 (88%)	17 (7%)	14 (6%)	1	11
55	XY	256/360 (71%)	222 (87%)	25 (10%)	9 (4%)	3	20
All	All	11925/12848 (93%)	11396 (96%)	459 (4%)	70 (1%)	21	56

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	R4	49	PHE
33	QB	16	HIS
33	QB	22	LYS
51	QT	95	ALA
55	QY	215	PRO

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%)	207 (97%)	7 (3%)	33	65
3	YD	215/218 (99%)	209 (97%)	6 (3%)	38	68
4	RE	164/166 (99%)	153 (93%)	11 (7%)	15	47
4	YE	164/166 (99%)	152 (93%)	12 (7%)	13	43
5	RF	160/166 (96%)	152 (95%)	8 (5%)	22	55
5	YF	159/166 (96%)	150 (94%)	9 (6%)	18	51
6	RG	144/156 (92%)	138 (96%)	6 (4%)	26	60
6	YG	142/156 (91%)	135 (95%)	7 (5%)	22	55
7	RH	144/148 (97%)	144 (100%)	0	100	100
7	YH	143/148 (97%)	134 (94%)	9 (6%)	16	48
8	RI	111/124 (90%)	100 (90%)	11 (10%)	7	31
8	YI	108/124 (87%)	99 (92%)	9 (8%)	10	38
9	RN	119/119 (100%)	111 (93%)	8 (7%)	15	47
9	YN	118/119 (99%)	112 (95%)	6 (5%)	21	54
10	RO	100/100 (100%)	98 (98%)	2 (2%)	48	72
10	YO	100/100 (100%)	97 (97%)	3 (3%)	36	66
11	RP	115/116 (99%)	111 (96%)	4 (4%)	32	64
11	YP	115/116 (99%)	112 (97%)	3 (3%)	40	69
12	RQ	111/111 (100%)	108 (97%)	3 (3%)	39	68
12	YQ	111/111 (100%)	106 (96%)	5 (4%)	24	58
13	RR	101/101 (100%)	94 (93%)	7 (7%)	14	45
13	YR	101/101 (100%)	95 (94%)	6 (6%)	18	50
14	RS	87/88 (99%)	85 (98%)	2 (2%)	44	70
14	YS	85/88 (97%)	84 (99%)	1 (1%)	63	79
15	RT	115/127 (91%)	113 (98%)	2 (2%)	53	75
15	YT	113/127 (89%)	112 (99%)	1 (1%)	70	81
16	RU	93/94 (99%)	90 (97%)	3 (3%)	34	65
16	YU	93/94 (99%)	91 (98%)	2 (2%)	45	71
17	RV	81/82 (99%)	76 (94%)	5 (6%)	16	49
17	YV	80/82 (98%)	77 (96%)	3 (4%)	29	62
18	RW	90/92 (98%)	87 (97%)	3 (3%)	33	65
18	YW	90/92 (98%)	89 (99%)	1 (1%)	65	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	RX	77/78 (99%)	76 (99%)	1 (1%)	61	78
19	YX	77/78 (99%)	76 (99%)	1 (1%)	61	78
20	RY	86/91 (94%)	84 (98%)	2 (2%)	44	70
20	YY	86/91 (94%)	85 (99%)	1 (1%)	63	79
21	RZ	159/179 (89%)	150 (94%)	9 (6%)	18	51
21	YZ	156/179 (87%)	150 (96%)	6 (4%)	29	62
22	R0	61/67 (91%)	59 (97%)	2 (3%)	33	65
22	Y0	61/67 (91%)	61 (100%)	0	100	100
23	R1	79/83 (95%)	78 (99%)	1 (1%)	61	78
23	Y1	81/83 (98%)	78 (96%)	3 (4%)	30	63
24	R2	65/67 (97%)	63 (97%)	2 (3%)	35	66
24	Y2	66/67 (98%)	63 (96%)	3 (4%)	24	58
25	R3	51/52 (98%)	49 (96%)	2 (4%)	28	62
25	Y3	50/52 (96%)	48 (96%)	2 (4%)	28	61
26	R4	58/63 (92%)	56 (97%)	2 (3%)	32	64
26	Y4	54/63 (86%)	51 (94%)	3 (6%)	19	52
27	R5	51/52 (98%)	48 (94%)	3 (6%)	18	50
27	Y5	50/52 (96%)	47 (94%)	3 (6%)	17	50
28	R6	51/52 (98%)	51 (100%)	0	100	100
28	Y6	50/52 (96%)	50 (100%)	0	100	100
29	R7	41/42 (98%)	38 (93%)	3 (7%)	13	43
29	Y7	41/42 (98%)	39 (95%)	2 (5%)	22	55
30	R8	54/55 (98%)	52 (96%)	2 (4%)	30	63
30	Y8	54/55 (98%)	52 (96%)	2 (4%)	30	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%)	181 (95%)	10 (5%)	21	54
33	XB	187/220 (85%)	177 (95%)	10 (5%)	20	53
34	QC	144/188 (77%)	143 (99%)	1 (1%)	76	83
34	XC	140/188 (74%)	138 (99%)	2 (1%)	59	77
35	QD	171/181 (94%)	168 (98%)	3 (2%)	51	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	XD	172/181 (95%)	168 (98%)	4 (2%)	44	70
36	QE	114/123 (93%)	111 (97%)	3 (3%)	40	69
36	XE	114/123 (93%)	112 (98%)	2 (2%)	51	74
37	QF	85/90 (94%)	85 (100%)	0	100	100
37	XF	85/90 (94%)	84 (99%)	1 (1%)	63	79
38	QG	120/127 (94%)	115 (96%)	5 (4%)	26	60
38	XG	119/127 (94%)	114 (96%)	5 (4%)	26	60
39	QH	116/119 (98%)	114 (98%)	2 (2%)	53	75
39	XH	114/119 (96%)	112 (98%)	2 (2%)	51	74
40	QI	91/99 (92%)	89 (98%)	2 (2%)	45	71
40	XI	88/99 (89%)	83 (94%)	5 (6%)	18	51
41	QJ	68/92 (74%)	67 (98%)	1 (2%)	57	76
41	XJ	68/92 (74%)	66 (97%)	2 (3%)	37	67
42	QK	83/99 (84%)	82 (99%)	1 (1%)	63	79
42	XK	83/99 (84%)	83 (100%)	0	100	100
43	QL	96/108 (89%)	95 (99%)	1 (1%)	68	80
43	XL	96/108 (89%)	95 (99%)	1 (1%)	68	80
44	QM	90/101 (89%)	87 (97%)	3 (3%)	33	65
44	XM	87/101 (86%)	83 (95%)	4 (5%)	24	58
45	QN	49/50 (98%)	47 (96%)	2 (4%)	27	60
45	XN	49/50 (98%)	47 (96%)	2 (4%)	27	60
46	QO	78/80 (98%)	76 (97%)	2 (3%)	40	69
46	XO	78/80 (98%)	76 (97%)	2 (3%)	40	69
47	QP	69/74 (93%)	69 (100%)	0	100	100
47	XP	68/74 (92%)	68 (100%)	0	100	100
48	QQ	94/97 (97%)	92 (98%)	2 (2%)	47	71
48	XQ	94/97 (97%)	92 (98%)	2 (2%)	47	71
49	QR	59/77 (77%)	57 (97%)	2 (3%)	32	64
49	XR	59/77 (77%)	58 (98%)	1 (2%)	53	75
50	QS	68/80 (85%)	65 (96%)	3 (4%)	25	59
50	XS	67/80 (84%)	66 (98%)	1 (2%)	57	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	QT	71/82 (87%)	66 (93%)	5 (7%)	14	45
51	XT	70/82 (85%)	68 (97%)	2 (3%)	37	67
52	QU	18/22 (82%)	18 (100%)	0	100	100
52	XU	18/22 (82%)	18 (100%)	0	100	100
55	QY	210/299 (70%)	201 (96%)	9 (4%)	26	59
55	XY	211/299 (71%)	192 (91%)	19 (9%)	9	34
All	All	9765/10662 (92%)	9421 (96%)	344 (4%)	32	64

5 of 344 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	YP	112	LEU
33	XB	224	GLN
13	YR	44	LEU
23	Y1	32	LYS
38	XG	144	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
51	QT	75	ASN
47	XP	14	ASN
11	YP	70	GLN
46	XO	62	GLN
38	XG	86	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	RA	2858/2915 (98%)	441 (15%)	27 (0%)
1	YA	2858/2915 (98%)	438 (15%)	25 (0%)
2	RB	119/122 (97%)	9 (7%)	0
2	YB	119/122 (97%)	10 (8%)	0
32	QA	1497/1521 (98%)	232 (15%)	16 (1%)
32	XA	1501/1521 (98%)	229 (15%)	19 (1%)
53	QV	76/77 (98%)	15 (19%)	0
53	XV	76/77 (98%)	15 (19%)	1 (1%)
54	QX	9/25 (36%)	2 (22%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	XX	8/25 (32%)	3 (37%)	0
All	All	9121/9320 (97%)	1394 (15%)	88 (0%)

5 of 1394 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	RA	10	G
1	RA	11	G
1	RA	12	U
1	RA	15	G
1	RA	45	C

5 of 88 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	YA	1076	C
32	XA	266	G
1	YA	1420	U
1	YA	2321	G
32	XA	748	C

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	5MC	XA	1404	32	19,22,23	4.08	8 (42%)	26,32,35	0.96	1 (3%)
1	4OC	YA	1920	1	19,22,24	3.13	7 (36%)	25,31,35	0.95	1 (4%)
1	4OC	RA	1920	1	19,22,24	3.15	7 (36%)	25,31,35	0.92	0
1	5MU	YA	1939	1,56	19,22,23	5.03	7 (36%)	27,32,35	4.12	9 (33%)
32	5MC	QA	1400	32	19,22,23	4.09	8 (42%)	26,32,35	0.97	1 (3%)
1	5MU	YA	1915	1,56	19,22,23	5.27	6 (31%)	27,32,35	4.11	11 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	0TD	XL	92	43	8,9,10	1.48	1 (12%)	6,11,13	2.37	3 (50%)
32	4OC	QA	1402	32	20,23,24	3.29	7 (35%)	25,32,35	0.98	2 (8%)
1	PSU	YA	2605	1	18,21,22	4.41	7 (38%)	21,30,33	2.12	6 (28%)
32	MA6	XA	1518	32	23,26,27	1.44	4 (17%)	33,38,41	3.43	12 (36%)
1	2MA	YA	2503	1,56	22,25,26	4.33	8 (36%)	32,37,40	3.10	12 (37%)
32	UR3	XA	1498	56,32	19,22,23	3.28	7 (36%)	26,32,35	1.73	2 (7%)
32	5MC	QA	1404	32	19,22,23	4.13	8 (42%)	26,32,35	0.96	1 (3%)
1	2MA	RA	2503	1,56	22,25,26	4.26	8 (36%)	32,37,40	2.95	11 (34%)
32	M2G	QA	966	32	24,27,28	2.81	7 (29%)	33,40,43	2.19	10 (30%)
32	5MC	XA	967	32	19,22,23	4.12	8 (42%)	26,32,35	0.93	1 (3%)
32	UR3	QA	1498	32	19,22,23	3.29	7 (36%)	26,32,35	1.72	2 (7%)
1	2MU	RA	2552	1,56	19,22,24	6.65	14 (73%)	25,31,36	2.82	7 (28%)
43	0TD	QL	92	43	8,9,10	1.48	1 (12%)	6,11,13	3.23	5 (83%)
32	2MG	XA	1207	32	23,26,27	2.84	7 (30%)	33,38,41	2.44	13 (39%)
32	7MG	XA	527	56,32	23,26,27	4.33	11 (47%)	27,39,42	2.23	11 (40%)
55	MEQ	XY	235	55	8,9,10	0.93	0	5,10,12	0.80	0
32	7MG	QA	527	56,32	23,26,27	4.31	11 (47%)	27,39,42	2.25	9 (33%)
32	2MG	QA	1207	56,32	23,26,27	2.86	8 (34%)	33,38,41	2.51	15 (45%)
32	4OC	XA	1402	32	20,23,24	3.11	8 (40%)	25,32,35	1.27	1 (4%)
1	5MU	RA	1939	1	19,22,23	5.03	7 (36%)	27,32,35	3.99	10 (37%)
32	5MC	QA	967	32	19,22,23	4.15	8 (42%)	26,32,35	0.91	1 (3%)
1	5MU	RA	1915	1	19,22,23	5.27	6 (31%)	27,32,35	4.09	13 (48%)
1	OMG	RA	2251	1,56,53	23,26,27	2.40	9 (39%)	32,38,41	2.27	15 (46%)
1	OMG	YA	2251	1,56,53	23,26,27	2.38	8 (34%)	32,38,41	2.20	15 (46%)
32	5MC	XA	1407	32	19,22,23	4.08	8 (42%)	26,32,35	0.89	1 (3%)
55	MEQ	QY	235	55	8,9,10	0.96	0	5,10,12	1.09	1 (20%)
32	MA6	XA	1519	32	23,26,27	1.46	4 (17%)	33,38,41	3.28	12 (36%)
1	PSU	RA	2605	1	18,21,22	4.47	7 (38%)	21,30,33	2.19	5 (23%)
32	5MC	QA	1407	32	19,22,23	4.07	8 (42%)	26,32,35	0.99	2 (7%)
1	2MU	YA	2552	1,56	19,22,24	6.69	14 (73%)	25,31,36	2.78	7 (28%)
32	MA6	QA	1519	32	23,26,27	1.43	4 (17%)	33,38,41	3.38	12 (36%)
32	5MC	XA	1400	32	19,22,23	4.05	8 (42%)	26,32,35	1.00	2 (7%)
1	5MC	YA	1942	1	19,22,23	4.10	8 (42%)	26,32,35	1.08	2 (7%)
1	5MC	YA	1962	1,56	19,22,23	4.04	8 (42%)	26,32,35	1.05	2 (7%)
1	5MC	RA	1962	1,56	19,22,23	4.04	8 (42%)	26,32,35	1.01	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	RA	1917	1	18,21,22	4.46	7 (38%)	21,30,33	1.90	4 (19%)
1	PSU	YA	1917	1	18,21,22	4.42	7 (38%)	21,30,33	2.01	4 (19%)
32	M2G	XA	966	32	24,27,28	2.74	7 (29%)	33,40,43	2.12	10 (30%)
32	MA6	QA	1518	32	23,26,27	1.45	4 (17%)	33,38,41	3.41	12 (36%)
1	PSU	YA	1911	1	18,21,22	4.39	7 (38%)	21,30,33	2.02	5 (23%)
1	5MC	RA	1942	1,56	19,22,23	4.10	8 (42%)	26,32,35	1.03	2 (7%)
1	PSU	RA	1911	1	18,21,22	4.45	7 (38%)	21,30,33	1.85	4 (19%)
32	PSU	XA	516	32	18,21,22	4.43	7 (38%)	21,30,33	2.09	6 (28%)
32	PSU	QA	516	56,32	18,21,22	4.49	7 (38%)	21,30,33	1.99	5 (23%)

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	5MC	XA	1404	32	-	0/7/25/26	0/2/2/2
1	4OC	YA	1920	1	-	1/9/27/30	0/2/2/2
1	4OC	RA	1920	1	-	0/9/27/30	0/2/2/2
1	5MU	YA	1939	1,56	-	0/7/25/26	0/2/2/2
32	5MC	QA	1400	32	-	2/7/25/26	0/2/2/2
1	5MU	YA	1915	1,56	-	4/7/25/26	0/2/2/2
43	0TD	XL	92	43	-	3/7/12/14	-
32	4OC	QA	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	YA	2605	1	-	0/7/25/26	0/2/2/2
32	MA6	XA	1518	32	-	0/11/29/30	0/3/3/3
1	2MA	YA	2503	1,56	-	0/7/25/26	0/3/3/3
32	UR3	XA	1498	56,32	-	0/7/25/26	0/2/2/2
32	5MC	QA	1404	32	-	0/7/25/26	0/2/2/2
1	2MA	RA	2503	1,56	-	0/7/25/26	0/3/3/3
32	M2G	QA	966	32	-	0/11/29/30	0/3/3/3
32	5MC	XA	967	32	-	0/7/25/26	0/2/2/2
32	UR3	QA	1498	32	-	0/7/25/26	0/2/2/2
1	2MU	RA	2552	1,56	-	0/9/27/28	0/2/2/2
43	0TD	QL	92	43	-	1/7/12/14	-
32	2MG	XA	1207	32	-	0/9/27/28	0/3/3/3
32	7MG	XA	527	56,32	-	2/7/37/38	0/3/3/3
55	MEQ	XY	235	55	-	4/8/9/11	-
32	7MG	QA	527	56,32	-	2/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	2MG	QA	1207	56,32	-	0/9/27/28	0/3/3/3
32	4OC	XA	1402	32	-	2/9/29/30	0/2/2/2
1	5MU	RA	1939	1	-	0/7/25/26	0/2/2/2
32	5MC	QA	967	32	-	0/7/25/26	0/2/2/2
1	5MU	RA	1915	1	-	4/7/25/26	0/2/2/2
1	OMG	RA	2251	1,56,53	-	0/9/27/28	0/3/3/3
1	OMG	YA	2251	1,56,53	-	0/9/27/28	0/3/3/3
32	5MC	XA	1407	32	-	0/7/25/26	0/2/2/2
55	MEQ	QY	235	55	-	2/8/9/11	-
32	MA6	XA	1519	32	-	2/11/29/30	0/3/3/3
1	PSU	RA	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	QA	1407	32	-	0/7/25/26	0/2/2/2
1	2MU	YA	2552	1,56	-	0/9/27/28	0/2/2/2
32	MA6	QA	1519	32	-	2/11/29/30	0/3/3/3
32	5MC	XA	1400	32	-	1/7/25/26	0/2/2/2
1	5MC	YA	1942	1	-	0/7/25/26	0/2/2/2
1	5MC	YA	1962	1,56	-	0/7/25/26	0/2/2/2
1	5MC	RA	1962	1,56	-	0/7/25/26	0/2/2/2
1	PSU	RA	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	YA	1917	1	-	0/7/25/26	0/2/2/2
32	M2G	XA	966	32	-	0/11/29/30	0/3/3/3
32	MA6	QA	1518	32	-	0/11/29/30	0/3/3/3
1	PSU	YA	1911	1	-	0/7/25/26	0/2/2/2
1	5MC	RA	1942	1,56	-	0/7/25/26	0/2/2/2
1	PSU	RA	1911	1	-	0/7/25/26	0/2/2/2
32	PSU	XA	516	32	-	0/7/25/26	0/2/2/2
32	PSU	QA	516	56,32	-	0/7/25/26	0/2/2/2

The worst 5 of 351 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	YA	2552	2MU	C5-C4	16.99	1.80	1.43
1	RA	2552	2MU	C5-C4	16.90	1.80	1.43
1	YA	2503	2MA	C4-N3	13.93	1.52	1.34
1	RA	2503	2MA	C4-N3	13.52	1.51	1.34
1	YA	1915	5MU	C6-N1	12.64	1.59	1.38

The worst 5 of 299 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	1915	5MU	C5-C4-N3	13.88	127.39	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	1939	5MU	C5-C4-N3	13.66	127.19	115.32
1	RA	1915	5MU	C5-C4-N3	13.25	126.84	115.32
1	RA	1939	5MU	C5-C4-N3	12.93	126.56	115.32
32	QA	1519	MA6	N1-C6-N6	-12.10	102.12	116.86

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	RA	1915	5MU	O4'-C1'-N1-C2
1	RA	1915	5MU	O4'-C1'-N1-C6
1	RA	1915	5MU	O4'-C4'-C5'-O5'
32	QA	1402	4OC	O4'-C4'-C5'-O5'
32	QA	1519	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

20 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	YA	1939	5MU	1	0
43	XL	92	0TD	1	0
32	QA	1402	4OC	2	0
32	XA	1518	MA6	2	0
1	YA	2503	2MA	2	0
32	QA	1404	5MC	1	0
1	RA	2503	2MA	2	0
32	QA	966	M2G	1	0
1	RA	2552	2MU	4	0
32	XA	1207	2MG	1	0
32	XA	1402	4OC	3	0
1	RA	1939	5MU	1	0
32	XA	1519	MA6	1	0
1	YA	2552	2MU	4	0
32	QA	1519	MA6	4	0
1	YA	1962	5MC	1	0
1	RA	1962	5MC	1	0
1	RA	1917	PSU	1	0
1	YA	1917	PSU	1	0
32	QA	1518	MA6	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2445 ligands modelled in this entry, 2443 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	-	-	-		
58	SF4	XD	301	-	0,12,12	-	-	-		

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

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

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	RA	2856/2915 (97%)	-0.42	19 (0%) 84 69	56, 90, 263, 484	0
1	YA	2856/2915 (97%)	-0.41	33 (1%) 76 58	42, 78, 256, 460	0
2	RB	120/122 (98%)	-0.28	0 100 100	100, 140, 172, 232	0
2	YB	120/122 (98%)	-0.32	0 100 100	73, 106, 131, 168	0
3	RD	275/276 (99%)	0.08	9 (3%) 49 30	55, 79, 112, 177	0
3	YD	275/276 (99%)	-0.09	3 (1%) 78 61	44, 66, 99, 194	0
4	RE	204/206 (99%)	0.07	5 (2%) 58 39	57, 85, 127, 179	0
4	YE	204/206 (99%)	0.00	2 (0%) 79 63	52, 86, 134, 194	0
5	RF	203/210 (96%)	0.08	1 (0%) 87 76	57, 101, 150, 184	0
5	YF	203/210 (96%)	0.03	1 (0%) 87 76	44, 82, 135, 179	0
6	RG	181/182 (99%)	0.45	7 (3%) 43 27	116, 143, 184, 216	0
6	YG	181/182 (99%)	0.28	5 (2%) 55 35	88, 114, 157, 215	0
7	RH	174/180 (96%)	0.57	10 (5%) 29 19	112, 177, 239, 281	0
7	YH	173/180 (96%)	0.33	5 (2%) 53 35	78, 99, 142, 222	0
8	RI	147/148 (99%)	0.81	16 (10%) 10 7	85, 136, 179, 213	0
8	YI	146/148 (98%)	0.37	4 (2%) 56 36	79, 121, 157, 177	0
9	RN	140/140 (100%)	0.17	2 (1%) 73 54	63, 99, 138, 189	0
9	YN	140/140 (100%)	0.09	1 (0%) 84 69	52, 88, 127, 165	0
10	RO	122/122 (100%)	0.03	3 (2%) 58 39	65, 83, 117, 168	0
10	YO	122/122 (100%)	-0.07	1 (0%) 82 67	58, 77, 108, 132	0
11	RP	149/150 (99%)	0.33	2 (1%) 75 55	63, 106, 149, 166	0
11	YP	149/150 (99%)	0.14	5 (3%) 48 30	52, 83, 122, 168	0
12	RQ	141/141 (100%)	0.12	4 (2%) 55 35	72, 103, 132, 152	0
12	YQ	141/141 (100%)	0.06	2 (1%) 73 54	62, 80, 107, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	RR	118/118 (100%)	0.12	0 100 100	60, 82, 102, 123	0
13	YR	118/118 (100%)	0.25	3 (2%) 58 39	56, 85, 115, 164	0
14	RS	110/112 (98%)	0.37	1 (0%) 81 64	102, 131, 166, 186	0
14	YS	110/112 (98%)	0.26	4 (3%) 46 28	88, 103, 137, 159	0
15	RT	131/146 (89%)	-0.01	3 (2%) 61 41	69, 92, 136, 203	0
15	YT	131/146 (89%)	0.05	0 100 100	65, 90, 135, 183	0
16	RU	116/118 (98%)	0.20	1 (0%) 81 64	60, 93, 130, 161	0
16	YU	116/118 (98%)	0.02	0 100 100	50, 82, 120, 174	0
17	RV	101/101 (100%)	-0.09	1 (0%) 79 63	62, 110, 148, 167	0
17	YV	101/101 (100%)	-0.03	0 100 100	48, 95, 136, 159	0
18	RW	112/113 (99%)	0.02	1 (0%) 81 64	59, 76, 118, 179	0
18	YW	112/113 (99%)	0.05	2 (1%) 67 48	51, 75, 114, 185	0
19	RX	95/96 (98%)	0.48	6 (6%) 26 17	78, 94, 127, 166	0
19	YX	95/96 (98%)	0.17	1 (1%) 78 61	60, 76, 112, 153	0
20	RY	107/110 (97%)	1.03	15 (14%) 6 5	89, 121, 173, 208	0
20	YY	107/110 (97%)	0.54	5 (4%) 36 23	73, 98, 163, 216	0
21	RZ	189/206 (91%)	0.17	1 (0%) 87 76	112, 140, 175, 196	0
21	YZ	189/206 (91%)	0.12	1 (0%) 87 76	88, 114, 158, 207	0
22	R0	77/85 (90%)	0.42	6 (7%) 19 12	83, 99, 134, 145	0
22	Y0	77/85 (90%)	-0.02	1 (1%) 75 55	64, 81, 123, 168	0
23	R1	97/98 (98%)	0.37	3 (3%) 51 32	61, 90, 128, 157	0
23	Y1	97/98 (98%)	-0.00	1 (1%) 79 63	51, 81, 125, 143	0
24	R2	70/72 (97%)	0.39	2 (2%) 53 35	86, 113, 148, 159	0
24	Y2	70/72 (97%)	0.49	3 (4%) 40 24	62, 85, 111, 181	0
25	R3	59/60 (98%)	0.31	1 (1%) 69 49	74, 100, 146, 208	0
25	Y3	59/60 (98%)	0.04	1 (1%) 69 49	65, 84, 137, 169	0
26	R4	69/71 (97%)	0.30	1 (1%) 73 54	134, 179, 227, 256	0
26	Y4	69/71 (97%)	0.32	4 (5%) 29 18	105, 155, 216, 228	0
27	R5	59/60 (98%)	-0.03	0 100 100	64, 88, 163, 204	0
27	Y5	59/60 (98%)	0.22	2 (3%) 48 30	51, 90, 192, 206	0
28	R6	53/54 (98%)	1.24	14 (26%) 1 1	255, 286, 320, 355	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	Y6	53/54 (98%)	1.51	16 (30%) 1 1	193, 240, 268, 295	0
29	R7	48/49 (97%)	0.31	4 (8%) 17 11	60, 70, 122, 166	0
29	Y7	48/49 (97%)	0.13	2 (4%) 40 25	50, 59, 116, 148	0
30	R8	64/65 (98%)	0.42	4 (6%) 26 17	70, 84, 115, 179	0
30	Y8	64/65 (98%)	0.29	5 (7%) 19 12	52, 71, 100, 170	0
31	R9	37/37 (100%)	3.18	25 (67%) 0 0	186, 218, 264, 281	0
31	Y9	37/37 (100%)	4.25	35 (94%) 0 0	162, 200, 247, 255	0
32	QA	1488/1521 (97%)	-0.09	21 (1%) 73 54	76, 131, 234, 406	0
32	XA	1492/1521 (98%)	-0.25	9 (0%) 85 73	57, 119, 220, 371	0
33	QB	231/256 (90%)	0.40	8 (3%) 47 29	126, 171, 212, 247	0
33	XB	231/256 (90%)	0.27	3 (1%) 75 55	102, 144, 191, 222	0
34	QC	206/239 (86%)	0.31	10 (4%) 35 22	137, 170, 218, 240	0
34	XC	206/239 (86%)	0.24	6 (2%) 53 35	109, 132, 172, 211	0
35	QD	208/209 (99%)	0.44	12 (5%) 29 18	107, 139, 175, 199	0
35	XD	208/209 (99%)	0.50	14 (6%) 24 15	98, 132, 170, 207	0
36	QE	148/162 (91%)	0.12	3 (2%) 65 45	101, 133, 163, 202	0
36	XE	148/162 (91%)	0.08	4 (2%) 56 36	95, 114, 153, 178	0
37	QF	100/101 (99%)	0.07	2 (2%) 65 45	111, 138, 175, 198	0
37	XF	100/101 (99%)	-0.09	0 100 100	84, 117, 154, 185	0
38	QG	155/156 (99%)	0.35	4 (2%) 57 37	127, 155, 192, 221	0
38	XG	155/156 (99%)	0.22	4 (2%) 57 37	112, 132, 173, 185	0
39	QH	137/138 (99%)	0.40	5 (3%) 46 28	102, 137, 168, 179	0
39	XH	137/138 (99%)	0.32	3 (2%) 62 42	88, 122, 152, 182	0
40	QI	127/128 (99%)	0.92	13 (10%) 12 8	124, 178, 212, 240	0
40	XI	126/128 (98%)	0.70	14 (11%) 10 7	95, 143, 179, 222	0
41	QJ	97/105 (92%)	0.81	9 (9%) 14 9	153, 181, 213, 225	0
41	XJ	96/105 (91%)	0.81	9 (9%) 14 9	112, 151, 189, 215	0
42	QK	114/129 (88%)	0.21	3 (2%) 57 37	104, 132, 159, 196	0
42	XK	114/129 (88%)	0.23	9 (7%) 18 12	85, 108, 140, 184	0
43	QL	121/132 (91%)	0.65	9 (7%) 20 13	91, 105, 132, 160	0
43	XL	121/132 (91%)	0.41	10 (8%) 17 11	81, 97, 129, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	QM	116/126 (92%)	0.67	13 (11%) 10 7	127, 161, 186, 212	0
44	XM	114/126 (90%)	0.55	9 (7%) 18 12	110, 143, 181, 203	0
45	QN	60/61 (98%)	0.87	8 (13%) 7 6	147, 168, 196, 220	0
45	XN	60/61 (98%)	0.86	4 (6%) 24 15	106, 125, 158, 173	0
46	QO	88/89 (98%)	0.31	1 (1%) 78 61	100, 120, 155, 182	0
46	XO	88/89 (98%)	0.32	4 (4%) 38 24	83, 113, 145, 169	0
47	QP	82/88 (93%)	0.52	4 (4%) 35 22	89, 118, 143, 174	0
47	XP	82/88 (93%)	0.57	3 (3%) 45 28	111, 135, 161, 189	0
48	QQ	99/105 (94%)	0.45	4 (4%) 42 26	84, 118, 159, 178	0
48	XQ	99/105 (94%)	0.34	4 (4%) 42 26	86, 114, 139, 175	0
49	QR	68/88 (77%)	0.34	1 (1%) 72 52	115, 142, 173, 212	0
49	XR	68/88 (77%)	0.07	2 (2%) 53 35	85, 114, 152, 157	0
50	QS	83/93 (89%)	0.54	6 (7%) 21 14	134, 172, 208, 233	0
50	XS	83/93 (89%)	0.78	6 (7%) 21 14	123, 152, 192, 267	0
51	QT	96/106 (90%)	0.97	12 (12%) 8 6	90, 114, 144, 179	0
51	XT	98/106 (92%)	1.01	18 (18%) 3 3	96, 129, 161, 188	0
52	QU	23/27 (85%)	1.52	7 (30%) 1 1	136, 154, 175, 184	0
52	XU	23/27 (85%)	1.70	7 (30%) 1 1	119, 136, 158, 174	0
53	QV	77/77 (100%)	-0.41	1 (1%) 75 55	100, 138, 189, 241	0
53	XV	77/77 (100%)	-0.43	1 (1%) 75 55	74, 121, 178, 229	0
54	QX	10/25 (40%)	1.46	3 (30%) 1 1	118, 149, 217, 231	0
54	XX	9/25 (36%)	1.36	3 (33%) 1 1	96, 111, 178, 193	0
55	QY	257/360 (71%)	0.66	29 (11%) 10 7	124, 163, 221, 279	0
55	XY	258/360 (71%)	0.56	28 (10%) 10 7	107, 136, 193, 241	0
All	All	21230/22168 (95%)	0.05	677 (3%) 50 31	42, 110, 202, 484	0

The worst 5 of 677 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
51	QT	9	ASN	9.4
31	Y9	26	ILE	8.9
31	Y9	37	GLY	8.8
55	XY	194	GLY	8.1
31	Y9	31	LYS	7.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	RA	1915	21/22	0.72	0.14	118,129,139,151	0
32	PSU	QA	516	20/21	0.83	0.09	121,124,134,144	0
32	2MG	QA	1207	24/25	0.85	0.10	153,161,175,176	0
1	PSU	RA	1917	20/21	0.89	0.09	78,100,113,119	0
32	PSU	XA	516	20/21	0.89	0.10	105,115,124,130	0
32	2MG	XA	1207	24/25	0.89	0.12	119,129,138,139	0
32	4OC	XA	1402	22/23	0.89	0.13	73,88,101,112	0
32	M2G	QA	966	25/26	0.91	0.14	119,125,137,151	0
32	7MG	QA	527	24/25	0.91	0.13	89,108,119,125	0
1	5MU	YA	1915	21/22	0.91	0.09	86,100,112,116	0
32	5MC	XA	967	21/22	0.92	0.12	91,107,118,120	0
1	PSU	RA	1911	20/21	0.92	0.09	96,104,111,112	0
1	4OC	RA	1920	21/23	0.92	0.13	96,107,119,126	0
32	5MC	QA	1400	21/22	0.93	0.14	103,118,125,129	0
1	PSU	YA	1917	20/21	0.93	0.09	59,70,94,115	0
32	5MC	XA	1404	21/22	0.93	0.13	60,72,81,98	0
32	UR3	XA	1498	21/22	0.93	0.13	57,79,99,112	0
32	7MG	XA	527	24/25	0.94	0.11	76,93,103,112	0
1	PSU	YA	1911	20/21	0.94	0.09	73,86,94,95	0
32	5MC	QA	967	21/22	0.94	0.11	114,122,132,133	0
43	0TD	QL	92	10/11	0.94	0.11	88,108,111,111	0
1	4OC	YA	1920	21/23	0.94	0.10	71,85,97,100	0
55	MEQ	QY	235	10/11	0.94	0.20	127,132,140,142	0
1	5MU	RA	1939	21/22	0.95	0.11	57,71,84,95	0
32	4OC	QA	1402	22/23	0.95	0.10	93,102,112,115	0
32	5MC	QA	1404	21/22	0.95	0.12	88,98,109,125	0
32	UR3	QA	1498	21/22	0.95	0.12	85,94,108,113	0
32	5MC	XA	1407	21/22	0.95	0.12	67,72,85,91	0
32	M2G	XA	966	25/26	0.95	0.10	93,101,131,140	0
43	0TD	XL	92	10/11	0.95	0.10	84,100,105,108	0
1	2MA	YA	2503	23/24	0.96	0.10	39,58,67,79	0
32	5MC	XA	1400	21/22	0.96	0.10	65,81,92,101	0
1	2MU	YA	2552	21/23	0.96	0.09	43,57,72,82	0
1	2MA	RA	2503	23/24	0.96	0.09	47,56,73,77	0
32	MA6	QA	1518	24/25	0.96	0.10	77,101,114,118	0
1	5MC	RA	1942	21/22	0.96	0.09	68,81,101,115	0
1	OMG	RA	2251	24/25	0.96	0.09	64,73,83,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MEQ	XY	235	10/11	0.96	0.20	113,113,129,136	0
32	5MC	QA	1407	21/22	0.97	0.07	68,80,94,102	0
1	PSU	RA	2605	20/21	0.97	0.08	47,62,74,78	0
1	5MC	RA	1962	21/22	0.97	0.07	61,72,82,98	0
32	MA6	QA	1519	24/25	0.97	0.11	90,100,106,107	0
1	2MU	RA	2552	21/23	0.97	0.08	56,69,83,86	0
32	MA6	XA	1518	24/25	0.97	0.09	58,73,92,95	0
32	MA6	XA	1519	24/25	0.97	0.10	62,72,79,85	0
1	5MU	YA	1939	21/22	0.97	0.08	43,56,71,85	0
1	5MC	YA	1942	21/22	0.97	0.07	54,65,71,83	0
1	PSU	YA	2605	20/21	0.98	0.07	36,50,56,58	0
1	5MC	YA	1962	21/22	0.98	0.06	48,56,69,81	0
1	OMG	YA	2251	24/25	0.98	0.07	45,50,64,78	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QD	304	1/1	-0.44	0.29	132,132,132,132	0
56	MG	QA	1792	1/1	-0.43	0.27	144,144,144,144	0
56	MG	YA	3476	1/1	-0.36	0.63	117,117,117,117	0
56	MG	RG	201	1/1	-0.27	0.14	175,175,175,175	0
56	MG	QN	103	1/1	-0.19	0.35	128,128,128,128	0
56	MG	RA	3260	1/1	-0.10	0.28	123,123,123,123	0
56	MG	YA	3333	1/1	-0.06	0.24	120,120,120,120	0
56	MG	R5	104	1/1	-0.06	0.18	137,137,137,137	0
56	MG	QA	1773	1/1	-0.05	0.29	113,113,113,113	0
56	MG	QA	1824	1/1	-0.05	0.23	139,139,139,139	0
56	MG	YA	3358	1/1	-0.01	0.15	118,118,118,118	0
56	MG	QA	1760	1/1	-0.00	0.22	132,132,132,132	0
56	MG	RA	3637	1/1	0.00	0.60	101,101,101,101	0
56	MG	RA	3782	1/1	-0.00	0.38	125,125,125,125	0
56	MG	RA	3468	1/1	0.03	0.22	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	QA	1798	1/1	0.03	0.28	106,106,106,106	0
56	MG	RB	210	1/1	0.03	0.20	123,123,123,123	0
56	MG	RA	3435	1/1	0.03	0.19	136,136,136,136	0
56	MG	QA	1772	1/1	0.05	0.39	109,109,109,109	0
56	MG	QA	1694	1/1	0.07	0.20	123,123,123,123	0
56	MG	RA	3188	1/1	0.07	0.23	129,129,129,129	0
56	MG	QA	1647	1/1	0.09	0.12	159,159,159,159	0
56	MG	YB	210	1/1	0.11	0.26	104,104,104,104	0
56	MG	RA	3193	1/1	0.12	0.28	141,141,141,141	0
56	MG	YA	3368	1/1	0.12	0.23	108,108,108,108	0
56	MG	XA	1704	1/1	0.12	0.27	112,112,112,112	0
56	MG	XA	1667	1/1	0.13	0.20	136,136,136,136	0
56	MG	QA	1747	1/1	0.15	0.28	152,152,152,152	0
56	MG	QA	1800	1/1	0.15	0.22	120,120,120,120	0
56	MG	QA	1758	1/1	0.15	0.19	119,119,119,119	0
56	MG	XA	1623	1/1	0.16	0.26	111,111,111,111	0
56	MG	QA	1748	1/1	0.16	0.39	129,129,129,129	0
56	MG	RA	3767	1/1	0.16	0.46	124,124,124,124	0
56	MG	RA	3486	1/1	0.17	0.24	88,88,88,88	0
56	MG	QA	1797	1/1	0.17	0.13	154,154,154,154	0
56	MG	RA	3626	1/1	0.17	0.25	119,119,119,119	0
56	MG	RG	203	1/1	0.18	0.26	99,99,99,99	0
56	MG	RA	3927	1/1	0.19	0.45	121,121,121,121	0
56	MG	XA	1777	1/1	0.19	0.30	134,134,134,134	0
56	MG	QA	1840	1/1	0.20	0.50	119,119,119,119	0
56	MG	RA	3425	1/1	0.20	0.24	132,132,132,132	0
56	MG	RA	3110	1/1	0.20	0.21	142,142,142,142	0
56	MG	YA	3338	1/1	0.21	0.26	78,78,78,78	0
56	MG	QA	1721	1/1	0.21	0.43	116,116,116,116	0
56	MG	XA	1636	1/1	0.21	0.21	108,108,108,108	0
56	MG	XA	1622	1/1	0.22	0.25	85,85,85,85	0
56	MG	RA	3034	1/1	0.22	0.30	112,112,112,112	0
56	MG	RA	3371	1/1	0.23	0.26	90,90,90,90	0
56	MG	QA	1784	1/1	0.23	0.33	132,132,132,132	0
56	MG	YA	3270	1/1	0.23	0.38	70,70,70,70	0
56	MG	QA	1757	1/1	0.24	0.25	110,110,110,110	0
56	MG	QA	1827	1/1	0.24	0.20	123,123,123,123	0
56	MG	RA	3843	1/1	0.24	0.17	139,139,139,139	0
57	ZN	R6	101	1/1	0.24	0.23	321,321,321,321	0
56	MG	RA	3950	1/1	0.25	0.36	130,130,130,130	0
56	MG	YB	208	1/1	0.25	0.31	97,97,97,97	0
56	MG	YA	3300	1/1	0.26	0.55	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3065	1/1	0.26	0.28	82,82,82,82	0
56	MG	QA	1656	1/1	0.26	0.36	135,135,135,135	0
56	MG	RA	3406	1/1	0.27	0.16	111,111,111,111	0
56	MG	YB	213	1/1	0.27	0.26	101,101,101,101	0
56	MG	YF	301	1/1	0.27	0.40	88,88,88,88	0
56	MG	YA	3508	1/1	0.27	0.21	146,146,146,146	0
56	MG	RA	3545	1/1	0.27	0.23	133,133,133,133	0
56	MG	RA	3908	1/1	0.28	0.39	86,86,86,86	0
56	MG	QA	1644	1/1	0.28	0.30	162,162,162,162	0
56	MG	XA	1769	1/1	0.28	0.50	117,117,117,117	0
56	MG	RA	3565	1/1	0.28	0.35	97,97,97,97	0
56	MG	QA	1736	1/1	0.28	0.37	104,104,104,104	0
56	MG	RA	3968	1/1	0.29	0.12	235,235,235,235	0
56	MG	YA	3486	1/1	0.29	0.30	97,97,97,97	0
56	MG	RA	3314	1/1	0.29	0.29	84,84,84,84	0
56	MG	YA	3612	1/1	0.29	0.30	123,123,123,123	0
56	MG	QA	1770	1/1	0.30	0.24	110,110,110,110	0
56	MG	RA	3244	1/1	0.30	0.27	93,93,93,93	0
56	MG	RA	3676	1/1	0.30	0.31	92,92,92,92	0
56	MG	YA	3454	1/1	0.30	0.53	108,108,108,108	0
56	MG	RA	3292	1/1	0.30	0.20	143,143,143,143	0
57	ZN	R9	101	1/1	0.30	0.36	309,309,309,309	0
56	MG	YA	3490	1/1	0.31	0.37	112,112,112,112	0
56	MG	RA	3743	1/1	0.31	0.37	123,123,123,123	0
56	MG	RB	211	1/1	0.31	0.16	129,129,129,129	0
56	MG	QA	1663	1/1	0.31	0.28	118,118,118,118	0
56	MG	RA	3245	1/1	0.32	0.31	95,95,95,95	0
56	MG	XA	1666	1/1	0.32	0.10	129,129,129,129	0
56	MG	RA	3151	1/1	0.33	0.23	114,114,114,114	0
56	MG	QA	1693	1/1	0.33	0.24	119,119,119,119	0
56	MG	RA	3713	1/1	0.33	0.17	96,96,96,96	0
56	MG	QA	1852	1/1	0.33	0.19	124,124,124,124	0
56	MG	RA	3929	1/1	0.34	0.18	137,137,137,137	0
56	MG	YA	3350	1/1	0.34	0.20	98,98,98,98	0
56	MG	YA	3312	1/1	0.34	0.22	88,88,88,88	0
56	MG	RA	3957	1/1	0.34	0.17	108,108,108,108	0
56	MG	YA	3424	1/1	0.34	0.33	101,101,101,101	0
56	MG	YA	3055	1/1	0.35	0.25	107,107,107,107	0
56	MG	QA	1681	1/1	0.35	0.15	155,155,155,155	0
56	MG	QA	1689	1/1	0.35	0.25	117,117,117,117	0
56	MG	RA	3357	1/1	0.35	0.20	113,113,113,113	0
56	MG	QA	1605	1/1	0.35	0.32	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3364	1/1	0.35	0.44	105,105,105,105	0
56	MG	RA	3825	1/1	0.36	0.25	127,127,127,127	0
56	MG	QA	1848	1/1	0.36	0.35	122,122,122,122	0
56	MG	RA	3937	1/1	0.36	0.11	149,149,149,149	0
56	MG	XA	1743	1/1	0.36	0.40	113,113,113,113	0
56	MG	YA	3075	1/1	0.36	0.33	93,93,93,93	0
56	MG	YA	3452	1/1	0.36	0.46	119,119,119,119	0
56	MG	YA	3257	1/1	0.36	0.46	130,130,130,130	0
56	MG	XA	1656	1/1	0.36	0.16	118,118,118,118	0
56	MG	RA	3609	1/1	0.37	0.28	118,118,118,118	0
56	MG	RA	3446	1/1	0.37	0.37	67,67,67,67	0
56	MG	QA	1710	1/1	0.37	0.20	115,115,115,115	0
56	MG	RA	3840	1/1	0.37	0.33	105,105,105,105	0
56	MG	RA	3841	1/1	0.37	0.26	101,101,101,101	0
56	MG	YA	3062	1/1	0.37	0.22	103,103,103,103	0
56	MG	RA	3459	1/1	0.37	0.20	73,73,73,73	0
56	MG	RA	3649	1/1	0.37	0.40	103,103,103,103	0
56	MG	YA	3455	1/1	0.38	0.41	74,74,74,74	0
56	MG	RA	3268	1/1	0.38	0.18	132,132,132,132	0
56	MG	RA	3673	1/1	0.38	0.20	114,114,114,114	0
56	MG	YA	3646	1/1	0.38	0.38	110,110,110,110	0
56	MG	QA	1752	1/1	0.39	0.39	106,106,106,106	0
56	MG	YA	3091	1/1	0.39	0.16	102,102,102,102	0
56	MG	YA	3226	1/1	0.39	0.31	111,111,111,111	0
56	MG	YA	3616	1/1	0.39	0.24	83,83,83,83	0
56	MG	RA	3749	1/1	0.39	0.15	102,102,102,102	0
56	MG	RA	3007	1/1	0.39	0.12	128,128,128,128	0
56	MG	RA	3711	1/1	0.39	0.20	90,90,90,90	0
56	MG	RA	3277	1/1	0.39	0.26	97,97,97,97	0
56	MG	YB	217	1/1	0.39	0.19	107,107,107,107	0
56	MG	RB	203	1/1	0.39	0.23	121,121,121,121	0
56	MG	RA	3630	1/1	0.39	0.37	106,106,106,106	0
56	MG	RA	3672	1/1	0.40	0.26	119,119,119,119	0
56	MG	QE	202	1/1	0.40	0.16	103,103,103,103	0
56	MG	RB	219	1/1	0.40	0.25	108,108,108,108	0
56	MG	RA	3808	1/1	0.40	0.27	121,121,121,121	0
56	MG	RA	3665	1/1	0.40	0.20	110,110,110,110	0
56	MG	QA	1802	1/1	0.41	0.35	109,109,109,109	0
56	MG	QA	1755	1/1	0.41	0.23	123,123,123,123	0
56	MG	QD	303	1/1	0.41	0.21	136,136,136,136	0
56	MG	QA	1825	1/1	0.41	0.30	125,125,125,125	0
56	MG	RF	302	1/1	0.41	0.21	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1832	1/1	0.41	0.40	98,98,98,98	0
56	MG	YA	3514	1/1	0.41	0.33	78,78,78,78	0
56	MG	QA	1732	1/1	0.41	0.37	95,95,95,95	0
56	MG	YA	3302	1/1	0.41	0.51	87,87,87,87	0
56	MG	YA	3621	1/1	0.42	0.59	138,138,138,138	0
56	MG	YE	301	1/1	0.42	0.63	122,122,122,122	0
56	MG	RA	3917	1/1	0.42	0.26	108,108,108,108	0
56	MG	XA	1707	1/1	0.42	0.23	108,108,108,108	0
56	MG	YA	3711	1/1	0.42	0.49	119,119,119,119	0
56	MG	RA	3581	1/1	0.42	0.18	108,108,108,108	0
56	MG	XA	1633	1/1	0.42	0.19	94,94,94,94	0
56	MG	QA	1809	1/1	0.42	0.26	90,90,90,90	0
56	MG	YA	3507	1/1	0.42	0.20	97,97,97,97	0
56	MG	RA	3348	1/1	0.43	0.28	124,124,124,124	0
56	MG	YA	3160	1/1	0.43	0.34	104,104,104,104	0
56	MG	RA	3487	1/1	0.43	0.30	98,98,98,98	0
56	MG	QA	1642	1/1	0.43	0.27	148,148,148,148	0
56	MG	QM	201	1/1	0.43	0.28	133,133,133,133	0
56	MG	YA	3299	1/1	0.43	0.30	54,54,54,54	0
56	MG	XA	1684	1/1	0.43	0.53	109,109,109,109	0
56	MG	YA	3054	1/1	0.44	0.31	95,95,95,95	0
56	MG	QA	1695	1/1	0.44	0.25	96,96,96,96	0
56	MG	YA	3725	1/1	0.44	0.20	79,79,79,79	0
56	MG	RA	3116	1/1	0.44	0.29	103,103,103,103	0
56	MG	QA	1716	1/1	0.44	0.42	101,101,101,101	0
56	MG	QA	1612	1/1	0.44	0.19	118,118,118,118	0
56	MG	XA	1779	1/1	0.44	0.47	102,102,102,102	0
56	MG	YA	3477	1/1	0.44	0.31	82,82,82,82	0
56	MG	QA	1683	1/1	0.44	0.25	122,122,122,122	0
56	MG	RA	3440	1/1	0.45	0.73	117,117,117,117	0
56	MG	QA	1614	1/1	0.45	0.25	87,87,87,87	0
56	MG	QA	1621	1/1	0.45	0.17	160,160,160,160	0
56	MG	QG	202	1/1	0.45	0.06	122,122,122,122	0
56	MG	YA	3234	1/1	0.45	0.53	96,96,96,96	0
56	MG	RA	3546	1/1	0.45	0.37	120,120,120,120	0
56	MG	RA	3812	1/1	0.45	0.23	104,104,104,104	0
56	MG	RA	3289	1/1	0.45	0.14	99,99,99,99	0
56	MG	XA	1775	1/1	0.45	0.41	124,124,124,124	0
56	MG	QA	1608	1/1	0.45	0.17	90,90,90,90	0
56	MG	QA	1805	1/1	0.45	0.25	107,107,107,107	0
56	MG	YA	3457	1/1	0.45	0.25	79,79,79,79	0
56	MG	YA	3695	1/1	0.45	0.29	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3518	1/1	0.46	0.22	84,84,84,84	0
56	MG	QA	1777	1/1	0.46	0.21	112,112,112,112	0
56	MG	QA	1712	1/1	0.46	0.23	117,117,117,117	0
56	MG	RA	3647	1/1	0.46	0.35	113,113,113,113	0
56	MG	RA	3515	1/1	0.46	0.20	62,62,62,62	0
56	MG	RA	3822	1/1	0.46	0.34	107,107,107,107	0
56	MG	YA	3522	1/1	0.46	0.23	71,71,71,71	0
56	MG	XA	1686	1/1	0.46	0.21	102,102,102,102	0
56	MG	XA	1703	1/1	0.46	0.17	110,110,110,110	0
56	MG	QA	1836	1/1	0.47	0.29	116,116,116,116	0
56	MG	RE	304	1/1	0.47	0.52	109,109,109,109	0
56	MG	YA	3292	1/1	0.47	0.22	148,148,148,148	0
56	MG	XA	1695	1/1	0.47	0.20	76,76,76,76	0
56	MG	YA	3433	1/1	0.47	0.47	118,118,118,118	0
56	MG	YA	3435	1/1	0.47	0.25	106,106,106,106	0
56	MG	RA	3965	1/1	0.47	0.20	124,124,124,124	0
56	MG	XA	1615	1/1	0.47	0.15	99,99,99,99	0
56	MG	QA	1775	1/1	0.47	0.51	131,131,131,131	0
56	MG	RA	3172	1/1	0.47	0.44	125,125,125,125	0
56	MG	RA	3030	1/1	0.47	0.40	108,108,108,108	0
56	MG	RA	3898	1/1	0.47	0.23	74,74,74,74	0
56	MG	RA	3557	1/1	0.47	0.37	117,117,117,117	0
56	MG	RA	3619	1/1	0.47	0.36	103,103,103,103	0
56	MG	YA	3192	1/1	0.48	0.20	103,103,103,103	0
56	MG	YA	3199	1/1	0.48	0.31	115,115,115,115	0
56	MG	XA	1689	1/1	0.48	0.26	102,102,102,102	0
56	MG	XA	1691	1/1	0.48	0.30	84,84,84,84	0
56	MG	YA	3330	1/1	0.48	0.31	110,110,110,110	0
56	MG	QA	1817	1/1	0.48	0.15	100,100,100,100	0
56	MG	RA	3250	1/1	0.48	0.39	118,118,118,118	0
56	MG	RA	3764	1/1	0.48	0.79	127,127,127,127	0
56	MG	RA	3616	1/1	0.48	0.33	109,109,109,109	0
56	MG	YA	3698	1/1	0.48	0.47	76,76,76,76	0
56	MG	RA	3061	1/1	0.48	0.16	116,116,116,116	0
56	MG	YA	3391	1/1	0.48	0.23	91,91,91,91	0
56	MG	XA	1663	1/1	0.48	0.13	117,117,117,117	0
56	MG	RA	3147	1/1	0.48	0.13	121,121,121,121	0
56	MG	RA	3444	1/1	0.48	0.27	92,92,92,92	0
56	MG	QV	104	1/1	0.49	0.13	109,109,109,109	0
56	MG	RA	3793	1/1	0.49	0.24	97,97,97,97	0
56	MG	QA	1841	1/1	0.49	0.34	124,124,124,124	0
56	MG	RA	3360	1/1	0.49	0.17	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3325	1/1	0.49	0.33	111,111,111,111	0
56	MG	QA	1768	1/1	0.49	0.14	114,114,114,114	0
56	MG	YA	3089	1/1	0.49	0.14	118,118,118,118	0
56	MG	QA	1820	1/1	0.49	0.41	118,118,118,118	0
56	MG	QA	1793	1/1	0.49	0.17	117,117,117,117	0
56	MG	RA	3750	1/1	0.49	0.22	85,85,85,85	0
56	MG	RA	3631	1/1	0.49	0.35	86,86,86,86	0
56	MG	QI	201	1/1	0.49	0.32	151,151,151,151	0
56	MG	XA	1624	1/1	0.49	0.14	122,122,122,122	0
56	MG	RA	3556	1/1	0.49	0.25	76,76,76,76	0
56	MG	RA	3424	1/1	0.49	0.27	115,115,115,115	0
56	MG	QV	101	1/1	0.49	0.13	124,124,124,124	0
56	MG	QV	103	1/1	0.49	0.25	119,119,119,119	0
56	MG	YA	3097	1/1	0.50	0.14	115,115,115,115	0
56	MG	QA	1822	1/1	0.50	0.18	96,96,96,96	0
56	MG	YA	3172	1/1	0.50	0.19	92,92,92,92	0
56	MG	YA	3185	1/1	0.50	0.12	135,135,135,135	0
56	MG	RA	3395	1/1	0.50	0.16	106,106,106,106	0
56	MG	XA	1713	1/1	0.50	0.39	96,96,96,96	0
56	MG	QR	101	1/1	0.50	0.14	116,116,116,116	0
56	MG	YA	3067	1/1	0.50	0.18	94,94,94,94	0
56	MG	RA	3222	1/1	0.50	0.38	116,116,116,116	0
56	MG	YA	3581	1/1	0.50	0.22	104,104,104,104	0
56	MG	RA	3627	1/1	0.50	0.13	124,124,124,124	0
56	MG	QA	1739	1/1	0.50	0.27	71,71,71,71	0
56	MG	YA	3462	1/1	0.50	0.27	78,78,78,78	0
56	MG	QA	1673	1/1	0.51	0.25	123,123,123,123	0
56	MG	YA	3159	1/1	0.51	0.21	86,86,86,86	0
56	MG	QA	1602	1/1	0.51	0.26	105,105,105,105	0
56	MG	QA	1718	1/1	0.51	0.37	120,120,120,120	0
56	MG	RA	3852	1/1	0.51	0.29	100,100,100,100	0
56	MG	QA	1643	1/1	0.51	0.28	126,126,126,126	0
56	MG	RA	3309	1/1	0.51	0.35	88,88,88,88	0
56	MG	XA	1621	1/1	0.51	0.34	90,90,90,90	0
56	MG	QA	1737	1/1	0.51	0.18	126,126,126,126	0
56	MG	YA	3644	1/1	0.51	0.26	73,73,73,73	0
56	MG	QA	1609	1/1	0.51	0.24	84,84,84,84	0
56	MG	XA	1718	1/1	0.51	0.25	95,95,95,95	0
56	MG	RA	3101	1/1	0.51	0.62	122,122,122,122	0
56	MG	RA	3146	1/1	0.51	0.20	82,82,82,82	0
56	MG	XA	1638	1/1	0.51	0.19	115,115,115,115	0
56	MG	XA	1652	1/1	0.51	0.24	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3362	1/1	0.51	0.30	78,78,78,78	0
56	MG	XA	1661	1/1	0.51	0.15	88,88,88,88	0
56	MG	YA	3283	1/1	0.51	0.30	99,99,99,99	0
56	MG	RA	3247	1/1	0.52	0.82	108,108,108,108	0
56	MG	RA	3129	1/1	0.52	0.15	100,100,100,100	0
56	MG	QA	1756	1/1	0.52	0.28	102,102,102,102	0
56	MG	RA	3113	1/1	0.52	0.45	96,96,96,96	0
56	MG	RB	209	1/1	0.52	0.15	141,141,141,141	0
56	MG	RA	3794	1/1	0.52	0.24	90,90,90,90	0
56	MG	QA	1670	1/1	0.52	0.45	93,93,93,93	0
56	MG	RA	3636	1/1	0.53	0.41	109,109,109,109	0
56	MG	QA	1708	1/1	0.53	0.31	112,112,112,112	0
56	MG	RA	3527	1/1	0.53	0.14	97,97,97,97	0
56	MG	RA	3334	1/1	0.53	0.26	77,77,77,77	0
56	MG	RA	3215	1/1	0.53	0.16	104,104,104,104	0
56	MG	RA	3300	1/1	0.53	0.17	136,136,136,136	0
56	MG	YA	3626	1/1	0.53	0.38	80,80,80,80	0
56	MG	YA	3641	1/1	0.53	0.35	80,80,80,80	0
56	MG	R0	102	1/1	0.53	0.21	99,99,99,99	0
56	MG	YA	3214	1/1	0.53	0.34	105,105,105,105	0
56	MG	YA	3658	1/1	0.53	0.20	78,78,78,78	0
56	MG	RA	3514	1/1	0.53	0.24	92,92,92,92	0
56	MG	XA	1650	1/1	0.53	0.17	99,99,99,99	0
56	MG	QA	1794	1/1	0.53	0.29	117,117,117,117	0
56	MG	YA	3250	1/1	0.53	0.42	100,100,100,100	0
56	MG	RA	3038	1/1	0.53	0.26	99,99,99,99	0
56	MG	RA	3290	1/1	0.53	0.37	89,89,89,89	0
56	MG	QN	102	1/1	0.53	0.18	129,129,129,129	0
56	MG	QA	1638	1/1	0.54	0.27	87,87,87,87	0
56	MG	RA	3035	1/1	0.54	0.14	84,84,84,84	0
56	MG	YA	3541	1/1	0.54	0.32	88,88,88,88	0
56	MG	QA	1743	1/1	0.54	0.32	113,113,113,113	0
56	MG	RB	222	1/1	0.54	0.28	120,120,120,120	0
56	MG	XA	1611	1/1	0.54	0.25	89,89,89,89	0
56	MG	RA	4038	1/1	0.54	0.23	141,141,141,141	0
56	MG	RA	3579	1/1	0.54	0.56	106,106,106,106	0
56	MG	RF	309	1/1	0.54	0.36	98,98,98,98	0
56	MG	QA	1660	1/1	0.54	0.43	118,118,118,118	0
56	MG	YA	3181	1/1	0.54	0.26	74,74,74,74	0
56	MG	RA	3696	1/1	0.54	0.46	93,93,93,93	0
56	MG	RA	3008	1/1	0.54	0.23	94,94,94,94	0
56	MG	RA	3564	1/1	0.54	0.32	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1626	1/1	0.54	0.29	97,97,97,97	0
56	MG	QA	1636	1/1	0.54	0.14	88,88,88,88	0
56	MG	YA	3712	1/1	0.54	0.23	78,78,78,78	0
57	ZN	RY	202	1/1	0.54	0.18	317,317,317,317	0
56	MG	YA	3227	1/1	0.54	0.26	101,101,101,101	0
56	MG	QA	1806	1/1	0.54	0.13	101,101,101,101	0
56	MG	QA	1646	1/1	0.55	0.26	90,90,90,90	0
56	MG	RA	3836	1/1	0.55	0.26	127,127,127,127	0
56	MG	YA	3210	1/1	0.55	0.29	107,107,107,107	0
56	MG	YO	201	1/1	0.55	0.35	126,126,126,126	0
56	MG	RA	3269	1/1	0.55	0.16	135,135,135,135	0
56	MG	RA	3027	1/1	0.55	0.22	116,116,116,116	0
56	MG	RA	3604	1/1	0.55	0.40	95,95,95,95	0
56	MG	QA	1640	1/1	0.55	0.25	112,112,112,112	0
56	MG	YA	3645	1/1	0.55	0.30	83,83,83,83	0
56	MG	RA	3530	1/1	0.55	0.29	74,74,74,74	0
56	MG	XA	1715	1/1	0.55	0.14	121,121,121,121	0
56	MG	QA	1675	1/1	0.55	0.25	115,115,115,115	0
56	MG	YA	3268	1/1	0.55	0.15	96,96,96,96	0
56	MG	XA	1764	1/1	0.55	0.42	79,79,79,79	0
56	MG	YA	3489	1/1	0.55	0.14	66,66,66,66	0
56	MG	QA	1676	1/1	0.55	0.17	92,92,92,92	0
56	MG	RA	3770	1/1	0.55	0.17	122,122,122,122	0
56	MG	RA	3644	1/1	0.55	0.33	101,101,101,101	0
56	MG	YA	3406	1/1	0.55	0.37	74,74,74,74	0
56	MG	YA	3419	1/1	0.55	0.47	107,107,107,107	0
56	MG	YA	3298	1/1	0.55	0.27	98,98,98,98	0
57	ZN	YY	201	1/1	0.55	0.22	329,329,329,329	0
56	MG	RA	3534	1/1	0.56	0.19	76,76,76,76	0
56	MG	YA	3637	1/1	0.56	0.28	78,78,78,78	0
56	MG	RA	3235	1/1	0.56	0.66	106,106,106,106	0
56	MG	YA	3149	1/1	0.56	0.10	124,124,124,124	0
56	MG	QA	1604	1/1	0.56	0.14	175,175,175,175	0
56	MG	RA	3520	1/1	0.56	0.31	102,102,102,102	0
56	MG	YA	3535	1/1	0.56	0.30	86,86,86,86	0
56	MG	XA	1744	1/1	0.56	0.28	80,80,80,80	0
56	MG	XA	1746	1/1	0.56	0.60	113,113,113,113	0
56	MG	YQ	202	1/1	0.56	0.21	76,76,76,76	0
56	MG	XA	1606	1/1	0.56	0.20	116,116,116,116	0
56	MG	YA	3692	1/1	0.56	0.25	103,103,103,103	0
56	MG	XA	1682	1/1	0.56	0.14	81,81,81,81	0
56	MG	QA	1849	1/1	0.56	0.29	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3477	1/1	0.56	0.14	100,100,100,100	0
56	MG	YA	3182	1/1	0.56	0.31	74,74,74,74	0
56	MG	RA	3206	1/1	0.56	0.32	101,101,101,101	0
56	MG	QA	1796	1/1	0.56	0.14	100,100,100,100	0
56	MG	QA	1672	1/1	0.57	0.17	92,92,92,92	0
56	MG	RA	3550	1/1	0.57	0.20	64,64,64,64	0
56	MG	RA	3417	1/1	0.57	0.48	108,108,108,108	0
56	MG	YA	3682	1/1	0.57	0.42	60,60,60,60	0
56	MG	YA	3201	1/1	0.57	0.38	92,92,92,92	0
56	MG	YA	3095	1/1	0.57	0.16	84,84,84,84	0
56	MG	QA	1707	1/1	0.57	0.16	122,122,122,122	0
56	MG	YA	3220	1/1	0.57	0.18	83,83,83,83	0
56	MG	XA	1717	1/1	0.57	0.23	80,80,80,80	0
56	MG	YA	3099	1/1	0.57	0.22	85,85,85,85	0
56	MG	XA	1720	1/1	0.57	0.15	89,89,89,89	0
56	MG	YA	3714	1/1	0.57	0.28	83,83,83,83	0
56	MG	YA	3544	1/1	0.57	0.24	53,53,53,53	0
56	MG	RA	3730	1/1	0.57	0.20	100,100,100,100	0
56	MG	RA	3539	1/1	0.57	0.42	110,110,110,110	0
56	MG	XA	1659	1/1	0.57	0.25	110,110,110,110	0
56	MG	RA	3310	1/1	0.57	0.26	65,65,65,65	0
56	MG	RA	3408	1/1	0.57	0.19	82,82,82,82	0
56	MG	YA	3357	1/1	0.57	0.41	123,123,123,123	0
56	MG	YE	303	1/1	0.57	0.52	109,109,109,109	0
56	MG	QA	1807	1/1	0.57	0.17	122,122,122,122	0
56	MG	YA	3484	1/1	0.57	0.26	78,78,78,78	0
56	MG	QA	1808	1/1	0.57	0.33	113,113,113,113	0
56	MG	RA	3393	1/1	0.58	0.43	97,97,97,97	0
56	MG	RA	3441	1/1	0.58	0.39	92,92,92,92	0
56	MG	QA	1613	1/1	0.58	0.29	103,103,103,103	0
56	MG	YA	3412	1/1	0.58	0.19	86,86,86,86	0
56	MG	RA	3203	1/1	0.58	0.27	104,104,104,104	0
56	MG	RA	3163	1/1	0.58	0.27	98,98,98,98	0
56	MG	RA	3857	1/1	0.58	0.23	82,82,82,82	0
56	MG	YA	3678	1/1	0.58	0.17	96,96,96,96	0
56	MG	YA	3034	1/1	0.58	0.25	93,93,93,93	0
56	MG	YA	3446	1/1	0.58	0.22	105,105,105,105	0
56	MG	RA	3896	1/1	0.58	0.35	72,72,72,72	0
56	MG	YA	3251	1/1	0.58	0.21	83,83,83,83	0
56	MG	QA	1766	1/1	0.58	0.26	118,118,118,118	0
56	MG	RB	220	1/1	0.58	0.15	117,117,117,117	0
56	MG	QA	1696	1/1	0.58	0.23	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3586	1/1	0.58	0.27	87,87,87,87	0
56	MG	YA	3289	1/1	0.58	0.32	66,66,66,66	0
56	MG	YA	3291	1/1	0.58	0.23	97,97,97,97	0
56	MG	QA	1828	1/1	0.58	0.18	107,107,107,107	0
56	MG	RA	3659	1/1	0.58	0.20	119,119,119,119	0
56	MG	RA	3307	1/1	0.58	0.22	243,243,243,243	0
56	MG	YA	3494	1/1	0.58	0.22	84,84,84,84	0
56	MG	RA	3060	1/1	0.58	0.09	122,122,122,122	0
56	MG	RA	3363	1/1	0.58	0.30	84,84,84,84	0
56	MG	RA	3932	1/1	0.58	0.46	122,122,122,122	0
56	MG	RA	3005	1/1	0.58	0.15	94,94,94,94	0
56	MG	RA	3427	1/1	0.58	0.34	108,108,108,108	0
56	MG	XA	1614	1/1	0.58	0.18	89,89,89,89	0
56	MG	QA	1795	1/1	0.58	0.28	102,102,102,102	0
56	MG	RA	3433	1/1	0.58	0.21	96,96,96,96	0
56	MG	QA	1665	1/1	0.58	0.10	128,128,128,128	0
56	MG	YA	3608	1/1	0.58	0.36	88,88,88,88	0
56	MG	RA	3130	1/1	0.58	0.11	90,90,90,90	0
56	MG	RA	3559	1/1	0.58	0.26	96,96,96,96	0
56	MG	RA	4035	1/1	0.58	0.27	120,120,120,120	0
56	MG	YA	3088	1/1	0.59	0.17	72,72,72,72	0
56	MG	YA	3673	1/1	0.59	0.43	114,114,114,114	0
56	MG	RA	3910	1/1	0.59	0.14	111,111,111,111	0
56	MG	QA	1671	1/1	0.59	0.22	105,105,105,105	0
56	MG	RQ	201	1/1	0.59	0.13	87,87,87,87	0
56	MG	RA	3894	1/1	0.59	0.46	94,94,94,94	0
56	MG	R0	103	1/1	0.59	0.47	99,99,99,99	0
56	MG	YA	3313	1/1	0.59	0.31	61,61,61,61	0
56	MG	YA	3131	1/1	0.59	0.27	89,89,89,89	0
56	MG	YA	3546	1/1	0.59	0.34	80,80,80,80	0
56	MG	RA	3366	1/1	0.59	0.53	110,110,110,110	0
56	MG	YA	3727	1/1	0.59	0.32	87,87,87,87	0
56	MG	YA	3024	1/1	0.59	0.59	139,139,139,139	0
56	MG	RB	208	1/1	0.59	0.12	114,114,114,114	0
56	MG	XA	1765	1/1	0.59	0.63	130,130,130,130	0
56	MG	YA	3170	1/1	0.59	0.12	116,116,116,116	0
56	MG	YA	3464	1/1	0.59	0.21	83,83,83,83	0
56	MG	RA	3960	1/1	0.59	0.33	83,83,83,83	0
56	MG	QA	1799	1/1	0.59	0.28	123,123,123,123	0
56	MG	RA	3051	1/1	0.59	0.40	126,126,126,126	0
56	MG	RA	3287	1/1	0.59	0.29	103,103,103,103	0
56	MG	YA	3381	1/1	0.59	0.23	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1779	1/1	0.59	0.29	90,90,90,90	0
56	MG	XA	1674	1/1	0.60	0.23	114,114,114,114	0
56	MG	YA	3414	1/1	0.60	0.14	117,117,117,117	0
56	MG	YA	3353	1/1	0.60	0.26	74,74,74,74	0
56	MG	QA	1816	1/1	0.60	0.26	89,89,89,89	0
56	MG	RA	3098	1/1	0.60	0.19	132,132,132,132	0
56	MG	RA	3771	1/1	0.60	0.09	90,90,90,90	0
56	MG	YA	3016	1/1	0.60	0.34	106,106,106,106	0
56	MG	QA	1653	1/1	0.60	0.21	101,101,101,101	0
56	MG	RA	3955	1/1	0.60	0.11	88,88,88,88	0
56	MG	YA	3402	1/1	0.60	0.39	94,94,94,94	0
56	MG	YA	3043	1/1	0.60	0.27	108,108,108,108	0
56	MG	YA	3407	1/1	0.60	0.34	111,111,111,111	0
56	MG	YA	3408	1/1	0.60	0.17	77,77,77,77	0
56	MG	QA	1713	1/1	0.60	0.30	73,73,73,73	0
56	MG	RA	3705	1/1	0.61	0.22	68,68,68,68	0
56	MG	RA	3558	1/1	0.61	0.34	93,93,93,93	0
56	MG	YA	3632	1/1	0.61	0.28	89,89,89,89	0
56	MG	YA	3033	1/1	0.61	0.48	87,87,87,87	0
56	MG	RQ	202	1/1	0.61	0.18	87,87,87,87	0
56	MG	RA	3930	1/1	0.61	0.18	88,88,88,88	0
56	MG	RA	3155	1/1	0.61	0.20	91,91,91,91	0
56	MG	RA	3560	1/1	0.61	0.17	90,90,90,90	0
56	MG	XA	1705	1/1	0.61	0.29	89,89,89,89	0
56	MG	YA	3651	1/1	0.61	0.09	118,118,118,118	0
56	MG	R8	101	1/1	0.61	0.25	118,118,118,118	0
56	MG	RA	3883	1/1	0.61	0.61	116,116,116,116	0
56	MG	RA	3540	1/1	0.61	0.16	108,108,108,108	0
56	MG	RA	3056	1/1	0.61	0.16	101,101,101,101	0
56	MG	QA	1606	1/1	0.61	0.11	124,124,124,124	0
56	MG	XA	1742	1/1	0.61	0.49	109,109,109,109	0
56	MG	RA	3281	1/1	0.61	0.50	126,126,126,126	0
56	MG	QA	1703	1/1	0.61	0.24	90,90,90,90	0
56	MG	XA	1646	1/1	0.61	0.21	119,119,119,119	0
56	MG	XA	1756	1/1	0.61	0.27	91,91,91,91	0
56	MG	YA	3534	1/1	0.61	0.44	104,104,104,104	0
56	MG	RA	3120	1/1	0.61	0.45	128,128,128,128	0
56	MG	YA	3436	1/1	0.61	0.32	127,127,127,127	0
56	MG	XA	1658	1/1	0.61	0.17	141,141,141,141	0
56	MG	RA	3513	1/1	0.61	0.32	106,106,106,106	0
56	MG	YA	3449	1/1	0.61	0.32	105,105,105,105	0
56	MG	YA	3450	1/1	0.61	0.16	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3974	1/1	0.61	0.45	109,109,109,109	0
56	MG	YA	3133	1/1	0.61	0.16	83,83,83,83	0
56	MG	RA	3145	1/1	0.61	0.32	105,105,105,105	0
56	MG	RA	3354	1/1	0.62	0.18	116,116,116,116	0
56	MG	RA	3715	1/1	0.62	0.27	77,77,77,77	0
56	MG	RA	3369	1/1	0.62	0.33	85,85,85,85	0
56	MG	YA	3418	1/1	0.62	0.27	84,84,84,84	0
56	MG	QA	1688	1/1	0.62	0.17	109,109,109,109	0
56	MG	QA	1717	1/1	0.62	0.31	102,102,102,102	0
56	MG	YA	3426	1/1	0.62	0.25	119,119,119,119	0
56	MG	RA	3587	1/1	0.62	0.21	104,104,104,104	0
56	MG	RA	3544	1/1	0.62	0.26	93,93,93,93	0
56	MG	RA	3863	1/1	0.62	0.36	87,87,87,87	0
56	MG	QA	1733	1/1	0.62	0.19	119,119,119,119	0
56	MG	RA	3109	1/1	0.62	0.58	143,143,143,143	0
56	MG	RA	3131	1/1	0.62	0.26	138,138,138,138	0
56	MG	RA	3946	1/1	0.62	0.26	98,98,98,98	0
56	MG	XA	1609	1/1	0.62	0.20	100,100,100,100	0
56	MG	QA	1704	1/1	0.62	0.19	79,79,79,79	0
56	MG	RA	3076	1/1	0.62	0.15	79,79,79,79	0
56	MG	XA	1778	1/1	0.62	0.11	114,114,114,114	0
56	MG	YA	3456	1/1	0.62	0.46	115,115,115,115	0
56	MG	YA	3223	1/1	0.62	0.41	100,100,100,100	0
56	MG	YA	3704	1/1	0.62	0.44	117,117,117,117	0
56	MG	YA	3710	1/1	0.62	0.26	113,113,113,113	0
56	MG	RA	3103	1/1	0.62	0.15	130,130,130,130	0
56	MG	RA	3494	1/1	0.63	0.31	81,81,81,81	0
56	MG	QA	1679	1/1	0.63	0.25	141,141,141,141	0
56	MG	RA	3503	1/1	0.63	0.23	147,147,147,147	0
56	MG	RA	3816	1/1	0.63	0.28	69,69,69,69	0
56	MG	RA	3504	1/1	0.63	0.29	88,88,88,88	0
56	MG	QA	1750	1/1	0.63	0.21	92,92,92,92	0
56	MG	YA	3467	1/1	0.63	0.40	114,114,114,114	0
56	MG	QA	1804	1/1	0.63	0.17	92,92,92,92	0
56	MG	RA	3542	1/1	0.63	0.31	101,101,101,101	0
56	MG	RA	3429	1/1	0.63	0.17	71,71,71,71	0
56	MG	RA	3633	1/1	0.63	0.11	96,96,96,96	0
56	MG	RA	3164	1/1	0.63	0.15	117,117,117,117	0
56	MG	RA	3362	1/1	0.63	0.24	71,71,71,71	0
56	MG	RN	202	1/1	0.63	0.12	88,88,88,88	0
56	MG	YA	3499	1/1	0.63	0.34	78,78,78,78	0
56	MG	YA	3022	1/1	0.63	0.52	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3639	1/1	0.63	0.25	97,97,97,97	0
56	MG	RA	3471	1/1	0.63	0.43	69,69,69,69	0
56	MG	YA	3516	1/1	0.63	0.31	86,86,86,86	0
56	MG	YA	3518	1/1	0.63	0.29	100,100,100,100	0
56	MG	RA	3762	1/1	0.63	0.29	91,91,91,91	0
56	MG	QA	1771	1/1	0.63	0.11	119,119,119,119	0
56	MG	RA	3591	1/1	0.63	0.24	102,102,102,102	0
56	MG	YA	3231	1/1	0.63	0.28	98,98,98,98	0
56	MG	XA	1733	1/1	0.63	0.25	84,84,84,84	0
56	MG	RA	3999	1/1	0.63	0.41	112,112,112,112	0
56	MG	Y0	101	1/1	0.63	0.31	78,78,78,78	0
56	MG	RA	3603	1/1	0.63	0.16	101,101,101,101	0
56	MG	YA	3063	1/1	0.63	0.22	82,82,82,82	0
56	MG	RA	3242	1/1	0.63	0.12	141,141,141,141	0
56	MG	YA	3261	1/1	0.63	0.26	60,60,60,60	0
56	MG	RA	3127	1/1	0.63	0.20	74,74,74,74	0
56	MG	RB	207	1/1	0.63	0.12	128,128,128,128	0
56	MG	YA	3622	1/1	0.63	0.23	86,86,86,86	0
56	MG	RA	3611	1/1	0.63	0.28	55,55,55,55	0
56	MG	QA	1843	1/1	0.63	0.16	101,101,101,101	0
56	MG	RA	3358	1/1	0.63	0.34	111,111,111,111	0
56	MG	YA	3096	1/1	0.63	0.19	124,124,124,124	0
56	MG	YA	3643	1/1	0.63	0.29	70,70,70,70	0
56	MG	RA	3675	1/1	0.63	0.22	105,105,105,105	0
56	MG	QA	1610	1/1	0.63	0.19	163,163,163,163	0
56	MG	RA	3341	1/1	0.64	0.33	96,96,96,96	0
56	MG	RA	3533	1/1	0.64	0.34	92,92,92,92	0
56	MG	RV	202	1/1	0.64	0.18	126,126,126,126	0
56	MG	QA	1764	1/1	0.64	0.23	108,108,108,108	0
56	MG	QA	1821	1/1	0.64	0.50	117,117,117,117	0
56	MG	XA	1673	1/1	0.64	0.19	106,106,106,106	0
56	MG	RA	3344	1/1	0.64	0.23	60,60,60,60	0
56	MG	RA	3443	1/1	0.64	0.20	127,127,127,127	0
56	MG	RA	3900	1/1	0.64	0.44	132,132,132,132	0
56	MG	RA	3801	1/1	0.64	0.26	114,114,114,114	0
56	MG	YA	3520	1/1	0.64	0.10	73,73,73,73	0
56	MG	YA	3239	1/1	0.64	0.27	100,100,100,100	0
56	MG	RA	3132	1/1	0.64	0.31	110,110,110,110	0
56	MG	XA	1699	1/1	0.64	0.26	90,90,90,90	0
56	MG	RA	3507	1/1	0.64	0.25	87,87,87,87	0
56	MG	RA	3220	1/1	0.64	0.14	96,96,96,96	0
56	MG	RA	3928	1/1	0.64	0.22	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3205	1/1	0.64	0.21	131,131,131,131	0
56	MG	YA	3430	1/1	0.64	0.29	100,100,100,100	0
56	MG	YA	3583	1/1	0.64	0.42	104,104,104,104	0
56	MG	QA	1726	1/1	0.64	0.17	72,72,72,72	0
56	MG	QA	1847	1/1	0.64	0.25	102,102,102,102	0
56	MG	QA	1729	1/1	0.64	0.21	117,117,117,117	0
56	MG	XA	1721	1/1	0.64	0.40	138,138,138,138	0
56	MG	XA	1723	1/1	0.64	0.19	110,110,110,110	0
56	MG	RA	3370	1/1	0.64	0.66	105,105,105,105	0
56	MG	XA	1741	1/1	0.64	0.12	91,91,91,91	0
56	MG	RA	3324	1/1	0.64	0.17	107,107,107,107	0
56	MG	RA	3519	1/1	0.64	0.22	104,104,104,104	0
56	MG	YA	3630	1/1	0.64	0.22	80,80,80,80	0
56	MG	RD	312	1/1	0.64	0.14	133,133,133,133	0
56	MG	QA	1680	1/1	0.64	0.22	105,105,105,105	0
56	MG	QA	1742	1/1	0.64	0.30	120,120,120,120	0
56	MG	RA	3359	1/1	0.64	0.35	84,84,84,84	0
56	MG	YA	3168	1/1	0.64	0.30	93,93,93,93	0
56	MG	RF	301	1/1	0.64	0.45	93,93,93,93	0
56	MG	XA	1776	1/1	0.64	0.33	98,98,98,98	0
56	MG	RA	3143	1/1	0.64	0.14	82,82,82,82	0
56	MG	XA	1641	1/1	0.64	0.15	86,86,86,86	0
56	MG	RA	3844	1/1	0.64	0.20	85,85,85,85	0
56	MG	XA	1782	1/1	0.64	0.10	105,105,105,105	0
56	MG	RA	3529	1/1	0.64	0.18	70,70,70,70	0
56	MG	QA	1754	1/1	0.64	0.18	111,111,111,111	0
56	MG	RA	3769	1/1	0.64	0.12	77,77,77,77	0
56	MG	RA	3620	1/1	0.64	0.21	53,53,53,53	0
56	MG	QA	1666	1/1	0.65	0.17	125,125,125,125	0
56	MG	YA	3396	1/1	0.65	0.25	44,44,44,44	0
56	MG	RB	223	1/1	0.65	0.12	89,89,89,89	0
56	MG	XA	1701	1/1	0.65	0.28	89,89,89,89	0
56	MG	RA	3327	1/1	0.65	0.14	92,92,92,92	0
56	MG	RA	3628	1/1	0.65	0.55	109,109,109,109	0
56	MG	YA	3642	1/1	0.65	0.21	87,87,87,87	0
56	MG	YA	3176	1/1	0.65	0.29	67,67,67,67	0
56	MG	YA	3048	1/1	0.65	0.20	76,76,76,76	0
56	MG	RA	3481	1/1	0.65	0.32	67,67,67,67	0
56	MG	QA	1851	1/1	0.65	0.12	105,105,105,105	0
56	MG	RA	3744	1/1	0.65	0.26	87,87,87,87	0
56	MG	RA	3522	1/1	0.65	0.45	97,97,97,97	0
56	MG	RA	3322	1/1	0.65	0.25	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3759	1/1	0.65	0.18	82,82,82,82	0
56	MG	YA	3213	1/1	0.65	0.38	131,131,131,131	0
56	MG	YA	3689	1/1	0.65	0.34	59,59,59,59	0
56	MG	RG	204	1/1	0.65	0.28	104,104,104,104	0
56	MG	YA	3329	1/1	0.65	0.19	97,97,97,97	0
56	MG	RA	3807	1/1	0.65	0.25	94,94,94,94	0
56	MG	RA	3653	1/1	0.65	0.27	99,99,99,99	0
56	MG	QA	1725	1/1	0.65	0.28	78,78,78,78	0
56	MG	XA	1657	1/1	0.65	0.14	116,116,116,116	0
56	MG	YA	3545	1/1	0.65	0.53	92,92,92,92	0
56	MG	YA	3340	1/1	0.65	0.32	73,73,73,73	0
56	MG	YA	3547	1/1	0.65	0.44	84,84,84,84	0
56	MG	YA	3572	1/1	0.65	0.17	96,96,96,96	0
56	MG	QA	1659	1/1	0.65	0.18	107,107,107,107	0
56	MG	QA	1727	1/1	0.65	0.24	110,110,110,110	0
56	MG	QA	1831	1/1	0.65	0.34	75,75,75,75	0
56	MG	RA	3634	1/1	0.65	0.31	98,98,98,98	0
56	MG	QA	1835	1/1	0.65	0.15	93,93,93,93	0
56	MG	YD	305	1/1	0.65	0.80	133,133,133,133	0
56	MG	RB	221	1/1	0.65	0.34	103,103,103,103	0
56	MG	RA	3254	1/1	0.65	0.59	147,147,147,147	0
56	MG	YA	3221	1/1	0.66	0.14	107,107,107,107	0
56	MG	RA	3402	1/1	0.66	0.14	103,103,103,103	0
56	MG	YA	3105	1/1	0.66	0.41	118,118,118,118	0
56	MG	YA	3124	1/1	0.66	0.15	96,96,96,96	0
56	MG	YA	3655	1/1	0.66	0.25	66,66,66,66	0
56	MG	RA	3335	1/1	0.66	0.31	74,74,74,74	0
56	MG	RA	3226	1/1	0.66	0.35	151,151,151,151	0
56	MG	XA	1616	1/1	0.66	0.13	88,88,88,88	0
56	MG	RA	3066	1/1	0.66	0.21	103,103,103,103	0
56	MG	RA	3909	1/1	0.66	0.19	89,89,89,89	0
56	MG	RA	3805	1/1	0.66	0.14	72,72,72,72	0
56	MG	RA	3430	1/1	0.66	0.28	82,82,82,82	0
56	MG	XA	1631	1/1	0.66	0.29	87,87,87,87	0
56	MG	RA	3918	1/1	0.66	0.26	119,119,119,119	0
56	MG	YA	3559	1/1	0.66	0.24	51,51,51,51	0
56	MG	YA	3703	1/1	0.66	0.13	95,95,95,95	0
56	MG	RB	227	1/1	0.66	0.10	140,140,140,140	0
56	MG	YA	3388	1/1	0.66	0.22	83,83,83,83	0
56	MG	RD	309	1/1	0.66	0.34	107,107,107,107	0
56	MG	YA	3606	1/1	0.66	0.30	91,91,91,91	0
56	MG	RA	3485	1/1	0.66	0.36	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3400	1/1	0.66	0.47	101,101,101,101	0
56	MG	RA	3739	1/1	0.66	0.19	86,86,86,86	0
56	MG	RA	3418	1/1	0.66	0.26	91,91,91,91	0
56	MG	YA	3187	1/1	0.66	0.21	122,122,122,122	0
56	MG	QA	1652	1/1	0.66	0.22	98,98,98,98	0
56	MG	RA	3867	1/1	0.66	0.16	79,79,79,79	0
56	MG	YD	302	1/1	0.66	0.25	74,74,74,74	0
56	MG	RF	304	1/1	0.66	0.23	67,67,67,67	0
56	MG	RA	3817	1/1	0.66	0.43	114,114,114,114	0
56	MG	RA	3692	1/1	0.66	0.22	91,91,91,91	0
56	MG	XA	1683	1/1	0.66	0.22	68,68,68,68	0
56	MG	QV	102	1/1	0.66	0.07	136,136,136,136	0
56	MG	XA	1685	1/1	0.66	0.37	106,106,106,106	0
56	MG	QA	1803	1/1	0.66	0.16	93,93,93,93	0
56	MG	XA	1688	1/1	0.66	0.40	87,87,87,87	0
57	ZN	Y6	101	1/1	0.66	0.28	307,307,307,307	0
56	MG	YA	3073	1/1	0.67	0.24	34,34,34,34	0
56	MG	YA	3560	1/1	0.67	0.25	67,67,67,67	0
56	MG	RA	3756	1/1	0.67	0.38	63,63,63,63	0
56	MG	YA	3174	1/1	0.67	0.32	91,91,91,91	0
56	MG	RA	3392	1/1	0.67	0.27	71,71,71,71	0
56	MG	YA	3600	1/1	0.67	0.38	75,75,75,75	0
56	MG	RA	3398	1/1	0.67	0.25	108,108,108,108	0
56	MG	YA	3007	1/1	0.67	0.20	69,69,69,69	0
56	MG	YA	3492	1/1	0.67	0.23	79,79,79,79	0
56	MG	YA	3092	1/1	0.67	0.17	123,123,123,123	0
56	MG	YA	3355	1/1	0.67	0.24	72,72,72,72	0
56	MG	YA	3502	1/1	0.67	0.39	95,95,95,95	0
56	MG	RA	3899	1/1	0.67	0.41	110,110,110,110	0
56	MG	RA	3681	1/1	0.67	0.37	124,124,124,124	0
56	MG	RB	215	1/1	0.67	0.11	95,95,95,95	0
56	MG	QA	1789	1/1	0.67	0.16	101,101,101,101	0
56	MG	YB	214	1/1	0.67	0.34	130,130,130,130	0
56	MG	YA	3639	1/1	0.67	0.36	83,83,83,83	0
56	MG	YA	3202	1/1	0.67	0.18	79,79,79,79	0
56	MG	RA	3552	1/1	0.67	0.41	120,120,120,120	0
56	MG	QA	1765	1/1	0.67	0.10	117,117,117,117	0
56	MG	QA	1633	1/1	0.67	0.15	136,136,136,136	0
56	MG	XA	1680	1/1	0.67	0.15	119,119,119,119	0
56	MG	RO	201	1/1	0.67	0.19	91,91,91,91	0
56	MG	QA	1813	1/1	0.67	0.18	88,88,88,88	0
56	MG	YA	3648	1/1	0.67	0.27	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RE	306	1/1	0.67	0.40	98,98,98,98	0
56	MG	XA	1781	1/1	0.67	0.33	76,76,76,76	0
56	MG	RA	3095	1/1	0.67	0.19	92,92,92,92	0
56	MG	QA	1846	1/1	0.67	0.14	127,127,127,127	0
56	MG	YA	3662	1/1	0.67	0.17	60,60,60,60	0
56	MG	YA	3664	1/1	0.67	0.28	56,56,56,56	0
56	MG	YA	3475	1/1	0.67	0.33	83,83,83,83	0
56	MG	YA	3550	1/1	0.67	0.28	93,93,93,93	0
56	MG	RA	3704	1/1	0.68	0.16	83,83,83,83	0
56	MG	YA	3057	1/1	0.68	0.20	78,78,78,78	0
56	MG	RA	3096	1/1	0.68	0.19	46,46,46,46	0
56	MG	XA	1709	1/1	0.68	0.26	73,73,73,73	0
56	MG	QL	201	1/1	0.68	0.11	89,89,89,89	0
56	MG	RA	3278	1/1	0.68	0.25	141,141,141,141	0
56	MG	YA	3633	1/1	0.68	0.28	99,99,99,99	0
56	MG	RA	3482	1/1	0.68	0.43	111,111,111,111	0
56	MG	RA	3049	1/1	0.68	0.60	122,122,122,122	0
56	MG	RA	3725	1/1	0.68	0.27	108,108,108,108	0
56	MG	RA	3365	1/1	0.68	0.23	61,61,61,61	0
56	MG	RA	3192	1/1	0.68	0.48	149,149,149,149	0
56	MG	RA	3784	1/1	0.68	0.27	108,108,108,108	0
56	MG	RB	225	1/1	0.68	0.11	131,131,131,131	0
56	MG	YD	307	1/1	0.68	0.32	83,83,83,83	0
56	MG	RA	3979	1/1	0.68	0.30	91,91,91,91	0
56	MG	RA	3983	1/1	0.68	0.23	130,130,130,130	0
56	MG	RA	3642	1/1	0.68	0.40	145,145,145,145	0
56	MG	XA	1761	1/1	0.68	0.31	85,85,85,85	0
56	MG	QA	1790	1/1	0.68	0.30	103,103,103,103	0
56	MG	YA	3551	1/1	0.68	0.20	73,73,73,73	0
56	MG	YA	3112	1/1	0.68	0.18	71,71,71,71	0
56	MG	YA	3482	1/1	0.68	0.27	90,90,90,90	0
56	MG	RA	3677	1/1	0.68	0.26	83,83,83,83	0
56	MG	YA	3324	1/1	0.68	0.24	55,55,55,55	0
56	MG	RA	3746	1/1	0.68	0.30	108,108,108,108	0
56	MG	RA	3493	1/1	0.68	0.23	122,122,122,122	0
56	MG	RA	3423	1/1	0.68	0.41	96,96,96,96	0
56	MG	XA	1617	1/1	0.68	0.26	72,72,72,72	0
56	MG	XJ	201	1/1	0.68	0.22	115,115,115,115	0
56	MG	YA	3154	1/1	0.68	0.34	88,88,88,88	0
56	MG	XA	1696	1/1	0.68	0.23	87,87,87,87	0
56	MG	YA	3611	1/1	0.68	0.22	65,65,65,65	0
56	MG	YA	3495	1/1	0.68	0.34	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	ZN	Y4	101	1/1	0.68	0.10	318,318,318,318	0
56	MG	RA	3350	1/1	0.68	0.13	76,76,76,76	0
56	MG	RA	3432	1/1	0.69	0.26	67,67,67,67	0
56	MG	YA	3697	1/1	0.69	0.31	57,57,57,57	0
56	MG	RA	3001	1/1	0.69	0.22	80,80,80,80	0
56	MG	RA	3735	1/1	0.69	0.26	93,93,93,93	0
56	MG	YA	3027	1/1	0.69	0.19	70,70,70,70	0
56	MG	RA	3873	1/1	0.69	0.20	86,86,86,86	0
56	MG	RA	3039	1/1	0.69	0.37	96,96,96,96	0
56	MG	RA	3741	1/1	0.69	0.30	59,59,59,59	0
56	MG	RA	3934	1/1	0.69	0.22	86,86,86,86	0
56	MG	YA	3722	1/1	0.69	0.25	84,84,84,84	0
56	MG	RB	205	1/1	0.69	0.12	102,102,102,102	0
56	MG	YA	3451	1/1	0.69	0.31	74,74,74,74	0
56	MG	YB	205	1/1	0.69	0.20	117,117,117,117	0
56	MG	XA	1737	1/1	0.69	0.32	74,74,74,74	0
56	MG	RA	3180	1/1	0.69	0.74	112,112,112,112	0
56	MG	QA	1740	1/1	0.69	0.15	92,92,92,92	0
56	MG	YB	212	1/1	0.69	0.32	89,89,89,89	0
56	MG	QA	1776	1/1	0.69	0.12	92,92,92,92	0
56	MG	RF	303	1/1	0.69	0.47	120,120,120,120	0
56	MG	YB	215	1/1	0.69	0.16	53,53,53,53	0
56	MG	RA	3195	1/1	0.69	0.14	148,148,148,148	0
56	MG	YD	301	1/1	0.69	0.29	95,95,95,95	0
56	MG	QA	1783	1/1	0.69	0.17	74,74,74,74	0
56	MG	QA	1744	1/1	0.69	0.16	104,104,104,104	0
56	MG	RA	3442	1/1	0.69	0.28	87,87,87,87	0
56	MG	RA	3951	1/1	0.69	0.25	77,77,77,77	0
56	MG	YA	3403	1/1	0.69	0.24	91,91,91,91	0
56	MG	YE	305	1/1	0.69	0.12	97,97,97,97	0
56	MG	RA	3706	1/1	0.69	0.37	68,68,68,68	0
56	MG	YG	202	1/1	0.69	0.13	99,99,99,99	0
56	MG	RA	3588	1/1	0.69	0.21	113,113,113,113	0
56	MG	YA	3562	1/1	0.69	0.27	107,107,107,107	0
56	MG	RB	216	1/1	0.69	0.14	95,95,95,95	0
56	MG	RA	3798	1/1	0.69	0.20	81,81,81,81	0
56	MG	RA	3196	1/1	0.69	0.24	123,123,123,123	0
56	MG	YA	3593	1/1	0.69	0.17	79,79,79,79	0
56	MG	RA	3421	1/1	0.69	0.28	123,123,123,123	0
56	MG	RA	3972	1/1	0.69	0.44	108,108,108,108	0
56	MG	RA	3050	1/1	0.70	0.39	115,115,115,115	0
56	MG	QA	1641	1/1	0.70	0.43	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3465	1/1	0.70	0.18	66,66,66,66	0
56	MG	YA	3023	1/1	0.70	0.13	87,87,87,87	0
56	MG	RA	3053	1/1	0.70	0.55	128,128,128,128	0
56	MG	YA	3098	1/1	0.70	0.26	85,85,85,85	0
56	MG	RA	3712	1/1	0.70	0.19	105,105,105,105	0
56	MG	RA	3125	1/1	0.70	0.15	91,91,91,91	0
56	MG	RN	201	1/1	0.70	0.44	130,130,130,130	0
56	MG	RA	3582	1/1	0.70	0.11	100,100,100,100	0
56	MG	YA	3215	1/1	0.70	0.32	84,84,84,84	0
56	MG	YA	3671	1/1	0.70	0.12	68,68,68,68	0
56	MG	YA	3127	1/1	0.70	0.32	94,94,94,94	0
56	MG	YA	3045	1/1	0.70	0.31	107,107,107,107	0
56	MG	YA	3680	1/1	0.70	0.26	66,66,66,66	0
56	MG	RA	3720	1/1	0.70	0.12	72,72,72,72	0
56	MG	YA	3687	1/1	0.70	0.21	87,87,87,87	0
56	MG	RA	3218	1/1	0.70	0.40	135,135,135,135	0
56	MG	RA	3727	1/1	0.70	0.24	109,109,109,109	0
56	MG	RB	212	1/1	0.70	0.46	95,95,95,95	0
56	MG	Y8	101	1/1	0.70	0.29	99,99,99,99	0
56	MG	XA	1772	1/1	0.70	0.23	49,49,49,49	0
56	MG	XA	1603	1/1	0.70	0.32	134,134,134,134	0
56	MG	RA	3655	1/1	0.70	0.22	95,95,95,95	0
56	MG	YA	3164	1/1	0.70	0.49	149,149,149,149	0
56	MG	YA	3242	1/1	0.70	0.28	115,115,115,115	0
56	MG	QA	1781	1/1	0.70	0.28	108,108,108,108	0
56	MG	RA	3912	1/1	0.70	0.23	79,79,79,79	0
56	MG	R5	103	1/1	0.70	0.24	75,75,75,75	0
56	MG	XF	201	1/1	0.70	0.12	107,107,107,107	0
56	MG	RA	3732	1/1	0.70	0.28	62,62,62,62	0
56	MG	XA	1697	1/1	0.70	0.16	100,100,100,100	0
56	MG	XA	1618	1/1	0.70	0.26	70,70,70,70	0
56	MG	YA	3530	1/1	0.70	0.27	67,67,67,67	0
56	MG	RA	4037	1/1	0.70	0.44	144,144,144,144	0
56	MG	YA	3001	1/1	0.70	0.35	142,142,142,142	0
56	MG	QA	1735	1/1	0.70	0.31	82,82,82,82	0
56	MG	YA	3281	1/1	0.71	0.54	97,97,97,97	0
56	MG	YA	3587	1/1	0.71	0.56	114,114,114,114	0
56	MG	QA	1826	1/1	0.71	0.25	79,79,79,79	0
56	MG	YA	3441	1/1	0.71	0.39	60,60,60,60	0
56	MG	QA	1759	1/1	0.71	0.24	113,113,113,113	0
56	MG	YA	3679	1/1	0.71	0.43	103,103,103,103	0
56	MG	YA	3448	1/1	0.71	0.23	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3367	1/1	0.71	0.23	80,80,80,80	0
56	MG	RA	3002	1/1	0.71	0.23	108,108,108,108	0
56	MG	YA	3613	1/1	0.71	0.30	92,92,92,92	0
56	MG	QA	1761	1/1	0.71	0.29	99,99,99,99	0
56	MG	YA	3694	1/1	0.71	0.28	76,76,76,76	0
56	MG	YA	3617	1/1	0.71	0.35	72,72,72,72	0
56	MG	RA	3651	1/1	0.71	0.20	109,109,109,109	0
56	MG	RA	3821	1/1	0.71	0.27	85,85,85,85	0
56	MG	RA	3669	1/1	0.71	0.24	70,70,70,70	0
56	MG	YA	3301	1/1	0.71	0.22	83,83,83,83	0
56	MG	RA	3924	1/1	0.71	0.20	84,84,84,84	0
56	MG	RA	3227	1/1	0.71	0.46	111,111,111,111	0
56	MG	YA	3175	1/1	0.71	0.22	77,77,77,77	0
56	MG	YA	3047	1/1	0.71	0.17	118,118,118,118	0
56	MG	XA	1690	1/1	0.71	0.33	89,89,89,89	0
56	MG	YA	3238	1/1	0.71	0.24	134,134,134,134	0
56	MG	RA	3738	1/1	0.71	0.32	68,68,68,68	0
56	MG	YA	3413	1/1	0.71	0.23	88,88,88,88	0
56	MG	YB	203	1/1	0.71	0.21	111,111,111,111	0
56	MG	RA	3839	1/1	0.71	0.19	113,113,113,113	0
56	MG	RA	3568	1/1	0.71	0.27	79,79,79,79	0
56	MG	XA	1625	1/1	0.71	0.51	92,92,92,92	0
56	MG	YA	3120	1/1	0.71	0.11	105,105,105,105	0
56	MG	RA	3963	1/1	0.71	0.24	159,159,159,159	0
56	MG	QA	1684	1/1	0.71	0.17	105,105,105,105	0
56	MG	QA	1687	1/1	0.71	0.18	131,131,131,131	0
56	MG	QA	1667	1/1	0.71	0.27	104,104,104,104	0
56	MG	YA	3684	1/1	0.72	0.29	76,76,76,76	0
56	MG	YA	3685	1/1	0.72	0.33	102,102,102,102	0
56	MG	YA	3280	1/1	0.72	0.30	51,51,51,51	0
56	MG	R0	104	1/1	0.72	0.32	105,105,105,105	0
56	MG	RA	3662	1/1	0.72	0.22	107,107,107,107	0
56	MG	RA	3407	1/1	0.72	0.23	61,61,61,61	0
56	MG	RA	3959	1/1	0.72	0.38	110,110,110,110	0
56	MG	QA	1690	1/1	0.72	0.23	126,126,126,126	0
56	MG	XA	1712	1/1	0.72	0.30	114,114,114,114	0
56	MG	YA	3082	1/1	0.72	0.13	111,111,111,111	0
56	MG	RA	3549	1/1	0.72	0.29	102,102,102,102	0
56	MG	RA	3853	1/1	0.72	0.39	63,63,63,63	0
56	MG	RA	3562	1/1	0.72	0.20	86,86,86,86	0
56	MG	RA	3815	1/1	0.72	0.12	78,78,78,78	0
56	MG	YA	3423	1/1	0.72	0.21	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RF	311	1/1	0.72	0.26	93,93,93,93	0
56	MG	YA	3504	1/1	0.72	0.43	86,86,86,86	0
56	MG	RA	3199	1/1	0.72	0.24	114,114,114,114	0
56	MG	RA	3276	1/1	0.72	0.37	134,134,134,134	0
56	MG	YA	3509	1/1	0.72	0.41	132,132,132,132	0
56	MG	RA	3781	1/1	0.72	0.38	106,106,106,106	0
56	MG	QA	1830	1/1	0.72	0.39	80,80,80,80	0
56	MG	RH	201	1/1	0.72	0.12	157,157,157,157	0
56	MG	XA	1754	1/1	0.72	0.10	82,82,82,82	0
56	MG	RA	3893	1/1	0.72	0.30	85,85,85,85	0
56	MG	RA	3517	1/1	0.72	0.18	72,72,72,72	0
56	MG	RA	3574	1/1	0.72	0.27	94,94,94,94	0
56	MG	QA	1839	1/1	0.72	0.22	106,106,106,106	0
56	MG	QA	1630	1/1	0.72	0.30	74,74,74,74	0
56	MG	RA	3576	1/1	0.72	0.11	82,82,82,82	0
56	MG	XA	1773	1/1	0.72	0.48	133,133,133,133	0
56	MG	YA	3145	1/1	0.72	0.21	86,86,86,86	0
56	MG	RA	3726	1/1	0.72	0.20	64,64,64,64	0
56	MG	QA	1677	1/1	0.72	0.22	99,99,99,99	0
56	MG	RT	202	1/1	0.72	0.26	94,94,94,94	0
56	MG	RD	306	1/1	0.72	0.26	115,115,115,115	0
56	MG	YA	3460	1/1	0.72	0.30	99,99,99,99	0
56	MG	RA	3466	1/1	0.72	0.29	77,77,77,77	0
56	MG	QA	1767	1/1	0.72	0.16	149,149,149,149	0
56	MG	YN	201	1/1	0.72	0.16	106,106,106,106	0
56	MG	XV	101	1/1	0.72	0.18	89,89,89,89	0
56	MG	YA	3674	1/1	0.72	0.20	73,73,73,73	0
57	ZN	R5	102	1/1	0.72	0.10	305,305,305,305	0
56	MG	QA	1730	1/1	0.72	0.17	102,102,102,102	0
56	MG	YA	3564	1/1	0.72	0.28	52,52,52,52	0
56	MG	Y1	101	1/1	0.72	0.26	65,65,65,65	0
56	MG	YA	3568	1/1	0.72	0.21	85,85,85,85	0
56	MG	RA	3488	1/1	0.72	0.26	88,88,88,88	0
56	MG	YA	3180	1/1	0.73	0.24	89,89,89,89	0
56	MG	RA	3941	1/1	0.73	0.32	87,87,87,87	0
56	MG	QA	1782	1/1	0.73	0.31	82,82,82,82	0
56	MG	XA	1645	1/1	0.73	0.26	124,124,124,124	0
56	MG	YA	3380	1/1	0.73	0.27	43,43,43,43	0
56	MG	QA	1648	1/1	0.73	0.12	112,112,112,112	0
56	MG	RA	3986	1/1	0.73	0.46	124,124,124,124	0
56	MG	YA	3282	1/1	0.73	0.39	88,88,88,88	0
56	MG	RA	3943	1/1	0.73	0.40	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3818	1/1	0.73	0.14	86,86,86,86	0
56	MG	YA	3401	1/1	0.73	0.35	68,68,68,68	0
56	MG	RA	3859	1/1	0.73	0.19	107,107,107,107	0
56	MG	RA	3457	1/1	0.73	0.29	92,92,92,92	0
56	MG	RA	3036	1/1	0.73	0.20	105,105,105,105	0
56	MG	YA	3580	1/1	0.73	0.13	50,50,50,50	0
56	MG	XA	1670	1/1	0.73	0.27	90,90,90,90	0
56	MG	RA	3956	1/1	0.73	0.19	86,86,86,86	0
56	MG	YA	3049	1/1	0.73	0.30	82,82,82,82	0
56	MG	RA	3201	1/1	0.73	0.25	104,104,104,104	0
56	MG	RW	202	1/1	0.73	0.31	101,101,101,101	0
56	MG	QA	1698	1/1	0.73	0.16	81,81,81,81	0
56	MG	YA	3152	1/1	0.73	0.21	76,76,76,76	0
56	MG	XA	1774	1/1	0.73	0.21	74,74,74,74	0
56	MG	RA	3372	1/1	0.73	0.11	48,48,48,48	0
56	MG	RA	3697	1/1	0.73	0.38	84,84,84,84	0
56	MG	QT	201	1/1	0.73	0.21	89,89,89,89	0
56	MG	RA	3650	1/1	0.73	0.25	88,88,88,88	0
56	MG	RA	3373	1/1	0.73	0.30	66,66,66,66	0
56	MG	YA	3336	1/1	0.73	0.23	99,99,99,99	0
56	MG	RA	3772	1/1	0.73	0.47	122,122,122,122	0
56	MG	RA	3728	1/1	0.73	0.18	98,98,98,98	0
56	MG	YA	3349	1/1	0.73	0.36	77,77,77,77	0
56	MG	XR	101	1/1	0.73	0.27	107,107,107,107	0
56	MG	YA	3442	1/1	0.73	0.40	92,92,92,92	0
56	MG	YA	3443	1/1	0.73	0.40	80,80,80,80	0
56	MG	YA	3243	1/1	0.73	0.18	120,120,120,120	0
56	MG	RA	3973	1/1	0.73	0.44	82,82,82,82	0
56	MG	YA	3528	1/1	0.73	0.21	67,67,67,67	0
56	MG	RA	3512	1/1	0.73	0.59	117,117,117,117	0
56	MG	RA	3241	1/1	0.73	0.55	117,117,117,117	0
56	MG	YA	3260	1/1	0.73	0.57	92,92,92,92	0
56	MG	RA	4002	1/1	0.74	0.25	102,102,102,102	0
56	MG	QA	1818	1/1	0.74	0.28	119,119,119,119	0
56	MG	YA	3118	1/1	0.74	0.25	48,48,48,48	0
56	MG	QA	1662	1/1	0.74	0.18	123,123,123,123	0
56	MG	RA	4010	1/1	0.74	0.24	127,127,127,127	0
56	MG	RA	3594	1/1	0.74	0.92	112,112,112,112	0
56	MG	RA	3179	1/1	0.74	0.58	133,133,133,133	0
56	MG	YA	3468	1/1	0.74	0.19	73,73,73,73	0
56	MG	RA	3022	1/1	0.74	0.11	83,83,83,83	0
56	MG	RA	3405	1/1	0.74	0.15	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3147	1/1	0.74	0.26	49,49,49,49	0
56	MG	YA	3709	1/1	0.74	0.34	82,82,82,82	0
56	MG	RA	3062	1/1	0.74	0.14	75,75,75,75	0
56	MG	YA	3150	1/1	0.74	0.30	117,117,117,117	0
56	MG	RA	3954	1/1	0.74	0.18	84,84,84,84	0
56	MG	YA	3262	1/1	0.74	0.17	79,79,79,79	0
56	MG	RA	3776	1/1	0.74	0.22	63,63,63,63	0
56	MG	YA	3155	1/1	0.74	0.38	141,141,141,141	0
56	MG	QA	1618	1/1	0.74	0.17	130,130,130,130	0
56	MG	RA	3838	1/1	0.74	0.14	71,71,71,71	0
56	MG	RA	3455	1/1	0.74	0.21	65,65,65,65	0
56	MG	RA	3618	1/1	0.74	0.27	110,110,110,110	0
56	MG	XA	1759	1/1	0.74	0.21	61,61,61,61	0
56	MG	RA	3190	1/1	0.74	0.51	160,160,160,160	0
56	MG	YA	3505	1/1	0.74	0.31	99,99,99,99	0
56	MG	QA	1635	1/1	0.74	0.21	88,88,88,88	0
56	MG	XA	1767	1/1	0.74	0.28	84,84,84,84	0
56	MG	RA	3084	1/1	0.74	0.27	84,84,84,84	0
56	MG	RA	3377	1/1	0.74	0.21	75,75,75,75	0
56	MG	YA	3510	1/1	0.74	0.21	49,49,49,49	0
56	MG	QA	1639	1/1	0.74	0.15	113,113,113,113	0
56	MG	RA	3434	1/1	0.74	0.17	101,101,101,101	0
56	MG	RA	3553	1/1	0.74	0.38	55,55,55,55	0
56	MG	XA	1675	1/1	0.74	0.27	80,80,80,80	0
56	MG	YA	3519	1/1	0.74	0.32	89,89,89,89	0
56	MG	RA	3010	1/1	0.74	0.14	97,97,97,97	0
56	MG	RA	3246	1/1	0.74	0.31	111,111,111,111	0
56	MG	RA	3977	1/1	0.74	0.37	99,99,99,99	0
56	MG	QA	1645	1/1	0.74	0.17	90,90,90,90	0
56	MG	RA	3666	1/1	0.74	0.19	74,74,74,74	0
56	MG	QA	1697	1/1	0.74	0.35	94,94,94,94	0
56	MG	RA	3298	1/1	0.74	0.41	104,104,104,104	0
56	MG	QA	1699	1/1	0.74	0.13	118,118,118,118	0
56	MG	RA	3723	1/1	0.74	0.18	91,91,91,91	0
56	MG	QA	1651	1/1	0.74	0.16	109,109,109,109	0
56	MG	RA	3987	1/1	0.74	0.22	114,114,114,114	0
56	MG	RA	3538	1/1	0.74	0.28	102,102,102,102	0
56	MG	RD	313	1/1	0.74	0.39	109,109,109,109	0
56	MG	RD	314	1/1	0.74	0.24	120,120,120,120	0
57	ZN	Y9	101	1/1	0.74	0.28	276,276,276,276	0
56	MG	YA	3039	1/1	0.75	0.16	77,77,77,77	0
56	MG	RA	3874	1/1	0.75	0.14	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1602	1/1	0.75	0.12	92,92,92,92	0
56	MG	RA	3187	1/1	0.75	0.14	64,64,64,64	0
56	MG	YA	3240	1/1	0.75	0.32	75,75,75,75	0
56	MG	RE	305	1/1	0.75	0.27	49,49,49,49	0
56	MG	RA	3892	1/1	0.75	0.21	91,91,91,91	0
56	MG	YA	3247	1/1	0.75	0.53	141,141,141,141	0
56	MG	QA	1720	1/1	0.75	0.30	105,105,105,105	0
56	MG	YA	3156	1/1	0.75	0.36	85,85,85,85	0
56	MG	RA	3238	1/1	0.75	0.27	102,102,102,102	0
56	MG	YA	3390	1/1	0.75	0.46	78,78,78,78	0
56	MG	XA	1619	1/1	0.75	0.13	139,139,139,139	0
56	MG	XA	1719	1/1	0.75	0.13	87,87,87,87	0
56	MG	RA	3286	1/1	0.75	0.22	131,131,131,131	0
56	MG	YA	3394	1/1	0.75	0.22	71,71,71,71	0
56	MG	YA	3582	1/1	0.75	0.17	71,71,71,71	0
56	MG	XA	1724	1/1	0.75	0.22	105,105,105,105	0
56	MG	RA	3623	1/1	0.75	0.52	170,170,170,170	0
56	MG	XA	1735	1/1	0.75	0.26	97,97,97,97	0
56	MG	QA	1603	1/1	0.75	0.28	125,125,125,125	0
56	MG	RA	3450	1/1	0.75	0.14	83,83,83,83	0
56	MG	QA	1812	1/1	0.75	0.13	90,90,90,90	0
56	MG	QA	1685	1/1	0.75	0.19	76,76,76,76	0
56	MG	RA	3451	1/1	0.75	0.21	79,79,79,79	0
56	MG	YA	3491	1/1	0.75	0.16	92,92,92,92	0
56	MG	XA	1642	1/1	0.75	0.11	108,108,108,108	0
56	MG	YA	3081	1/1	0.75	0.17	125,125,125,125	0
56	MG	RA	3510	1/1	0.75	0.29	70,70,70,70	0
56	MG	XA	1647	1/1	0.75	0.17	163,163,163,163	0
56	MG	RA	3901	1/1	0.75	0.15	79,79,79,79	0
56	MG	RA	3716	1/1	0.75	0.26	91,91,91,91	0
56	MG	YA	3726	1/1	0.75	0.39	105,105,105,105	0
56	MG	YA	3619	1/1	0.75	0.22	89,89,89,89	0
56	MG	QA	1692	1/1	0.75	0.11	135,135,135,135	0
56	MG	RA	3003	1/1	0.75	0.08	55,55,55,55	0
56	MG	YA	3190	1/1	0.75	0.35	130,130,130,130	0
56	MG	QA	1654	1/1	0.75	0.13	120,120,120,120	0
56	MG	YA	3631	1/1	0.75	0.34	71,71,71,71	0
56	MG	RA	4001	1/1	0.75	0.31	74,74,74,74	0
56	MG	RA	3274	1/1	0.75	0.12	90,90,90,90	0
56	MG	RA	3174	1/1	0.75	0.52	120,120,120,120	0
56	MG	YA	3208	1/1	0.75	0.12	78,78,78,78	0
56	MG	RA	3783	1/1	0.75	0.29	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1783	1/1	0.75	0.11	141,141,141,141	0
56	MG	RA	3232	1/1	0.75	0.17	98,98,98,98	0
56	MG	YA	3439	1/1	0.75	0.08	84,84,84,84	0
56	MG	QA	1749	1/1	0.75	0.31	111,111,111,111	0
56	MG	QA	1622	1/1	0.75	0.15	97,97,97,97	0
56	MG	RA	3921	1/1	0.75	0.28	49,49,49,49	0
56	MG	RQ	206	1/1	0.75	0.23	88,88,88,88	0
56	MG	RD	311	1/1	0.75	0.17	103,103,103,103	0
56	MG	YA	3028	1/1	0.75	0.16	51,51,51,51	0
56	MG	YA	3656	1/1	0.75	0.34	38,38,38,38	0
56	MG	RB	202	1/1	0.75	0.17	118,118,118,118	0
56	MG	YA	3543	1/1	0.75	0.24	84,84,84,84	0
56	MG	RA	3490	1/1	0.75	0.29	54,54,54,54	0
56	MG	XA	1708	1/1	0.76	0.38	89,89,89,89	0
56	MG	QE	201	1/1	0.76	0.26	105,105,105,105	0
56	MG	YA	3036	1/1	0.76	0.33	127,127,127,127	0
56	MG	YA	3038	1/1	0.76	0.09	73,73,73,73	0
56	MG	RA	3717	1/1	0.76	0.14	79,79,79,79	0
56	MG	RA	3976	1/1	0.76	0.34	101,101,101,101	0
56	MG	YA	3717	1/1	0.76	0.24	50,50,50,50	0
56	MG	RA	3097	1/1	0.76	0.15	92,92,92,92	0
56	MG	QA	1723	1/1	0.76	0.17	87,87,87,87	0
56	MG	YA	3196	1/1	0.76	0.36	114,114,114,114	0
56	MG	YA	3377	1/1	0.76	0.16	84,84,84,84	0
56	MG	RA	3243	1/1	0.76	0.13	106,106,106,106	0
56	MG	RA	3317	1/1	0.76	0.23	86,86,86,86	0
56	MG	YA	3382	1/1	0.76	0.12	112,112,112,112	0
56	MG	RA	3661	1/1	0.76	0.23	98,98,98,98	0
56	MG	RA	3707	1/1	0.76	0.18	94,94,94,94	0
56	MG	YA	3056	1/1	0.76	0.13	90,90,90,90	0
56	MG	RA	3256	1/1	0.76	0.24	132,132,132,132	0
56	MG	XA	1654	1/1	0.76	0.13	119,119,119,119	0
56	MG	YA	3461	1/1	0.76	0.26	84,84,84,84	0
56	MG	RA	3755	1/1	0.76	0.38	107,107,107,107	0
56	MG	YA	3399	1/1	0.76	0.23	108,108,108,108	0
56	MG	YA	3296	1/1	0.76	0.27	109,109,109,109	0
56	MG	QA	1706	1/1	0.76	0.15	100,100,100,100	0
56	MG	XA	1762	1/1	0.76	0.14	125,125,125,125	0
56	MG	YA	3216	1/1	0.76	0.28	132,132,132,132	0
56	MG	YA	3473	1/1	0.76	0.23	59,59,59,59	0
56	MG	YE	302	1/1	0.76	0.24	83,83,83,83	0
56	MG	RA	3166	1/1	0.76	0.13	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1770	1/1	0.76	0.35	86,86,86,86	0
56	MG	RB	218	1/1	0.76	0.30	64,64,64,64	0
56	MG	QA	1787	1/1	0.76	0.24	84,84,84,84	0
56	MG	YF	302	1/1	0.76	0.12	69,69,69,69	0
56	MG	YG	201	1/1	0.76	0.14	111,111,111,111	0
56	MG	YA	3478	1/1	0.76	0.21	115,115,115,115	0
56	MG	YA	3305	1/1	0.76	0.21	85,85,85,85	0
56	MG	RA	3854	1/1	0.76	0.24	55,55,55,55	0
56	MG	QA	1814	1/1	0.76	0.22	81,81,81,81	0
56	MG	YT	201	1/1	0.76	0.16	96,96,96,96	0
56	MG	YA	3083	1/1	0.76	0.42	85,85,85,85	0
56	MG	YA	3415	1/1	0.76	0.32	81,81,81,81	0
56	MG	YA	3084	1/1	0.76	0.14	85,85,85,85	0
56	MG	YA	3591	1/1	0.76	0.30	88,88,88,88	0
56	MG	XA	1694	1/1	0.76	0.31	66,66,66,66	0
56	MG	QA	1763	1/1	0.76	0.24	102,102,102,102	0
56	MG	YA	3493	1/1	0.76	0.20	89,89,89,89	0
56	MG	YA	3693	1/1	0.76	0.36	58,58,58,58	0
56	MG	QA	1791	1/1	0.76	0.30	111,111,111,111	0
56	MG	RA	3690	1/1	0.76	0.18	72,72,72,72	0
56	MG	RA	3458	1/1	0.76	0.28	87,87,87,87	0
56	MG	RA	3615	1/1	0.76	0.20	59,59,59,59	0
56	MG	YA	3246	1/1	0.76	0.46	100,100,100,100	0
56	MG	RA	3795	1/1	0.76	0.11	90,90,90,90	0
56	MG	YA	3343	1/1	0.77	0.33	64,64,64,64	0
56	MG	QA	1674	1/1	0.77	0.16	144,144,144,144	0
56	MG	YA	3142	1/1	0.77	0.35	106,106,106,106	0
56	MG	YA	3037	1/1	0.77	0.26	99,99,99,99	0
56	MG	RA	3869	1/1	0.77	0.32	56,56,56,56	0
56	MG	RA	3566	1/1	0.77	0.64	111,111,111,111	0
56	MG	RA	3810	1/1	0.77	0.14	145,145,145,145	0
56	MG	RA	3414	1/1	0.77	0.33	43,43,43,43	0
56	MG	QA	1850	1/1	0.77	0.41	96,96,96,96	0
56	MG	RA	3571	1/1	0.77	0.21	69,69,69,69	0
56	MG	RA	3719	1/1	0.77	0.25	109,109,109,109	0
56	MG	R3	101	1/1	0.77	0.33	97,97,97,97	0
56	MG	RA	3763	1/1	0.77	0.20	86,86,86,86	0
56	MG	RA	3017	1/1	0.77	0.29	103,103,103,103	0
56	MG	RA	3279	1/1	0.77	0.15	144,144,144,144	0
56	MG	RA	3339	1/1	0.77	0.26	69,69,69,69	0
56	MG	XA	1750	1/1	0.77	0.18	89,89,89,89	0
56	MG	QH	201	1/1	0.77	0.28	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3554	1/1	0.77	0.22	69,69,69,69	0
56	MG	RA	3691	1/1	0.77	0.33	80,80,80,80	0
56	MG	YA	3561	1/1	0.77	0.34	63,63,63,63	0
56	MG	RA	3456	1/1	0.77	0.30	58,58,58,58	0
56	MG	RA	3729	1/1	0.77	0.19	103,103,103,103	0
56	MG	RF	308	1/1	0.77	0.56	127,127,127,127	0
56	MG	YI	201	1/1	0.77	0.07	103,103,103,103	0
56	MG	XA	1678	1/1	0.77	0.22	117,117,117,117	0
56	MG	QA	1778	1/1	0.77	0.41	93,93,93,93	0
56	MG	RA	3693	1/1	0.77	0.26	86,86,86,86	0
56	MG	QA	1741	1/1	0.77	0.32	84,84,84,84	0
56	MG	RA	3169	1/1	0.77	0.19	72,72,72,72	0
56	MG	YX	101	1/1	0.77	0.28	60,60,60,60	0
56	MG	RA	3080	1/1	0.77	0.36	142,142,142,142	0
56	MG	QA	1661	1/1	0.77	0.26	121,121,121,121	0
56	MG	YA	3094	1/1	0.77	0.16	63,63,63,63	0
56	MG	RA	3184	1/1	0.77	0.41	142,142,142,142	0
56	MG	RA	3590	1/1	0.77	0.46	129,129,129,129	0
56	MG	RA	3267	1/1	0.77	0.56	144,144,144,144	0
56	MG	YA	3019	1/1	0.77	0.42	99,99,99,99	0
56	MG	YA	3421	1/1	0.77	0.33	100,100,100,100	0
56	MG	YA	3699	1/1	0.77	0.39	99,99,99,99	0
56	MG	RA	3428	1/1	0.77	0.14	71,71,71,71	0
56	MG	RA	3709	1/1	0.77	0.13	84,84,84,84	0
56	MG	YA	3110	1/1	0.77	0.18	109,109,109,109	0
56	MG	QA	1753	1/1	0.77	0.23	79,79,79,79	0
56	MG	RA	3501	1/1	0.77	0.14	83,83,83,83	0
56	MG	RA	3332	1/1	0.77	0.28	101,101,101,101	0
56	MG	YA	3030	1/1	0.77	0.46	115,115,115,115	0
56	MG	YA	3625	1/1	0.77	0.35	102,102,102,102	0
56	MG	RB	224	1/1	0.77	0.11	127,127,127,127	0
56	MG	RA	3670	1/1	0.77	0.24	78,78,78,78	0
56	MG	YA	3053	1/1	0.78	0.24	79,79,79,79	0
56	MG	YA	3667	1/1	0.78	0.24	54,54,54,54	0
56	MG	RA	3090	1/1	0.78	0.18	111,111,111,111	0
56	MG	RA	3617	1/1	0.78	0.18	105,105,105,105	0
56	MG	YA	3361	1/1	0.78	0.28	67,67,67,67	0
56	MG	Y7	101	1/1	0.78	0.29	79,79,79,79	0
56	MG	Y7	102	1/1	0.78	0.45	147,147,147,147	0
56	MG	RA	3397	1/1	0.78	0.14	61,61,61,61	0
56	MG	RA	3186	1/1	0.78	0.15	97,97,97,97	0
56	MG	RA	3137	1/1	0.78	0.12	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3842	1/1	0.78	0.19	76,76,76,76	0
56	MG	RA	3058	1/1	0.78	0.18	113,113,113,113	0
56	MG	RA	3167	1/1	0.78	0.12	96,96,96,96	0
56	MG	QA	1823	1/1	0.78	0.14	106,106,106,106	0
56	MG	YA	3566	1/1	0.78	0.40	147,147,147,147	0
56	MG	RA	3126	1/1	0.78	0.19	75,75,75,75	0
56	MG	YA	3571	1/1	0.78	0.14	70,70,70,70	0
56	MG	RA	3437	1/1	0.78	0.21	92,92,92,92	0
56	MG	QA	1788	1/1	0.78	0.18	102,102,102,102	0
56	MG	XA	1620	1/1	0.78	0.12	81,81,81,81	0
56	MG	YA	3277	1/1	0.78	0.17	72,72,72,72	0
56	MG	RA	3337	1/1	0.78	0.29	76,76,76,76	0
56	MG	RA	3171	1/1	0.78	0.21	83,83,83,83	0
56	MG	QV	106	1/1	0.78	0.13	112,112,112,112	0
56	MG	YA	3480	1/1	0.78	0.23	87,87,87,87	0
56	MG	YA	3706	1/1	0.78	0.11	105,105,105,105	0
56	MG	RA	3194	1/1	0.78	0.26	76,76,76,76	0
56	MG	RA	3753	1/1	0.78	0.30	63,63,63,63	0
56	MG	RA	3077	1/1	0.78	0.63	90,90,90,90	0
56	MG	RA	3420	1/1	0.78	0.29	90,90,90,90	0
56	MG	RQ	203	1/1	0.78	0.16	85,85,85,85	0
56	MG	XA	1758	1/1	0.78	0.36	65,65,65,65	0
56	MG	RA	3042	1/1	0.78	0.13	68,68,68,68	0
56	MG	RT	201	1/1	0.78	0.21	110,110,110,110	0
56	MG	YA	3723	1/1	0.78	0.14	92,92,92,92	0
56	MG	YA	3615	1/1	0.78	0.19	78,78,78,78	0
56	MG	RA	3175	1/1	0.78	0.58	120,120,120,120	0
56	MG	RA	3721	1/1	0.78	0.28	111,111,111,111	0
56	MG	YA	3106	1/1	0.78	0.15	66,66,66,66	0
56	MG	YA	3497	1/1	0.78	0.26	94,94,94,94	0
56	MG	YA	3303	1/1	0.78	0.21	55,55,55,55	0
56	MG	YA	3624	1/1	0.78	0.33	73,73,73,73	0
56	MG	YB	211	1/1	0.78	0.24	88,88,88,88	0
56	MG	QA	1845	1/1	0.78	0.14	124,124,124,124	0
56	MG	YA	3309	1/1	0.78	0.22	50,50,50,50	0
56	MG	YA	3422	1/1	0.78	0.31	58,58,58,58	0
56	MG	RA	3532	1/1	0.78	0.13	147,147,147,147	0
56	MG	RA	3682	1/1	0.78	0.41	114,114,114,114	0
56	MG	RA	3176	1/1	0.78	0.19	91,91,91,91	0
56	MG	YA	3123	1/1	0.78	0.11	84,84,84,84	0
56	MG	YA	3432	1/1	0.78	0.15	68,68,68,68	0
56	MG	YA	3219	1/1	0.78	0.21	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3018	1/1	0.78	0.44	150,150,150,150	0
56	MG	XK	201	1/1	0.78	0.11	82,82,82,82	0
56	MG	RE	302	1/1	0.78	0.50	105,105,105,105	0
56	MG	RA	3099	1/1	0.78	0.41	114,114,114,114	0
56	MG	RA	3828	1/1	0.78	0.16	115,115,115,115	0
56	MG	YA	3134	1/1	0.78	0.17	78,78,78,78	0
56	MG	QA	1854	1/1	0.78	0.09	97,97,97,97	0
56	MG	YA	3346	1/1	0.78	0.27	72,72,72,72	0
56	MG	R7	102	1/1	0.78	0.18	69,69,69,69	0
56	MG	YA	3536	1/1	0.78	0.29	72,72,72,72	0
56	MG	RB	206	1/1	0.78	0.13	123,123,123,123	0
56	MG	QA	1649	1/1	0.78	0.21	83,83,83,83	0
56	MG	RA	3239	1/1	0.79	0.56	155,155,155,155	0
56	MG	RA	3938	1/1	0.79	0.19	79,79,79,79	0
56	MG	RA	3280	1/1	0.79	0.19	98,98,98,98	0
56	MG	YA	3093	1/1	0.79	0.16	59,59,59,59	0
56	MG	RA	3860	1/1	0.79	0.23	87,87,87,87	0
56	MG	RA	3531	1/1	0.79	0.41	104,104,104,104	0
56	MG	QQ	201	1/1	0.79	0.10	103,103,103,103	0
56	MG	RA	3734	1/1	0.79	0.26	151,151,151,151	0
56	MG	RA	3596	1/1	0.79	0.48	137,137,137,137	0
56	MG	YA	3487	1/1	0.79	0.13	77,77,77,77	0
56	MG	QT	202	1/1	0.79	0.33	87,87,87,87	0
56	MG	QA	1811	1/1	0.79	0.18	93,93,93,93	0
56	MG	RA	3599	1/1	0.79	0.28	102,102,102,102	0
56	MG	RA	3011	1/1	0.79	0.18	107,107,107,107	0
56	MG	RA	3882	1/1	0.79	0.18	41,41,41,41	0
56	MG	QA	1700	1/1	0.79	0.28	73,73,73,73	0
56	MG	YA	3393	1/1	0.79	0.23	97,97,97,97	0
56	MG	YA	3241	1/1	0.79	0.18	107,107,107,107	0
56	MG	RA	3698	1/1	0.79	0.54	130,130,130,130	0
56	MG	YA	3006	1/1	0.79	0.15	72,72,72,72	0
56	MG	RA	3885	1/1	0.79	0.26	119,119,119,119	0
56	MG	XA	1714	1/1	0.79	0.33	99,99,99,99	0
56	MG	RA	3886	1/1	0.79	0.38	66,66,66,66	0
56	MG	RA	3887	1/1	0.79	0.21	80,80,80,80	0
56	MG	RA	3699	1/1	0.79	0.54	85,85,85,85	0
56	MG	RA	3967	1/1	0.79	0.42	109,109,109,109	0
56	MG	YA	3136	1/1	0.79	0.25	100,100,100,100	0
56	MG	YA	3512	1/1	0.79	0.47	141,141,141,141	0
56	MG	QA	1711	1/1	0.79	0.15	136,136,136,136	0
56	MG	YA	3515	1/1	0.79	0.30	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1655	1/1	0.79	0.21	87,87,87,87	0
56	MG	YA	3263	1/1	0.79	0.30	66,66,66,66	0
56	MG	XA	1610	1/1	0.79	0.42	85,85,85,85	0
56	MG	RA	3283	1/1	0.79	0.19	147,147,147,147	0
56	MG	RA	3608	1/1	0.79	0.23	61,61,61,61	0
56	MG	YA	3416	1/1	0.79	0.31	83,83,83,83	0
56	MG	RA	3141	1/1	0.79	0.23	110,110,110,110	0
56	MG	RA	3225	1/1	0.79	0.31	137,137,137,137	0
56	MG	XA	1747	1/1	0.79	0.28	65,65,65,65	0
56	MG	RA	3752	1/1	0.79	0.40	76,76,76,76	0
56	MG	RA	3142	1/1	0.79	0.09	59,59,59,59	0
56	MG	RA	3379	1/1	0.79	0.41	62,62,62,62	0
56	MG	YA	3284	1/1	0.79	0.26	65,65,65,65	0
56	MG	RA	3567	1/1	0.79	0.33	97,97,97,97	0
56	MG	RA	3328	1/1	0.79	0.35	47,47,47,47	0
56	MG	YA	3161	1/1	0.79	0.29	110,110,110,110	0
56	MG	RA	3543	1/1	0.79	0.26	77,77,77,77	0
56	MG	QA	1728	1/1	0.79	0.14	72,72,72,72	0
56	MG	YA	3696	1/1	0.79	0.36	65,65,65,65	0
56	MG	RA	3154	1/1	0.79	0.19	106,106,106,106	0
56	MG	YA	3171	1/1	0.79	0.26	125,125,125,125	0
56	MG	QA	1844	1/1	0.79	0.31	94,94,94,94	0
56	MG	YA	3050	1/1	0.79	0.36	100,100,100,100	0
56	MG	RA	4000	1/1	0.79	0.26	77,77,77,77	0
56	MG	YA	3445	1/1	0.79	0.28	75,75,75,75	0
56	MG	YA	3707	1/1	0.79	0.15	109,109,109,109	0
56	MG	RA	3484	1/1	0.79	0.27	83,83,83,83	0
56	MG	YA	3178	1/1	0.79	0.17	89,89,89,89	0
56	MG	RA	3578	1/1	0.79	0.13	112,112,112,112	0
56	MG	QA	1734	1/1	0.79	0.25	89,89,89,89	0
56	MG	YA	3319	1/1	0.79	0.18	84,84,84,84	0
56	MG	QA	1615	1/1	0.79	0.12	123,123,123,123	0
56	MG	RA	3012	1/1	0.79	0.26	106,106,106,106	0
56	MG	RA	3162	1/1	0.79	0.51	132,132,132,132	0
56	MG	RA	3722	1/1	0.79	0.23	79,79,79,79	0
56	MG	QA	1623	1/1	0.79	0.08	172,172,172,172	0
56	MG	RA	3248	1/1	0.79	0.34	116,116,116,116	0
56	MG	XV	103	1/1	0.79	0.20	77,77,77,77	0
56	MG	YB	202	1/1	0.79	0.12	88,88,88,88	0
56	MG	YA	3197	1/1	0.79	0.17	65,65,65,65	0
56	MG	RA	3400	1/1	0.79	0.13	90,90,90,90	0
56	MG	YB	206	1/1	0.79	0.47	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3632	1/1	0.79	0.22	77,77,77,77	0
56	MG	QA	1634	1/1	0.79	0.08	110,110,110,110	0
56	MG	RA	3074	1/1	0.79	0.17	60,60,60,60	0
56	MG	RA	3491	1/1	0.79	0.36	65,65,65,65	0
56	MG	RA	3306	1/1	0.80	0.56	139,139,139,139	0
56	MG	RA	3465	1/1	0.80	0.38	60,60,60,60	0
56	MG	RA	3401	1/1	0.80	0.29	67,67,67,67	0
56	MG	RA	3104	1/1	0.80	0.41	134,134,134,134	0
56	MG	RA	3282	1/1	0.80	0.20	90,90,90,90	0
56	MG	XA	1698	1/1	0.80	0.20	90,90,90,90	0
56	MG	RA	3217	1/1	0.80	0.13	89,89,89,89	0
56	MG	R1	101	1/1	0.80	0.49	120,120,120,120	0
56	MG	RA	3436	1/1	0.80	0.28	85,85,85,85	0
56	MG	RA	3311	1/1	0.80	0.33	107,107,107,107	0
56	MG	RA	3820	1/1	0.80	0.14	106,106,106,106	0
56	MG	XA	1706	1/1	0.80	0.18	62,62,62,62	0
56	MG	QA	1715	1/1	0.80	0.35	60,60,60,60	0
56	MG	RA	3971	1/1	0.80	0.19	53,53,53,53	0
56	MG	RA	3313	1/1	0.80	0.17	48,48,48,48	0
56	MG	YA	3345	1/1	0.80	0.27	72,72,72,72	0
56	MG	QA	1601	1/1	0.80	0.22	136,136,136,136	0
56	MG	RA	3526	1/1	0.80	0.12	78,78,78,78	0
56	MG	RA	3823	1/1	0.80	0.25	116,116,116,116	0
56	MG	RA	3233	1/1	0.80	0.22	88,88,88,88	0
56	MG	RA	3612	1/1	0.80	0.14	71,71,71,71	0
56	MG	RA	3004	1/1	0.80	0.19	123,123,123,123	0
56	MG	RA	3375	1/1	0.80	0.28	54,54,54,54	0
56	MG	RA	3985	1/1	0.80	0.12	71,71,71,71	0
56	MG	YA	3700	1/1	0.80	0.34	100,100,100,100	0
56	MG	RA	3318	1/1	0.80	0.14	67,67,67,67	0
56	MG	RA	3445	1/1	0.80	0.19	63,63,63,63	0
56	MG	YA	3143	1/1	0.80	0.11	79,79,79,79	0
56	MG	RA	3919	1/1	0.80	0.30	98,98,98,98	0
56	MG	XA	1738	1/1	0.80	0.25	55,55,55,55	0
56	MG	YA	3146	1/1	0.80	0.43	101,101,101,101	0
56	MG	RA	3768	1/1	0.80	0.15	69,69,69,69	0
56	MG	XA	1626	1/1	0.80	0.10	93,93,93,93	0
56	MG	XA	1629	1/1	0.80	0.17	89,89,89,89	0
56	MG	YA	3041	1/1	0.80	0.17	71,71,71,71	0
56	MG	RA	3183	1/1	0.80	0.28	104,104,104,104	0
56	MG	XA	1635	1/1	0.80	0.14	98,98,98,98	0
56	MG	QA	1616	1/1	0.80	0.16	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3255	1/1	0.80	0.17	77,77,77,77	0
56	MG	YA	3392	1/1	0.80	0.31	38,38,38,38	0
56	MG	RA	3492	1/1	0.80	0.27	50,50,50,50	0
56	MG	XA	1643	1/1	0.80	0.20	84,84,84,84	0
56	MG	RA	4009	1/1	0.80	0.25	73,73,73,73	0
56	MG	RA	3449	1/1	0.80	0.26	73,73,73,73	0
56	MG	RA	4014	1/1	0.80	0.16	83,83,83,83	0
56	MG	XA	1648	1/1	0.80	0.29	100,100,100,100	0
56	MG	XA	1649	1/1	0.80	0.29	105,105,105,105	0
56	MG	YA	3733	1/1	0.80	0.30	38,38,38,38	0
56	MG	RA	3625	1/1	0.80	0.72	98,98,98,98	0
56	MG	RA	3387	1/1	0.80	0.52	52,52,52,52	0
56	MG	QA	1853	1/1	0.80	0.12	133,133,133,133	0
56	MG	RA	3041	1/1	0.80	0.28	109,109,109,109	0
56	MG	YA	3169	1/1	0.80	0.15	112,112,112,112	0
56	MG	RA	3223	1/1	0.80	0.44	157,157,157,157	0
56	MG	YA	3058	1/1	0.80	0.20	83,83,83,83	0
56	MG	YA	3410	1/1	0.80	0.30	74,74,74,74	0
56	MG	QA	1746	1/1	0.80	0.32	95,95,95,95	0
56	MG	RA	3678	1/1	0.80	0.19	82,82,82,82	0
56	MG	RA	3157	1/1	0.80	0.32	119,119,119,119	0
56	MG	XA	1671	1/1	0.80	0.32	140,140,140,140	0
56	MG	RA	3506	1/1	0.80	0.18	76,76,76,76	0
56	MG	RA	3683	1/1	0.80	0.15	74,74,74,74	0
56	MG	RA	3685	1/1	0.80	0.22	72,72,72,72	0
56	MG	RA	3947	1/1	0.80	0.17	91,91,91,91	0
56	MG	YA	3513	1/1	0.80	0.32	76,76,76,76	0
56	MG	RA	3583	1/1	0.80	0.21	87,87,87,87	0
56	MG	YA	3184	1/1	0.80	0.53	133,133,133,133	0
56	MG	RA	3331	1/1	0.80	0.24	96,96,96,96	0
56	MG	RR	202	1/1	0.80	0.51	114,114,114,114	0
56	MG	RA	3082	1/1	0.80	0.47	140,140,140,140	0
56	MG	YA	3304	1/1	0.80	0.26	80,80,80,80	0
56	MG	YA	3191	1/1	0.80	0.16	105,105,105,105	0
56	MG	YA	3525	1/1	0.80	0.20	40,40,40,40	0
56	MG	RA	3903	1/1	0.81	0.24	78,78,78,78	0
56	MG	RA	3904	1/1	0.81	0.23	64,64,64,64	0
56	MG	YA	3629	1/1	0.81	0.33	103,103,103,103	0
56	MG	RA	3308	1/1	0.81	0.27	61,61,61,61	0
56	MG	YA	3521	1/1	0.81	0.25	90,90,90,90	0
56	MG	RA	3694	1/1	0.81	0.32	110,110,110,110	0
56	MG	YA	3741	1/1	0.81	0.28	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3285	1/1	0.81	0.34	59,59,59,59	0
56	MG	XA	1632	1/1	0.81	0.25	71,71,71,71	0
56	MG	YA	3140	1/1	0.81	0.15	94,94,94,94	0
56	MG	RA	3500	1/1	0.81	0.35	63,63,63,63	0
56	MG	RX	101	1/1	0.81	0.25	81,81,81,81	0
56	MG	RA	3229	1/1	0.81	0.46	146,146,146,146	0
56	MG	YA	3003	1/1	0.81	0.33	92,92,92,92	0
56	MG	RA	3778	1/1	0.81	0.28	101,101,101,101	0
56	MG	XA	1732	1/1	0.81	0.23	77,77,77,77	0
56	MG	RA	3645	1/1	0.81	0.19	75,75,75,75	0
56	MG	RA	3602	1/1	0.81	0.32	116,116,116,116	0
56	MG	QA	1774	1/1	0.81	0.10	101,101,101,101	0
56	MG	RA	3871	1/1	0.81	0.26	91,91,91,91	0
56	MG	YB	216	1/1	0.81	0.18	87,87,87,87	0
56	MG	RA	3751	1/1	0.81	0.18	56,56,56,56	0
56	MG	YA	3549	1/1	0.81	0.28	87,87,87,87	0
56	MG	YA	3087	1/1	0.81	0.23	97,97,97,97	0
56	MG	XA	1653	1/1	0.81	0.33	99,99,99,99	0
56	MG	YA	3158	1/1	0.81	0.18	54,54,54,54	0
56	MG	YA	3663	1/1	0.81	0.17	75,75,75,75	0
56	MG	RA	3701	1/1	0.81	0.28	97,97,97,97	0
56	MG	QA	1709	1/1	0.81	0.26	87,87,87,87	0
56	MG	RA	3881	1/1	0.81	0.31	73,73,73,73	0
56	MG	XA	1660	1/1	0.81	0.14	116,116,116,116	0
56	MG	QA	1780	1/1	0.81	0.35	85,85,85,85	0
56	MG	YA	3485	1/1	0.81	0.30	85,85,85,85	0
56	MG	RA	3789	1/1	0.81	0.19	89,89,89,89	0
56	MG	YF	303	1/1	0.81	0.26	104,104,104,104	0
56	MG	XA	1766	1/1	0.81	0.26	75,75,75,75	0
56	MG	RA	3831	1/1	0.81	0.20	78,78,78,78	0
56	MG	YA	3570	1/1	0.81	0.56	82,82,82,82	0
56	MG	RA	3390	1/1	0.81	0.21	40,40,40,40	0
56	MG	RB	217	1/1	0.81	0.15	107,107,107,107	0
56	MG	YA	3245	1/1	0.81	0.09	135,135,135,135	0
56	MG	XA	1676	1/1	0.81	0.21	90,90,90,90	0
56	MG	RA	3252	1/1	0.81	0.40	120,120,120,120	0
56	MG	RA	3521	1/1	0.81	0.34	83,83,83,83	0
56	MG	XA	1681	1/1	0.81	0.14	112,112,112,112	0
56	MG	YA	3040	1/1	0.81	0.39	103,103,103,103	0
56	MG	YA	3586	1/1	0.81	0.21	39,39,39,39	0
56	MG	XA	1780	1/1	0.81	0.12	86,86,86,86	0
56	MG	RA	3299	1/1	0.81	0.11	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3496	1/1	0.81	0.34	78,78,78,78	0
56	MG	YA	3428	1/1	0.81	0.26	69,69,69,69	0
56	MG	RA	3312	1/1	0.81	0.27	99,99,99,99	0
56	MG	YA	3108	1/1	0.81	0.24	76,76,76,76	0
56	MG	RA	3509	1/1	0.81	0.23	95,95,95,95	0
56	MG	YA	3046	1/1	0.81	0.45	119,119,119,119	0
56	MG	YA	3113	1/1	0.81	0.31	112,112,112,112	0
56	MG	RA	3262	1/1	0.81	0.06	181,181,181,181	0
56	MG	YA	3614	1/1	0.81	0.24	47,47,47,47	0
56	MG	YA	3267	1/1	0.81	0.26	68,68,68,68	0
56	MG	RA	3476	1/1	0.81	0.24	61,61,61,61	0
56	MG	RA	3851	1/1	0.81	0.29	47,47,47,47	0
56	MG	YA	3364	1/1	0.81	0.28	77,77,77,77	0
56	MG	YA	3274	1/1	0.81	0.30	68,68,68,68	0
57	ZN	Y5	102	1/1	0.81	0.14	277,277,277,277	0
56	MG	RA	3263	1/1	0.81	0.13	101,101,101,101	0
56	MG	RA	3023	1/1	0.81	0.38	110,110,110,110	0
56	MG	YA	3012	1/1	0.82	0.23	90,90,90,90	0
56	MG	QA	1627	1/1	0.82	0.48	126,126,126,126	0
56	MG	QA	1629	1/1	0.82	0.09	86,86,86,86	0
56	MG	RW	201	1/1	0.82	0.12	83,83,83,83	0
56	MG	YA	3327	1/1	0.82	0.39	30,30,30,30	0
56	MG	YA	3420	1/1	0.82	0.22	65,65,65,65	0
56	MG	RA	3872	1/1	0.82	0.42	78,78,78,78	0
56	MG	RA	3495	1/1	0.82	0.23	96,96,96,96	0
56	MG	RA	3773	1/1	0.82	0.14	91,91,91,91	0
56	MG	YA	3501	1/1	0.82	0.37	89,89,89,89	0
56	MG	RA	3774	1/1	0.82	0.12	89,89,89,89	0
56	MG	QA	1724	1/1	0.82	0.27	82,82,82,82	0
56	MG	RA	3075	1/1	0.82	0.47	112,112,112,112	0
56	MG	RA	3777	1/1	0.82	0.25	65,65,65,65	0
56	MG	RA	3119	1/1	0.82	0.27	103,103,103,103	0
56	MG	XA	1630	1/1	0.82	0.19	85,85,85,85	0
56	MG	YA	3101	1/1	0.82	0.56	167,167,167,167	0
56	MG	RA	3656	1/1	0.82	0.18	110,110,110,110	0
56	MG	QA	1855	1/1	0.82	0.12	152,152,152,152	0
56	MG	YA	3259	1/1	0.82	0.28	94,94,94,94	0
56	MG	RA	3333	1/1	0.82	0.33	48,48,48,48	0
56	MG	RA	3889	1/1	0.82	0.24	60,60,60,60	0
56	MG	RA	3410	1/1	0.82	0.19	47,47,47,47	0
56	MG	YA	3517	1/1	0.82	0.19	81,81,81,81	0
56	MG	RA	3641	1/1	0.82	0.10	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3148	1/1	0.82	0.31	107,107,107,107	0
56	MG	YB	209	1/1	0.82	0.26	76,76,76,76	0
56	MG	YA	3189	1/1	0.82	0.24	80,80,80,80	0
56	MG	RB	214	1/1	0.82	0.10	93,93,93,93	0
56	MG	RA	3855	1/1	0.82	0.35	90,90,90,90	0
56	MG	YA	3373	1/1	0.82	0.23	65,65,65,65	0
56	MG	RA	3936	1/1	0.82	0.32	89,89,89,89	0
56	MG	YA	3529	1/1	0.82	0.24	90,90,90,90	0
56	MG	YA	3453	1/1	0.82	0.25	70,70,70,70	0
56	MG	YA	3379	1/1	0.82	0.39	57,57,57,57	0
56	MG	XA	1760	1/1	0.82	0.18	74,74,74,74	0
56	MG	YA	3195	1/1	0.82	0.14	69,69,69,69	0
56	MG	RA	3897	1/1	0.82	0.14	79,79,79,79	0
56	MG	XA	1763	1/1	0.82	0.28	81,81,81,81	0
56	MG	QA	1607	1/1	0.82	0.15	98,98,98,98	0
56	MG	YA	3458	1/1	0.82	0.29	79,79,79,79	0
56	MG	YA	3198	1/1	0.82	0.24	91,91,91,91	0
56	MG	XA	1662	1/1	0.82	0.14	119,119,119,119	0
56	MG	RA	3161	1/1	0.82	0.24	114,114,114,114	0
56	MG	XA	1665	1/1	0.82	0.13	81,81,81,81	0
56	MG	RA	3940	1/1	0.82	0.31	85,85,85,85	0
56	MG	RA	3088	1/1	0.82	0.15	117,117,117,117	0
56	MG	XA	1668	1/1	0.82	0.24	72,72,72,72	0
56	MG	YA	3665	1/1	0.82	0.33	58,58,58,58	0
56	MG	RA	3480	1/1	0.82	0.18	47,47,47,47	0
56	MG	YA	3668	1/1	0.82	0.20	42,42,42,42	0
56	MG	RA	3826	1/1	0.82	0.32	78,78,78,78	0
56	MG	RA	3902	1/1	0.82	0.27	67,67,67,67	0
56	MG	YA	3471	1/1	0.82	0.40	69,69,69,69	0
56	MG	YA	3398	1/1	0.82	0.44	66,66,66,66	0
56	MG	RA	3170	1/1	0.82	0.21	80,80,80,80	0
56	MG	YQ	201	1/1	0.82	0.21	84,84,84,84	0
56	MG	RA	3198	1/1	0.82	0.34	118,118,118,118	0
56	MG	YR	201	1/1	0.82	0.25	93,93,93,93	0
56	MG	QA	1617	1/1	0.82	0.11	129,129,129,129	0
56	MG	XL	201	1/1	0.82	0.16	78,78,78,78	0
56	MG	YT	203	1/1	0.82	0.24	94,94,94,94	0
56	MG	XT	201	1/1	0.82	0.28	93,93,93,93	0
56	MG	YA	3683	1/1	0.82	0.46	123,123,123,123	0
56	MG	YA	3218	1/1	0.82	0.19	92,92,92,92	0
56	MG	RB	226	1/1	0.82	0.21	82,82,82,82	0
56	MG	RA	3906	1/1	0.82	0.37	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3483	1/1	0.82	0.18	65,65,65,65	0
56	MG	RD	302	1/1	0.82	0.38	90,90,90,90	0
56	MG	YA	3574	1/1	0.82	0.20	62,62,62,62	0
56	MG	RA	3803	1/1	0.82	0.13	50,50,50,50	0
56	MG	YA	3306	1/1	0.82	0.12	46,46,46,46	0
56	MG	RA	4017	1/1	0.82	0.23	110,110,110,110	0
56	MG	YA	3010	1/1	0.82	0.23	101,101,101,101	0
56	MG	YA	3387	1/1	0.83	0.24	70,70,70,70	0
56	MG	XA	1716	1/1	0.83	0.16	103,103,103,103	0
56	MG	YA	3537	1/1	0.83	0.36	94,94,94,94	0
56	MG	XA	1640	1/1	0.83	0.15	85,85,85,85	0
56	MG	RA	3057	1/1	0.83	0.41	97,97,97,97	0
56	MG	RA	3100	1/1	0.83	0.48	144,144,144,144	0
56	MG	YA	3203	1/1	0.83	0.15	78,78,78,78	0
56	MG	RA	3687	1/1	0.83	0.31	74,74,74,74	0
56	MG	YA	3005	1/1	0.83	0.29	115,115,115,115	0
56	MG	QA	1762	1/1	0.83	0.12	84,84,84,84	0
56	MG	YA	3293	1/1	0.83	0.13	56,56,56,56	0
56	MG	YA	3294	1/1	0.83	0.10	67,67,67,67	0
56	MG	RA	3523	1/1	0.83	0.26	91,91,91,91	0
56	MG	RA	3791	1/1	0.83	0.27	90,90,90,90	0
56	MG	RA	3302	1/1	0.83	0.17	107,107,107,107	0
56	MG	RA	3439	1/1	0.83	0.39	48,48,48,48	0
56	MG	QA	1691	1/1	0.83	0.32	87,87,87,87	0
56	MG	RA	3403	1/1	0.83	0.36	43,43,43,43	0
56	MG	XA	1745	1/1	0.83	0.17	67,67,67,67	0
56	MG	RA	3926	1/1	0.83	0.26	87,87,87,87	0
56	MG	RA	3660	1/1	0.83	0.13	104,104,104,104	0
56	MG	YA	3569	1/1	0.83	0.21	82,82,82,82	0
56	MG	QA	1657	1/1	0.83	0.07	159,159,159,159	0
56	MG	RE	303	1/1	0.83	0.41	112,112,112,112	0
56	MG	RA	3367	1/1	0.83	0.23	64,64,64,64	0
56	MG	RA	3577	1/1	0.83	0.33	76,76,76,76	0
56	MG	YA	3235	1/1	0.83	0.19	93,93,93,93	0
56	MG	YO	202	1/1	0.83	0.14	86,86,86,86	0
56	MG	YA	3686	1/1	0.83	0.41	72,72,72,72	0
56	MG	YA	3167	1/1	0.83	0.44	111,111,111,111	0
56	MG	RA	3153	1/1	0.83	0.46	159,159,159,159	0
56	MG	RA	3635	1/1	0.83	0.24	103,103,103,103	0
56	MG	RA	3391	1/1	0.83	0.15	52,52,52,52	0
56	MG	QA	1631	1/1	0.83	0.17	118,118,118,118	0
56	MG	RA	3009	1/1	0.83	0.28	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3244	1/1	0.83	0.17	119,119,119,119	0
56	MG	XA	1679	1/1	0.83	0.13	95,95,95,95	0
56	MG	QA	1669	1/1	0.83	0.15	106,106,106,106	0
56	MG	RA	3638	1/1	0.83	0.45	130,130,130,130	0
56	MG	RA	3118	1/1	0.83	0.17	131,131,131,131	0
56	MG	YA	3429	1/1	0.83	0.26	77,77,77,77	0
56	MG	YA	3248	1/1	0.83	0.27	100,100,100,100	0
56	MG	RA	3535	1/1	0.83	0.13	85,85,85,85	0
56	MG	YA	3111	1/1	0.83	0.39	101,101,101,101	0
56	MG	YA	3252	1/1	0.83	0.27	108,108,108,108	0
56	MG	YA	3708	1/1	0.83	0.21	76,76,76,76	0
56	MG	RA	3584	1/1	0.83	0.18	56,56,56,56	0
56	MG	RA	3994	1/1	0.83	0.42	111,111,111,111	0
56	MG	QO	101	1/1	0.83	0.14	93,93,93,93	0
56	MG	YA	3119	1/1	0.83	0.25	98,98,98,98	0
56	MG	YA	3186	1/1	0.83	0.20	88,88,88,88	0
56	MG	RA	3284	1/1	0.83	0.31	114,114,114,114	0
56	MG	RA	3448	1/1	0.83	0.17	85,85,85,85	0
56	MG	RA	3349	1/1	0.83	0.21	62,62,62,62	0
56	MG	YA	3628	1/1	0.83	0.23	68,68,68,68	0
56	MG	RA	3905	1/1	0.83	0.22	91,91,91,91	0
56	MG	YA	3130	1/1	0.83	0.38	151,151,151,151	0
56	MG	RA	3374	1/1	0.83	0.22	44,44,44,44	0
56	MG	YA	3375	1/1	0.83	0.32	55,55,55,55	0
56	MG	YA	3275	1/1	0.83	0.12	74,74,74,74	0
56	MG	QA	1719	1/1	0.83	0.17	81,81,81,81	0
56	MG	RA	3747	1/1	0.83	0.15	84,84,84,84	0
56	MG	QA	1837	1/1	0.83	0.27	122,122,122,122	0
56	MG	YA	3137	1/1	0.83	0.33	75,75,75,75	0
56	MG	YA	3385	1/1	0.83	0.36	82,82,82,82	0
56	MG	RD	315	1/1	0.84	0.32	122,122,122,122	0
56	MG	RA	3462	1/1	0.84	0.32	84,84,84,84	0
56	MG	XA	1727	1/1	0.84	0.12	75,75,75,75	0
56	MG	XA	1731	1/1	0.84	0.24	84,84,84,84	0
56	MG	QF	201	1/1	0.84	0.10	101,101,101,101	0
56	MG	YA	3224	1/1	0.84	0.33	98,98,98,98	0
56	MG	RA	3346	1/1	0.84	0.29	128,128,128,128	0
56	MG	RA	3800	1/1	0.84	0.28	77,77,77,77	0
56	MG	RA	3419	1/1	0.84	0.30	59,59,59,59	0
56	MG	RA	3802	1/1	0.84	0.22	50,50,50,50	0
56	MG	RA	3525	1/1	0.84	0.17	76,76,76,76	0
56	MG	YW	202	1/1	0.84	0.15	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3523	1/1	0.84	0.18	34,34,34,34	0
56	MG	YA	3107	1/1	0.84	0.24	83,83,83,83	0
56	MG	R7	101	1/1	0.84	0.24	111,111,111,111	0
56	MG	RA	3975	1/1	0.84	0.11	60,60,60,60	0
56	MG	RA	3467	1/1	0.84	0.16	67,67,67,67	0
56	MG	RA	3845	1/1	0.84	0.25	69,69,69,69	0
56	MG	XA	1755	1/1	0.84	0.29	71,71,71,71	0
56	MG	YA	3310	1/1	0.84	0.28	41,41,41,41	0
56	MG	RA	3394	1/1	0.84	0.37	47,47,47,47	0
56	MG	RA	3736	1/1	0.84	0.16	79,79,79,79	0
56	MG	XA	1607	1/1	0.84	0.07	119,119,119,119	0
56	MG	XA	1608	1/1	0.84	0.22	78,78,78,78	0
56	MG	RA	3984	1/1	0.84	0.13	86,86,86,86	0
56	MG	RA	3128	1/1	0.84	0.10	91,91,91,91	0
56	MG	RG	202	1/1	0.84	0.21	112,112,112,112	0
56	MG	RA	3177	1/1	0.84	0.29	106,106,106,106	0
56	MG	RA	3813	1/1	0.84	0.12	81,81,81,81	0
56	MG	YA	3128	1/1	0.84	0.19	98,98,98,98	0
56	MG	YA	3332	1/1	0.84	0.21	48,48,48,48	0
56	MG	YA	3188	1/1	0.84	0.25	87,87,87,87	0
56	MG	QV	105	1/1	0.84	0.07	120,120,120,120	0
56	MG	RA	3988	1/1	0.84	0.41	88,88,88,88	0
56	MG	YA	3061	1/1	0.84	0.13	85,85,85,85	0
56	MG	RA	3221	1/1	0.84	0.18	140,140,140,140	0
56	MG	XA	1693	1/1	0.84	0.17	67,67,67,67	0
56	MG	RA	3178	1/1	0.84	0.07	134,134,134,134	0
56	MG	RA	3173	1/1	0.84	0.17	79,79,79,79	0
56	MG	RA	3210	1/1	0.84	0.30	130,130,130,130	0
56	MG	YA	3141	1/1	0.84	0.26	86,86,86,86	0
56	MG	RA	3315	1/1	0.84	0.28	44,44,44,44	0
56	MG	RA	3303	1/1	0.84	0.19	98,98,98,98	0
56	MG	RA	3657	1/1	0.84	0.20	73,73,73,73	0
56	MG	XE	201	1/1	0.84	0.12	109,109,109,109	0
56	MG	RA	3213	1/1	0.84	0.33	111,111,111,111	0
56	MG	YA	3207	1/1	0.84	0.15	114,114,114,114	0
56	MG	RA	3383	1/1	0.84	0.22	85,85,85,85	0
56	MG	RA	3340	1/1	0.84	0.20	44,44,44,44	0
56	MG	RA	4036	1/1	0.84	0.42	78,78,78,78	0
56	MG	XA	1639	1/1	0.84	0.11	85,85,85,85	0
56	MG	RA	3026	1/1	0.84	0.46	128,128,128,128	0
56	MG	YA	3370	1/1	0.84	0.22	38,38,38,38	0
56	MG	QD	301	1/1	0.84	0.24	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3374	1/1	0.84	0.16	43,43,43,43	0
56	MG	RA	3025	1/1	0.84	0.53	98,98,98,98	0
56	MG	YA	3029	1/1	0.84	0.31	76,76,76,76	0
56	MG	YA	3603	1/1	0.84	0.23	75,75,75,75	0
56	MG	YA	3290	1/1	0.84	0.13	70,70,70,70	0
56	MG	YA	3607	1/1	0.84	0.21	69,69,69,69	0
56	MG	YA	3691	1/1	0.84	0.29	123,123,123,123	0
56	MG	RA	3345	1/1	0.84	0.18	97,97,97,97	0
56	MG	YA	3734	1/1	0.85	0.42	120,120,120,120	0
56	MG	YA	3735	1/1	0.85	0.20	64,64,64,64	0
56	MG	YA	3025	1/1	0.85	0.13	69,69,69,69	0
56	MG	YA	3026	1/1	0.85	0.17	52,52,52,52	0
56	MG	R3	102	1/1	0.85	0.71	131,131,131,131	0
56	MG	XA	1634	1/1	0.85	0.19	60,60,60,60	0
56	MG	YA	3638	1/1	0.85	0.31	62,62,62,62	0
56	MG	YA	3166	1/1	0.85	0.36	142,142,142,142	0
56	MG	YA	3531	1/1	0.85	0.08	68,68,68,68	0
56	MG	YA	3533	1/1	0.85	0.20	64,64,64,64	0
56	MG	R5	101	1/1	0.85	0.27	130,130,130,130	0
56	MG	YA	3459	1/1	0.85	0.23	41,41,41,41	0
56	MG	QB	301	1/1	0.85	0.14	146,146,146,146	0
56	MG	QA	1682	1/1	0.85	0.24	128,128,128,128	0
56	MG	RA	3742	1/1	0.85	0.21	77,77,77,77	0
56	MG	YA	3463	1/1	0.85	0.34	92,92,92,92	0
56	MG	RA	3338	1/1	0.85	0.23	88,88,88,88	0
56	MG	RA	3806	1/1	0.85	0.28	98,98,98,98	0
56	MG	YB	218	1/1	0.85	0.16	51,51,51,51	0
56	MG	RA	3258	1/1	0.85	0.17	96,96,96,96	0
56	MG	RA	3664	1/1	0.85	0.28	90,90,90,90	0
56	MG	YA	3470	1/1	0.85	0.21	35,35,35,35	0
56	MG	YA	3311	1/1	0.85	0.13	32,32,32,32	0
56	MG	XA	1655	1/1	0.85	0.18	89,89,89,89	0
56	MG	RA	3850	1/1	0.85	0.33	70,70,70,70	0
56	MG	YA	3666	1/1	0.85	0.22	84,84,84,84	0
56	MG	XA	1751	1/1	0.85	0.20	77,77,77,77	0
56	MG	XA	1752	1/1	0.85	0.20	98,98,98,98	0
56	MG	RA	3935	1/1	0.85	0.31	103,103,103,103	0
56	MG	RF	310	1/1	0.85	0.65	112,112,112,112	0
56	MG	YA	3405	1/1	0.85	0.32	110,110,110,110	0
56	MG	RA	3809	1/1	0.85	0.23	72,72,72,72	0
56	MG	YA	3117	1/1	0.85	0.13	99,99,99,99	0
56	MG	YA	3677	1/1	0.85	0.12	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3326	1/1	0.85	0.25	62,62,62,62	0
56	MG	QL	202	1/1	0.85	0.22	95,95,95,95	0
56	MG	RA	3775	1/1	0.85	0.26	90,90,90,90	0
56	MG	RA	3569	1/1	0.85	0.39	86,86,86,86	0
56	MG	RA	3593	1/1	0.85	0.60	91,91,91,91	0
56	MG	RA	3622	1/1	0.85	0.54	82,82,82,82	0
56	MG	RA	3989	1/1	0.85	0.24	112,112,112,112	0
56	MG	RA	3779	1/1	0.85	0.16	124,124,124,124	0
56	MG	RA	3475	1/1	0.85	0.17	37,37,37,37	0
56	MG	RA	3399	1/1	0.85	0.23	51,51,51,51	0
56	MG	YT	204	1/1	0.85	0.19	93,93,93,93	0
56	MG	YA	3344	1/1	0.85	0.20	94,94,94,94	0
56	MG	RA	3123	1/1	0.85	0.17	72,72,72,72	0
56	MG	RA	3384	1/1	0.85	0.27	72,72,72,72	0
56	MG	YA	3264	1/1	0.85	0.16	66,66,66,66	0
56	MG	RA	3032	1/1	0.85	0.24	86,86,86,86	0
56	MG	YA	3498	1/1	0.85	0.41	108,108,108,108	0
56	MG	YA	3427	1/1	0.85	0.24	70,70,70,70	0
56	MG	YA	3352	1/1	0.85	0.33	36,36,36,36	0
56	MG	RA	3388	1/1	0.85	0.23	58,58,58,58	0
56	MG	RA	3652	1/1	0.85	0.50	162,162,162,162	0
56	MG	YA	3431	1/1	0.85	0.29	50,50,50,50	0
56	MG	RA	3087	1/1	0.85	0.20	148,148,148,148	0
56	MG	RA	4029	1/1	0.85	0.43	150,150,150,150	0
56	MG	RA	3914	1/1	0.85	0.30	129,129,129,129	0
56	MG	YA	3204	1/1	0.85	0.29	132,132,132,132	0
56	MG	RA	3237	1/1	0.85	0.28	136,136,136,136	0
56	MG	YA	3366	1/1	0.85	0.22	50,50,50,50	0
56	MG	RA	3796	1/1	0.85	0.30	48,48,48,48	0
56	MG	RA	3361	1/1	0.85	0.23	76,76,76,76	0
56	MG	RB	201	1/1	0.85	0.11	88,88,88,88	0
56	MG	YA	3715	1/1	0.85	0.13	61,61,61,61	0
56	MG	RA	3016	1/1	0.85	0.41	76,76,76,76	0
56	MG	QA	1632	1/1	0.85	0.09	102,102,102,102	0
56	MG	YA	3018	1/1	0.85	0.35	146,146,146,146	0
56	MG	RA	3336	1/1	0.85	0.35	61,61,61,61	0
56	MG	RA	3925	1/1	0.85	0.24	100,100,100,100	0
56	MG	R1	104	1/1	0.85	0.21	74,74,74,74	0
56	MG	RA	3070	1/1	0.85	0.69	110,110,110,110	0
56	MG	RA	3766	1/1	0.86	0.26	92,92,92,92	0
56	MG	RA	3499	1/1	0.86	0.17	41,41,41,41	0
56	MG	RA	3848	1/1	0.86	0.14	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3676	1/1	0.86	0.23	58,58,58,58	0
56	MG	RA	4016	1/1	0.86	0.56	115,115,115,115	0
56	MG	YA	3100	1/1	0.86	0.10	70,70,70,70	0
56	MG	XA	1700	1/1	0.86	0.20	86,86,86,86	0
56	MG	YA	3553	1/1	0.86	0.22	43,43,43,43	0
56	MG	XA	1702	1/1	0.86	0.20	67,67,67,67	0
56	MG	RA	3804	1/1	0.86	0.23	42,42,42,42	0
56	MG	YA	3013	1/1	0.86	0.09	35,35,35,35	0
56	MG	RA	4028	1/1	0.86	0.42	151,151,151,151	0
56	MG	RA	3953	1/1	0.86	0.14	49,49,49,49	0
56	MG	XA	1604	1/1	0.86	0.14	92,92,92,92	0
56	MG	RA	4031	1/1	0.86	0.22	79,79,79,79	0
56	MG	RA	3605	1/1	0.86	0.19	63,63,63,63	0
56	MG	XA	1711	1/1	0.86	0.20	90,90,90,90	0
56	MG	RE	307	1/1	0.86	0.17	67,67,67,67	0
56	MG	YA	3474	1/1	0.86	0.28	56,56,56,56	0
56	MG	RE	308	1/1	0.86	0.18	75,75,75,75	0
56	MG	QA	1838	1/1	0.86	0.20	96,96,96,96	0
56	MG	XA	1612	1/1	0.86	0.13	97,97,97,97	0
56	MG	RA	3404	1/1	0.86	0.16	36,36,36,36	0
56	MG	YA	3573	1/1	0.86	0.15	48,48,48,48	0
56	MG	RA	3396	1/1	0.86	0.26	34,34,34,34	0
56	MG	RA	3064	1/1	0.86	0.15	97,97,97,97	0
56	MG	QA	1664	1/1	0.86	0.14	148,148,148,148	0
56	MG	RA	3122	1/1	0.86	0.08	85,85,85,85	0
56	MG	YA	3032	1/1	0.86	0.22	102,102,102,102	0
56	MG	RA	3614	1/1	0.86	0.22	63,63,63,63	0
56	MG	XA	1728	1/1	0.86	0.28	86,86,86,86	0
56	MG	YA	3701	1/1	0.86	0.27	86,86,86,86	0
56	MG	RA	3962	1/1	0.86	0.12	88,88,88,88	0
56	MG	RA	3585	1/1	0.86	0.17	72,72,72,72	0
56	MG	QA	1786	1/1	0.86	0.22	93,93,93,93	0
56	MG	YA	3599	1/1	0.86	0.29	33,33,33,33	0
56	MG	QA	1611	1/1	0.86	0.10	132,132,132,132	0
56	MG	RA	3089	1/1	0.86	0.27	102,102,102,102	0
56	MG	RA	3966	1/1	0.86	0.14	62,62,62,62	0
56	MG	YA	3411	1/1	0.86	0.10	48,48,48,48	0
56	MG	RA	3409	1/1	0.86	0.15	37,37,37,37	0
56	MG	YA	3610	1/1	0.86	0.16	42,42,42,42	0
56	MG	RA	3508	1/1	0.86	0.15	52,52,52,52	0
56	MG	RA	3473	1/1	0.86	0.30	94,94,94,94	0
56	MG	YA	3718	1/1	0.86	0.20	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3271	1/1	0.86	0.33	148,148,148,148	0
56	MG	RA	3679	1/1	0.86	0.51	114,114,114,114	0
56	MG	YA	3320	1/1	0.86	0.37	29,29,29,29	0
56	MG	YA	3322	1/1	0.86	0.23	49,49,49,49	0
56	MG	QA	1620	1/1	0.86	0.10	171,171,171,171	0
56	MG	YA	3230	1/1	0.86	0.23	131,131,131,131	0
56	MG	RA	3621	1/1	0.86	0.40	112,112,112,112	0
56	MG	RA	3592	1/1	0.86	0.21	98,98,98,98	0
56	MG	YA	3737	1/1	0.86	0.23	51,51,51,51	0
56	MG	YA	3623	1/1	0.86	0.28	92,92,92,92	0
56	MG	RP	201	1/1	0.86	0.48	128,128,128,128	0
56	MG	RA	3879	1/1	0.86	0.25	69,69,69,69	0
56	MG	YB	204	1/1	0.86	0.15	154,154,154,154	0
56	MG	RA	3412	1/1	0.86	0.14	70,70,70,70	0
56	MG	RA	3786	1/1	0.86	0.44	137,137,137,137	0
56	MG	QA	1686	1/1	0.86	0.23	117,117,117,117	0
56	MG	RQ	205	1/1	0.86	0.23	118,118,118,118	0
56	MG	RA	3980	1/1	0.86	0.79	122,122,122,122	0
56	MG	RA	3156	1/1	0.86	0.41	153,153,153,153	0
56	MG	RR	203	1/1	0.86	0.16	70,70,70,70	0
56	MG	RA	3790	1/1	0.86	0.35	103,103,103,103	0
56	MG	RA	3686	1/1	0.86	0.27	119,119,119,119	0
56	MG	QA	1810	1/1	0.86	0.26	176,176,176,176	0
56	MG	YA	3640	1/1	0.86	0.24	76,76,76,76	0
56	MG	RU	201	1/1	0.86	0.16	79,79,79,79	0
56	MG	RA	3037	1/1	0.86	0.18	78,78,78,78	0
56	MG	RA	3837	1/1	0.86	0.22	46,46,46,46	0
56	MG	YA	3524	1/1	0.86	0.14	41,41,41,41	0
56	MG	YA	3444	1/1	0.86	0.17	69,69,69,69	0
56	MG	YA	3354	1/1	0.86	0.20	46,46,46,46	0
56	MG	RA	3291	1/1	0.86	0.09	113,113,113,113	0
56	MG	YA	3649	1/1	0.86	0.26	54,54,54,54	0
56	MG	YA	3650	1/1	0.86	0.27	55,55,55,55	0
56	MG	QA	1815	1/1	0.86	0.25	92,92,92,92	0
56	MG	YA	3653	1/1	0.86	0.19	46,46,46,46	0
56	MG	YA	3654	1/1	0.86	0.18	44,44,44,44	0
56	MG	RA	3600	1/1	0.86	0.13	103,103,103,103	0
56	MG	RA	3761	1/1	0.86	0.10	81,81,81,81	0
56	MG	XV	104	1/1	0.86	0.11	92,92,92,92	0
56	MG	YA	3090	1/1	0.86	0.12	43,43,43,43	0
56	MG	YA	3659	1/1	0.86	0.25	47,47,47,47	0
56	MG	RA	3629	1/1	0.86	0.25	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3365	1/1	0.86	0.24	87,87,87,87	0
56	MG	RA	3555	1/1	0.86	0.15	78,78,78,78	0
56	MG	RA	3942	1/1	0.86	0.34	84,84,84,84	0
56	MG	YA	3265	1/1	0.86	0.31	86,86,86,86	0
56	MG	R1	103	1/1	0.86	0.17	89,89,89,89	0
56	MG	RA	3498	1/1	0.86	0.17	30,30,30,30	0
56	MG	YA	3647	1/1	0.87	0.30	58,58,58,58	0
56	MG	RA	3536	1/1	0.87	0.24	119,119,119,119	0
56	MG	YA	3162	1/1	0.87	0.12	54,54,54,54	0
56	MG	RA	3537	1/1	0.87	0.19	71,71,71,71	0
56	MG	QA	1650	1/1	0.87	0.09	92,92,92,92	0
56	MG	YA	3554	1/1	0.87	0.27	65,65,65,65	0
56	MG	YA	3555	1/1	0.87	0.18	50,50,50,50	0
56	MG	XA	1722	1/1	0.87	0.23	81,81,81,81	0
56	MG	RA	3255	1/1	0.87	0.26	127,127,127,127	0
56	MG	RA	3452	1/1	0.87	0.15	92,92,92,92	0
56	MG	RA	3453	1/1	0.87	0.30	62,62,62,62	0
56	MG	QA	1751	1/1	0.87	0.39	91,91,91,91	0
56	MG	XA	1730	1/1	0.87	0.15	61,61,61,61	0
56	MG	YA	3661	1/1	0.87	0.27	62,62,62,62	0
56	MG	RA	3640	1/1	0.87	0.22	64,64,64,64	0
56	MG	YA	3565	1/1	0.87	0.25	38,38,38,38	0
56	MG	RA	3541	1/1	0.87	0.25	65,65,65,65	0
56	MG	RA	3200	1/1	0.87	0.30	108,108,108,108	0
56	MG	RA	3849	1/1	0.87	0.28	71,71,71,71	0
56	MG	XA	1740	1/1	0.87	0.27	81,81,81,81	0
56	MG	RA	3944	1/1	0.87	0.25	50,50,50,50	0
56	MG	RA	3740	1/1	0.87	0.21	103,103,103,103	0
56	MG	YA	3670	1/1	0.87	0.22	26,26,26,26	0
56	MG	YA	3254	1/1	0.87	0.26	122,122,122,122	0
56	MG	RA	3422	1/1	0.87	0.35	84,84,84,84	0
56	MG	YA	3256	1/1	0.87	0.24	100,100,100,100	0
56	MG	RA	3378	1/1	0.87	0.21	55,55,55,55	0
56	MG	YA	3425	1/1	0.87	0.23	72,72,72,72	0
56	MG	YA	3035	1/1	0.87	0.32	67,67,67,67	0
56	MG	RA	3189	1/1	0.87	0.30	135,135,135,135	0
56	MG	RA	3380	1/1	0.87	0.33	39,39,39,39	0
56	MG	RD	305	1/1	0.87	0.06	66,66,66,66	0
56	MG	RA	3680	1/1	0.87	0.62	140,140,140,140	0
56	MG	XA	1757	1/1	0.87	0.26	67,67,67,67	0
56	MG	RA	3240	1/1	0.87	0.28	118,118,118,118	0
56	MG	RA	3858	1/1	0.87	0.48	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	4023	1/1	0.87	0.36	106,106,106,106	0
56	MG	YA	3044	1/1	0.87	0.11	77,77,77,77	0
56	MG	YA	3688	1/1	0.87	0.14	50,50,50,50	0
56	MG	YA	3604	1/1	0.87	0.15	44,44,44,44	0
56	MG	RV	203	1/1	0.87	0.18	91,91,91,91	0
56	MG	YA	3437	1/1	0.87	0.23	87,87,87,87	0
56	MG	QA	1624	1/1	0.87	0.09	130,130,130,130	0
56	MG	QA	1769	1/1	0.87	0.22	94,94,94,94	0
56	MG	RA	3748	1/1	0.87	0.24	47,47,47,47	0
56	MG	YA	3279	1/1	0.87	0.27	80,80,80,80	0
56	MG	XA	1771	1/1	0.87	0.32	77,77,77,77	0
56	MG	QA	1722	1/1	0.87	0.20	70,70,70,70	0
56	MG	RA	3202	1/1	0.87	0.32	86,86,86,86	0
56	MG	RA	3601	1/1	0.87	0.21	125,125,125,125	0
56	MG	RY	201	1/1	0.87	0.28	119,119,119,119	0
56	MG	RZ	301	1/1	0.87	0.05	80,80,80,80	0
56	MG	RA	3961	1/1	0.87	0.21	74,74,74,74	0
56	MG	YA	3205	1/1	0.87	0.23	91,91,91,91	0
56	MG	RA	3684	1/1	0.87	0.80	160,160,160,160	0
56	MG	YA	3138	1/1	0.87	0.18	34,34,34,34	0
56	MG	RA	3916	1/1	0.87	0.15	121,121,121,121	0
56	MG	YA	3059	1/1	0.87	0.16	84,84,84,84	0
56	MG	RA	3165	1/1	0.87	0.17	72,72,72,72	0
56	MG	RA	3204	1/1	0.87	0.37	149,149,149,149	0
56	MG	YA	3144	1/1	0.87	0.27	94,94,94,94	0
56	MG	RA	3431	1/1	0.87	0.43	53,53,53,53	0
56	MG	RA	3389	1/1	0.87	0.29	47,47,47,47	0
56	MG	YA	3069	1/1	0.87	0.29	91,91,91,91	0
56	MG	RA	3606	1/1	0.87	0.28	51,51,51,51	0
56	MG	YA	3721	1/1	0.87	0.13	115,115,115,115	0
56	MG	RA	3876	1/1	0.87	0.14	50,50,50,50	0
56	MG	YA	3077	1/1	0.87	0.36	112,112,112,112	0
56	MG	YA	3538	1/1	0.87	0.23	83,83,83,83	0
56	MG	YA	3540	1/1	0.87	0.18	66,66,66,66	0
57	ZN	R4	101	1/1	0.87	0.12	297,297,297,297	0
56	MG	RA	3829	1/1	0.87	0.15	68,68,68,68	0
56	MG	YA	3729	1/1	0.87	0.17	156,156,156,156	0
56	MG	RA	3760	1/1	0.87	0.19	49,49,49,49	0
56	MG	RA	3835	1/1	0.87	0.20	93,93,93,93	0
56	MG	XA	1627	1/1	0.87	0.11	78,78,78,78	0
56	MG	RA	3158	1/1	0.87	0.13	82,82,82,82	0
56	MG	RA	3353	1/1	0.87	0.09	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3610	1/1	0.87	0.29	61,61,61,61	0
56	MG	RA	3870	1/1	0.88	0.42	59,59,59,59	0
56	MG	XA	1726	1/1	0.88	0.22	106,106,106,106	0
56	MG	RA	3570	1/1	0.88	0.11	71,71,71,71	0
56	MG	RA	3832	1/1	0.88	0.33	75,75,75,75	0
56	MG	RA	3295	1/1	0.88	0.51	148,148,148,148	0
56	MG	RA	3915	1/1	0.88	0.30	84,84,84,84	0
56	MG	RA	4013	1/1	0.88	0.32	115,115,115,115	0
56	MG	RA	3230	1/1	0.88	0.27	91,91,91,91	0
56	MG	YA	3690	1/1	0.88	0.32	62,62,62,62	0
56	MG	RA	3745	1/1	0.88	0.14	66,66,66,66	0
56	MG	YA	3177	1/1	0.88	0.18	109,109,109,109	0
56	MG	RD	301	1/1	0.88	0.21	91,91,91,91	0
56	MG	RA	3516	1/1	0.88	0.28	79,79,79,79	0
56	MG	RA	4018	1/1	0.88	0.34	153,153,153,153	0
56	MG	RA	4021	1/1	0.88	0.06	101,101,101,101	0
56	MG	RA	3880	1/1	0.88	0.17	55,55,55,55	0
56	MG	XA	1664	1/1	0.88	0.14	89,89,89,89	0
56	MG	YA	3469	1/1	0.88	0.21	37,37,37,37	0
56	MG	RA	3112	1/1	0.88	0.32	113,113,113,113	0
56	MG	RA	3922	1/1	0.88	0.09	59,59,59,59	0
56	MG	YA	3539	1/1	0.88	0.20	72,72,72,72	0
56	MG	YA	3472	1/1	0.88	0.26	45,45,45,45	0
56	MG	YA	3121	1/1	0.88	0.28	92,92,92,92	0
56	MG	XA	1672	1/1	0.88	0.17	78,78,78,78	0
56	MG	RA	3014	1/1	0.88	0.12	74,74,74,74	0
56	MG	RA	4032	1/1	0.88	0.20	100,100,100,100	0
56	MG	RA	3071	1/1	0.88	0.26	97,97,97,97	0
56	MG	RA	3351	1/1	0.88	0.26	42,42,42,42	0
56	MG	QA	1625	1/1	0.88	0.14	106,106,106,106	0
56	MG	RA	3106	1/1	0.88	0.40	124,124,124,124	0
56	MG	RA	3646	1/1	0.88	0.24	63,63,63,63	0
56	MG	XA	1605	1/1	0.88	0.18	104,104,104,104	0
56	MG	RA	3674	1/1	0.88	0.29	83,83,83,83	0
56	MG	RA	3052	1/1	0.88	0.31	142,142,142,142	0
56	MG	YA	3716	1/1	0.88	0.50	108,108,108,108	0
56	MG	YA	3347	1/1	0.88	0.31	38,38,38,38	0
56	MG	YA	3015	1/1	0.88	0.32	111,111,111,111	0
56	MG	YA	3200	1/1	0.88	0.33	99,99,99,99	0
56	MG	YA	3072	1/1	0.88	0.07	70,70,70,70	0
56	MG	XA	1613	1/1	0.88	0.07	73,73,73,73	0
56	MG	RA	3045	1/1	0.88	0.31	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3017	1/1	0.88	0.25	116,116,116,116	0
56	MG	RA	3702	1/1	0.88	0.26	74,74,74,74	0
56	MG	YA	3278	1/1	0.88	0.24	57,57,57,57	0
56	MG	YA	3078	1/1	0.88	0.34	92,92,92,92	0
56	MG	YA	3360	1/1	0.88	0.24	41,41,41,41	0
56	MG	YA	3079	1/1	0.88	0.09	78,78,78,78	0
56	MG	YA	3080	1/1	0.88	0.40	126,126,126,126	0
56	MG	RA	3785	1/1	0.88	0.08	102,102,102,102	0
56	MG	YA	3657	1/1	0.88	0.25	51,51,51,51	0
56	MG	RA	3607	1/1	0.88	0.27	42,42,42,42	0
56	MG	RA	3787	1/1	0.88	0.19	91,91,91,91	0
56	MG	RA	3150	1/1	0.88	0.17	84,84,84,84	0
56	MG	RF	305	1/1	0.88	0.32	79,79,79,79	0
56	MG	RA	3939	1/1	0.88	0.19	72,72,72,72	0
56	MG	RA	3185	1/1	0.88	0.43	164,164,164,164	0
56	MG	RA	3469	1/1	0.88	0.17	57,57,57,57	0
56	MG	RA	3294	1/1	0.88	0.12	36,36,36,36	0
56	MG	RA	3472	1/1	0.88	0.26	38,38,38,38	0
56	MG	XV	102	1/1	0.88	0.07	107,107,107,107	0
56	MG	YA	3588	1/1	0.88	0.27	28,28,28,28	0
56	MG	YA	3031	1/1	0.88	0.14	60,60,60,60	0
56	MG	YA	3592	1/1	0.88	0.21	52,52,52,52	0
56	MG	RA	3548	1/1	0.88	0.36	60,60,60,60	0
56	MG	YA	3594	1/1	0.88	0.20	53,53,53,53	0
56	MG	RA	3329	1/1	0.88	0.20	69,69,69,69	0
56	MG	YA	3228	1/1	0.88	0.31	150,150,150,150	0
56	MG	RA	3797	1/1	0.88	0.27	105,105,105,105	0
56	MG	QA	1819	1/1	0.88	0.23	92,92,92,92	0
56	MG	YA	3605	1/1	0.88	0.14	65,65,65,65	0
56	MG	YA	3681	1/1	0.88	0.20	40,40,40,40	0
56	MG	RA	3830	1/1	0.88	0.62	76,76,76,76	0
56	MG	YA	3225	1/1	0.89	0.21	100,100,100,100	0
56	MG	YA	3597	1/1	0.89	0.24	72,72,72,72	0
56	MG	RA	3489	1/1	0.89	0.34	98,98,98,98	0
56	MG	RA	3305	1/1	0.89	0.13	117,117,117,117	0
56	MG	RA	3325	1/1	0.89	0.15	68,68,68,68	0
56	MG	XA	1651	1/1	0.89	0.35	119,119,119,119	0
56	MG	YA	3447	1/1	0.89	0.21	74,74,74,74	0
56	MG	RD	303	1/1	0.89	0.35	79,79,79,79	0
56	MG	YA	3102	1/1	0.89	0.17	53,53,53,53	0
56	MG	YA	3233	1/1	0.89	0.28	114,114,114,114	0
56	MG	XA	1736	1/1	0.89	0.27	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3438	1/1	0.89	0.32	52,52,52,52	0
56	MG	RA	3249	1/1	0.89	0.26	101,101,101,101	0
56	MG	XA	1739	1/1	0.89	0.33	54,54,54,54	0
56	MG	YA	3383	1/1	0.89	0.29	44,44,44,44	0
56	MG	RA	3780	1/1	0.89	0.42	88,88,88,88	0
56	MG	YA	3386	1/1	0.89	0.11	31,31,31,31	0
56	MG	RA	3054	1/1	0.89	0.47	138,138,138,138	0
56	MG	QA	1738	1/1	0.89	0.14	108,108,108,108	0
56	MG	YA	3308	1/1	0.89	0.20	41,41,41,41	0
56	MG	RA	3102	1/1	0.89	0.28	123,123,123,123	0
56	MG	RA	3140	1/1	0.89	0.12	78,78,78,78	0
56	MG	YA	3532	1/1	0.89	0.22	53,53,53,53	0
56	MG	RA	3067	1/1	0.89	0.16	75,75,75,75	0
56	MG	RA	3068	1/1	0.89	0.19	89,89,89,89	0
56	MG	XA	1669	1/1	0.89	0.20	52,52,52,52	0
56	MG	RA	3933	1/1	0.89	0.46	115,115,115,115	0
56	MG	YA	3314	1/1	0.89	0.11	35,35,35,35	0
56	MG	RA	3046	1/1	0.89	0.09	42,42,42,42	0
56	MG	QA	1745	1/1	0.89	0.14	124,124,124,124	0
56	MG	YA	3321	1/1	0.89	0.18	45,45,45,45	0
56	MG	YA	3705	1/1	0.89	0.38	154,154,154,154	0
56	MG	QA	1619	1/1	0.89	0.08	145,145,145,145	0
56	MG	YA	3323	1/1	0.89	0.25	33,33,33,33	0
56	MG	RA	3502	1/1	0.89	0.13	49,49,49,49	0
56	MG	RA	3667	1/1	0.89	0.41	72,72,72,72	0
56	MG	YA	3126	1/1	0.89	0.12	56,56,56,56	0
56	MG	RA	3856	1/1	0.89	0.24	56,56,56,56	0
56	MG	YA	3409	1/1	0.89	0.20	57,57,57,57	0
56	MG	QA	1705	1/1	0.89	0.22	73,73,73,73	0
56	MG	YA	3008	1/1	0.89	0.14	68,68,68,68	0
56	MG	RA	3078	1/1	0.89	0.36	147,147,147,147	0
56	MG	RA	3168	1/1	0.89	0.34	124,124,124,124	0
56	MG	RA	3792	1/1	0.89	0.10	85,85,85,85	0
56	MG	YA	3719	1/1	0.89	0.28	72,72,72,72	0
56	MG	RA	3234	1/1	0.89	0.79	100,100,100,100	0
56	MG	YA	3339	1/1	0.89	0.18	44,44,44,44	0
56	MG	RA	3316	1/1	0.89	0.19	38,38,38,38	0
56	MG	QA	1668	1/1	0.89	0.23	107,107,107,107	0
56	MG	QA	1801	1/1	0.89	0.15	96,96,96,96	0
56	MG	RA	3865	1/1	0.89	0.22	73,73,73,73	0
56	MG	RA	3866	1/1	0.89	0.30	68,68,68,68	0
56	MG	RA	3945	1/1	0.89	0.24	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3907	1/1	0.89	0.25	107,107,107,107	0
56	MG	RA	3385	1/1	0.89	0.23	46,46,46,46	0
56	MG	YA	3206	1/1	0.89	0.17	82,82,82,82	0
56	MG	YA	3738	1/1	0.89	0.38	146,146,146,146	0
56	MG	RA	3949	1/1	0.89	0.25	105,105,105,105	0
56	MG	YA	3743	1/1	0.89	0.26	89,89,89,89	0
56	MG	YA	3085	1/1	0.89	0.22	105,105,105,105	0
56	MG	QA	1856	1/1	0.89	0.17	125,125,125,125	0
56	MG	YA	3660	1/1	0.89	0.15	47,47,47,47	0
56	MG	RA	3737	1/1	0.89	0.19	80,80,80,80	0
56	MG	YA	3575	1/1	0.89	0.20	55,55,55,55	0
56	MG	YA	3578	1/1	0.89	0.18	56,56,56,56	0
56	MG	RA	3121	1/1	0.89	0.12	64,64,64,64	0
56	MG	QA	1637	1/1	0.89	0.23	90,90,90,90	0
56	MG	QA	1678	1/1	0.89	0.30	98,98,98,98	0
56	MG	YA	3503	1/1	0.89	0.23	43,43,43,43	0
56	MG	RA	3013	1/1	0.89	0.10	57,57,57,57	0
56	MG	RA	3563	1/1	0.89	0.07	72,72,72,72	0
56	MG	RA	3319	1/1	0.89	0.25	37,37,37,37	0
56	MG	RA	3285	1/1	0.89	0.31	125,125,125,125	0
56	MG	RA	3323	1/1	0.89	0.22	81,81,81,81	0
56	MG	RA	3411	1/1	0.89	0.20	56,56,56,56	0
56	MG	YA	3652	1/1	0.90	0.12	49,49,49,49	0
56	MG	RF	307	1/1	0.90	0.16	72,72,72,72	0
56	MG	YA	3151	1/1	0.90	0.35	114,114,114,114	0
56	MG	XA	1601	1/1	0.90	0.60	109,109,109,109	0
56	MG	QA	1842	1/1	0.90	0.26	65,65,65,65	0
56	MG	RA	3668	1/1	0.90	0.23	66,66,66,66	0
56	MG	RA	3320	1/1	0.90	0.18	64,64,64,64	0
56	MG	QA	1658	1/1	0.90	0.22	106,106,106,106	0
56	MG	RA	3015	1/1	0.90	0.26	112,112,112,112	0
56	MG	YA	3589	1/1	0.90	0.22	47,47,47,47	0
56	MG	YA	3728	1/1	0.90	0.26	55,55,55,55	0
56	MG	YA	3271	1/1	0.90	0.21	28,28,28,28	0
56	MG	XA	1748	1/1	0.90	0.19	41,41,41,41	0
56	MG	QA	1731	1/1	0.90	0.23	63,63,63,63	0
56	MG	RA	3083	1/1	0.90	0.32	107,107,107,107	0
56	MG	YA	3276	1/1	0.90	0.31	38,38,38,38	0
56	MG	YA	3736	1/1	0.90	0.23	99,99,99,99	0
56	MG	RA	3913	1/1	0.90	0.06	67,67,67,67	0
56	MG	YA	3598	1/1	0.90	0.25	39,39,39,39	0
56	MG	YA	3342	1/1	0.90	0.11	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3111	1/1	0.90	0.27	74,74,74,74	0
56	MG	YA	3744	1/1	0.90	0.15	91,91,91,91	0
56	MG	RA	3765	1/1	0.90	0.34	65,65,65,65	0
56	MG	RA	3108	1/1	0.90	0.26	106,106,106,106	0
56	MG	RA	3474	1/1	0.90	0.15	44,44,44,44	0
56	MG	RA	3888	1/1	0.90	0.47	109,109,109,109	0
56	MG	QA	1702	1/1	0.90	0.29	66,66,66,66	0
56	MG	YA	3114	1/1	0.90	0.07	66,66,66,66	0
56	MG	RA	3454	1/1	0.90	0.17	96,96,96,96	0
56	MG	RA	3381	1/1	0.90	0.22	52,52,52,52	0
56	MG	YA	3173	1/1	0.90	0.26	128,128,128,128	0
56	MG	YA	3068	1/1	0.90	0.31	110,110,110,110	0
56	MG	YA	3356	1/1	0.90	0.16	74,74,74,74	0
56	MG	YA	3479	1/1	0.90	0.17	46,46,46,46	0
56	MG	RD	308	1/1	0.90	0.08	63,63,63,63	0
56	MG	YA	3542	1/1	0.90	0.14	62,62,62,62	0
56	MG	RA	3861	1/1	0.90	0.29	134,134,134,134	0
56	MG	RA	3426	1/1	0.90	0.21	40,40,40,40	0
56	MG	RA	3597	1/1	0.90	0.17	88,88,88,88	0
56	MG	YA	3125	1/1	0.90	0.12	55,55,55,55	0
56	MG	YA	3363	1/1	0.90	0.30	54,54,54,54	0
56	MG	YA	3548	1/1	0.90	0.19	50,50,50,50	0
56	MG	YA	3076	1/1	0.90	0.29	120,120,120,120	0
56	MG	RQ	204	1/1	0.90	0.19	78,78,78,78	0
56	MG	RA	3479	1/1	0.90	0.35	43,43,43,43	0
56	MG	RA	3304	1/1	0.90	0.14	97,97,97,97	0
56	MG	RA	3356	1/1	0.90	0.21	63,63,63,63	0
56	MG	RA	3997	1/1	0.90	0.24	96,96,96,96	0
56	MG	QA	1714	1/1	0.90	0.29	86,86,86,86	0
56	MG	YA	3634	1/1	0.90	0.22	62,62,62,62	0
56	MG	RA	3270	1/1	0.90	0.60	145,145,145,145	0
56	MG	RA	3134	1/1	0.90	0.27	104,104,104,104	0
56	MG	RA	3846	1/1	0.90	0.40	128,128,128,128	0
56	MG	RA	3273	1/1	0.90	0.17	116,116,116,116	0
56	MG	RA	4003	1/1	0.90	0.36	127,127,127,127	0
56	MG	QA	1833	1/1	0.90	0.30	78,78,78,78	0
56	MG	XX	101	1/1	0.90	0.22	129,129,129,129	0
56	MG	RA	4007	1/1	0.90	0.25	43,43,43,43	0
56	MG	RA	3216	1/1	0.90	0.52	104,104,104,104	0
56	MG	YA	3315	1/1	0.90	0.31	51,51,51,51	0
56	MG	YA	3318	1/1	0.90	0.23	39,39,39,39	0
56	MG	XA	1729	1/1	0.90	0.12	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3964	1/1	0.90	0.22	109,109,109,109	0
56	MG	RA	3875	1/1	0.90	0.28	91,91,91,91	0
56	MG	RA	3191	1/1	0.90	0.43	124,124,124,124	0
56	MG	YA	3148	1/1	0.90	0.31	91,91,91,91	0
56	MG	RA	3878	1/1	0.90	0.15	85,85,85,85	0
56	MG	RA	3718	1/1	0.91	0.14	52,52,52,52	0
56	MG	YT	202	1/1	0.91	0.12	88,88,88,88	0
56	MG	RA	3952	1/1	0.91	0.22	56,56,56,56	0
56	MG	RA	3688	1/1	0.91	0.12	79,79,79,79	0
56	MG	YA	3295	1/1	0.91	0.09	34,34,34,34	0
56	MG	YA	3065	1/1	0.91	0.35	83,83,83,83	0
56	MG	YA	3297	1/1	0.91	0.18	76,76,76,76	0
56	MG	YA	3116	1/1	0.91	0.15	106,106,106,106	0
56	MG	Y5	101	1/1	0.91	0.20	126,126,126,126	0
56	MG	YA	3066	1/1	0.91	0.13	79,79,79,79	0
56	MG	RA	3920	1/1	0.91	0.09	57,57,57,57	0
56	MG	RA	3352	1/1	0.91	0.07	47,47,47,47	0
56	MG	Y8	102	1/1	0.91	0.47	77,77,77,77	0
56	MG	YA	3438	1/1	0.91	0.19	79,79,79,79	0
56	MG	RA	3643	1/1	0.91	0.07	75,75,75,75	0
56	MG	YA	3071	1/1	0.91	0.29	100,100,100,100	0
56	MG	RA	3923	1/1	0.91	0.09	48,48,48,48	0
56	MG	RA	4004	1/1	0.91	0.16	146,146,146,146	0
56	MG	YA	3074	1/1	0.91	0.19	97,97,97,97	0
56	MG	YA	3378	1/1	0.91	0.25	87,87,87,87	0
56	MG	YA	3511	1/1	0.91	0.31	60,60,60,60	0
56	MG	RA	4005	1/1	0.91	0.18	93,93,93,93	0
56	MG	YA	3183	1/1	0.91	0.58	119,119,119,119	0
56	MG	QA	1785	1/1	0.91	0.06	85,85,85,85	0
56	MG	RA	3890	1/1	0.91	0.28	90,90,90,90	0
56	MG	YA	3129	1/1	0.91	0.34	140,140,140,140	0
56	MG	RA	3624	1/1	0.91	0.26	67,67,67,67	0
56	MG	RA	3464	1/1	0.91	0.15	53,53,53,53	0
56	MG	RA	3833	1/1	0.91	0.28	66,66,66,66	0
56	MG	RA	3862	1/1	0.91	0.36	83,83,83,83	0
56	MG	QA	1829	1/1	0.91	0.18	83,83,83,83	0
56	MG	YB	201	1/1	0.91	0.13	136,136,136,136	0
56	MG	XA	1768	1/1	0.91	0.36	85,85,85,85	0
56	MG	RA	3138	1/1	0.91	0.35	127,127,127,127	0
56	MG	YA	3194	1/1	0.91	0.13	73,73,73,73	0
56	MG	YA	3602	1/1	0.91	0.18	46,46,46,46	0
56	MG	RA	3671	1/1	0.91	0.09	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3139	1/1	0.91	0.09	72,72,72,72	0
56	MG	RA	3524	1/1	0.91	0.51	100,100,100,100	0
56	MG	RA	3149	1/1	0.91	0.09	122,122,122,122	0
56	MG	RA	3868	1/1	0.91	0.28	66,66,66,66	0
56	MG	RA	4026	1/1	0.91	0.21	122,122,122,122	0
56	MG	YA	3609	1/1	0.91	0.17	39,39,39,39	0
56	MG	RA	3447	1/1	0.91	0.30	55,55,55,55	0
56	MG	RA	3355	1/1	0.91	0.22	70,70,70,70	0
56	MG	RA	3047	1/1	0.91	0.17	75,75,75,75	0
56	MG	RA	3386	1/1	0.91	0.19	40,40,40,40	0
56	MG	YA	3334	1/1	0.91	0.22	53,53,53,53	0
56	MG	RA	3654	1/1	0.91	0.20	80,80,80,80	0
56	MG	RA	3814	1/1	0.91	0.29	64,64,64,64	0
56	MG	YA	3273	1/1	0.91	0.09	28,28,28,28	0
56	MG	RA	3124	1/1	0.91	0.29	131,131,131,131	0
56	MG	YA	3341	1/1	0.91	0.32	42,42,42,42	0
56	MG	RA	3275	1/1	0.91	0.13	101,101,101,101	0
56	MG	RA	3152	1/1	0.91	0.26	106,106,106,106	0
56	MG	XA	1644	1/1	0.91	0.10	81,81,81,81	0
56	MG	RA	3347	1/1	0.91	0.07	85,85,85,85	0
56	MG	YA	3051	1/1	0.91	0.08	62,62,62,62	0
56	MG	RA	3251	1/1	0.91	0.21	110,110,110,110	0
56	MG	YA	3627	1/1	0.91	0.23	42,42,42,42	0
56	MG	YA	3417	1/1	0.91	0.11	58,58,58,58	0
56	MG	RA	3376	1/1	0.91	0.18	58,58,58,58	0
56	MG	YA	3217	1/1	0.91	0.07	106,106,106,106	0
56	MG	YA	3103	1/1	0.91	0.07	53,53,53,53	0
56	MG	YA	3104	1/1	0.91	0.25	78,78,78,78	0
56	MG	RA	3159	1/1	0.91	0.31	88,88,88,88	0
56	MG	RA	3948	1/1	0.91	0.15	60,60,60,60	0
56	MG	RA	3253	1/1	0.91	0.34	120,120,120,120	0
56	MG	RA	3031	1/1	0.91	0.20	72,72,72,72	0
56	MG	RA	3991	1/1	0.91	0.30	135,135,135,135	0
56	MG	YA	3193	1/1	0.92	0.23	121,121,121,121	0
56	MG	RA	3708	1/1	0.92	0.07	59,59,59,59	0
56	MG	YA	3064	1/1	0.92	0.51	105,105,105,105	0
56	MG	RA	3330	1/1	0.92	0.08	67,67,67,67	0
56	MG	RA	3710	1/1	0.92	0.14	84,84,84,84	0
56	MG	RA	3824	1/1	0.92	0.28	119,119,119,119	0
56	MG	RA	3992	1/1	0.92	0.20	134,134,134,134	0
56	MG	RE	301	1/1	0.92	0.19	57,57,57,57	0
56	MG	XA	1628	1/1	0.92	0.06	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3070	1/1	0.92	0.22	85,85,85,85	0
56	MG	RA	3931	1/1	0.92	0.13	72,72,72,72	0
56	MG	YA	3157	1/1	0.92	0.13	80,80,80,80	0
56	MG	RA	3995	1/1	0.92	0.26	116,116,116,116	0
56	MG	RA	3733	1/1	0.92	0.12	51,51,51,51	0
56	MG	YA	3527	1/1	0.92	0.30	66,66,66,66	0
56	MG	YA	3115	1/1	0.92	0.12	153,153,153,153	0
56	MG	RA	3877	1/1	0.92	0.18	34,34,34,34	0
56	MG	RA	3754	1/1	0.92	0.28	54,54,54,54	0
56	MG	RA	3219	1/1	0.92	0.55	103,103,103,103	0
56	MG	RA	3029	1/1	0.92	0.60	144,144,144,144	0
56	MG	RA	3758	1/1	0.92	0.28	89,89,89,89	0
56	MG	YA	3372	1/1	0.92	0.17	110,110,110,110	0
56	MG	RA	3105	1/1	0.92	0.48	127,127,127,127	0
56	MG	YA	3601	1/1	0.92	0.15	46,46,46,46	0
56	MG	R0	101	1/1	0.92	0.15	106,106,106,106	0
56	MG	YA	3269	1/1	0.92	0.31	34,34,34,34	0
56	MG	RA	3085	1/1	0.92	0.50	130,130,130,130	0
56	MG	RA	3117	1/1	0.92	0.16	116,116,116,116	0
56	MG	XA	1710	1/1	0.92	0.22	56,56,56,56	0
56	MG	YV	201	1/1	0.92	0.23	92,92,92,92	0
56	MG	YW	201	1/1	0.92	0.26	116,116,116,116	0
56	MG	RA	3969	1/1	0.92	0.17	98,98,98,98	0
56	MG	RA	3834	1/1	0.92	0.17	56,56,56,56	0
56	MG	YA	3434	1/1	0.92	0.20	70,70,70,70	0
56	MG	RA	3224	1/1	0.92	0.56	142,142,142,142	0
56	MG	RA	3264	1/1	0.92	0.09	69,69,69,69	0
56	MG	RA	3107	1/1	0.92	0.20	89,89,89,89	0
56	MG	YA	3004	1/1	0.92	0.12	42,42,42,42	0
56	MG	YA	3132	1/1	0.92	0.20	92,92,92,92	0
56	MG	RA	3094	1/1	0.92	0.16	109,109,109,109	0
56	MG	YA	3675	1/1	0.92	0.20	49,49,49,49	0
56	MG	RA	3891	1/1	0.92	0.14	45,45,45,45	0
56	MG	RA	4020	1/1	0.92	0.28	88,88,88,88	0
56	MG	XA	1725	1/1	0.92	0.36	72,72,72,72	0
56	MG	RA	3296	1/1	0.92	0.41	113,113,113,113	0
56	MG	YA	3337	1/1	0.92	0.16	33,33,33,33	0
56	MG	RA	3978	1/1	0.92	0.13	91,91,91,91	0
56	MG	RA	3580	1/1	0.92	0.13	87,87,87,87	0
56	MG	YA	3558	1/1	0.92	0.22	41,41,41,41	0
56	MG	YA	3395	1/1	0.92	0.27	43,43,43,43	0
56	MG	YA	3287	1/1	0.92	0.14	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3703	1/1	0.92	0.20	53,53,53,53	0
56	MG	XA	1734	1/1	0.92	0.15	80,80,80,80	0
56	MG	RA	3982	1/1	0.92	0.18	74,74,74,74	0
56	MG	RA	3478	1/1	0.92	0.18	33,33,33,33	0
56	MG	RA	3086	1/1	0.92	0.50	130,130,130,130	0
56	MG	RA	4033	1/1	0.92	0.37	119,119,119,119	0
56	MG	YA	3567	1/1	0.92	0.19	40,40,40,40	0
56	MG	RA	3048	1/1	0.92	0.13	71,71,71,71	0
56	MG	RA	3063	1/1	0.92	0.09	67,67,67,67	0
56	MG	YA	3348	1/1	0.92	0.16	75,75,75,75	0
56	MG	RA	3970	1/1	0.93	0.12	37,37,37,37	0
56	MG	YA	3590	1/1	0.93	0.23	43,43,43,43	0
56	MG	RA	3595	1/1	0.93	0.35	126,126,126,126	0
56	MG	RA	4012	1/1	0.93	0.80	126,126,126,126	0
56	MG	RF	312	1/1	0.93	0.12	84,84,84,84	0
56	MG	YA	3222	1/1	0.93	0.17	89,89,89,89	0
56	MG	YA	3596	1/1	0.93	0.07	51,51,51,51	0
56	MG	YA	3731	1/1	0.93	0.19	104,104,104,104	0
56	MG	YA	3732	1/1	0.93	0.12	78,78,78,78	0
56	MG	RA	3069	1/1	0.93	0.21	98,98,98,98	0
56	MG	YA	3466	1/1	0.93	0.31	37,37,37,37	0
56	MG	RA	3757	1/1	0.93	0.22	44,44,44,44	0
56	MG	RA	3483	1/1	0.93	0.07	34,34,34,34	0
56	MG	RA	3911	1/1	0.93	0.23	59,59,59,59	0
56	MG	RA	3231	1/1	0.93	0.31	115,115,115,115	0
56	MG	RA	4019	1/1	0.93	0.25	136,136,136,136	0
56	MG	XA	1753	1/1	0.93	0.21	62,62,62,62	0
56	MG	RA	3788	1/1	0.93	0.23	145,145,145,145	0
56	MG	RA	3575	1/1	0.93	0.11	85,85,85,85	0
56	MG	RA	3505	1/1	0.93	0.26	57,57,57,57	0
56	MG	RA	4024	1/1	0.93	0.18	116,116,116,116	0
56	MG	RA	3884	1/1	0.93	0.20	43,43,43,43	0
56	MG	YA	3236	1/1	0.93	0.45	98,98,98,98	0
56	MG	RA	3293	1/1	0.93	0.12	76,76,76,76	0
56	MG	RA	3415	1/1	0.93	0.38	47,47,47,47	0
56	MG	RA	4030	1/1	0.93	0.26	115,115,115,115	0
56	MG	YA	3135	1/1	0.93	0.09	65,65,65,65	0
56	MG	RA	3257	1/1	0.93	0.40	87,87,87,87	0
56	MG	RA	3079	1/1	0.93	0.27	135,135,135,135	0
56	MG	YA	3042	1/1	0.93	0.10	33,33,33,33	0
56	MG	QA	1701	1/1	0.93	0.27	66,66,66,66	0
56	MG	RA	3272	1/1	0.93	0.34	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3135	1/1	0.93	0.29	112,112,112,112	0
56	MG	RA	3326	1/1	0.93	0.22	74,74,74,74	0
56	MG	YA	3249	1/1	0.93	0.30	100,100,100,100	0
56	MG	QA	1834	1/1	0.93	0.35	61,61,61,61	0
56	MG	RA	3114	1/1	0.93	0.23	162,162,162,162	0
56	MG	RA	3342	1/1	0.93	0.29	37,37,37,37	0
56	MG	YD	303	1/1	0.93	0.29	74,74,74,74	0
56	MG	YA	3556	1/1	0.93	0.07	37,37,37,37	0
56	MG	YD	306	1/1	0.93	0.12	85,85,85,85	0
56	MG	RA	4039	1/1	0.93	0.14	95,95,95,95	0
56	MG	RV	204	1/1	0.93	0.18	79,79,79,79	0
56	MG	RA	3714	1/1	0.93	0.09	74,74,74,74	0
56	MG	RA	3181	1/1	0.93	0.33	92,92,92,92	0
56	MG	YE	304	1/1	0.93	0.16	24,24,24,24	0
56	MG	YA	3440	1/1	0.93	0.13	59,59,59,59	0
56	MG	YA	3258	1/1	0.93	0.28	85,85,85,85	0
56	MG	RA	3301	1/1	0.93	0.19	144,144,144,144	0
56	MG	YA	3636	1/1	0.93	0.33	52,52,52,52	0
56	MG	RA	3996	1/1	0.93	0.31	122,122,122,122	0
56	MG	YA	3702	1/1	0.93	0.24	74,74,74,74	0
56	MG	RA	3663	1/1	0.93	0.32	66,66,66,66	0
56	MG	YA	3153	1/1	0.93	0.13	73,73,73,73	0
56	MG	YA	3506	1/1	0.93	0.28	146,146,146,146	0
56	MG	RA	3613	1/1	0.93	0.26	40,40,40,40	0
56	MG	RA	3496	1/1	0.93	0.29	43,43,43,43	0
56	MG	RA	3497	1/1	0.93	0.36	41,41,41,41	0
56	MG	RA	3115	1/1	0.93	0.25	112,112,112,112	0
56	MG	YA	3328	1/1	0.93	0.29	28,28,28,28	0
56	MG	RA	3266	1/1	0.93	0.18	103,103,103,103	0
56	MG	YA	3209	1/1	0.93	0.14	36,36,36,36	0
56	MG	RA	3695	1/1	0.93	0.24	58,58,58,58	0
56	MG	YA	3212	1/1	0.93	0.30	98,98,98,98	0
56	MG	RB	213	1/1	0.93	0.29	71,71,71,71	0
56	MG	RF	306	1/1	0.93	0.17	106,106,106,106	0
56	MG	RA	3460	1/1	0.93	0.14	73,73,73,73	0
56	MG	YA	3163	1/1	0.93	0.15	119,119,119,119	0
56	MG	RA	3214	1/1	0.93	0.25	122,122,122,122	0
56	MG	RA	3895	1/1	0.94	0.42	73,73,73,73	0
56	MG	XA	1687	1/1	0.94	0.28	67,67,67,67	0
56	MG	RA	3059	1/1	0.94	0.10	47,47,47,47	0
56	MG	RA	3136	1/1	0.94	0.29	83,83,83,83	0
56	MG	RA	3799	1/1	0.94	0.23	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3547	1/1	0.94	0.30	68,68,68,68	0
56	MG	RA	4006	1/1	0.94	0.15	81,81,81,81	0
56	MG	RA	3055	1/1	0.94	0.23	117,117,117,117	0
56	MG	YA	3060	1/1	0.94	0.07	59,59,59,59	0
56	MG	YA	3371	1/1	0.94	0.14	47,47,47,47	0
56	MG	RA	4008	1/1	0.94	0.28	109,109,109,109	0
56	MG	RA	3259	1/1	0.94	0.27	121,121,121,121	0
56	MG	YA	3672	1/1	0.94	0.23	53,53,53,53	0
56	MG	YP	201	1/1	0.94	0.18	86,86,86,86	0
56	MG	RA	3827	1/1	0.94	0.09	48,48,48,48	0
56	MG	RA	3040	1/1	0.94	0.18	76,76,76,76	0
56	MG	RA	3261	1/1	0.94	0.22	101,101,101,101	0
56	MG	YA	3730	1/1	0.94	0.42	82,82,82,82	0
56	MG	YA	3331	1/1	0.94	0.16	45,45,45,45	0
56	MG	QA	1628	1/1	0.94	0.05	123,123,123,123	0
56	MG	RA	3139	1/1	0.94	0.65	102,102,102,102	0
56	MG	YA	3211	1/1	0.94	0.29	96,96,96,96	0
56	MG	RA	3700	1/1	0.94	0.46	105,105,105,105	0
56	MG	RA	3589	1/1	0.94	0.15	42,42,42,42	0
56	MG	YA	3253	1/1	0.94	0.51	136,136,136,136	0
56	MG	RA	3958	1/1	0.94	0.22	53,53,53,53	0
56	MG	YA	3739	1/1	0.94	0.35	131,131,131,131	0
56	MG	YA	3740	1/1	0.94	0.12	70,70,70,70	0
56	MG	RA	3072	1/1	0.94	0.37	108,108,108,108	0
56	MG	RA	3073	1/1	0.94	0.09	69,69,69,69	0
56	MG	RA	3724	1/1	0.94	0.22	66,66,66,66	0
56	MG	YA	3635	1/1	0.94	0.37	38,38,38,38	0
56	MG	RA	3811	1/1	0.94	0.46	77,77,77,77	0
56	MG	YA	3584	1/1	0.94	0.38	77,77,77,77	0
56	MG	RA	3990	1/1	0.94	0.15	101,101,101,101	0
56	MG	RA	4025	1/1	0.94	0.41	150,150,150,150	0
56	MG	RA	3382	1/1	0.94	0.14	48,48,48,48	0
56	MG	YB	207	1/1	0.94	0.13	110,110,110,110	0
56	MG	RA	3265	1/1	0.94	0.14	116,116,116,116	0
56	MG	RA	3044	1/1	0.94	0.28	131,131,131,131	0
56	MG	YA	3488	1/1	0.94	0.11	39,39,39,39	0
56	MG	YA	3397	1/1	0.94	0.14	54,54,54,54	0
56	MG	RA	3024	1/1	0.94	0.05	63,63,63,63	0
56	MG	RA	3133	1/1	0.94	0.11	97,97,97,97	0
56	MG	YA	3595	1/1	0.94	0.09	46,46,46,46	0
56	MG	YA	3307	1/1	0.94	0.17	39,39,39,39	0
56	MG	YA	3266	1/1	0.94	0.17	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3689	1/1	0.94	0.19	141,141,141,141	0
56	MG	RA	3091	1/1	0.94	0.21	142,142,142,142	0
56	MG	YA	3404	1/1	0.94	0.61	67,67,67,67	0
56	MG	XA	1677	1/1	0.94	0.30	60,60,60,60	0
56	MG	RA	3598	1/1	0.94	0.38	89,89,89,89	0
56	MG	QG	201	1/1	0.94	0.09	96,96,96,96	0
56	MG	YA	3122	1/1	0.94	0.22	135,135,135,135	0
56	MG	YA	3500	1/1	0.94	0.14	39,39,39,39	0
56	MG	YA	3359	1/1	0.94	0.19	59,59,59,59	0
56	MG	YD	308	1/1	0.94	0.21	92,92,92,92	0
56	MG	YA	3272	1/1	0.94	0.21	71,71,71,71	0
56	MG	YA	3052	1/1	0.94	0.07	54,54,54,54	0
56	MG	RA	3321	1/1	0.95	0.12	38,38,38,38	0
56	MG	RA	4022	1/1	0.95	0.33	82,82,82,82	0
56	MG	RA	3416	1/1	0.95	0.07	50,50,50,50	0
56	MG	RA	3197	1/1	0.95	0.28	117,117,117,117	0
56	MG	RA	3368	1/1	0.95	0.29	76,76,76,76	0
56	MG	RA	3561	1/1	0.95	0.21	38,38,38,38	0
56	MG	RD	307	1/1	0.95	0.12	114,114,114,114	0
56	MG	RA	4027	1/1	0.95	0.14	105,105,105,105	0
56	MG	YA	3165	1/1	0.95	0.22	131,131,131,131	0
56	MG	YA	3086	1/1	0.95	0.21	95,95,95,95	0
56	MG	RV	201	1/1	0.95	0.10	90,90,90,90	0
56	MG	RA	3461	1/1	0.95	0.19	32,32,32,32	0
56	MG	YA	3316	1/1	0.95	0.30	30,30,30,30	0
56	MG	YA	3317	1/1	0.95	0.15	37,37,37,37	0
56	MG	YA	3669	1/1	0.95	0.26	37,37,37,37	0
56	MG	YA	3009	1/1	0.95	0.15	65,65,65,65	0
56	MG	YA	3286	1/1	0.95	0.22	40,40,40,40	0
56	MG	YA	3557	1/1	0.95	0.41	51,51,51,51	0
56	MG	YA	3389	1/1	0.95	0.23	32,32,32,32	0
56	MG	XF	202	1/1	0.95	0.04	90,90,90,90	0
56	MG	RA	3160	1/1	0.95	0.32	102,102,102,102	0
56	MG	RA	3463	1/1	0.95	0.12	39,39,39,39	0
56	MG	YA	3713	1/1	0.95	0.13	26,26,26,26	0
56	MG	RA	3020	1/1	0.95	0.40	145,145,145,145	0
56	MG	YA	3526	1/1	0.95	0.10	35,35,35,35	0
56	MG	YA	3563	1/1	0.95	0.32	60,60,60,60	0
56	MG	RA	3208	1/1	0.95	0.20	114,114,114,114	0
56	MG	RA	3093	1/1	0.95	0.33	117,117,117,117	0
56	MG	RA	3043	1/1	0.95	0.17	53,53,53,53	0
56	MG	RA	3551	1/1	0.95	0.17	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3297	1/1	0.95	0.28	86,86,86,86	0
56	MG	RA	3288	1/1	0.95	0.17	99,99,99,99	0
56	MG	YA	3237	1/1	0.95	0.32	127,127,127,127	0
56	MG	YA	3179	1/1	0.95	0.18	97,97,97,97	0
56	MG	RA	3033	1/1	0.95	0.19	135,135,135,135	0
56	MG	RA	3413	1/1	0.95	0.13	66,66,66,66	0
56	MG	RA	3648	1/1	0.95	0.28	127,127,127,127	0
56	MG	RA	3144	1/1	0.95	0.10	79,79,79,79	0
56	MG	YD	309	1/1	0.95	0.13	45,45,45,45	0
56	MG	RB	204	1/1	0.95	0.08	102,102,102,102	0
58	SF4	QD	302	8/8	0.95	0.06	107,119,141,144	0
56	MG	YA	3585	1/1	0.96	0.28	43,43,43,43	0
56	MG	YA	3369	1/1	0.96	0.08	22,22,22,22	0
56	MG	RA	3847	1/1	0.96	0.26	38,38,38,38	0
56	MG	YA	3618	1/1	0.96	0.44	63,63,63,63	0
56	MG	RA	3470	1/1	0.96	0.04	65,65,65,65	0
56	MG	YA	3620	1/1	0.96	0.06	55,55,55,55	0
56	MG	RD	304	1/1	0.96	0.36	92,92,92,92	0
56	MG	RA	3572	1/1	0.96	0.14	52,52,52,52	0
56	MG	RA	3182	1/1	0.96	0.24	118,118,118,118	0
56	MG	XA	1749	1/1	0.96	0.09	47,47,47,47	0
56	MG	RA	3864	1/1	0.96	0.35	51,51,51,51	0
56	MG	RA	3343	1/1	0.96	0.09	56,56,56,56	0
56	MG	RA	3993	1/1	0.96	0.23	102,102,102,102	0
56	MG	YA	3109	1/1	0.96	0.09	32,32,32,32	0
56	MG	RD	310	1/1	0.96	0.36	125,125,125,125	0
56	MG	RA	3207	1/1	0.96	0.28	153,153,153,153	0
56	MG	RA	3092	1/1	0.96	0.06	99,99,99,99	0
56	MG	RA	3209	1/1	0.96	0.08	106,106,106,106	0
56	MG	YA	3229	1/1	0.96	0.28	111,111,111,111	0
56	MG	RA	3021	1/1	0.96	0.23	109,109,109,109	0
56	MG	RR	201	1/1	0.96	0.44	72,72,72,72	0
56	MG	YA	3232	1/1	0.96	0.43	129,129,129,129	0
56	MG	R1	102	1/1	0.96	0.18	65,65,65,65	0
56	MG	YA	3002	1/1	0.96	0.04	54,54,54,54	0
56	MG	RA	3819	1/1	0.96	0.30	29,29,29,29	0
56	MG	YA	3576	1/1	0.96	0.20	39,39,39,39	0
56	MG	YA	3577	1/1	0.96	0.20	52,52,52,52	0
56	MG	RA	3731	1/1	0.96	0.08	46,46,46,46	0
56	MG	RA	3211	1/1	0.96	0.14	113,113,113,113	0
56	MG	RA	4034	1/1	0.96	0.15	96,96,96,96	0
56	MG	YA	3552	1/1	0.96	0.14	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1637	1/1	0.96	0.11	156,156,156,156	0
56	MG	RA	3028	1/1	0.96	0.27	118,118,118,118	0
56	MG	RU	202	1/1	0.96	0.60	104,104,104,104	0
56	MG	RA	3006	1/1	0.97	0.07	76,76,76,76	0
56	MG	YA	3481	1/1	0.97	0.25	34,34,34,34	0
56	MG	RA	3236	1/1	0.97	0.23	113,113,113,113	0
56	MG	YA	3351	1/1	0.97	0.25	36,36,36,36	0
56	MG	XA	1692	1/1	0.97	0.26	52,52,52,52	0
56	MG	RA	3658	1/1	0.97	0.22	54,54,54,54	0
56	MG	RA	3528	1/1	0.97	0.05	81,81,81,81	0
56	MG	YA	3288	1/1	0.97	0.33	38,38,38,38	0
56	MG	RA	3081	1/1	0.97	0.23	111,111,111,111	0
56	MG	RA	3981	1/1	0.97	0.06	106,106,106,106	0
56	MG	RA	3019	1/1	0.97	0.45	102,102,102,102	0
56	MG	YA	3021	1/1	0.97	0.10	49,49,49,49	0
56	MG	YA	3376	1/1	0.97	0.24	55,55,55,55	0
56	MG	YA	3742	1/1	0.97	0.48	105,105,105,105	0
56	MG	RA	3228	1/1	0.97	0.37	132,132,132,132	0
56	MG	YA	3720	1/1	0.97	0.23	112,112,112,112	0
56	MG	RA	3212	1/1	0.97	0.15	102,102,102,102	0
56	MG	RA	3573	1/1	0.97	0.27	77,77,77,77	0
56	MG	RA	3511	1/1	0.97	0.27	35,35,35,35	0
56	MG	RA	3998	1/1	0.97	0.14	134,134,134,134	0
56	MG	RA	4011	1/1	0.97	0.22	124,124,124,124	0
56	MG	YA	3011	1/1	0.97	0.09	68,68,68,68	0
56	MG	YA	3579	1/1	0.97	0.24	28,28,28,28	0
56	MG	YA	3384	1/1	0.97	0.18	28,28,28,28	0
56	MG	YD	304	1/1	0.98	0.16	118,118,118,118	0
56	MG	YA	3335	1/1	0.98	0.28	29,29,29,29	0
56	MG	RA	4015	1/1	0.98	0.37	117,117,117,117	0
56	MG	YA	3724	1/1	0.98	0.36	141,141,141,141	0
56	MG	YA	3020	1/1	0.98	0.22	134,134,134,134	0
57	ZN	QN	101	1/1	0.98	0.04	142,142,142,142	0
58	SF4	XD	301	8/8	0.98	0.04	97,108,130,131	0
56	MG	YA	3014	1/1	0.99	0.04	57,57,57,57	0
57	ZN	XN	101	1/1	0.99	0.04	114,114,114,114	0

6.5 Other polymers

There are no such residues in this entry.