



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 04:38 AM EDT

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

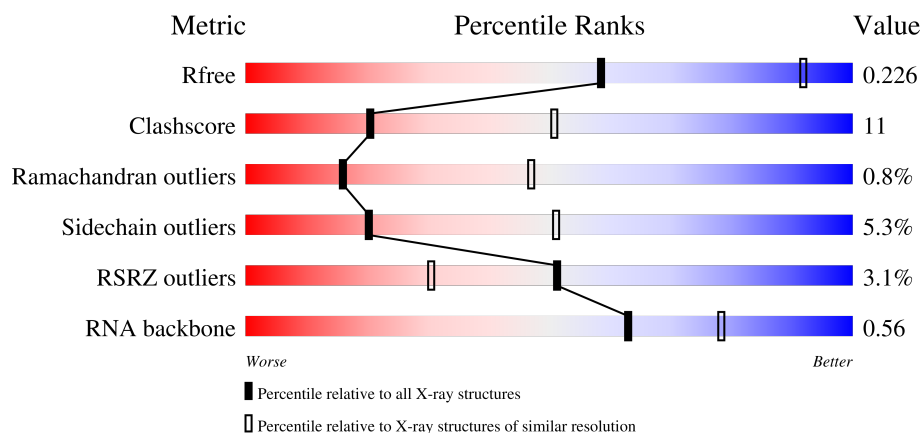
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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

Mol	Chain	Length	Quality of chain
1	QV	77	3% 58% 34% 6%
1	XV	77	3% 65% 26% 9%
2	QX	25	12% 24% 12% 60%
2	XX	25	12% 20% 12% 8% 60%

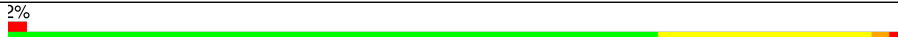
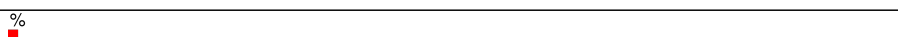
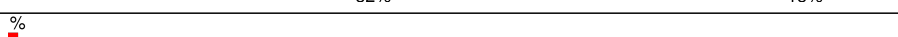
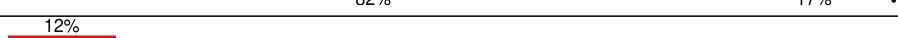
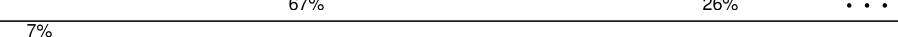
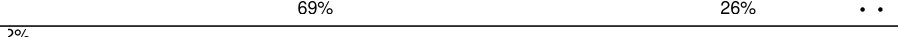
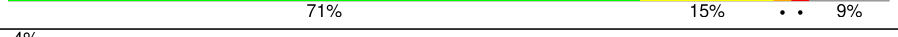
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Mol	Chain	Length	Quality of chain
3	QY	380	
3	XY	380	
4	RA	2915	
4	YA	2915	
5	RB	122	
5	YB	122	
6	RD	276	
6	YD	276	
7	RE	206	
7	YE	206	
8	RF	210	
8	YF	210	
9	RG	182	
9	YG	182	
10	RH	180	
10	YH	180	
11	RI	148	
11	YI	148	
12	RN	140	
12	YN	140	
13	RO	122	
13	YO	122	
14	RP	150	
14	YP	150	
15	RQ	141	

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Mol	Chain	Length	Quality of chain
15	YQ	141	
16	RR	118	
16	YR	118	
17	RS	112	
17	YS	112	
18	RT	146	
18	YT	146	
19	RU	118	
19	YU	118	
20	RV	101	
20	YV	101	
21	RW	113	
21	YW	113	
22	RX	96	
22	YX	96	
23	RY	110	
23	YY	110	
24	RZ	206	
24	YZ	206	
25	R0	85	
25	Y0	85	
26	R1	98	
26	Y1	98	
27	R2	72	
27	Y2	72	

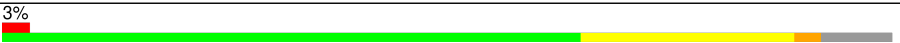
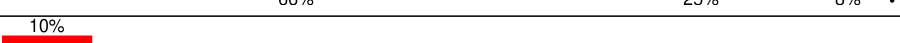
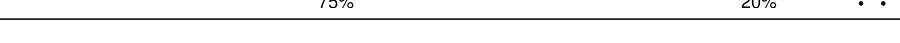
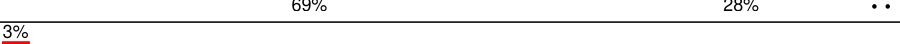
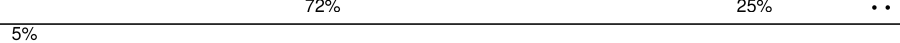
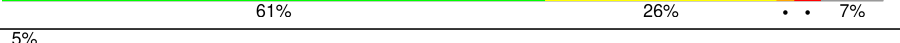
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Mol	Chain	Length	Quality of chain
28	R3	60	
28	Y3	60	
29	R4	71	
29	Y4	71	
30	R5	60	
30	Y5	60	
31	R6	54	
31	Y6	54	
32	R7	49	
32	Y7	49	
33	R8	65	
33	Y8	65	
34	R9	37	
34	Y9	37	
35	QA	1521	
35	XA	1521	
36	QB	256	
36	XB	256	
37	QC	239	
37	XC	239	
38	QD	209	
38	XD	209	
39	QE	162	
39	XE	162	
40	QF	101	

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Mol	Chain	Length	Quality of chain
40	XF	101	
41	QG	156	
41	XG	156	
42	QH	138	
42	XH	138	
43	QI	128	
43	XI	128	
44	QJ	105	
44	XJ	105	
45	QK	129	
45	XK	129	
46	QL	132	
46	XL	132	
47	QM	126	
47	XM	126	
48	QN	61	
48	XN	61	
49	QO	89	
49	XO	89	
50	QP	88	
50	XP	88	
51	QQ	105	
51	XQ	105	
52	QR	88	
52	XR	88	

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

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

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

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

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

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

2 Entry composition

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

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

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

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

- Molecule 2 is a RNA chain called messenger RNA.

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

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

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

There are 30 discrepancies between the modelled and reference sequences:

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

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

- Molecule 4 is a RNA chain called T23S rRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	YR	1	Total 1	Mg 1	0	0
56	YT	3	Total 3	Mg 3	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	1	Total 1	Mg 1	0	0
56	Y8	2	Total 2	Mg 2	0	0
56	XA	190	Total 190	Mg 190	0	0
56	XE	2	Total 2	Mg 2	0	0
56	XF	4	Total 4	Mg 4	0	0
56	XH	1	Total 1	Mg 1	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	QA	279	Total 279	Mg 279	0	0
56	QB	1	Total 1	Mg 1	0	0

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

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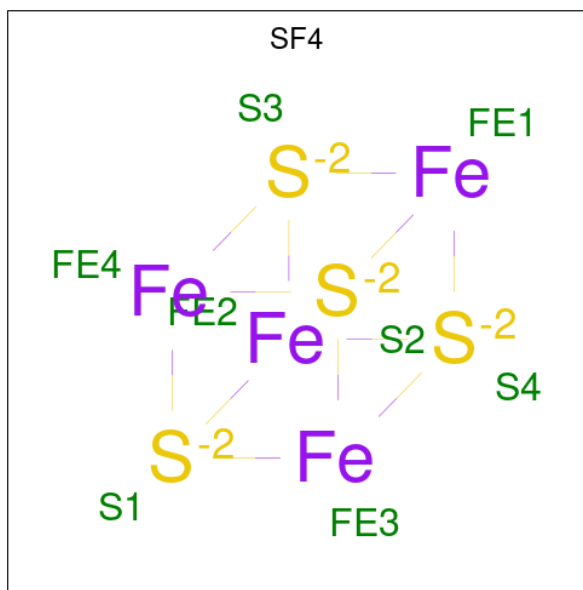
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	RN	3	Total 3	Mg 3	0	0
56	RO	1	Total 1	Mg 1	0	0
56	RP	2	Total 2	Mg 2	0	0
56	RQ	4	Total 4	Mg 4	0	0
56	RR	5	Total 5	Mg 5	0	0
56	RT	3	Total 3	Mg 3	0	0
56	RU	3	Total 3	Mg 3	0	0
56	RV	4	Total 4	Mg 4	0	0
56	RW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

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

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

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



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

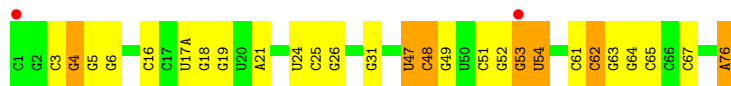
3 Residue-property plots [i](#)

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

- Molecule 1: P-site tRNA fMet



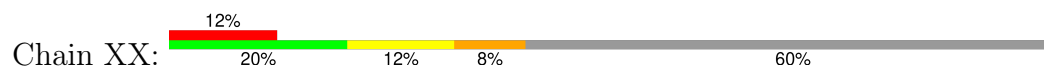
- Molecule 1: P-site tRNA fMet



- Molecule 2: messenger RNA

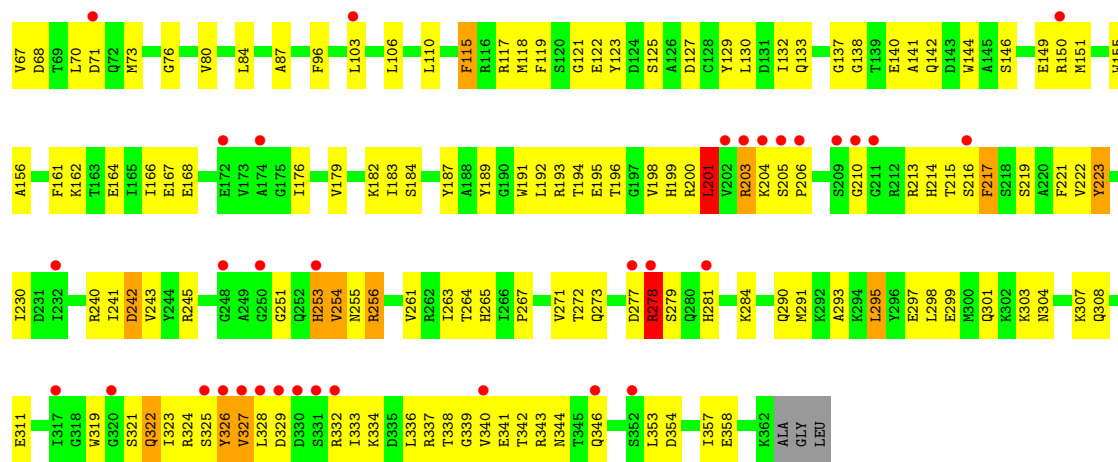


- Molecule 2: messenger RNA

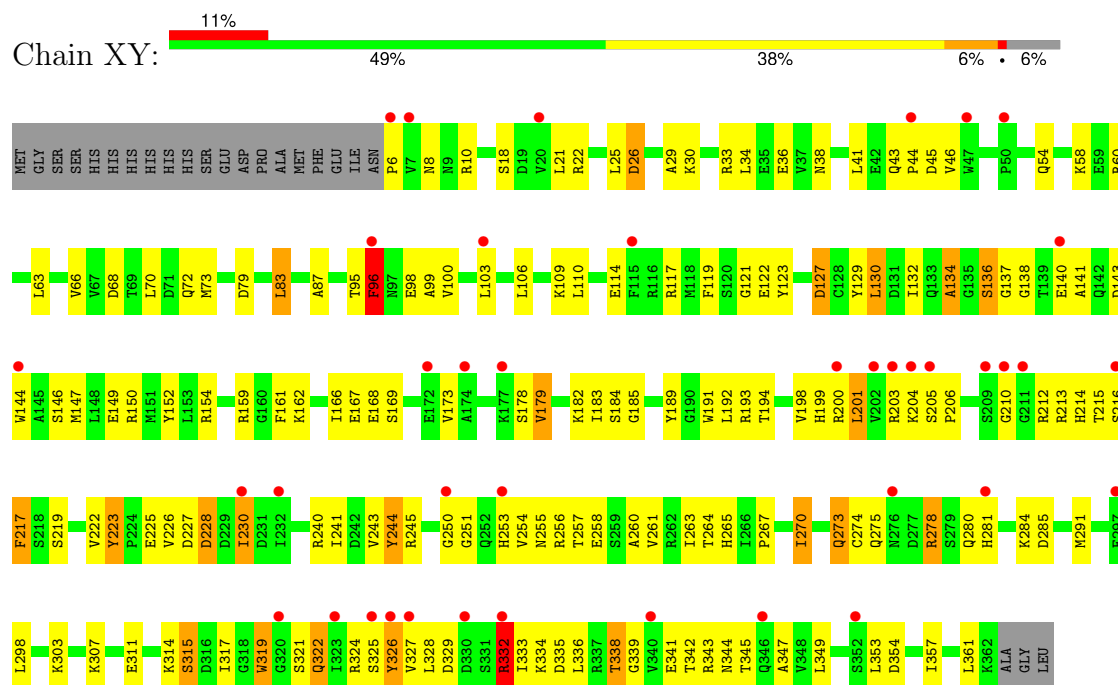


- Molecule 3: Peptide chain release factor 2

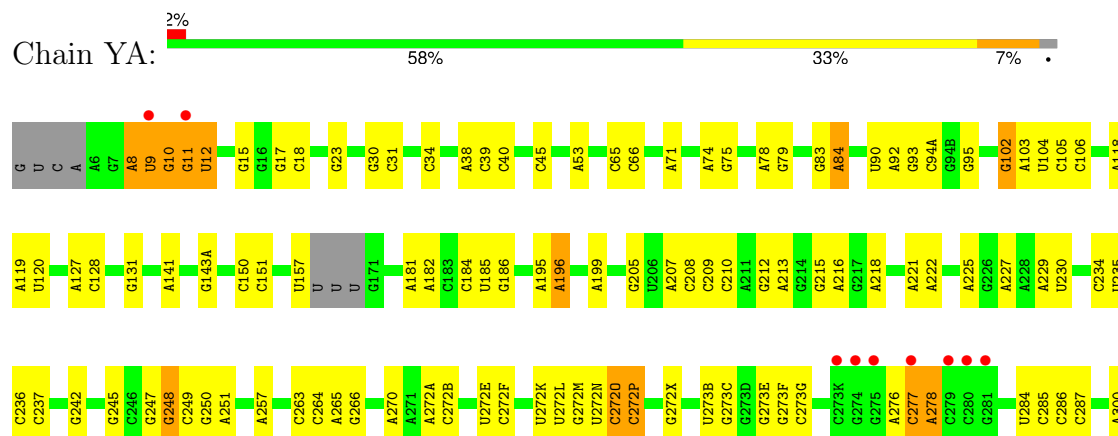




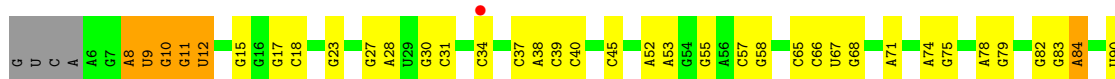
• Molecule 3: Peptide chain release factor 2



• Molecule 4: T23S rRNA



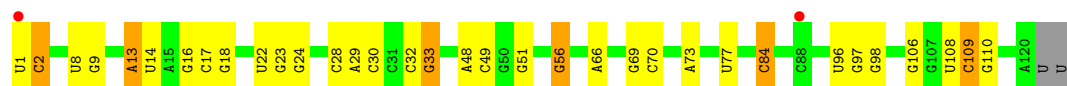
U1590	C1501	A1379	A1269	G1164	A1084	U1012	A917	G831	G707	G638	G561	C455	G301
G1591	C1502	G1380	C1270	U1165	A1085	C1013	A918	G832	G717	U639	U562	C456	C302
C1592	U1503	A1271	G1271	C1166	G1087	U1017	G919	U833	A718	C641	G563	A457	U303
G1594	C1504	A1272	U1273	U1167	A1088	G1017	U922	A835	C719	G642	U566	G458	U305
A1507	A1508	C1386	U1278	G1171	G1089	A1021	C923	G836	C720	A643	A567	G467	U306
A1509	C1509A	C1387	G1279	A	U1090	G1022	C924	C837	C721	U644	U568	G468	G307
A1509B	A1509C	U1397	U1287	U	G1091	G1025	C925	U839	A722	C645	U569	G469	G308
G1510	C1511	U1397	U1288	G	U1094	U1026	C932	C840	C730	A646	A572	A470	A311
C1514	U1514	G1400	U1289	A	A1095	A1027	G944	G848	C731	A652C	A573	G476	A320
G1515	G1515	G1401	C1289	C1178	U1096	A1028	A941	A849	C732	G652D	C574	G476	A320
U1629	U1630	U1405	C1290	C1179	U1097	A1029	G945	C855	C733	G652E	C575	G481	G321
G1630	C1407	U1406	C1293	C1181	A1098	G1030	A946	C857	G738	G	C576	G482	A322
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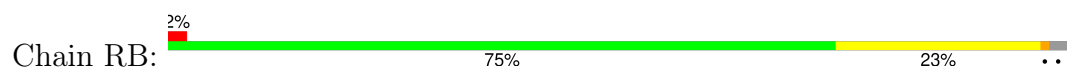
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A2927	A2809	U2496	A2378	A2295	C2130	U2130	A2041	A1651	U1807	C1667	A1552
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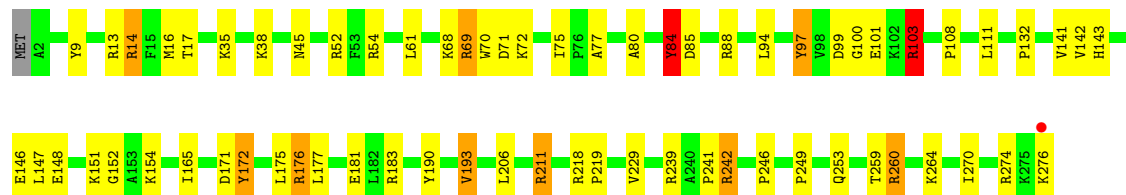
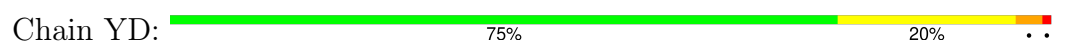
- Molecule 5: 5S rRNA



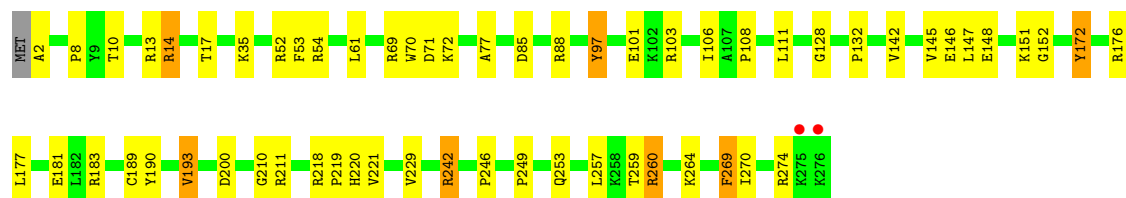
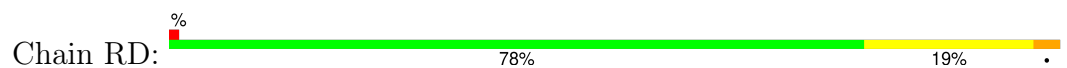
- Molecule 5: 5S rRNA



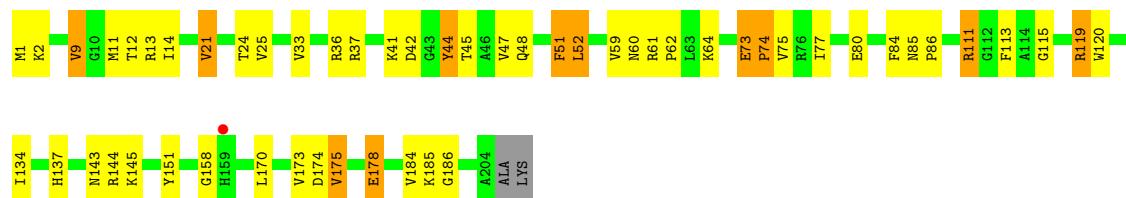
- Molecule 6: 50S ribosomal protein L2



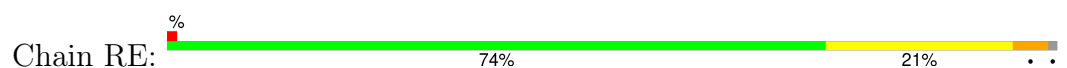
- Molecule 6: 50S ribosomal protein L2

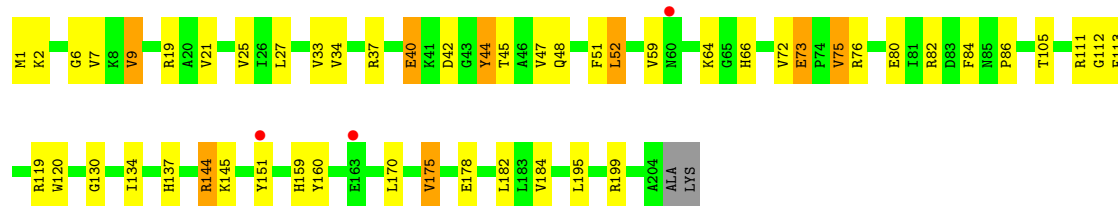


- Molecule 7: 50S ribosomal protein L3



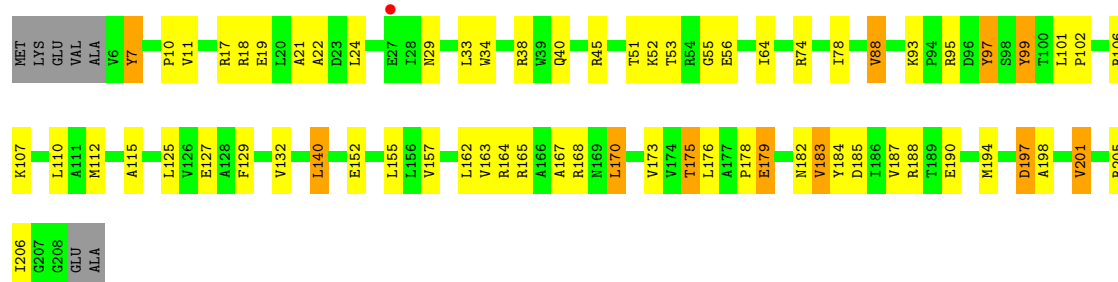
- Molecule 7: 50S ribosomal protein L3





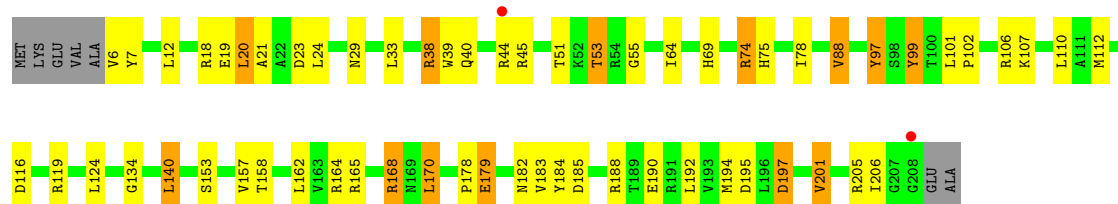
• Molecule 8: 50S ribosomal protein L4

Chain YF: 64% 27% 5% .



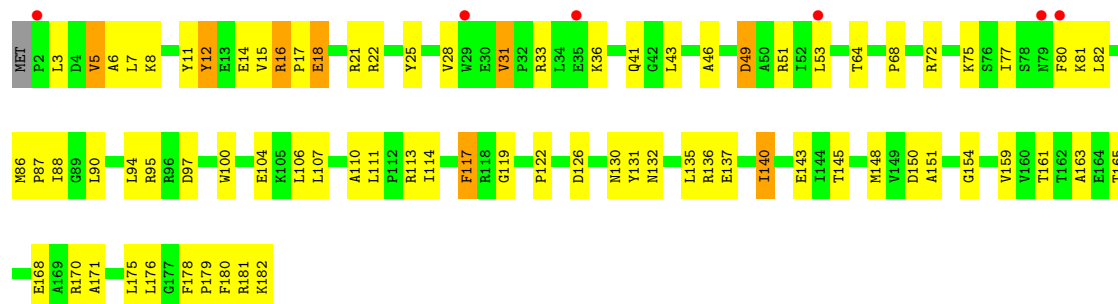
• Molecule 8: 50S ribosomal protein L4

Chain RF: 68% 23% 6% .



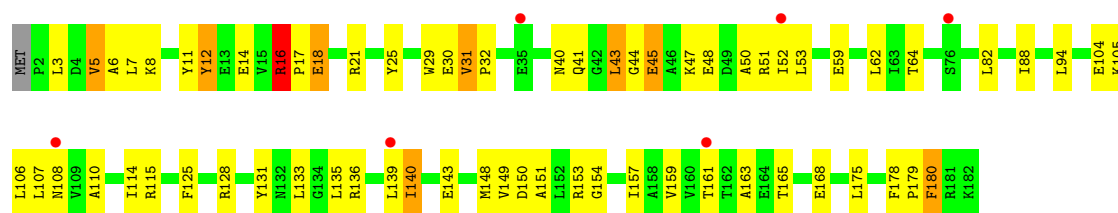
• Molecule 9: 50S ribosomal protein L5

Chain YG: 56% 39% 3% . .

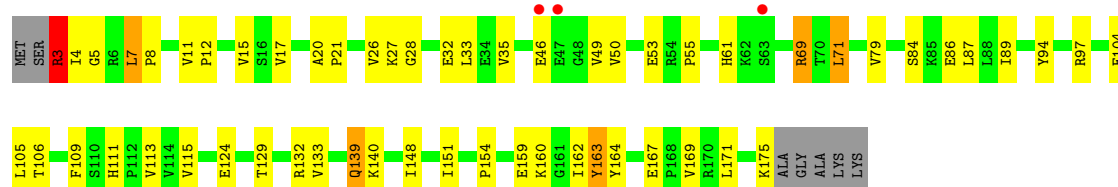


• Molecule 9: 50S ribosomal protein L5

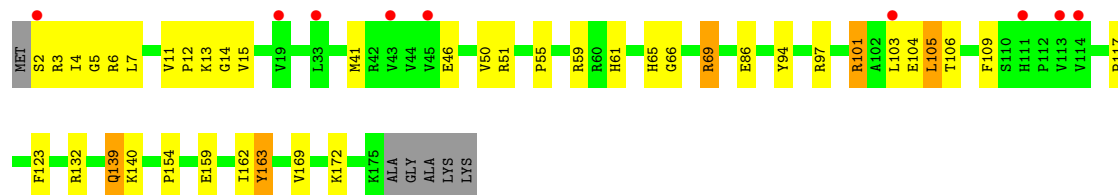
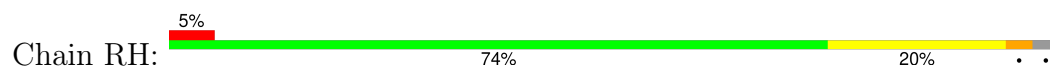
Chain RG: 63% 32% . .



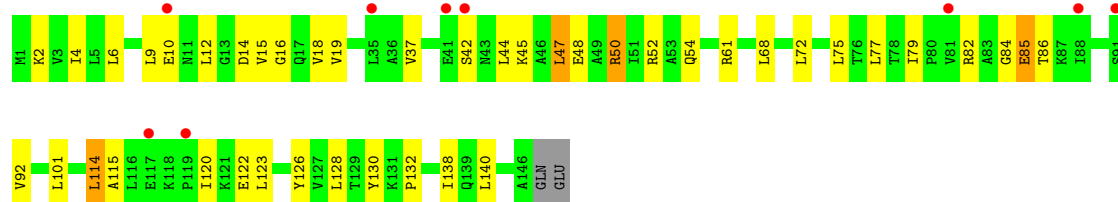
• Molecule 10: 50S ribosomal protein L6



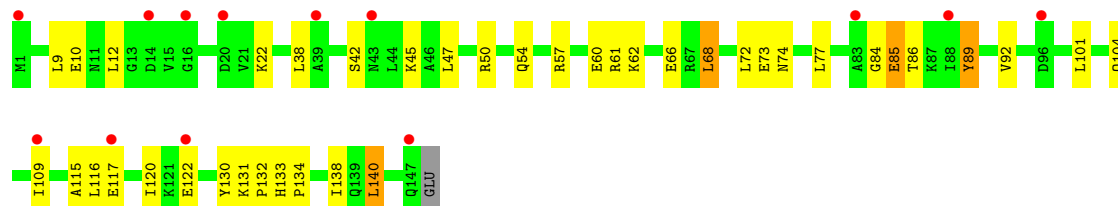
• Molecule 10: 50S ribosomal protein L6



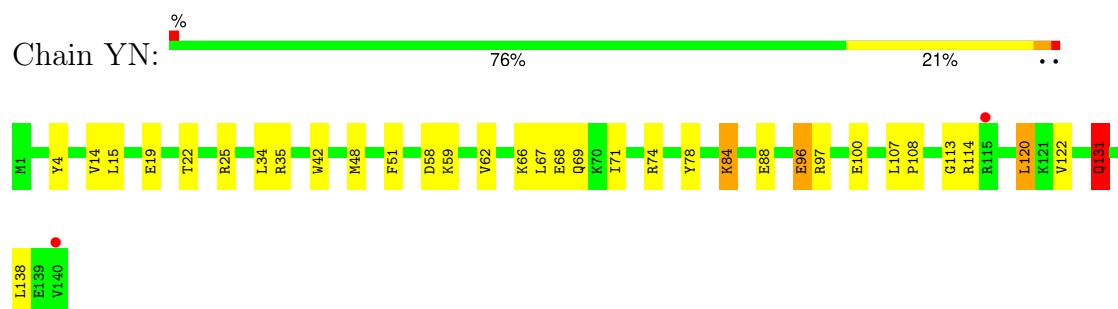
• Molecule 11: 50S ribosomal protein L9



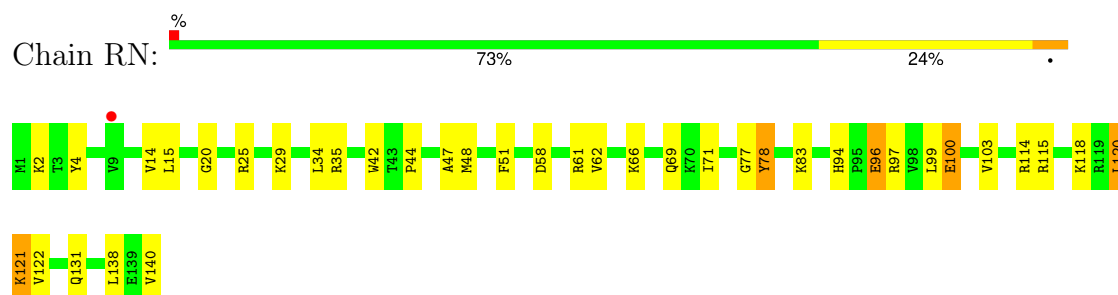
• Molecule 11: 50S ribosomal protein L9



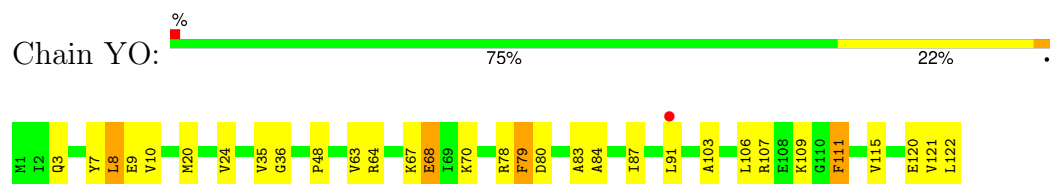
- Molecule 12: 50S ribosomal protein L13



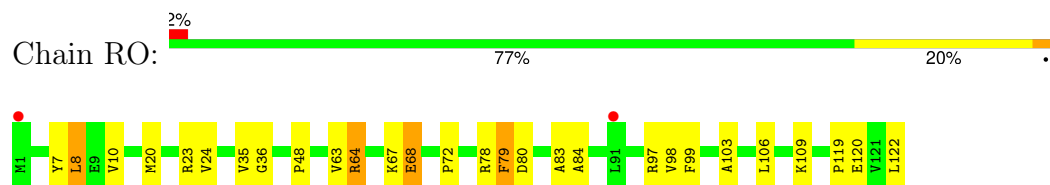
- Molecule 12: 50S ribosomal protein L13



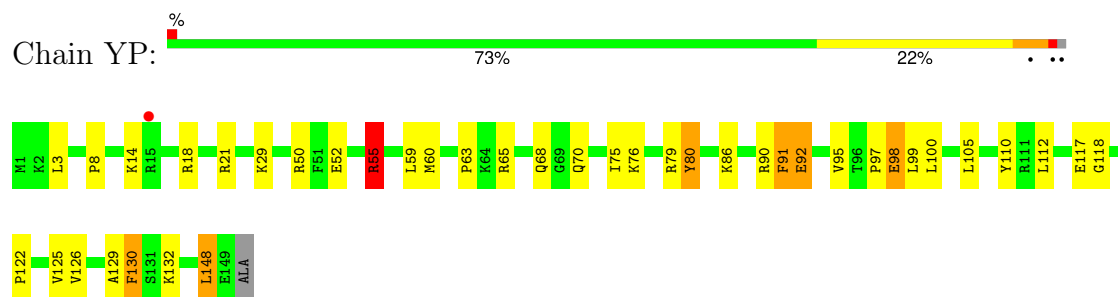
- Molecule 13: 50S ribosomal protein L14



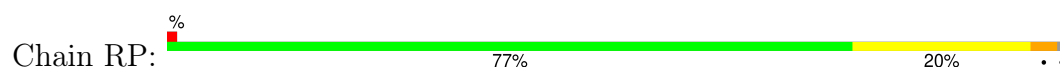
- Molecule 13: 50S ribosomal protein L14

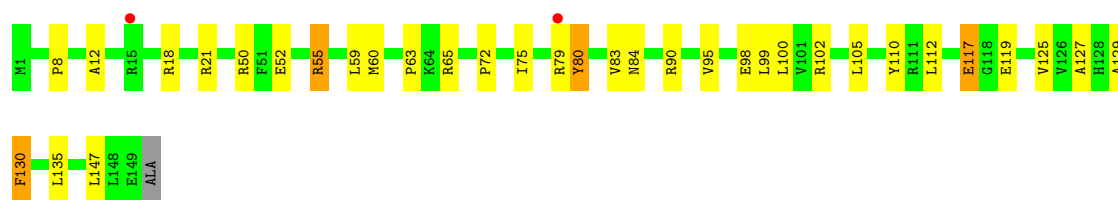


- Molecule 14: 50S ribosomal protein L15

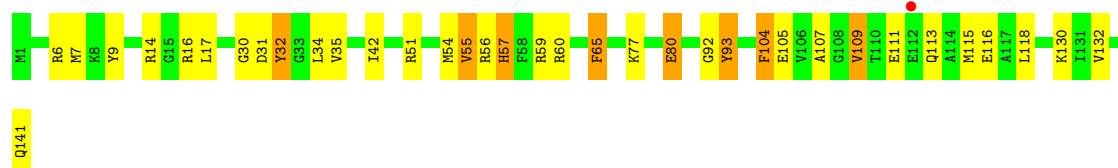
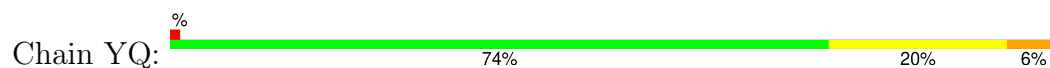


- Molecule 14: 50S ribosomal protein L15

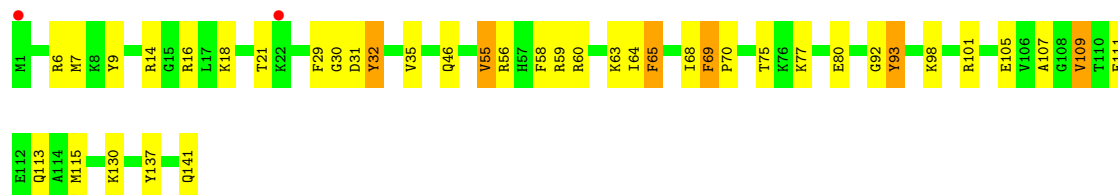
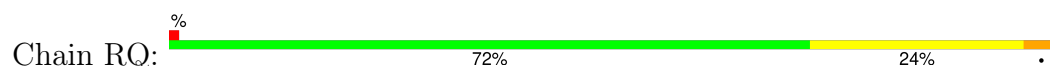




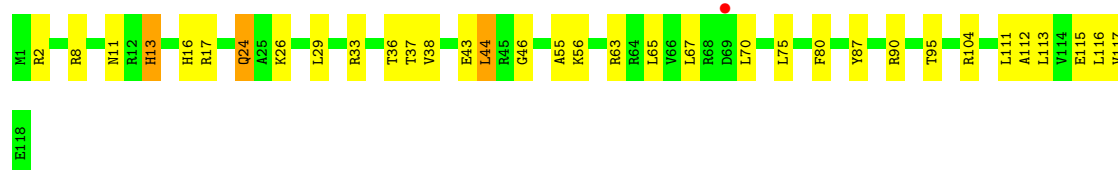
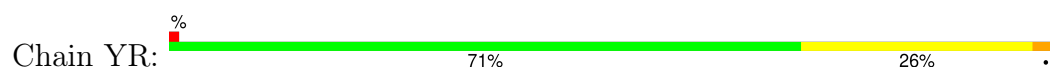
- Molecule 15: 50S ribosomal protein L16



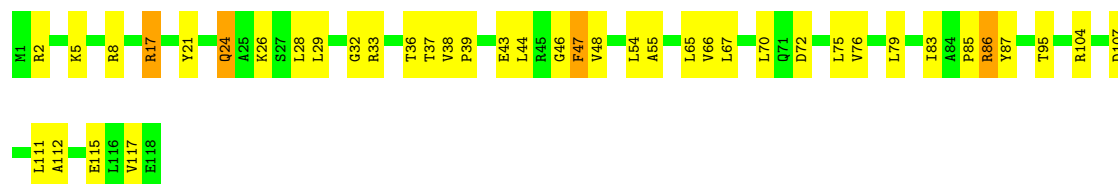
- Molecule 15: 50S ribosomal protein L16



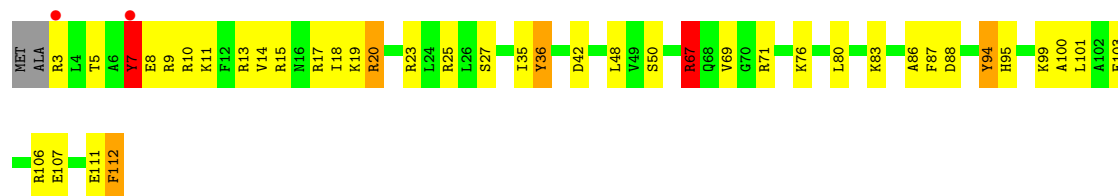
- Molecule 16: 50S ribosomal protein L17



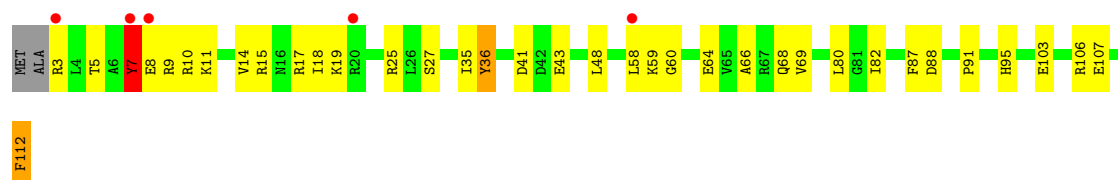
- Molecule 16: 50S ribosomal protein L17



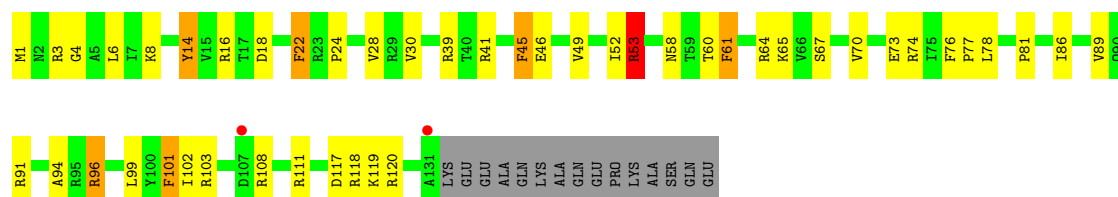
- Molecule 17: 50S ribosomal protein L18



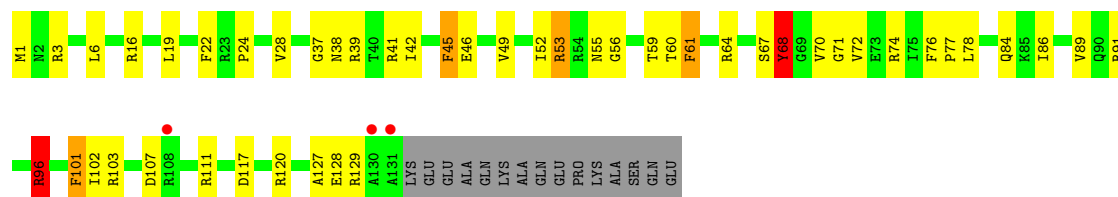
- Molecule 17: 50S ribosomal protein L18



- Molecule 18: 50S ribosomal protein L19



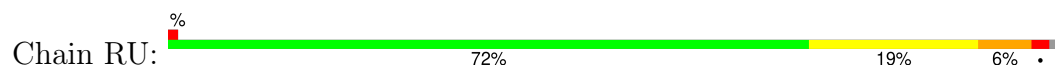
- Molecule 18: 50S ribosomal protein L19



- Molecule 19: 50S ribosomal protein L20

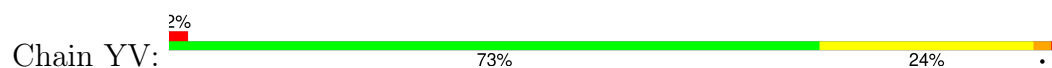


- Molecule 19: 50S ribosomal protein L20

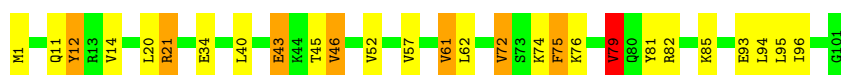




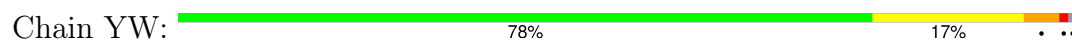
- Molecule 20: 50S ribosomal protein L21



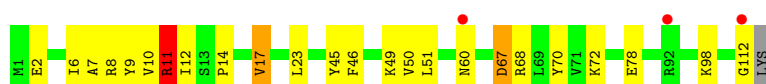
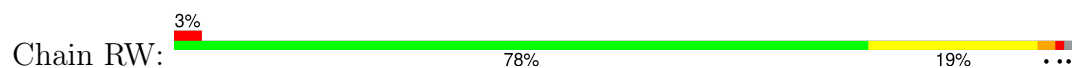
- Molecule 20: 50S ribosomal protein L21



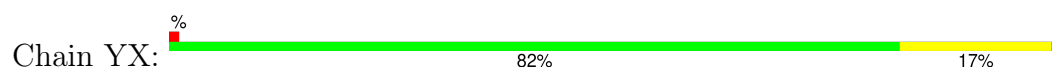
- Molecule 21: 50S ribosomal protein L22



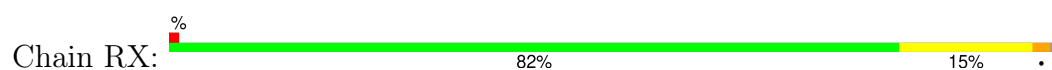
- Molecule 21: 50S ribosomal protein L22



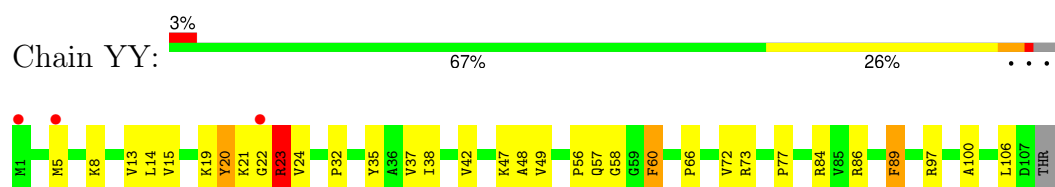
- Molecule 22: 50S ribosomal protein L23



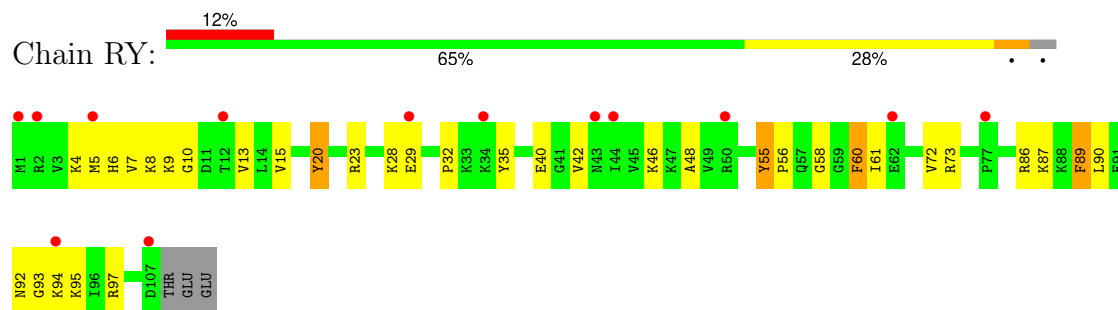
- Molecule 22: 50S ribosomal protein L23



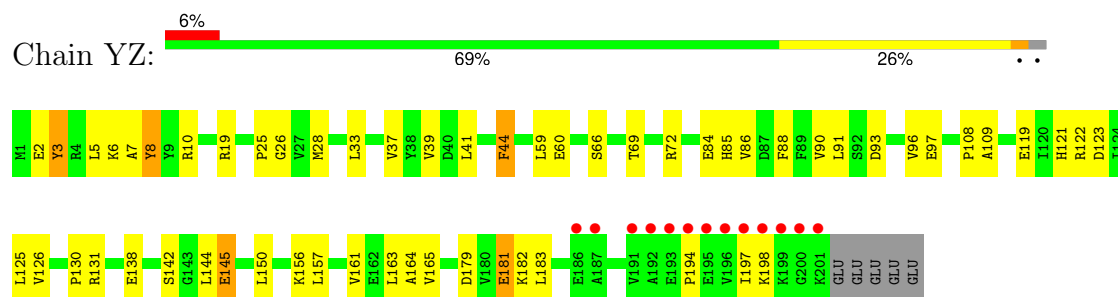
- Molecule 23: 50S ribosomal protein L24



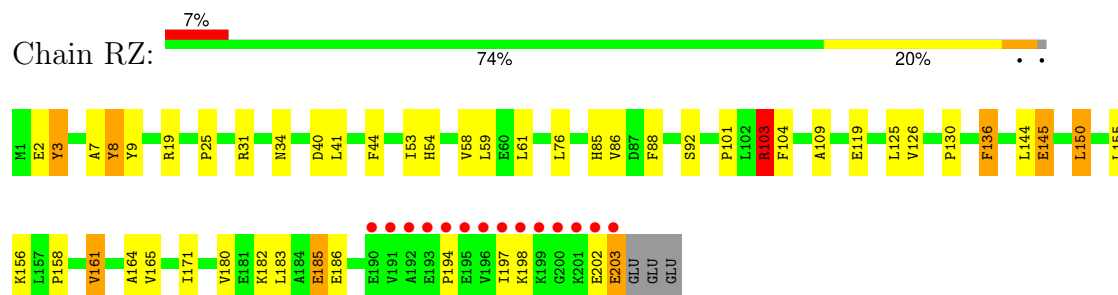
- Molecule 23: 50S ribosomal protein L24



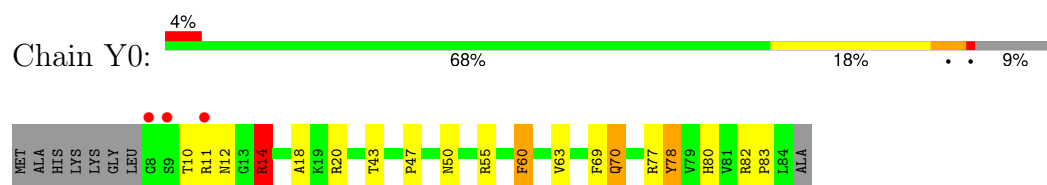
- Molecule 24: 50S ribosomal protein L25



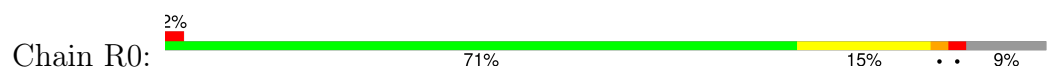
- Molecule 24: 50S ribosomal protein L25



- Molecule 25: 50S ribosomal protein L27



- Molecule 25: 50S ribosomal protein L27





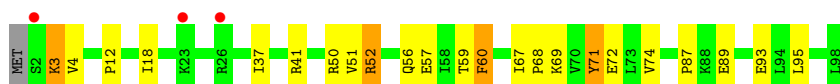
- Molecule 26: 50S ribosomal protein L28

Chain Y1: 64% 29% 5% ..



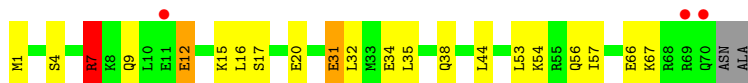
- Molecule 26: 50S ribosomal protein L28

Chain R1: 3% 76% 19% ..



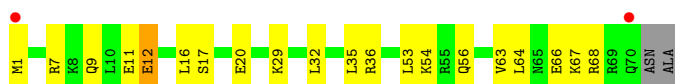
- Molecule 27: 50S ribosomal protein L29

Chain Y2: 4% 68% 25% ..



- Molecule 27: 50S ribosomal protein L29

Chain R2: 3% 69% 26% ..



- Molecule 28: 50S ribosomal protein L30

Chain Y3: 3% 82% 15% ..

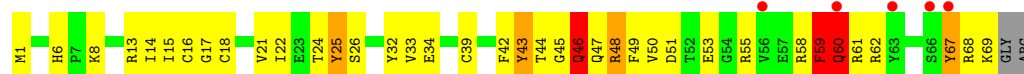
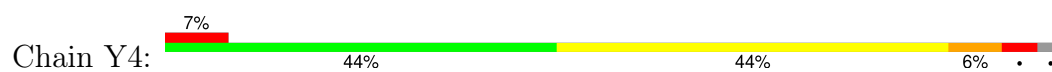


- Molecule 28: 50S ribosomal protein L30

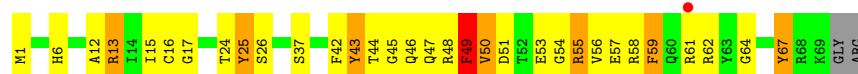
Chain R3: 2% 80% 18% ..



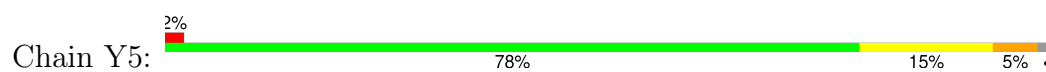
- Molecule 29: 50S ribosomal protein L31



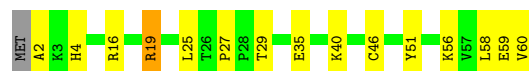
- Molecule 29: 50S ribosomal protein L31



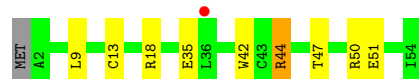
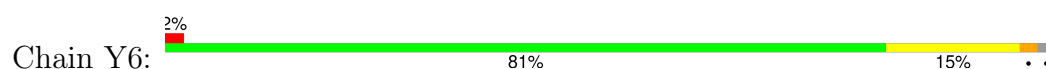
- Molecule 30: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L32



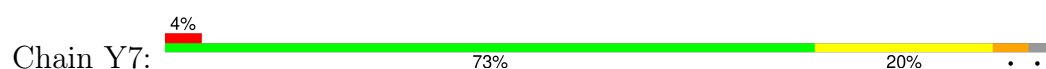
- Molecule 31: 50S ribosomal protein L33



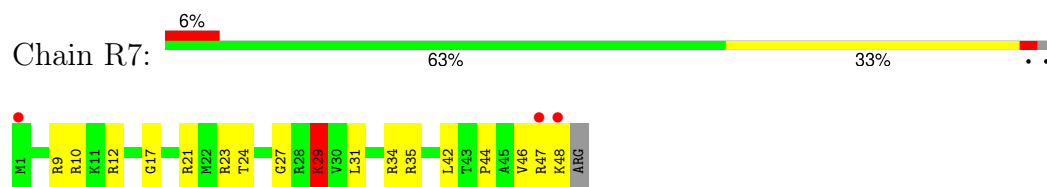
- Molecule 31: 50S ribosomal protein L33



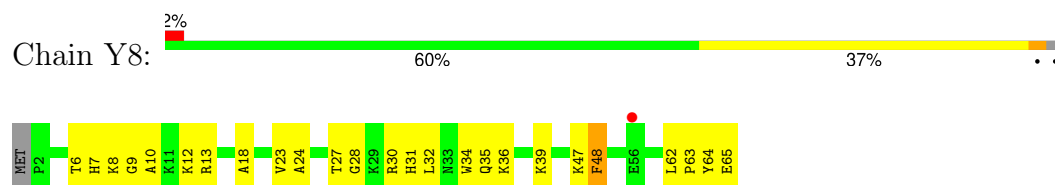
- Molecule 32: 50S ribosomal protein L34



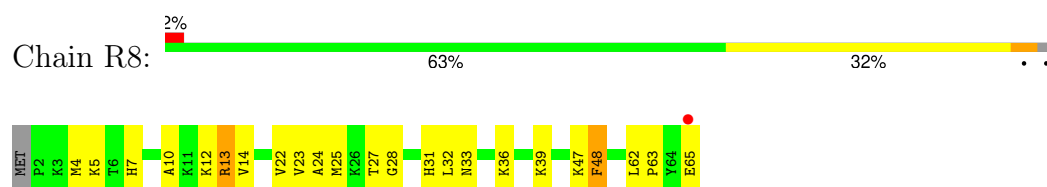
- Molecule 32: 50S ribosomal protein L34



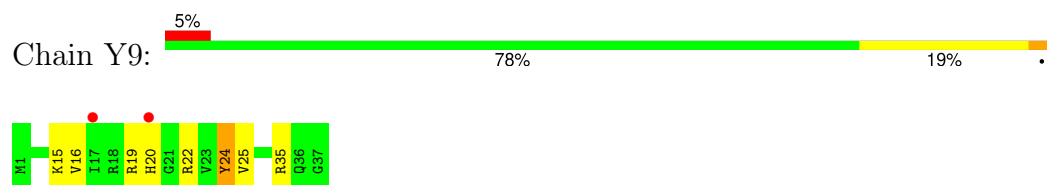
- Molecule 33: 50S ribosomal protein L35



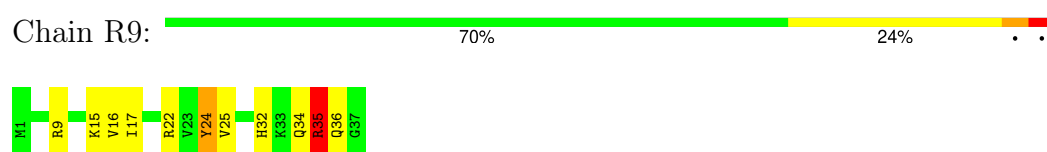
- Molecule 33: 50S ribosomal protein L35



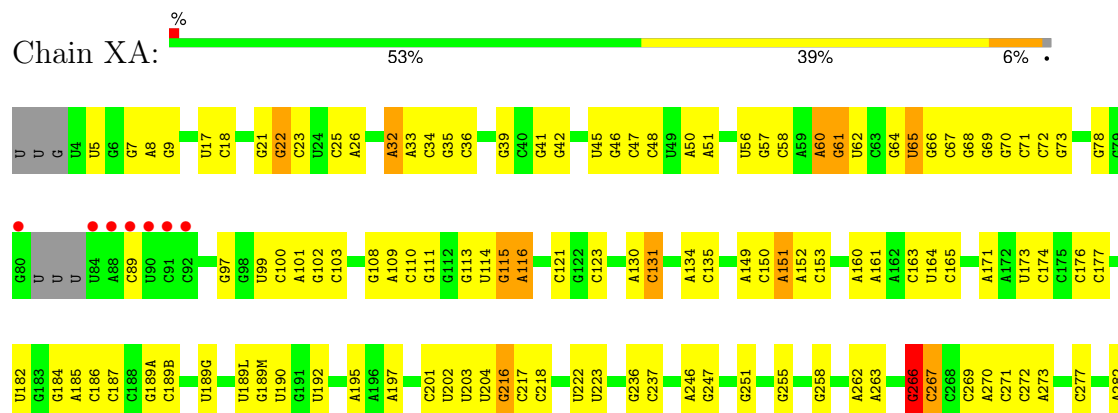
- Molecule 34: 50S ribosomal protein L36

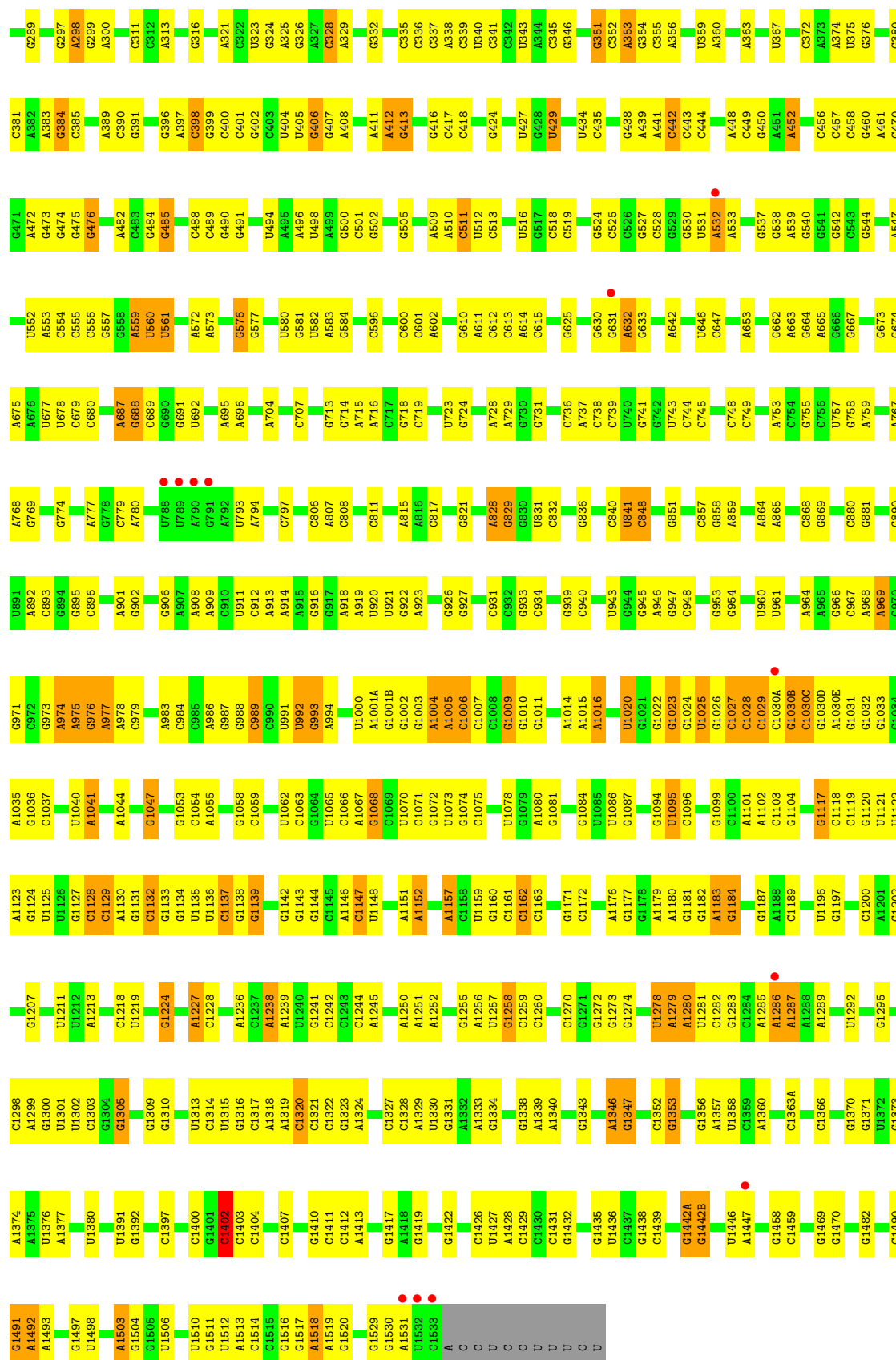


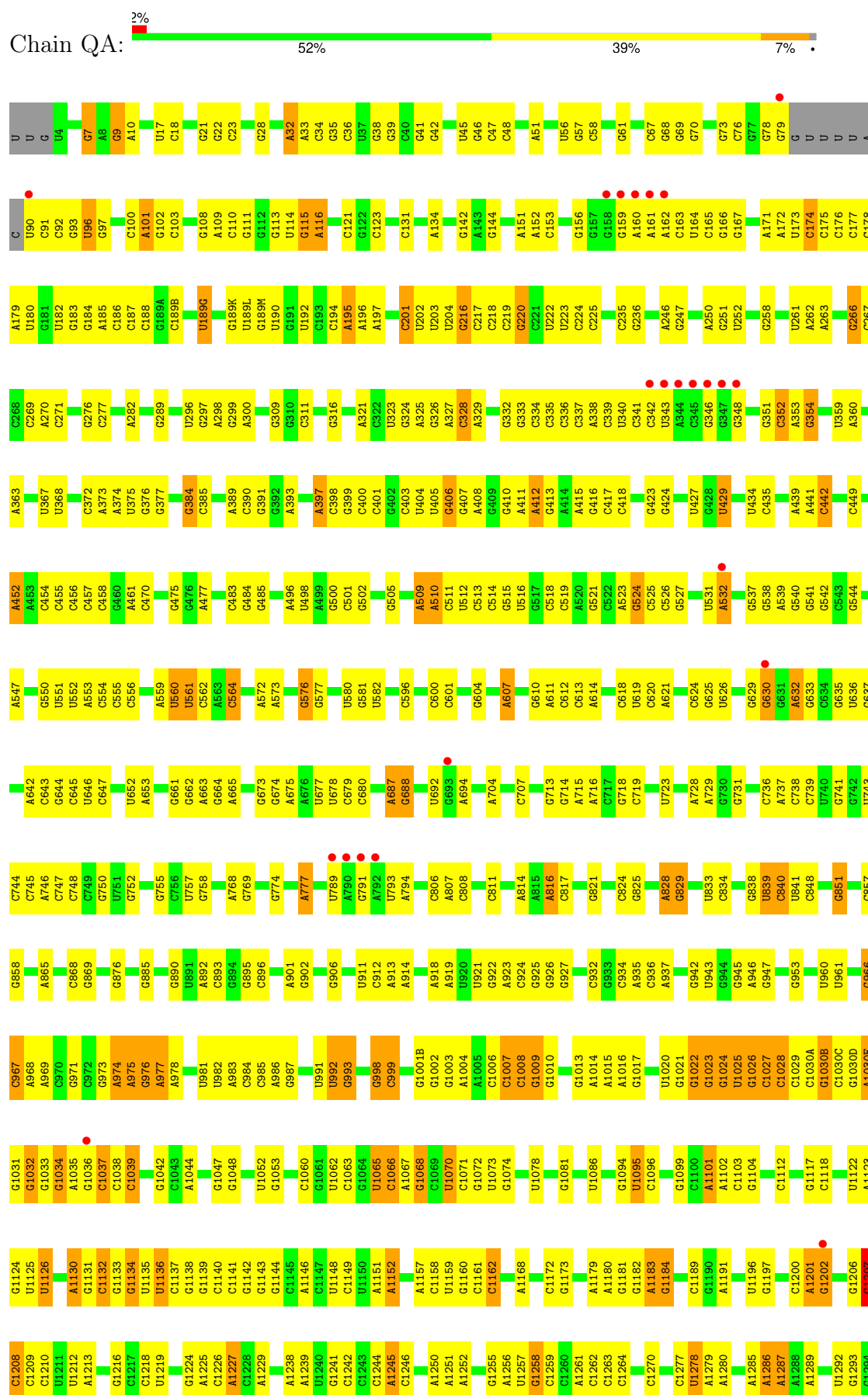
- Molecule 34: 50S ribosomal protein L36

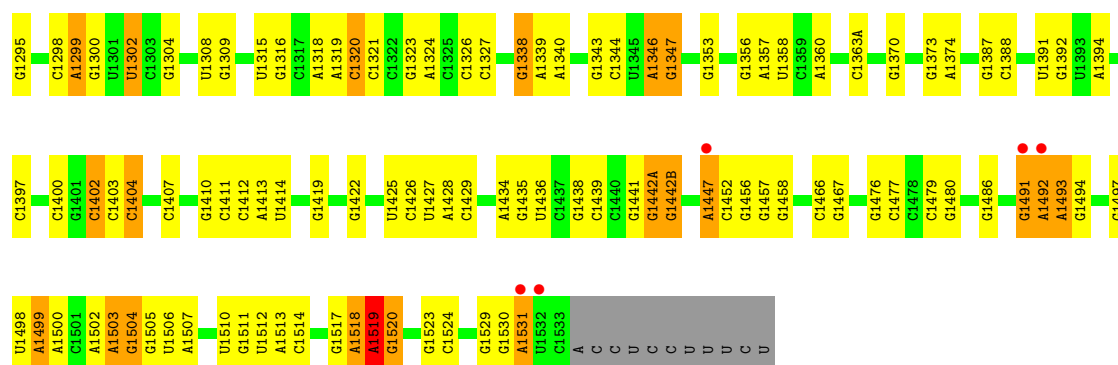


- Molecule 35: 16S rRNA

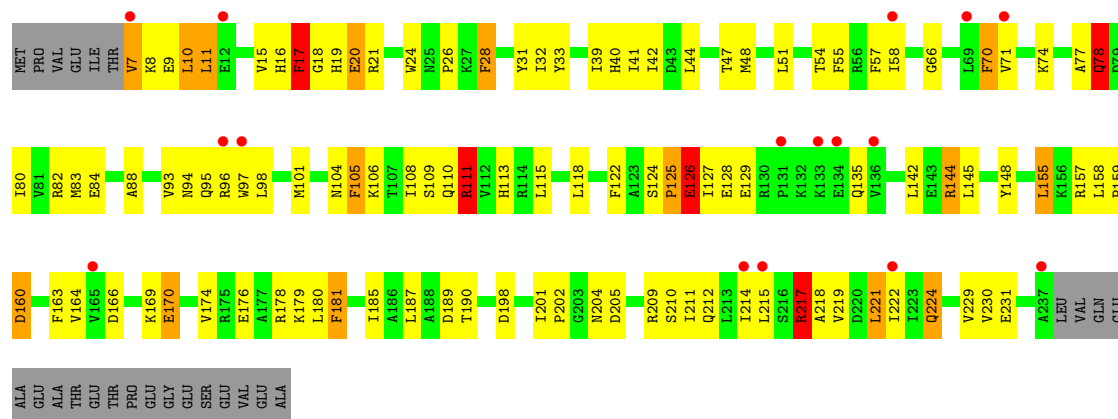




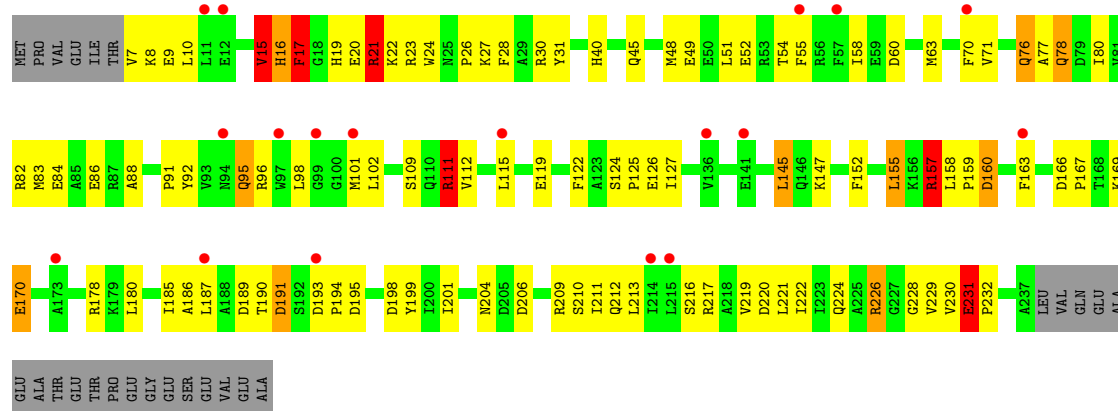




• Molecule 36: 30S ribosomal protein S2

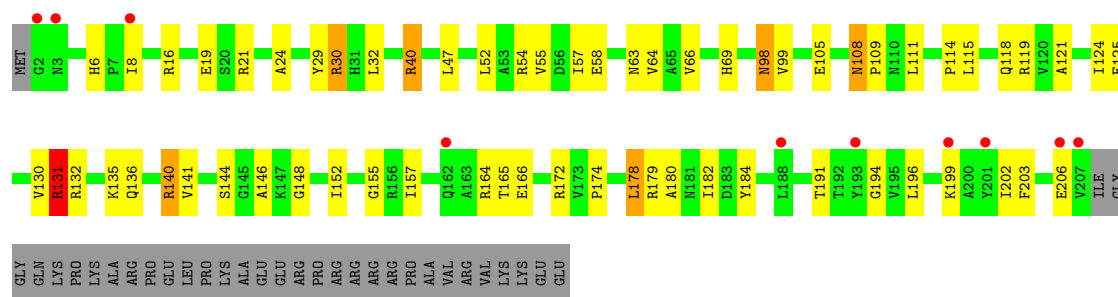


• Molecule 36: 30S ribosomal protein S2

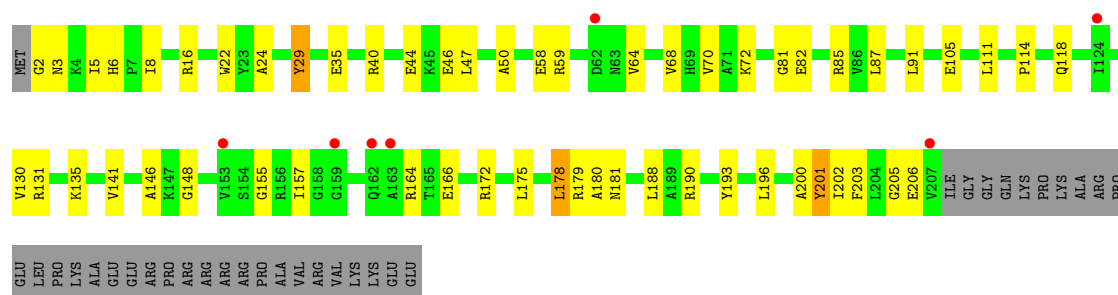


• Molecule 37: 30S ribosomal protein S3

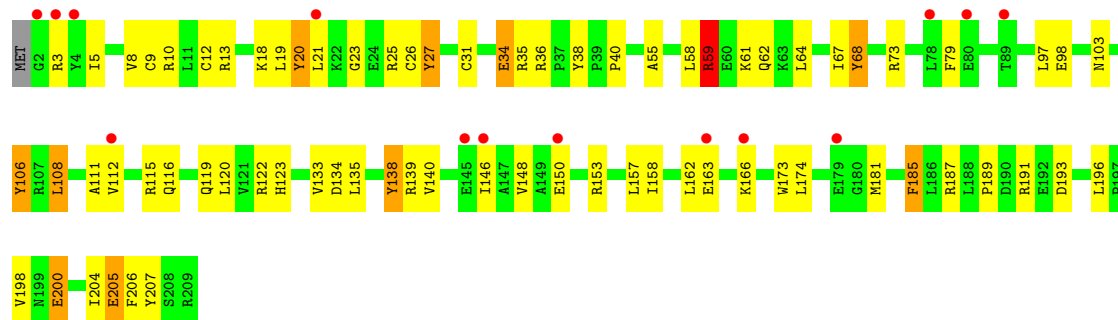




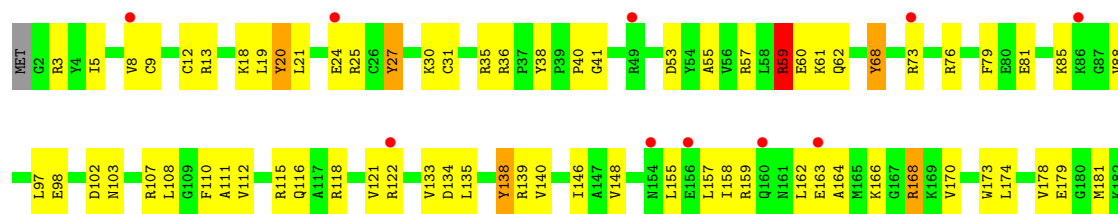
• Molecule 37: 30S ribosomal protein S3

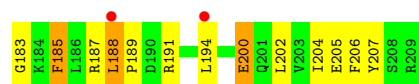


• Molecule 38: 30S ribosomal protein S4

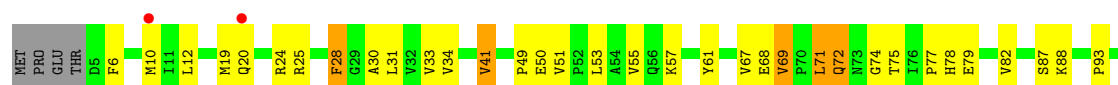


• Molecule 38: 30S ribosomal protein S4





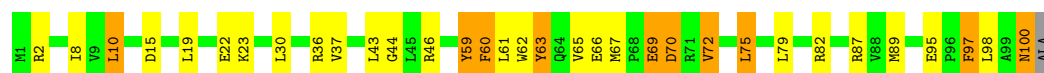
- Molecule 39: 30S ribosomal protein S5



- Molecule 39: 30S ribosomal protein S5



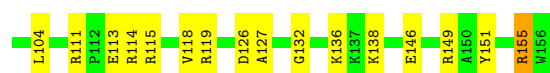
- Molecule 40: 30S ribosomal protein S6



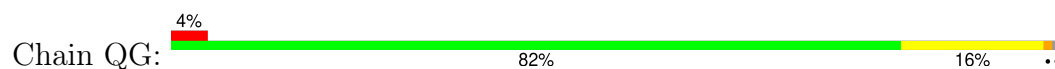
- Molecule 40: 30S ribosomal protein S6



- Molecule 41: 30S ribosomal protein S7



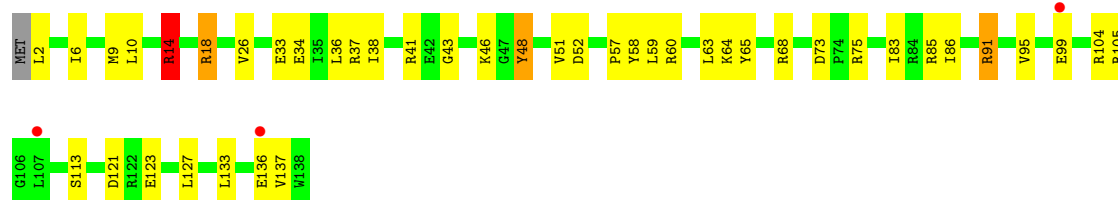
- Molecule 41: 30S ribosomal protein S7



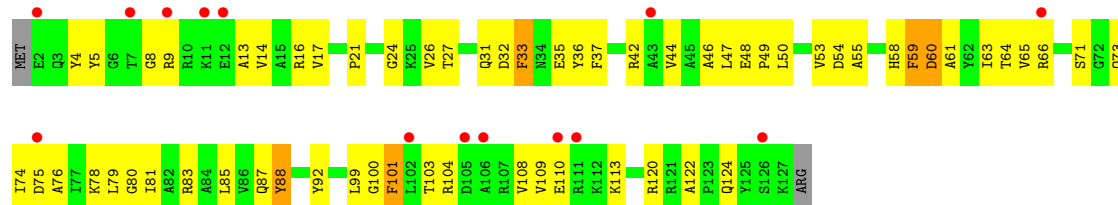
- Molecule 42: 30S ribosomal protein S8



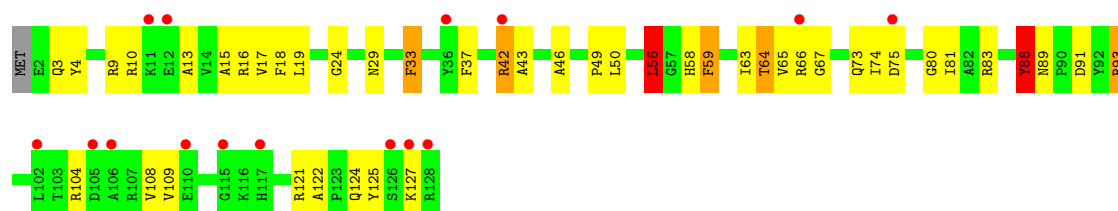
- Molecule 42: 30S ribosomal protein S8



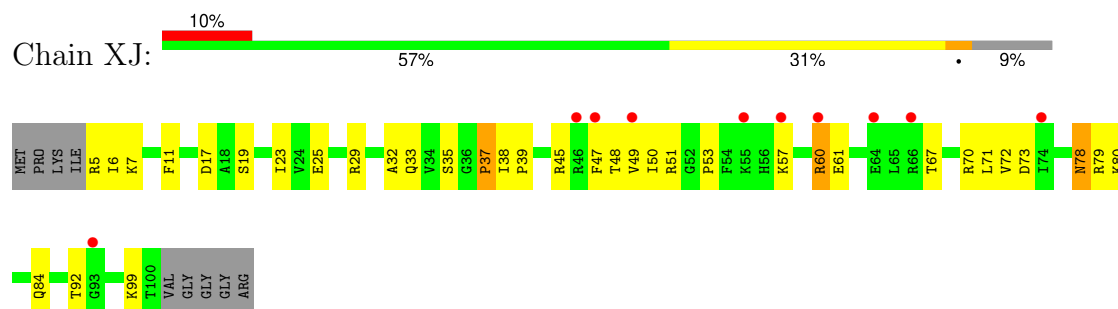
- Molecule 43: 30S ribosomal protein S9



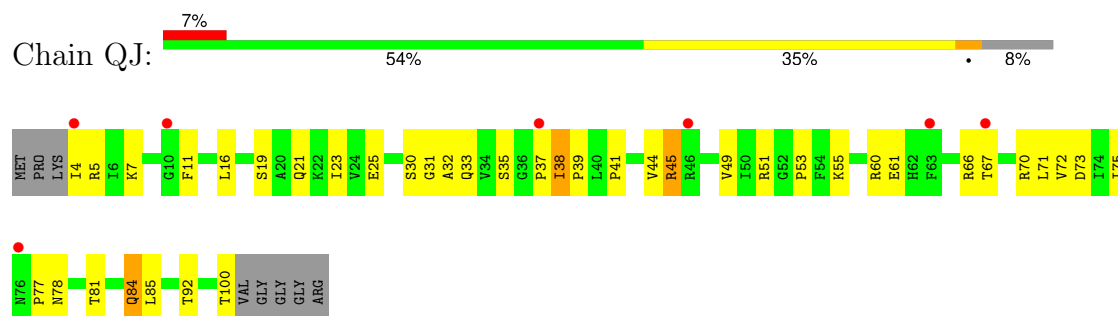
- Molecule 43: 30S ribosomal protein S9



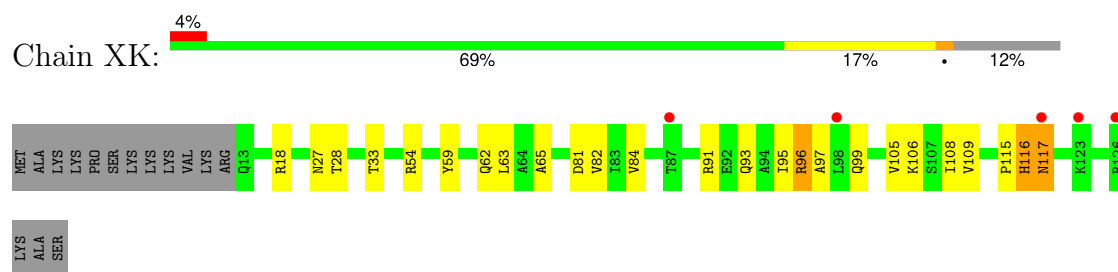
• Molecule 44: 30S ribosomal protein S10



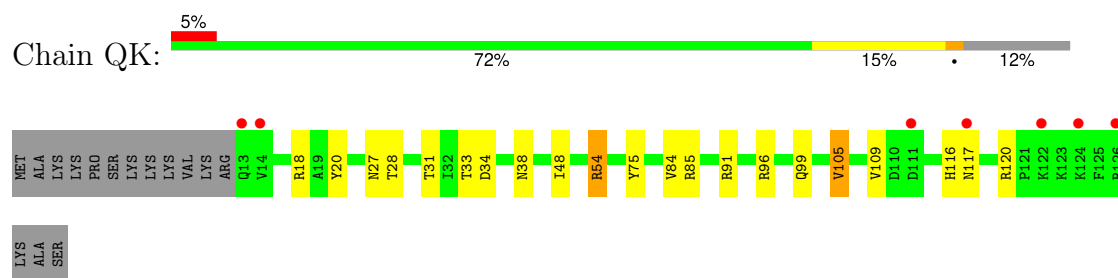
• Molecule 44: 30S ribosomal protein S10



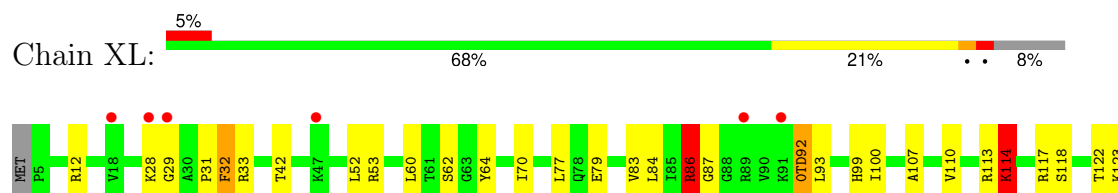
• Molecule 45: 30S ribosomal protein S11

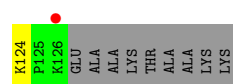


• Molecule 45: 30S ribosomal protein S11

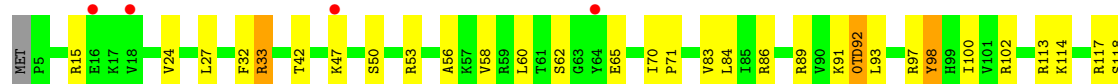


• Molecule 46: 30S ribosomal protein S12

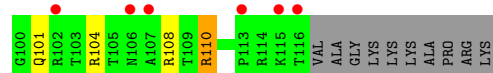




- Molecule 46: 30S ribosomal protein S12



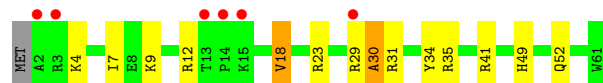
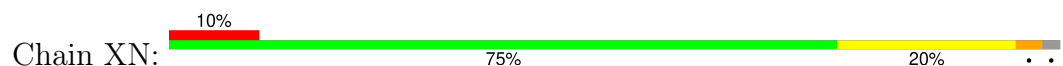
- Molecule 47: 30S ribosomal protein S13



- Molecule 47: 30S ribosomal protein S13



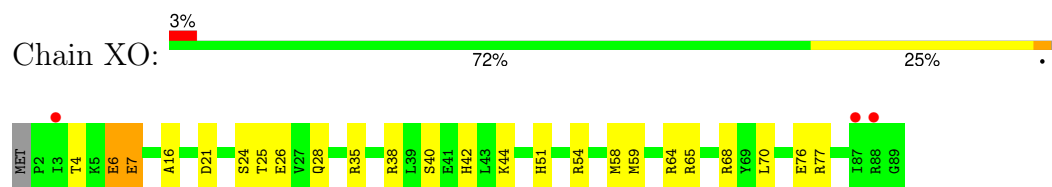
- Molecule 48: 30S ribosomal protein S14 type Z



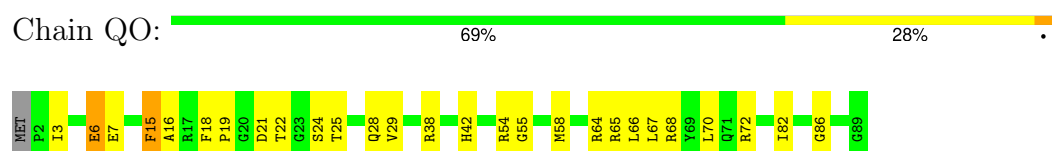
- Molecule 48: 30S ribosomal protein S14 type Z



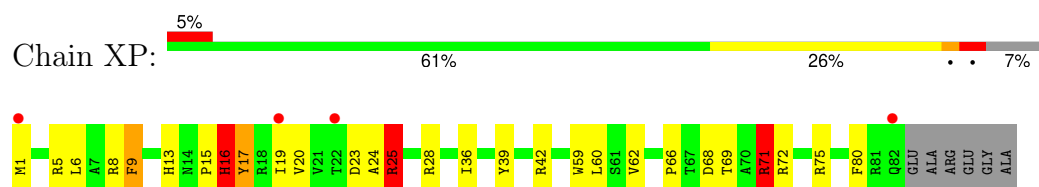
- Molecule 49: 30S ribosomal protein S15



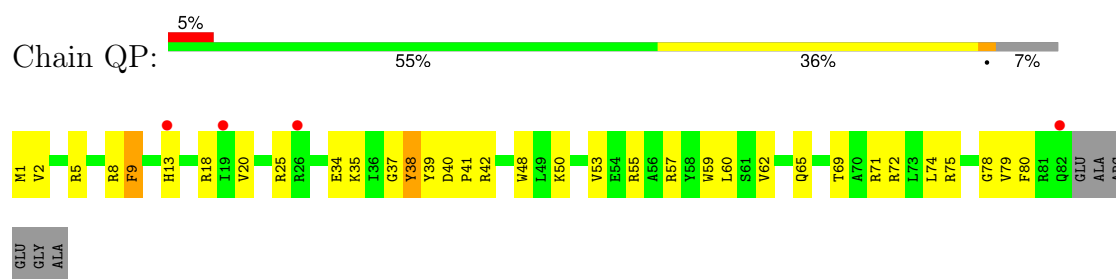
- Molecule 49: 30S ribosomal protein S15



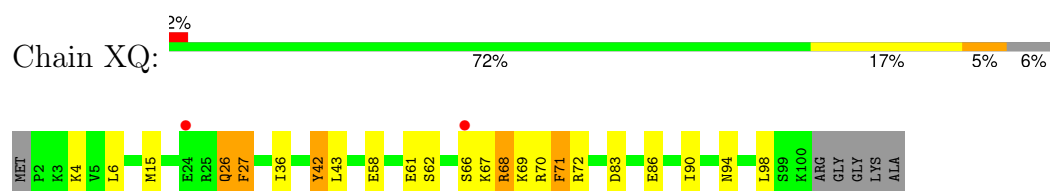
- Molecule 50: 30S ribosomal protein S16



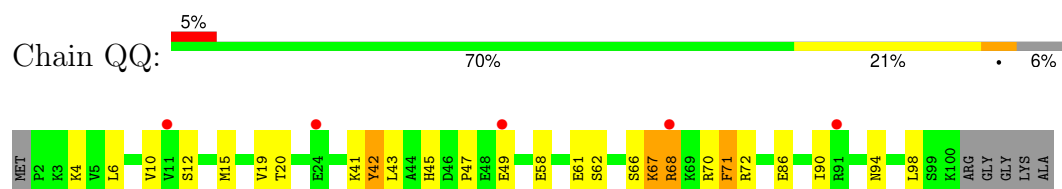
- Molecule 50: 30S ribosomal protein S16



- Molecule 51: 30S ribosomal protein S17

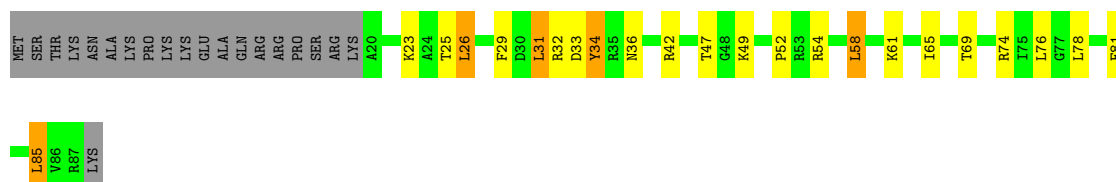


- Molecule 51: 30S ribosomal protein S17



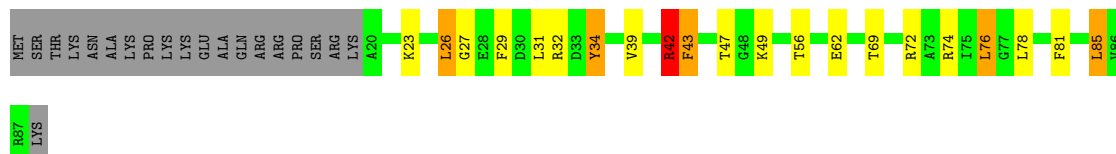
- Molecule 52: 30S ribosomal protein S18





- Molecule 52: 30S ribosomal protein S18

Chain QR: 53% 17% 6% 23%



- Molecule 53: 30S ribosomal protein S19

Chain XS: 8% 60% 28% 11%



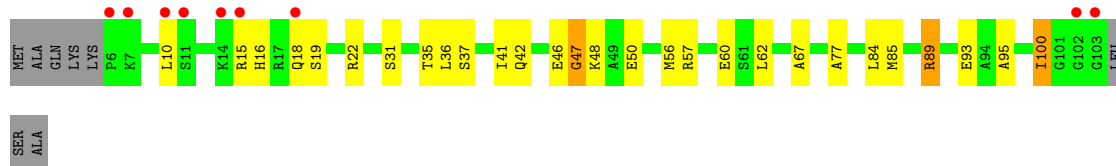
- Molecule 53: 30S ribosomal protein S19

Chain QS: 8% 66% 20% 11%



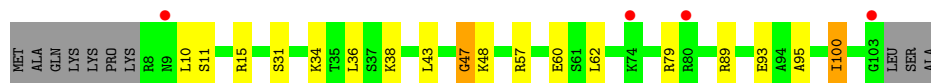
- Molecule 54: 30S ribosomal protein S20

Chain XT: 8% 66% 24% 8%

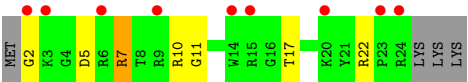


- Molecule 54: 30S ribosomal protein S20

Chain QT: 4% 74% 15% 9%



- Molecule 55: 30S ribosomal protein Thx



• Molecule 55: 30S ribosomal protein Thx



4 Data and refinement statistics

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

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

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: OMG, MG, UR3, PSU, M2G, 2MG, 7MG, MA6, 2MU, 4OC, 5MU, 2MA, ZN, SF4, 5MC, 0TD

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

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

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

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

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

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

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

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

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

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

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

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

5.2 Too-close contacts

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

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

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

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

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

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

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

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

The worst 5 of 5505 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

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

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

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

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

5 of 103 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

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

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

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

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

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

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

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

Mol	Chain	Res	Type
53	QS	47	HIS

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

5.3.3 RNA ⓘ

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

5 of 1428 RNA backbone outliers are listed below:

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

5 of 88 RNA pucker outliers are listed below:

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
35	5MC	QA	1404	35	19,22,23	1.66	2 (10%)	26,32,35	1.07	2 (7%)
4	5MU	YA	1939	4,56	19,22,23	1.41	6 (31%)	27,32,35	2.20	6 (22%)
35	5MC	QA	1400	35	19,22,23	1.69	3 (15%)	26,32,35	1.12	2 (7%)
4	2MU	RA	2552	4,56	19,22,24	1.25	3 (15%)	25,31,36	1.89	5 (20%)
4	PSU	RA	2605	4	18,21,22	1.35	2 (11%)	21,30,33	2.03	4 (19%)
4	5MC	RA	1962	4,56	19,22,23	1.65	3 (15%)	26,32,35	1.10	2 (7%)
4	PSU	YA	1917	4	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
35	MA6	QA	1519	35	23,26,27	1.55	5 (21%)	33,38,41	2.30	13 (39%)
4	2MU	YA	2552	4,56	19,22,24	1.25	3 (15%)	25,31,36	1.91	6 (24%)
4	PSU	YA	2605	4	18,21,22	1.36	2 (11%)	21,30,33	2.00	4 (19%)
4	PSU	RA	1911	4	18,21,22	1.36	2 (11%)	21,30,33	2.04	4 (19%)
35	2MG	QA	1207	35,56	23,26,27	1.26	4 (17%)	33,38,41	2.29	7 (21%)
4	OMG	RA	2251	1,4,56	23,26,27	1.19	3 (13%)	32,38,41	1.99	6 (18%)
4	4OC	YA	1920	4	19,22,24	0.78	0	25,31,35	0.91	1 (4%)
35	5MC	XA	967	35	19,22,23	1.67	3 (15%)	26,32,35	1.12	2 (7%)
35	MA6	XA	1519	35	23,26,27	1.55	3 (13%)	33,38,41	2.38	13 (39%)
35	5MC	QA	1407	35	19,22,23	1.64	3 (15%)	26,32,35	1.16	3 (11%)
4	OMG	YA	2251	1,4,56	23,26,27	1.23	3 (13%)	32,38,41	2.00	6 (18%)
35	M2G	XA	966	35	24,27,28	1.28	4 (16%)	33,40,43	1.86	6 (18%)
35	7MG	QA	527	35,56	23,26,27	1.30	3 (13%)	27,39,42	2.66	7 (25%)
4	PSU	RA	1917	4	18,21,22	1.39	2 (11%)	21,30,33	1.97	3 (14%)
35	4OC	XA	1402	35	20,23,24	0.76	0	25,32,35	0.97	1 (4%)
35	MA6	QA	1518	35	23,26,27	1.57	5 (21%)	33,38,41	2.25	13 (39%)
4	5MU	RA	1939	4	19,22,23	1.38	4 (21%)	27,32,35	2.13	6 (22%)
4	4OC	RA	1920	4	19,22,24	0.80	0	25,31,35	0.98	1 (4%)
4	2MA	YA	2503	4,56	22,25,26	1.50	4 (18%)	32,37,40	2.33	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	5MC	XA	1407	35	19,22,23	1.58	3 (15%)	26,32,35	1.14	3 (11%)
35	PSU	QA	516	35,56	18,21,22	1.37	2 (11%)	21,30,33	2.01	4 (19%)
35	5MC	XA	1404	35	19,22,23	1.66	3 (15%)	26,32,35	1.12	2 (7%)
4	5MC	RA	1942	4,56	19,22,23	1.64	3 (15%)	26,32,35	1.08	2 (7%)
35	UR3	QA	1498	35	19,22,23	1.00	1 (5%)	26,32,35	1.74	2 (7%)
4	5MC	YA	1962	4,56	19,22,23	1.64	3 (15%)	26,32,35	1.13	2 (7%)
4	5MC	YA	1942	4	19,22,23	1.55	3 (15%)	26,32,35	1.09	2 (7%)
35	5MC	XA	1400	35	19,22,23	1.61	3 (15%)	26,32,35	1.16	3 (11%)
35	M2G	QA	966	35	24,27,28	1.29	4 (16%)	33,40,43	1.84	6 (18%)
35	7MG	XA	527	35	23,26,27	1.34	3 (13%)	27,39,42	2.62	7 (25%)
35	PSU	XA	516	35	18,21,22	1.36	2 (11%)	21,30,33	2.02	5 (23%)
35	2MG	XA	1207	35	23,26,27	1.24	4 (17%)	33,38,41	2.22	6 (18%)
46	0TD	XL	92	46	8,9,10	2.52	2 (25%)	6,11,13	2.14	3 (50%)
4	PSU	YA	1911	4	18,21,22	1.39	2 (11%)	21,30,33	2.03	4 (19%)
35	4OC	QA	1402	35	20,23,24	0.77	0	25,32,35	0.96	1 (4%)
4	5MU	RA	1915	4,56	19,22,23	1.43	5 (26%)	27,32,35	2.20	8 (29%)
4	2MA	RA	2503	4,56	22,25,26	1.48	4 (18%)	32,37,40	2.31	9 (28%)
46	0TD	QL	92	46	8,9,10	2.37	1 (12%)	6,11,13	2.36	3 (50%)
35	UR3	XA	1498	35,56	19,22,23	1.02	2 (10%)	26,32,35	1.74	2 (7%)
35	5MC	QA	967	35	19,22,23	1.66	3 (15%)	26,32,35	1.10	2 (7%)
35	MA6	XA	1518	35	23,26,27	1.52	4 (17%)	33,38,41	2.31	13 (39%)
4	5MU	YA	1915	4	19,22,23	1.48	5 (26%)	27,32,35	2.11	8 (29%)

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
35	5MC	QA	1404	35	-	0/7/25/26	0/2/2/2
4	5MU	YA	1939	4,56	-	0/7/25/26	0/2/2/2
35	5MC	QA	1400	35	-	1/7/25/26	0/2/2/2
4	2MU	RA	2552	4,56	-	0/9/27/28	0/2/2/2
4	PSU	RA	2605	4	-	0/7/25/26	0/2/2/2
4	5MC	RA	1962	4,56	-	0/7/25/26	0/2/2/2
4	PSU	YA	1917	4	-	0/7/25/26	0/2/2/2
35	MA6	QA	1519	35	-	3/11/29/30	0/3/3/3

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

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

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

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

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

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

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

There are no ring outliers.

20 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	QA	1404	5MC	1	0
4	RA	2552	2MU	1	0
4	RA	1962	5MC	1	0
35	QA	1519	MA6	2	0
35	QA	1207	2MG	2	0
4	YA	1920	4OC	1	0
4	YA	2251	OMG	1	0
35	XA	1402	4OC	1	0
35	QA	1518	MA6	2	0
4	RA	1939	5MU	1	0
4	RA	1920	4OC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	RA	1942	5MC	2	0
4	YA	1962	5MC	1	0
35	QA	966	M2G	1	0
46	XL	92	0TD	1	0
35	QA	1402	4OC	1	0
46	QL	92	0TD	2	0
35	QA	967	5MC	1	0
35	XA	1518	MA6	1	0
4	YA	1915	5MU	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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

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

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

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

The worst 5 of 669 RSRZ outliers are listed below:

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

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	5MU	RA	1915	21/22	0.81	0.12	92,100,114,117	0
35	2MG	QA	1207	24/25	0.88	0.10	101,124,131,134	0
35	2MG	XA	1207	24/25	0.88	0.11	85,98,106,107	0
4	PSU	RA	1917	20/21	0.88	0.10	53,73,89,103	0
46	0TD	XL	92	10/11	0.89	0.13	58,67,84,87	0
46	0TD	QL	92	10/11	0.89	0.13	59,72,74,78	0
4	PSU	YA	1917	20/21	0.90	0.09	51,62,88,91	0
4	5MU	YA	1915	21/22	0.91	0.10	52,76,85,87	0
35	PSU	QA	516	20/21	0.91	0.08	71,77,87,88	0
35	PSU	XA	516	20/21	0.92	0.08	75,86,95,95	0
35	M2G	QA	966	25/26	0.92	0.12	71,80,92,93	0
35	M2G	XA	966	25/26	0.93	0.13	56,75,94,105	0
35	7MG	QA	527	24/25	0.93	0.12	51,70,76,76	0
35	5MC	XA	967	21/22	0.93	0.11	62,75,84,92	0
35	5MC	QA	967	21/22	0.93	0.11	71,84,95,99	0
35	4OC	XA	1402	22/23	0.94	0.11	45,57,67,81	0
4	PSU	YA	1911	20/21	0.94	0.08	45,57,62,63	0
4	4OC	RA	1920	21/23	0.94	0.10	55,62,85,94	0
35	5MC	XA	1400	21/22	0.95	0.10	50,65,74,85	0
35	7MG	XA	527	24/25	0.95	0.09	54,63,74,79	0
35	5MC	XA	1404	21/22	0.95	0.11	34,45,58,63	0
35	4OC	QA	1402	22/23	0.95	0.10	55,67,72,74	0
4	PSU	RA	1911	20/21	0.96	0.07	55,66,73,74	0
35	5MC	XA	1407	21/22	0.96	0.09	46,49,58,59	0
35	MA6	QA	1518	24/25	0.96	0.09	48,58,67,72	0
35	5MC	QA	1400	21/22	0.96	0.10	66,75,85,88	0
4	5MU	YA	1939	21/22	0.97	0.07	15,27,36,48	0
35	5MC	QA	1404	21/22	0.97	0.09	55,62,67,73	0
4	5MC	YA	1942	21/22	0.97	0.07	25,38,47,50	0
35	MA6	QA	1519	24/25	0.97	0.12	41,56,68,79	0
4	OMG	YA	2251	24/25	0.97	0.07	13,25,35,41	0
4	4OC	YA	1920	21/23	0.97	0.07	40,47,55,60	0
35	UR3	XA	1498	21/22	0.97	0.07	34,43,57,66	0
35	MA6	XA	1518	24/25	0.97	0.09	31,41,46,52	0
35	MA6	XA	1519	24/25	0.97	0.08	28,45,53,54	0
4	5MU	RA	1939	21/22	0.97	0.07	23,37,44,52	0
4	5MC	RA	1942	21/22	0.97	0.08	41,50,62,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	5MC	YA	1962	21/22	0.98	0.06	25,33,47,55	0
35	5MC	QA	1407	21/22	0.98	0.06	44,51,62,68	0
35	UR3	QA	1498	21/22	0.98	0.07	44,57,69,72	0
4	2MA	YA	2503	23/24	0.98	0.06	8,22,36,38	0
4	2MU	YA	2552	21/23	0.98	0.06	19,28,42,46	0
4	PSU	YA	2605	20/21	0.98	0.07	10,25,42,59	0
4	5MC	RA	1962	21/22	0.98	0.06	39,46,52,62	0
4	OMG	RA	2251	24/25	0.98	0.07	31,38,50,55	0
4	2MA	RA	2503	23/24	0.98	0.06	16,24,31,37	0
4	2MU	RA	2552	21/23	0.98	0.05	19,33,40,48	0
4	PSU	RA	2605	20/21	0.98	0.07	19,36,47,48	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1673	1/1	-0.17	0.18	103,103,103,103	0
56	MG	QA	1647	1/1	-0.15	0.26	134,134,134,134	0
56	MG	QA	1612	1/1	-0.07	0.37	97,97,97,97	0
56	MG	QA	1839	1/1	-0.06	0.21	93,93,93,93	0
56	MG	XA	1773	1/1	-0.05	0.65	96,96,96,96	0
56	MG	QA	1698	1/1	-0.04	0.28	100,100,100,100	0
56	MG	QG	203	1/1	-0.03	0.17	100,100,100,100	0
56	MG	QA	1799	1/1	-0.01	0.24	83,83,83,83	0
56	MG	QA	1858	1/1	0.01	1.04	115,115,115,115	0
56	MG	QA	1751	1/1	0.01	0.28	83,83,83,83	0
56	MG	XA	1669	1/1	0.04	0.21	103,103,103,103	0
56	MG	QA	1683	1/1	0.05	0.18	112,112,112,112	0
56	MG	RA	3112	1/1	0.06	0.27	117,117,117,117	0
56	MG	Y1	101	1/1	0.09	0.18	104,104,104,104	0
56	MG	RA	3994	1/1	0.09	0.31	88,88,88,88	0
56	MG	YA	3637	1/1	0.12	0.67	101,101,101,101	0
56	MG	QA	1736	1/1	0.14	0.40	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3344	1/1	0.16	0.26	80,80,80,80	0
56	MG	QI	201	1/1	0.16	0.26	106,106,106,106	0
56	MG	RH	201	1/1	0.16	0.12	88,88,88,88	0
56	MG	QY	401	1/1	0.17	0.38	111,111,111,111	0
56	MG	XA	1783	1/1	0.18	0.41	99,99,99,99	0
56	MG	RA	3983	1/1	0.18	0.20	84,84,84,84	0
56	MG	XA	1725	1/1	0.19	0.48	87,87,87,87	0
56	MG	XA	1727	1/1	0.19	0.26	84,84,84,84	0
56	MG	RA	3546	1/1	0.19	0.33	111,111,111,111	0
56	MG	YA	3185	1/1	0.22	0.41	105,105,105,105	0
56	MG	RG	201	1/1	0.22	0.12	121,121,121,121	0
56	MG	QA	1785	1/1	0.22	0.36	84,84,84,84	0
56	MG	QA	1686	1/1	0.23	0.21	103,103,103,103	0
56	MG	QA	1783	1/1	0.24	0.19	77,77,77,77	0
56	MG	QA	1603	1/1	0.25	0.32	105,105,105,105	0
56	MG	RA	3196	1/1	0.25	0.32	104,104,104,104	0
56	MG	QD	304	1/1	0.25	0.35	111,111,111,111	0
56	MG	RA	3727	1/1	0.25	0.51	108,108,108,108	0
56	MG	QA	1757	1/1	0.26	0.32	86,86,86,86	0
56	MG	RA	3951	1/1	0.26	0.43	87,87,87,87	0
56	MG	QA	1685	1/1	0.26	0.34	91,91,91,91	0
56	MG	RA	3875	1/1	0.27	0.34	90,90,90,90	0
56	MG	QA	1829	1/1	0.27	0.21	94,94,94,94	0
56	MG	QA	1657	1/1	0.28	0.45	98,98,98,98	0
56	MG	XA	1637	1/1	0.29	0.22	89,89,89,89	0
56	MG	RB	208	1/1	0.30	0.24	90,90,90,90	0
56	MG	QU	101	1/1	0.31	0.21	81,81,81,81	0
56	MG	QA	1768	1/1	0.31	0.26	91,91,91,91	0
56	MG	RB	223	1/1	0.32	0.41	102,102,102,102	0
56	MG	QA	1693	1/1	0.32	0.24	88,88,88,88	0
56	MG	QA	1764	1/1	0.32	0.31	101,101,101,101	0
56	MG	XE	201	1/1	0.33	0.31	79,79,79,79	0
56	MG	XF	203	1/1	0.33	0.31	109,109,109,109	0
56	MG	XA	1753	1/1	0.34	0.42	99,99,99,99	0
56	MG	RA	3115	1/1	0.34	0.39	92,92,92,92	0
56	MG	QA	1867	1/1	0.34	0.16	99,99,99,99	0
56	MG	RA	3410	1/1	0.34	0.28	76,76,76,76	0
56	MG	RA	3452	1/1	0.34	0.28	78,78,78,78	0
56	MG	XA	1662	1/1	0.35	0.25	80,80,80,80	0
56	MG	YA	3270	1/1	0.35	0.29	83,83,83,83	0
56	MG	QE	202	1/1	0.35	0.16	91,91,91,91	0
56	MG	RH	202	1/1	0.35	0.12	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3524	1/1	0.36	0.25	96,96,96,96	0
56	MG	QA	1871	1/1	0.37	0.18	100,100,100,100	0
56	MG	RA	3358	1/1	0.37	0.18	99,99,99,99	0
56	MG	YN	201	1/1	0.37	0.18	87,87,87,87	0
56	MG	YA	3459	1/1	0.38	0.30	85,85,85,85	0
56	MG	YG	201	1/1	0.38	0.24	116,116,116,116	0
56	MG	YI	201	1/1	0.38	0.14	110,110,110,110	0
56	MG	QA	1633	1/1	0.38	0.11	95,95,95,95	0
56	MG	QA	1780	1/1	0.38	0.23	92,92,92,92	0
56	MG	YA	3628	1/1	0.39	0.36	105,105,105,105	0
56	MG	XA	1639	1/1	0.39	0.32	98,98,98,98	0
56	MG	RA	3058	1/1	0.39	0.70	88,88,88,88	0
56	MG	QD	301	1/1	0.39	0.30	90,90,90,90	0
56	MG	RA	3271	1/1	0.40	0.22	93,93,93,93	0
56	MG	XA	1692	1/1	0.40	0.39	75,75,75,75	0
56	MG	RA	3961	1/1	0.40	0.33	114,114,114,114	0
56	MG	RA	3572	1/1	0.40	0.42	83,83,83,83	0
56	MG	YA	3491	1/1	0.40	0.36	53,53,53,53	0
56	MG	RA	3011	1/1	0.41	0.24	84,84,84,84	0
56	MG	QA	1731	1/1	0.41	0.33	71,71,71,71	0
56	MG	QA	1832	1/1	0.41	0.29	92,92,92,92	0
56	MG	YA	3467	1/1	0.41	0.55	82,82,82,82	0
56	MG	RA	3654	1/1	0.41	0.39	87,87,87,87	0
56	MG	QA	1712	1/1	0.41	0.22	87,87,87,87	0
56	MG	QA	1715	1/1	0.41	0.29	77,77,77,77	0
56	MG	QA	1725	1/1	0.41	0.63	90,90,90,90	0
56	MG	QA	1682	1/1	0.42	0.25	93,93,93,93	0
56	MG	QA	1727	1/1	0.42	0.18	100,100,100,100	0
56	MG	RA	3105	1/1	0.42	0.14	71,71,71,71	0
56	MG	YA	3177	1/1	0.43	0.22	71,71,71,71	0
56	MG	RA	3100	1/1	0.43	0.30	93,93,93,93	0
56	MG	RA	3987	1/1	0.43	0.39	80,80,80,80	0
56	MG	YA	3505	1/1	0.44	0.39	88,88,88,88	0
56	MG	QA	1842	1/1	0.44	0.24	84,84,84,84	0
56	MG	YA	3174	1/1	0.44	0.25	95,95,95,95	0
56	MG	RA	3439	1/1	0.44	0.20	89,89,89,89	0
56	MG	QA	1674	1/1	0.45	0.21	85,85,85,85	0
56	MG	RB	217	1/1	0.45	0.26	94,94,94,94	0
56	MG	XA	1754	1/1	0.45	0.58	86,86,86,86	0
56	MG	XA	1711	1/1	0.46	0.30	92,92,92,92	0
56	MG	RA	3982	1/1	0.46	0.36	83,83,83,83	0
56	MG	RA	3519	1/1	0.46	0.28	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3523	1/1	0.46	0.26	64,64,64,64	0
56	MG	YA	3193	1/1	0.46	0.37	101,101,101,101	0
56	MG	YB	209	1/1	0.46	0.44	102,102,102,102	0
56	MG	RA	3635	1/1	0.46	0.17	112,112,112,112	0
56	MG	QA	1789	1/1	0.46	0.39	99,99,99,99	0
56	MG	RA	3099	1/1	0.46	0.33	102,102,102,102	0
56	MG	QA	1848	1/1	0.46	0.34	68,68,68,68	0
56	MG	QA	1748	1/1	0.46	0.28	92,92,92,92	0
56	MG	R9	101	1/1	0.46	0.40	92,92,92,92	0
56	MG	XA	1609	1/1	0.47	0.51	88,88,88,88	0
56	MG	RA	3922	1/1	0.47	0.30	70,70,70,70	0
56	MG	QA	1844	1/1	0.47	0.22	80,80,80,80	0
56	MG	RA	3062	1/1	0.47	0.19	82,82,82,82	0
56	MG	RA	3733	1/1	0.47	0.47	96,96,96,96	0
56	MG	XA	1608	1/1	0.48	0.25	76,76,76,76	0
56	MG	XA	1787	1/1	0.48	0.56	84,84,84,84	0
56	MG	RA	3780	1/1	0.48	0.47	74,74,74,74	0
56	MG	RA	3198	1/1	0.48	0.15	84,84,84,84	0
56	MG	YA	3415	1/1	0.48	0.35	84,84,84,84	0
56	MG	YA	3488	1/1	0.48	0.18	105,105,105,105	0
56	MG	RA	3634	1/1	0.48	0.18	81,81,81,81	0
56	MG	YA	3028	1/1	0.48	0.23	51,51,51,51	0
56	MG	XA	1654	1/1	0.48	0.33	89,89,89,89	0
56	MG	QA	1812	1/1	0.49	0.41	68,68,68,68	0
56	MG	QA	1713	1/1	0.49	0.29	79,79,79,79	0
56	MG	YA	3662	1/1	0.49	0.56	91,91,91,91	0
56	MG	YA	3379	1/1	0.49	0.32	70,70,70,70	0
56	MG	RA	4004	1/1	0.49	0.56	93,93,93,93	0
56	MG	R4	102	1/1	0.49	0.12	88,88,88,88	0
56	MG	QA	1608	1/1	0.49	0.21	110,110,110,110	0
57	ZN	Y4	101	1/1	0.49	0.14	305,305,305,305	0
56	MG	RA	3553	1/1	0.50	0.38	87,87,87,87	0
56	MG	QA	1798	1/1	0.50	0.33	119,119,119,119	0
56	MG	RA	3511	1/1	0.50	0.41	62,62,62,62	0
56	MG	YA	3057	1/1	0.50	0.38	99,99,99,99	0
56	MG	RA	3942	1/1	0.50	0.26	104,104,104,104	0
56	MG	YA	3632	1/1	0.50	0.27	62,62,62,62	0
56	MG	YA	3421	1/1	0.50	0.30	75,75,75,75	0
56	MG	RA	3552	1/1	0.51	0.23	97,97,97,97	0
56	MG	XA	1709	1/1	0.51	0.26	72,72,72,72	0
56	MG	QA	1601	1/1	0.51	0.72	129,129,129,129	0
56	MG	YA	3293	1/1	0.51	0.36	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3437	1/1	0.51	0.26	77,77,77,77	0
56	MG	RA	3540	1/1	0.51	0.28	73,73,73,73	0
56	MG	QA	1606	1/1	0.51	0.24	93,93,93,93	0
56	MG	RA	3993	1/1	0.52	0.26	86,86,86,86	0
56	MG	YA	3528	1/1	0.52	0.56	104,104,104,104	0
56	MG	RA	3752	1/1	0.52	0.43	102,102,102,102	0
56	MG	QA	1756	1/1	0.52	0.36	114,114,114,114	0
56	MG	RB	215	1/1	0.52	0.25	91,91,91,91	0
56	MG	RA	3293	1/1	0.52	0.12	128,128,128,128	0
56	MG	YA	3396	1/1	0.52	0.36	94,94,94,94	0
56	MG	XA	1651	1/1	0.52	0.21	90,90,90,90	0
56	MG	YA	3414	1/1	0.52	0.50	83,83,83,83	0
56	MG	YA	3242	1/1	0.52	0.53	88,88,88,88	0
56	MG	YA	3253	1/1	0.52	0.28	98,98,98,98	0
56	MG	R5	104	1/1	0.52	0.15	67,67,67,67	0
56	MG	QA	1738	1/1	0.52	0.29	98,98,98,98	0
56	MG	YA	3037	1/1	0.52	0.29	88,88,88,88	0
56	MG	XJ	201	1/1	0.53	0.17	97,97,97,97	0
56	MG	RA	3786	1/1	0.53	0.17	87,87,87,87	0
56	MG	YA	3347	1/1	0.53	0.35	99,99,99,99	0
56	MG	RA	3481	1/1	0.53	0.18	81,81,81,81	0
56	MG	RA	3595	1/1	0.53	0.23	84,84,84,84	0
56	MG	QA	1876	1/1	0.53	0.13	84,84,84,84	0
56	MG	QA	1651	1/1	0.54	0.32	89,89,89,89	0
56	MG	RB	211	1/1	0.54	0.19	95,95,95,95	0
56	MG	QA	1745	1/1	0.54	0.32	98,98,98,98	0
56	MG	XA	1660	1/1	0.54	0.17	99,99,99,99	0
56	MG	QY	403	1/1	0.54	0.45	81,81,81,81	0
56	MG	RD	310	1/1	0.54	0.23	94,94,94,94	0
56	MG	RA	3688	1/1	0.54	0.24	90,90,90,90	0
56	MG	QA	1697	1/1	0.54	0.25	76,76,76,76	0
56	MG	YA	3058	1/1	0.54	0.17	75,75,75,75	0
56	MG	YA	3462	1/1	0.54	0.38	75,75,75,75	0
56	MG	RA	3563	1/1	0.54	0.29	66,66,66,66	0
56	MG	RA	3781	1/1	0.54	0.27	60,60,60,60	0
56	MG	RA	3490	1/1	0.54	0.33	86,86,86,86	0
56	MG	QM	201	1/1	0.55	0.20	85,85,85,85	0
56	MG	RA	3525	1/1	0.55	0.29	65,65,65,65	0
56	MG	QA	1840	1/1	0.55	0.32	89,89,89,89	0
56	MG	QA	1875	1/1	0.55	0.25	75,75,75,75	0
56	MG	QA	1665	1/1	0.55	0.27	102,102,102,102	0
56	MG	YE	303	1/1	0.55	0.58	103,103,103,103	0

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1759	1/1	0.58	0.23	78,78,78,78	0
56	MG	QA	1814	1/1	0.58	0.20	97,97,97,97	0
56	MG	XA	1781	1/1	0.58	0.51	110,110,110,110	0
56	MG	RA	3289	1/1	0.58	0.22	83,83,83,83	0
56	MG	RA	3401	1/1	0.59	0.12	44,44,44,44	0
56	MG	RA	3828	1/1	0.59	0.15	94,94,94,94	0
56	MG	RA	3847	1/1	0.59	0.21	102,102,102,102	0
56	MG	RA	3851	1/1	0.59	0.22	91,91,91,91	0
56	MG	QD	303	1/1	0.59	0.16	79,79,79,79	0
56	MG	YA	3370	1/1	0.59	0.33	67,67,67,67	0
56	MG	QA	1690	1/1	0.59	0.15	72,72,72,72	0
56	MG	YB	205	1/1	0.59	0.24	89,89,89,89	0
56	MG	QA	1694	1/1	0.59	0.40	97,97,97,97	0
56	MG	QA	1720	1/1	0.59	0.43	97,97,97,97	0
56	MG	RA	3217	1/1	0.59	0.18	88,88,88,88	0
56	MG	RN	202	1/1	0.59	0.18	98,98,98,98	0
56	MG	RA	3777	1/1	0.59	0.52	93,93,93,93	0
56	MG	QA	1878	1/1	0.59	0.34	108,108,108,108	0
56	MG	RA	3367	1/1	0.59	0.40	74,74,74,74	0
56	MG	YA	3501	1/1	0.59	0.52	115,115,115,115	0
56	MG	QA	1826	1/1	0.60	0.20	74,74,74,74	0
56	MG	XA	1703	1/1	0.60	0.22	60,60,60,60	0
56	MG	XA	1610	1/1	0.60	0.30	79,79,79,79	0
56	MG	QA	1837	1/1	0.60	0.28	69,69,69,69	0
56	MG	RA	3031	1/1	0.60	0.34	75,75,75,75	0
56	MG	QA	1664	1/1	0.60	0.34	92,92,92,92	0
56	MG	RA	3611	1/1	0.60	0.22	80,80,80,80	0
56	MG	YA	3561	1/1	0.60	0.26	45,45,45,45	0
56	MG	YA	3455	1/1	0.60	0.48	79,79,79,79	0
56	MG	RW	202	1/1	0.60	0.38	89,89,89,89	0
56	MG	YA	3120	1/1	0.60	0.21	72,72,72,72	0
56	MG	QA	1652	1/1	0.60	0.20	83,83,83,83	0
56	MG	QA	1816	1/1	0.60	0.44	76,76,76,76	0
56	MG	RA	3249	1/1	0.60	0.69	94,94,94,94	0
56	MG	RA	3625	1/1	0.61	0.44	91,91,91,91	0
56	MG	RA	3756	1/1	0.61	0.29	83,83,83,83	0
56	MG	RA	3375	1/1	0.61	0.27	73,73,73,73	0
56	MG	QA	1739	1/1	0.61	0.17	87,87,87,87	0
56	MG	YA	3466	1/1	0.61	0.38	80,80,80,80	0
56	MG	RA	3782	1/1	0.61	0.48	94,94,94,94	0
56	MG	XA	1721	1/1	0.61	0.39	86,86,86,86	0
56	MG	YA	3261	1/1	0.61	0.17	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3701	1/1	0.61	0.36	64,64,64,64	0
56	MG	RA	3429	1/1	0.61	0.21	89,89,89,89	0
56	MG	RA	3589	1/1	0.61	0.22	100,100,100,100	0
56	MG	QA	1856	1/1	0.61	0.30	89,89,89,89	0
56	MG	YA	3364	1/1	0.61	0.35	67,67,67,67	0
56	MG	RA	3422	1/1	0.62	0.33	84,84,84,84	0
56	MG	QA	1675	1/1	0.62	0.19	94,94,94,94	0
56	MG	RA	3577	1/1	0.62	0.29	94,94,94,94	0
56	MG	RA	3431	1/1	0.62	0.35	88,88,88,88	0
56	MG	QA	1805	1/1	0.62	0.15	76,76,76,76	0
56	MG	QA	1810	1/1	0.62	0.29	69,69,69,69	0
56	MG	YA	3478	1/1	0.62	0.23	67,67,67,67	0
56	MG	RA	3823	1/1	0.62	0.32	97,97,97,97	0
56	MG	YA	3131	1/1	0.62	0.31	88,88,88,88	0
56	MG	QL	201	1/1	0.62	0.17	66,66,66,66	0
56	MG	YD	302	1/1	0.62	0.30	71,71,71,71	0
56	MG	RF	312	1/1	0.62	0.18	62,62,62,62	0
56	MG	QA	1822	1/1	0.62	0.36	65,65,65,65	0
56	MG	XA	1719	1/1	0.62	0.41	95,95,95,95	0
56	MG	RA	3028	1/1	0.62	0.26	69,69,69,69	0
56	MG	RA	3943	1/1	0.62	0.31	86,86,86,86	0
56	MG	RT	203	1/1	0.62	0.11	88,88,88,88	0
56	MG	XA	1616	1/1	0.62	0.16	115,115,115,115	0
56	MG	RA	3203	1/1	0.62	0.43	97,97,97,97	0
56	MG	QA	1615	1/1	0.62	0.12	107,107,107,107	0
56	MG	XA	1603	1/1	0.62	0.23	76,76,76,76	0
56	MG	QA	1642	1/1	0.62	0.23	83,83,83,83	0
56	MG	RB	216	1/1	0.63	0.13	59,59,59,59	0
56	MG	RA	3878	1/1	0.63	0.40	81,81,81,81	0
56	MG	YA	3340	1/1	0.63	0.24	59,59,59,59	0
56	MG	QA	1752	1/1	0.63	0.24	77,77,77,77	0
56	MG	XA	1784	1/1	0.63	0.40	72,72,72,72	0
56	MG	RA	3154	1/1	0.63	0.23	88,88,88,88	0
56	MG	RA	3256	1/1	0.63	0.49	103,103,103,103	0
56	MG	QA	1861	1/1	0.63	0.31	75,75,75,75	0
56	MG	YB	218	1/1	0.63	0.21	80,80,80,80	0
56	MG	RA	3278	1/1	0.63	0.37	83,83,83,83	0
56	MG	QA	1726	1/1	0.63	0.38	81,81,81,81	0
56	MG	RA	3549	1/1	0.63	0.29	78,78,78,78	0
56	MG	RA	4001	1/1	0.63	0.34	58,58,58,58	0
56	MG	RA	3187	1/1	0.63	0.51	106,106,106,106	0
56	MG	XA	1648	1/1	0.63	0.18	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1819	1/1	0.63	0.15	65,65,65,65	0
56	MG	YA	3099	1/1	0.63	0.23	106,106,106,106	0
56	MG	QA	1843	1/1	0.64	0.16	89,89,89,89	0
56	MG	RA	3675	1/1	0.64	0.31	75,75,75,75	0
56	MG	RA	3364	1/1	0.64	0.23	96,96,96,96	0
56	MG	YA	3544	1/1	0.64	0.40	81,81,81,81	0
56	MG	RA	3370	1/1	0.64	0.58	88,88,88,88	0
56	MG	RA	3036	1/1	0.64	0.19	69,69,69,69	0
56	MG	YA	3134	1/1	0.64	0.37	89,89,89,89	0
56	MG	RA	3205	1/1	0.64	0.22	76,76,76,76	0
56	MG	QA	1769	1/1	0.64	0.16	95,95,95,95	0
56	MG	RA	3746	1/1	0.64	0.38	112,112,112,112	0
56	MG	YA	3247	1/1	0.64	0.33	106,106,106,106	0
56	MG	QA	1750	1/1	0.64	0.24	67,67,67,67	0
56	MG	RA	3343	1/1	0.64	0.22	68,68,68,68	0
56	MG	YA	3427	1/1	0.64	0.24	75,75,75,75	0
56	MG	YA	3095	1/1	0.65	0.18	68,68,68,68	0
56	MG	QA	1708	1/1	0.65	0.26	77,77,77,77	0
56	MG	QA	1802	1/1	0.65	0.28	79,79,79,79	0
56	MG	YA	3302	1/1	0.65	0.38	72,72,72,72	0
56	MG	RA	3491	1/1	0.65	0.35	81,81,81,81	0
56	MG	QA	1849	1/1	0.65	0.47	81,81,81,81	0
56	MG	RF	302	1/1	0.65	0.20	73,73,73,73	0
56	MG	RA	3051	1/1	0.65	0.28	83,83,83,83	0
56	MG	RA	3404	1/1	0.65	0.18	81,81,81,81	0
56	MG	RA	3644	1/1	0.65	0.29	84,84,84,84	0
56	MG	QA	1831	1/1	0.65	0.43	93,93,93,93	0
56	MG	YA	3308	1/1	0.65	0.25	64,64,64,64	0
56	MG	YA	3740	1/1	0.65	0.23	52,52,52,52	0
56	MG	YA	3107	1/1	0.65	0.34	80,80,80,80	0
56	MG	RA	4019	1/1	0.65	0.43	87,87,87,87	0
56	MG	QA	1766	1/1	0.65	0.36	71,71,71,71	0
56	MG	QA	1874	1/1	0.65	0.27	74,74,74,74	0
56	MG	QN	103	1/1	0.65	0.49	80,80,80,80	0
56	MG	QA	1862	1/1	0.66	0.25	101,101,101,101	0
56	MG	QA	1835	1/1	0.66	0.29	89,89,89,89	0
56	MG	XA	1689	1/1	0.66	0.17	64,64,64,64	0
56	MG	YA	3439	1/1	0.66	0.27	80,80,80,80	0
56	MG	RA	3729	1/1	0.66	0.19	59,59,59,59	0
56	MG	QA	1777	1/1	0.66	0.14	81,81,81,81	0
56	MG	RA	3489	1/1	0.66	0.39	50,50,50,50	0
56	MG	RA	3122	1/1	0.66	0.35	92,92,92,92	0

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

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

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

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

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1649	1/1	0.74	0.20	92,92,92,92	0
56	MG	RA	3077	1/1	0.74	0.17	70,70,70,70	0
56	MG	RA	3453	1/1	0.74	0.31	64,64,64,64	0
56	MG	RA	4015	1/1	0.74	0.51	89,89,89,89	0
56	MG	RA	3261	1/1	0.74	0.27	82,82,82,82	0
56	MG	YA	3260	1/1	0.74	0.31	71,71,71,71	0
56	MG	YA	3468	1/1	0.74	0.42	58,58,58,58	0
56	MG	RA	3272	1/1	0.74	0.14	83,83,83,83	0
56	MG	RA	3102	1/1	0.74	0.32	107,107,107,107	0
56	MG	XA	1686	1/1	0.74	0.25	68,68,68,68	0
56	MG	XA	1747	1/1	0.74	0.28	59,59,59,59	0
56	MG	RA	3283	1/1	0.74	0.33	101,101,101,101	0
56	MG	YA	3523	1/1	0.74	0.20	56,56,56,56	0
56	MG	RA	3839	1/1	0.74	0.13	72,72,72,72	0
56	MG	RA	3514	1/1	0.74	0.22	87,87,87,87	0
56	MG	YA	3198	1/1	0.74	0.19	80,80,80,80	0
56	MG	YB	215	1/1	0.74	0.27	92,92,92,92	0
56	MG	YA	3566	1/1	0.74	0.24	60,60,60,60	0
56	MG	YD	301	1/1	0.74	0.23	60,60,60,60	0
56	MG	YA	3167	1/1	0.74	0.36	88,88,88,88	0
56	MG	RA	3171	1/1	0.74	0.19	89,89,89,89	0
56	MG	XA	1663	1/1	0.74	0.23	107,107,107,107	0
56	MG	RA	3537	1/1	0.74	0.27	93,93,93,93	0
56	MG	RA	3916	1/1	0.74	0.28	72,72,72,72	0
56	MG	RA	3357	1/1	0.74	0.17	61,61,61,61	0
56	MG	XA	1620	1/1	0.74	0.14	63,63,63,63	0
56	MG	QT	201	1/1	0.74	0.38	65,65,65,65	0
56	MG	RA	3940	1/1	0.74	0.18	83,83,83,83	0
56	MG	QA	1808	1/1	0.74	0.28	54,54,54,54	0
56	MG	QA	1809	1/1	0.74	0.16	67,67,67,67	0
56	MG	RT	201	1/1	0.74	0.23	77,77,77,77	0
56	MG	RA	3015	1/1	0.74	0.23	72,72,72,72	0
56	MG	XA	1668	1/1	0.74	0.28	87,87,87,87	0
56	MG	QA	1854	1/1	0.74	0.23	67,67,67,67	0
56	MG	R0	102	1/1	0.74	0.18	84,84,84,84	0
56	MG	R0	104	1/1	0.74	0.30	90,90,90,90	0
56	MG	YA	3154	1/1	0.74	0.28	86,86,86,86	0
56	MG	XA	1625	1/1	0.74	0.19	74,74,74,74	0
56	MG	XA	1715	1/1	0.74	0.27	55,55,55,55	0
56	MG	QA	1733	1/1	0.74	0.25	60,60,60,60	0
56	MG	QA	1765	1/1	0.74	0.26	83,83,83,83	0
56	MG	QA	1636	1/1	0.74	0.27	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	ZN	R4	101	1/1	0.74	0.18	269,269,269,269	0
56	MG	RA	3731	1/1	0.75	0.23	83,83,83,83	0
56	MG	XL	201	1/1	0.75	0.36	85,85,85,85	0
56	MG	QA	1847	1/1	0.75	0.43	64,64,64,64	0
56	MG	XA	1647	1/1	0.75	0.31	92,92,92,92	0
56	MG	YA	3445	1/1	0.75	0.24	72,72,72,72	0
56	MG	QA	1818	1/1	0.75	0.19	63,63,63,63	0
56	MG	QA	1661	1/1	0.75	0.41	81,81,81,81	0
56	MG	QA	1784	1/1	0.75	0.24	64,64,64,64	0
56	MG	QA	1753	1/1	0.75	0.22	71,71,71,71	0
56	MG	QN	102	1/1	0.75	0.15	68,68,68,68	0
56	MG	YA	3657	1/1	0.75	0.26	34,34,34,34	0
56	MG	QA	1639	1/1	0.75	0.22	79,79,79,79	0
56	MG	RA	3957	1/1	0.75	0.13	66,66,66,66	0
56	MG	XA	1698	1/1	0.75	0.32	66,66,66,66	0
56	MG	RA	3126	1/1	0.75	0.28	79,79,79,79	0
56	MG	YA	3190	1/1	0.75	0.12	78,78,78,78	0
56	MG	RA	3542	1/1	0.75	0.34	76,76,76,76	0
56	MG	QA	1864	1/1	0.75	0.29	90,90,90,90	0
56	MG	RA	3785	1/1	0.75	0.21	56,56,56,56	0
56	MG	QA	1672	1/1	0.75	0.34	45,45,45,45	0
56	MG	QA	1709	1/1	0.75	0.30	53,53,53,53	0
56	MG	YA	3492	1/1	0.75	0.39	63,63,63,63	0
56	MG	XA	1704	1/1	0.75	0.17	83,83,83,83	0
56	MG	YA	3249	1/1	0.75	0.34	72,72,72,72	0
56	MG	RA	3039	1/1	0.75	0.27	76,76,76,76	0
56	MG	QA	1611	1/1	0.75	0.48	89,89,89,89	0
56	MG	RA	3193	1/1	0.75	0.42	94,94,94,94	0
56	MG	R1	102	1/1	0.75	0.43	71,71,71,71	0
56	MG	RA	3710	1/1	0.75	0.49	70,70,70,70	0
56	MG	RA	3312	1/1	0.75	0.12	124,124,124,124	0
56	MG	XA	1643	1/1	0.75	0.11	80,80,80,80	0
56	MG	RA	3057	1/1	0.75	0.24	93,93,93,93	0
56	MG	XA	1645	1/1	0.75	0.24	93,93,93,93	0
56	MG	RA	3331	1/1	0.75	0.42	73,73,73,73	0
56	MG	QA	1770	1/1	0.75	0.15	73,73,73,73	0
56	MG	RA	3507	1/1	0.76	0.26	109,109,109,109	0
56	MG	XA	1723	1/1	0.76	0.21	75,75,75,75	0
56	MG	XA	1724	1/1	0.76	0.29	65,65,65,65	0
56	MG	YA	3712	1/1	0.76	0.34	51,51,51,51	0
56	MG	RA	3997	1/1	0.76	0.07	98,98,98,98	0
56	MG	YA	3082	1/1	0.76	0.25	78,78,78,78	0

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

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3179	1/1	0.77	0.26	69,69,69,69	0
56	MG	YA	3223	1/1	0.77	0.28	91,91,91,91	0
56	MG	RA	4058	1/1	0.77	0.42	120,120,120,120	0
56	MG	RA	3550	1/1	0.77	0.28	70,70,70,70	0
56	MG	RA	3444	1/1	0.77	0.69	83,83,83,83	0
56	MG	YA	3469	1/1	0.77	0.42	88,88,88,88	0
56	MG	QB	301	1/1	0.78	0.18	91,91,91,91	0
56	MG	XA	1665	1/1	0.78	0.15	73,73,73,73	0
56	MG	RA	3825	1/1	0.78	0.18	98,98,98,98	0
56	MG	RB	224	1/1	0.78	0.28	78,78,78,78	0
56	MG	XA	1644	1/1	0.78	0.19	61,61,61,61	0
56	MG	YA	3678	1/1	0.78	0.30	50,50,50,50	0
56	MG	RA	3248	1/1	0.78	0.16	56,56,56,56	0
56	MG	YA	3745	1/1	0.78	0.33	67,67,67,67	0
56	MG	RA	3251	1/1	0.78	0.33	69,69,69,69	0
56	MG	XA	1731	1/1	0.78	0.22	65,65,65,65	0
56	MG	RA	3486	1/1	0.78	0.44	78,78,78,78	0
56	MG	YE	301	1/1	0.78	0.38	95,95,95,95	0
56	MG	XA	1744	1/1	0.78	0.27	59,59,59,59	0
56	MG	YA	3086	1/1	0.78	0.34	95,95,95,95	0
56	MG	RA	3265	1/1	0.78	0.08	111,111,111,111	0
56	MG	RA	3663	1/1	0.78	0.29	77,77,77,77	0
56	MG	RA	3374	1/1	0.78	0.78	92,92,92,92	0
56	MG	YA	3695	1/1	0.78	0.44	76,76,76,76	0
56	MG	RA	3924	1/1	0.78	0.20	65,65,65,65	0
56	MG	RA	3510	1/1	0.78	0.13	38,38,38,38	0
56	MG	QA	1797	1/1	0.78	0.30	95,95,95,95	0
56	MG	YA	3303	1/1	0.78	0.23	85,85,85,85	0
56	MG	RA	4024	1/1	0.78	0.29	59,59,59,59	0
56	MG	YA	3173	1/1	0.78	0.34	85,85,85,85	0
56	MG	QA	1616	1/1	0.78	0.10	92,92,92,92	0
56	MG	RU	202	1/1	0.78	0.19	78,78,78,78	0
56	MG	RA	4046	1/1	0.78	0.43	86,86,86,86	0
56	MG	RA	4049	1/1	0.78	0.14	92,92,92,92	0
56	MG	QA	1804	1/1	0.78	0.29	71,71,71,71	0
56	MG	QA	1621	1/1	0.78	0.12	71,71,71,71	0
56	MG	RA	3790	1/1	0.78	0.21	82,82,82,82	0
56	MG	YA	3474	1/1	0.78	0.30	72,72,72,72	0
56	MG	RB	209	1/1	0.78	0.08	92,92,92,92	0
56	MG	YA	3255	1/1	0.78	0.20	88,88,88,88	0
56	MG	YB	214	1/1	0.78	0.20	45,45,45,45	0
56	MG	YA	3070	1/1	0.78	0.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3667	1/1	0.78	0.20	90,90,90,90	0
56	MG	YA	3085	1/1	0.78	0.14	86,86,86,86	0
56	MG	XA	1623	1/1	0.79	0.36	73,73,73,73	0
56	MG	QA	1667	1/1	0.79	0.12	67,67,67,67	0
56	MG	YA	3042	1/1	0.79	0.20	61,61,61,61	0
56	MG	RA	3653	1/1	0.79	0.19	75,75,75,75	0
56	MG	RA	3934	1/1	0.79	0.07	62,62,62,62	0
56	MG	RA	3768	1/1	0.79	0.32	76,76,76,76	0
56	MG	QA	1760	1/1	0.79	0.40	77,77,77,77	0
56	MG	RA	3142	1/1	0.79	0.13	76,76,76,76	0
56	MG	RA	3661	1/1	0.79	0.20	89,89,89,89	0
56	MG	QA	1813	1/1	0.79	0.36	83,83,83,83	0
56	MG	RA	3665	1/1	0.79	0.34	77,77,77,77	0
56	MG	YA	3005	1/1	0.79	0.25	63,63,63,63	0
56	MG	RA	3299	1/1	0.79	0.41	96,96,96,96	0
56	MG	RA	3302	1/1	0.79	0.16	92,92,92,92	0
56	MG	RA	3956	1/1	0.79	0.35	77,77,77,77	0
56	MG	QA	1744	1/1	0.79	0.22	65,65,65,65	0
56	MG	RB	228	1/1	0.79	0.09	93,93,93,93	0
56	MG	RA	3679	1/1	0.79	0.27	54,54,54,54	0
56	MG	RA	3591	1/1	0.79	0.36	77,77,77,77	0
56	MG	YA	3718	1/1	0.79	0.13	60,60,60,60	0
56	MG	RA	3596	1/1	0.79	0.17	83,83,83,83	0
56	MG	RA	3522	1/1	0.79	0.18	55,55,55,55	0
56	MG	RA	3316	1/1	0.79	0.38	84,84,84,84	0
56	MG	RA	3607	1/1	0.79	0.33	98,98,98,98	0
56	MG	RA	3977	1/1	0.79	0.31	62,62,62,62	0
56	MG	YA	3726	1/1	0.79	0.36	81,81,81,81	0
56	MG	RA	3706	1/1	0.79	0.26	58,58,58,58	0
56	MG	RA	3241	1/1	0.79	0.35	108,108,108,108	0
56	MG	QA	1730	1/1	0.79	0.27	49,49,49,49	0
56	MG	XA	1772	1/1	0.79	0.35	51,51,51,51	0
56	MG	RA	3181	1/1	0.79	0.15	90,90,90,90	0
56	MG	RA	3841	1/1	0.79	0.33	64,64,64,64	0
56	MG	RA	3845	1/1	0.79	0.27	94,94,94,94	0
56	MG	XA	1722	1/1	0.79	0.08	67,67,67,67	0
56	MG	YA	3069	1/1	0.79	0.24	78,78,78,78	0
56	MG	YA	3646	1/1	0.79	0.17	69,69,69,69	0
56	MG	RA	3456	1/1	0.79	0.22	58,58,58,58	0
56	MG	RA	3195	1/1	0.79	0.34	115,115,115,115	0
56	MG	QA	1773	1/1	0.79	0.11	71,71,71,71	0
56	MG	YA	3418	1/1	0.79	0.38	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	4018	1/1	0.79	0.29	70,70,70,70	0
56	MG	QA	1830	1/1	0.79	0.18	85,85,85,85	0
56	MG	RA	3883	1/1	0.79	0.30	93,93,93,93	0
56	MG	RA	3890	1/1	0.79	0.41	57,57,57,57	0
56	MG	RA	3898	1/1	0.79	0.11	48,48,48,48	0
56	MG	RA	3558	1/1	0.79	0.33	82,82,82,82	0
56	MG	RA	3907	1/1	0.79	0.32	78,78,78,78	0
56	MG	YA	3737	1/1	0.79	0.72	107,107,107,107	0
56	MG	QA	1637	1/1	0.80	0.28	93,93,93,93	0
56	MG	RA	3227	1/1	0.80	0.26	93,93,93,93	0
56	MG	RA	3346	1/1	0.80	0.38	72,72,72,72	0
56	MG	RA	3704	1/1	0.80	0.34	91,91,91,91	0
56	MG	RA	4038	1/1	0.80	0.26	66,66,66,66	0
56	MG	RA	3593	1/1	0.80	0.29	66,66,66,66	0
56	MG	YA	3698	1/1	0.80	0.46	77,77,77,77	0
56	MG	RA	3713	1/1	0.80	0.27	47,47,47,47	0
56	MG	RA	3715	1/1	0.80	0.30	76,76,76,76	0
56	MG	RA	3719	1/1	0.80	0.19	55,55,55,55	0
56	MG	RA	3498	1/1	0.80	0.25	58,58,58,58	0
56	MG	RB	207	1/1	0.80	0.13	82,82,82,82	0
56	MG	YA	3645	1/1	0.80	0.26	67,67,67,67	0
56	MG	RA	3891	1/1	0.80	0.25	59,59,59,59	0
56	MG	RA	3505	1/1	0.80	0.16	64,64,64,64	0
56	MG	QA	1767	1/1	0.80	0.20	90,90,90,90	0
56	MG	RA	3362	1/1	0.80	0.31	93,93,93,93	0
56	MG	RA	3912	1/1	0.80	0.78	76,76,76,76	0
56	MG	YA	3251	1/1	0.80	0.26	100,100,100,100	0
56	MG	RA	3512	1/1	0.80	0.41	80,80,80,80	0
56	MG	YA	3649	1/1	0.80	0.28	60,60,60,60	0
56	MG	XA	1601	1/1	0.80	0.28	75,75,75,75	0
56	MG	RA	3629	1/1	0.80	0.30	60,60,60,60	0
56	MG	RA	3741	1/1	0.80	0.12	61,61,61,61	0
56	MG	QA	1860	1/1	0.80	0.19	100,100,100,100	0
56	MG	YA	3653	1/1	0.80	0.32	55,55,55,55	0
56	MG	RA	3017	1/1	0.80	0.42	68,68,68,68	0
56	MG	YA	3204	1/1	0.80	0.13	42,42,42,42	0
56	MG	QA	1696	1/1	0.80	0.12	73,73,73,73	0
56	MG	YA	3599	1/1	0.80	0.31	70,70,70,70	0
56	MG	XA	1718	1/1	0.80	0.29	73,73,73,73	0
56	MG	RA	3764	1/1	0.80	0.28	60,60,60,60	0
56	MG	XA	1680	1/1	0.80	0.17	77,77,77,77	0
56	MG	RA	3038	1/1	0.80	0.25	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3642	1/1	0.80	0.18	70,70,70,70	0
56	MG	YA	3052	1/1	0.80	0.18	45,45,45,45	0
56	MG	YA	3186	1/1	0.80	0.14	39,39,39,39	0
56	MG	RG	202	1/1	0.80	0.16	85,85,85,85	0
56	MG	RA	3646	1/1	0.80	0.34	92,92,92,92	0
56	MG	QA	1660	1/1	0.80	0.21	77,77,77,77	0
56	MG	XA	1775	1/1	0.80	0.43	72,72,72,72	0
56	MG	YA	3732	1/1	0.80	0.38	73,73,73,73	0
56	MG	QA	1795	1/1	0.80	0.33	61,61,61,61	0
56	MG	XA	1687	1/1	0.80	0.21	101,101,101,101	0
56	MG	YA	3456	1/1	0.80	0.38	68,68,68,68	0
56	MG	RA	3557	1/1	0.80	0.23	63,63,63,63	0
56	MG	XA	1619	1/1	0.80	0.10	74,74,74,74	0
56	MG	RA	3667	1/1	0.80	0.19	60,60,60,60	0
56	MG	RA	3801	1/1	0.80	0.15	74,74,74,74	0
56	MG	YA	3197	1/1	0.80	0.23	77,77,77,77	0
56	MG	R0	103	1/1	0.80	0.54	81,81,81,81	0
56	MG	RA	3812	1/1	0.80	0.22	106,106,106,106	0
56	MG	YA	3676	1/1	0.80	0.44	73,73,73,73	0
56	MG	YA	3228	1/1	0.80	0.14	75,75,75,75	0
56	MG	RA	3317	1/1	0.80	0.27	73,73,73,73	0
56	MG	RA	3207	1/1	0.80	0.31	69,69,69,69	0
56	MG	RA	3459	1/1	0.80	0.40	78,78,78,78	0
56	MG	YA	3020	1/1	0.80	0.45	80,80,80,80	0
56	MG	XA	1790	1/1	0.80	0.11	98,98,98,98	0
56	MG	YA	3314	1/1	0.80	0.32	55,55,55,55	0
56	MG	RA	3310	1/1	0.81	0.19	96,96,96,96	0
56	MG	YA	3463	1/1	0.81	0.14	47,47,47,47	0
56	MG	YA	3419	1/1	0.81	0.33	66,66,66,66	0
56	MG	RA	3995	1/1	0.81	0.37	111,111,111,111	0
56	MG	YA	3103	1/1	0.81	0.16	63,63,63,63	0
56	MG	RA	3998	1/1	0.81	0.25	87,87,87,87	0
56	MG	YA	3567	1/1	0.81	0.26	42,42,42,42	0
56	MG	RA	3182	1/1	0.81	0.47	85,85,85,85	0
56	MG	RA	3019	1/1	0.81	0.39	113,113,113,113	0
56	MG	QA	1859	1/1	0.81	0.29	50,50,50,50	0
56	MG	RA	4008	1/1	0.81	0.51	86,86,86,86	0
56	MG	YA	3424	1/1	0.81	0.08	27,27,27,27	0
56	MG	RA	3806	1/1	0.81	0.36	78,78,78,78	0
56	MG	XA	1712	1/1	0.81	0.27	61,61,61,61	0
56	MG	YA	3001	1/1	0.81	0.25	90,90,90,90	0
56	MG	YA	3511	1/1	0.81	0.39	60,60,60,60	0

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

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1622	1/1	0.82	0.16	62,62,62,62	0
56	MG	RA	3921	1/1	0.82	0.38	88,88,88,88	0
56	MG	XA	1622	1/1	0.82	0.12	42,42,42,42	0
56	MG	YA	3588	1/1	0.82	0.23	76,76,76,76	0
56	MG	YA	3122	1/1	0.82	0.29	60,60,60,60	0
56	MG	YA	3731	1/1	0.82	0.25	32,32,32,32	0
56	MG	RA	3929	1/1	0.82	0.28	65,65,65,65	0
56	MG	QA	1742	1/1	0.82	0.23	58,58,58,58	0
56	MG	XA	1627	1/1	0.82	0.20	62,62,62,62	0
56	MG	XA	1632	1/1	0.82	0.31	59,59,59,59	0
56	MG	YA	3046	1/1	0.82	0.30	75,75,75,75	0
56	MG	QA	1791	1/1	0.82	0.38	96,96,96,96	0
56	MG	RA	3340	1/1	0.82	0.31	52,52,52,52	0
56	MG	RA	3088	1/1	0.82	0.54	89,89,89,89	0
56	MG	YA	3507	1/1	0.82	0.25	44,44,44,44	0
56	MG	RA	3093	1/1	0.82	0.11	72,72,72,72	0
56	MG	YG	202	1/1	0.82	0.16	78,78,78,78	0
56	MG	XA	1685	1/1	0.82	0.23	65,65,65,65	0
56	MG	RA	3224	1/1	0.82	0.27	96,96,96,96	0
56	MG	YA	3078	1/1	0.82	0.29	60,60,60,60	0
56	MG	YA	3422	1/1	0.82	0.23	122,122,122,122	0
56	MG	QA	1648	1/1	0.82	0.11	67,67,67,67	0
56	MG	RA	3535	1/1	0.82	0.25	57,57,57,57	0
56	MG	YA	3742	1/1	0.82	0.22	36,36,36,36	0
56	MG	RA	3788	1/1	0.82	0.18	75,75,75,75	0
56	MG	RA	3968	1/1	0.82	0.29	66,66,66,66	0
56	MG	YA	3222	1/1	0.82	0.33	71,71,71,71	0
56	MG	RA	3240	1/1	0.82	0.27	92,92,92,92	0
56	MG	YA	3304	1/1	0.82	0.29	56,56,56,56	0
56	MG	RA	3794	1/1	0.82	0.44	86,86,86,86	0
56	MG	RA	3246	1/1	0.82	0.26	69,69,69,69	0
56	MG	RA	3397	1/1	0.82	0.35	65,65,65,65	0
56	MG	RA	3121	1/1	0.82	0.28	83,83,83,83	0
56	MG	YA	3755	1/1	0.82	0.19	80,80,80,80	0
56	MG	RV	202	1/1	0.82	0.14	55,55,55,55	0
56	MG	YA	3146	1/1	0.82	0.19	60,60,60,60	0
56	MG	YA	3130	1/1	0.82	0.38	65,65,65,65	0
56	MG	RZ	301	1/1	0.82	0.09	66,66,66,66	0
56	MG	RA	3130	1/1	0.82	0.14	69,69,69,69	0
56	MG	RA	3556	1/1	0.82	0.30	75,75,75,75	0
56	MG	QA	1857	1/1	0.82	0.44	71,71,71,71	0
56	MG	RA	3005	1/1	0.82	0.26	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3700	1/1	0.82	0.28	71,71,71,71	0
56	MG	RA	3826	1/1	0.82	0.21	62,62,62,62	0
56	MG	RA	3827	1/1	0.82	0.30	57,57,57,57	0
56	MG	YA	3437	1/1	0.82	0.34	85,85,85,85	0
56	MG	QA	1723	1/1	0.82	0.17	50,50,50,50	0
56	MG	RA	3152	1/1	0.82	0.19	106,106,106,106	0
56	MG	RA	3569	1/1	0.82	0.30	64,64,64,64	0
56	MG	XA	1626	1/1	0.83	0.52	77,77,77,77	0
56	MG	RA	3584	1/1	0.83	0.13	45,45,45,45	0
56	MG	YR	201	1/1	0.83	0.21	66,66,66,66	0
56	MG	RA	3059	1/1	0.83	0.21	76,76,76,76	0
56	MG	YT	202	1/1	0.83	0.25	84,84,84,84	0
56	MG	RA	3592	1/1	0.83	0.32	56,56,56,56	0
56	MG	YT	203	1/1	0.83	0.19	78,78,78,78	0
56	MG	YB	207	1/1	0.83	0.48	110,110,110,110	0
56	MG	RA	3726	1/1	0.83	0.24	53,53,53,53	0
56	MG	RA	4047	1/1	0.83	0.45	117,117,117,117	0
56	MG	XA	1778	1/1	0.83	0.29	60,60,60,60	0
56	MG	RA	4052	1/1	0.83	0.17	90,90,90,90	0
56	MG	RA	3074	1/1	0.83	0.10	52,52,52,52	0
56	MG	QA	1825	1/1	0.83	0.26	74,74,74,74	0
56	MG	YA	3161	1/1	0.83	0.30	76,76,76,76	0
56	MG	QA	1776	1/1	0.83	0.29	80,80,80,80	0
56	MG	YA	3464	1/1	0.83	0.33	73,73,73,73	0
56	MG	RB	202	1/1	0.83	0.13	55,55,55,55	0
56	MG	YA	3208	1/1	0.83	0.29	60,60,60,60	0
56	MG	RA	3737	1/1	0.83	0.22	77,77,77,77	0
56	MG	YA	3687	1/1	0.83	0.23	75,75,75,75	0
56	MG	QA	1833	1/1	0.83	0.26	51,51,51,51	0
56	MG	RA	3354	1/1	0.83	0.19	61,61,61,61	0
56	MG	YA	3210	1/1	0.83	0.27	65,65,65,65	0
56	MG	RA	3747	1/1	0.83	0.38	96,96,96,96	0
56	MG	YA	3641	1/1	0.83	0.41	86,86,86,86	0
56	MG	YA	3733	1/1	0.83	0.17	62,62,62,62	0
56	MG	QL	203	1/1	0.83	0.14	60,60,60,60	0
56	MG	RA	3755	1/1	0.83	0.34	71,71,71,71	0
56	MG	RA	3518	1/1	0.83	0.32	82,82,82,82	0
56	MG	QA	1741	1/1	0.83	0.30	45,45,45,45	0
56	MG	XA	1728	1/1	0.83	0.19	101,101,101,101	0
56	MG	RA	3760	1/1	0.83	0.18	74,74,74,74	0
56	MG	YA	3214	1/1	0.83	0.25	111,111,111,111	0
56	MG	QA	1641	1/1	0.83	0.34	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3245	1/1	0.83	0.14	81,81,81,81	0
56	MG	RA	3526	1/1	0.83	0.30	51,51,51,51	0
56	MG	RD	304	1/1	0.83	0.35	86,86,86,86	0
56	MG	RA	3772	1/1	0.83	0.25	57,57,57,57	0
56	MG	XF	202	1/1	0.83	0.10	73,73,73,73	0
56	MG	XA	1691	1/1	0.83	0.30	60,60,60,60	0
56	MG	QA	1747	1/1	0.83	0.35	72,72,72,72	0
56	MG	YA	3263	1/1	0.83	0.50	81,81,81,81	0
56	MG	YD	310	1/1	0.83	0.11	64,64,64,64	0
56	MG	XA	1653	1/1	0.83	0.33	79,79,79,79	0
56	MG	RF	309	1/1	0.83	0.34	68,68,68,68	0
56	MG	QA	1801	1/1	0.83	0.23	78,78,78,78	0
56	MG	RA	3652	1/1	0.83	0.33	88,88,88,88	0
56	MG	XK	201	1/1	0.83	0.09	53,53,53,53	0
56	MG	QA	1703	1/1	0.83	0.13	60,60,60,60	0
56	MG	XA	1613	1/1	0.83	0.10	51,51,51,51	0
56	MG	QA	1806	1/1	0.83	0.17	73,73,73,73	0
56	MG	RA	3425	1/1	0.83	0.29	94,94,94,94	0
56	MG	YA	3104	1/1	0.83	0.35	85,85,85,85	0
56	MG	YA	3101	1/1	0.83	0.34	70,70,70,70	0
56	MG	RO	201	1/1	0.83	0.21	93,93,93,93	0
56	MG	YA	3053	1/1	0.83	0.36	77,77,77,77	0
56	MG	RA	3670	1/1	0.83	0.17	80,80,80,80	0
56	MG	RA	3805	1/1	0.83	0.33	98,98,98,98	0
56	MG	RA	3034	1/1	0.83	0.34	100,100,100,100	0
56	MG	RA	3166	1/1	0.83	0.28	68,68,68,68	0
56	MG	RA	3169	1/1	0.83	0.19	82,82,82,82	0
56	MG	RA	3816	1/1	0.83	0.34	102,102,102,102	0
56	MG	QA	1655	1/1	0.83	0.20	64,64,64,64	0
56	MG	YA	3138	1/1	0.83	0.23	61,61,61,61	0
56	MG	R0	101	1/1	0.83	0.27	94,94,94,94	0
56	MG	RA	3996	1/1	0.83	0.40	73,73,73,73	0
56	MG	YA	3065	1/1	0.83	0.27	88,88,88,88	0
56	MG	YA	3288	1/1	0.83	0.30	53,53,53,53	0
56	MG	YA	3292	1/1	0.83	0.64	81,81,81,81	0
56	MG	QA	1724	1/1	0.83	0.25	76,76,76,76	0
56	MG	RA	3042	1/1	0.83	0.19	80,80,80,80	0
56	MG	RA	3831	1/1	0.83	0.23	65,65,65,65	0
56	MG	RA	4005	1/1	0.83	0.19	58,58,58,58	0
56	MG	YA	3555	1/1	0.83	0.34	77,77,77,77	0
56	MG	RA	3702	1/1	0.83	0.25	67,67,67,67	0
56	MG	RA	3458	1/1	0.83	0.23	74,74,74,74	0

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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	0.84	0.27	86,86,86,86	0
56	MG	RA	3842	1/1	0.84	0.21	72,72,72,72	0
56	MG	RA	3294	1/1	0.84	0.23	61,61,61,61	0
56	MG	RA	4021	1/1	0.84	0.14	56,56,56,56	0
56	MG	YA	3295	1/1	0.84	0.23	44,44,44,44	0
56	MG	YA	3525	1/1	0.84	0.33	86,86,86,86	0
56	MG	RA	3587	1/1	0.84	0.39	53,53,53,53	0
56	MG	RA	3095	1/1	0.84	0.40	88,88,88,88	0
56	MG	RA	3862	1/1	0.84	0.24	79,79,79,79	0
56	MG	YA	3562	1/1	0.84	0.25	70,70,70,70	0
56	MG	XA	1606	1/1	0.84	0.06	95,95,95,95	0
56	MG	RA	3311	1/1	0.84	0.37	100,100,100,100	0
56	MG	YA	3050	1/1	0.84	0.16	85,85,85,85	0
56	MG	YA	3238	1/1	0.84	0.24	91,91,91,91	0
56	MG	RA	4056	1/1	0.84	0.39	70,70,70,70	0
56	MG	YA	3470	1/1	0.84	0.18	59,59,59,59	0
56	MG	RA	3485	1/1	0.84	0.51	65,65,65,65	0
56	MG	RA	3881	1/1	0.84	0.48	68,68,68,68	0
56	MG	RA	3111	1/1	0.84	0.30	106,106,106,106	0
56	MG	RA	3214	1/1	0.84	0.23	59,59,59,59	0
56	MG	RA	3601	1/1	0.84	0.54	87,87,87,87	0
56	MG	QA	1630	1/1	0.84	0.16	81,81,81,81	0
56	MG	RA	3739	1/1	0.84	0.31	78,78,78,78	0
56	MG	QA	1677	1/1	0.84	0.35	94,94,94,94	0
56	MG	YA	3570	1/1	0.84	0.36	59,59,59,59	0
56	MG	QA	1771	1/1	0.84	0.13	57,57,57,57	0
56	MG	YA	3531	1/1	0.84	0.25	66,66,66,66	0
56	MG	XA	1733	1/1	0.84	0.16	72,72,72,72	0
56	MG	YB	202	1/1	0.84	0.15	56,56,56,56	0
56	MG	RA	3925	1/1	0.84	0.30	83,83,83,83	0
56	MG	RA	3352	1/1	0.84	0.29	65,65,65,65	0
56	MG	RA	3628	1/1	0.84	0.25	65,65,65,65	0
56	MG	QA	1865	1/1	0.84	0.29	75,75,75,75	0
56	MG	XA	1739	1/1	0.84	0.34	61,61,61,61	0
56	MG	XA	1656	1/1	0.84	0.25	80,80,80,80	0
56	MG	RA	3134	1/1	0.84	0.28	83,83,83,83	0
56	MG	RA	3244	1/1	0.84	0.16	71,71,71,71	0
56	MG	RA	3939	1/1	0.84	0.27	58,58,58,58	0
56	MG	XA	1618	1/1	0.84	0.36	72,72,72,72	0
56	MG	RA	3365	1/1	0.84	0.26	61,61,61,61	0
56	MG	XA	1701	1/1	0.84	0.30	51,51,51,51	0
56	MG	RA	3143	1/1	0.84	0.11	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3769	1/1	0.84	0.36	46,46,46,46	0
56	MG	RA	3949	1/1	0.84	0.18	80,80,80,80	0
56	MG	YA	3135	1/1	0.84	0.50	89,89,89,89	0
56	MG	QA	1827	1/1	0.84	0.21	52,52,52,52	0
56	MG	RA	3371	1/1	0.84	0.37	75,75,75,75	0
56	MG	RA	3779	1/1	0.84	0.31	86,86,86,86	0
56	MG	YA	3051	1/1	0.84	0.18	64,64,64,64	0
56	MG	YA	3351	1/1	0.84	0.30	51,51,51,51	0
56	MG	RA	3380	1/1	0.84	0.24	43,43,43,43	0
56	MG	XT	201	1/1	0.84	0.13	65,65,65,65	0
56	MG	RA	3396	1/1	0.84	0.31	58,58,58,58	0
56	MG	RG	204	1/1	0.84	0.16	67,67,67,67	0
56	MG	RA	3258	1/1	0.84	0.35	96,96,96,96	0
56	MG	YA	3257	1/1	0.84	0.36	84,84,84,84	0
56	MG	YA	3115	1/1	0.84	0.24	52,52,52,52	0
56	MG	QA	1792	1/1	0.84	0.22	69,69,69,69	0
56	MG	YX	101	1/1	0.84	0.25	31,31,31,31	0
56	MG	RP	201	1/1	0.84	0.50	72,72,72,72	0
56	MG	RA	3407	1/1	0.84	0.35	34,34,34,34	0
56	MG	Y0	101	1/1	0.84	0.40	65,65,65,65	0
56	MG	RT	202	1/1	0.84	0.17	65,65,65,65	0
56	MG	RA	3176	1/1	0.84	0.43	96,96,96,96	0
56	MG	QG	201	1/1	0.84	0.21	91,91,91,91	0
56	MG	RA	3555	1/1	0.84	0.55	68,68,68,68	0
56	MG	QA	1711	1/1	0.84	0.17	63,63,63,63	0
56	MG	RA	3180	1/1	0.84	0.22	75,75,75,75	0
56	MG	RA	3279	1/1	0.84	0.31	103,103,103,103	0
56	MG	RX	101	1/1	0.84	0.24	51,51,51,51	0
56	MG	YA	3133	1/1	0.84	0.28	91,91,91,91	0
56	MG	YA	3330	1/1	0.84	0.26	62,62,62,62	0
56	MG	YA	3616	1/1	0.84	0.38	53,53,53,53	0
56	MG	RA	3566	1/1	0.84	0.21	57,57,57,57	0
56	MG	RA	3689	1/1	0.84	0.45	70,70,70,70	0
56	MG	RA	3285	1/1	0.84	0.20	85,85,85,85	0
56	MG	R1	103	1/1	0.84	0.13	55,55,55,55	0
56	MG	XA	1771	1/1	0.84	0.32	62,62,62,62	0
56	MG	RA	3696	1/1	0.84	0.36	74,74,74,74	0
56	MG	YA	3248	1/1	0.84	0.21	105,105,105,105	0
56	MG	YA	3493	1/1	0.84	0.21	74,74,74,74	0
56	MG	RA	3703	1/1	0.84	0.33	71,71,71,71	0
56	MG	RA	3837	1/1	0.84	0.19	59,59,59,59	0
56	MG	RA	3448	1/1	0.84	0.28	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3865	1/1	0.85	0.30	51,51,51,51	0
56	MG	RA	3866	1/1	0.85	0.11	76,76,76,76	0
56	MG	RA	3867	1/1	0.85	0.17	63,63,63,63	0
56	MG	YA	3551	1/1	0.85	0.31	60,60,60,60	0
56	MG	RA	3603	1/1	0.85	0.38	101,101,101,101	0
56	MG	RA	3129	1/1	0.85	0.19	45,45,45,45	0
56	MG	XA	1713	1/1	0.85	0.24	49,49,49,49	0
56	MG	YA	3693	1/1	0.85	0.25	60,60,60,60	0
56	MG	YA	3359	1/1	0.85	0.25	72,72,72,72	0
56	MG	YA	3622	1/1	0.85	0.30	49,49,49,49	0
56	MG	RA	3136	1/1	0.85	0.29	84,84,84,84	0
56	MG	XA	1629	1/1	0.85	0.13	51,51,51,51	0
56	MG	XA	1720	1/1	0.85	0.33	63,63,63,63	0
56	MG	QA	1868	1/1	0.85	0.35	58,58,58,58	0
56	MG	YA	3519	1/1	0.85	0.44	79,79,79,79	0
56	MG	RA	3250	1/1	0.85	0.29	69,69,69,69	0
56	MG	RA	3151	1/1	0.85	0.27	59,59,59,59	0
56	MG	RA	3918	1/1	0.85	0.40	71,71,71,71	0
56	MG	YA	3420	1/1	0.85	0.13	39,39,39,39	0
56	MG	YA	3218	1/1	0.85	0.39	89,89,89,89	0
56	MG	RA	3759	1/1	0.85	0.26	67,67,67,67	0
56	MG	YB	208	1/1	0.85	0.15	81,81,81,81	0
56	MG	RA	3259	1/1	0.85	0.11	87,87,87,87	0
56	MG	RA	3377	1/1	0.85	0.29	42,42,42,42	0
56	MG	QA	1679	1/1	0.85	0.19	64,64,64,64	0
56	MG	RA	3528	1/1	0.85	0.31	76,76,76,76	0
56	MG	RA	3530	1/1	0.85	0.19	75,75,75,75	0
56	MG	QA	1632	1/1	0.85	0.15	70,70,70,70	0
56	MG	RA	3163	1/1	0.85	0.69	93,93,93,93	0
56	MG	RA	3536	1/1	0.85	0.30	64,64,64,64	0
56	MG	RA	3268	1/1	0.85	0.26	95,95,95,95	0
56	MG	RA	3650	1/1	0.85	0.32	69,69,69,69	0
56	MG	RA	3053	1/1	0.85	0.35	89,89,89,89	0
56	MG	QA	1877	1/1	0.85	0.19	94,94,94,94	0
56	MG	XA	1642	1/1	0.85	0.22	55,55,55,55	0
56	MG	YA	3497	1/1	0.85	0.21	63,63,63,63	0
56	MG	RA	3950	1/1	0.85	0.26	87,87,87,87	0
56	MG	YA	3450	1/1	0.85	0.36	79,79,79,79	0
56	MG	RA	3952	1/1	0.85	0.26	49,49,49,49	0
56	MG	YA	3565	1/1	0.85	0.34	85,85,85,85	0
56	MG	YA	3368	1/1	0.85	0.25	62,62,62,62	0
56	MG	RA	3415	1/1	0.85	0.28	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QE	201	1/1	0.85	0.27	84,84,84,84	0
56	MG	QA	1689	1/1	0.85	0.29	80,80,80,80	0
56	MG	YA	3502	1/1	0.85	0.29	79,79,79,79	0
56	MG	QA	1691	1/1	0.85	0.27	104,104,104,104	0
56	MG	YA	3176	1/1	0.85	0.22	102,102,102,102	0
56	MG	YA	3221	1/1	0.85	0.40	77,77,77,77	0
56	MG	RA	3290	1/1	0.85	0.27	74,74,74,74	0
56	MG	RA	3086	1/1	0.85	0.49	124,124,124,124	0
56	MG	YA	3375	1/1	0.85	0.36	55,55,55,55	0
56	MG	RA	3810	1/1	0.85	0.18	75,75,75,75	0
56	MG	RA	3440	1/1	0.85	0.32	57,57,57,57	0
56	MG	RA	3978	1/1	0.85	0.35	55,55,55,55	0
56	MG	RA	3981	1/1	0.85	0.08	69,69,69,69	0
56	MG	RA	3089	1/1	0.85	0.21	67,67,67,67	0
56	MG	YA	3124	1/1	0.85	0.26	54,54,54,54	0
56	MG	YA	3541	1/1	0.85	0.24	20,20,20,20	0
56	MG	QA	1700	1/1	0.85	0.26	66,66,66,66	0
56	MG	YA	3485	1/1	0.85	0.50	77,77,77,77	0
56	MG	RA	3305	1/1	0.85	0.17	98,98,98,98	0
56	MG	RA	3578	1/1	0.85	0.21	60,60,60,60	0
56	MG	XA	1655	1/1	0.85	0.28	84,84,84,84	0
56	MG	YA	3384	1/1	0.85	0.24	38,38,38,38	0
56	MG	YA	3043	1/1	0.85	0.28	62,62,62,62	0
56	MG	RA	3835	1/1	0.85	0.38	56,56,56,56	0
56	MG	RA	3208	1/1	0.85	0.15	70,70,70,70	0
56	MG	YA	3609	1/1	0.85	0.18	51,51,51,51	0
56	MG	YA	3682	1/1	0.85	0.13	37,37,37,37	0
56	MG	RA	3466	1/1	0.85	0.34	56,56,56,56	0
56	MG	QA	1758	1/1	0.85	0.36	76,76,76,76	0
56	MG	RA	3476	1/1	0.85	0.30	30,30,30,30	0
56	MG	YA	3683	1/1	0.85	0.30	39,39,39,39	0
56	MG	RA	3849	1/1	0.85	0.12	52,52,52,52	0
56	MG	RA	4013	1/1	0.85	0.22	76,76,76,76	0
56	MG	R5	101	1/1	0.85	0.37	105,105,105,105	0
56	MG	QA	1714	1/1	0.85	0.13	42,42,42,42	0
56	MG	RA	3329	1/1	0.85	0.16	86,86,86,86	0
56	MG	YA	3026	1/1	0.85	0.29	93,93,93,93	0
56	MG	XA	1760	1/1	0.85	0.30	71,71,71,71	0
56	MG	YA	3688	1/1	0.85	0.30	62,62,62,62	0
56	MG	YD	305	1/1	0.86	0.33	82,82,82,82	0
56	MG	YA	3264	1/1	0.86	0.21	88,88,88,88	0
56	MG	RA	3520	1/1	0.86	0.19	34,34,34,34	0

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1772	1/1	0.86	0.36	79,79,79,79	0
56	MG	YA	3039	1/1	0.86	0.31	73,73,73,73	0
56	MG	YA	3140	1/1	0.86	0.35	65,65,65,65	0
56	MG	XA	1646	1/1	0.86	0.21	63,63,63,63	0
56	MG	XA	1696	1/1	0.86	0.23	67,67,67,67	0
56	MG	QA	1778	1/1	0.86	0.27	61,61,61,61	0
56	MG	RN	201	1/1	0.86	0.25	85,85,85,85	0
56	MG	YA	3706	1/1	0.86	0.28	79,79,79,79	0
56	MG	YA	3004	1/1	0.86	0.08	43,43,43,43	0
56	MG	QA	1669	1/1	0.86	0.29	71,71,71,71	0
56	MG	YA	3169	1/1	0.86	0.28	91,91,91,91	0
56	MG	QA	1673	1/1	0.86	0.13	52,52,52,52	0
56	MG	RQ	203	1/1	0.86	0.27	82,82,82,82	0
56	MG	RR	3203	1/1	0.86	0.32	84,84,84,84	0
56	MG	YA	3127	1/1	0.86	0.13	50,50,50,50	0
56	MG	YA	3713	1/1	0.86	0.50	67,67,67,67	0
56	MG	RA	3219	1/1	0.86	0.16	66,66,66,66	0
56	MG	RA	3104	1/1	0.86	0.17	57,57,57,57	0
56	MG	QA	1613	1/1	0.86	0.10	97,97,97,97	0
56	MG	YA	3716	1/1	0.86	0.27	65,65,65,65	0
56	MG	RA	3332	1/1	0.86	0.13	53,53,53,53	0
56	MG	RA	3334	1/1	0.86	0.26	46,46,46,46	0
56	MG	RA	4006	1/1	0.86	0.26	81,81,81,81	0
56	MG	RA	3338	1/1	0.86	0.36	38,38,38,38	0
56	MG	RA	4010	1/1	0.86	0.23	76,76,76,76	0
56	MG	QR	101	1/1	0.86	0.17	71,71,71,71	0
56	MG	XA	1764	1/1	0.86	0.33	52,52,52,52	0
56	MG	RA	3229	1/1	0.86	0.36	82,82,82,82	0
56	MG	RA	3344	1/1	0.86	0.29	51,51,51,51	0
56	MG	YA	3360	1/1	0.86	0.27	53,53,53,53	0
56	MG	RA	3351	1/1	0.86	0.18	70,70,70,70	0
56	MG	YA	3526	1/1	0.86	0.21	43,43,43,43	0
56	MG	YA	3056	1/1	0.86	0.26	81,81,81,81	0
56	MG	RA	3753	1/1	0.86	0.35	48,48,48,48	0
56	MG	YA	3097	1/1	0.86	0.20	37,37,37,37	0
56	MG	RA	3009	1/1	0.86	0.11	53,53,53,53	0
56	MG	RA	4040	1/1	0.86	0.29	69,69,69,69	0
56	MG	RA	3243	1/1	0.86	0.25	73,73,73,73	0
56	MG	RA	3342	1/1	0.87	0.33	60,60,60,60	0
56	MG	YA	3031	1/1	0.87	0.24	46,46,46,46	0
56	MG	RA	3859	1/1	0.87	0.31	72,72,72,72	0
56	MG	RA	3462	1/1	0.87	0.21	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	4026	1/1	0.87	0.25	71,71,71,71	0
56	MG	YA	3748	1/1	0.87	0.30	95,95,95,95	0
56	MG	RA	4031	1/1	0.87	0.29	102,102,102,102	0
56	MG	RA	4034	1/1	0.87	0.22	73,73,73,73	0
56	MG	QA	1836	1/1	0.87	0.27	89,89,89,89	0
56	MG	YA	3479	1/1	0.87	0.24	50,50,50,50	0
56	MG	RA	3475	1/1	0.87	0.40	46,46,46,46	0
56	MG	YA	3623	1/1	0.87	0.25	54,54,54,54	0
56	MG	RA	3868	1/1	0.87	0.25	48,48,48,48	0
56	MG	QH	201	1/1	0.87	0.28	76,76,76,76	0
56	MG	RA	3484	1/1	0.87	0.25	30,30,30,30	0
56	MG	RA	3599	1/1	0.87	0.22	66,66,66,66	0
56	MG	RA	3167	1/1	0.87	0.10	69,69,69,69	0
56	MG	RA	4053	1/1	0.87	0.20	74,74,74,74	0
56	MG	YA	3624	1/1	0.87	0.42	71,71,71,71	0
56	MG	RA	4055	1/1	0.87	0.25	86,86,86,86	0
56	MG	RA	3360	1/1	0.87	0.33	66,66,66,66	0
56	MG	YA	3482	1/1	0.87	0.29	65,65,65,65	0
56	MG	RA	3887	1/1	0.87	0.22	53,53,53,53	0
56	MG	XA	1681	1/1	0.87	0.19	106,106,106,106	0
56	MG	RA	3363	1/1	0.87	0.22	50,50,50,50	0
56	MG	YA	3372	1/1	0.87	0.33	49,49,49,49	0
56	MG	YA	3109	1/1	0.87	0.19	35,35,35,35	0
56	MG	RA	3178	1/1	0.87	0.28	79,79,79,79	0
56	MG	RA	3909	1/1	0.87	0.25	73,73,73,73	0
56	MG	RA	3911	1/1	0.87	0.18	46,46,46,46	0
56	MG	YA	3012	1/1	0.87	0.14	56,56,56,56	0
56	MG	RA	3914	1/1	0.87	0.25	56,56,56,56	0
56	MG	YA	3639	1/1	0.87	0.33	74,74,74,74	0
56	MG	RA	3083	1/1	0.87	0.25	80,80,80,80	0
56	MG	YA	3116	1/1	0.87	0.19	58,58,58,58	0
56	MG	YA	3231	1/1	0.87	0.21	59,59,59,59	0
56	MG	RA	3373	1/1	0.87	0.28	44,44,44,44	0
56	MG	QA	1699	1/1	0.87	0.15	65,65,65,65	0
56	MG	RB	220	1/1	0.87	0.36	47,47,47,47	0
56	MG	YB	213	1/1	0.87	0.28	57,57,57,57	0
56	MG	YA	3392	1/1	0.87	0.28	54,54,54,54	0
56	MG	RA	3379	1/1	0.87	0.33	44,44,44,44	0
56	MG	YA	3181	1/1	0.87	0.22	66,66,66,66	0
56	MG	RA	3386	1/1	0.87	0.23	26,26,26,26	0
56	MG	RA	3282	1/1	0.87	0.26	109,109,109,109	0
56	MG	RA	3389	1/1	0.87	0.24	23,23,23,23	0

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1714	1/1	0.87	0.16	58,58,58,58	0
56	MG	RA	3450	1/1	0.87	0.48	53,53,53,53	0
56	MG	RA	3836	1/1	0.87	0.26	91,91,91,91	0
56	MG	YA	3316	1/1	0.87	0.17	53,53,53,53	0
56	MG	RA	3575	1/1	0.87	0.25	62,62,62,62	0
56	MG	RA	3840	1/1	0.87	0.16	83,83,83,83	0
56	MG	YA	3324	1/1	0.87	0.35	39,39,39,39	0
56	MG	R5	103	1/1	0.87	0.25	59,59,59,59	0
56	MG	RA	3052	1/1	0.87	0.26	85,85,85,85	0
56	MG	QA	1779	1/1	0.87	0.12	80,80,80,80	0
56	MG	YA	3447	1/1	0.87	0.26	68,68,68,68	0
56	MG	QA	1627	1/1	0.87	0.10	42,42,42,42	0
56	MG	RA	3586	1/1	0.87	0.26	73,73,73,73	0
56	MG	XA	1630	1/1	0.88	0.18	62,62,62,62	0
56	MG	QA	1705	1/1	0.88	0.21	37,37,37,37	0
56	MG	QA	1670	1/1	0.88	0.24	81,81,81,81	0
56	MG	YA	3454	1/1	0.88	0.49	52,52,52,52	0
56	MG	YA	3024	1/1	0.88	0.43	59,59,59,59	0
56	MG	RA	3732	1/1	0.88	0.11	54,54,54,54	0
56	MG	RD	301	1/1	0.88	0.41	76,76,76,76	0
56	MG	YA	3309	1/1	0.88	0.14	37,37,37,37	0
56	MG	RA	3428	1/1	0.88	0.16	60,60,60,60	0
56	MG	RD	311	1/1	0.88	0.24	70,70,70,70	0
56	MG	RD	312	1/1	0.88	0.18	76,76,76,76	0
56	MG	YA	3520	1/1	0.88	0.20	68,68,68,68	0
56	MG	RA	3815	1/1	0.88	0.11	68,68,68,68	0
56	MG	YA	3178	1/1	0.88	0.15	62,62,62,62	0
56	MG	RA	3085	1/1	0.88	0.17	76,76,76,76	0
56	MG	RE	306	1/1	0.88	0.17	59,59,59,59	0
56	MG	YA	3438	1/1	0.88	0.21	45,45,45,45	0
56	MG	RA	3819	1/1	0.88	0.19	33,33,33,33	0
56	MG	RA	3657	1/1	0.88	0.22	65,65,65,65	0
56	MG	RA	3742	1/1	0.88	0.12	81,81,81,81	0
56	MG	RA	3931	1/1	0.88	0.31	73,73,73,73	0
56	MG	RA	3223	1/1	0.88	0.14	63,63,63,63	0
56	MG	RA	3026	1/1	0.88	0.28	72,72,72,72	0
56	MG	QA	1815	1/1	0.88	0.24	65,65,65,65	0
56	MG	RA	3750	1/1	0.88	0.44	66,66,66,66	0
56	MG	XA	1786	1/1	0.88	0.13	72,72,72,72	0
56	MG	RA	3033	1/1	0.88	0.36	91,91,91,91	0
56	MG	RA	3164	1/1	0.88	0.25	87,87,87,87	0
56	MG	RA	3832	1/1	0.88	0.12	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1695	1/1	0.88	0.34	52,52,52,52	0
56	MG	RA	3097	1/1	0.88	0.28	93,93,93,93	0
56	MG	RA	3449	1/1	0.88	0.20	45,45,45,45	0
56	MG	RA	4045	1/1	0.88	0.26	71,71,71,71	0
56	MG	RA	3295	1/1	0.88	0.12	73,73,73,73	0
56	MG	RA	3674	1/1	0.88	0.35	77,77,77,77	0
56	MG	YA	3017	1/1	0.88	0.33	60,60,60,60	0
56	MG	RQ	202	1/1	0.88	0.11	51,51,51,51	0
56	MG	YA	3709	1/1	0.88	0.24	58,58,58,58	0
56	MG	RR	3202	1/1	0.88	0.26	69,69,69,69	0
56	MG	RA	3101	1/1	0.88	0.21	68,68,68,68	0
56	MG	YA	3045	1/1	0.88	0.14	27,27,27,27	0
56	MG	YA	3040	1/1	0.88	0.20	66,66,66,66	0
56	MG	XE	202	1/1	0.88	0.10	67,67,67,67	0
56	MG	RA	3959	1/1	0.88	0.10	43,43,43,43	0
56	MG	QA	1619	1/1	0.88	0.12	75,75,75,75	0
56	MG	QL	202	1/1	0.88	0.16	68,68,68,68	0
56	MG	RA	3048	1/1	0.88	0.25	78,78,78,78	0
56	MG	RA	3612	1/1	0.88	0.33	64,64,64,64	0
56	MG	YA	3049	1/1	0.88	0.31	78,78,78,78	0
56	MG	RA	3695	1/1	0.88	0.14	52,52,52,52	0
56	MG	RA	3547	1/1	0.88	0.21	74,74,74,74	0
56	MG	YA	3378	1/1	0.88	0.22	53,53,53,53	0
56	MG	YA	3643	1/1	0.88	0.34	36,36,36,36	0
56	MG	QA	1794	1/1	0.88	0.22	79,79,79,79	0
56	MG	R1	101	1/1	0.88	0.27	82,82,82,82	0
56	MG	XA	1766	1/1	0.88	0.44	52,52,52,52	0
56	MG	RA	3480	1/1	0.88	0.28	42,42,42,42	0
56	MG	YA	3644	1/1	0.88	0.31	57,57,57,57	0
56	MG	R3	102	1/1	0.88	0.32	80,80,80,80	0
56	MG	RA	3709	1/1	0.88	0.25	75,75,75,75	0
56	MG	YA	3355	1/1	0.88	0.30	75,75,75,75	0
56	MG	YE	304	1/1	0.88	0.22	51,51,51,51	0
56	MG	YA	3084	1/1	0.88	0.20	66,66,66,66	0
56	MG	RA	3336	1/1	0.88	0.22	66,66,66,66	0
56	MG	QA	1635	1/1	0.88	0.10	58,58,58,58	0
57	ZN	YY	201	1/1	0.88	0.11	221,221,221,221	0
56	MG	YA	3068	1/1	0.88	0.12	65,65,65,65	0
57	ZN	RY	201	1/1	0.88	0.15	210,210,210,210	0
56	MG	YA	3535	1/1	0.88	0.35	75,75,75,75	0
56	MG	RA	3608	1/1	0.89	0.18	104,104,104,104	0
56	MG	RA	3270	1/1	0.89	0.33	103,103,103,103	0

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

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

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3441	1/1	0.90	0.17	61,61,61,61	0
56	MG	RA	4064	1/1	0.90	0.19	64,64,64,64	0
56	MG	RA	3185	1/1	0.90	0.30	94,94,94,94	0
56	MG	RA	3445	1/1	0.90	0.17	58,58,58,58	0
56	MG	XA	1743	1/1	0.90	0.32	44,44,44,44	0
56	MG	RA	3447	1/1	0.90	0.13	57,57,57,57	0
56	MG	RA	3582	1/1	0.90	0.34	72,72,72,72	0
56	MG	RA	3189	1/1	0.90	0.10	39,39,39,39	0
56	MG	RA	3892	1/1	0.90	0.35	55,55,55,55	0
56	MG	RA	3190	1/1	0.90	0.28	62,62,62,62	0
56	MG	RA	3308	1/1	0.90	0.13	64,64,64,64	0
56	MG	RA	3902	1/1	0.90	0.16	49,49,49,49	0
56	MG	RA	3451	1/1	0.90	0.27	27,27,27,27	0
56	MG	RA	3071	1/1	0.90	0.27	63,63,63,63	0
56	MG	RA	3192	1/1	0.90	0.26	92,92,92,92	0
56	MG	YA	3074	1/1	0.90	0.21	63,63,63,63	0
56	MG	YA	3307	1/1	0.90	0.31	73,73,73,73	0
56	MG	YA	3703	1/1	0.90	0.23	35,35,35,35	0
56	MG	RB	219	1/1	0.90	0.14	57,57,57,57	0
56	MG	YA	3634	1/1	0.90	0.42	48,48,48,48	0
56	MG	YA	3552	1/1	0.90	0.37	52,52,52,52	0
56	MG	YA	3636	1/1	0.90	0.15	45,45,45,45	0
56	MG	RA	3325	1/1	0.90	0.26	42,42,42,42	0
56	MG	RA	3200	1/1	0.90	0.29	99,99,99,99	0
56	MG	XA	1621	1/1	0.90	0.29	68,68,68,68	0
56	MG	QA	1684	1/1	0.90	0.17	97,97,97,97	0
56	MG	YD	303	1/1	0.90	0.25	44,44,44,44	0
56	MG	YA	3044	1/1	0.90	0.13	35,35,35,35	0
56	MG	RA	3471	1/1	0.90	0.22	42,42,42,42	0
56	MG	RA	3335	1/1	0.90	0.19	46,46,46,46	0
56	MG	QA	1687	1/1	0.90	0.14	97,97,97,97	0
56	MG	RA	3091	1/1	0.90	0.27	104,104,104,104	0
56	MG	RD	305	1/1	0.90	0.18	86,86,86,86	0
56	MG	RD	307	1/1	0.90	0.27	83,83,83,83	0
56	MG	RA	3478	1/1	0.90	0.26	34,34,34,34	0
56	MG	YA	3354	1/1	0.90	0.38	47,47,47,47	0
56	MG	YA	3472	1/1	0.90	0.28	23,23,23,23	0
56	MG	RA	3937	1/1	0.90	0.11	38,38,38,38	0
56	MG	YA	3441	1/1	0.90	0.23	34,34,34,34	0
56	MG	XA	1761	1/1	0.90	0.18	38,38,38,38	0
56	MG	RA	3766	1/1	0.90	0.23	29,29,29,29	0
56	MG	YA	3275	1/1	0.90	0.27	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3276	1/1	0.90	0.33	67,67,67,67	0
56	MG	YA	3564	1/1	0.90	0.19	42,42,42,42	0
56	MG	YA	3262	1/1	0.90	0.27	88,88,88,88	0
56	MG	RA	3492	1/1	0.90	0.26	68,68,68,68	0
56	MG	QA	1629	1/1	0.90	0.11	51,51,51,51	0
56	MG	RF	308	1/1	0.90	0.27	74,74,74,74	0
56	MG	XA	1633	1/1	0.90	0.22	51,51,51,51	0
56	MG	RA	3496	1/1	0.90	0.20	16,16,16,16	0
56	MG	RA	3225	1/1	0.90	0.31	109,109,109,109	0
56	MG	YE	307	1/1	0.90	0.07	64,64,64,64	0
56	MG	XA	1636	1/1	0.90	0.06	60,60,60,60	0
56	MG	RA	3640	1/1	0.90	0.16	48,48,48,48	0
56	MG	YA	3149	1/1	0.90	0.21	56,56,56,56	0
56	MG	YA	3182	1/1	0.90	0.15	68,68,68,68	0
56	MG	RA	3509	1/1	0.90	0.35	69,69,69,69	0
56	MG	RA	3233	1/1	0.90	0.24	72,72,72,72	0
56	MG	RA	3234	1/1	0.90	0.12	64,64,64,64	0
56	MG	RA	3966	1/1	0.90	0.32	65,65,65,65	0
56	MG	RA	3113	1/1	0.90	0.30	65,65,65,65	0
56	MG	YA	3366	1/1	0.90	0.26	59,59,59,59	0
56	MG	QA	1841	1/1	0.90	0.20	28,28,28,28	0
56	MG	RA	3117	1/1	0.90	0.17	64,64,64,64	0
56	MG	RQ	201	1/1	0.90	0.12	47,47,47,47	0
56	MG	RA	3651	1/1	0.90	0.11	41,41,41,41	0
56	MG	YA	3573	1/1	0.90	0.35	38,38,38,38	0
56	MG	RA	3120	1/1	0.90	0.11	63,63,63,63	0
56	MG	QA	1775	1/1	0.90	0.27	72,72,72,72	0
56	MG	RR	3204	1/1	0.90	0.32	83,83,83,83	0
56	MG	RA	3013	1/1	0.90	0.37	71,71,71,71	0
56	MG	YA	3522	1/1	0.90	0.29	65,65,65,65	0
56	MG	YA	3577	1/1	0.90	0.36	53,53,53,53	0
56	MG	YA	3250	1/1	0.90	0.14	45,45,45,45	0
56	MG	YA	3660	1/1	0.90	0.21	34,34,34,34	0
56	MG	YA	3483	1/1	0.90	0.27	26,26,26,26	0
56	MG	RA	3989	1/1	0.90	0.07	39,39,39,39	0
56	MG	XA	1780	1/1	0.90	0.34	40,40,40,40	0
56	MG	YA	3315	1/1	0.90	0.34	62,62,62,62	0
56	MG	RA	3666	1/1	0.90	0.23	69,69,69,69	0
56	MG	RA	3529	1/1	0.90	0.27	77,77,77,77	0
56	MG	YT	201	1/1	0.90	0.12	57,57,57,57	0
56	MG	RA	3531	1/1	0.90	0.10	34,34,34,34	0
56	MG	YA	3291	1/1	0.90	0.28	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3029	1/1	0.90	0.33	66,66,66,66	0
56	MG	RA	3140	1/1	0.90	0.24	93,93,93,93	0
56	MG	YA	3323	1/1	0.90	0.18	37,37,37,37	0
56	MG	RA	3264	1/1	0.90	0.34	63,63,63,63	0
56	MG	RA	3680	1/1	0.90	0.21	46,46,46,46	0
56	MG	RA	3681	1/1	0.90	0.14	119,119,119,119	0
56	MG	YA	3741	1/1	0.90	0.20	57,57,57,57	0
56	MG	RA	3148	1/1	0.90	0.17	66,66,66,66	0
56	MG	RA	3149	1/1	0.90	0.08	39,39,39,39	0
56	MG	RA	3686	1/1	0.90	0.28	62,62,62,62	0
56	MG	RA	3544	1/1	0.90	0.36	78,78,78,78	0
56	MG	R7	102	1/1	0.90	0.24	72,72,72,72	0
56	MG	YA	3593	1/1	0.90	0.23	28,28,28,28	0
56	MG	YA	3266	1/1	0.90	0.33	70,70,70,70	0
56	MG	RA	4017	1/1	0.90	0.28	90,90,90,90	0
56	MG	YA	3377	1/1	0.90	0.35	52,52,52,52	0
56	MG	YA	3189	1/1	0.90	0.24	96,96,96,96	0
56	MG	YA	3751	1/1	0.90	0.14	39,39,39,39	0
56	MG	YA	3209	1/1	0.91	0.21	48,48,48,48	0
56	MG	YA	3738	1/1	0.91	0.11	68,68,68,68	0
56	MG	YA	3548	1/1	0.91	0.27	32,32,32,32	0
56	MG	YA	3407	1/1	0.91	0.32	18,18,18,18	0
56	MG	RA	3500	1/1	0.91	0.28	25,25,25,25	0
56	MG	RA	3504	1/1	0.91	0.32	38,38,38,38	0
56	MG	XA	1676	1/1	0.91	0.25	42,42,42,42	0
56	MG	YA	3007	1/1	0.91	0.17	63,63,63,63	0
56	MG	YA	3512	1/1	0.91	0.28	62,62,62,62	0
56	MG	RA	3708	1/1	0.91	0.18	54,54,54,54	0
56	MG	RA	3125	1/1	0.91	0.14	36,36,36,36	0
56	MG	RA	3300	1/1	0.91	0.31	68,68,68,68	0
56	MG	YA	3061	1/1	0.91	0.25	57,57,57,57	0
56	MG	RA	3958	1/1	0.91	0.32	104,104,104,104	0
56	MG	YA	3556	1/1	0.91	0.17	41,41,41,41	0
56	MG	RA	3303	1/1	0.91	0.41	79,79,79,79	0
56	MG	RA	3716	1/1	0.91	0.12	52,52,52,52	0
56	MG	RA	3218	1/1	0.91	0.15	65,65,65,65	0
56	MG	RA	3609	1/1	0.91	0.12	71,71,71,71	0
56	MG	RA	3830	1/1	0.91	0.15	66,66,66,66	0
56	MG	XA	1737	1/1	0.91	0.23	47,47,47,47	0
56	MG	QA	1649	1/1	0.91	0.15	50,50,50,50	0
56	MG	RA	3613	1/1	0.91	0.19	35,35,35,35	0
56	MG	XA	1684	1/1	0.91	0.29	40,40,40,40	0

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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	0.91	0.15	56,56,56,56	0
56	MG	YA	3558	1/1	0.91	0.09	25,25,25,25	0
56	MG	RA	3424	1/1	0.91	0.24	80,80,80,80	0
56	MG	YA	3287	1/1	0.91	0.36	35,35,35,35	0
56	MG	XA	1745	1/1	0.91	0.25	44,44,44,44	0
56	MG	RA	3427	1/1	0.91	0.29	78,78,78,78	0
56	MG	RA	3843	1/1	0.91	0.20	72,72,72,72	0
56	MG	YA	3758	1/1	0.91	0.19	76,76,76,76	0
56	MG	RE	305	1/1	0.91	0.13	33,33,33,33	0
56	MG	YA	3416	1/1	0.91	0.44	39,39,39,39	0
56	MG	YA	3234	1/1	0.91	0.15	76,76,76,76	0
56	MG	YA	3235	1/1	0.91	0.24	91,91,91,91	0
56	MG	YB	204	1/1	0.91	0.14	99,99,99,99	0
56	MG	RA	3991	1/1	0.91	0.18	73,73,73,73	0
56	MG	RA	3235	1/1	0.91	0.19	70,70,70,70	0
56	MG	RA	3852	1/1	0.91	0.14	47,47,47,47	0
56	MG	RA	3856	1/1	0.91	0.19	33,33,33,33	0
56	MG	RA	3436	1/1	0.91	0.31	56,56,56,56	0
56	MG	YA	3521	1/1	0.91	0.27	95,95,95,95	0
56	MG	YA	3145	1/1	0.91	0.22	59,59,59,59	0
56	MG	YA	3451	1/1	0.91	0.28	64,64,64,64	0
56	MG	RA	3643	1/1	0.91	0.36	71,71,71,71	0
56	MG	YA	3062	1/1	0.91	0.12	57,57,57,57	0
56	MG	RA	3748	1/1	0.91	0.12	61,61,61,61	0
56	MG	YA	3113	1/1	0.91	0.18	104,104,104,104	0
56	MG	RA	3541	1/1	0.91	0.22	74,74,74,74	0
56	MG	YA	3114	1/1	0.91	0.22	90,90,90,90	0
56	MG	RA	3072	1/1	0.91	0.43	93,93,93,93	0
56	MG	YA	3575	1/1	0.91	0.25	30,30,30,30	0
56	MG	RA	3873	1/1	0.91	0.27	31,31,31,31	0
56	MG	RA	3159	1/1	0.91	0.29	107,107,107,107	0
56	MG	QA	1781	1/1	0.91	0.24	54,54,54,54	0
56	MG	YA	3297	1/1	0.91	0.25	19,19,19,19	0
56	MG	QA	1729	1/1	0.91	0.27	50,50,50,50	0
56	MG	RA	3080	1/1	0.91	0.22	81,81,81,81	0
56	MG	RQ	204	1/1	0.91	0.25	72,72,72,72	0
56	MG	YA	3381	1/1	0.91	0.17	11,11,11,11	0
56	MG	RA	3253	1/1	0.91	0.14	66,66,66,66	0
56	MG	RA	3889	1/1	0.91	0.26	48,48,48,48	0
56	MG	RA	3658	1/1	0.91	0.47	95,95,95,95	0
56	MG	RA	3082	1/1	0.91	0.33	62,62,62,62	0
56	MG	RA	3554	1/1	0.91	0.30	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1607	1/1	0.91	0.17	47,47,47,47	0
56	MG	RA	3084	1/1	0.91	0.23	79,79,79,79	0
56	MG	QA	1786	1/1	0.91	0.14	54,54,54,54	0
56	MG	XA	1707	1/1	0.91	0.25	58,58,58,58	0
56	MG	RA	3087	1/1	0.91	0.37	99,99,99,99	0
56	MG	YA	3425	1/1	0.91	0.15	49,49,49,49	0
56	MG	YA	3580	1/1	0.91	0.29	27,27,27,27	0
56	MG	QA	1617	1/1	0.91	0.11	61,61,61,61	0
56	MG	YA	3581	1/1	0.91	0.29	24,24,24,24	0
56	MG	YA	3029	1/1	0.91	0.37	57,57,57,57	0
56	MG	YA	3243	1/1	0.91	0.14	67,67,67,67	0
56	MG	RA	3470	1/1	0.91	0.23	34,34,34,34	0
56	MG	YA	3079	1/1	0.91	0.30	91,91,91,91	0
56	MG	RA	3098	1/1	0.91	0.07	12,12,12,12	0
56	MG	QA	1680	1/1	0.91	0.24	64,64,64,64	0
56	MG	YA	3226	1/1	0.91	0.35	75,75,75,75	0
56	MG	RA	3372	1/1	0.91	0.26	61,61,61,61	0
56	MG	RA	4057	1/1	0.91	0.23	77,77,77,77	0
56	MG	YA	3025	1/1	0.91	0.15	55,55,55,55	0
56	MG	QA	1625	1/1	0.91	0.17	61,61,61,61	0
56	MG	QA	1800	1/1	0.91	0.23	41,41,41,41	0
56	MG	YA	3010	1/1	0.91	0.14	41,41,41,41	0
56	MG	YA	3402	1/1	0.91	0.25	32,32,32,32	0
56	MG	YA	3119	1/1	0.91	0.27	78,78,78,78	0
56	MG	RA	3381	1/1	0.91	0.23	39,39,39,39	0
56	MG	YA	3027	1/1	0.91	0.19	45,45,45,45	0
56	MG	YA	3669	1/1	0.91	0.22	15,15,15,15	0
56	MG	YA	3252	1/1	0.91	0.32	70,70,70,70	0
56	MG	YA	3608	1/1	0.91	0.30	44,44,44,44	0
56	MG	YA	3554	1/1	0.92	0.21	44,44,44,44	0
56	MG	RA	3623	1/1	0.92	0.21	34,34,34,34	0
56	MG	RA	4050	1/1	0.92	0.30	59,59,59,59	0
56	MG	YA	3444	1/1	0.92	0.30	27,27,27,27	0
56	MG	RA	3626	1/1	0.92	0.10	68,68,68,68	0
56	MG	YA	3373	1/1	0.92	0.23	41,41,41,41	0
56	MG	YW	201	1/1	0.92	0.19	75,75,75,75	0
56	MG	YA	3121	1/1	0.92	0.27	47,47,47,47	0
56	MG	YA	3749	1/1	0.92	0.16	54,54,54,54	0
56	MG	RA	3632	1/1	0.92	0.26	55,55,55,55	0
56	MG	RA	3383	1/1	0.92	0.34	40,40,40,40	0
56	MG	YA	3376	1/1	0.92	0.22	58,58,58,58	0
56	MG	YA	3752	1/1	0.92	0.06	52,52,52,52	0

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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	0.92	0.19	84,84,84,84	0
56	MG	YA	3343	1/1	0.92	0.22	21,21,21,21	0
56	MG	YA	3280	1/1	0.92	0.24	14,14,14,14	0
56	MG	RA	3174	1/1	0.92	0.14	62,62,62,62	0
56	MG	RA	3392	1/1	0.92	0.22	28,28,28,28	0
56	MG	YA	3692	1/1	0.92	0.15	39,39,39,39	0
56	MG	RA	3915	1/1	0.92	0.20	41,41,41,41	0
56	MG	YA	3035	1/1	0.92	0.24	73,73,73,73	0
56	MG	YA	3630	1/1	0.92	0.20	32,32,32,32	0
56	MG	YA	3487	1/1	0.92	0.31	46,46,46,46	0
56	MG	YA	3633	1/1	0.92	0.32	47,47,47,47	0
56	MG	YA	3137	1/1	0.92	0.18	40,40,40,40	0
56	MG	YA	3489	1/1	0.92	0.24	15,15,15,15	0
56	MG	YA	3224	1/1	0.92	0.12	66,66,66,66	0
56	MG	RA	3408	1/1	0.92	0.23	24,24,24,24	0
56	MG	XA	1664	1/1	0.92	0.23	67,67,67,67	0
56	MG	YA	3386	1/1	0.92	0.26	23,23,23,23	0
56	MG	YA	3638	1/1	0.92	0.23	65,65,65,65	0
56	MG	RA	3288	1/1	0.92	0.24	95,95,95,95	0
56	MG	RA	3783	1/1	0.92	0.16	42,42,42,42	0
56	MG	YA	3387	1/1	0.92	0.28	37,37,37,37	0
56	MG	YA	3708	1/1	0.92	0.31	37,37,37,37	0
56	MG	XA	1614	1/1	0.92	0.17	60,60,60,60	0
56	MG	RA	3938	1/1	0.92	0.24	100,100,100,100	0
56	MG	RA	3787	1/1	0.92	0.48	105,105,105,105	0
56	MG	XA	1670	1/1	0.92	0.17	80,80,80,80	0
56	MG	YA	3458	1/1	0.92	0.30	46,46,46,46	0
56	MG	YA	3389	1/1	0.92	0.19	50,50,50,50	0
56	MG	QA	1755	1/1	0.92	0.21	69,69,69,69	0
56	MG	XA	1741	1/1	0.92	0.23	67,67,67,67	0
56	MG	RD	303	1/1	0.92	0.10	41,41,41,41	0
56	MG	XA	1742	1/1	0.92	0.25	52,52,52,52	0
56	MG	YA	3390	1/1	0.92	0.36	33,33,33,33	0
56	MG	YA	3289	1/1	0.92	0.25	38,38,38,38	0
56	MG	YA	3714	1/1	0.92	0.44	80,80,80,80	0
56	MG	RA	3202	1/1	0.92	0.21	92,92,92,92	0
56	MG	YA	3165	1/1	0.92	0.15	73,73,73,73	0
56	MG	XA	1678	1/1	0.92	0.18	81,81,81,81	0
56	MG	XA	1679	1/1	0.92	0.26	52,52,52,52	0
56	MG	YA	3268	1/1	0.92	0.28	73,73,73,73	0
56	MG	QA	1618	1/1	0.92	0.10	96,96,96,96	0
56	MG	YA	3080	1/1	0.92	0.37	80,80,80,80	0

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

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

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

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

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

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3675	1/1	0.94	0.20	29,29,29,29	0
56	MG	RA	3393	1/1	0.94	0.20	14,14,14,14	0
56	MG	RA	3508	1/1	0.94	0.18	42,42,42,42	0
56	MG	YA	3066	1/1	0.94	0.24	50,50,50,50	0
56	MG	RA	3615	1/1	0.94	0.27	34,34,34,34	0
56	MG	YA	3098	1/1	0.94	0.10	49,49,49,49	0
56	MG	RA	3618	1/1	0.94	0.25	48,48,48,48	0
56	MG	YA	3734	1/1	0.94	0.27	41,41,41,41	0
56	MG	RA	3116	1/1	0.94	0.21	104,104,104,104	0
56	MG	RA	3298	1/1	0.94	0.11	24,24,24,24	0
56	MG	YF	303	1/1	0.94	0.27	85,85,85,85	0
56	MG	QA	1671	1/1	0.94	0.10	64,64,64,64	0
56	MG	RA	3738	1/1	0.94	0.29	53,53,53,53	0
56	MG	YA	3356	1/1	0.94	0.38	50,50,50,50	0
56	MG	YA	3213	1/1	0.94	0.24	67,67,67,67	0
56	MG	YA	3023	1/1	0.94	0.09	16,16,16,16	0
56	MG	RA	3124	1/1	0.94	0.06	46,46,46,46	0
56	MG	RA	3743	1/1	0.94	0.14	35,35,35,35	0
56	MG	QA	1740	1/1	0.94	0.28	55,55,55,55	0
56	MG	RA	3213	1/1	0.94	0.22	105,105,105,105	0
56	MG	YA	3397	1/1	0.94	0.34	68,68,68,68	0
56	MG	RA	3309	1/1	0.94	0.11	63,63,63,63	0
56	MG	YA	3579	1/1	0.94	0.22	36,36,36,36	0
56	MG	YA	3326	1/1	0.94	0.27	27,27,27,27	0
56	MG	QA	1870	1/1	0.94	0.26	47,47,47,47	0
56	MG	RR	3201	1/1	0.94	0.28	62,62,62,62	0
56	MG	RA	3044	1/1	0.94	0.08	29,29,29,29	0
56	MG	YA	3743	1/1	0.94	0.29	43,43,43,43	0
56	MG	XA	1699	1/1	0.94	0.32	44,44,44,44	0
56	MG	YQ	201	1/1	0.94	0.13	33,33,33,33	0
56	MG	YA	3744	1/1	0.94	0.27	33,33,33,33	0
56	MG	RA	3534	1/1	0.94	0.11	44,44,44,44	0
56	MG	RA	3135	1/1	0.94	0.13	77,77,77,77	0
56	MG	YA	3328	1/1	0.94	0.20	15,15,15,15	0
56	MG	RA	3321	1/1	0.94	0.17	19,19,19,19	0
56	MG	YA	3365	1/1	0.94	0.23	48,48,48,48	0
56	MG	RA	4022	1/1	0.94	0.12	73,73,73,73	0
56	MG	RA	3539	1/1	0.94	0.31	39,39,39,39	0
56	MG	RA	3138	1/1	0.94	0.21	53,53,53,53	0
56	MG	YA	3583	1/1	0.94	0.23	29,29,29,29	0
56	MG	RA	3767	1/1	0.94	0.28	37,37,37,37	0
56	MG	RA	3899	1/1	0.94	0.16	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3900	1/1	0.94	0.16	30,30,30,30	0
56	MG	YA	3274	1/1	0.94	0.21	48,48,48,48	0
56	MG	QA	1879	1/1	0.94	0.26	78,78,78,78	0
56	MG	YA	3691	1/1	0.94	0.23	38,38,38,38	0
56	MG	YA	3543	1/1	0.94	0.22	36,36,36,36	0
56	MG	YA	3640	1/1	0.94	0.30	40,40,40,40	0
56	MG	YA	3299	1/1	0.94	0.25	10,10,10,10	0
56	MG	RA	3333	1/1	0.94	0.29	24,24,24,24	0
56	MG	YA	3753	1/1	0.94	0.18	54,54,54,54	0
56	MG	YA	3506	1/1	0.94	0.14	53,53,53,53	0
56	MG	RA	3913	1/1	0.94	0.27	43,43,43,43	0
56	MG	YA	3301	1/1	0.94	0.20	42,42,42,42	0
56	MG	RA	3238	1/1	0.94	0.25	106,106,106,106	0
56	MG	YA	3259	1/1	0.94	0.23	66,66,66,66	0
56	MG	YA	3333	1/1	0.94	0.24	26,26,26,26	0
56	MG	YA	3408	1/1	0.94	0.24	17,17,17,17	0
56	MG	RA	3668	1/1	0.94	0.24	49,49,49,49	0
56	MG	RA	3068	1/1	0.94	0.19	79,79,79,79	0
56	MG	RA	3069	1/1	0.94	0.10	55,55,55,55	0
56	MG	XA	1717	1/1	0.94	0.28	59,59,59,59	0
56	MG	YA	3760	1/1	0.94	0.18	85,85,85,85	0
56	MG	RA	3673	1/1	0.94	0.22	45,45,45,45	0
56	MG	RA	3792	1/1	0.94	0.21	35,35,35,35	0
56	MG	RA	3073	1/1	0.94	0.20	64,64,64,64	0
56	MG	RA	3622	1/1	0.95	0.19	20,20,20,20	0
56	MG	RA	3141	1/1	0.95	0.47	93,93,93,93	0
56	MG	RA	3255	1/1	0.95	0.22	100,100,100,100	0
56	MG	XA	1757	1/1	0.95	0.16	30,30,30,30	0
56	MG	RA	3627	1/1	0.95	0.26	76,76,76,76	0
56	MG	YA	3724	1/1	0.95	0.28	51,51,51,51	0
56	MG	YA	3014	1/1	0.95	0.07	39,39,39,39	0
56	MG	RA	3793	1/1	0.95	0.28	38,38,38,38	0
56	MG	YA	3571	1/1	0.95	0.21	23,23,23,23	0
56	MG	YA	3430	1/1	0.95	0.05	20,20,20,20	0
56	MG	YA	3144	1/1	0.95	0.22	57,57,57,57	0
56	MG	RA	3262	1/1	0.95	0.20	80,80,80,80	0
56	MG	RA	3893	1/1	0.95	0.28	34,34,34,34	0
56	MG	YA	3286	1/1	0.95	0.08	35,35,35,35	0
56	MG	RA	3799	1/1	0.95	0.16	54,54,54,54	0
56	MG	YA	3157	1/1	0.95	0.14	44,44,44,44	0
56	MG	RA	3999	1/1	0.95	0.13	21,21,21,21	0
56	MG	RA	3096	1/1	0.95	0.12	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3266	1/1	0.95	0.14	74,74,74,74	0
56	MG	RA	3803	1/1	0.95	0.11	64,64,64,64	0
56	MG	RA	3267	1/1	0.95	0.11	47,47,47,47	0
56	MG	RA	3718	1/1	0.95	0.18	62,62,62,62	0
56	MG	YA	3618	1/1	0.95	0.18	24,24,24,24	0
56	MG	RA	3269	1/1	0.95	0.11	74,74,74,74	0
56	MG	RA	3483	1/1	0.95	0.23	21,21,21,21	0
56	MG	YA	3237	1/1	0.95	0.20	69,69,69,69	0
56	MG	RA	4009	1/1	0.95	0.11	70,70,70,70	0
56	MG	YA	3518	1/1	0.95	0.22	16,16,16,16	0
56	MG	YA	3357	1/1	0.95	0.20	39,39,39,39	0
56	MG	RA	3813	1/1	0.95	0.23	23,23,23,23	0
56	MG	YB	216	1/1	0.95	0.26	45,45,45,45	0
56	MG	RA	3409	1/1	0.95	0.17	33,33,33,33	0
56	MG	YA	3736	1/1	0.95	0.10	39,39,39,39	0
56	MG	RF	307	1/1	0.95	0.26	65,65,65,65	0
56	MG	YA	3158	1/1	0.95	0.29	49,49,49,49	0
56	MG	YA	3076	1/1	0.95	0.19	4,4,4,4	0
56	MG	RA	3919	1/1	0.95	0.27	47,47,47,47	0
56	MG	YA	3440	1/1	0.95	0.14	29,29,29,29	0
56	MG	RA	3820	1/1	0.95	0.14	28,28,28,28	0
56	MG	YA	3702	1/1	0.95	0.13	30,30,30,30	0
56	MG	RA	3923	1/1	0.95	0.25	79,79,79,79	0
56	MG	XA	1730	1/1	0.95	0.14	47,47,47,47	0
56	MG	YA	3625	1/1	0.95	0.19	19,19,19,19	0
56	MG	RA	3417	1/1	0.95	0.11	42,42,42,42	0
56	MG	RA	3221	1/1	0.95	0.24	63,63,63,63	0
56	MG	RA	3928	1/1	0.95	0.30	59,59,59,59	0
56	MG	YA	3077	1/1	0.95	0.09	35,35,35,35	0
56	MG	YA	3705	1/1	0.95	0.17	32,32,32,32	0
56	MG	RA	3502	1/1	0.95	0.19	20,20,20,20	0
56	MG	RA	3503	1/1	0.95	0.16	21,21,21,21	0
56	MG	YA	3212	1/1	0.95	0.14	62,62,62,62	0
56	MG	RA	3353	1/1	0.95	0.21	35,35,35,35	0
56	MG	RA	3506	1/1	0.95	0.14	26,26,26,26	0
56	MG	RA	4039	1/1	0.95	0.16	73,73,73,73	0
56	MG	RA	3170	1/1	0.95	0.14	66,66,66,66	0
56	MG	YA	3054	1/1	0.95	0.14	27,27,27,27	0
56	MG	YA	3033	1/1	0.95	0.07	13,13,13,13	0
56	MG	YA	3587	1/1	0.95	0.14	31,31,31,31	0
56	MG	YA	3125	1/1	0.95	0.14	58,58,58,58	0
56	MG	RA	3359	1/1	0.95	0.12	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3513	1/1	0.95	0.07	14,14,14,14	0
56	MG	YE	306	1/1	0.95	0.21	13,13,13,13	0
56	MG	RA	3001	1/1	0.95	0.17	68,68,68,68	0
56	MG	QA	1719	1/1	0.95	0.28	32,32,32,32	0
56	MG	YA	3002	1/1	0.95	0.12	64,64,64,64	0
56	MG	YA	3342	1/1	0.95	0.17	20,20,20,20	0
56	MG	RA	3006	1/1	0.95	0.10	33,33,33,33	0
56	MG	RA	3848	1/1	0.95	0.30	50,50,50,50	0
56	MG	QA	1722	1/1	0.95	0.24	61,61,61,61	0
56	MG	YA	3319	1/1	0.95	0.21	20,20,20,20	0
56	MG	YA	3399	1/1	0.95	0.29	36,36,36,36	0
56	MG	YA	3371	1/1	0.95	0.21	14,14,14,14	0
56	MG	YA	3321	1/1	0.95	0.26	29,29,29,29	0
56	MG	YA	3088	1/1	0.95	0.07	42,42,42,42	0
56	MG	RA	3765	1/1	0.95	0.29	40,40,40,40	0
56	MG	YA	3009	1/1	0.95	0.13	37,37,37,37	0
56	MG	XF	201	1/1	0.95	0.11	39,39,39,39	0
56	MG	RA	3306	1/1	0.95	0.34	66,66,66,66	0
56	MG	RA	3016	1/1	0.95	0.34	77,77,77,77	0
56	MG	RA	3770	1/1	0.95	0.21	22,22,22,22	0
56	MG	RA	3771	1/1	0.95	0.08	45,45,45,45	0
56	MG	YA	3325	1/1	0.95	0.17	20,20,20,20	0
56	MG	YA	3759	1/1	0.95	0.38	64,64,64,64	0
56	MG	RA	3378	1/1	0.95	0.22	25,25,25,25	0
56	MG	YA	3602	1/1	0.95	0.22	16,16,16,16	0
56	MG	RA	3455	1/1	0.95	0.27	48,48,48,48	0
56	MG	YA	3205	1/1	0.95	0.21	58,58,58,58	0
56	MG	RA	3194	1/1	0.95	0.16	67,67,67,67	0
56	MG	RA	3870	1/1	0.95	0.23	24,24,24,24	0
56	MG	XA	1710	1/1	0.95	0.20	66,66,66,66	0
56	MG	YA	3604	1/1	0.95	0.23	11,11,11,11	0
56	MG	RA	3619	1/1	0.95	0.23	27,27,27,27	0
56	MG	RA	3874	1/1	0.95	0.24	25,25,25,25	0
56	MG	RA	3025	1/1	0.95	0.06	23,23,23,23	0
57	ZN	Y6	101	1/1	0.95	0.18	169,169,169,169	0
56	MG	YA	3569	1/1	0.95	0.29	32,32,32,32	0
56	MG	RA	3877	1/1	0.95	0.19	23,23,23,23	0
57	ZN	R6	101	1/1	0.95	0.15	160,160,160,160	0
56	MG	RA	3633	1/1	0.96	0.28	74,74,74,74	0
56	MG	RA	3778	1/1	0.96	0.28	41,41,41,41	0
56	MG	XA	1738	1/1	0.96	0.29	58,58,58,58	0
56	MG	YA	3011	1/1	0.96	0.15	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3435	1/1	0.96	0.31	23,23,23,23	0
56	MG	YA	3686	1/1	0.96	0.20	15,15,15,15	0
56	MG	YA	3352	1/1	0.96	0.26	11,11,11,11	0
56	MG	RA	3047	1/1	0.96	0.04	12,12,12,12	0
56	MG	YA	3647	1/1	0.96	0.20	27,27,27,27	0
56	MG	RA	3570	1/1	0.96	0.13	35,35,35,35	0
56	MG	RA	3049	1/1	0.96	0.13	48,48,48,48	0
56	MG	YA	3172	1/1	0.96	0.17	69,69,69,69	0
56	MG	YA	3615	1/1	0.96	0.24	11,11,11,11	0
56	MG	RA	4030	1/1	0.96	0.25	71,71,71,71	0
56	MG	RA	3324	1/1	0.96	0.18	14,14,14,14	0
56	MG	RA	3160	1/1	0.96	0.28	83,83,83,83	0
56	MG	RA	4033	1/1	0.96	0.18	17,17,17,17	0
56	MG	RA	3576	1/1	0.96	0.21	43,43,43,43	0
56	MG	YA	3096	1/1	0.96	0.14	26,26,26,26	0
56	MG	RA	4036	1/1	0.96	0.23	85,85,85,85	0
56	MG	RA	3720	1/1	0.96	0.08	33,33,33,33	0
56	MG	YA	3617	1/1	0.96	0.13	17,17,17,17	0
56	MG	RA	3004	1/1	0.96	0.06	29,29,29,29	0
56	MG	YA	3063	1/1	0.96	0.10	35,35,35,35	0
56	MG	QA	1706	1/1	0.96	0.24	35,35,35,35	0
56	MG	YA	3152	1/1	0.96	0.14	50,50,50,50	0
56	MG	YA	3022	1/1	0.96	0.16	62,62,62,62	0
56	MG	RA	3060	1/1	0.96	0.06	21,21,21,21	0
56	MG	YA	3696	1/1	0.96	0.21	17,17,17,17	0
56	MG	RA	3879	1/1	0.96	0.14	29,29,29,29	0
56	MG	YA	3015	1/1	0.96	0.17	23,23,23,23	0
56	MG	YA	3090	1/1	0.96	0.18	54,54,54,54	0
56	MG	YA	3296	1/1	0.96	0.35	32,32,32,32	0
56	MG	YA	3533	1/1	0.96	0.16	48,48,48,48	0
56	MG	YA	3560	1/1	0.96	0.07	6,6,6,6	0
56	MG	RA	3885	1/1	0.96	0.20	66,66,66,66	0
56	MG	RA	3119	1/1	0.96	0.12	74,74,74,74	0
56	MG	RA	3400	1/1	0.96	0.28	21,21,21,21	0
56	MG	YA	3132	1/1	0.96	0.21	86,86,86,86	0
56	MG	YA	3627	1/1	0.96	0.28	38,38,38,38	0
56	MG	RA	3465	1/1	0.96	0.20	27,27,27,27	0
56	MG	YA	3006	1/1	0.96	0.11	18,18,18,18	0
56	MG	RA	3467	1/1	0.96	0.20	21,21,21,21	0
56	MG	RA	3894	1/1	0.96	0.23	23,23,23,23	0
56	MG	RA	3895	1/1	0.96	0.20	54,54,54,54	0
56	MG	RA	3070	1/1	0.96	0.24	78,78,78,78	0

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3431	1/1	0.97	0.12	57,57,57,57	0
56	MG	RA	3676	1/1	0.97	0.13	86,86,86,86	0
56	MG	RA	3430	1/1	0.97	0.12	9,9,9,9	0
56	MG	YD	306	1/1	0.97	0.14	53,53,53,53	0
56	MG	YA	3337	1/1	0.97	0.17	35,35,35,35	0
56	MG	YA	3433	1/1	0.97	0.14	19,19,19,19	0
56	MG	YA	3374	1/1	0.97	0.27	34,34,34,34	0
56	MG	YA	3128	1/1	0.97	0.06	26,26,26,26	0
56	MG	YA	3452	1/1	0.97	0.09	46,46,46,46	0
56	MG	RA	3147	1/1	0.97	0.15	39,39,39,39	0
56	MG	YA	3320	1/1	0.97	0.20	26,26,26,26	0
56	MG	RA	3585	1/1	0.97	0.30	59,59,59,59	0
56	MG	YA	3141	1/1	0.97	0.21	23,23,23,23	0
56	MG	YA	3129	1/1	0.97	0.06	31,31,31,31	0
56	MG	RA	3395	1/1	0.97	0.06	22,22,22,22	0
56	MG	RA	3904	1/1	0.97	0.10	24,24,24,24	0
56	MG	RA	3443	1/1	0.97	0.29	20,20,20,20	0
56	MG	Y8	102	1/1	0.97	0.28	41,41,41,41	0
56	MG	RA	3964	1/1	0.97	0.08	44,44,44,44	0
56	MG	YA	3670	1/1	0.97	0.19	12,12,12,12	0
56	MG	RA	3041	1/1	0.97	0.05	44,44,44,44	0
56	MG	RA	3745	1/1	0.97	0.13	21,21,21,21	0
56	MG	YA	3527	1/1	0.97	0.27	50,50,50,50	0
56	MG	RA	3855	1/1	0.97	0.45	62,62,62,62	0
56	MG	RA	3273	1/1	0.97	0.23	76,76,76,76	0
56	MG	RA	3971	1/1	0.97	0.20	19,19,19,19	0
56	MG	QA	1631	1/1	0.97	0.03	34,34,34,34	0
56	MG	YA	3605	1/1	0.97	0.18	19,19,19,19	0
56	MG	YA	3697	1/1	0.97	0.36	38,38,38,38	0
56	MG	YA	3091	1/1	0.97	0.06	36,36,36,36	0
56	MG	QA	1695	1/1	0.97	0.31	48,48,48,48	0
56	MG	RA	3501	1/1	0.97	0.32	22,22,22,22	0
56	MG	YA	3282	1/1	0.97	0.18	10,10,10,10	0
56	MG	RA	3979	1/1	0.97	0.16	37,37,37,37	0
56	MG	RA	3808	1/1	0.97	0.16	56,56,56,56	0
56	MG	RA	3014	1/1	0.97	0.12	38,38,38,38	0
56	MG	QA	1790	1/1	0.97	0.33	56,56,56,56	0
56	MG	YA	3290	1/1	0.97	0.24	47,47,47,47	0
56	MG	RA	4044	1/1	0.97	0.18	95,95,95,95	0
56	MG	RA	3655	1/1	0.97	0.16	25,25,25,25	0
56	MG	XA	1635	1/1	0.97	0.14	29,29,29,29	0
56	MG	YA	3106	1/1	0.97	0.06	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3385	1/1	0.97	0.20	23,23,23,23	0
56	MG	RA	3168	1/1	0.97	0.10	71,71,71,71	0
56	MG	RA	3020	1/1	0.97	0.27	89,89,89,89	0
56	MG	RA	3092	1/1	0.97	0.15	79,79,79,79	0
56	MG	RA	3056	1/1	0.97	0.14	70,70,70,70	0
56	MG	XA	1694	1/1	0.97	0.26	30,30,30,30	0
56	MG	YA	3358	1/1	0.97	0.28	18,18,18,18	0
56	MG	RA	3420	1/1	0.97	0.07	19,19,19,19	0
56	MG	YA	3284	1/1	0.97	0.14	8,8,8,8	0
56	MG	YA	3728	1/1	0.97	0.12	8,8,8,8	0
56	MG	YB	219	1/1	0.97	0.23	31,31,31,31	0
56	MG	RA	3337	1/1	0.97	0.26	81,81,81,81	0
56	MG	RA	4060	1/1	0.97	0.20	82,82,82,82	0
58	SF4	XD	301	8/8	0.97	0.06	58,74,100,102	0
56	MG	RA	3323	1/1	0.98	0.07	38,38,38,38	0
56	MG	YA	3143	1/1	0.98	0.10	56,56,56,56	0
56	MG	YA	3542	1/1	0.98	0.17	21,21,21,21	0
56	MG	YA	3016	1/1	0.98	0.06	29,29,29,29	0
56	MG	YA	3151	1/1	0.98	0.03	8,8,8,8	0
56	MG	RA	4028	1/1	0.98	0.11	78,78,78,78	0
56	MG	YA	3041	1/1	0.98	0.05	35,35,35,35	0
56	MG	RA	3123	1/1	0.98	0.12	30,30,30,30	0
56	MG	RE	303	1/1	0.98	0.11	15,15,15,15	0
56	MG	YA	3503	1/1	0.98	0.10	18,18,18,18	0
56	MG	RB	205	1/1	0.98	0.07	47,47,47,47	0
56	MG	YA	3353	1/1	0.98	0.12	14,14,14,14	0
56	MG	RA	3597	1/1	0.98	0.12	19,19,19,19	0
56	MG	YB	210	1/1	0.98	0.36	57,57,57,57	0
56	MG	YA	3195	1/1	0.98	0.07	33,33,33,33	0
56	MG	YA	3685	1/1	0.98	0.24	19,19,19,19	0
56	MG	YA	3317	1/1	0.98	0.07	24,24,24,24	0
56	MG	YA	3595	1/1	0.98	0.27	12,12,12,12	0
56	MG	YA	3480	1/1	0.98	0.21	17,17,17,17	0
56	MG	RA	3888	1/1	0.98	0.28	24,24,24,24	0
56	MG	YA	3008	1/1	0.98	0.11	47,47,47,47	0
56	MG	YA	3013	1/1	0.98	0.06	23,23,23,23	0
56	MG	YA	3651	1/1	0.98	0.32	15,15,15,15	0
56	MG	YA	3652	1/1	0.98	0.29	24,24,24,24	0
56	MG	YA	3112	1/1	0.98	0.10	9,9,9,9	0
56	MG	YA	3673	1/1	0.98	0.15	13,13,13,13	0
56	MG	YA	3382	1/1	0.98	0.19	29,29,29,29	0
56	MG	YD	304	1/1	0.98	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3601	1/1	0.98	0.30	29,29,29,29	0
56	MG	YA	3739	1/1	0.98	0.35	79,79,79,79	0
56	MG	RA	3579	1/1	0.98	0.15	24,24,24,24	0
56	MG	RA	3348	1/1	0.98	0.14	34,34,34,34	0
56	MG	XA	1746	1/1	0.98	0.30	35,35,35,35	0
56	MG	RA	3318	1/1	0.98	0.16	19,19,19,19	0
56	MG	YA	3460	1/1	0.98	0.10	28,28,28,28	0
56	MG	YD	308	1/1	0.98	0.10	71,71,71,71	0
56	MG	QA	1628	1/1	0.98	0.26	49,49,49,49	0
56	MG	YD	309	1/1	0.98	0.10	14,14,14,14	0
57	ZN	Y9	101	1/1	0.98	0.07	107,107,107,107	0
56	MG	RA	3833	1/1	0.98	0.20	29,29,29,29	0
56	MG	RA	3419	1/1	0.98	0.24	17,17,17,17	0
56	MG	RD	306	1/1	0.98	0.07	33,33,33,33	0
56	MG	RA	3946	1/1	0.98	0.04	18,18,18,18	0
58	SF4	QD	302	8/8	0.98	0.07	51,57,76,106	0
56	MG	YA	3612	1/1	0.99	0.09	23,23,23,23	0
56	MG	RA	3838	1/1	0.99	0.27	17,17,17,17	0
56	MG	RA	3516	1/1	0.99	0.23	13,13,13,13	0
56	MG	YA	3306	1/1	0.99	0.12	9,9,9,9	0
57	ZN	Y5	102	1/1	0.99	0.06	119,119,119,119	0
56	MG	YA	3362	1/1	0.99	0.25	18,18,18,18	0
56	MG	YA	3363	1/1	0.99	0.29	11,11,11,11	0
57	ZN	XN	101	1/1	0.99	0.02	94,94,94,94	0
57	ZN	QN	101	1/1	0.99	0.03	105,105,105,105	0
56	MG	YA	3380	1/1	0.99	0.14	7,7,7,7	0
56	MG	RA	3773	1/1	0.99	0.18	25,25,25,25	0
57	ZN	R5	102	1/1	0.99	0.03	119,119,119,119	0
56	MG	RA	3153	1/1	0.99	0.04	35,35,35,35	0
57	ZN	R9	102	1/1	0.99	0.07	92,92,92,92	0
56	MG	YA	3346	1/1	0.99	0.30	16,16,16,16	0
56	MG	RA	3442	1/1	0.99	0.26	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.