



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 25, 2026 – 02:31 PM UTC

PDB ID : 5J3C / pdb_00005j3c
Title : Thermus thermophilus 70S termination complex containing E. coli RF1
Authors : Hoffer, E.D.; Dunham, C.M.
Deposited on : 2016-03-30
Resolution : 3.04 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

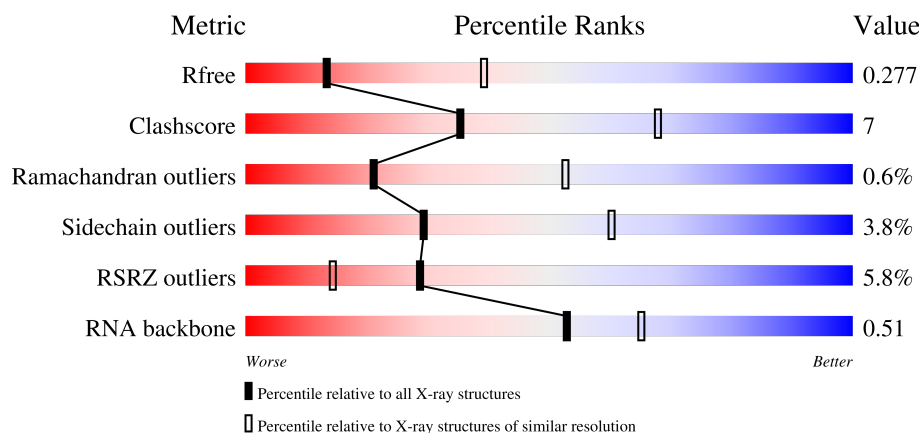
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)
RNA backbone	3983	1163 (3.28-2.80)

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

Mol	Chain	Length	Quality of chain
1	RA	2915	2% 61% 31% 7%
1	YA	2915	3% 62% 30% 6%
2	RB	122	2% 77% 18%
2	YB	122	% 77% 19%

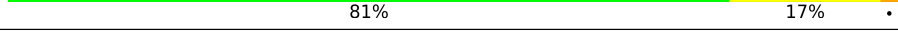
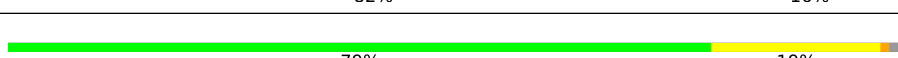
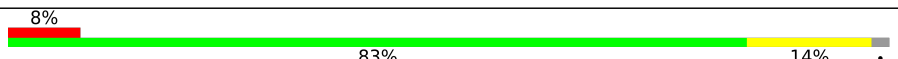
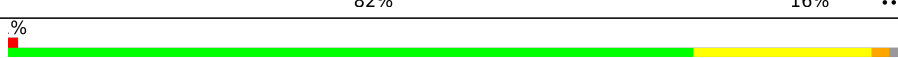
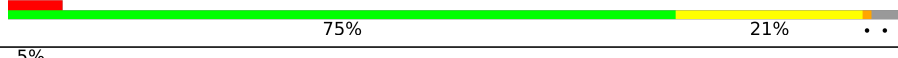
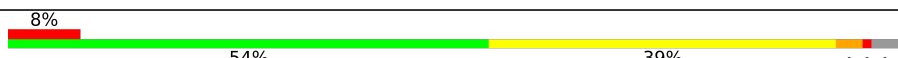
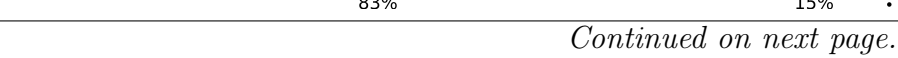
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Mol	Chain	Length	Quality of chain
3	RD	276	81% 17% .
3	YD	276	81% 16% .
4	RE	206	2% 76% 21% ..
4	YE	206	74% 22% ..
5	RF	210	72% 21% . .
5	YF	210	69% 26% . .
6	RG	182	9% 74% 25% ..
6	YG	182	3% 69% 28% ..
7	RH	180	16% 79% 17% ..
7	YH	180	5% 67% 28% . .
8	RI	148	16% 80% 18% ..
8	YI	148	3% 80% 17% ..
9	RN	140	4% 82% 16% .
9	YN	140	84% 15% .
10	RO	122	75% 24% .
10	YO	122	80% 19% .
11	RP	150	76% 21% ..
11	YP	150	75% 21% ..
12	RQ	141	81% 17% .
12	YQ	141	3% 77% 21% .
13	RR	118	72% 23% 5%
13	YR	118	79% 20% .
14	RS	112	6% 81% 14% ..
14	YS	112	4% 81% 17% .
15	RT	146	2% 65% 23% . 10%

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

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

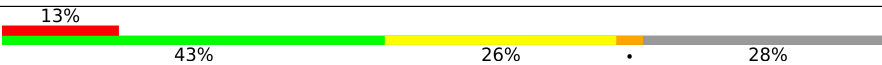
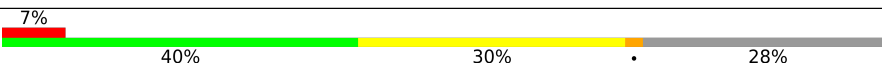
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Mol	Chain	Length	Quality of chain
40	XI	128	
41	QJ	105	
41	XJ	105	
42	QK	129	
42	XK	129	
43	QL	132	
43	XL	132	
44	QM	126	
44	XM	126	
45	QN	61	
45	XN	61	
46	QO	89	
46	XO	89	
47	QP	88	
47	XP	88	
48	QQ	105	
48	XQ	105	
49	QR	88	
49	XR	88	
50	QS	93	
50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

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Mol	Chain	Length	Quality of chain
53	QV	77	
53	XV	77	
54	QX	25	
54	XX	25	
55	QY	360	
55	XY	360	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	QA	1711	-	-	-	X
56	MG	QA	1755	-	-	-	X
56	MG	QA	1828	-	-	-	X
56	MG	QA	1855	-	-	-	X
56	MG	R1	103	-	-	-	X
56	MG	R3	102	-	-	-	X
56	MG	RA	3026	-	-	-	X
56	MG	RA	3049	-	-	-	X
56	MG	RA	3051	-	-	-	X
56	MG	RA	3057	-	-	-	X
56	MG	RA	3064	-	-	-	X
56	MG	RA	3067	-	-	-	X
56	MG	RA	3080	-	-	-	X
56	MG	RA	3082	-	-	-	X
56	MG	RA	3083	-	-	-	X
56	MG	RA	3087	-	-	-	X
56	MG	RA	3100	-	-	-	X
56	MG	RA	3106	-	-	-	X
56	MG	RA	3116	-	-	-	X
56	MG	RA	3163	-	-	-	X
56	MG	RA	3176	-	-	-	X
56	MG	RA	3184	-	-	-	X
56	MG	RA	3189	-	-	-	X
56	MG	RA	3192	-	-	-	X
56	MG	RA	3207	-	-	-	X
56	MG	RA	3226	-	-	-	X
56	MG	RA	3232	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3244	-	-	-	X
56	MG	RA	3247	-	-	-	X
56	MG	RA	3249	-	-	-	X
56	MG	RA	3251	-	-	-	X
56	MG	RA	3257	-	-	-	X
56	MG	RA	3289	-	-	-	X
56	MG	RA	3295	-	-	-	X
56	MG	RA	3355	-	-	-	X
56	MG	RA	3430	-	-	-	X
56	MG	RA	3462	-	-	-	X
56	MG	RA	3514	-	-	-	X
56	MG	RA	3516	-	-	-	X
56	MG	RA	3525	-	-	-	X
56	MG	RA	3535	-	-	-	X
56	MG	RA	3559	-	-	-	X
56	MG	RA	3580	-	-	-	X
56	MG	RA	3587	-	-	-	X
56	MG	RA	3597	-	-	-	X
56	MG	RA	3616	-	-	-	X
56	MG	RA	3618	-	-	-	X
56	MG	RA	3633	-	-	-	X
56	MG	RA	3637	-	-	-	X
56	MG	RA	3676	-	-	-	X
56	MG	RA	3677	-	-	-	X
56	MG	RA	3682	-	-	-	X
56	MG	RA	3690	-	-	-	X
56	MG	RA	3757	-	-	-	X
56	MG	RA	3793	-	-	-	X
56	MG	RA	3820	-	-	-	X
56	MG	RA	3821	-	-	-	X
56	MG	RA	3829	-	-	-	X
56	MG	RA	3861	-	-	-	X
56	MG	RA	3875	-	-	-	X
56	MG	RA	3916	-	-	-	X
56	MG	RA	3966	-	-	-	X
56	MG	RA	3977	-	-	-	X
56	MG	RA	3998	-	-	-	X
56	MG	RA	4018	-	-	-	X
56	MG	RA	4024	-	-	-	X
56	MG	RA	4026	-	-	-	X
56	MG	RA	4029	-	-	-	X
56	MG	RD	307	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RF	303	-	-	-	X
56	MG	RW	202	-	-	-	X
56	MG	XA	1601	-	-	-	X
56	MG	XA	1675	-	-	-	X
56	MG	XA	1694	-	-	-	X
56	MG	XA	1704	-	-	-	X
56	MG	XA	1713	-	-	-	X
56	MG	XA	1749	-	-	-	X
56	MG	XY	401	-	-	-	X
56	MG	YA	3016	-	-	-	X
56	MG	YA	3018	-	-	-	X
56	MG	YA	3068	-	-	-	X
56	MG	YA	3080	-	-	-	X
56	MG	YA	3100	-	-	-	X
56	MG	YA	3104	-	-	-	X
56	MG	YA	3128	-	-	-	X
56	MG	YA	3151	-	-	-	X
56	MG	YA	3166	-	-	-	X
56	MG	YA	3183	-	-	-	X
56	MG	YA	3240	-	-	-	X
56	MG	YA	3241	-	-	-	X
56	MG	YA	3249	-	-	-	X
56	MG	YA	3252	-	-	-	X
56	MG	YA	3421	-	-	-	X
56	MG	YA	3455	-	-	-	X
56	MG	YA	3456	-	-	-	X
56	MG	YA	3473	-	-	-	X
56	MG	YA	3500	-	-	-	X
56	MG	YA	3509	-	-	-	X
56	MG	YA	3517	-	-	-	X
56	MG	YA	3626	-	-	-	X
56	MG	YA	3661	-	-	-	X
56	MG	YA	3709	-	-	-	X
56	MG	YA	3717	-	-	-	X
56	MG	YA	3720	-	-	-	X
56	MG	YA	3727	-	-	-	X
56	MG	YA	3747	-	-	-	X
57	ZN	R9	102	-	-	-	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 294929 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	QV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
53	XV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 54 is a RNA chain called messenger RNA.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	QY	259	Total	C	N	O	S	0	0	0
			2014	1235	382	389	8			
55	XY	260	Total	C	N	O	S	0	0	0
			2022	1241	383	390	8			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	RA	1032	Total	Mg	0	0
			1032	1032		
56	RB	22	Total	Mg	0	0
			22	22		
56	RD	15	Total	Mg	0	0
			15	15		
56	RE	7	Total	Mg	0	0
			7	7		
56	RF	11	Total	Mg	0	0
			11	11		
56	RG	4	Total	Mg	0	0
			4	4		
56	RN	2	Total	Mg	0	0
			2	2		
56	RO	1	Total	Mg	0	0
			1	1		
56	RP	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	RQ	5	Total 5	Mg 5	0	0
56	RR	4	Total 4	Mg 4	0	0
56	RS	1	Total 1	Mg 1	0	0
56	RT	3	Total 3	Mg 3	0	0
56	RU	3	Total 3	Mg 3	0	0
56	RV	3	Total 3	Mg 3	0	0
56	RW	2	Total 2	Mg 2	0	0
56	RX	1	Total 1	Mg 1	0	0
56	RY	1	Total 1	Mg 1	0	0
56	R0	7	Total 7	Mg 7	0	0
56	R1	5	Total 5	Mg 5	0	0
56	R3	2	Total 2	Mg 2	0	0
56	R5	1	Total 1	Mg 1	0	0
56	R7	3	Total 3	Mg 3	0	0
56	R9	1	Total 1	Mg 1	0	0
56	QA	262	Total 262	Mg 262	0	0
56	QB	1	Total 1	Mg 1	0	0
56	QD	2	Total 2	Mg 2	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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QH	1	Total 1	Mg 1	0	0
56	QI	1	Total 1	Mg 1	0	0
56	QJ	1	Total 1	Mg 1	0	0
56	QL	2	Total 2	Mg 2	0	0
56	QN	1	Total 1	Mg 1	0	0
56	QO	1	Total 1	Mg 1	0	0
56	QQ	1	Total 1	Mg 1	0	0
56	QR	1	Total 1	Mg 1	0	0
56	QT	1	Total 1	Mg 1	0	0
56	QV	6	Total 6	Mg 6	0	0
56	YA	749	Total 749	Mg 749	0	0
56	YB	20	Total 20	Mg 20	0	0
56	YD	9	Total 9	Mg 9	0	0
56	YE	6	Total 6	Mg 6	0	0
56	YF	2	Total 2	Mg 2	0	0
56	YG	2	Total 2	Mg 2	0	0
56	YI	1	Total 1	Mg 1	0	0
56	YN	1	Total 1	Mg 1	0	0
56	YO	1	Total 1	Mg 1	0	0
56	YP	1	Total 1	Mg 1	0	0
56	YQ	3	Total 3	Mg 3	0	0

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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	2	Total 2	Mg 2	0	0
56	Y7	1	Total 1	Mg 1	0	0
56	Y8	2	Total 2	Mg 2	0	0
56	XA	187	Total 187	Mg 187	0	0
56	XE	2	Total 2	Mg 2	0	0
56	XF	4	Total 4	Mg 4	0	0
56	XJ	1	Total 1	Mg 1	0	0
56	XL	1	Total 1	Mg 1	0	0
56	XT	1	Total 1	Mg 1	0	0
56	XV	4	Total 4	Mg 4	0	0
56	XY	1	Total 1	Mg 1	0	0

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

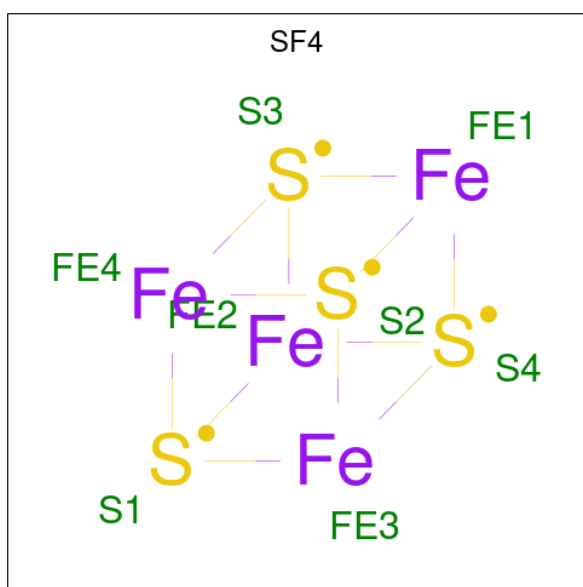
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	RY	1	Total 1	Zn 1	0	0

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

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

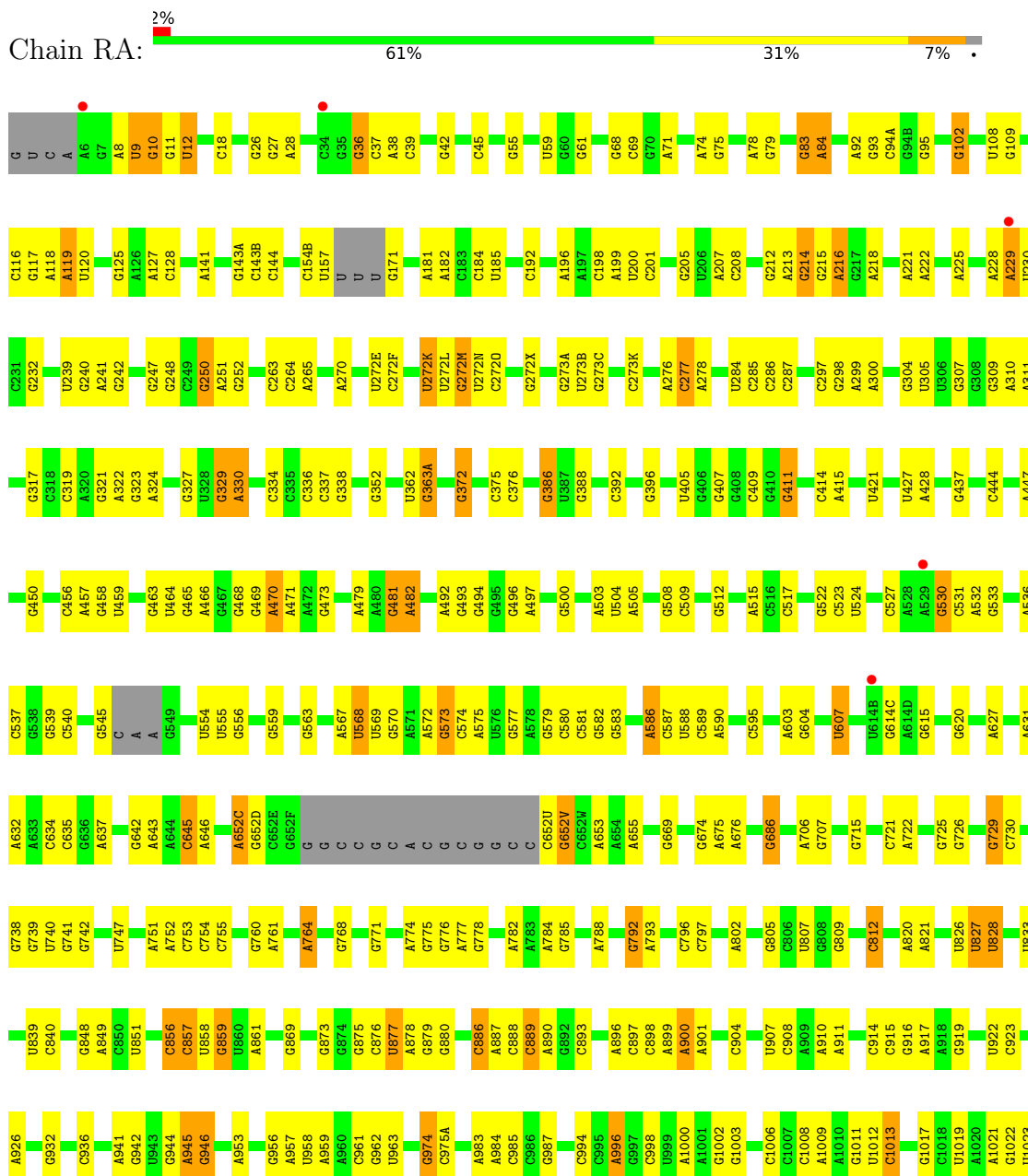


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	QD	1	Total 8	Fe 4	S 4	0	0
58	XD	1	Total 8	Fe 4	S 4	0	0

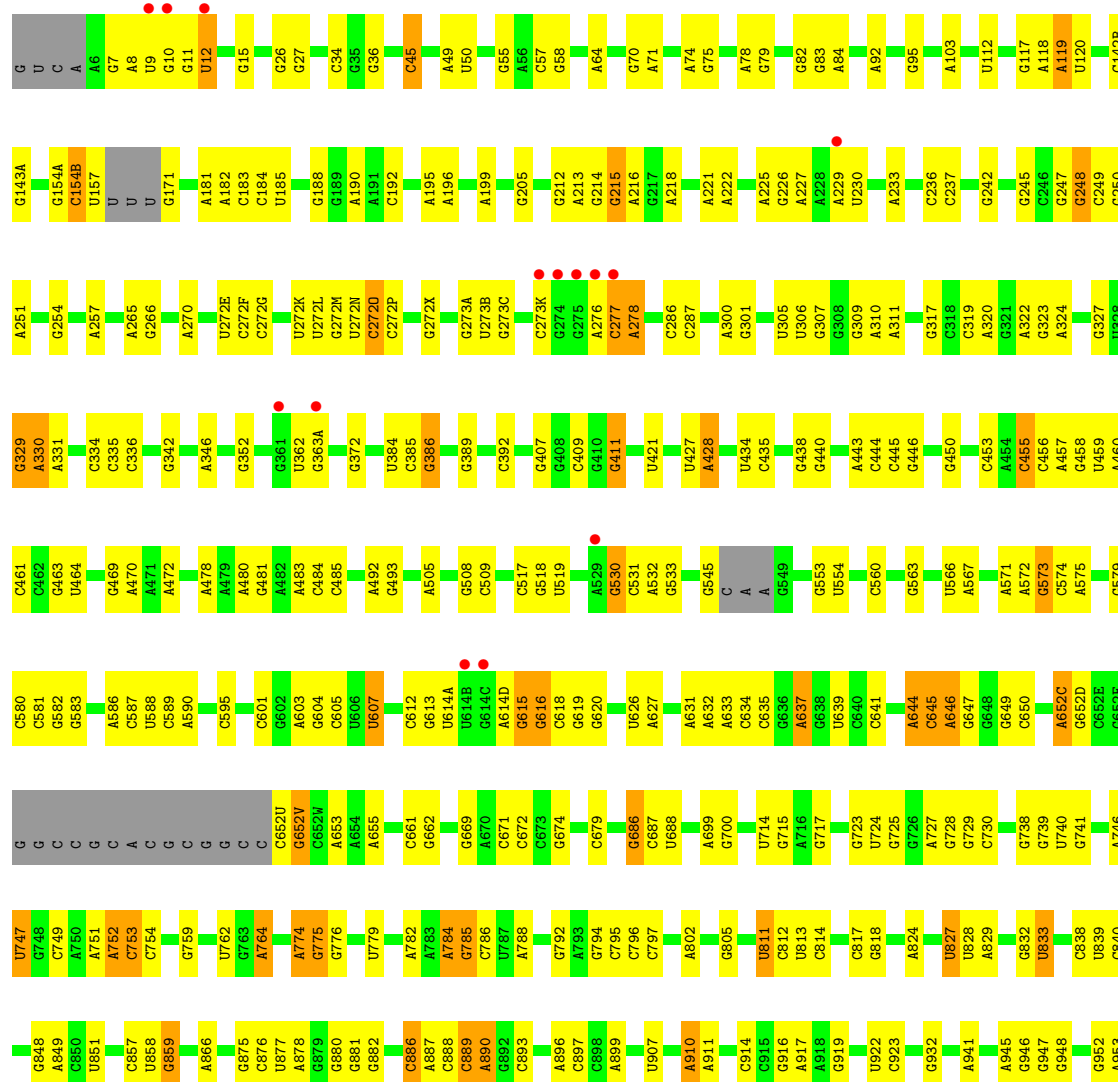
3 Residue-property plots

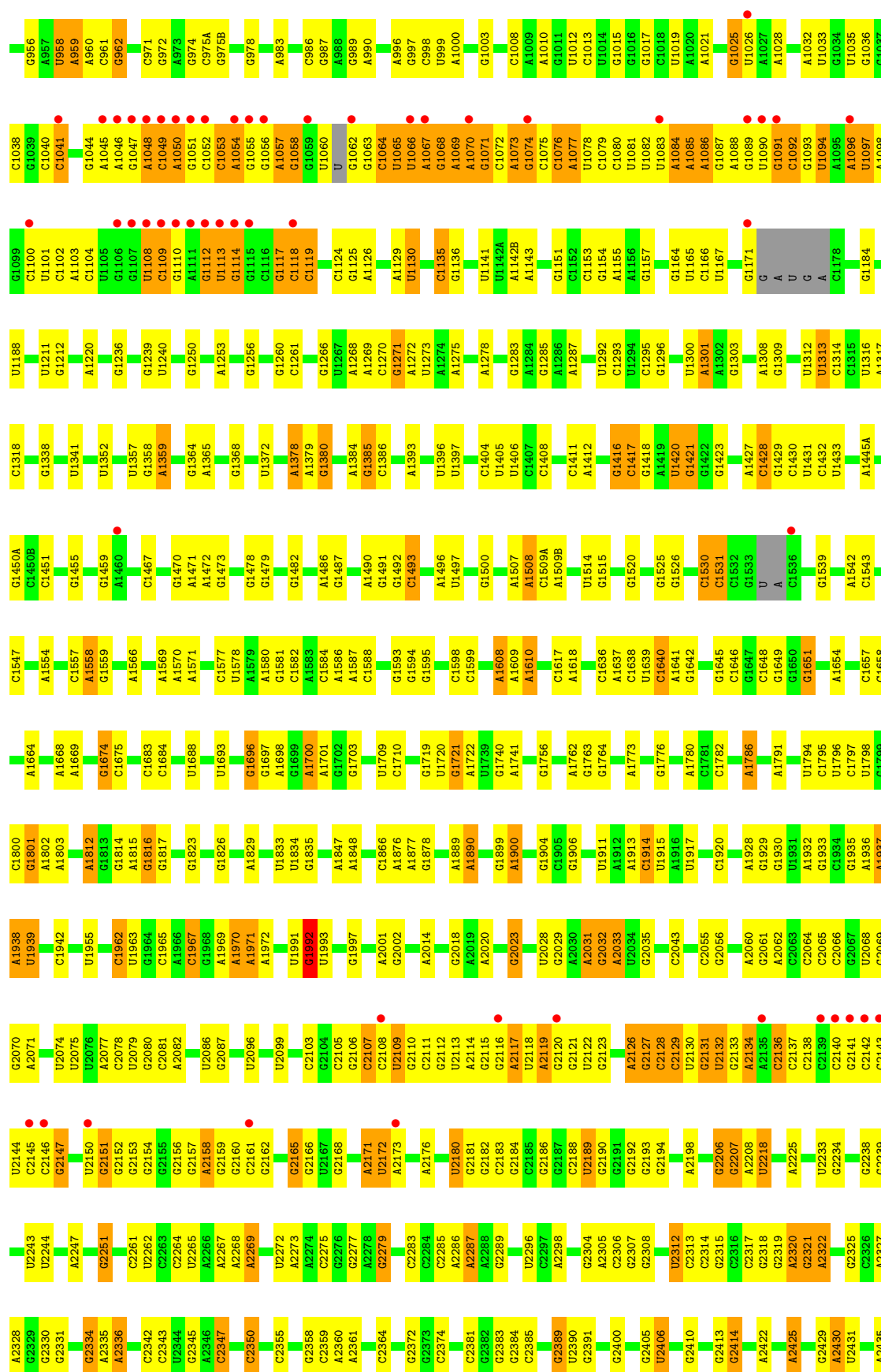
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

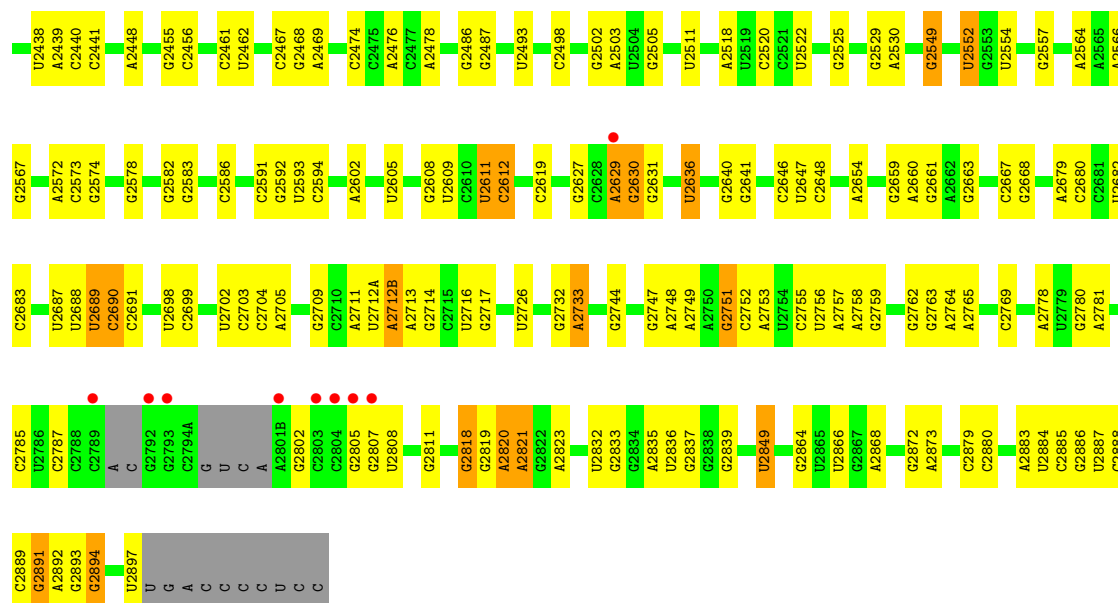
• Molecule 1: 23S rRNA



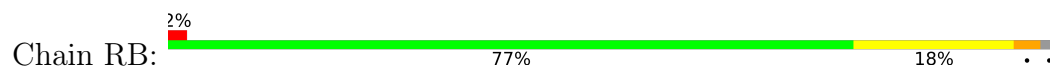




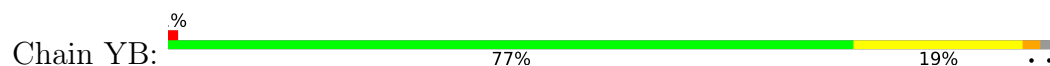




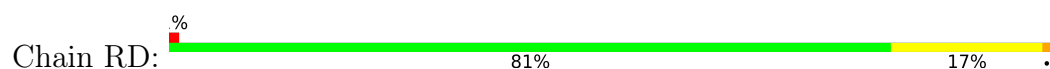
- Molecule 2: 5S rRNA



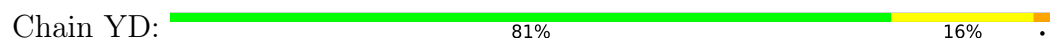
- Molecule 2: 5S rRNA



- Molecule 3: 50S ribosomal protein L2

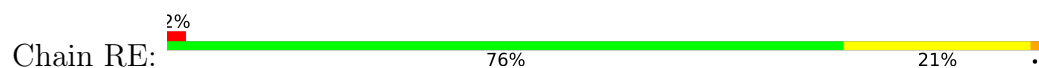


- Molecule 3: 50S ribosomal protein L2

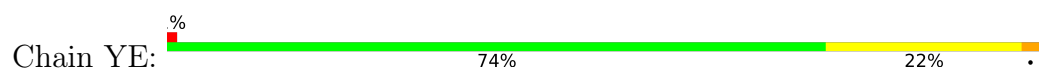




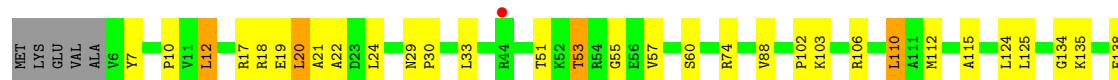
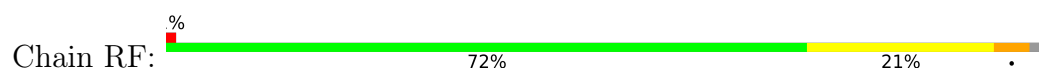
- Molecule 4: 50S ribosomal protein L3



- Molecule 4: 50S ribosomal protein L3



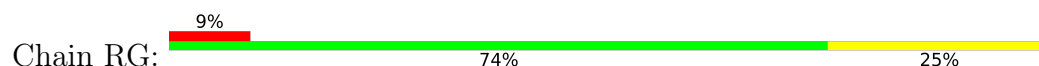
- Molecule 5: 50S ribosomal protein L4

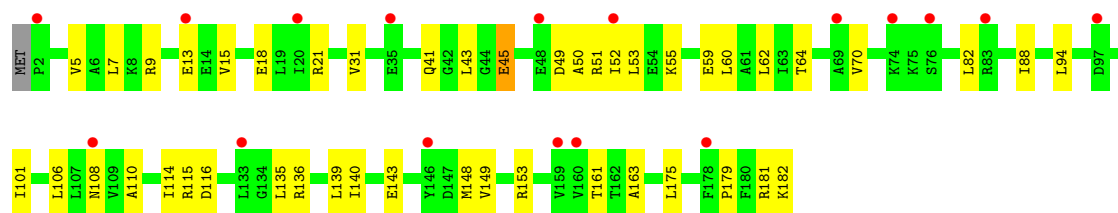


- Molecule 5: 50S ribosomal protein L4

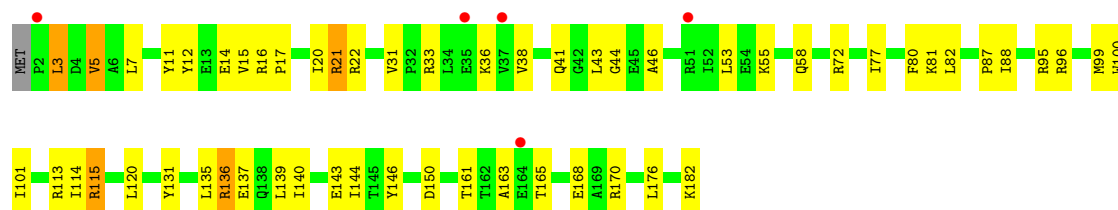


- Molecule 6: 50S ribosomal protein L5

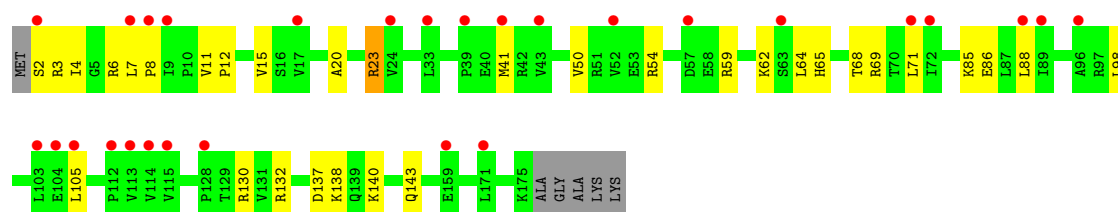
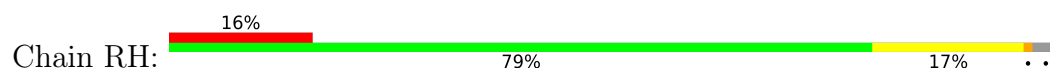




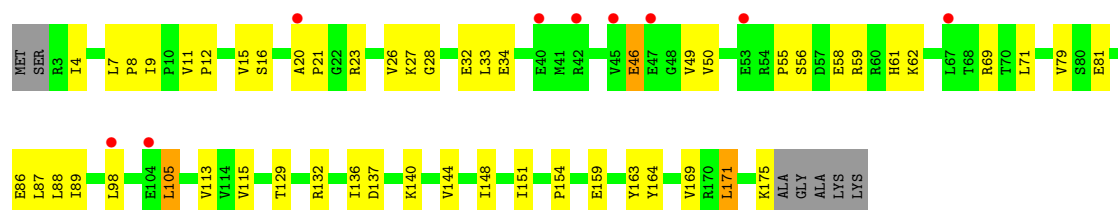
• Molecule 6: 50S ribosomal protein L5



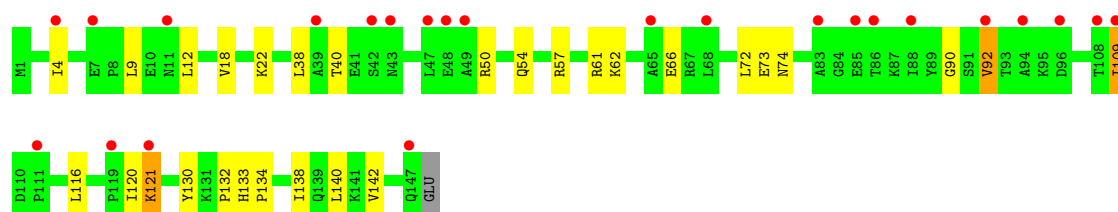
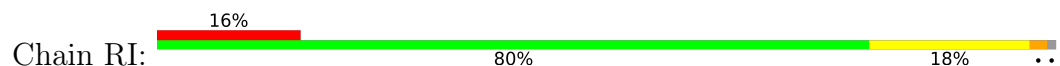
• Molecule 7: 50S ribosomal protein L6



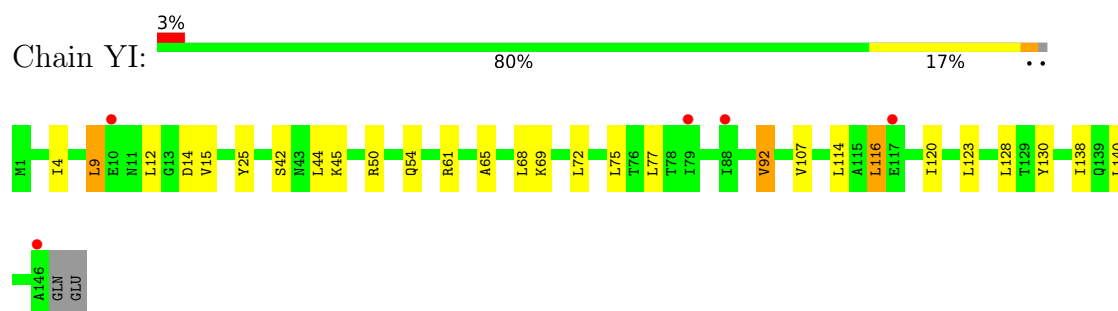
• Molecule 7: 50S ribosomal protein L6



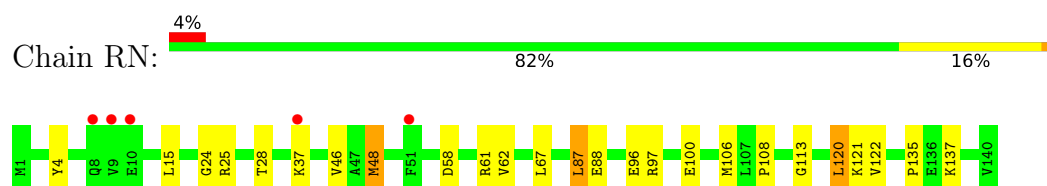
• Molecule 8: 50S ribosomal protein L9



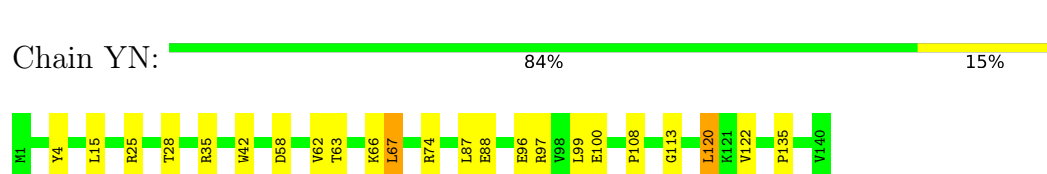
- Molecule 8: 50S ribosomal protein L9



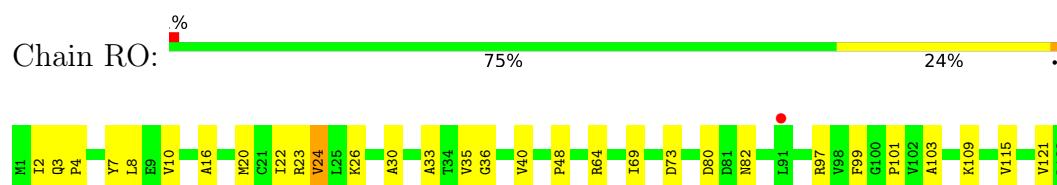
- Molecule 9: 50S ribosomal protein L13



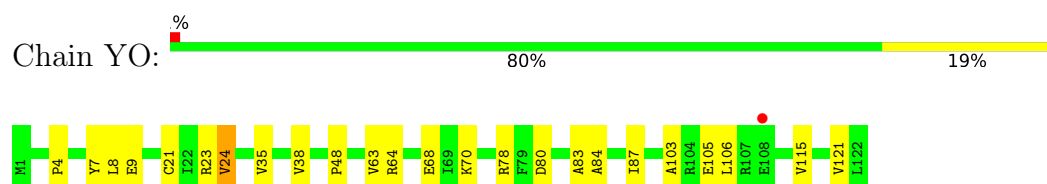
- Molecule 9: 50S ribosomal protein L13



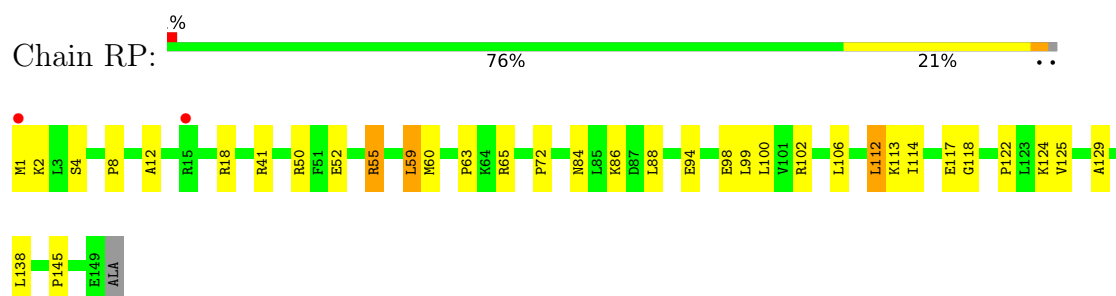
- Molecule 10: 50S ribosomal protein L14



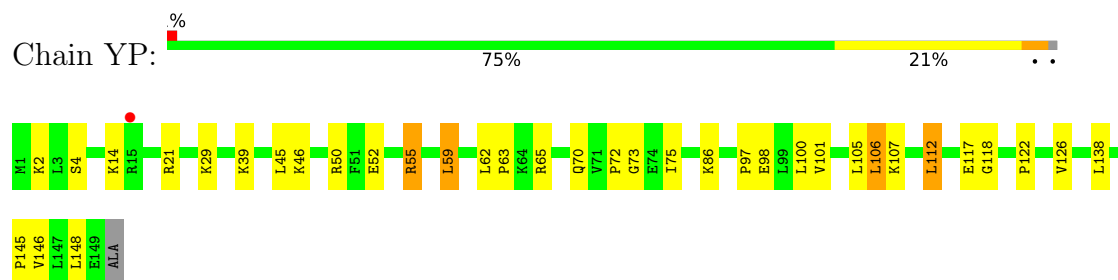
- Molecule 10: 50S ribosomal protein L14



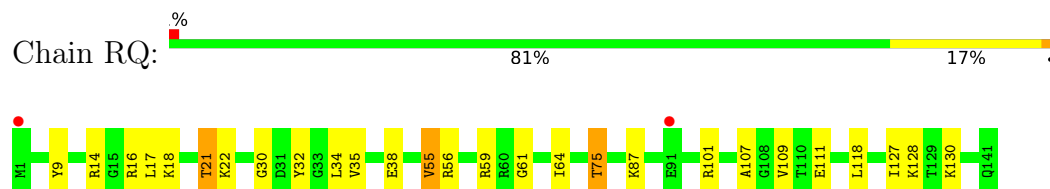
- Molecule 11: 50S ribosomal protein L15



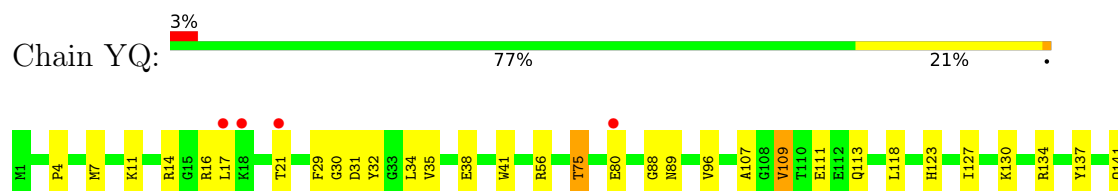
- Molecule 11: 50S ribosomal protein L15



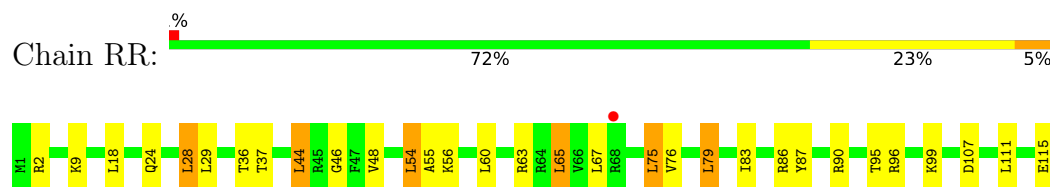
- Molecule 12: 50S ribosomal protein L16



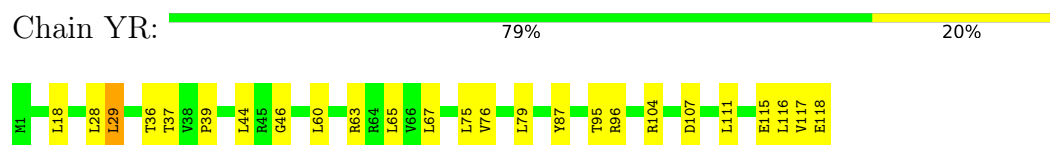
- Molecule 12: 50S ribosomal protein L16



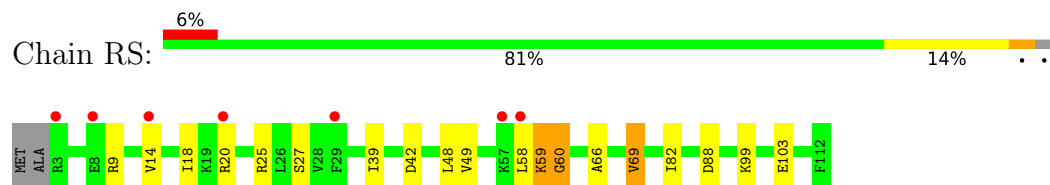
- Molecule 13: 50S ribosomal protein L17



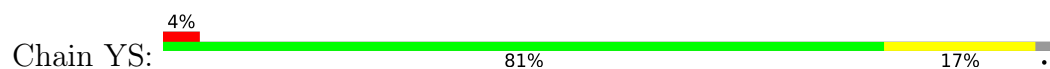
- Molecule 13: 50S ribosomal protein L17

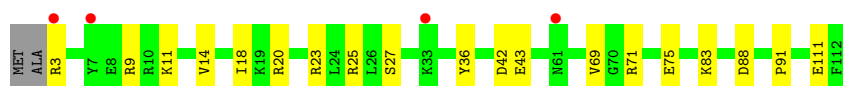


- Molecule 14: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L18

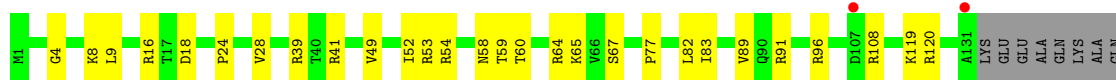
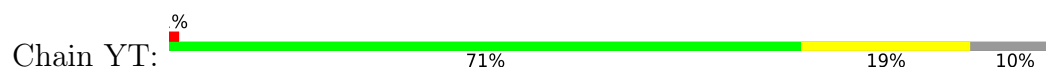




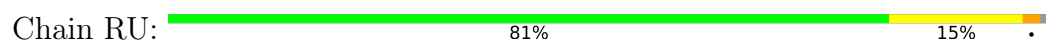
- Molecule 15: 50S ribosomal protein L19



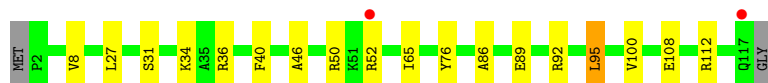
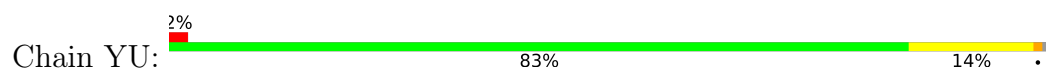
- Molecule 15: 50S ribosomal protein L19



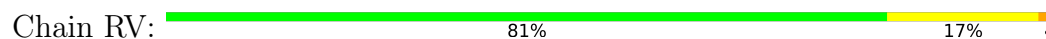
- Molecule 16: 50S ribosomal protein L20



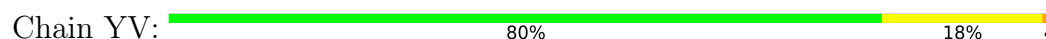
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21

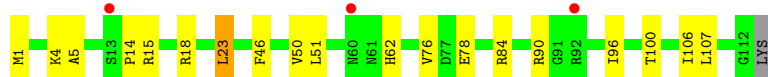
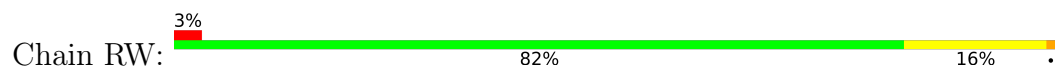


- Molecule 17: 50S ribosomal protein L21

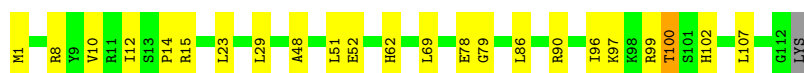
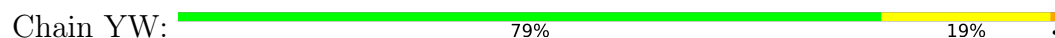




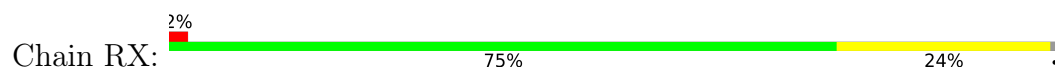
- Molecule 18: 50S ribosomal protein L22



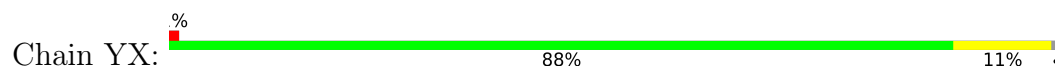
- Molecule 18: 50S ribosomal protein L22



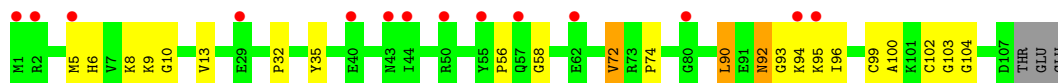
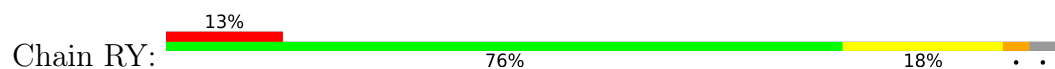
- Molecule 19: 50S ribosomal protein L23



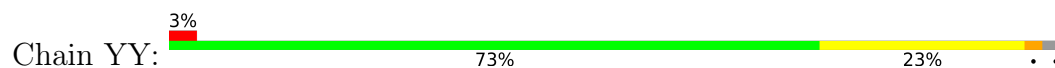
- Molecule 19: 50S ribosomal protein L23



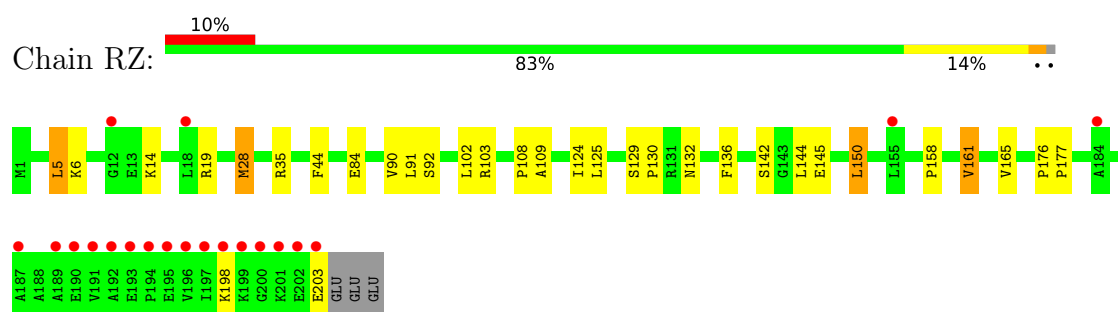
- Molecule 20: 50S ribosomal protein L24



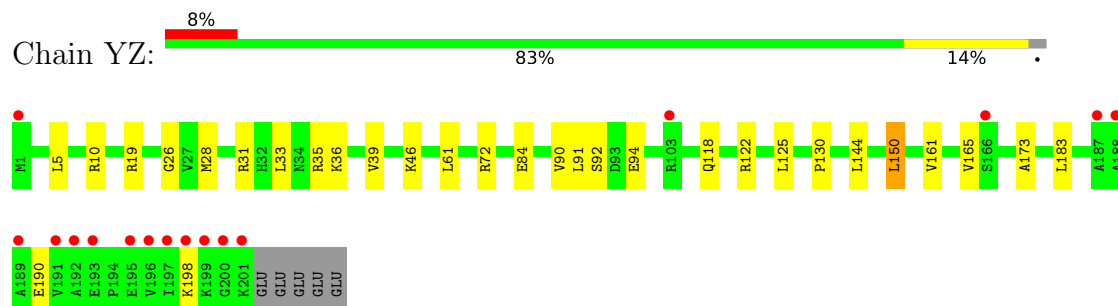
- Molecule 20: 50S ribosomal protein L24



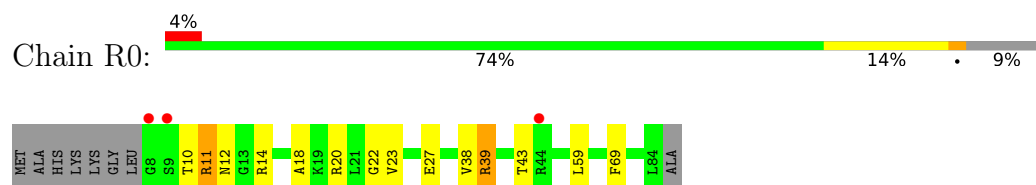
- Molecule 21: 50S ribosomal protein L25



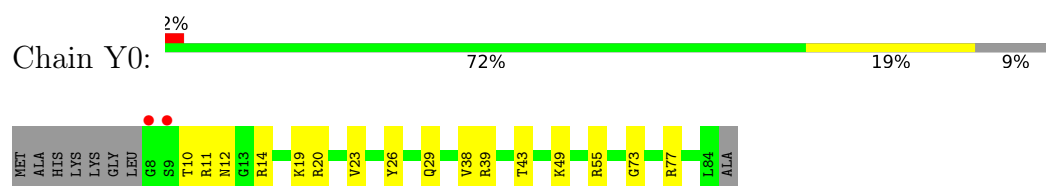
- Molecule 21: 50S ribosomal protein L25



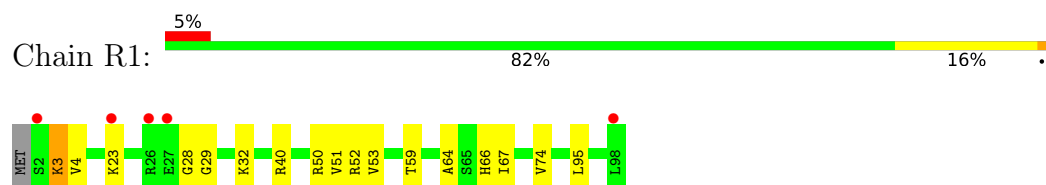
- Molecule 22: 50S ribosomal protein L27



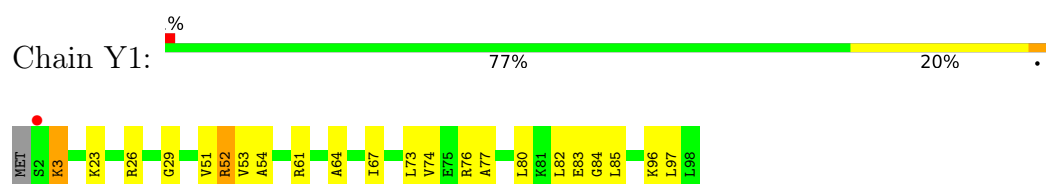
- Molecule 22: 50S ribosomal protein L27



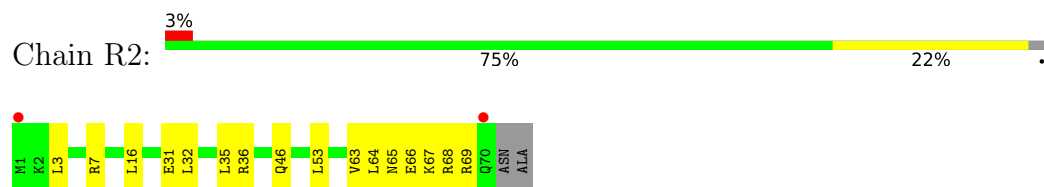
- Molecule 23: 50S ribosomal protein L28



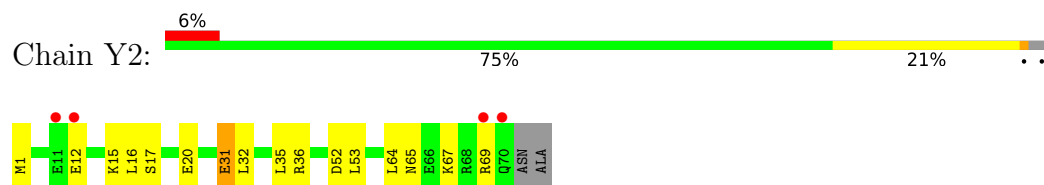
- Molecule 23: 50S ribosomal protein L28



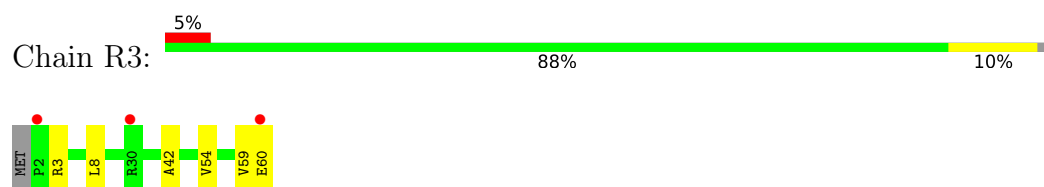
- Molecule 24: 50S ribosomal protein L29



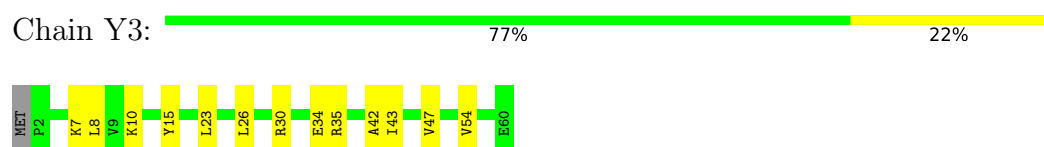
- Molecule 24: 50S ribosomal protein L29



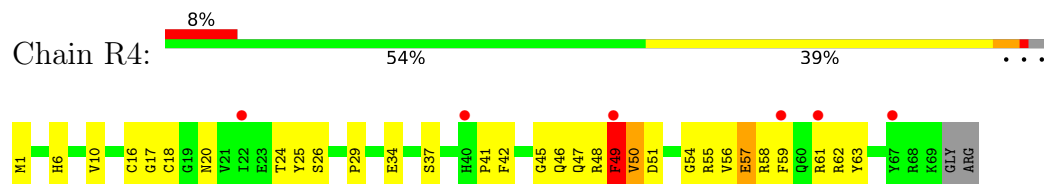
- Molecule 25: 50S ribosomal protein L30



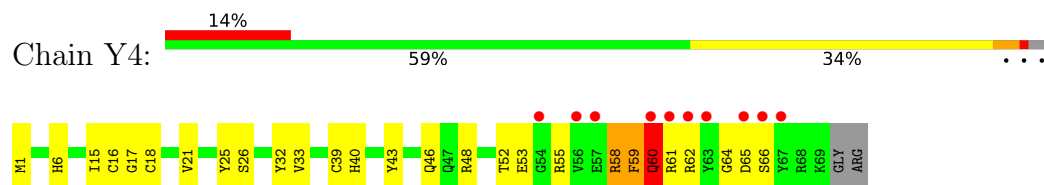
- Molecule 25: 50S ribosomal protein L30



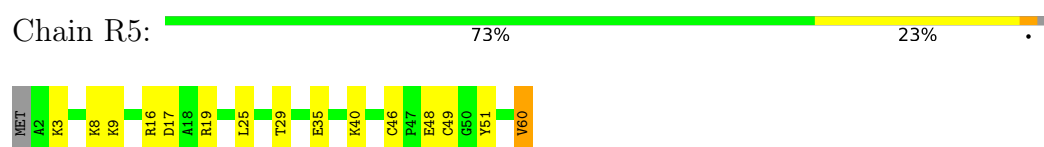
- Molecule 26: 50S ribosomal protein L31



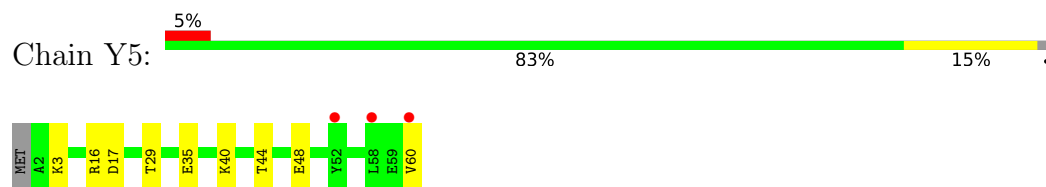
- Molecule 26: 50S ribosomal protein L31



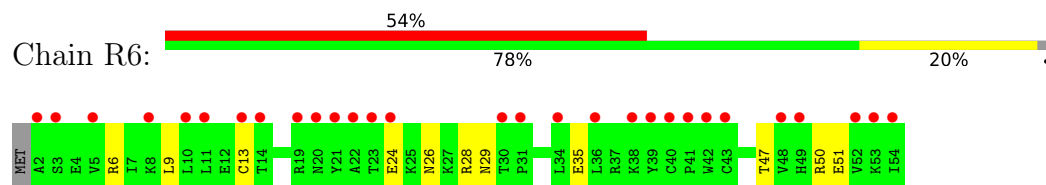
- Molecule 27: 50S ribosomal protein L32



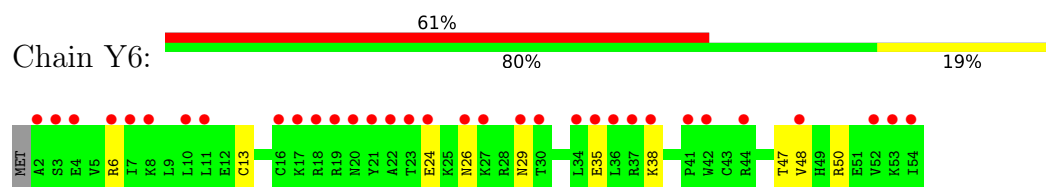
- Molecule 27: 50S ribosomal protein L32



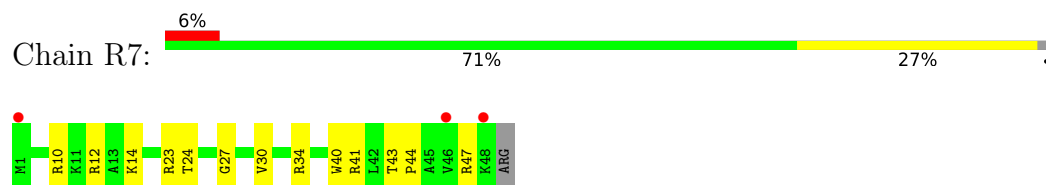
- Molecule 28: 50S ribosomal protein L33



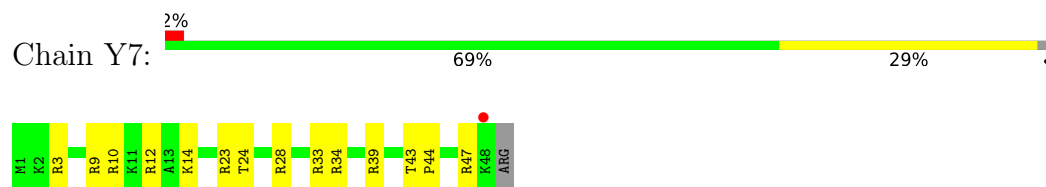
- Molecule 28: 50S ribosomal protein L33



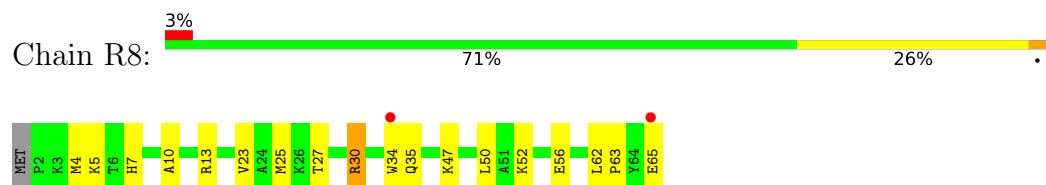
- Molecule 29: 50S ribosomal protein L34



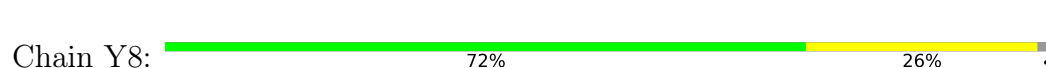
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35





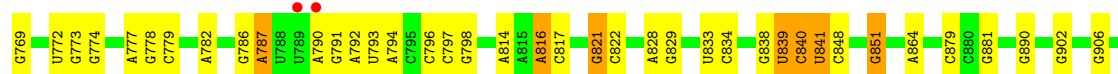
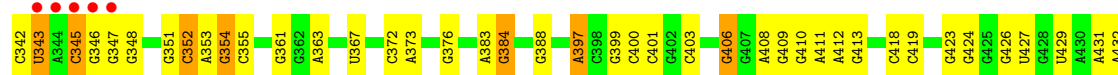
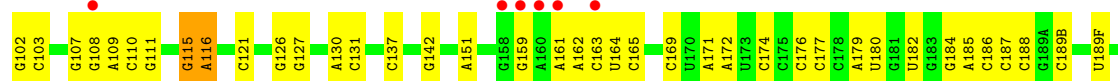
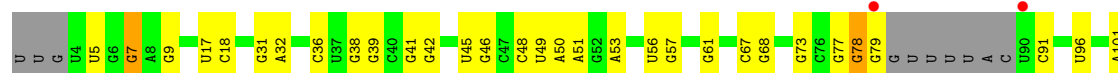
- Molecule 31: 50S ribosomal protein L36

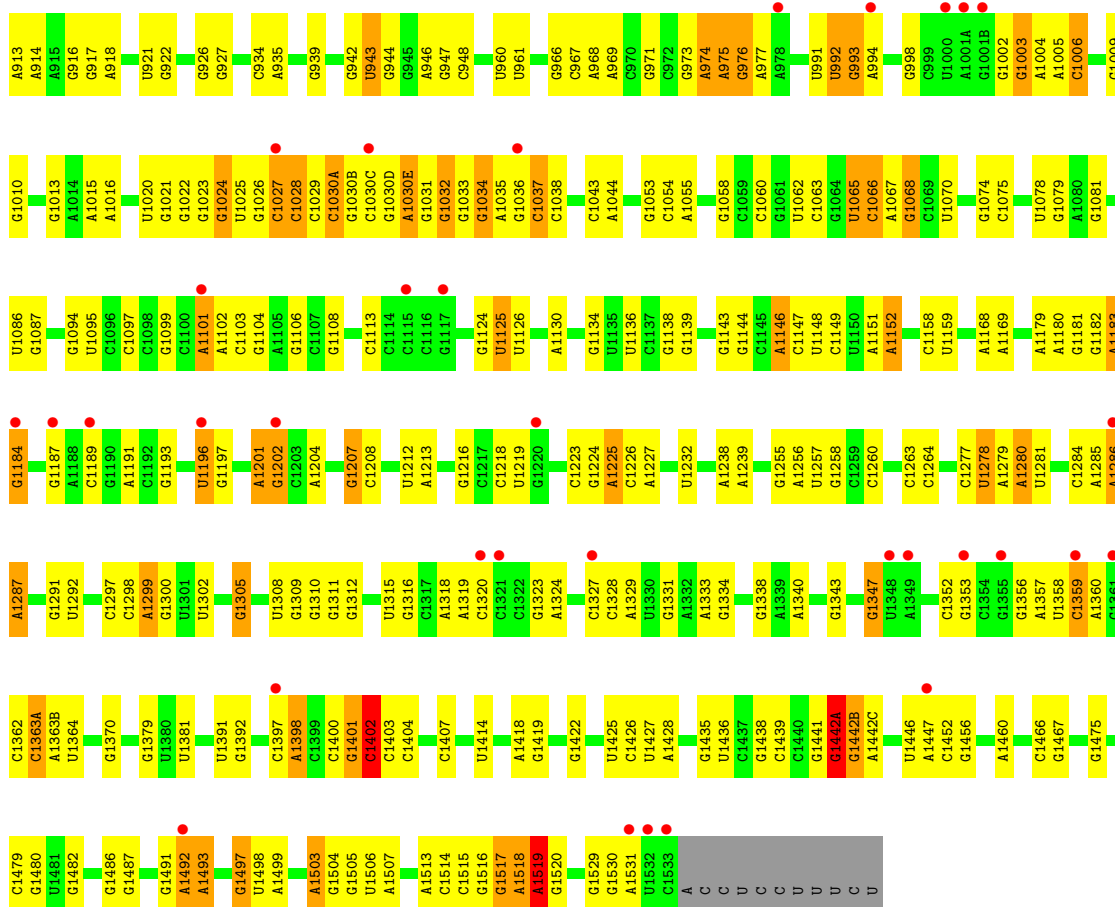


- Molecule 31: 50S ribosomal protein L36



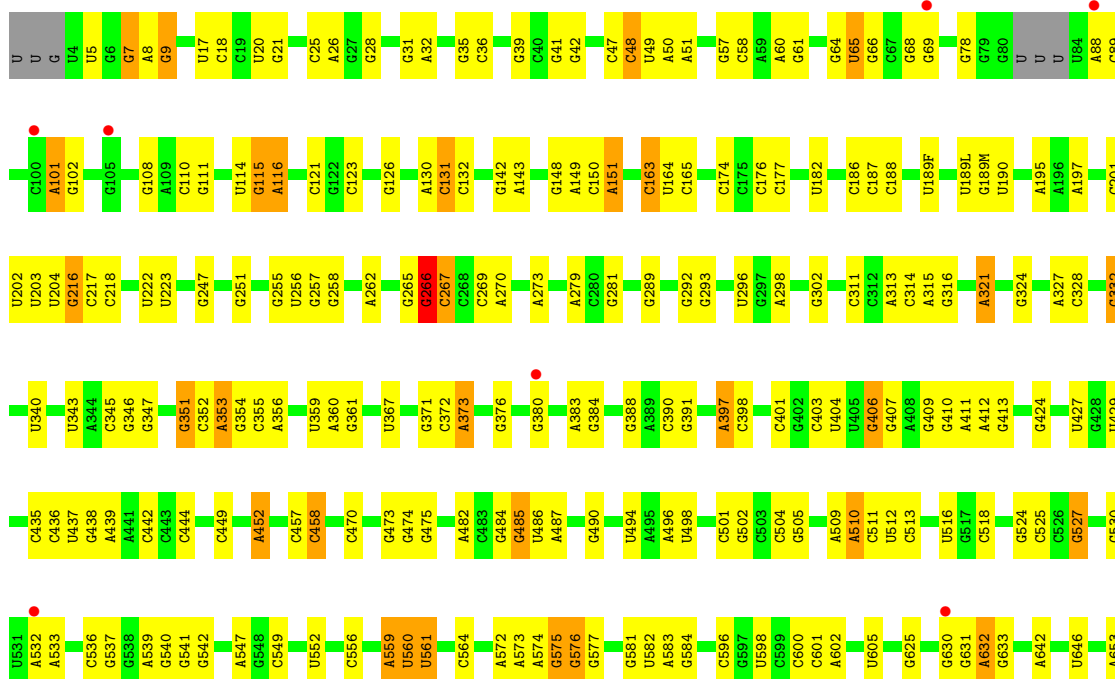
- Molecule 32: 16S rRNA

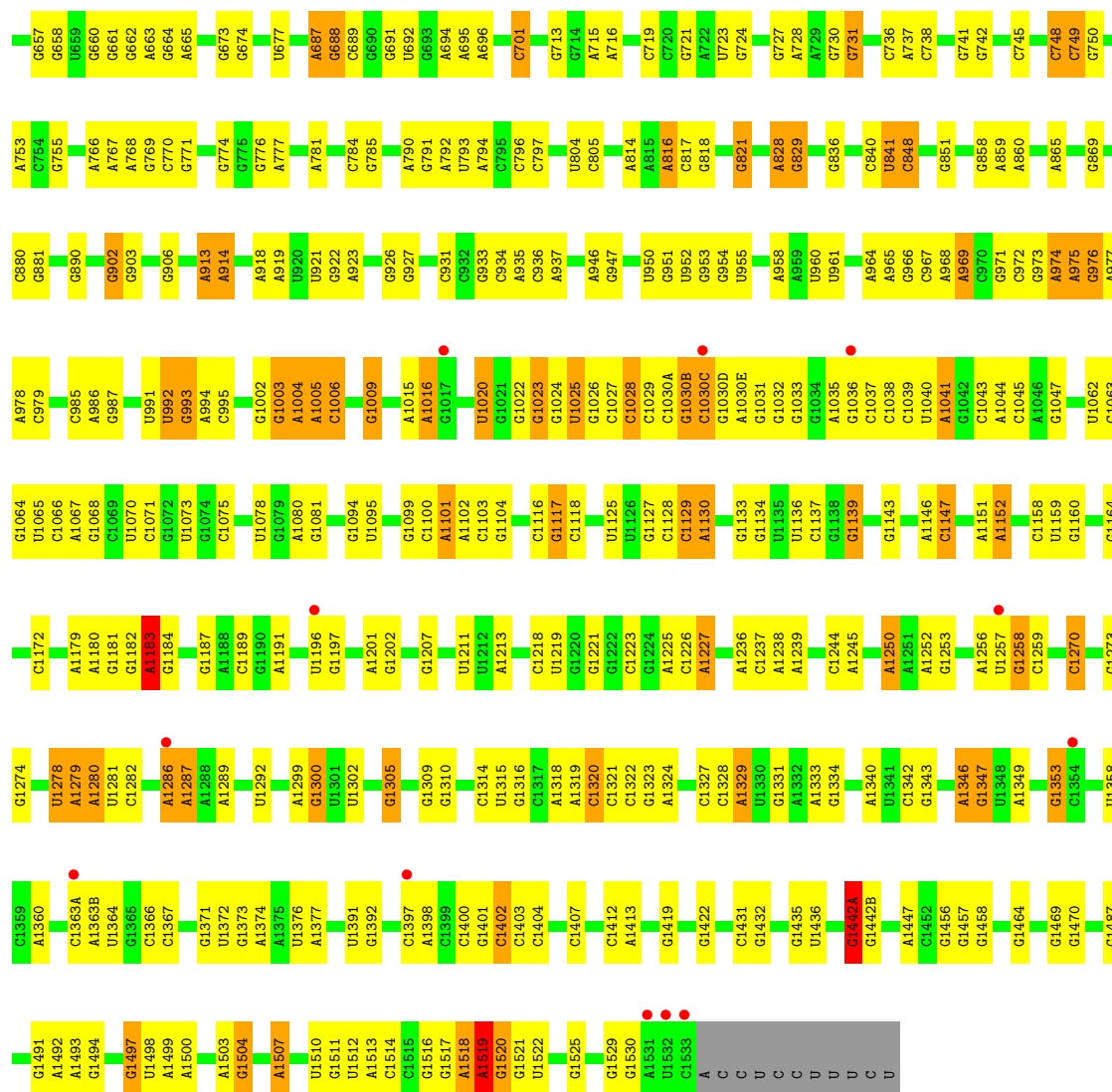


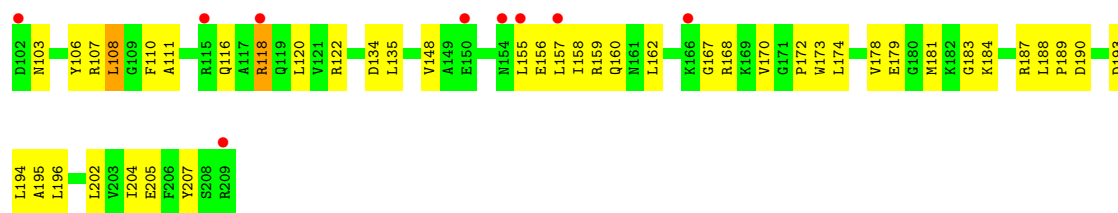


• Molecule 32: 16S rRNA

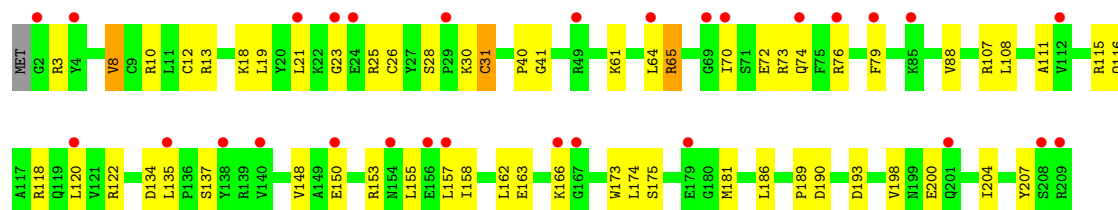
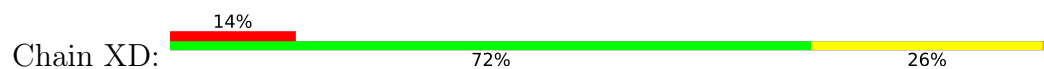
Chain XA: %



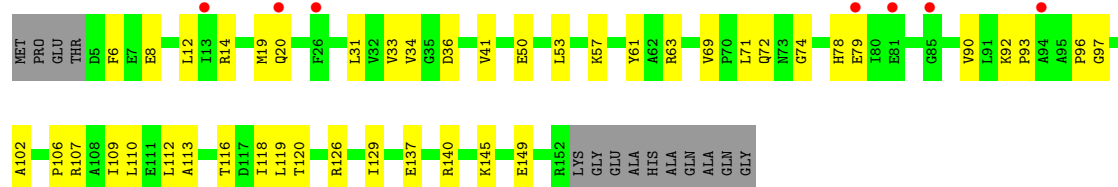




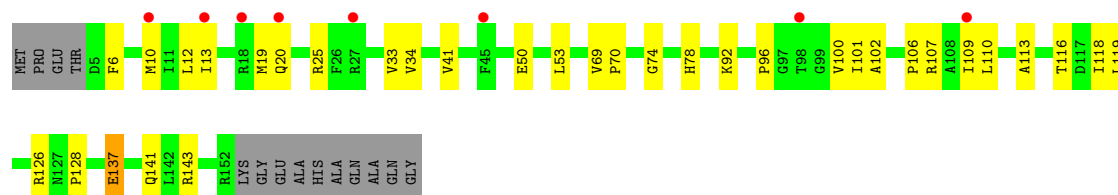
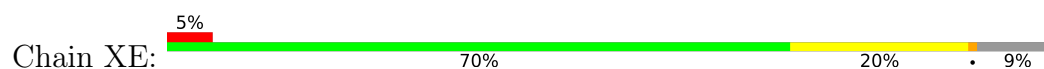
• Molecule 35: 30S ribosomal protein S4



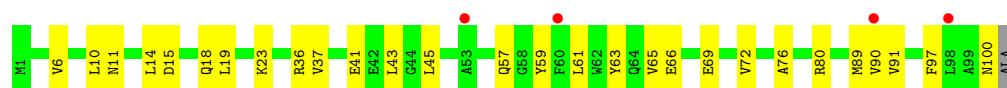
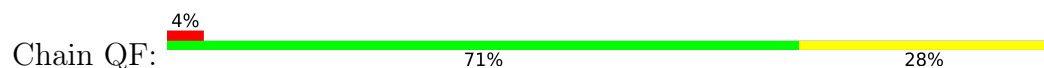
• Molecule 36: 30S ribosomal protein S5



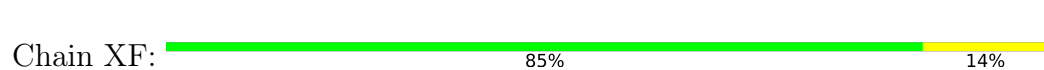
• Molecule 36: 30S ribosomal protein S5



• Molecule 37: 30S ribosomal protein S6

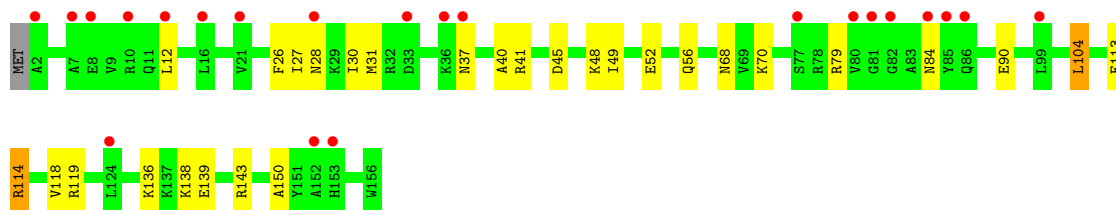


• Molecule 37: 30S ribosomal protein S6



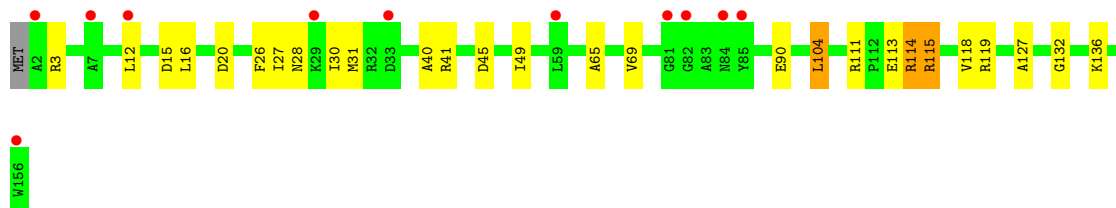
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- Molecule 38: 30S ribosomal protein S7

Chain QG: 14% 81% 17% ..



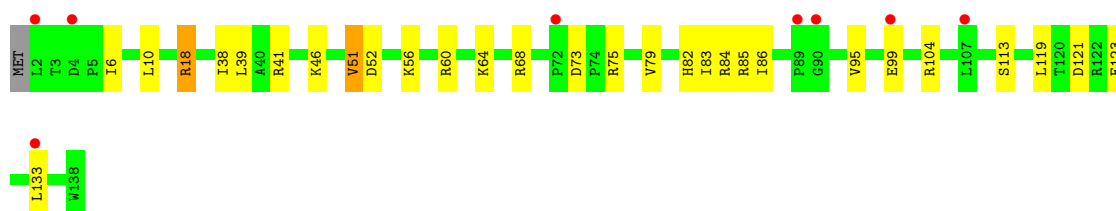
- Molecule 38: 30S ribosomal protein S7

Chain XG: 7% 82% 15% ..



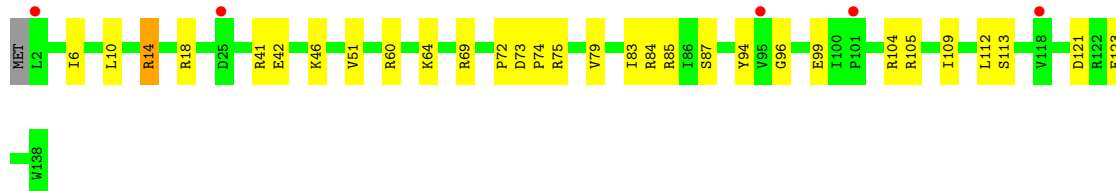
- Molecule 39: 30S ribosomal protein S8

Chain QH: 6% 78% 20% ..



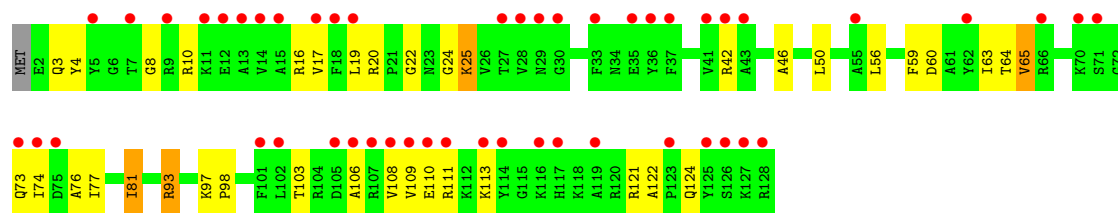
- Molecule 39: 30S ribosomal protein S8

Chain XH: 4% 78% 21% ..

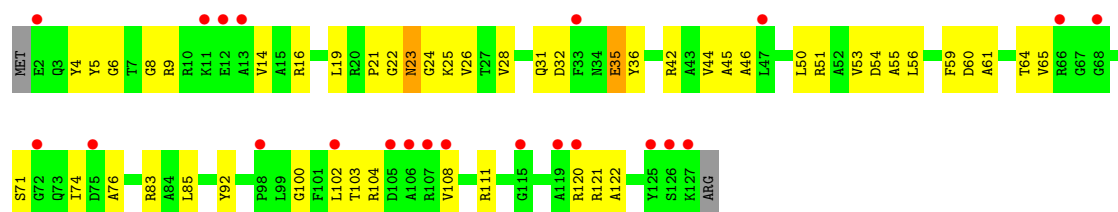


- Molecule 40: 30S ribosomal protein S9

Chain QI: 38% 70% 27% ..



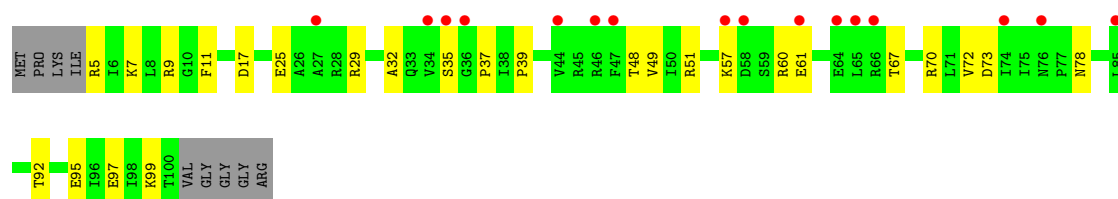
- Molecule 40: 30S ribosomal protein S9



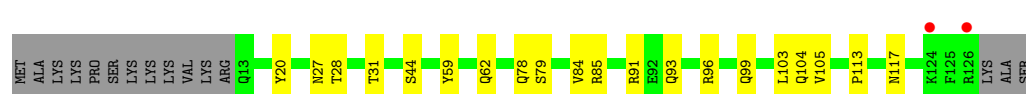
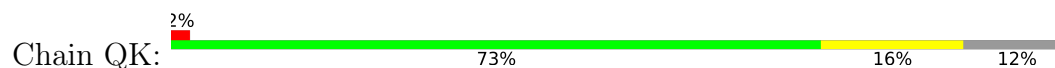
- Molecule 41: 30S ribosomal protein S10



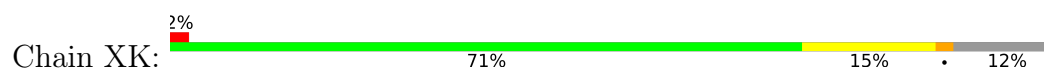
- Molecule 41: 30S ribosomal protein S10

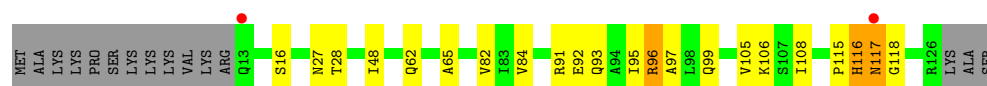


- Molecule 42: 30S ribosomal protein S11

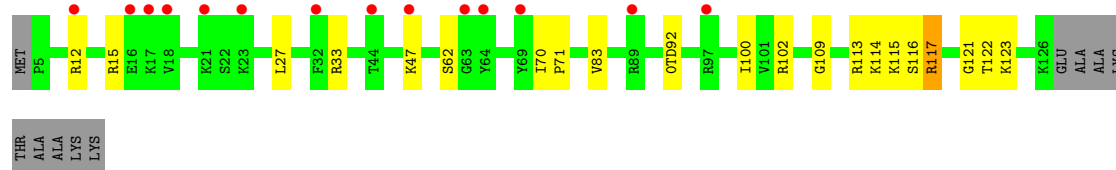
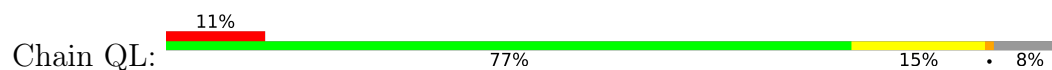


- Molecule 42: 30S ribosomal protein S11

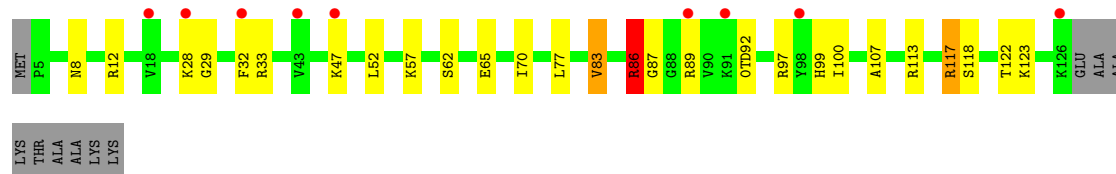
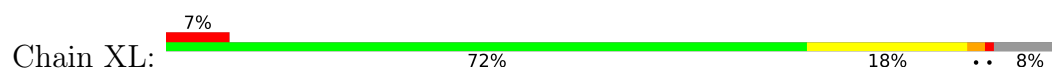




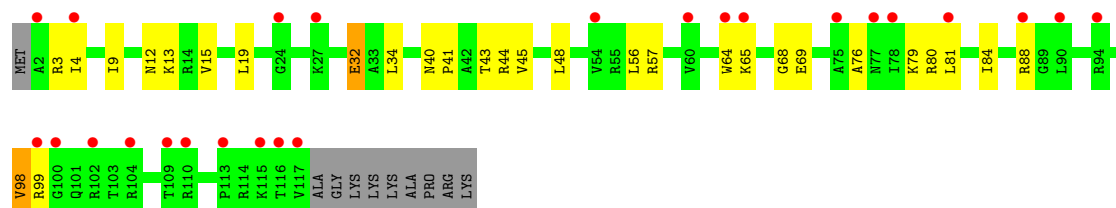
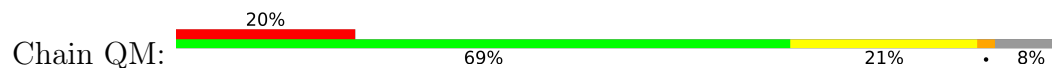
- Molecule 43: 30S ribosomal protein S12



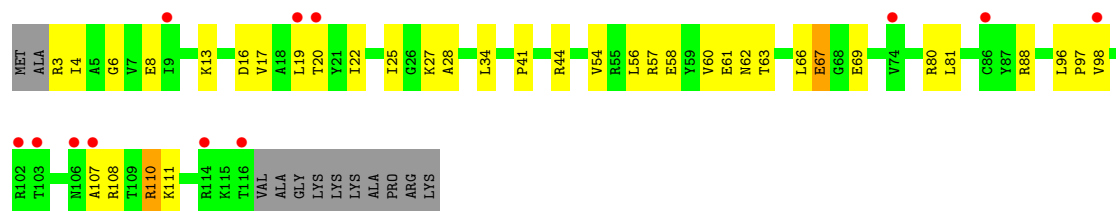
- Molecule 43: 30S ribosomal protein S12



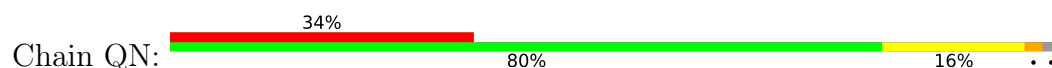
- Molecule 44: 30S ribosomal protein S13

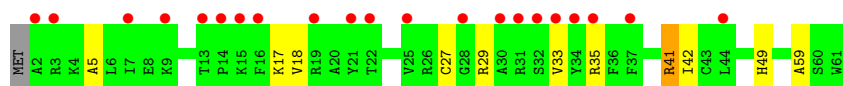


- Molecule 44: 30S ribosomal protein S13

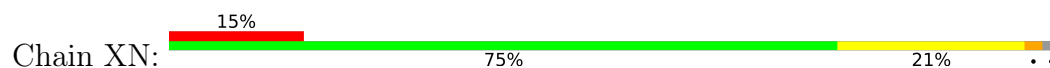


- Molecule 45: 30S ribosomal protein S14 type Z

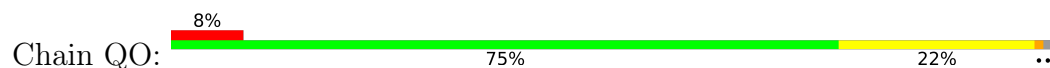




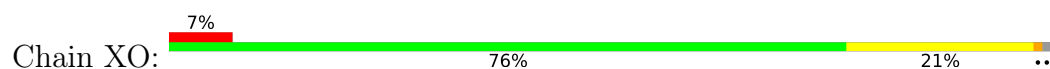
- Molecule 45: 30S ribosomal protein S14 type Z



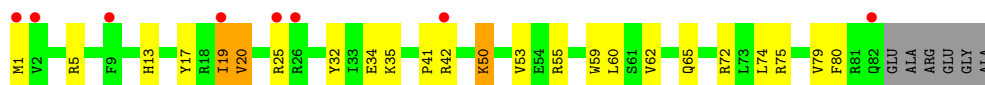
- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15



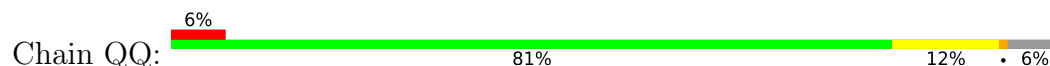
- Molecule 47: 30S ribosomal protein S16



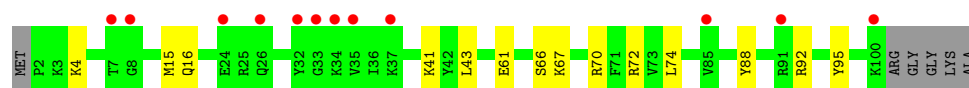
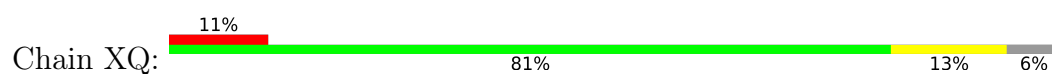
- Molecule 47: 30S ribosomal protein S16



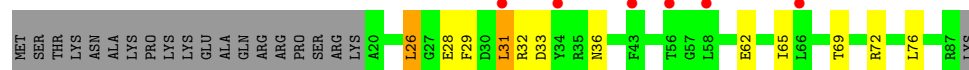
- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



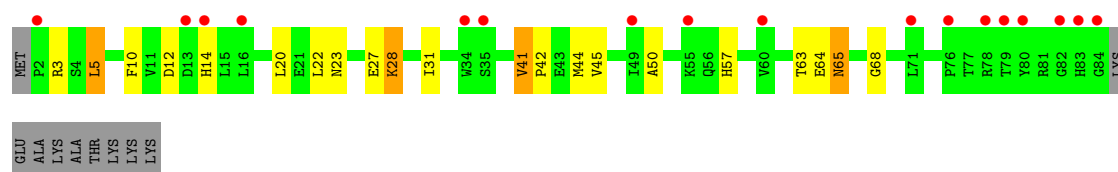
- Molecule 49: 30S ribosomal protein S18



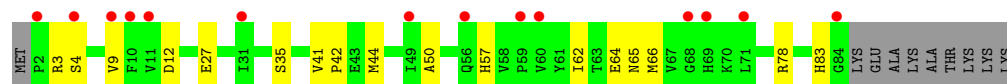
- Molecule 49: 30S ribosomal protein S18



- Molecule 50: 30S ribosomal protein S19



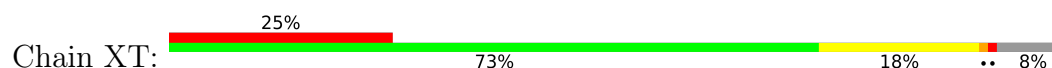
- Molecule 50: 30S ribosomal protein S19

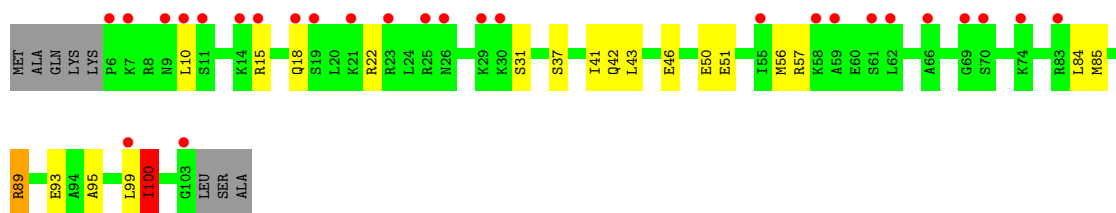


- Molecule 51: 30S ribosomal protein S20

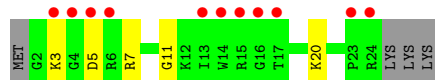
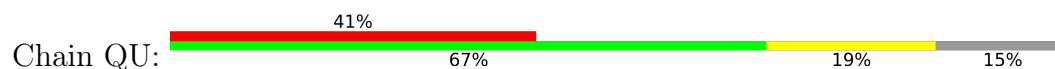


- Molecule 51: 30S ribosomal protein S20

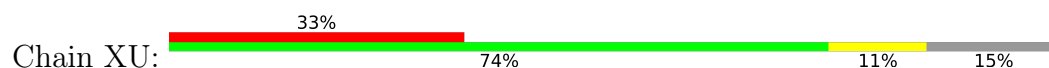




- Molecule 52: 30S ribosomal protein Thx



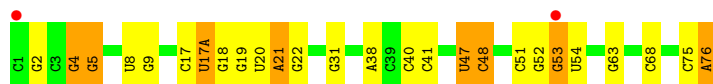
- Molecule 52: 30S ribosomal protein Thx



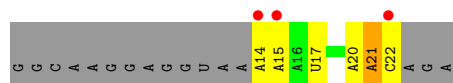
- Molecule 53: P-site tRNA fMet



- Molecule 53: P-site tRNA fMet

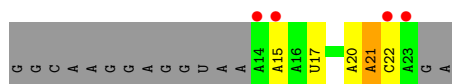


- Molecule 54: messenger RNA

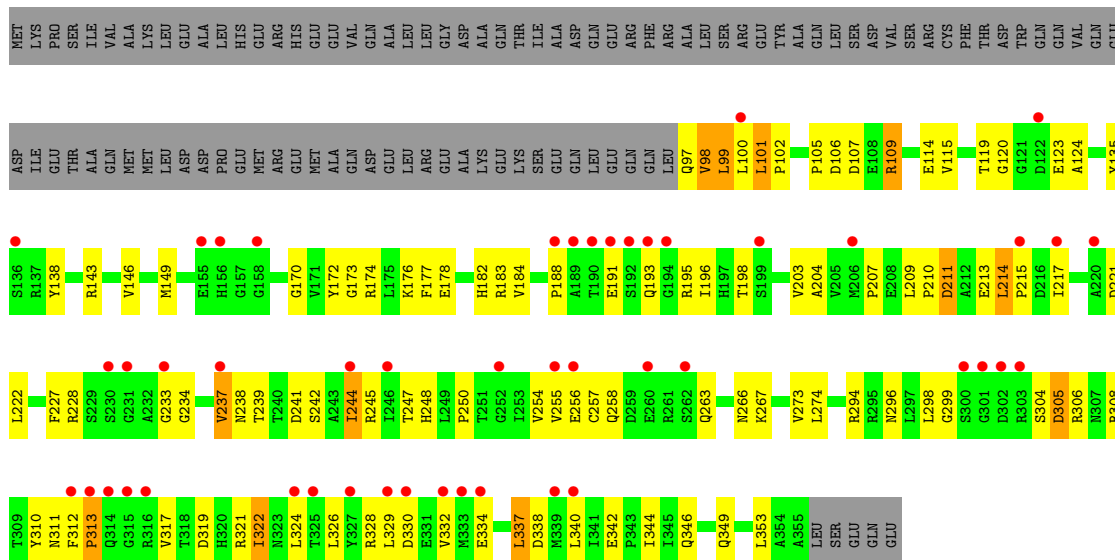
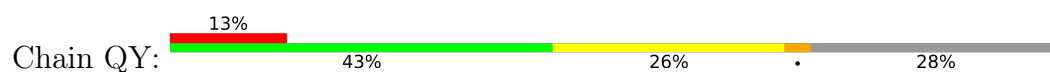


- Molecule 54: messenger RNA

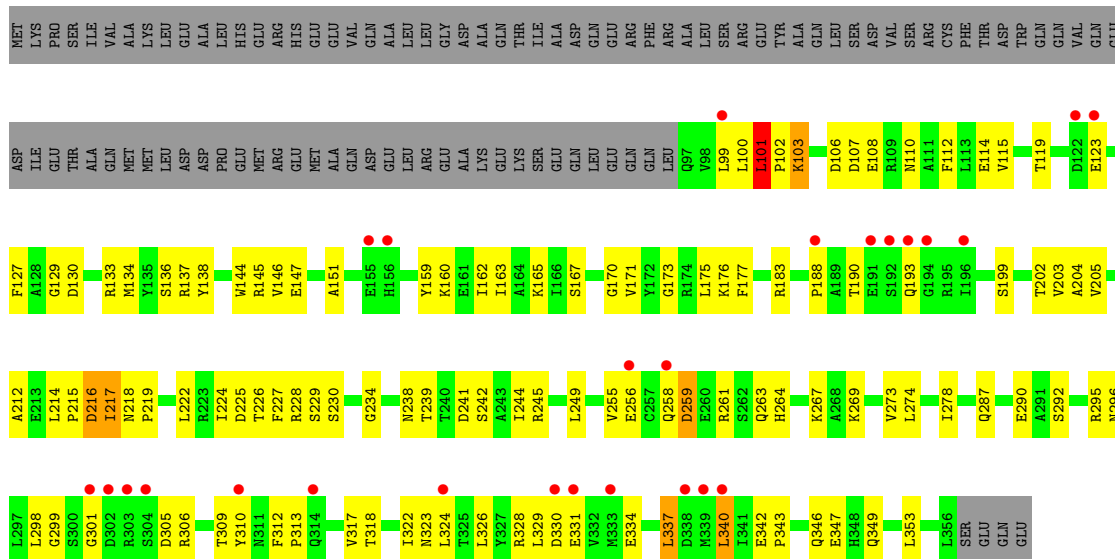




• Molecule 55: Peptide chain release factor 1



• Molecule 55: Peptide chain release factor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.51Å 450.89Å 622.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.86 – 3.04 49.86 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.86-3.04) 99.3 (49.86-3.04)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.07Å)	Xtriage
Refinement program	PHENIX, PHENIX	Depositor
R, R_{free}	0.246 , 0.279 0.246 , 0.277	Depositor DCC
R_{free} test set	52117 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	294929	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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, 0TD, 5MU, M2G, ZN, MA6, 2MG, 5MC, MG, 7MG, UR3, PSU, 2MA, 2MU, 4OC, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	RA	0.24	0/68901	0.42	1/107544 (0.0%)
1	YA	0.28	0/68901	0.47	1/107544 (0.0%)
2	RB	0.19	0/2876	0.35	0/4486
2	YB	0.24	0/2878	0.41	0/4490
3	RD	0.31	0/2181	0.57	0/2940
3	YD	0.34	0/2186	0.62	1/2944 (0.0%)
4	RE	0.30	0/1592	0.55	0/2149
4	YE	0.33	0/1592	0.60	2/2149 (0.1%)
5	RF	0.27	0/1619	0.53	0/2193
5	YF	0.36	0/1615	0.59	0/2188
6	RG	0.23	0/1451	0.49	0/1961
6	YG	0.27	0/1449	0.56	0/1957
7	RH	0.23	0/1356	0.44	0/1834
7	YH	0.29	0/1350	0.53	0/1826
8	RI	0.23	0/1109	0.49	0/1512
8	YI	0.29	0/1091	0.49	0/1490
9	RN	0.28	0/1148	0.51	0/1547
9	YN	0.29	0/1144	0.50	0/1543
10	RO	0.27	0/943	0.51	0/1269
10	YO	0.32	0/943	0.54	0/1269
11	RP	0.29	0/1152	0.56	0/1533
11	YP	0.35	0/1152	0.61	0/1533
12	RQ	0.27	0/1143	0.53	0/1527
12	YQ	0.34	0/1143	0.58	0/1527
13	RR	0.33	0/982	0.56	0/1312
13	YR	0.33	0/982	0.55	0/1312
14	RS	0.27	0/887	0.58	0/1180
14	YS	0.30	0/880	0.59	0/1172
15	RT	0.31	0/1105	0.57	0/1477
15	YT	0.29	0/1097	0.54	0/1468
16	RU	0.26	0/977	0.51	0/1301
16	YU	0.31	0/977	0.52	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	RV	0.27	0/786	0.49	0/1053
17	YV	0.30	0/782	0.53	0/1049
18	RW	0.28	0/897	0.52	0/1205
18	YW	0.30	0/897	0.53	0/1205
19	RX	0.30	0/764	0.53	0/1025
19	YX	0.33	0/764	0.57	0/1025
20	RY	0.28	0/823	0.57	1/1099 (0.1%)
20	YY	0.32	0/823	0.58	0/1100
21	RZ	0.30	1/1620 (0.1%)	0.48	1/2200 (0.0%)
21	YZ	0.28	0/1590	0.51	0/2162
22	R0	0.33	0/616	0.60	1/821 (0.1%)
22	Y0	0.37	0/616	0.69	1/821 (0.1%)
23	R1	0.30	0/761	0.52	0/1013
23	Y1	0.31	0/766	0.53	0/1018
24	R2	0.23	0/590	0.48	0/781
24	Y2	0.30	0/594	0.51	0/785
25	R3	0.28	0/474	0.52	0/635
25	Y3	0.30	0/469	0.57	0/630
26	R4	0.37	0/559	0.80	1/754 (0.1%)
26	Y4	0.34	0/549	0.79	5/741 (0.7%)
27	R5	0.37	0/473	0.57	0/639
27	Y5	0.37	0/469	0.57	0/635
28	R6	0.23	0/460	0.43	0/613
28	Y6	0.23	0/456	0.44	0/608
29	R7	0.38	0/426	0.65	0/561
29	Y7	0.38	0/426	0.69	0/561
30	R8	0.31	0/525	0.53	0/691
30	Y8	0.34	0/525	0.55	0/691
31	R9	0.30	0/310	0.58	0/407
31	Y9	0.29	0/310	0.54	0/407
32	QA	0.19	0/35795	0.36	1/55864 (0.0%)
32	XA	0.20	2/35890 (0.0%)	0.37	4/56012 (0.0%)
33	QB	0.29	0/1876	0.56	1/2533 (0.0%)
33	XB	0.28	0/1860	0.58	0/2518
34	QC	0.22	0/1582	0.48	0/2137
34	XC	0.30	1/1566 (0.1%)	0.53	0/2119
35	QD	0.26	0/1695	0.54	0/2274
35	XD	0.25	0/1698	0.51	0/2277
36	QE	0.26	0/1149	0.48	0/1548
36	XE	0.26	0/1149	0.47	0/1548
37	QF	0.24	0/827	0.44	0/1120
37	XF	0.26	0/829	0.51	0/1123
38	QG	0.22	0/1254	0.44	0/1683

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	XG	0.23	0/1248	0.45	0/1676
39	QH	0.22	0/1118	0.47	0/1506
39	XH	0.26	0/1108	0.52	0/1494
40	QI	0.27	0/1005	0.57	0/1351
40	XI	0.24	0/985	0.51	0/1329
41	QJ	0.23	0/732	0.47	0/993
41	XJ	0.24	0/723	0.52	1/984 (0.1%)
42	QK	0.24	0/849	0.46	0/1150
42	XK	0.25	0/848	0.53	1/1149 (0.1%)
43	QL	0.30	0/937	0.51	0/1260
43	XL	0.29	0/937	0.60	0/1260
44	QM	0.24	0/924	0.54	0/1242
44	XM	0.25	0/905	0.53	0/1217
45	QN	0.27	0/501	0.50	0/664
45	XN	0.27	0/501	0.54	0/664
46	QO	0.25	0/739	0.49	0/985
46	XO	0.28	0/739	0.57	0/985
47	QP	0.24	0/697	0.49	0/939
47	XP	0.24	0/693	0.48	0/935
48	QQ	0.25	0/836	0.48	0/1117
48	XQ	0.23	0/836	0.48	0/1117
49	QR	0.25	0/560	0.48	0/746
49	XR	0.25	0/560	0.49	0/746
50	QS	0.23	0/663	0.54	1/895 (0.1%)
50	XS	0.20	0/660	0.45	0/893
51	QT	0.27	0/734	0.55	0/969
51	XT	0.25	0/736	0.48	0/976
52	QU	0.25	0/203	0.58	0/266
52	XU	0.23	0/203	0.67	0/266
53	QV	0.19	0/1832	0.39	0/2855
53	XV	0.20	0/1836	0.39	0/2859
54	QX	0.24	0/216	0.40	0/334
54	XX	0.27	0/241	0.51	0/373
55	QY	0.33	0/2046	0.65	0/2759
55	XY	0.39	0/2054	0.68	0/2770
All	All	0.26	4/316497 (0.0%)	0.46	24/472893 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	RS	0	1
33	QB	0	1
43	XL	0	1
55	QY	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	RZ	176	PRO	CA-C	6.72	1.56	1.52
34	XC	173	VAL	C-N	5.43	1.46	1.33
32	XA	1498	UR3	O3'-P	5.36	1.61	1.56
32	XA	68	G	O3'-P	-5.23	1.53	1.61

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	RY	92	ASN	N-CA-C	7.26	120.11	111.33
41	XJ	32	ALA	N-CA-C	-6.14	101.38	110.46
21	RZ	176	PRO	O-C-N	6.10	124.02	121.15
32	QA	1442(A)	G	P-O3'-C3'	5.95	126.83	119.70
42	XK	116	HIS	N-CA-C	5.81	120.75	111.81

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	QB	231	GLU	Peptide
55	QY	305	ASP	Peptide
14	RS	58	LEU	Peptide
43	XL	86	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	RA	61758	0	31144	594	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	YA	61758	0	31147	611	1
2	RB	2572	0	1305	12	0
2	YB	2573	0	1306	13	0
3	RD	2131	0	2207	52	0
3	YD	2136	0	2218	52	0
4	RE	1559	0	1618	36	0
4	YE	1559	0	1618	41	0
5	RF	1584	0	1625	38	0
5	YF	1580	0	1619	48	0
6	RG	1426	0	1445	31	0
6	YG	1424	0	1441	42	0
7	RH	1330	0	1407	25	0
7	YH	1324	0	1402	33	0
8	RI	1094	0	1127	22	0
8	YI	1076	0	1093	14	0
9	RN	1121	0	1195	16	0
9	YN	1117	0	1184	16	0
10	RO	933	0	996	18	0
10	YO	933	0	996	15	0
11	RP	1135	0	1212	23	0
11	YP	1135	0	1212	33	0
12	RQ	1122	0	1179	20	0
12	YQ	1122	0	1179	21	0
13	RR	968	0	1033	22	0
13	YR	968	0	1033	14	0
14	RS	877	0	938	12	0
14	YS	870	0	923	13	0
15	RT	1091	0	1151	26	0
15	YT	1083	0	1136	19	0
16	RU	959	0	1019	16	0
16	YU	959	0	1019	18	0
17	RV	775	0	841	14	0
17	YV	771	0	830	13	0
18	RW	886	0	940	13	0
18	YW	886	0	940	13	0
19	RX	750	0	814	16	0
19	YX	750	0	814	6	0
20	RY	810	0	894	16	0
20	YY	810	0	891	19	0
21	RZ	1587	0	1598	24	0
21	YZ	1557	0	1564	25	0
22	R0	608	0	622	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	Y0	608	0	622	15	0
23	R1	754	0	823	10	0
23	Y1	759	0	837	18	0
24	R2	588	0	643	11	1
24	Y2	592	0	654	8	0
25	R3	469	0	518	5	0
25	Y3	464	0	514	6	0
26	R4	546	0	523	29	0
26	Y4	536	0	516	27	0
27	R5	459	0	477	12	0
27	Y5	455	0	467	5	0
28	R6	453	0	475	7	0
28	Y6	449	0	471	7	0
29	R7	418	0	467	11	0
29	Y7	418	0	467	8	0
30	R8	517	0	582	18	0
30	Y8	517	0	582	20	0
31	R9	307	0	336	13	0
31	Y9	307	0	336	11	0
32	QA	32246	0	16294	308	0
32	XA	32331	0	16338	348	0
33	QB	1842	0	1862	56	0
33	XB	1825	0	1828	64	0
34	QC	1558	0	1557	33	0
34	XC	1542	0	1517	32	0
35	QD	1665	0	1690	61	0
35	XD	1668	0	1706	42	0
36	QE	1133	0	1191	29	0
36	XE	1133	0	1191	25	0
37	QF	814	0	808	19	0
37	XF	816	0	807	8	0
38	QG	1235	0	1249	20	0
38	XG	1229	0	1238	16	0
39	QH	1098	0	1143	20	0
39	XH	1088	0	1126	21	0
40	QI	986	0	990	28	0
40	XI	966	0	953	35	0
41	QJ	719	0	672	28	0
41	XJ	710	0	661	20	0
42	QK	834	0	838	12	0
42	XK	833	0	836	13	0
43	QL	932	0	981	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	XL	932	0	981	25	0
44	QM	914	0	954	23	0
44	XM	895	0	920	25	0
45	QN	492	0	529	11	0
45	XN	492	0	529	14	0
46	QO	728	0	760	13	0
46	XO	728	0	760	14	0
47	QP	681	0	697	19	0
47	XP	677	0	686	19	0
48	QQ	823	0	891	9	0
48	XQ	823	0	891	10	0
49	QR	555	0	618	11	0
49	XR	555	0	618	10	0
50	QS	648	0	658	17	0
50	XS	645	0	635	19	0
51	QT	732	0	809	15	0
51	XT	733	0	795	14	0
52	QU	199	0	208	4	0
52	XU	199	0	208	1	0
53	QV	1640	0	837	15	0
53	XV	1644	0	836	15	0
54	QX	193	0	98	5	0
54	XX	215	0	108	2	0
55	QY	2014	0	1980	74	0
55	XY	2022	0	1991	86	0
56	QA	262	0	0	0	0
56	QB	1	0	0	0	0
56	QD	2	0	0	0	0
56	QE	2	0	0	0	0
56	QF	1	0	0	0	0
56	QG	3	0	0	0	0
56	QH	1	0	0	0	0
56	QI	1	0	0	0	0
56	QJ	1	0	0	0	0
56	QL	2	0	0	0	0
56	QN	1	0	0	0	0
56	QO	1	0	0	0	0
56	QQ	1	0	0	0	0
56	QR	1	0	0	0	0
56	QT	1	0	0	0	0
56	QV	6	0	0	0	0
56	R0	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	R1	5	0	0	0	0
56	R3	2	0	0	0	0
56	R5	1	0	0	0	0
56	R7	3	0	0	0	0
56	R9	1	0	0	0	0
56	RA	1032	0	0	0	0
56	RB	22	0	0	0	0
56	RD	15	0	0	0	0
56	RE	7	0	0	0	0
56	RF	11	0	0	0	0
56	RG	4	0	0	0	0
56	RN	2	0	0	0	0
56	RO	1	0	0	0	0
56	RP	2	0	0	0	0
56	RQ	5	0	0	0	0
56	RR	4	0	0	0	0
56	RS	1	0	0	0	0
56	RT	3	0	0	0	0
56	RU	3	0	0	0	0
56	RV	3	0	0	0	0
56	RW	2	0	0	0	0
56	RX	1	0	0	0	0
56	RY	1	0	0	0	0
56	XA	187	0	0	0	0
56	XE	2	0	0	0	0
56	XF	4	0	0	0	0
56	XJ	1	0	0	0	0
56	XL	1	0	0	0	0
56	XT	1	0	0	0	0
56	XV	4	0	0	0	0
56	XY	1	0	0	0	0
56	Y0	1	0	0	0	0
56	Y1	1	0	0	0	0
56	Y5	2	0	0	0	0
56	Y7	1	0	0	0	0
56	Y8	2	0	0	0	0
56	YA	749	0	0	0	0
56	YB	20	0	0	0	0
56	YD	9	0	0	0	0
56	YE	6	0	0	0	0
56	YF	2	0	0	0	0
56	YG	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	0	0	0	0
56	YR	1	0	0	0	0
56	YT	3	0	0	0	0
56	YV	1	0	0	0	0
56	YW	2	0	0	0	0
56	YX	1	0	0	0	0
57	QN	1	0	0	0	0
57	R4	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R9	1	0	0	0	0
57	RY	1	0	0	0	0
57	XN	1	0	0	0	0
57	Y4	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YY	1	0	0	0	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
All	All	294929	0	198658	3486	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 3486 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:2552:2MU:C5	1:RA:2552:2MU:C4	1.74	1.65
1:YA:2552:2MU:C4	1:YA:2552:2MU:C5	1.75	1.56
32:XA:1003:G:H2'	32:XA:1004:A:H4'	1.40	1.03
1:YA:2131:G:H5''	1:YA:2132:U:H5'	1.46	0.98
26:Y4:59:PHE:HA	26:Y4:61:ARG:H	1.26	0.97

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:R2:46:GLN:OE1	1:YA:277:C:O2'[3_555]	2.02	0.18

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	RD	273/276 (99%)	263 (96%)	10 (4%)	0	100	100
3	YD	273/276 (99%)	262 (96%)	11 (4%)	0	100	100
4	RE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	24	57
4	YE	202/206 (98%)	194 (96%)	8 (4%)	0	100	100
5	RF	201/210 (96%)	196 (98%)	5 (2%)	0	100	100
5	YF	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	24	57
6	RG	179/182 (98%)	168 (94%)	9 (5%)	2 (1%)	11	39
6	YG	179/182 (98%)	169 (94%)	9 (5%)	1 (1%)	21	53
7	RH	172/180 (96%)	164 (95%)	8 (5%)	0	100	100
7	YH	171/180 (95%)	163 (95%)	8 (5%)	0	100	100
8	RI	145/148 (98%)	134 (92%)	10 (7%)	1 (1%)	18	49
8	YI	144/148 (97%)	136 (94%)	8 (6%)	0	100	100
9	RN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	YN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
10	RO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	YO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
11	RP	147/150 (98%)	141 (96%)	5 (3%)	1 (1%)	18	49
11	YP	147/150 (98%)	141 (96%)	5 (3%)	1 (1%)	18	49
12	RQ	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
12	YQ	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
13	RR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	YR	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	RS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	14	44
14	YS	108/112 (96%)	105 (97%)	3 (3%)	0	100	100
15	RT	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
15	YT	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
16	RU	114/118 (97%)	114 (100%)	0	0	100	100
16	YU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	RV	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
17	YV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12	41
18	RW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	YW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	RX	93/96 (97%)	92 (99%)	1 (1%)	0	100	100
19	YX	93/96 (97%)	92 (99%)	0	1 (1%)	11	39
20	RY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
20	YY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
21	RZ	201/206 (98%)	196 (98%)	5 (2%)	0	100	100
21	YZ	199/206 (97%)	194 (98%)	5 (2%)	0	100	100
22	R0	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
22	Y0	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
23	R1	95/98 (97%)	94 (99%)	0	1 (1%)	11	39
23	Y1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	39
24	R2	68/72 (94%)	68 (100%)	0	0	100	100
24	Y2	68/72 (94%)	68 (100%)	0	0	100	100
25	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	R4	67/71 (94%)	55 (82%)	7 (10%)	5 (8%)	1	3
26	Y4	67/71 (94%)	56 (84%)	9 (13%)	2 (3%)	3	17
27	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	Y5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	R7	46/49 (94%)	46 (100%)	0	0	100	100
29	Y7	46/49 (94%)	46 (100%)	0	0	100	100
30	R8	62/65 (95%)	62 (100%)	0	0	100	100
30	Y8	62/65 (95%)	62 (100%)	0	0	100	100
31	R9	35/37 (95%)	35 (100%)	0	0	100	100
31	Y9	35/37 (95%)	35 (100%)	0	0	100	100
33	QB	229/256 (90%)	204 (89%)	17 (7%)	8 (4%)	3	14
33	XB	229/256 (90%)	203 (89%)	21 (9%)	5 (2%)	5	23
34	QC	204/239 (85%)	191 (94%)	13 (6%)	0	100	100
34	XC	204/239 (85%)	189 (93%)	14 (7%)	1 (0%)	24	57
35	QD	206/209 (99%)	196 (95%)	10 (5%)	0	100	100
35	XD	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
36	QE	146/162 (90%)	145 (99%)	1 (1%)	0	100	100
36	XE	146/162 (90%)	145 (99%)	1 (1%)	0	100	100
37	QF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	XF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	QG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
38	XG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
39	QH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
39	XH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
40	QI	125/128 (98%)	116 (93%)	9 (7%)	0	100	100
40	XI	124/128 (97%)	113 (91%)	9 (7%)	2 (2%)	7	30
41	QJ	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	3	16
41	XJ	94/105 (90%)	83 (88%)	10 (11%)	1 (1%)	11	39
42	QK	112/129 (87%)	105 (94%)	7 (6%)	0	100	100
42	XK	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	14	44
43	QL	119/132 (90%)	118 (99%)	1 (1%)	0	100	100
43	XL	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
44	QM	114/126 (90%)	105 (92%)	8 (7%)	1 (1%)	14	44
44	XM	112/126 (89%)	104 (93%)	7 (6%)	1 (1%)	14	44
45	QN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	XN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
46	QO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
46	XO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
47	QP	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
47	XP	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
48	QQ	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
48	XQ	97/105 (92%)	95 (98%)	2 (2%)	0	100	100
49	QR	66/88 (75%)	66 (100%)	0	0	100	100
49	XR	66/88 (75%)	66 (100%)	0	0	100	100
50	QS	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
50	XS	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
51	QT	94/106 (89%)	90 (96%)	3 (3%)	1 (1%)	11	39
51	XT	96/106 (91%)	90 (94%)	4 (4%)	2 (2%)	5	24
52	QU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	XU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
55	QY	257/360 (71%)	218 (85%)	21 (8%)	18 (7%)	1	4
55	XY	258/360 (72%)	215 (83%)	30 (12%)	13 (5%)	1	9
All	All	11955/12848 (93%)	11397 (95%)	481 (4%)	77 (1%)	21	53

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	R4	47	GLN
26	R4	49	PHE
33	QB	16	HIS
55	QY	98	VAL
55	QY	210	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	RD	214/218 (98%)	209 (98%)	5 (2%)	44	70
3	YD	215/218 (99%)	207 (96%)	8 (4%)	30	61
4	RE	164/166 (99%)	157 (96%)	7 (4%)	26	57
4	YE	164/166 (99%)	156 (95%)	8 (5%)	22	53
5	RF	160/166 (96%)	148 (92%)	12 (8%)	12	38
5	YF	159/166 (96%)	151 (95%)	8 (5%)	22	53
6	RG	144/156 (92%)	138 (96%)	6 (4%)	26	58
6	YG	142/156 (91%)	136 (96%)	6 (4%)	26	58
7	RH	144/148 (97%)	140 (97%)	4 (3%)	38	67
7	YH	143/148 (97%)	133 (93%)	10 (7%)	14	41
8	RI	111/124 (90%)	106 (96%)	5 (4%)	24	56
8	YI	108/124 (87%)	99 (92%)	9 (8%)	10	34
9	RN	119/119 (100%)	113 (95%)	6 (5%)	22	53
9	YN	118/119 (99%)	114 (97%)	4 (3%)	32	63
10	RO	100/100 (100%)	98 (98%)	2 (2%)	48	73
10	YO	100/100 (100%)	99 (99%)	1 (1%)	68	81
11	RP	115/116 (99%)	109 (95%)	6 (5%)	21	51
11	YP	115/116 (99%)	110 (96%)	5 (4%)	26	57
12	RQ	111/111 (100%)	107 (96%)	4 (4%)	31	62
12	YQ	111/111 (100%)	108 (97%)	3 (3%)	39	68
13	RR	101/101 (100%)	92 (91%)	9 (9%)	9	32
13	YR	101/101 (100%)	93 (92%)	8 (8%)	11	36
14	RS	87/88 (99%)	85 (98%)	2 (2%)	44	70
14	YS	85/88 (97%)	83 (98%)	2 (2%)	43	70
15	RT	115/127 (91%)	110 (96%)	5 (4%)	26	57
15	YT	113/127 (89%)	109 (96%)	4 (4%)	32	62
16	RU	93/94 (99%)	90 (97%)	3 (3%)	34	64
16	YU	93/94 (99%)	91 (98%)	2 (2%)	45	71
17	RV	81/82 (99%)	76 (94%)	5 (6%)	16	45
17	YV	80/82 (98%)	77 (96%)	3 (4%)	29	60
18	RW	90/92 (98%)	86 (96%)	4 (4%)	25	56
18	YW	90/92 (98%)	86 (96%)	4 (4%)	25	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	RX	77/78 (99%)	75 (97%)	2 (3%)	40	69
19	YX	77/78 (99%)	76 (99%)	1 (1%)	61	79
20	RY	86/91 (94%)	84 (98%)	2 (2%)	44	70
20	YY	86/91 (94%)	84 (98%)	2 (2%)	44	70
21	RZ	169/179 (94%)	164 (97%)	5 (3%)	36	66
21	YZ	165/179 (92%)	161 (98%)	4 (2%)	43	70
22	R0	61/67 (91%)	59 (97%)	2 (3%)	33	64
22	Y0	61/67 (91%)	61 (100%)	0	100	100
23	R1	79/83 (95%)	77 (98%)	2 (2%)	42	69
23	Y1	81/83 (98%)	78 (96%)	3 (4%)	30	61
24	R2	65/67 (97%)	65 (100%)	0	100	100
24	Y2	66/67 (98%)	64 (97%)	2 (3%)	36	66
25	R3	51/52 (98%)	49 (96%)	2 (4%)	28	59
25	Y3	50/52 (96%)	47 (94%)	3 (6%)	17	47
26	R4	58/63 (92%)	56 (97%)	2 (3%)	32	63
26	Y4	54/63 (86%)	51 (94%)	3 (6%)	19	49
27	R5	51/52 (98%)	49 (96%)	2 (4%)	28	59
27	Y5	50/52 (96%)	48 (96%)	2 (4%)	28	59
28	R6	51/52 (98%)	50 (98%)	1 (2%)	48	73
28	Y6	50/52 (96%)	49 (98%)	1 (2%)	48	73
29	R7	41/42 (98%)	39 (95%)	2 (5%)	22	53
29	Y7	41/42 (98%)	39 (95%)	2 (5%)	22	53
30	R8	54/55 (98%)	53 (98%)	1 (2%)	50	73
30	Y8	54/55 (98%)	54 (100%)	0	100	100
31	R9	34/34 (100%)	34 (100%)	0	100	100
31	Y9	34/34 (100%)	34 (100%)	0	100	100
33	QB	191/220 (87%)	179 (94%)	12 (6%)	16	45
33	XB	187/220 (85%)	178 (95%)	9 (5%)	23	54
34	QC	144/188 (77%)	138 (96%)	6 (4%)	26	58
34	XC	140/188 (74%)	136 (97%)	4 (3%)	37	67
35	QD	171/181 (94%)	164 (96%)	7 (4%)	27	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	XD	172/181 (95%)	164 (95%)	8 (5%)	23	55
36	QE	114/123 (93%)	112 (98%)	2 (2%)	51	74
36	XE	114/123 (93%)	112 (98%)	2 (2%)	51	74
37	QF	85/90 (94%)	84 (99%)	1 (1%)	63	79
37	XF	85/90 (94%)	83 (98%)	2 (2%)	43	70
38	QG	120/127 (94%)	115 (96%)	5 (4%)	26	58
38	XG	119/127 (94%)	115 (97%)	4 (3%)	32	63
39	QH	116/119 (98%)	112 (97%)	4 (3%)	32	63
39	XH	114/119 (96%)	111 (97%)	3 (3%)	40	69
40	QI	91/99 (92%)	85 (93%)	6 (7%)	15	43
40	XI	88/99 (89%)	83 (94%)	5 (6%)	18	49
41	QJ	68/92 (74%)	67 (98%)	1 (2%)	57	77
41	XJ	68/92 (74%)	68 (100%)	0	100	100
42	QK	83/99 (84%)	81 (98%)	2 (2%)	43	70
42	XK	83/99 (84%)	81 (98%)	2 (2%)	43	70
43	QL	96/108 (89%)	94 (98%)	2 (2%)	47	72
43	XL	96/108 (89%)	92 (96%)	4 (4%)	26	58
44	QM	90/101 (89%)	87 (97%)	3 (3%)	33	64
44	XM	87/101 (86%)	83 (95%)	4 (5%)	24	55
45	QN	49/50 (98%)	46 (94%)	3 (6%)	17	46
45	XN	49/50 (98%)	47 (96%)	2 (4%)	27	58
46	QO	78/80 (98%)	77 (99%)	1 (1%)	61	79
46	XO	78/80 (98%)	76 (97%)	2 (3%)	40	69
47	QP	69/74 (93%)	65 (94%)	4 (6%)	18	48
47	XP	68/74 (92%)	64 (94%)	4 (6%)	18	47
48	QQ	94/97 (97%)	92 (98%)	2 (2%)	47	72
48	XQ	94/97 (97%)	92 (98%)	2 (2%)	47	72
49	QR	59/77 (77%)	56 (95%)	3 (5%)	21	52
49	XR	59/77 (77%)	57 (97%)	2 (3%)	32	63
50	QS	68/80 (85%)	65 (96%)	3 (4%)	25	56
50	XS	67/80 (84%)	66 (98%)	1 (2%)	57	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	QT	71/82 (87%)	67 (94%)	4 (6%)	19	49
51	XT	70/82 (85%)	66 (94%)	4 (6%)	18	49
52	QU	18/22 (82%)	18 (100%)	0	100	100
52	XU	18/22 (82%)	17 (94%)	1 (6%)	19	49
55	QY	210/300 (70%)	204 (97%)	6 (3%)	37	67
55	XY	211/300 (70%)	202 (96%)	9 (4%)	26	57
All	All	9784/10664 (92%)	9417 (96%)	367 (4%)	29	60

5 of 367 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	YI	116	LEU
26	Y4	58	ARG
10	YO	24	VAL
15	YT	96	ARG
33	XB	222	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
46	QO	9	GLN
7	YH	158	HIS
48	XQ	93	GLN
40	XI	89	ASN
50	QS	65	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	RA	2858/2915 (98%)	494 (17%)	22 (0%)
1	YA	2858/2915 (98%)	483 (16%)	24 (0%)
2	RB	119/122 (97%)	14 (11%)	0
2	YB	119/122 (97%)	13 (10%)	0
32	QA	1497/1521 (98%)	259 (17%)	15 (1%)
32	XA	1501/1521 (98%)	236 (15%)	16 (1%)
53	QV	76/77 (98%)	16 (21%)	0
53	XV	76/77 (98%)	16 (21%)	1 (1%)
54	QX	8/25 (32%)	4 (50%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	XX	9/25 (36%)	4 (44%)	0
All	All	9121/9320 (97%)	1539 (16%)	78 (0%)

5 of 1539 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	RA	10	G
1	RA	12	U
1	RA	36	G
1	RA	45	C
1	RA	59	U

5 of 78 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	YA	2172	U
32	XA	992	U
1	YA	2430	A
32	XA	560	U
32	XA	1256	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
32	5MC	XA	1404	32	19,22,23	4.32	7 (36%)	26,32,35	1.59	4 (15%)
32	7MG	QA	527	56,32	23,26,27	5.54	11 (47%)	27,39,42	4.06	12 (44%)
32	PSU	QA	516	56,32	18,21,22	1.19	1 (5%)	21,30,33	1.60	5 (23%)
32	2MG	XA	1207	32	23,26,27	3.11	7 (30%)	33,38,41	3.69	13 (39%)
32	M2G	QA	966	32	24,27,28	2.75	6 (25%)	33,40,43	2.38	9 (27%)
32	5MC	XA	967	32	19,22,23	4.22	7 (36%)	26,32,35	1.55	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4OC	RA	1920	1	19,22,24	3.28	7 (36%)	25,31,35	1.28	3 (12%)
43	0TD	XL	92	43	8,9,10	1.45	1 (12%)	6,11,13	2.71	4 (66%)
32	7MG	XA	527	56,32	23,26,27	5.41	11 (47%)	27,39,42	3.88	12 (44%)
1	5MC	RA	1942	56,1	19,22,23	4.14	7 (36%)	26,32,35	1.34	3 (11%)
43	0TD	QL	92	43	8,9,10	2.48	1 (12%)	6,11,13	3.31	4 (66%)
32	MA6	QA	1518	32	23,26,27	1.62	4 (17%)	33,38,41	2.90	9 (27%)
32	M2G	XA	966	32	24,27,28	2.59	6 (25%)	33,40,43	2.46	9 (27%)
1	PSU	YA	1911	1	18,21,22	1.10	1 (5%)	21,30,33	1.73	5 (23%)
1	5MU	YA	1915	1	19,22,23	5.20	6 (31%)	27,32,35	3.55	11 (40%)
1	2MA	YA	2503	56,1	22,25,26	4.10	8 (36%)	32,37,40	3.48	13 (40%)
32	5MC	XA	1407	32	19,22,23	4.17	7 (36%)	26,32,35	1.78	6 (23%)
32	UR3	QA	1498	32	19,22,23	3.16	6 (31%)	26,32,35	2.02	7 (26%)
1	5MC	RA	1962	56,1	19,22,23	4.05	7 (36%)	26,32,35	1.28	3 (11%)
1	OMG	YA	2251	53,56,1	23,26,27	2.55	7 (30%)	32,38,41	3.14	16 (50%)
32	2MG	QA	1207	32	23,26,27	3.19	7 (30%)	33,38,41	3.78	13 (39%)
32	MA6	XA	1519	32	23,26,27	1.65	4 (17%)	33,38,41	3.82	14 (42%)
1	2MU	RA	2552	56,1	19,22,24	6.09	12 (63%)	25,31,36	3.32	10 (40%)
1	OMG	RA	2251	53,56,1	23,26,27	2.54	7 (30%)	32,38,41	3.05	15 (46%)
1	5MC	YA	1962	56,1	19,22,23	3.84	7 (36%)	26,32,35	1.34	3 (11%)
1	5MU	RA	1915	1	19,22,23	5.15	7 (36%)	27,32,35	3.45	10 (37%)
1	5MU	YA	1939	56,1	19,22,23	4.91	5 (26%)	27,32,35	4.05	9 (33%)
1	5MC	YA	1942	1	19,22,23	4.12	7 (36%)	26,32,35	1.59	5 (19%)
1	PSU	YA	2605	1	18,21,22	1.04	1 (5%)	21,30,33	1.51	3 (14%)
32	4OC	XA	1402	32	20,23,24	3.11	7 (35%)	25,32,35	1.37	4 (16%)
1	2MU	YA	2552	56,1	19,22,24	6.14	12 (63%)	25,31,36	3.47	10 (40%)
32	UR3	XA	1498	56,32	19,22,23	3.10	6 (31%)	26,32,35	1.88	4 (15%)
32	5MC	QA	1400	32	19,22,23	4.24	7 (36%)	26,32,35	1.38	3 (11%)
32	5MC	QA	1407	32	19,22,23	4.27	7 (36%)	26,32,35	1.48	3 (11%)
1	PSU	RA	1917	1	18,21,22	1.11	1 (5%)	21,30,33	1.62	4 (19%)
32	MA6	QA	1519	32	23,26,27	1.53	7 (30%)	33,38,41	2.92	9 (27%)
32	PSU	XA	516	32	18,21,22	1.06	1 (5%)	21,30,33	1.69	5 (23%)
32	5MC	QA	1404	32	19,22,23	4.33	7 (36%)	26,32,35	1.54	4 (15%)
32	MA6	XA	1518	32	23,26,27	1.42	4 (17%)	33,38,41	3.01	10 (30%)
32	5MC	XA	1400	32	19,22,23	4.21	7 (36%)	26,32,35	1.68	5 (19%)
1	5MU	RA	1939	1	19,22,23	4.84	5 (26%)	27,32,35	3.68	8 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	YA	1917	1	18,21,22	0.99	1 (5%)	21,30,33	1.83	5 (23%)
1	PSU	RA	2605	1	18,21,22	1.09	1 (5%)	21,30,33	1.97	3 (14%)
1	4OC	YA	1920	1	19,22,24	3.11	7 (36%)	25,31,35	1.23	3 (12%)
1	PSU	RA	1911	1	18,21,22	1.04	1 (5%)	21,30,33	1.64	4 (19%)
32	4OC	QA	1402	32	20,23,24	3.26	7 (35%)	25,32,35	1.23	2 (8%)
1	2MA	RA	2503	56,1	22,25,26	4.22	8 (36%)	32,37,40	3.38	13 (40%)
32	5MC	QA	967	32	19,22,23	4.30	7 (36%)	26,32,35	1.48	4 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	XA	1404	32	-	0/7/25/26	0/2/2/2
32	7MG	QA	527	56,32	-	2/7/37/38	0/3/3/3
32	PSU	QA	516	56,32	-	0/7/25/26	0/2/2/2
32	2MG	XA	1207	32	-	0/9/27/28	0/3/3/3
32	M2G	QA	966	32	-	0/11/29/30	0/3/3/3
32	5MC	XA	967	32	-	1/7/25/26	0/2/2/2
1	4OC	RA	1920	1	-	0/9/27/30	0/2/2/2
43	0TD	XL	92	43	-	3/7/12/14	-
32	7MG	XA	527	56,32	-	2/7/37/38	0/3/3/3
1	5MC	RA	1942	56,1	-	0/7/25/26	0/2/2/2
43	0TD	QL	92	43	-	1/7/12/14	-
32	MA6	QA	1518	32	-	0/11/29/30	0/3/3/3
32	M2G	XA	966	32	-	0/11/29/30	0/3/3/3
1	PSU	YA	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	YA	1915	1	-	2/7/25/26	0/2/2/2
1	2MA	YA	2503	56,1	-	1/7/25/26	0/3/3/3
32	5MC	XA	1407	32	-	0/7/25/26	0/2/2/2
32	UR3	QA	1498	32	-	0/7/25/26	0/2/2/2
1	5MC	RA	1962	56,1	-	0/7/25/26	0/2/2/2
1	OMG	YA	2251	53,56,1	-	0/9/27/28	0/3/3/3
32	2MG	QA	1207	32	-	0/9/27/28	0/3/3/3
32	MA6	XA	1519	32	-	2/11/29/30	0/3/3/3
1	2MU	RA	2552	56,1	-	0/9/27/28	0/2/2/2
1	OMG	RA	2251	53,56,1	-	0/9/27/28	0/3/3/3
1	5MC	YA	1962	56,1	-	0/7/25/26	0/2/2/2
1	5MU	RA	1915	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	YA	1939	56,1	-	0/7/25/26	0/2/2/2
1	5MC	YA	1942	1	-	0/7/25/26	0/2/2/2
1	PSU	YA	2605	1	-	0/7/25/26	0/2/2/2
32	4OC	XA	1402	32	-	2/9/29/30	0/2/2/2
1	2MU	YA	2552	56,1	-	0/9/27/28	0/2/2/2
32	UR3	XA	1498	56,32	-	0/7/25/26	0/2/2/2
32	5MC	QA	1400	32	-	2/7/25/26	0/2/2/2
32	5MC	QA	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	RA	1917	1	-	0/7/25/26	0/2/2/2
32	MA6	QA	1519	32	-	3/11/29/30	0/3/3/3
32	PSU	XA	516	32	-	0/7/25/26	0/2/2/2
32	5MC	QA	1404	32	-	0/7/25/26	0/2/2/2
32	MA6	XA	1518	32	-	1/11/29/30	0/3/3/3
32	5MC	XA	1400	32	-	2/7/25/26	0/2/2/2
1	5MU	RA	1939	1	-	2/7/25/26	0/2/2/2
1	PSU	YA	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	RA	2605	1	-	0/7/25/26	0/2/2/2
1	4OC	YA	1920	1	-	1/9/27/30	0/2/2/2
1	PSU	RA	1911	1	-	0/7/25/26	0/2/2/2
32	4OC	QA	1402	32	-	2/9/29/30	0/2/2/2
1	2MA	RA	2503	56,1	-	0/7/25/26	0/3/3/3
32	5MC	QA	967	32	-	0/7/25/26	0/2/2/2

The worst 5 of 278 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	QA	527	7MG	C8-N9	17.08	1.56	1.45
32	XA	527	7MG	C8-N9	16.34	1.56	1.45
1	YA	2552	2MU	C5-C4	14.41	1.75	1.43
1	RA	2552	2MU	C5-C4	14.35	1.74	1.43
1	YA	2503	2MA	C4-N3	13.42	1.51	1.34

The worst 5 of 337 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	XA	1519	MA6	N1-C6-N6	-14.34	99.39	116.86
1	YA	1939	5MU	C5-C4-N3	14.33	127.77	115.32
1	RA	1939	5MU	C5-C4-N3	13.01	126.63	115.32
1	YA	1915	5MU	C5-C4-N3	12.31	126.02	115.32
32	QA	1207	2MG	C2-N3-C4	12.00	127.00	112.00

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	RA	1915	5MU	O4'-C1'-N1-C2
1	RA	1915	5MU	O4'-C1'-N1-C6
32	QA	1402	4OC	O4'-C4'-C5'-O5'
32	QA	1519	MA6	O4'-C4'-C5'-O5'
32	QA	1519	MA6	C5-C6-N6-C9

There are no ring outliers.

17 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	RA	1920	4OC	1	0
1	RA	1942	5MC	1	0
32	QA	1518	MA6	1	0
1	RA	1962	5MC	1	0
1	YA	2251	OMG	1	0
32	XA	1519	MA6	4	0
1	RA	2552	2MU	3	0
1	RA	2251	OMG	1	0
1	YA	1962	5MC	2	0
1	YA	1939	5MU	2	0
1	YA	2552	2MU	3	0
1	RA	1917	PSU	1	0
32	QA	1519	MA6	2	0
32	XA	1518	MA6	5	0
1	RA	1939	5MU	1	0
32	QA	1402	4OC	1	0
1	RA	2503	2MA	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2450 ligands modelled in this entry, 2448 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	SF4	XD	301	35	0,12,12	-	-	-		
58	SF4	QD	302	35	0,12,12	-	-	-		

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	RA	2856/2915 (97%)	-0.08	66 (2%) 61 37	25, 61, 221, 314	0
1	YA	2856/2915 (97%)	-0.22	76 (2%) 56 32	15, 48, 188, 299	0
2	RB	120/122 (98%)	0.21	2 (1%) 69 45	64, 96, 118, 154	0
2	YB	120/122 (98%)	-0.19	1 (0%) 82 63	40, 67, 84, 108	0
3	RD	275/276 (99%)	0.05	3 (1%) 78 56	24, 49, 69, 101	0
3	YD	275/276 (99%)	-0.11	1 (0%) 88 76	19, 40, 60, 93	0
4	RE	204/206 (99%)	0.28	5 (2%) 58 34	29, 62, 92, 103	0
4	YE	204/206 (99%)	0.22	3 (1%) 72 48	20, 62, 91, 101	0
5	RF	203/210 (96%)	0.35	2 (0%) 79 58	30, 69, 104, 113	0
5	YF	203/210 (96%)	0.03	0 100 100	17, 51, 81, 93	0
6	RG	181/182 (99%)	1.05	17 (9%) 14 7	80, 108, 127, 140	0
6	YG	181/182 (99%)	0.46	5 (2%) 55 31	60, 78, 108, 131	0
7	RH	174/180 (96%)	1.26	28 (16%) 4 3	96, 141, 180, 185	0
7	YH	173/180 (96%)	0.62	9 (5%) 33 16	49, 76, 96, 123	0
8	RI	147/148 (99%)	1.16	24 (16%) 4 3	60, 110, 130, 141	0
8	YI	146/148 (98%)	0.75	5 (3%) 48 27	52, 90, 117, 125	0
9	RN	140/140 (100%)	0.62	5 (3%) 46 25	44, 71, 100, 121	0
9	YN	140/140 (100%)	0.15	0 100 100	27, 58, 90, 104	0
10	RO	122/122 (100%)	0.06	1 (0%) 82 63	35, 56, 73, 85	0
10	YO	122/122 (100%)	0.04	1 (0%) 82 63	30, 53, 72, 81	0
11	RP	149/150 (99%)	0.46	2 (1%) 75 52	33, 73, 98, 111	0
11	YP	149/150 (99%)	0.18	1 (0%) 84 66	21, 52, 80, 96	0
12	RQ	141/141 (100%)	0.49	2 (1%) 73 50	46, 71, 88, 100	0
12	YQ	141/141 (100%)	0.20	4 (2%) 55 31	33, 51, 67, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	RR	118/118 (100%)	0.23	1 (0%) 82 63	30, 55, 72, 83	0
13	YR	118/118 (100%)	0.30	0 100 100	30, 55, 77, 97	0
14	RS	110/112 (98%)	0.96	7 (6%) 25 13	72, 91, 105, 116	0
14	YS	110/112 (98%)	0.31	4 (3%) 46 25	43, 63, 80, 88	0
15	RT	131/146 (89%)	0.23	3 (2%) 61 37	43, 64, 99, 117	0
15	YT	131/146 (89%)	0.36	2 (1%) 72 48	42, 66, 91, 117	0
16	RU	116/118 (98%)	0.30	0 100 100	33, 62, 91, 97	0
16	YU	116/118 (98%)	0.14	2 (1%) 69 45	23, 48, 88, 104	0
17	RV	101/101 (100%)	0.31	0 100 100	40, 82, 103, 115	0
17	YV	101/101 (100%)	0.12	0 100 100	25, 62, 86, 105	0
18	RW	112/113 (99%)	0.27	3 (2%) 56 32	36, 52, 84, 102	0
18	YW	112/113 (99%)	0.16	0 100 100	32, 47, 75, 107	0
19	RX	95/96 (98%)	0.58	2 (2%) 63 39	38, 65, 82, 91	0
19	YX	95/96 (98%)	0.08	1 (1%) 78 56	24, 42, 70, 91	0
20	RY	107/110 (97%)	1.25	14 (13%) 7 4	58, 92, 119, 129	0
20	YY	107/110 (97%)	0.59	3 (2%) 55 31	43, 68, 93, 107	0
21	RZ	203/206 (98%)	1.06	20 (9%) 13 7	78, 109, 144, 170	0
21	YZ	201/206 (97%)	0.58	16 (7%) 18 9	54, 78, 116, 163	0
22	R0	77/85 (90%)	0.58	3 (3%) 43 23	47, 64, 81, 96	0
22	Y0	77/85 (90%)	0.10	2 (2%) 57 33	28, 43, 72, 95	0
23	R1	97/98 (98%)	0.46	5 (5%) 33 16	31, 60, 90, 100	0
23	Y1	97/98 (98%)	0.23	1 (1%) 79 58	28, 50, 91, 106	0
24	R2	70/72 (97%)	0.56	2 (2%) 53 30	58, 81, 97, 108	0
24	Y2	70/72 (97%)	0.34	4 (5%) 29 15	32, 57, 77, 91	0
25	R3	59/60 (98%)	0.56	3 (5%) 33 17	43, 70, 100, 125	0
25	Y3	59/60 (98%)	0.25	0 100 100	30, 48, 92, 99	0
26	R4	69/71 (97%)	1.09	6 (8%) 16 8	104, 142, 170, 174	0
26	Y4	69/71 (97%)	1.05	10 (14%) 6 3	67, 117, 168, 175	0
27	R5	59/60 (98%)	0.27	0 100 100	30, 60, 109, 116	0
27	Y5	59/60 (98%)	0.41	3 (5%) 33 17	24, 56, 129, 138	0
28	R6	53/54 (98%)	2.41	29 (54%) 0 0	144, 186, 208, 215	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	Y6	53/54 (98%)	2.44	33 (62%) 0 0	119, 157, 178, 184	0
29	R7	48/49 (97%)	0.38	3 (6%) 26 13	29, 41, 65, 82	0
29	Y7	48/49 (97%)	-0.14	1 (2%) 63 39	19, 27, 57, 82	0
30	R8	64/65 (98%)	0.53	2 (3%) 51 29	41, 54, 70, 90	0
30	Y8	64/65 (98%)	0.08	0 100 100	18, 42, 63, 81	0
31	R9	37/37 (100%)	4.18	33 (89%) 0 0	122, 170, 195, 206	0
31	Y9	37/37 (100%)	4.07	35 (94%) 0 0	120, 136, 170, 177	0
32	QA	1488/1521 (97%)	0.40	52 (3%) 47 26	45, 96, 172, 287	0
32	XA	1492/1521 (98%)	0.24	19 (1%) 75 52	29, 91, 170, 268	0
33	QB	231/256 (90%)	1.13	31 (13%) 7 4	98, 130, 151, 163	0
33	XB	231/256 (90%)	0.94	25 (10%) 11 6	84, 114, 143, 160	0
34	QC	206/239 (86%)	0.98	24 (11%) 9 5	97, 123, 151, 165	0
34	XC	206/239 (86%)	0.79	19 (9%) 14 7	75, 99, 124, 139	0
35	QD	208/209 (99%)	0.89	20 (9%) 13 7	76, 97, 116, 125	0
35	XD	208/209 (99%)	1.23	29 (13%) 6 4	76, 104, 129, 135	0
36	QE	148/162 (91%)	0.65	7 (4%) 36 19	69, 91, 107, 127	0
36	XE	148/162 (91%)	0.54	8 (5%) 31 15	65, 89, 109, 119	0
37	QF	100/101 (99%)	0.87	4 (4%) 42 23	87, 105, 116, 119	0
37	XF	100/101 (99%)	0.39	0 100 100	61, 86, 105, 109	0
38	QG	155/156 (99%)	1.03	22 (14%) 6 4	93, 112, 135, 142	0
38	XG	155/156 (99%)	0.67	11 (7%) 22 11	80, 99, 115, 128	0
39	QH	137/138 (99%)	0.83	8 (5%) 29 14	80, 96, 114, 119	0
39	XH	137/138 (99%)	0.77	5 (3%) 46 25	74, 95, 107, 112	0
40	QI	127/128 (99%)	1.74	49 (38%) 1 1	88, 129, 153, 159	0
40	XI	126/128 (98%)	1.28	22 (17%) 4 2	75, 114, 131, 139	0
41	QJ	97/105 (92%)	1.55	24 (24%) 2 1	99, 126, 146, 152	0
41	XJ	96/105 (91%)	1.34	16 (16%) 4 3	82, 113, 133, 138	0
42	QK	114/129 (88%)	0.59	2 (1%) 67 43	65, 94, 108, 121	0
42	XK	114/129 (88%)	0.32	2 (1%) 67 43	52, 76, 93, 108	0
43	QL	121/132 (91%)	0.81	14 (11%) 9 5	52, 73, 86, 92	0
43	XL	121/132 (91%)	0.72	9 (7%) 20 10	57, 72, 86, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	QM	116/126 (92%)	1.40	25 (21%) 2 1	101, 122, 138, 148	0
44	XM	114/126 (90%)	1.08	12 (10%) 11 6	83, 108, 119, 122	0
45	QN	60/61 (98%)	1.75	21 (35%) 1 1	104, 115, 129, 132	0
45	XN	60/61 (98%)	1.19	9 (15%) 5 3	72, 93, 109, 114	0
46	QO	88/89 (98%)	0.76	7 (7%) 18 9	70, 87, 118, 129	0
46	XO	88/89 (98%)	0.68	6 (6%) 23 12	52, 79, 109, 113	0
47	QP	82/88 (93%)	0.89	8 (9%) 13 7	62, 83, 105, 118	0
47	XP	82/88 (93%)	1.36	15 (18%) 3 2	73, 103, 125, 138	0
48	QQ	99/105 (94%)	0.82	6 (6%) 27 13	60, 83, 101, 111	0
48	XQ	99/105 (94%)	0.88	12 (12%) 8 5	59, 82, 100, 107	0
49	QR	68/88 (77%)	0.89	6 (8%) 15 8	87, 108, 120, 131	0
49	XR	68/88 (77%)	0.49	0 100 100	54, 86, 108, 112	0
50	QS	83/93 (89%)	1.39	17 (20%) 2 2	103, 125, 135, 141	0
50	XS	83/93 (89%)	1.40	14 (16%) 4 2	90, 109, 140, 145	0
51	QT	96/106 (90%)	1.00	11 (11%) 9 5	58, 80, 103, 108	0
51	XT	98/106 (92%)	1.52	27 (27%) 1 1	81, 98, 112, 123	0
52	QU	23/27 (85%)	2.30	11 (47%) 0 0	95, 114, 119, 121	0
52	XU	23/27 (85%)	1.81	9 (39%) 1 1	90, 96, 103, 111	0
53	QV	77/77 (100%)	0.17	3 (3%) 43 23	63, 93, 134, 144	0
53	XV	77/77 (100%)	0.07	2 (2%) 57 33	48, 85, 126, 147	0
54	QX	9/25 (36%)	1.34	3 (33%) 1 1	78, 91, 116, 129	0
54	XX	10/25 (40%)	1.70	4 (40%) 1 1	62, 78, 125, 136	0
55	QY	259/360 (71%)	1.19	48 (18%) 3 2	71, 111, 149, 181	0
55	XY	260/360 (72%)	0.90	26 (10%) 12 6	54, 94, 135, 143	0
All	All	21260/22168 (95%)	0.41	1240 (5%) 29 14	15, 78, 147, 314	0

The worst 5 of 1240 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	R9	26	ILE	10.4
31	R9	15	LYS	7.7
31	R9	23	VAL	7.6
31	Y9	33	LYS	7.4
22	Y0	8	GLY	7.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	5MU	RA	1915	21/22	0.82	0.13	88,92,95,97	0
32	2MG	QA	1207	24/25	0.85	0.12	117,127,138,140	0
32	2MG	XA	1207	24/25	0.86	0.14	91,97,111,112	0
32	PSU	QA	516	20/21	0.87	0.10	90,93,97,97	0
1	5MU	YA	1915	21/22	0.88	0.11	71,75,78,80	0
1	PSU	RA	1917	20/21	0.88	0.11	66,77,85,87	0
32	M2G	QA	966	25/26	0.89	0.15	81,89,103,104	0
32	7MG	QA	527	24/25	0.89	0.13	69,74,78,83	0
1	4OC	RA	1920	21/23	0.90	0.14	69,81,86,87	0
43	0TD	QL	92	10/11	0.90	0.14	73,80,84,86	0
32	5MC	XA	967	21/22	0.91	0.15	73,77,82,83	0
32	M2G	XA	966	25/26	0.91	0.13	75,80,91,94	0
32	4OC	XA	1402	22/23	0.91	0.12	45,54,61,64	0
43	0TD	XL	92	10/11	0.91	0.13	75,79,89,89	0
32	5MC	QA	1400	21/22	0.92	0.14	74,86,88,91	0
1	PSU	YA	1917	20/21	0.92	0.09	53,61,62,64	0
32	PSU	XA	516	20/21	0.92	0.09	73,80,84,87	0
1	PSU	RA	1911	20/21	0.92	0.10	71,79,83,85	0
32	5MC	QA	1404	21/22	0.93	0.13	61,66,69,71	0
1	4OC	YA	1920	21/23	0.93	0.12	44,53,55,57	0
32	5MC	QA	967	21/22	0.93	0.12	86,91,94,98	0
32	5MC	XA	1404	21/22	0.93	0.12	32,41,48,52	0
32	4OC	QA	1402	22/23	0.93	0.11	63,70,75,79	0
32	MA6	QA	1518	24/25	0.94	0.11	58,65,69,70	0
1	5MU	RA	1939	21/22	0.94	0.11	38,41,46,48	0
32	UR3	QA	1498	21/22	0.94	0.13	59,62,65,69	0
1	5MC	RA	1942	21/22	0.95	0.10	48,52,62,65	0
1	PSU	YA	1911	20/21	0.95	0.08	50,60,64,64	0
32	UR3	XA	1498	21/22	0.95	0.11	36,47,58,62	0
32	MA6	XA	1519	24/25	0.95	0.13	41,49,53,53	0
32	7MG	XA	527	24/25	0.95	0.12	57,64,66,70	0
32	5MC	QA	1407	21/22	0.96	0.09	47,55,67,79	0
1	5MC	RA	1962	21/22	0.96	0.09	38,42,46,50	0
1	OMG	RA	2251	24/25	0.96	0.09	33,39,42,43	0
32	5MC	XA	1400	21/22	0.96	0.10	42,52,62,66	0
1	5MU	YA	1939	21/22	0.96	0.09	15,24,29,30	0
1	5MC	YA	1942	21/22	0.96	0.09	30,37,42,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MC	YA	1962	21/22	0.96	0.09	32,37,43,46	0
32	MA6	XA	1518	24/25	0.96	0.11	43,49,54,56	0
1	2MA	RA	2503	23/24	0.96	0.09	25,28,37,43	0
1	2MU	RA	2552	21/23	0.96	0.09	34,37,46,47	0
1	OMG	YA	2251	24/25	0.97	0.08	22,28,32,33	0
32	5MC	XA	1407	21/22	0.97	0.07	35,42,46,47	0
1	2MA	YA	2503	23/24	0.97	0.07	14,22,27,32	0
1	2MU	YA	2552	21/23	0.97	0.08	27,31,37,38	0
1	PSU	RA	2605	20/21	0.97	0.07	23,33,39,43	0
32	MA6	QA	1519	24/25	0.97	0.10	53,60,63,63	0
1	PSU	YA	2605	20/21	0.98	0.07	16,25,28,30	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	1678	1/1	-0.18	0.28	85,85,85,85	0
56	MG	QA	1844	1/1	-0.05	0.27	82,82,82,82	0
56	MG	QA	1827	1/1	-0.04	0.23	109,109,109,109	0
56	MG	QA	1855	1/1	0.01	0.50	85,85,85,85	0
56	MG	QA	1828	1/1	0.01	0.65	112,112,112,112	0
56	MG	XA	1670	1/1	0.02	0.32	101,101,101,101	0
56	MG	QA	1644	1/1	0.03	0.34	107,107,107,107	0
56	MG	QA	1766	1/1	0.04	0.35	94,94,94,94	0
56	MG	QA	1659	1/1	0.05	0.37	104,104,104,104	0
56	MG	RA	3441	1/1	0.07	0.39	75,75,75,75	0
56	MG	QA	1697	1/1	0.08	0.20	85,85,85,85	0
56	MG	RA	3193	1/1	0.08	0.28	97,97,97,97	0
56	MG	R9	101	1/1	0.11	0.34	94,94,94,94	0
56	MG	QA	1830	1/1	0.14	0.22	86,86,86,86	0
56	MG	YA	3056	1/1	0.15	0.23	82,82,82,82	0
56	MG	XA	1657	1/1	0.15	0.16	91,91,91,91	0
56	MG	RG	201	1/1	0.16	0.23	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1748	1/1	0.18	0.28	88,88,88,88	0
56	MG	QA	1765	1/1	0.19	0.20	88,88,88,88	0
56	MG	RF	303	1/1	0.19	0.45	95,95,95,95	0
56	MG	RA	3911	1/1	0.20	0.25	95,95,95,95	0
56	MG	RN	202	1/1	0.21	0.18	86,86,86,86	0
56	MG	RA	3620	1/1	0.23	0.17	119,119,119,119	0
56	MG	YA	3188	1/1	0.23	0.29	88,88,88,88	0
56	MG	QA	1617	1/1	0.23	0.16	105,105,105,105	0
57	ZN	R9	102	1/1	0.24	0.48	203,203,203,203	0
56	MG	RA	3346	1/1	0.25	0.28	95,95,95,95	0
56	MG	RA	3558	1/1	0.25	0.32	68,68,68,68	0
56	MG	XA	1719	1/1	0.27	0.30	61,61,61,61	0
56	MG	YA	3626	1/1	0.27	0.49	94,94,94,94	0
56	MG	RA	3669	1/1	0.27	0.32	71,71,71,71	0
56	MG	RA	3184	1/1	0.30	0.79	94,94,94,94	0
56	MG	XA	1778	1/1	0.31	0.26	90,90,90,90	0
56	MG	RA	3552	1/1	0.31	0.19	79,79,79,79	0
56	MG	RB	208	1/1	0.32	0.18	87,87,87,87	0
56	MG	RA	3242	1/1	0.32	0.18	60,60,60,60	0
56	MG	RA	3699	1/1	0.33	0.21	72,72,72,72	0
56	MG	RD	315	1/1	0.33	0.35	69,69,69,69	0
56	MG	QA	1805	1/1	0.33	0.24	82,82,82,82	0
56	MG	RA	3535	1/1	0.33	0.45	90,90,90,90	0
56	MG	QA	1610	1/1	0.33	0.21	76,76,76,76	0
56	MG	QA	1720	1/1	0.33	0.31	72,72,72,72	0
56	MG	RA	3851	1/1	0.34	0.39	74,74,74,74	0
56	MG	YB	212	1/1	0.34	0.28	73,73,73,73	0
56	MG	RA	3803	1/1	0.34	0.37	83,83,83,83	0
56	MG	RA	3034	1/1	0.35	0.26	81,81,81,81	0
56	MG	RA	3415	1/1	0.35	0.22	87,87,87,87	0
56	MG	RG	204	1/1	0.35	0.26	97,97,97,97	0
56	MG	QD	303	1/1	0.36	0.24	83,83,83,83	0
56	MG	RA	3355	1/1	0.36	0.48	88,88,88,88	0
56	MG	RA	3519	1/1	0.37	0.18	57,57,57,57	0
56	MG	QA	1791	1/1	0.37	0.17	63,63,63,63	0
56	MG	RB	221	1/1	0.37	0.18	89,89,89,89	0
56	MG	RA	3116	1/1	0.37	0.67	89,89,89,89	0
56	MG	QA	1751	1/1	0.38	0.25	99,99,99,99	0
56	MG	RA	3099	1/1	0.38	0.25	79,79,79,79	0
56	MG	RA	3073	1/1	0.38	0.35	73,73,73,73	0
56	MG	RA	3737	1/1	0.38	0.22	64,64,64,64	0
56	MG	YB	203	1/1	0.38	0.16	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3666	1/1	0.38	0.18	93,93,93,93	0
56	MG	YB	216	1/1	0.38	0.31	85,85,85,85	0
56	MG	RA	3056	1/1	0.39	0.29	89,89,89,89	0
56	MG	RA	3619	1/1	0.39	0.19	90,90,90,90	0
56	MG	RA	3345	1/1	0.39	0.17	69,69,69,69	0
56	MG	RA	3087	1/1	0.39	0.58	59,59,59,59	0
56	MG	QA	1797	1/1	0.40	0.18	83,83,83,83	0
56	MG	QA	1711	1/1	0.40	0.41	91,91,91,91	0
56	MG	RA	3449	1/1	0.40	0.28	65,65,65,65	0
56	MG	YQ	203	1/1	0.41	0.20	62,62,62,62	0
56	MG	QA	1808	1/1	0.41	0.29	84,84,84,84	0
56	MG	YA	3455	1/1	0.41	0.54	88,88,88,88	0
56	MG	QA	1709	1/1	0.41	0.26	72,72,72,72	0
56	MG	RT	203	1/1	0.42	0.15	96,96,96,96	0
56	MG	RA	3501	1/1	0.42	0.18	78,78,78,78	0
56	MG	YA	3498	1/1	0.42	0.36	86,86,86,86	0
56	MG	RA	3633	1/1	0.43	0.81	110,110,110,110	0
56	MG	RA	3007	1/1	0.43	0.15	83,83,83,83	0
56	MG	RA	3597	1/1	0.43	0.42	68,68,68,68	0
56	MG	RA	3622	1/1	0.43	0.29	53,53,53,53	0
56	MG	RA	3717	1/1	0.43	0.23	81,81,81,81	0
56	MG	QA	1817	1/1	0.44	0.14	67,67,67,67	0
56	MG	RA	3665	1/1	0.44	0.32	71,71,71,71	0
56	MG	QA	1698	1/1	0.44	0.25	73,73,73,73	0
56	MG	QE	202	1/1	0.44	0.19	77,77,77,77	0
56	MG	RA	3244	1/1	0.44	0.70	86,86,86,86	0
56	MG	QA	1715	1/1	0.45	0.15	68,68,68,68	0
56	MG	XA	1713	1/1	0.45	0.46	83,83,83,83	0
56	MG	RA	3353	1/1	0.45	0.36	56,56,56,56	0
56	MG	YA	3199	1/1	0.46	0.27	77,77,77,77	0
56	MG	RA	3916	1/1	0.46	0.42	98,98,98,98	0
56	MG	XA	1705	1/1	0.46	0.23	58,58,58,58	0
56	MG	R1	103	1/1	0.46	0.42	65,65,65,65	0
56	MG	XA	1613	1/1	0.47	0.20	81,81,81,81	0
56	MG	YA	3016	1/1	0.47	0.41	108,108,108,108	0
56	MG	RB	207	1/1	0.47	0.20	80,80,80,80	0
56	MG	YA	3566	1/1	0.47	0.35	94,94,94,94	0
56	MG	YA	3223	1/1	0.47	0.13	80,80,80,80	0
56	MG	QA	1762	1/1	0.48	0.25	92,92,92,92	0
56	MG	RA	3150	1/1	0.48	0.33	94,94,94,94	0
56	MG	XA	1636	1/1	0.48	0.18	71,71,71,71	0
56	MG	RA	3247	1/1	0.48	0.40	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1666	1/1	0.48	0.10	95,95,95,95	0
56	MG	YA	3451	1/1	0.48	0.19	68,68,68,68	0
56	MG	RA	3804	1/1	0.48	0.19	72,72,72,72	0
56	MG	RA	3658	1/1	0.48	0.17	62,62,62,62	0
56	MG	QA	1800	1/1	0.48	0.28	75,75,75,75	0
56	MG	RA	3259	1/1	0.48	0.08	102,102,102,102	0
56	MG	RW	202	1/1	0.48	0.44	76,76,76,76	0
56	MG	QA	1695	1/1	0.48	0.20	85,85,85,85	0
56	MG	YA	3159	1/1	0.48	0.25	70,70,70,70	0
56	MG	RA	3837	1/1	0.49	0.21	59,59,59,59	0
56	MG	XA	1671	1/1	0.49	0.16	70,70,70,70	0
56	MG	RA	3596	1/1	0.49	0.20	81,81,81,81	0
56	MG	RA	3782	1/1	0.49	0.20	93,93,93,93	0
56	MG	YA	3505	1/1	0.49	0.28	53,53,53,53	0
56	MG	RA	3066	1/1	0.49	0.25	85,85,85,85	0
56	MG	RA	3101	1/1	0.49	0.26	87,87,87,87	0
56	MG	XA	1659	1/1	0.49	0.14	73,73,73,73	0
56	MG	QA	1684	1/1	0.49	0.13	90,90,90,90	0
56	MG	YA	3692	1/1	0.50	0.24	79,79,79,79	0
56	MG	RA	3808	1/1	0.50	0.21	63,63,63,63	0
56	MG	RA	3281	1/1	0.50	0.16	70,70,70,70	0
56	MG	RA	3801	1/1	0.50	0.29	66,66,66,66	0
56	MG	RA	3302	1/1	0.50	0.28	44,44,44,44	0
56	MG	XA	1610	1/1	0.50	0.40	87,87,87,87	0
56	MG	RW	201	1/1	0.50	0.21	65,65,65,65	0
56	MG	QA	1646	1/1	0.50	0.13	81,81,81,81	0
56	MG	RA	3689	1/1	0.50	0.37	56,56,56,56	0
56	MG	QA	1836	1/1	0.50	0.27	46,46,46,46	0
57	ZN	Y5	103	1/1	0.50	0.18	214,214,214,214	0
56	MG	YA	3523	1/1	0.51	0.21	61,61,61,61	0
56	MG	RA	3177	1/1	0.51	0.23	77,77,77,77	0
56	MG	QT	201	1/1	0.51	0.29	64,64,64,64	0
56	MG	YA	3351	1/1	0.51	0.19	57,57,57,57	0
56	MG	XA	1746	1/1	0.51	0.28	49,49,49,49	0
56	MG	RA	3424	1/1	0.51	0.19	72,72,72,72	0
56	MG	RY	201	1/1	0.51	0.23	76,76,76,76	0
56	MG	RA	3945	1/1	0.51	0.24	62,62,62,62	0
56	MG	RA	3241	1/1	0.51	0.35	76,76,76,76	0
56	MG	RA	3593	1/1	0.52	0.28	71,71,71,71	0
56	MG	YA	3331	1/1	0.52	0.28	67,67,67,67	0
56	MG	RA	3953	1/1	0.52	0.23	67,67,67,67	0
56	MG	RA	3856	1/1	0.52	0.24	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	RA	3340	1/1	0.52	0.15	70,70,70,70	0
56	MG	XA	1608	1/1	0.52	0.17	89,89,89,89	0
56	MG	RA	3131	1/1	0.52	0.22	72,72,72,72	0
56	MG	RA	3928	1/1	0.52	0.15	72,72,72,72	0
56	MG	YA	3172	1/1	0.52	0.11	78,78,78,78	0
56	MG	QA	1653	1/1	0.52	0.20	73,73,73,73	0
56	MG	XE	201	1/1	0.52	0.19	47,47,47,47	0
56	MG	RA	3938	1/1	0.52	0.15	42,42,42,42	0
56	MG	XA	1661	1/1	0.52	0.15	61,61,61,61	0
56	MG	XA	1689	1/1	0.53	0.28	83,83,83,83	0
56	MG	YA	3512	1/1	0.53	0.19	69,69,69,69	0
56	MG	RA	3648	1/1	0.53	0.39	100,100,100,100	0
56	MG	RA	3512	1/1	0.53	0.30	67,67,67,67	0
56	MG	RA	3731	1/1	0.53	0.23	71,71,71,71	0
56	MG	QA	1640	1/1	0.54	0.24	59,59,59,59	0
56	MG	RA	3816	1/1	0.54	0.28	106,106,106,106	0
56	MG	RA	3641	1/1	0.54	0.28	55,55,55,55	0
56	MG	QA	1730	1/1	0.54	0.21	77,77,77,77	0
56	MG	RA	3690	1/1	0.54	0.60	65,65,65,65	0
56	MG	R0	107	1/1	0.54	0.23	69,69,69,69	0
56	MG	RA	3038	1/1	0.54	0.32	77,77,77,77	0
56	MG	RB	206	1/1	0.54	0.16	95,95,95,95	0
56	MG	QA	1608	1/1	0.54	0.24	85,85,85,85	0
56	MG	RA	3757	1/1	0.54	0.59	80,80,80,80	0
56	MG	RA	3764	1/1	0.54	0.20	82,82,82,82	0
56	MG	YA	3712	1/1	0.55	0.21	49,49,49,49	0
56	MG	RA	3384	1/1	0.55	0.39	71,71,71,71	0
56	MG	RA	3273	1/1	0.55	0.23	73,73,73,73	0
56	MG	YA	3405	1/1	0.55	0.22	54,54,54,54	0
56	MG	RA	3810	1/1	0.55	0.14	81,81,81,81	0
56	MG	RA	3616	1/1	0.55	0.70	65,65,65,65	0
56	MG	YA	3096	1/1	0.55	0.17	81,81,81,81	0
56	MG	RA	3704	1/1	0.55	0.14	50,50,50,50	0
56	MG	QA	1850	1/1	0.55	0.31	98,98,98,98	0
56	MG	RA	3637	1/1	0.55	0.41	98,98,98,98	0
56	MG	RA	3289	1/1	0.55	0.85	114,114,114,114	0
56	MG	QE	201	1/1	0.55	0.15	60,60,60,60	0
56	MG	YA	3258	1/1	0.55	0.17	48,48,48,48	0
56	MG	RA	3838	1/1	0.56	0.26	76,76,76,76	0
56	MG	RB	217	1/1	0.56	0.30	88,88,88,88	0
56	MG	YA	3261	1/1	0.56	0.30	96,96,96,96	0
56	MG	RA	3258	1/1	0.56	0.26	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3257	1/1	0.56	0.47	52,52,52,52	0
56	MG	YA	3587	1/1	0.56	0.27	56,56,56,56	0
56	MG	XA	1646	1/1	0.56	0.18	77,77,77,77	0
56	MG	RF	301	1/1	0.56	0.18	57,57,57,57	0
56	MG	QG	203	1/1	0.56	0.12	81,81,81,81	0
56	MG	YA	3454	1/1	0.56	0.40	73,73,73,73	0
56	MG	RA	3898	1/1	0.56	0.23	62,62,62,62	0
56	MG	YA	3466	1/1	0.56	0.23	69,69,69,69	0
56	MG	RA	3425	1/1	0.57	0.16	73,73,73,73	0
56	MG	QA	1656	1/1	0.57	0.29	72,72,72,72	0
56	MG	RA	3362	1/1	0.57	0.17	69,69,69,69	0
56	MG	XA	1616	1/1	0.57	0.28	83,83,83,83	0
56	MG	YA	3642	1/1	0.57	0.25	61,61,61,61	0
56	MG	RA	3448	1/1	0.57	0.37	77,77,77,77	0
56	MG	YA	3149	1/1	0.57	0.16	101,101,101,101	0
56	MG	YA	3272	1/1	0.57	0.37	45,45,45,45	0
56	MG	QA	1763	1/1	0.57	0.09	67,67,67,67	0
56	MG	XA	1664	1/1	0.57	0.13	74,74,74,74	0
56	MG	RA	3037	1/1	0.57	0.26	69,69,69,69	0
56	MG	YA	3359	1/1	0.57	0.18	72,72,72,72	0
56	MG	RA	3051	1/1	0.58	0.52	110,110,110,110	0
56	MG	QI	201	1/1	0.58	0.12	74,74,74,74	0
56	MG	RA	3317	1/1	0.58	0.34	85,85,85,85	0
56	MG	RA	3973	1/1	0.58	0.20	42,42,42,42	0
56	MG	YA	3691	1/1	0.58	0.38	60,60,60,60	0
56	MG	QA	1833	1/1	0.58	0.28	74,74,74,74	0
56	MG	RA	3149	1/1	0.58	0.34	63,63,63,63	0
56	MG	YA	3104	1/1	0.58	0.42	96,96,96,96	0
56	MG	QA	1801	1/1	0.58	0.11	63,63,63,63	0
56	MG	XA	1690	1/1	0.58	0.14	61,61,61,61	0
56	MG	XA	1704	1/1	0.58	0.41	79,79,79,79	0
56	MG	YA	3155	1/1	0.58	0.39	92,92,92,92	0
56	MG	RQ	204	1/1	0.58	0.36	76,76,76,76	0
56	MG	YA	3464	1/1	0.58	0.34	64,64,64,64	0
56	MG	YA	3162	1/1	0.58	0.35	94,94,94,94	0
56	MG	RA	3570	1/1	0.58	0.14	58,58,58,58	0
56	MG	XA	1614	1/1	0.58	0.14	60,60,60,60	0
56	MG	QA	1815	1/1	0.58	0.40	92,92,92,92	0
56	MG	RV	202	1/1	0.58	0.15	83,83,83,83	0
56	MG	QA	1826	1/1	0.58	0.15	92,92,92,92	0
56	MG	XA	1663	1/1	0.59	0.18	61,61,61,61	0
56	MG	RA	3707	1/1	0.59	0.19	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	3789	1/1	0.59	0.30	95,95,95,95	0
56	MG	QA	1806	1/1	0.59	0.14	49,49,49,49	0
56	MG	RA	3396	1/1	0.59	0.12	67,67,67,67	0
56	MG	QA	1710	1/1	0.59	0.18	92,92,92,92	0
56	MG	QQ	201	1/1	0.60	0.12	63,63,63,63	0
56	MG	YA	3196	1/1	0.60	0.11	71,71,71,71	0
56	MG	RA	3333	1/1	0.60	0.26	39,39,39,39	0
56	MG	RA	3802	1/1	0.60	0.23	81,81,81,81	0
56	MG	YA	3044	1/1	0.60	0.14	72,72,72,72	0
56	MG	QA	1673	1/1	0.60	0.39	58,58,58,58	0
56	MG	YA	3264	1/1	0.60	0.39	70,70,70,70	0
56	MG	QA	1683	1/1	0.60	0.19	60,60,60,60	0
56	MG	YA	3097	1/1	0.60	0.32	82,82,82,82	0
56	MG	RA	3926	1/1	0.60	0.33	69,69,69,69	0
56	MG	YA	3354	1/1	0.60	0.21	43,43,43,43	0
56	MG	XA	1695	1/1	0.60	0.19	52,52,52,52	0
56	MG	YA	3118	1/1	0.60	0.26	72,72,72,72	0
56	MG	QA	1822	1/1	0.60	0.14	70,70,70,70	0
56	MG	YA	3426	1/1	0.60	0.22	65,65,65,65	0
56	MG	YA	3428	1/1	0.60	0.30	100,100,100,100	0
56	MG	YA	3154	1/1	0.60	0.20	45,45,45,45	0
56	MG	RA	3232	1/1	0.60	0.44	73,73,73,73	0
56	MG	XA	1767	1/1	0.60	0.28	55,55,55,55	0
56	MG	QA	1723	1/1	0.60	0.33	54,54,54,54	0
56	MG	RA	3350	1/1	0.60	0.27	66,66,66,66	0
56	MG	YA	3166	1/1	0.60	0.44	86,86,86,86	0
56	MG	QA	1746	1/1	0.60	0.25	84,84,84,84	0
56	MG	YA	3444	1/1	0.61	0.39	67,67,67,67	0
56	MG	YA	3747	1/1	0.61	0.42	71,71,71,71	0
56	MG	QA	1807	1/1	0.61	0.27	53,53,53,53	0
56	MG	YA	3066	1/1	0.61	0.19	52,52,52,52	0
56	MG	RA	3454	1/1	0.61	0.22	41,41,41,41	0
56	MG	YA	3241	1/1	0.61	0.61	81,81,81,81	0
56	MG	XA	1694	1/1	0.61	0.41	79,79,79,79	0
56	MG	RA	3668	1/1	0.61	0.19	76,76,76,76	0
56	MG	RA	3839	1/1	0.61	0.20	74,74,74,74	0
56	MG	RA	3719	1/1	0.61	0.23	75,75,75,75	0
56	MG	RA	3961	1/1	0.61	0.23	82,82,82,82	0
56	MG	RA	3372	1/1	0.61	0.33	50,50,50,50	0
56	MG	XA	1723	1/1	0.61	0.16	64,64,64,64	0
56	MG	RA	3510	1/1	0.61	0.16	42,42,42,42	0
56	MG	RA	3561	1/1	0.61	0.20	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	QR	101	1/1	0.61	0.21	67,67,67,67	0
56	MG	RA	3316	1/1	0.61	0.24	66,66,66,66	0
56	MG	XA	1785	1/1	0.61	0.23	73,73,73,73	0
56	MG	YA	3683	1/1	0.61	0.19	60,60,60,60	0
56	MG	RA	3147	1/1	0.61	0.18	45,45,45,45	0
56	MG	QA	1842	1/1	0.61	0.22	67,67,67,67	0
56	MG	QA	1755	1/1	0.62	0.56	100,100,100,100	0
56	MG	RA	3010	1/1	0.62	0.13	62,62,62,62	0
56	MG	RA	3788	1/1	0.62	0.25	75,75,75,75	0
56	MG	RA	3305	1/1	0.62	0.24	69,69,69,69	0
56	MG	RA	3549	1/1	0.62	0.23	50,50,50,50	0
56	MG	YE	303	1/1	0.62	0.19	59,59,59,59	0
56	MG	QA	1773	1/1	0.62	0.16	100,100,100,100	0
56	MG	RA	3251	1/1	0.62	0.41	83,83,83,83	0
56	MG	RA	3557	1/1	0.62	0.17	61,61,61,61	0
56	MG	RA	3948	1/1	0.62	0.25	58,58,58,58	0
56	MG	YA	3570	1/1	0.62	0.33	82,82,82,82	0
56	MG	XA	1615	1/1	0.62	0.15	61,61,61,61	0
56	MG	RA	3447	1/1	0.62	0.30	44,44,44,44	0
56	MG	RA	3874	1/1	0.62	0.23	85,85,85,85	0
56	MG	XA	1638	1/1	0.62	0.13	76,76,76,76	0
56	MG	XA	1759	1/1	0.62	0.23	63,63,63,63	0
56	MG	YA	3185	1/1	0.62	0.13	70,70,70,70	0
56	MG	YA	3663	1/1	0.62	0.20	44,44,44,44	0
56	MG	YA	3048	1/1	0.62	0.17	69,69,69,69	0
56	MG	RA	3256	1/1	0.62	0.31	93,93,93,93	0
56	MG	RA	3980	1/1	0.62	0.36	95,95,95,95	0
56	MG	YA	3702	1/1	0.62	0.33	54,54,54,54	0
56	MG	XA	1624	1/1	0.63	0.23	84,84,84,84	0
56	MG	YA	3144	1/1	0.63	0.26	76,76,76,76	0
56	MG	YA	3717	1/1	0.63	0.43	62,62,62,62	0
56	MG	YA	3517	1/1	0.63	0.44	78,78,78,78	0
56	MG	XA	1651	1/1	0.63	0.24	83,83,83,83	0
56	MG	YA	3018	1/1	0.63	0.44	67,67,67,67	0
56	MG	RA	3202	1/1	0.63	0.26	73,73,73,73	0
56	MG	QA	1784	1/1	0.63	0.22	62,62,62,62	0
56	MG	YA	3252	1/1	0.63	0.45	88,88,88,88	0
56	MG	QA	1675	1/1	0.63	0.21	66,66,66,66	0
56	MG	RA	3894	1/1	0.63	0.31	52,52,52,52	0
56	MG	XA	1769	1/1	0.63	0.30	66,66,66,66	0
56	MG	RA	3063	1/1	0.63	0.16	57,57,57,57	0
56	MG	RA	3194	1/1	0.63	0.31	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3182	1/1	0.63	0.17	35,35,35,35	0
57	ZN	R5	101	1/1	0.63	0.14	214,214,214,214	0
56	MG	RA	3543	1/1	0.63	0.20	50,50,50,50	0
56	MG	RP	201	1/1	0.63	0.21	58,58,58,58	0
56	MG	RA	3113	1/1	0.64	0.35	73,73,73,73	0
56	MG	YA	3181	1/1	0.64	0.23	53,53,53,53	0
56	MG	XA	1710	1/1	0.64	0.29	56,56,56,56	0
56	MG	QA	1609	1/1	0.64	0.24	64,64,64,64	0
56	MG	QA	1846	1/1	0.64	0.29	84,84,84,84	0
56	MG	YA	3123	1/1	0.64	0.18	66,66,66,66	0
56	MG	RA	3784	1/1	0.64	0.39	84,84,84,84	0
56	MG	YA	3369	1/1	0.64	0.22	63,63,63,63	0
56	MG	YA	3382	1/1	0.64	0.26	69,69,69,69	0
56	MG	QA	1756	1/1	0.64	0.36	69,69,69,69	0
56	MG	RA	3744	1/1	0.64	0.29	62,62,62,62	0
56	MG	YA	3236	1/1	0.64	0.32	72,72,72,72	0
56	MG	RA	3057	1/1	0.64	0.50	81,81,81,81	0
56	MG	YA	3245	1/1	0.64	0.20	94,94,94,94	0
56	MG	RA	3708	1/1	0.64	0.23	43,43,43,43	0
56	MG	RA	4029	1/1	0.64	0.50	69,69,69,69	0
56	MG	RB	204	1/1	0.64	0.13	69,69,69,69	0
56	MG	QA	1612	1/1	0.65	0.21	103,103,103,103	0
56	MG	QA	1809	1/1	0.65	0.19	71,71,71,71	0
56	MG	RA	3508	1/1	0.65	0.19	58,58,58,58	0
56	MG	YA	3414	1/1	0.65	0.19	56,56,56,56	0
56	MG	RB	218	1/1	0.65	0.16	86,86,86,86	0
56	MG	RA	3875	1/1	0.65	0.55	85,85,85,85	0
56	MG	RA	3300	1/1	0.65	0.21	93,93,93,93	0
56	MG	RA	3137	1/1	0.65	0.24	66,66,66,66	0
56	MG	XA	1722	1/1	0.65	0.19	76,76,76,76	0
56	MG	RA	3821	1/1	0.65	0.41	90,90,90,90	0
56	MG	RA	3176	1/1	0.65	0.45	87,87,87,87	0
56	MG	YA	3710	1/1	0.65	0.20	65,65,65,65	0
56	MG	RA	3520	1/1	0.65	0.17	49,49,49,49	0
56	MG	RA	3118	1/1	0.65	0.18	62,62,62,62	0
56	MG	YA	3482	1/1	0.65	0.31	82,82,82,82	0
56	MG	QA	1802	1/1	0.65	0.21	40,40,40,40	0
56	MG	RA	3100	1/1	0.65	0.46	89,89,89,89	0
56	MG	YA	3055	1/1	0.65	0.25	77,77,77,77	0
56	MG	RA	3780	1/1	0.65	0.11	60,60,60,60	0
56	MG	YA	3521	1/1	0.65	0.23	48,48,48,48	0
56	MG	QA	1611	1/1	0.65	0.13	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	YA	3720	1/1	0.66	0.48	78,78,78,78	0
56	MG	YA	3285	1/1	0.66	0.39	68,68,68,68	0
56	MG	YA	3484	1/1	0.66	0.28	63,63,63,63	0
56	MG	YA	3306	1/1	0.66	0.19	53,53,53,53	0
56	MG	RA	3621	1/1	0.66	0.35	65,65,65,65	0
56	MG	RA	3141	1/1	0.66	0.30	85,85,85,85	0
56	MG	RA	3756	1/1	0.66	0.23	66,66,66,66	0
56	MG	RA	3338	1/1	0.66	0.15	56,56,56,56	0
56	MG	RA	3077	1/1	0.66	0.28	57,57,57,57	0
56	MG	YA	3549	1/1	0.66	0.28	51,51,51,51	0
56	MG	RA	3295	1/1	0.66	0.48	75,75,75,75	0
56	MG	RA	3642	1/1	0.66	0.37	86,86,86,86	0
56	MG	RA	3726	1/1	0.66	0.15	50,50,50,50	0
56	MG	XA	1622	1/1	0.66	0.21	68,68,68,68	0
56	MG	QA	1823	1/1	0.66	0.22	69,69,69,69	0
56	MG	RA	3064	1/1	0.66	0.44	79,79,79,79	0
56	MG	YA	3432	1/1	0.66	0.18	59,59,59,59	0
56	MG	YA	3667	1/1	0.66	0.28	60,60,60,60	0
56	MG	RA	3976	1/1	0.66	0.16	67,67,67,67	0
56	MG	RA	3822	1/1	0.66	0.38	69,69,69,69	0
56	MG	YA	3452	1/1	0.66	0.15	45,45,45,45	0
56	MG	RA	4018	1/1	0.66	0.45	110,110,110,110	0
56	MG	QA	1670	1/1	0.66	0.19	53,53,53,53	0
56	MG	QA	1835	1/1	0.66	0.26	50,50,50,50	0
56	MG	QA	1603	1/1	0.66	0.22	62,62,62,62	0
56	MG	YA	3249	1/1	0.67	0.44	75,75,75,75	0
56	MG	RA	3538	1/1	0.67	0.16	72,72,72,72	0
56	MG	RA	3539	1/1	0.67	0.25	76,76,76,76	0
56	MG	RA	3812	1/1	0.67	0.28	85,85,85,85	0
56	MG	RA	3514	1/1	0.67	0.48	79,79,79,79	0
56	MG	RA	3583	1/1	0.67	0.37	82,82,82,82	0
56	MG	YA	3284	1/1	0.67	0.36	72,72,72,72	0
56	MG	QG	202	1/1	0.67	0.18	76,76,76,76	0
56	MG	RA	3307	1/1	0.67	0.24	57,57,57,57	0
56	MG	RA	3906	1/1	0.67	0.26	49,49,49,49	0
56	MG	YA	3160	1/1	0.67	0.23	67,67,67,67	0
56	MG	R7	103	1/1	0.67	0.21	66,66,66,66	0
56	MG	RA	3275	1/1	0.67	0.21	90,90,90,90	0
56	MG	RA	3996	1/1	0.67	0.20	68,68,68,68	0
56	MG	RF	309	1/1	0.67	0.34	69,69,69,69	0
56	MG	RA	3998	1/1	0.67	0.52	80,80,80,80	0
56	MG	RA	3636	1/1	0.67	0.14	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1632	1/1	0.67	0.27	71,71,71,71	0
56	MG	YA	3647	1/1	0.67	0.17	64,64,64,64	0
56	MG	RA	4021	1/1	0.67	0.17	79,79,79,79	0
56	MG	QA	1707	1/1	0.67	0.30	60,60,60,60	0
56	MG	RA	3439	1/1	0.67	0.19	69,69,69,69	0
56	MG	RA	3847	1/1	0.67	0.26	71,71,71,71	0
56	MG	XA	1658	1/1	0.67	0.25	71,71,71,71	0
56	MG	QA	1622	1/1	0.67	0.11	61,61,61,61	0
56	MG	QA	1712	1/1	0.67	0.21	60,60,60,60	0
56	MG	YA	3100	1/1	0.67	0.43	105,105,105,105	0
56	MG	QA	1686	1/1	0.68	0.19	54,54,54,54	0
56	MG	QA	1691	1/1	0.68	0.18	52,52,52,52	0
56	MG	RD	314	1/1	0.68	0.22	64,64,64,64	0
56	MG	YA	3688	1/1	0.68	0.31	84,84,84,84	0
56	MG	QG	201	1/1	0.68	0.36	96,96,96,96	0
56	MG	RA	3402	1/1	0.68	0.18	76,76,76,76	0
56	MG	RA	3414	1/1	0.68	0.21	74,74,74,74	0
56	MG	RA	3126	1/1	0.68	0.18	47,47,47,47	0
56	MG	RA	3553	1/1	0.68	0.15	54,54,54,54	0
56	MG	XA	1680	1/1	0.68	0.17	46,46,46,46	0
56	MG	XA	1684	1/1	0.68	0.25	102,102,102,102	0
56	MG	RA	3319	1/1	0.68	0.14	48,48,48,48	0
56	MG	RA	3041	1/1	0.68	0.18	58,58,58,58	0
56	MG	RA	3860	1/1	0.68	0.30	74,74,74,74	0
56	MG	RA	3559	1/1	0.68	0.47	79,79,79,79	0
56	MG	RA	3274	1/1	0.68	0.35	77,77,77,77	0
56	MG	QA	1721	1/1	0.68	0.26	70,70,70,70	0
56	MG	XA	1706	1/1	0.68	0.16	64,64,64,64	0
56	MG	RA	3189	1/1	0.68	0.45	94,94,94,94	0
56	MG	QA	1651	1/1	0.68	0.16	58,58,58,58	0
56	MG	RA	3444	1/1	0.68	0.34	58,58,58,58	0
56	MG	RA	3031	1/1	0.68	0.16	58,58,58,58	0
56	MG	RA	3537	1/1	0.68	0.29	66,66,66,66	0
56	MG	QA	1667	1/1	0.68	0.19	95,95,95,95	0
56	MG	RA	3392	1/1	0.68	0.11	56,56,56,56	0
56	MG	RA	3609	1/1	0.68	0.30	85,85,85,85	0
56	MG	RA	3060	1/1	0.68	0.09	68,68,68,68	0
56	MG	YA	3130	1/1	0.68	0.25	62,62,62,62	0
56	MG	YA	3320	1/1	0.68	0.20	60,60,60,60	0
56	MG	QA	1682	1/1	0.68	0.13	59,59,59,59	0
56	MG	RA	3823	1/1	0.68	0.15	62,62,62,62	0
56	MG	XY	401	1/1	0.68	0.54	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1781	1/1	0.68	0.29	76,76,76,76	0
56	MG	YA	3646	1/1	0.68	0.25	37,37,37,37	0
56	MG	RA	3835	1/1	0.68	0.27	78,78,78,78	0
56	MG	QA	1638	1/1	0.69	0.17	48,48,48,48	0
56	MG	YA	3656	1/1	0.69	0.19	81,81,81,81	0
56	MG	RA	3722	1/1	0.69	0.11	74,74,74,74	0
56	MG	QF	201	1/1	0.69	0.12	80,80,80,80	0
56	MG	RA	3585	1/1	0.69	0.23	73,73,73,73	0
56	MG	RA	3467	1/1	0.69	0.23	46,46,46,46	0
56	MG	RA	3883	1/1	0.69	0.31	65,65,65,65	0
56	MG	XA	1675	1/1	0.69	0.42	99,99,99,99	0
56	MG	RB	213	1/1	0.69	0.11	49,49,49,49	0
56	MG	QA	1655	1/1	0.69	0.20	48,48,48,48	0
56	MG	YA	3438	1/1	0.69	0.23	53,53,53,53	0
56	MG	RA	3736	1/1	0.69	0.23	68,68,68,68	0
56	MG	RA	3974	1/1	0.69	0.27	60,60,60,60	0
56	MG	QA	1664	1/1	0.69	0.38	105,105,105,105	0
56	MG	YA	3205	1/1	0.69	0.29	59,59,59,59	0
56	MG	QA	1819	1/1	0.69	0.17	38,38,38,38	0
56	MG	YA	3228	1/1	0.69	0.14	61,61,61,61	0
56	MG	QA	1736	1/1	0.69	0.18	82,82,82,82	0
56	MG	RA	3130	1/1	0.69	0.14	61,61,61,61	0
56	MG	R1	105	1/1	0.69	0.36	87,87,87,87	0
56	MG	RA	3240	1/1	0.69	0.16	75,75,75,75	0
56	MG	RA	3994	1/1	0.69	0.15	51,51,51,51	0
56	MG	RA	3534	1/1	0.69	0.21	39,39,39,39	0
56	MG	YA	3513	1/1	0.69	0.14	43,43,43,43	0
56	MG	RA	3291	1/1	0.69	0.16	73,73,73,73	0
56	MG	RF	306	1/1	0.69	0.32	76,76,76,76	0
56	MG	RA	3761	1/1	0.69	0.32	56,56,56,56	0
56	MG	YA	3539	1/1	0.69	0.28	63,63,63,63	0
56	MG	QA	1687	1/1	0.69	0.17	55,55,55,55	0
56	MG	XA	1782	1/1	0.69	0.25	51,51,51,51	0
56	MG	QA	1777	1/1	0.69	0.11	62,62,62,62	0
56	MG	RA	3280	1/1	0.69	0.24	69,69,69,69	0
56	MG	RA	4024	1/1	0.69	0.51	84,84,84,84	0
56	MG	RA	3677	1/1	0.69	0.82	91,91,91,91	0
56	MG	QA	1860	1/1	0.69	0.27	64,64,64,64	0
56	MG	RA	4030	1/1	0.69	0.23	60,60,60,60	0
56	MG	RA	3215	1/1	0.70	0.29	103,103,103,103	0
56	MG	YA	3546	1/1	0.70	0.16	34,34,34,34	0
56	MG	QA	1774	1/1	0.70	0.09	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	3357	1/1	0.70	0.32	54,54,54,54	0
56	MG	RA	3697	1/1	0.70	0.31	64,64,64,64	0
56	MG	YA	3298	1/1	0.70	0.24	61,61,61,61	0
56	MG	QA	1625	1/1	0.70	0.23	72,72,72,72	0
56	MG	YA	3142	1/1	0.70	0.15	66,66,66,66	0
56	MG	RA	3781	1/1	0.70	0.40	80,80,80,80	0
56	MG	RA	3255	1/1	0.70	0.33	70,70,70,70	0
56	MG	RA	3223	1/1	0.70	0.26	98,98,98,98	0
56	MG	XA	1669	1/1	0.70	0.10	65,65,65,65	0
56	MG	RA	3186	1/1	0.70	0.13	60,60,60,60	0
56	MG	RA	3156	1/1	0.70	0.25	72,72,72,72	0
56	MG	RA	3712	1/1	0.70	0.16	59,59,59,59	0
56	MG	RA	3296	1/1	0.70	0.24	61,61,61,61	0
56	MG	YA	3408	1/1	0.70	0.27	45,45,45,45	0
56	MG	RA	3718	1/1	0.70	0.30	57,57,57,57	0
56	MG	RA	3192	1/1	0.70	0.40	108,108,108,108	0
56	MG	YA	3709	1/1	0.70	0.51	101,101,101,101	0
56	MG	RA	3464	1/1	0.70	0.22	72,72,72,72	0
56	MG	QA	1812	1/1	0.70	0.11	73,73,73,73	0
56	MG	QA	1733	1/1	0.70	0.20	61,61,61,61	0
56	MG	RA	3133	1/1	0.70	0.17	48,48,48,48	0
56	MG	YA	3725	1/1	0.70	0.21	57,57,57,57	0
56	MG	YA	3727	1/1	0.70	0.45	81,81,81,81	0
56	MG	YA	3735	1/1	0.70	0.20	44,44,44,44	0
56	MG	XA	1714	1/1	0.70	0.21	91,91,91,91	0
56	MG	RA	3544	1/1	0.70	0.20	60,60,60,60	0
56	MG	RA	3732	1/1	0.70	0.19	54,54,54,54	0
56	MG	YA	3032	1/1	0.70	0.28	70,70,70,70	0
56	MG	XA	1743	1/1	0.70	0.14	50,50,50,50	0
56	MG	YA	3216	1/1	0.70	0.28	81,81,81,81	0
56	MG	YA	3218	1/1	0.70	0.25	49,49,49,49	0
56	MG	YE	306	1/1	0.70	0.19	68,68,68,68	0
56	MG	RA	3121	1/1	0.70	0.23	57,57,57,57	0
56	MG	RA	3423	1/1	0.70	0.20	59,59,59,59	0
56	MG	YA	3234	1/1	0.70	0.30	69,69,69,69	0
56	MG	XA	1779	1/1	0.70	0.31	77,77,77,77	0
56	MG	RA	3738	1/1	0.70	0.20	57,57,57,57	0
56	MG	RA	3670	1/1	0.70	0.16	42,42,42,42	0
56	MG	RA	3067	1/1	0.70	0.41	98,98,98,98	0
56	MG	YA	3068	1/1	0.70	0.42	82,82,82,82	0
56	MG	YA	3082	1/1	0.70	0.15	70,70,70,70	0
56	MG	RA	3683	1/1	0.70	0.14	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1769	1/1	0.70	0.11	63,63,63,63	0
56	MG	YA	3520	1/1	0.71	0.09	39,39,39,39	0
56	MG	QA	1771	1/1	0.71	0.15	79,79,79,79	0
56	MG	RA	3694	1/1	0.71	0.23	41,41,41,41	0
56	MG	QA	1816	1/1	0.71	0.16	49,49,49,49	0
56	MG	RA	3765	1/1	0.71	0.10	42,42,42,42	0
56	MG	RA	3646	1/1	0.71	0.18	64,64,64,64	0
56	MG	QA	1778	1/1	0.71	0.24	59,59,59,59	0
56	MG	RA	3957	1/1	0.71	0.32	77,77,77,77	0
56	MG	YA	3275	1/1	0.71	0.26	34,34,34,34	0
56	MG	RA	3279	1/1	0.71	0.19	86,86,86,86	0
56	MG	QA	1693	1/1	0.71	0.24	65,65,65,65	0
56	MG	RA	3132	1/1	0.71	0.18	49,49,49,49	0
56	MG	YA	3456	1/1	0.71	0.49	88,88,88,88	0
56	MG	RA	3104	1/1	0.71	0.24	83,83,83,83	0
56	MG	RX	101	1/1	0.71	0.27	65,65,65,65	0
56	MG	RA	3195	1/1	0.71	0.11	71,71,71,71	0
56	MG	YA	3672	1/1	0.71	0.21	40,40,40,40	0
56	MG	RA	3443	1/1	0.71	0.23	86,86,86,86	0
56	MG	RA	3793	1/1	0.71	0.54	73,73,73,73	0
56	MG	XV	101	1/1	0.71	0.21	73,73,73,73	0
56	MG	QA	1634	1/1	0.71	0.14	66,66,66,66	0
56	MG	QA	1635	1/1	0.71	0.10	90,90,90,90	0
56	MG	YA	3240	1/1	0.71	0.45	94,94,94,94	0
56	MG	RA	3797	1/1	0.71	0.18	66,66,66,66	0
56	MG	YA	3540	1/1	0.72	0.25	38,38,38,38	0
56	MG	RA	3618	1/1	0.72	0.60	70,70,70,70	0
56	MG	QA	1742	1/1	0.72	0.23	53,53,53,53	0
56	MG	RA	3532	1/1	0.72	0.23	64,64,64,64	0
56	MG	YA	3174	1/1	0.72	0.26	69,69,69,69	0
56	MG	QA	1750	1/1	0.72	0.23	68,68,68,68	0
56	MG	YA	3620	1/1	0.72	0.18	46,46,46,46	0
56	MG	RA	3676	1/1	0.72	0.43	98,98,98,98	0
56	MG	YA	3635	1/1	0.72	0.19	66,66,66,66	0
56	MG	RA	3468	1/1	0.72	0.15	64,64,64,64	0
56	MG	YA	3386	1/1	0.72	0.32	80,80,80,80	0
56	MG	RA	3859	1/1	0.72	0.24	75,75,75,75	0
56	MG	RA	3472	1/1	0.72	0.30	40,40,40,40	0
56	MG	RA	3861	1/1	0.72	0.46	91,91,91,91	0
56	MG	YA	3422	1/1	0.72	0.17	34,34,34,34	0
56	MG	YA	3423	1/1	0.72	0.40	77,77,77,77	0
56	MG	YA	3424	1/1	0.72	0.20	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3494	1/1	0.72	0.25	69,69,69,69	0
56	MG	YA	3210	1/1	0.72	0.13	66,66,66,66	0
56	MG	XA	1686	1/1	0.72	0.18	69,69,69,69	0
56	MG	YA	3212	1/1	0.72	0.16	62,62,62,62	0
56	MG	YA	3437	1/1	0.72	0.21	55,55,55,55	0
56	MG	YA	3706	1/1	0.72	0.31	64,64,64,64	0
56	MG	RA	3562	1/1	0.72	0.33	64,64,64,64	0
56	MG	XA	1699	1/1	0.72	0.21	64,64,64,64	0
56	MG	YA	3440	1/1	0.72	0.23	76,76,76,76	0
56	MG	RA	3567	1/1	0.72	0.22	56,56,56,56	0
56	MG	RA	3748	1/1	0.72	0.17	65,65,65,65	0
56	MG	RO	201	1/1	0.72	0.28	71,71,71,71	0
56	MG	RA	3174	1/1	0.72	0.35	101,101,101,101	0
56	MG	RA	3580	1/1	0.72	0.47	97,97,97,97	0
56	MG	YA	3731	1/1	0.72	0.20	43,43,43,43	0
56	MG	XA	1720	1/1	0.72	0.17	63,63,63,63	0
56	MG	QA	1840	1/1	0.72	0.24	69,69,69,69	0
56	MG	RA	3143	1/1	0.72	0.16	49,49,49,49	0
56	MG	XA	1739	1/1	0.72	0.27	43,43,43,43	0
56	MG	RA	3304	1/1	0.72	0.23	73,73,73,73	0
56	MG	YA	3480	1/1	0.72	0.23	39,39,39,39	0
56	MG	YA	3115	1/1	0.72	0.28	77,77,77,77	0
56	MG	YD	309	1/1	0.72	0.20	38,38,38,38	0
56	MG	RA	3218	1/1	0.72	0.27	81,81,81,81	0
56	MG	RA	3545	1/1	0.72	0.40	84,84,84,84	0
56	MG	YA	3500	1/1	0.72	0.44	83,83,83,83	0
56	MG	XA	1601	1/1	0.72	0.46	68,68,68,68	0
56	MG	RA	3932	1/1	0.72	0.09	55,55,55,55	0
56	MG	QA	1799	1/1	0.72	0.19	77,77,77,77	0
56	MG	QA	1654	1/1	0.72	0.15	87,87,87,87	0
56	MG	RA	3400	1/1	0.72	0.20	34,34,34,34	0
56	MG	RB	212	1/1	0.72	0.13	52,52,52,52	0
56	MG	RA	3197	1/1	0.72	0.17	51,51,51,51	0
56	MG	RA	3271	1/1	0.72	0.23	76,76,76,76	0
56	MG	QA	1666	1/1	0.72	0.15	72,72,72,72	0
56	MG	XA	1649	1/1	0.73	0.24	88,88,88,88	0
56	MG	RA	3243	1/1	0.73	0.37	79,79,79,79	0
56	MG	RA	3806	1/1	0.73	0.11	69,69,69,69	0
56	MG	YA	3156	1/1	0.73	0.23	49,49,49,49	0
56	MG	RA	3148	1/1	0.73	0.11	70,70,70,70	0
56	MG	RA	3230	1/1	0.73	0.19	50,50,50,50	0
56	MG	QA	1785	1/1	0.73	0.19	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3164	1/1	0.73	0.29	65,65,65,65	0
56	MG	RA	3674	1/1	0.73	0.34	71,71,71,71	0
56	MG	RA	3516	1/1	0.73	0.62	58,58,58,58	0
56	MG	RA	3818	1/1	0.73	0.26	60,60,60,60	0
56	MG	RA	3163	1/1	0.73	0.47	100,100,100,100	0
56	MG	RA	3299	1/1	0.73	0.35	80,80,80,80	0
56	MG	XA	1677	1/1	0.73	0.20	78,78,78,78	0
56	MG	RA	3526	1/1	0.73	0.14	42,42,42,42	0
56	MG	QJ	201	1/1	0.73	0.25	69,69,69,69	0
56	MG	RA	3339	1/1	0.73	0.26	59,59,59,59	0
56	MG	RA	3970	1/1	0.73	0.39	83,83,83,83	0
56	MG	QA	1716	1/1	0.73	0.34	45,45,45,45	0
56	MG	QV	103	1/1	0.73	0.15	68,68,68,68	0
56	MG	RA	3239	1/1	0.73	0.09	73,73,73,73	0
56	MG	RA	3276	1/1	0.73	0.27	84,84,84,84	0
56	MG	RA	3575	1/1	0.73	0.12	71,71,71,71	0
56	MG	YA	3222	1/1	0.73	0.14	39,39,39,39	0
56	MG	QA	1652	1/1	0.73	0.12	68,68,68,68	0
56	MG	RA	3771	1/1	0.73	0.18	34,34,34,34	0
56	MG	YA	3231	1/1	0.73	0.24	69,69,69,69	0
56	MG	RA	3986	1/1	0.73	0.32	73,73,73,73	0
56	MG	YA	3473	1/1	0.73	0.41	68,68,68,68	0
56	MG	RA	3207	1/1	0.73	0.47	82,82,82,82	0
56	MG	RA	3706	1/1	0.73	0.27	57,57,57,57	0
56	MG	YB	214	1/1	0.73	0.21	71,71,71,71	0
56	MG	RA	3644	1/1	0.73	0.19	46,46,46,46	0
56	MG	YA	3487	1/1	0.73	0.22	59,59,59,59	0
56	MG	RA	4003	1/1	0.73	0.34	38,38,38,38	0
56	MG	QA	1665	1/1	0.73	0.21	87,87,87,87	0
56	MG	RA	4004	1/1	0.73	0.22	62,62,62,62	0
56	MG	YA	3509	1/1	0.73	0.49	66,66,66,66	0
56	MG	RA	3349	1/1	0.73	0.19	74,74,74,74	0
56	MG	RA	3094	1/1	0.73	0.23	55,55,55,55	0
56	MG	YA	3110	1/1	0.73	0.35	63,63,63,63	0
56	MG	RA	3714	1/1	0.73	0.19	56,56,56,56	0
56	MG	XA	1781	1/1	0.73	0.27	53,53,53,53	0
56	MG	RA	3657	1/1	0.73	0.34	84,84,84,84	0
56	MG	RA	3352	1/1	0.73	0.17	42,42,42,42	0
56	MG	QA	1841	1/1	0.73	0.12	49,49,49,49	0
56	MG	RA	3083	1/1	0.73	0.41	81,81,81,81	0
56	MG	YA	3302	1/1	0.73	0.18	48,48,48,48	0
56	MG	RA	3315	1/1	0.73	0.23	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	RA	3667	1/1	0.73	0.33	73,73,73,73	0
56	MG	YA	3151	1/1	0.73	0.42	86,86,86,86	0
56	MG	RA	3829	1/1	0.74	0.73	79,79,79,79	0
56	MG	YA	3326	1/1	0.74	0.27	68,68,68,68	0
56	MG	YA	3191	1/1	0.74	0.21	88,88,88,88	0
56	MG	XA	1672	1/1	0.74	0.25	63,63,63,63	0
56	MG	R0	105	1/1	0.74	0.13	52,52,52,52	0
56	MG	RA	3187	1/1	0.74	0.13	54,54,54,54	0
56	MG	YA	3203	1/1	0.74	0.21	53,53,53,53	0
56	MG	RA	3632	1/1	0.74	0.22	63,63,63,63	0
56	MG	XA	1683	1/1	0.74	0.22	68,68,68,68	0
56	MG	YA	3109	1/1	0.74	0.22	76,76,76,76	0
56	MG	RA	3206	1/1	0.74	0.17	63,63,63,63	0
56	MG	YA	3214	1/1	0.74	0.28	68,68,68,68	0
56	MG	RA	3711	1/1	0.74	0.20	63,63,63,63	0
56	MG	XA	1693	1/1	0.74	0.24	63,63,63,63	0
56	MG	RA	3090	1/1	0.74	0.18	90,90,90,90	0
56	MG	RA	3848	1/1	0.74	0.36	64,64,64,64	0
56	MG	RA	3517	1/1	0.74	0.16	54,54,54,54	0
56	MG	RG	202	1/1	0.74	0.15	98,98,98,98	0
56	MG	YI	201	1/1	0.74	0.20	108,108,108,108	0
56	MG	RA	3462	1/1	0.74	0.42	55,55,55,55	0
56	MG	RA	3175	1/1	0.74	0.39	81,81,81,81	0
56	MG	QA	1780	1/1	0.74	0.13	69,69,69,69	0
56	MG	RA	3363	1/1	0.74	0.12	41,41,41,41	0
56	MG	QA	1669	1/1	0.74	0.18	87,87,87,87	0
56	MG	QA	1614	1/1	0.74	0.28	69,69,69,69	0
56	MG	RA	3039	1/1	0.74	0.30	64,64,64,64	0
56	MG	YA	3033	1/1	0.74	0.23	36,36,36,36	0
56	MG	XA	1621	1/1	0.74	0.27	80,80,80,80	0
56	MG	RA	3152	1/1	0.74	0.13	67,67,67,67	0
56	MG	XA	1745	1/1	0.74	0.22	60,60,60,60	0
56	MG	RA	3047	1/1	0.74	0.19	63,63,63,63	0
56	MG	XA	1625	1/1	0.74	0.38	69,69,69,69	0
56	MG	YA	3052	1/1	0.74	0.14	58,58,58,58	0
56	MG	YA	3668	1/1	0.74	0.22	65,65,65,65	0
56	MG	RA	3395	1/1	0.74	0.17	42,42,42,42	0
56	MG	XA	1775	1/1	0.74	0.33	42,42,42,42	0
56	MG	RA	3887	1/1	0.74	0.22	54,54,54,54	0
56	MG	YA	3175	1/1	0.74	0.27	51,51,51,51	0
56	MG	YA	3467	1/1	0.74	0.22	38,38,38,38	0
56	MG	RA	3049	1/1	0.74	0.48	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	3697	1/1	0.74	0.26	63,63,63,63	0
56	MG	YA	3293	1/1	0.74	0.33	66,66,66,66	0
56	MG	XA	1660	1/1	0.74	0.13	83,83,83,83	0
56	MG	RA	3253	1/1	0.74	0.11	42,42,42,42	0
57	ZN	RY	202	1/1	0.74	0.22	187,187,187,187	0
56	MG	YA	3708	1/1	0.74	0.34	76,76,76,76	0
56	MG	YA	3183	1/1	0.74	0.50	108,108,108,108	0
56	MG	QA	1753	1/1	0.74	0.23	73,73,73,73	0
57	ZN	Y6	101	1/1	0.74	0.31	193,193,193,193	0
56	MG	QA	1641	1/1	0.75	0.15	63,63,63,63	0
56	MG	YA	3676	1/1	0.75	0.16	68,68,68,68	0
56	MG	QA	1754	1/1	0.75	0.27	56,56,56,56	0
56	MG	QA	1688	1/1	0.75	0.27	61,61,61,61	0
56	MG	YA	3146	1/1	0.75	0.19	58,58,58,58	0
56	MG	RA	3524	1/1	0.75	0.19	85,85,85,85	0
56	MG	QA	1814	1/1	0.75	0.19	55,55,55,55	0
56	MG	R1	101	1/1	0.75	0.39	101,101,101,101	0
56	MG	YA	3458	1/1	0.75	0.23	68,68,68,68	0
56	MG	QA	1649	1/1	0.75	0.13	68,68,68,68	0
56	MG	RA	3249	1/1	0.75	0.43	70,70,70,70	0
56	MG	RA	3563	1/1	0.75	0.24	69,69,69,69	0
56	MG	QA	1768	1/1	0.75	0.20	57,57,57,57	0
56	MG	RA	3955	1/1	0.75	0.19	42,42,42,42	0
56	MG	QA	1825	1/1	0.75	0.18	54,54,54,54	0
56	MG	RA	4026	1/1	0.75	0.57	104,104,104,104	0
56	MG	YA	3290	1/1	0.75	0.39	34,34,34,34	0
56	MG	YA	3494	1/1	0.75	0.23	62,62,62,62	0
56	MG	YA	3733	1/1	0.75	0.25	50,50,50,50	0
56	MG	RA	3030	1/1	0.75	0.35	52,52,52,52	0
56	MG	RA	3451	1/1	0.75	0.15	46,46,46,46	0
56	MG	YA	3748	1/1	0.75	0.21	68,68,68,68	0
56	MG	QA	1776	1/1	0.75	0.20	62,62,62,62	0
56	MG	RA	3967	1/1	0.75	0.33	81,81,81,81	0
56	MG	YA	3313	1/1	0.75	0.12	50,50,50,50	0
56	MG	YA	3314	1/1	0.75	0.28	34,34,34,34	0
56	MG	RA	3484	1/1	0.75	0.12	59,59,59,59	0
56	MG	RA	3910	1/1	0.75	0.13	70,70,70,70	0
56	MG	QA	1839	1/1	0.75	0.22	90,90,90,90	0
56	MG	YA	3349	1/1	0.75	0.21	65,65,65,65	0
56	MG	XA	1721	1/1	0.75	0.11	52,52,52,52	0
56	MG	YA	3538	1/1	0.75	0.27	65,65,65,65	0
56	MG	Y7	101	1/1	0.75	0.24	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	RA	3536	1/1	0.75	0.16	49,49,49,49	0
56	MG	XA	1605	1/1	0.75	0.20	60,60,60,60	0
56	MG	RA	3327	1/1	0.75	0.24	61,61,61,61	0
56	MG	YA	3092	1/1	0.75	0.18	75,75,75,75	0
56	MG	QA	1722	1/1	0.75	0.27	63,63,63,63	0
56	MG	YA	3200	1/1	0.75	0.21	55,55,55,55	0
56	MG	YA	3569	1/1	0.75	0.27	34,34,34,34	0
56	MG	RA	3918	1/1	0.75	0.23	63,63,63,63	0
56	MG	QA	1620	1/1	0.75	0.15	102,102,102,102	0
56	MG	RA	3446	1/1	0.75	0.22	71,71,71,71	0
56	MG	RA	3626	1/1	0.75	0.14	45,45,45,45	0
56	MG	YA	3631	1/1	0.75	0.27	59,59,59,59	0
56	MG	XA	1627	1/1	0.75	0.18	60,60,60,60	0
56	MG	RA	3631	1/1	0.75	0.31	86,86,86,86	0
56	MG	YA	3112	1/1	0.75	0.14	44,44,44,44	0
56	MG	YA	3217	1/1	0.75	0.35	92,92,92,92	0
56	MG	RA	3374	1/1	0.75	0.19	46,46,46,46	0
56	MG	RA	3943	1/1	0.75	0.28	42,42,42,42	0
56	MG	YA	3661	1/1	0.75	0.42	34,34,34,34	0
56	MG	YA	3119	1/1	0.75	0.10	59,59,59,59	0
56	MG	YA	3120	1/1	0.75	0.37	66,66,66,66	0
56	MG	R0	106	1/1	0.75	0.26	52,52,52,52	0
56	MG	RA	3977	1/1	0.76	0.66	81,81,81,81	0
56	MG	RA	3430	1/1	0.76	0.46	72,72,72,72	0
56	MG	RA	3984	1/1	0.76	0.28	87,87,87,87	0
56	MG	RA	3518	1/1	0.76	0.18	34,34,34,34	0
56	MG	YA	3213	1/1	0.76	0.21	58,58,58,58	0
56	MG	RA	3373	1/1	0.76	0.22	34,34,34,34	0
56	MG	QA	1618	1/1	0.76	0.10	91,91,91,91	0
56	MG	RA	3023	1/1	0.76	0.28	61,61,61,61	0
56	MG	RA	3540	1/1	0.76	0.34	61,61,61,61	0
56	MG	QA	1770	1/1	0.76	0.16	50,50,50,50	0
56	MG	RA	3523	1/1	0.76	0.33	63,63,63,63	0
56	MG	RA	3927	1/1	0.76	0.19	42,42,42,42	0
56	MG	RA	3796	1/1	0.76	0.32	55,55,55,55	0
56	MG	RA	3844	1/1	0.76	0.22	53,53,53,53	0
56	MG	YA	3235	1/1	0.76	0.17	43,43,43,43	0
56	MG	QA	1699	1/1	0.76	0.19	59,59,59,59	0
56	MG	YA	3116	1/1	0.76	0.18	55,55,55,55	0
56	MG	RA	3383	1/1	0.76	0.22	54,54,54,54	0
56	MG	QA	1779	1/1	0.76	0.25	77,77,77,77	0
56	MG	YA	3475	1/1	0.76	0.23	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	RA	3180	1/1	0.76	0.36	75,75,75,75	0
56	MG	YA	3481	1/1	0.76	0.30	64,64,64,64	0
56	MG	RA	3671	1/1	0.76	0.21	62,62,62,62	0
56	MG	YA	3128	1/1	0.76	0.54	62,62,62,62	0
56	MG	RA	3754	1/1	0.76	0.28	64,64,64,64	0
56	MG	YA	3489	1/1	0.76	0.25	62,62,62,62	0
56	MG	QA	1861	1/1	0.76	0.08	62,62,62,62	0
56	MG	YB	206	1/1	0.76	0.18	76,76,76,76	0
56	MG	RA	3294	1/1	0.76	0.26	90,90,90,90	0
56	MG	RA	3805	1/1	0.76	0.24	57,57,57,57	0
56	MG	QA	1794	1/1	0.76	0.15	57,57,57,57	0
56	MG	XA	1718	1/1	0.76	0.18	74,74,74,74	0
56	MG	RA	3323	1/1	0.76	0.21	65,65,65,65	0
56	MG	QA	1719	1/1	0.76	0.18	62,62,62,62	0
56	MG	RA	3713	1/1	0.76	0.28	92,92,92,92	0
56	MG	RA	3964	1/1	0.76	0.17	77,77,77,77	0
56	MG	RA	3966	1/1	0.76	0.56	119,119,119,119	0
56	MG	RB	216	1/1	0.76	0.22	83,83,83,83	0
56	MG	RA	3050	1/1	0.76	0.35	65,65,65,65	0
56	MG	R3	102	1/1	0.76	0.44	89,89,89,89	0
56	MG	RA	3679	1/1	0.76	0.36	75,75,75,75	0
56	MG	QV	101	1/1	0.76	0.27	79,79,79,79	0
56	MG	XA	1753	1/1	0.76	0.16	58,58,58,58	0
56	MG	RA	3769	1/1	0.76	0.17	60,60,60,60	0
56	MG	YA	3338	1/1	0.76	0.30	34,34,34,34	0
56	MG	XA	1768	1/1	0.76	0.31	68,68,68,68	0
56	MG	YA	3003	1/1	0.76	0.26	66,66,66,66	0
56	MG	YA	3180	1/1	0.76	0.15	59,59,59,59	0
56	MG	QA	1811	1/1	0.76	0.11	65,65,65,65	0
56	MG	QA	1743	1/1	0.76	0.34	79,79,79,79	0
56	MG	XA	1780	1/1	0.76	0.24	73,73,73,73	0
56	MG	YA	3613	1/1	0.76	0.27	34,34,34,34	0
56	MG	YA	3026	1/1	0.76	0.20	42,42,42,42	0
56	MG	RD	307	1/1	0.76	0.41	77,77,77,77	0
56	MG	QA	1668	1/1	0.76	0.11	94,94,94,94	0
56	MG	XL	201	1/1	0.76	0.18	57,57,57,57	0
56	MG	YA	3038	1/1	0.76	0.13	64,64,64,64	0
56	MG	YA	3407	1/1	0.76	0.29	81,81,81,81	0
56	MG	QA	1606	1/1	0.76	0.11	74,74,74,74	0
56	MG	XA	1647	1/1	0.76	0.16	84,84,84,84	0
56	MG	RA	3682	1/1	0.76	0.40	107,107,107,107	0
56	MG	XA	1650	1/1	0.76	0.18	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	3650	1/1	0.76	0.24	76,76,76,76	0
56	MG	RU	203	1/1	0.77	0.17	56,56,56,56	0
56	MG	RA	3005	1/1	0.77	0.12	43,43,43,43	0
56	MG	XA	1679	1/1	0.77	0.18	52,52,52,52	0
56	MG	YA	3553	1/1	0.77	0.19	52,52,52,52	0
56	MG	QA	1789	1/1	0.77	0.22	71,71,71,71	0
56	MG	YB	218	1/1	0.77	0.22	79,79,79,79	0
56	MG	QA	1676	1/1	0.77	0.24	84,84,84,84	0
56	MG	RA	3574	1/1	0.77	0.18	64,64,64,64	0
56	MG	RA	3123	1/1	0.77	0.14	37,37,37,37	0
56	MG	YA	3601	1/1	0.77	0.16	40,40,40,40	0
56	MG	YQ	202	1/1	0.77	0.20	41,41,41,41	0
56	MG	RA	3165	1/1	0.77	0.11	88,88,88,88	0
56	MG	YX	101	1/1	0.77	0.22	42,42,42,42	0
56	MG	YA	3253	1/1	0.77	0.19	63,63,63,63	0
56	MG	YA	3057	1/1	0.77	0.19	61,61,61,61	0
56	MG	YA	3260	1/1	0.77	0.22	88,88,88,88	0
56	MG	RA	3978	1/1	0.77	0.15	64,64,64,64	0
56	MG	QA	1639	1/1	0.77	0.14	50,50,50,50	0
56	MG	RA	3979	1/1	0.77	0.22	67,67,67,67	0
56	MG	YA	3177	1/1	0.77	0.36	96,96,96,96	0
56	MG	QA	1804	1/1	0.77	0.16	52,52,52,52	0
56	MG	YA	3094	1/1	0.77	0.19	39,39,39,39	0
56	MG	RA	3475	1/1	0.77	0.23	70,70,70,70	0
56	MG	RA	3863	1/1	0.77	0.21	64,64,64,64	0
56	MG	YA	3098	1/1	0.77	0.17	57,57,57,57	0
56	MG	XA	1737	1/1	0.77	0.18	60,60,60,60	0
56	MG	YA	3300	1/1	0.77	0.17	58,58,58,58	0
56	MG	RA	3939	1/1	0.77	0.23	53,53,53,53	0
56	MG	XA	1744	1/1	0.77	0.32	57,57,57,57	0
56	MG	YA	3103	1/1	0.77	0.29	68,68,68,68	0
56	MG	QA	1759	1/1	0.77	0.21	65,65,65,65	0
56	MG	RA	3867	1/1	0.77	0.23	54,54,54,54	0
56	MG	XA	1642	1/1	0.77	0.11	75,75,75,75	0
56	MG	XA	1643	1/1	0.77	0.15	68,68,68,68	0
56	MG	XA	1765	1/1	0.77	0.12	65,65,65,65	0
56	MG	RA	3629	1/1	0.77	0.26	94,94,94,94	0
56	MG	YA	3486	1/1	0.77	0.19	44,44,44,44	0
56	MG	YA	3324	1/1	0.77	0.37	34,34,34,34	0
56	MG	RA	3483	1/1	0.77	0.33	42,42,42,42	0
56	MG	QA	1701	1/1	0.77	0.13	42,42,42,42	0
56	MG	RA	3169	1/1	0.77	0.17	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3074	1/1	0.77	0.18	56,56,56,56	0
56	MG	RA	3497	1/1	0.77	0.14	47,47,47,47	0
56	MG	RA	3958	1/1	0.77	0.17	64,64,64,64	0
56	MG	RA	3960	1/1	0.77	0.11	65,65,65,65	0
56	MG	XA	1662	1/1	0.77	0.11	52,52,52,52	0
56	MG	RA	3324	1/1	0.77	0.19	76,76,76,76	0
56	MG	RA	3768	1/1	0.77	0.13	84,84,84,84	0
56	MG	XV	102	1/1	0.77	0.19	107,107,107,107	0
56	MG	RA	3728	1/1	0.77	0.12	40,40,40,40	0
56	MG	RB	202	1/1	0.77	0.16	80,80,80,80	0
56	MG	RA	3308	1/1	0.77	0.27	34,34,34,34	0
56	MG	RA	3525	1/1	0.77	0.41	67,67,67,67	0
56	MG	RU	201	1/1	0.77	0.17	56,56,56,56	0
56	MG	YA	3421	1/1	0.77	0.42	87,87,87,87	0
56	MG	RA	3178	1/1	0.78	0.25	76,76,76,76	0
56	MG	RA	3394	1/1	0.78	0.18	34,34,34,34	0
56	MG	YA	3410	1/1	0.78	0.16	34,34,34,34	0
56	MG	RA	3944	1/1	0.78	0.14	58,58,58,58	0
56	MG	YA	3136	1/1	0.78	0.35	58,58,58,58	0
56	MG	YA	3551	1/1	0.78	0.29	51,51,51,51	0
56	MG	QA	1821	1/1	0.78	0.16	57,57,57,57	0
56	MG	RA	3862	1/1	0.78	0.30	50,50,50,50	0
56	MG	RA	4008	1/1	0.78	0.40	89,89,89,89	0
56	MG	RA	4011	1/1	0.78	0.23	76,76,76,76	0
56	MG	YA	3427	1/1	0.78	0.26	53,53,53,53	0
56	MG	YA	3595	1/1	0.78	0.32	69,69,69,69	0
56	MG	XA	1703	1/1	0.78	0.19	62,62,62,62	0
56	MG	Y1	101	1/1	0.78	0.21	42,42,42,42	0
56	MG	YA	3243	1/1	0.78	0.20	37,37,37,37	0
56	MG	YA	3610	1/1	0.78	0.22	45,45,45,45	0
56	MG	RA	3779	1/1	0.78	0.18	76,76,76,76	0
56	MG	YA	3619	1/1	0.78	0.16	47,47,47,47	0
56	MG	YA	3031	1/1	0.78	0.17	36,36,36,36	0
56	MG	RA	3326	1/1	0.78	0.23	34,34,34,34	0
56	MG	RA	3868	1/1	0.78	0.22	53,53,53,53	0
56	MG	YA	3256	1/1	0.78	0.11	41,41,41,41	0
56	MG	RA	3026	1/1	0.78	0.43	105,105,105,105	0
56	MG	YA	3043	1/1	0.78	0.23	34,34,34,34	0
56	MG	RA	3061	1/1	0.78	0.12	61,61,61,61	0
56	MG	XA	1730	1/1	0.78	0.23	60,60,60,60	0
56	MG	RA	3076	1/1	0.78	0.17	57,57,57,57	0
56	MG	QA	1786	1/1	0.78	0.23	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3054	1/1	0.78	0.23	61,61,61,61	0
56	MG	XA	1628	1/1	0.78	0.11	48,48,48,48	0
56	MG	QA	1787	1/1	0.78	0.18	69,69,69,69	0
56	MG	QA	1677	1/1	0.78	0.19	84,84,84,84	0
56	MG	RA	3623	1/1	0.78	0.17	61,61,61,61	0
56	MG	XA	1749	1/1	0.78	0.41	66,66,66,66	0
56	MG	RA	3120	1/1	0.78	0.40	111,111,111,111	0
56	MG	RA	3577	1/1	0.78	0.26	66,66,66,66	0
56	MG	YA	3080	1/1	0.78	0.48	106,106,106,106	0
56	MG	QA	1747	1/1	0.78	0.17	40,40,40,40	0
56	MG	QA	1848	1/1	0.78	0.11	44,44,44,44	0
56	MG	RA	3902	1/1	0.78	0.30	65,65,65,65	0
56	MG	QA	1854	1/1	0.78	0.16	65,65,65,65	0
56	MG	XA	1654	1/1	0.78	0.21	66,66,66,66	0
56	MG	RA	3188	1/1	0.78	0.20	77,77,77,77	0
56	MG	RA	3068	1/1	0.78	0.16	51,51,51,51	0
56	MG	YA	3493	1/1	0.78	0.11	57,57,57,57	0
56	MG	RA	3798	1/1	0.78	0.28	34,34,34,34	0
56	MG	RA	3913	1/1	0.78	0.12	49,49,49,49	0
56	MG	RA	3842	1/1	0.78	0.08	66,66,66,66	0
56	MG	XE	202	1/1	0.78	0.09	73,73,73,73	0
56	MG	RA	3584	1/1	0.78	0.15	45,45,45,45	0
56	MG	RA	3106	1/1	0.78	0.42	71,71,71,71	0
56	MG	RA	3556	1/1	0.78	0.08	56,56,56,56	0
56	MG	QA	1810	1/1	0.78	0.13	53,53,53,53	0
56	MG	RA	3140	1/1	0.78	0.10	65,65,65,65	0
56	MG	YA	3519	1/1	0.78	0.23	46,46,46,46	0
56	MG	QA	1706	1/1	0.78	0.18	47,47,47,47	0
56	MG	RA	3463	1/1	0.78	0.30	34,34,34,34	0
56	MG	RA	3154	1/1	0.78	0.36	111,111,111,111	0
56	MG	QA	1831	1/1	0.79	0.13	77,77,77,77	0
56	MG	YA	3327	1/1	0.79	0.19	45,45,45,45	0
56	MG	QA	1631	1/1	0.79	0.13	58,58,58,58	0
56	MG	RA	3254	1/1	0.79	0.23	122,122,122,122	0
56	MG	RA	3115	1/1	0.79	0.38	87,87,87,87	0
56	MG	RQ	205	1/1	0.79	0.25	73,73,73,73	0
56	MG	RA	3734	1/1	0.79	0.18	73,73,73,73	0
56	MG	YA	3072	1/1	0.79	0.15	78,78,78,78	0
56	MG	XA	1688	1/1	0.79	0.27	38,38,38,38	0
56	MG	RA	3624	1/1	0.79	0.39	58,58,58,58	0
56	MG	RA	3418	1/1	0.79	0.21	69,69,69,69	0
56	MG	YD	307	1/1	0.79	0.18	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	3364	1/1	0.79	0.21	39,39,39,39	0
56	MG	QA	1645	1/1	0.79	0.22	69,69,69,69	0
56	MG	RA	3371	1/1	0.79	0.38	34,34,34,34	0
56	MG	XA	1700	1/1	0.79	0.18	55,55,55,55	0
56	MG	RA	3080	1/1	0.79	0.55	102,102,102,102	0
56	MG	YA	3215	1/1	0.79	0.26	72,72,72,72	0
56	MG	QA	1851	1/1	0.79	0.23	93,93,93,93	0
56	MG	QA	1852	1/1	0.79	0.33	77,77,77,77	0
56	MG	RA	3427	1/1	0.79	0.26	71,71,71,71	0
56	MG	RA	3288	1/1	0.79	0.22	34,34,34,34	0
56	MG	RA	3082	1/1	0.79	0.49	95,95,95,95	0
56	MG	RA	3196	1/1	0.79	0.37	102,102,102,102	0
56	MG	RA	3817	1/1	0.79	0.15	70,70,70,70	0
56	MG	RA	3581	1/1	0.79	0.09	68,68,68,68	0
56	MG	RA	3219	1/1	0.79	0.17	73,73,73,73	0
56	MG	RA	3136	1/1	0.79	0.29	59,59,59,59	0
56	MG	RA	3351	1/1	0.79	0.17	81,81,81,81	0
56	MG	RA	3226	1/1	0.79	0.48	80,80,80,80	0
56	MG	RB	222	1/1	0.79	0.07	57,57,57,57	0
56	MG	RA	3228	1/1	0.79	0.36	78,78,78,78	0
56	MG	RA	3004	1/1	0.79	0.24	88,88,88,88	0
56	MG	YA	3453	1/1	0.79	0.17	45,45,45,45	0
56	MG	QO	101	1/1	0.79	0.16	52,52,52,52	0
56	MG	YA	3660	1/1	0.79	0.17	42,42,42,42	0
56	MG	RA	3605	1/1	0.79	0.16	43,43,43,43	0
56	MG	QA	1672	1/1	0.79	0.10	72,72,72,72	0
56	MG	RA	3922	1/1	0.79	0.13	36,36,36,36	0
56	MG	XA	1639	1/1	0.79	0.17	80,80,80,80	0
56	MG	XA	1763	1/1	0.79	0.16	44,44,44,44	0
56	MG	YA	3462	1/1	0.79	0.26	78,78,78,78	0
56	MG	YA	3669	1/1	0.79	0.35	44,44,44,44	0
56	MG	RA	3985	1/1	0.79	0.35	78,78,78,78	0
56	MG	QV	102	1/1	0.79	0.07	62,62,62,62	0
56	MG	YA	3682	1/1	0.79	0.21	40,40,40,40	0
56	MG	RA	3450	1/1	0.79	0.23	42,42,42,42	0
56	MG	RF	308	1/1	0.79	0.35	95,95,95,95	0
56	MG	XA	1652	1/1	0.79	0.35	91,91,91,91	0
56	MG	YA	3006	1/1	0.79	0.13	59,59,59,59	0
56	MG	QA	1758	1/1	0.79	0.13	46,46,46,46	0
56	MG	YA	3017	1/1	0.79	0.23	76,76,76,76	0
56	MG	QA	1681	1/1	0.79	0.24	56,56,56,56	0
56	MG	RA	3203	1/1	0.79	0.22	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3555	1/1	0.79	0.16	50,50,50,50	0
56	MG	RA	3929	1/1	0.79	0.14	49,49,49,49	0
56	MG	RA	3453	1/1	0.79	0.35	71,71,71,71	0
56	MG	QA	1621	1/1	0.79	0.14	100,100,100,100	0
56	MG	RA	3408	1/1	0.79	0.20	60,60,60,60	0
56	MG	RA	3457	1/1	0.79	0.15	39,39,39,39	0
56	MG	YA	3499	1/1	0.79	0.39	86,86,86,86	0
57	ZN	YY	201	1/1	0.79	0.17	157,157,157,157	0
56	MG	QA	1626	1/1	0.79	0.23	62,62,62,62	0
56	MG	QA	1628	1/1	0.79	0.08	87,87,87,87	0
56	MG	RA	3179	1/1	0.80	0.37	88,88,88,88	0
56	MG	YA	3368	1/1	0.80	0.24	63,63,63,63	0
56	MG	RA	3832	1/1	0.80	0.25	53,53,53,53	0
56	MG	YA	3374	1/1	0.80	0.15	34,34,34,34	0
56	MG	RA	3767	1/1	0.80	0.17	73,73,73,73	0
56	MG	RA	3337	1/1	0.80	0.26	49,49,49,49	0
56	MG	YB	202	1/1	0.80	0.17	80,80,80,80	0
56	MG	YA	3122	1/1	0.80	0.16	87,87,87,87	0
56	MG	YA	3535	1/1	0.80	0.24	38,38,38,38	0
56	MG	RA	3931	1/1	0.80	0.21	42,42,42,42	0
56	MG	RA	3663	1/1	0.80	0.14	45,45,45,45	0
56	MG	YB	215	1/1	0.80	0.10	34,34,34,34	0
56	MG	RA	3664	1/1	0.80	0.23	99,99,99,99	0
56	MG	YA	3133	1/1	0.80	0.12	60,60,60,60	0
56	MG	YB	219	1/1	0.80	0.11	50,50,50,50	0
56	MG	RA	3487	1/1	0.80	0.30	36,36,36,36	0
56	MG	XA	1698	1/1	0.80	0.23	44,44,44,44	0
56	MG	YA	3024	1/1	0.80	0.28	85,85,85,85	0
56	MG	RA	3146	1/1	0.80	0.18	67,67,67,67	0
56	MG	RA	3495	1/1	0.80	0.22	52,52,52,52	0
56	MG	YA	3567	1/1	0.80	0.34	51,51,51,51	0
56	MG	YN	201	1/1	0.80	0.12	51,51,51,51	0
56	MG	RA	3221	1/1	0.80	0.31	57,57,57,57	0
56	MG	XA	1709	1/1	0.80	0.13	61,61,61,61	0
56	MG	RA	3065	1/1	0.80	0.20	55,55,55,55	0
56	MG	YA	3576	1/1	0.80	0.10	63,63,63,63	0
56	MG	YA	3582	1/1	0.80	0.19	40,40,40,40	0
56	MG	XA	1716	1/1	0.80	0.17	76,76,76,76	0
56	MG	YA	3584	1/1	0.80	0.12	34,34,34,34	0
56	MG	RA	3949	1/1	0.80	0.30	54,54,54,54	0
56	MG	XA	1602	1/1	0.80	0.23	62,62,62,62	0
56	MG	XA	1603	1/1	0.80	0.24	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	3951	1/1	0.80	0.22	62,62,62,62	0
56	MG	RA	3265	1/1	0.80	0.12	78,78,78,78	0
56	MG	XA	1727	1/1	0.80	0.40	62,62,62,62	0
56	MG	YA	3157	1/1	0.80	0.21	56,56,56,56	0
56	MG	RA	3723	1/1	0.80	0.21	43,43,43,43	0
56	MG	RA	3032	1/1	0.80	0.22	79,79,79,79	0
56	MG	RA	3455	1/1	0.80	0.18	44,44,44,44	0
56	MG	RA	3014	1/1	0.80	0.15	63,63,63,63	0
56	MG	RA	3012	1/1	0.80	0.34	87,87,87,87	0
56	MG	YA	3171	1/1	0.80	0.17	51,51,51,51	0
56	MG	RA	3322	1/1	0.80	0.17	42,42,42,42	0
56	MG	QA	1604	1/1	0.80	0.10	67,67,67,67	0
56	MG	RA	3298	1/1	0.80	0.13	94,94,94,94	0
56	MG	YA	3069	1/1	0.80	0.43	87,87,87,87	0
56	MG	XA	1762	1/1	0.80	0.27	44,44,44,44	0
56	MG	RA	3587	1/1	0.80	0.67	88,88,88,88	0
56	MG	RD	306	1/1	0.80	0.12	43,43,43,43	0
56	MG	RA	3097	1/1	0.80	0.26	34,34,34,34	0
56	MG	YA	3471	1/1	0.80	0.30	41,41,41,41	0
56	MG	YA	3301	1/1	0.80	0.22	34,34,34,34	0
56	MG	XA	1774	1/1	0.80	0.38	62,62,62,62	0
56	MG	RA	3740	1/1	0.80	0.12	55,55,55,55	0
56	MG	RA	3742	1/1	0.80	0.11	53,53,53,53	0
56	MG	RA	3098	1/1	0.80	0.19	67,67,67,67	0
56	MG	RA	3747	1/1	0.80	0.26	55,55,55,55	0
56	MG	RA	3471	1/1	0.80	0.18	34,34,34,34	0
56	MG	YA	3684	1/1	0.80	0.29	47,47,47,47	0
56	MG	RA	3398	1/1	0.80	0.14	45,45,45,45	0
56	MG	RA	3698	1/1	0.80	0.32	38,38,38,38	0
56	MG	RA	3607	1/1	0.80	0.22	37,37,37,37	0
56	MG	YA	3204	1/1	0.80	0.14	52,52,52,52	0
56	MG	YA	3333	1/1	0.80	0.26	37,37,37,37	0
56	MG	RA	3820	1/1	0.80	0.77	90,90,90,90	0
56	MG	YA	3347	1/1	0.80	0.21	58,58,58,58	0
56	MG	RA	3025	1/1	0.80	0.20	49,49,49,49	0
56	MG	YA	3503	1/1	0.80	0.32	55,55,55,55	0
56	MG	RA	3763	1/1	0.80	0.20	52,52,52,52	0
56	MG	YA	3506	1/1	0.80	0.24	67,67,67,67	0
56	MG	RA	3655	1/1	0.80	0.13	54,54,54,54	0
56	MG	YA	3511	1/1	0.80	0.20	50,50,50,50	0
56	MG	RA	3029	1/1	0.81	0.51	69,69,69,69	0
56	MG	YA	3047	1/1	0.81	0.15	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3886	1/1	0.81	0.23	38,38,38,38	0
56	MG	YA	3545	1/1	0.81	0.25	51,51,51,51	0
56	MG	RA	3420	1/1	0.81	0.20	38,38,38,38	0
56	MG	RA	3659	1/1	0.81	0.18	53,53,53,53	0
56	MG	RA	3422	1/1	0.81	0.29	49,49,49,49	0
56	MG	RA	3314	1/1	0.81	0.14	34,34,34,34	0
56	MG	XA	1687	1/1	0.81	0.24	55,55,55,55	0
56	MG	YA	3555	1/1	0.81	0.18	48,48,48,48	0
56	MG	RA	3834	1/1	0.81	0.13	60,60,60,60	0
56	MG	RA	3965	1/1	0.81	0.09	63,63,63,63	0
56	MG	YA	3568	1/1	0.81	0.28	35,35,35,35	0
56	MG	YD	305	1/1	0.81	0.44	83,83,83,83	0
56	MG	YA	3067	1/1	0.81	0.16	64,64,64,64	0
56	MG	XA	1697	1/1	0.81	0.15	52,52,52,52	0
56	MG	RA	3628	1/1	0.81	0.32	70,70,70,70	0
56	MG	YA	3572	1/1	0.81	0.15	53,53,53,53	0
56	MG	YA	3263	1/1	0.81	0.46	59,59,59,59	0
56	MG	YF	301	1/1	0.81	0.30	57,57,57,57	0
56	MG	RA	3452	1/1	0.81	0.32	34,34,34,34	0
56	MG	RA	3185	1/1	0.81	0.29	106,106,106,106	0
56	MG	RA	3746	1/1	0.81	0.23	41,41,41,41	0
56	MG	YA	3591	1/1	0.81	0.28	56,56,56,56	0
56	MG	YA	3280	1/1	0.81	0.23	41,41,41,41	0
56	MG	RA	3053	1/1	0.81	0.29	70,70,70,70	0
56	MG	YA	3179	1/1	0.81	0.16	54,54,54,54	0
56	MG	YA	3611	1/1	0.81	0.23	57,57,57,57	0
56	MG	XA	1717	1/1	0.81	0.08	56,56,56,56	0
56	MG	YA	3457	1/1	0.81	0.31	46,46,46,46	0
56	MG	RA	3009	1/1	0.81	0.13	42,42,42,42	0
56	MG	XA	1604	1/1	0.81	0.20	80,80,80,80	0
56	MG	YA	3093	1/1	0.81	0.17	34,34,34,34	0
56	MG	QA	1692	1/1	0.81	0.15	44,44,44,44	0
56	MG	RA	3498	1/1	0.81	0.23	54,54,54,54	0
56	MG	XA	1611	1/1	0.81	0.12	59,59,59,59	0
56	MG	QA	1694	1/1	0.81	0.25	58,58,58,58	0
56	MG	RA	3158	1/1	0.81	0.56	108,108,108,108	0
56	MG	RB	220	1/1	0.81	0.15	55,55,55,55	0
56	MG	RA	3342	1/1	0.81	0.18	83,83,83,83	0
56	MG	YA	3198	1/1	0.81	0.17	50,50,50,50	0
56	MG	RA	3855	1/1	0.81	0.25	34,34,34,34	0
56	MG	R1	104	1/1	0.81	0.15	49,49,49,49	0
56	MG	QA	1772	1/1	0.81	0.18	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	3675	1/1	0.81	0.35	98,98,98,98	0
56	MG	YA	3328	1/1	0.81	0.38	34,34,34,34	0
56	MG	YA	3488	1/1	0.81	0.13	43,43,43,43	0
56	MG	RA	3343	1/1	0.81	0.24	40,40,40,40	0
56	MG	YA	3673	1/1	0.81	0.27	35,35,35,35	0
56	MG	YA	3207	1/1	0.81	0.34	84,84,84,84	0
56	MG	YA	3679	1/1	0.81	0.24	59,59,59,59	0
56	MG	RA	3511	1/1	0.81	0.21	77,77,77,77	0
56	MG	RA	3809	1/1	0.81	0.19	59,59,59,59	0
56	MG	YA	3010	1/1	0.81	0.18	70,70,70,70	0
56	MG	QA	1602	1/1	0.81	0.15	73,73,73,73	0
56	MG	YA	3690	1/1	0.81	0.24	55,55,55,55	0
56	MG	RA	3102	1/1	0.81	0.31	83,83,83,83	0
56	MG	RA	3024	1/1	0.81	0.08	41,41,41,41	0
56	MG	QA	1661	1/1	0.81	0.35	77,77,77,77	0
56	MG	YA	3700	1/1	0.81	0.16	50,50,50,50	0
56	MG	RA	3119	1/1	0.81	0.41	121,121,121,121	0
56	MG	RF	307	1/1	0.81	0.32	60,60,60,60	0
56	MG	RA	3727	1/1	0.81	0.20	47,47,47,47	0
56	MG	YA	3140	1/1	0.81	0.16	43,43,43,43	0
56	MG	YA	3395	1/1	0.81	0.22	62,62,62,62	0
56	MG	RA	4006	1/1	0.81	0.48	111,111,111,111	0
56	MG	RA	3684	1/1	0.81	0.15	46,46,46,46	0
56	MG	XA	1665	1/1	0.81	0.21	76,76,76,76	0
56	MG	YA	3041	1/1	0.81	0.24	54,54,54,54	0
56	MG	RA	3181	1/1	0.81	0.32	48,48,48,48	0
56	MG	YA	3527	1/1	0.81	0.14	56,56,56,56	0
56	MG	YA	3530	1/1	0.81	0.31	34,34,34,34	0
56	MG	YA	3239	1/1	0.81	0.46	94,94,94,94	0
56	MG	YA	3040	1/1	0.82	0.21	55,55,55,55	0
56	MG	YA	3685	1/1	0.82	0.30	45,45,45,45	0
56	MG	YA	3294	1/1	0.82	0.20	81,81,81,81	0
56	MG	YA	3689	1/1	0.82	0.24	62,62,62,62	0
56	MG	RD	304	1/1	0.82	0.29	55,55,55,55	0
56	MG	RA	3022	1/1	0.82	0.12	54,54,54,54	0
56	MG	YA	3492	1/1	0.82	0.15	34,34,34,34	0
56	MG	RA	3509	1/1	0.82	0.12	43,43,43,43	0
56	MG	RD	308	1/1	0.82	0.55	98,98,98,98	0
56	MG	YA	3701	1/1	0.82	0.29	44,44,44,44	0
56	MG	RA	3309	1/1	0.82	0.26	34,34,34,34	0
56	MG	YA	3705	1/1	0.82	0.28	58,58,58,58	0
56	MG	YA	3049	1/1	0.82	0.14	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	3707	1/1	0.82	0.09	49,49,49,49	0
56	MG	RA	3988	1/1	0.82	0.33	110,110,110,110	0
56	MG	XA	1676	1/1	0.82	0.18	37,37,37,37	0
56	MG	QA	1832	1/1	0.82	0.12	61,61,61,61	0
56	MG	RE	306	1/1	0.82	0.18	37,37,37,37	0
56	MG	RA	3269	1/1	0.82	0.36	100,100,100,100	0
56	MG	YA	3714	1/1	0.82	0.25	48,48,48,48	0
56	MG	RF	302	1/1	0.82	0.31	93,93,93,93	0
56	MG	RA	3541	1/1	0.82	0.31	50,50,50,50	0
56	MG	QA	1615	1/1	0.82	0.11	105,105,105,105	0
56	MG	RF	304	1/1	0.82	0.23	46,46,46,46	0
56	MG	YA	3194	1/1	0.82	0.52	112,112,112,112	0
56	MG	YA	3518	1/1	0.82	0.25	57,57,57,57	0
56	MG	YA	3345	1/1	0.82	0.26	71,71,71,71	0
56	MG	RA	3997	1/1	0.82	0.33	95,95,95,95	0
56	MG	RA	3270	1/1	0.82	0.21	88,88,88,88	0
56	MG	RA	3751	1/1	0.82	0.16	55,55,55,55	0
56	MG	YA	3525	1/1	0.82	0.08	36,36,36,36	0
56	MG	QA	1689	1/1	0.82	0.16	62,62,62,62	0
56	MG	YA	3202	1/1	0.82	0.24	58,58,58,58	0
56	MG	YA	3084	1/1	0.82	0.15	50,50,50,50	0
56	MG	RA	3045	1/1	0.82	0.22	66,66,66,66	0
56	MG	QA	1623	1/1	0.82	0.13	84,84,84,84	0
56	MG	YA	3378	1/1	0.82	0.13	48,48,48,48	0
56	MG	RA	3272	1/1	0.82	0.30	79,79,79,79	0
56	MG	YA	3383	1/1	0.82	0.16	90,90,90,90	0
56	MG	RA	3170	1/1	0.82	0.37	114,114,114,114	0
56	MG	RA	3086	1/1	0.82	0.46	113,113,113,113	0
56	MG	YA	3400	1/1	0.82	0.35	54,54,54,54	0
56	MG	YE	304	1/1	0.82	0.23	64,64,64,64	0
56	MG	YA	3404	1/1	0.82	0.18	43,43,43,43	0
56	MG	RA	4017	1/1	0.82	0.29	54,54,54,54	0
56	MG	RA	3201	1/1	0.82	0.28	85,85,85,85	0
56	MG	RA	3672	1/1	0.82	0.43	76,76,76,76	0
56	MG	QA	1636	1/1	0.82	0.12	51,51,51,51	0
56	MG	RA	4022	1/1	0.82	0.37	72,72,72,72	0
56	MG	RA	3096	1/1	0.82	0.38	65,65,65,65	0
56	MG	Y0	101	1/1	0.82	0.27	45,45,45,45	0
56	MG	YA	3221	1/1	0.82	0.22	53,53,53,53	0
56	MG	RA	3638	1/1	0.82	0.13	73,73,73,73	0
56	MG	Y8	102	1/1	0.82	0.27	44,44,44,44	0
56	MG	RA	3489	1/1	0.82	0.24	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	QA	1798	1/1	0.82	0.14	66,66,66,66	0
56	MG	RA	3224	1/1	0.82	0.31	51,51,51,51	0
56	MG	RB	201	1/1	0.82	0.09	54,54,54,54	0
56	MG	QA	1713	1/1	0.82	0.22	57,57,57,57	0
56	MG	YA	3434	1/1	0.82	0.13	49,49,49,49	0
56	MG	RA	3183	1/1	0.82	0.28	72,72,72,72	0
56	MG	QA	1647	1/1	0.82	0.14	60,60,60,60	0
56	MG	QA	1648	1/1	0.82	0.19	35,35,35,35	0
56	MG	RA	3124	1/1	0.82	0.19	57,57,57,57	0
56	MG	RB	205	1/1	0.82	0.13	52,52,52,52	0
56	MG	RA	3901	1/1	0.82	0.18	51,51,51,51	0
56	MG	RA	3434	1/1	0.82	0.13	51,51,51,51	0
56	MG	YA	3251	1/1	0.82	0.17	47,47,47,47	0
56	MG	XA	1623	1/1	0.82	0.11	47,47,47,47	0
56	MG	YA	3644	1/1	0.82	0.30	54,54,54,54	0
56	MG	RA	3285	1/1	0.82	0.24	52,52,52,52	0
56	MG	RA	3686	1/1	0.82	0.25	56,56,56,56	0
56	MG	YA	3255	1/1	0.82	0.27	76,76,76,76	0
56	MG	RA	3503	1/1	0.82	0.40	34,34,34,34	0
56	MG	XA	1633	1/1	0.82	0.09	50,50,50,50	0
56	MG	XA	1634	1/1	0.82	0.16	43,43,43,43	0
56	MG	QA	1658	1/1	0.82	0.17	45,45,45,45	0
56	MG	YA	3150	1/1	0.82	0.29	75,75,75,75	0
56	MG	RA	3836	1/1	0.82	0.26	34,34,34,34	0
56	MG	QA	1660	1/1	0.82	0.08	82,82,82,82	0
56	MG	RA	3656	1/1	0.82	0.23	50,50,50,50	0
56	MG	YA	3671	1/1	0.82	0.12	46,46,46,46	0
56	MG	YA	3029	1/1	0.82	0.26	43,43,43,43	0
56	MG	RA	3505	1/1	0.82	0.34	76,76,76,76	0
56	MG	RA	3792	1/1	0.82	0.31	34,34,34,34	0
56	MG	RA	3695	1/1	0.82	0.22	38,38,38,38	0
56	MG	RA	3739	1/1	0.82	0.27	65,65,65,65	0
56	MG	YA	3163	1/1	0.82	0.20	89,89,89,89	0
56	MG	RA	3016	1/1	0.83	0.62	79,79,79,79	0
56	MG	RA	3222	1/1	0.83	0.15	97,97,97,97	0
56	MG	YA	3315	1/1	0.83	0.20	34,34,34,34	0
56	MG	RA	3409	1/1	0.83	0.22	34,34,34,34	0
56	MG	RA	3546	1/1	0.83	0.37	46,46,46,46	0
56	MG	YA	3186	1/1	0.83	0.13	49,49,49,49	0
56	MG	YA	3073	1/1	0.83	0.35	34,34,34,34	0
56	MG	YA	3076	1/1	0.83	0.32	79,79,79,79	0
56	MG	YA	3192	1/1	0.83	0.14	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	YA	3078	1/1	0.83	0.37	78,78,78,78	0
56	MG	RA	3205	1/1	0.83	0.38	76,76,76,76	0
56	MG	YA	3197	1/1	0.83	0.15	34,34,34,34	0
56	MG	YA	3346	1/1	0.83	0.22	34,34,34,34	0
56	MG	RA	3478	1/1	0.83	0.17	70,70,70,70	0
56	MG	RA	3857	1/1	0.83	0.47	69,69,69,69	0
56	MG	YA	3522	1/1	0.83	0.17	52,52,52,52	0
56	MG	RA	3002	1/1	0.83	0.15	58,58,58,58	0
56	MG	RA	3604	1/1	0.83	0.21	37,37,37,37	0
56	MG	YA	3740	1/1	0.83	0.15	40,40,40,40	0
56	MG	RA	3260	1/1	0.83	0.18	63,63,63,63	0
56	MG	YA	3365	1/1	0.83	0.28	57,57,57,57	0
56	MG	RA	3162	1/1	0.83	0.28	85,85,85,85	0
56	MG	RA	3212	1/1	0.83	0.09	70,70,70,70	0
56	MG	YB	205	1/1	0.83	0.38	66,66,66,66	0
56	MG	RA	3614	1/1	0.83	0.42	68,68,68,68	0
56	MG	YB	207	1/1	0.83	0.11	50,50,50,50	0
56	MG	RA	3745	1/1	0.83	0.28	38,38,38,38	0
56	MG	RA	3615	1/1	0.83	0.44	61,61,61,61	0
56	MG	RA	3491	1/1	0.83	0.47	70,70,70,70	0
56	MG	QA	1717	1/1	0.83	0.28	62,62,62,62	0
56	MG	RA	3702	1/1	0.83	0.13	57,57,57,57	0
56	MG	R1	102	1/1	0.83	0.24	71,71,71,71	0
56	MG	RA	3617	1/1	0.83	0.27	51,51,51,51	0
56	MG	RA	3972	1/1	0.83	0.23	46,46,46,46	0
56	MG	YA	3117	1/1	0.83	0.31	45,45,45,45	0
56	MG	RA	3391	1/1	0.83	0.26	41,41,41,41	0
56	MG	RA	3888	1/1	0.83	0.60	61,61,61,61	0
56	MG	YE	305	1/1	0.83	0.25	34,34,34,34	0
56	MG	XA	1711	1/1	0.83	0.31	59,59,59,59	0
56	MG	YA	3226	1/1	0.83	0.19	39,39,39,39	0
56	MG	YA	3227	1/1	0.83	0.28	90,90,90,90	0
56	MG	XA	1715	1/1	0.83	0.34	61,61,61,61	0
56	MG	R7	101	1/1	0.83	0.36	41,41,41,41	0
56	MG	QA	1734	1/1	0.83	0.16	40,40,40,40	0
56	MG	RA	3975	1/1	0.83	0.25	96,96,96,96	0
56	MG	YA	3585	1/1	0.83	0.19	75,75,75,75	0
56	MG	RA	3814	1/1	0.83	0.12	54,54,54,54	0
56	MG	YA	3590	1/1	0.83	0.28	34,34,34,34	0
56	MG	YA	3007	1/1	0.83	0.16	38,38,38,38	0
56	MG	RA	3329	1/1	0.83	0.25	38,38,38,38	0
56	MG	XA	1724	1/1	0.83	0.36	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1725	1/1	0.83	0.14	79,79,79,79	0
56	MG	YA	3431	1/1	0.83	0.20	47,47,47,47	0
56	MG	RA	3200	1/1	0.83	0.15	62,62,62,62	0
56	MG	RA	3758	1/1	0.83	0.36	59,59,59,59	0
56	MG	RA	3052	1/1	0.83	0.40	88,88,88,88	0
56	MG	YA	3023	1/1	0.83	0.10	55,55,55,55	0
56	MG	RA	3566	1/1	0.83	0.18	60,60,60,60	0
56	MG	YA	3250	1/1	0.83	0.18	64,64,64,64	0
56	MG	YA	3448	1/1	0.83	0.23	73,73,73,73	0
56	MG	QA	1752	1/1	0.83	0.39	85,85,85,85	0
56	MG	RA	3500	1/1	0.83	0.26	40,40,40,40	0
56	MG	RA	3235	1/1	0.83	0.25	95,95,95,95	0
56	MG	RA	3827	1/1	0.83	0.07	66,66,66,66	0
56	MG	RA	3766	1/1	0.83	0.29	67,67,67,67	0
56	MG	RA	3715	1/1	0.83	0.15	70,70,70,70	0
56	MG	RA	3459	1/1	0.83	0.13	47,47,47,47	0
56	MG	QA	1678	1/1	0.83	0.15	64,64,64,64	0
56	MG	RA	3236	1/1	0.83	0.31	90,90,90,90	0
56	MG	YA	3666	1/1	0.83	0.20	43,43,43,43	0
56	MG	RA	3027	1/1	0.83	0.20	64,64,64,64	0
56	MG	RA	3673	1/1	0.83	0.81	57,57,57,57	0
56	MG	QA	1767	1/1	0.83	0.09	62,62,62,62	0
56	MG	YA	3470	1/1	0.83	0.15	59,59,59,59	0
56	MG	YA	3279	1/1	0.83	0.12	37,37,37,37	0
56	MG	YA	3165	1/1	0.83	0.32	78,78,78,78	0
56	MG	RA	3401	1/1	0.83	0.19	38,38,38,38	0
56	MG	YA	3169	1/1	0.83	0.11	64,64,64,64	0
56	MG	XA	1787	1/1	0.83	0.20	64,64,64,64	0
56	MG	YA	3287	1/1	0.83	0.38	48,48,48,48	0
56	MG	YA	3170	1/1	0.83	0.15	107,107,107,107	0
56	MG	XA	1645	1/1	0.83	0.07	54,54,54,54	0
56	MG	YA	3292	1/1	0.83	0.13	40,40,40,40	0
56	MG	RF	311	1/1	0.83	0.15	70,70,70,70	0
56	MG	YA	3687	1/1	0.83	0.44	43,43,43,43	0
56	MG	RA	3724	1/1	0.83	0.26	44,44,44,44	0
56	MG	RA	3442	1/1	0.83	0.22	52,52,52,52	0
56	MG	RA	4013	1/1	0.83	0.28	88,88,88,88	0
56	MG	QA	1627	1/1	0.83	0.27	83,83,83,83	0
56	MG	YA	3065	1/1	0.83	0.21	47,47,47,47	0
56	MG	RN	201	1/1	0.83	0.19	70,70,70,70	0
56	MG	RA	3001	1/1	0.84	0.18	39,39,39,39	0
56	MG	YA	3075	1/1	0.84	0.12	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	3199	1/1	0.84	0.16	54,54,54,54	0
56	MG	RA	3891	1/1	0.84	0.17	39,39,39,39	0
56	MG	QA	1725	1/1	0.84	0.15	55,55,55,55	0
56	MG	RA	3892	1/1	0.84	0.24	69,69,69,69	0
56	MG	RA	4023	1/1	0.84	0.44	108,108,108,108	0
56	MG	RA	3075	1/1	0.84	0.34	88,88,88,88	0
56	MG	RA	3588	1/1	0.84	0.55	78,78,78,78	0
56	MG	YA	3288	1/1	0.84	0.30	34,34,34,34	0
56	MG	YB	220	1/1	0.84	0.21	36,36,36,36	0
56	MG	YD	301	1/1	0.84	0.19	44,44,44,44	0
56	MG	QA	1671	1/1	0.84	0.29	84,84,84,84	0
56	MG	RA	3388	1/1	0.84	0.14	35,35,35,35	0
56	MG	RA	3490	1/1	0.84	0.19	34,34,34,34	0
56	MG	RA	3905	1/1	0.84	0.17	43,43,43,43	0
56	MG	RA	3661	1/1	0.84	0.25	34,34,34,34	0
56	MG	RA	3907	1/1	0.84	0.22	61,61,61,61	0
56	MG	RA	3211	1/1	0.84	0.38	83,83,83,83	0
56	MG	RA	3598	1/1	0.84	0.15	34,34,34,34	0
56	MG	YA	3630	1/1	0.84	0.31	58,58,58,58	0
56	MG	RA	3599	1/1	0.84	0.24	45,45,45,45	0
56	MG	RA	3696	1/1	0.84	0.17	66,66,66,66	0
56	MG	RV	201	1/1	0.84	0.11	58,58,58,58	0
56	MG	YT	203	1/1	0.84	0.22	76,76,76,76	0
56	MG	YA	3009	1/1	0.84	0.14	35,35,35,35	0
56	MG	RA	3917	1/1	0.84	0.19	89,89,89,89	0
56	MG	YA	3323	1/1	0.84	0.22	41,41,41,41	0
56	MG	YA	3655	1/1	0.84	0.25	34,34,34,34	0
56	MG	Y8	101	1/1	0.84	0.21	53,53,53,53	0
56	MG	RA	3730	1/1	0.84	0.30	43,43,43,43	0
56	MG	RB	215	1/1	0.84	0.34	48,48,48,48	0
56	MG	YA	3209	1/1	0.84	0.08	59,59,59,59	0
56	MG	RA	3320	1/1	0.84	0.10	55,55,55,55	0
56	MG	QA	1764	1/1	0.84	0.08	62,62,62,62	0
56	MG	QA	1824	1/1	0.84	0.17	46,46,46,46	0
56	MG	YA	3334	1/1	0.84	0.11	40,40,40,40	0
56	MG	YA	3127	1/1	0.84	0.13	59,59,59,59	0
56	MG	YA	3340	1/1	0.84	0.17	34,34,34,34	0
56	MG	RA	3419	1/1	0.84	0.10	38,38,38,38	0
56	MG	YA	3496	1/1	0.84	0.18	39,39,39,39	0
56	MG	RA	3293	1/1	0.84	0.15	34,34,34,34	0
56	MG	XA	1726	1/1	0.84	0.16	62,62,62,62	0
56	MG	RA	3020	1/1	0.84	0.34	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	XA	1620	1/1	0.84	0.11	76,76,76,76	0
56	MG	RA	3214	1/1	0.84	0.12	68,68,68,68	0
56	MG	RA	3775	1/1	0.84	0.40	86,86,86,86	0
56	MG	RD	303	1/1	0.84	0.36	85,85,85,85	0
56	MG	YA	3358	1/1	0.84	0.19	46,46,46,46	0
56	MG	YA	3143	1/1	0.84	0.43	84,84,84,84	0
56	MG	RA	3777	1/1	0.84	0.11	57,57,57,57	0
56	MG	RA	3991	1/1	0.84	0.10	42,42,42,42	0
56	MG	RA	3058	1/1	0.84	0.10	62,62,62,62	0
56	MG	YA	3229	1/1	0.84	0.31	77,77,77,77	0
56	MG	QA	1702	1/1	0.84	0.07	51,51,51,51	0
56	MG	YA	3694	1/1	0.84	0.28	34,34,34,34	0
56	MG	RA	3311	1/1	0.84	0.17	43,43,43,43	0
56	MG	RA	3941	1/1	0.84	0.20	51,51,51,51	0
56	MG	RA	3942	1/1	0.84	0.18	56,56,56,56	0
56	MG	YA	3394	1/1	0.84	0.36	34,34,34,34	0
56	MG	RA	3160	1/1	0.84	0.32	89,89,89,89	0
56	MG	XA	1771	1/1	0.84	0.31	64,64,64,64	0
56	MG	QA	1601	1/1	0.84	0.16	57,57,57,57	0
56	MG	RA	3645	1/1	0.84	0.28	54,54,54,54	0
56	MG	XA	1648	1/1	0.84	0.09	76,76,76,76	0
56	MG	QA	1782	1/1	0.84	0.13	53,53,53,53	0
56	MG	YA	3533	1/1	0.84	0.20	54,54,54,54	0
56	MG	YA	3406	1/1	0.84	0.39	38,38,38,38	0
56	MG	YA	3536	1/1	0.84	0.23	35,35,35,35	0
56	MG	XA	1653	1/1	0.84	0.18	79,79,79,79	0
56	MG	YA	3161	1/1	0.84	0.29	73,73,73,73	0
56	MG	YA	3248	1/1	0.84	0.27	52,52,52,52	0
56	MG	QA	1657	1/1	0.84	0.12	71,71,71,71	0
56	MG	XF	203	1/1	0.84	0.28	80,80,80,80	0
56	MG	YA	3722	1/1	0.84	0.11	49,49,49,49	0
56	MG	YA	3061	1/1	0.84	0.13	47,47,47,47	0
56	MG	RA	3527	1/1	0.84	0.18	55,55,55,55	0
56	MG	XV	104	1/1	0.84	0.20	52,52,52,52	0
56	MG	RA	3881	1/1	0.84	0.27	41,41,41,41	0
56	MG	RA	3785	1/1	0.84	0.29	66,66,66,66	0
56	MG	QA	1788	1/1	0.84	0.24	48,48,48,48	0
56	MG	RA	3428	1/1	0.84	0.32	34,34,34,34	0
56	MG	YA	3070	1/1	0.84	0.19	63,63,63,63	0
56	MG	QA	1662	1/1	0.84	0.15	51,51,51,51	0
56	MG	YA	3173	1/1	0.84	0.27	77,77,77,77	0
56	MG	QA	1738	1/1	0.85	0.27	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	3412	1/1	0.85	0.21	48,48,48,48	0
56	MG	YA	3713	1/1	0.85	0.28	56,56,56,56	0
56	MG	QA	1741	1/1	0.85	0.08	57,57,57,57	0
56	MG	YA	3715	1/1	0.85	0.20	44,44,44,44	0
56	MG	YA	3716	1/1	0.85	0.35	34,34,34,34	0
56	MG	RR	201	1/1	0.85	0.30	79,79,79,79	0
56	MG	QA	1624	1/1	0.85	0.09	77,77,77,77	0
56	MG	RR	204	1/1	0.85	0.16	65,65,65,65	0
56	MG	YA	3091	1/1	0.85	0.13	66,66,66,66	0
56	MG	RA	3268	1/1	0.85	0.30	68,68,68,68	0
56	MG	QL	202	1/1	0.85	0.27	65,65,65,65	0
56	MG	YA	3554	1/1	0.85	0.24	68,68,68,68	0
56	MG	YA	3281	1/1	0.85	0.21	49,49,49,49	0
56	MG	YA	3561	1/1	0.85	0.44	50,50,50,50	0
56	MG	YA	3562	1/1	0.85	0.24	34,34,34,34	0
56	MG	YA	3563	1/1	0.85	0.21	35,35,35,35	0
56	MG	YB	201	1/1	0.85	0.21	51,51,51,51	0
56	MG	YA	3565	1/1	0.85	0.28	40,40,40,40	0
56	MG	YA	3282	1/1	0.85	0.27	34,34,34,34	0
56	MG	RA	3341	1/1	0.85	0.23	42,42,42,42	0
56	MG	RA	3865	1/1	0.85	0.18	46,46,46,46	0
56	MG	RA	3930	1/1	0.85	0.15	57,57,57,57	0
56	MG	RA	3011	1/1	0.85	0.17	66,66,66,66	0
56	MG	YA	3439	1/1	0.85	0.21	65,65,65,65	0
56	MG	YA	3574	1/1	0.85	0.31	41,41,41,41	0
56	MG	RA	3028	1/1	0.85	0.38	58,58,58,58	0
56	MG	RA	3204	1/1	0.85	0.31	86,86,86,86	0
56	MG	YA	3583	1/1	0.85	0.33	34,34,34,34	0
56	MG	QA	1813	1/1	0.85	0.23	55,55,55,55	0
56	MG	QV	105	1/1	0.85	0.09	84,84,84,84	0
56	MG	RA	3370	1/1	0.85	0.36	53,53,53,53	0
56	MG	QA	1757	1/1	0.85	0.17	81,81,81,81	0
56	MG	RA	3089	1/1	0.85	0.22	73,73,73,73	0
56	MG	R0	103	1/1	0.85	0.39	72,72,72,72	0
56	MG	YA	3598	1/1	0.85	0.31	34,34,34,34	0
56	MG	RA	3749	1/1	0.85	0.31	36,36,36,36	0
56	MG	YA	3604	1/1	0.85	0.37	66,66,66,66	0
56	MG	YA	3308	1/1	0.85	0.24	34,34,34,34	0
56	MG	YG	201	1/1	0.85	0.11	40,40,40,40	0
56	MG	RA	3542	1/1	0.85	0.36	73,73,73,73	0
56	MG	RA	3995	1/1	0.85	0.27	47,47,47,47	0
56	MG	YA	3616	1/1	0.85	0.13	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	3752	1/1	0.85	0.25	54,54,54,54	0
56	MG	YA	3465	1/1	0.85	0.28	60,60,60,60	0
56	MG	YA	3121	1/1	0.85	0.32	78,78,78,78	0
56	MG	RA	3691	1/1	0.85	0.30	49,49,49,49	0
56	MG	RA	3568	1/1	0.85	0.29	78,78,78,78	0
56	MG	YA	3325	1/1	0.85	0.25	37,37,37,37	0
56	MG	YA	3636	1/1	0.85	0.43	62,62,62,62	0
56	MG	YA	3025	1/1	0.85	0.13	43,43,43,43	0
56	MG	YA	3643	1/1	0.85	0.36	39,39,39,39	0
56	MG	RA	3634	1/1	0.85	0.11	48,48,48,48	0
56	MG	RA	3173	1/1	0.85	0.19	44,44,44,44	0
56	MG	RA	4005	1/1	0.85	0.32	70,70,70,70	0
56	MG	XA	1733	1/1	0.85	0.25	58,58,58,58	0
56	MG	YA	3651	1/1	0.85	0.16	44,44,44,44	0
56	MG	QA	1703	1/1	0.85	0.25	41,41,41,41	0
56	MG	XA	1609	1/1	0.85	0.20	45,45,45,45	0
56	MG	YA	3139	1/1	0.85	0.22	80,80,80,80	0
56	MG	RA	3952	1/1	0.85	0.10	49,49,49,49	0
56	MG	YA	3037	1/1	0.85	0.32	88,88,88,88	0
56	MG	XA	1747	1/1	0.85	0.18	37,37,37,37	0
56	MG	RA	3033	1/1	0.85	0.25	90,90,90,90	0
56	MG	RA	3954	1/1	0.85	0.28	45,45,45,45	0
56	MG	XA	1750	1/1	0.85	0.25	37,37,37,37	0
56	MG	RA	4012	1/1	0.85	0.23	66,66,66,66	0
56	MG	XA	1757	1/1	0.85	0.10	58,58,58,58	0
56	MG	RA	3841	1/1	0.85	0.20	53,53,53,53	0
56	MG	XA	1760	1/1	0.85	0.21	44,44,44,44	0
56	MG	RA	3762	1/1	0.85	0.29	59,59,59,59	0
56	MG	RA	3318	1/1	0.85	0.17	56,56,56,56	0
56	MG	RA	3404	1/1	0.85	0.37	35,35,35,35	0
56	MG	RA	3429	1/1	0.85	0.42	34,34,34,34	0
56	MG	YA	3363	1/1	0.85	0.25	48,48,48,48	0
56	MG	XA	1626	1/1	0.85	0.08	55,55,55,55	0
56	MG	RA	3850	1/1	0.85	0.31	37,37,37,37	0
56	MG	RA	3482	1/1	0.85	0.20	34,34,34,34	0
56	MG	XA	1629	1/1	0.85	0.15	44,44,44,44	0
56	MG	XA	1631	1/1	0.85	0.13	41,41,41,41	0
56	MG	RA	3735	1/1	0.85	0.22	56,56,56,56	0
56	MG	RA	4027	1/1	0.85	0.37	99,99,99,99	0
56	MG	YA	3510	1/1	0.85	0.38	97,97,97,97	0
56	MG	RA	3528	1/1	0.85	0.17	58,58,58,58	0
56	MG	YA	3381	1/1	0.85	0.24	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	3059	1/1	0.85	0.20	39,39,39,39	0
56	MG	QA	1724	1/1	0.85	0.23	77,77,77,77	0
56	MG	RA	4031	1/1	0.85	0.19	58,58,58,58	0
56	MG	QA	1858	1/1	0.85	0.09	84,84,84,84	0
56	MG	RA	3770	1/1	0.85	0.22	39,39,39,39	0
56	MG	YA	3396	1/1	0.85	0.31	61,61,61,61	0
56	MG	YA	3698	1/1	0.85	0.38	43,43,43,43	0
56	MG	XV	103	1/1	0.85	0.08	55,55,55,55	0
56	MG	YA	3398	1/1	0.85	0.33	34,34,34,34	0
56	MG	QA	1795	1/1	0.85	0.20	42,42,42,42	0
56	MG	QB	301	1/1	0.85	0.14	72,72,72,72	0
56	MG	YA	3526	1/1	0.85	0.21	49,49,49,49	0
56	MG	YA	3254	1/1	0.85	0.35	45,45,45,45	0
56	MG	RA	3919	1/1	0.85	0.15	41,41,41,41	0
56	MG	RA	3114	1/1	0.85	0.23	110,110,110,110	0
56	MG	RA	3586	1/1	0.85	0.68	89,89,89,89	0
56	MG	YA	3366	1/1	0.86	0.16	58,58,58,58	0
56	MG	RA	3138	1/1	0.86	0.43	110,110,110,110	0
56	MG	YA	3225	1/1	0.86	0.17	56,56,56,56	0
56	MG	RA	3693	1/1	0.86	0.13	51,51,51,51	0
56	MG	RA	3361	1/1	0.86	0.36	59,59,59,59	0
56	MG	YA	3021	1/1	0.86	0.12	34,34,34,34	0
56	MG	YA	3129	1/1	0.86	0.32	69,69,69,69	0
56	MG	RA	3017	1/1	0.86	0.26	49,49,49,49	0
56	MG	YA	3233	1/1	0.86	0.27	100,100,100,100	0
56	MG	RA	3277	1/1	0.86	0.28	81,81,81,81	0
56	MG	YA	3719	1/1	0.86	0.31	74,74,74,74	0
56	MG	RA	3813	1/1	0.86	0.32	52,52,52,52	0
56	MG	RA	3238	1/1	0.86	0.25	79,79,79,79	0
56	MG	RA	3412	1/1	0.86	0.20	74,74,74,74	0
56	MG	XA	1673	1/1	0.86	0.19	38,38,38,38	0
56	MG	XA	1674	1/1	0.86	0.16	52,52,52,52	0
56	MG	RA	3896	1/1	0.86	0.20	42,42,42,42	0
56	MG	YA	3729	1/1	0.86	0.24	34,34,34,34	0
56	MG	YA	3402	1/1	0.86	0.29	51,51,51,51	0
56	MG	QA	1674	1/1	0.86	0.08	50,50,50,50	0
56	MG	RA	3594	1/1	0.86	0.32	54,54,54,54	0
56	MG	YA	3736	1/1	0.86	0.14	65,65,65,65	0
56	MG	YA	3557	1/1	0.86	0.20	34,34,34,34	0
56	MG	YA	3244	1/1	0.86	0.21	67,67,67,67	0
56	MG	YA	3035	1/1	0.86	0.07	47,47,47,47	0
56	MG	YA	3749	1/1	0.86	0.17	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3247	1/1	0.86	0.11	88,88,88,88	0
56	MG	RA	3899	1/1	0.86	0.23	55,55,55,55	0
56	MG	RA	3368	1/1	0.86	0.22	49,49,49,49	0
56	MG	RA	3092	1/1	0.86	0.12	89,89,89,89	0
56	MG	QA	1679	1/1	0.86	0.11	69,69,69,69	0
56	MG	QA	1761	1/1	0.86	0.17	68,68,68,68	0
56	MG	XA	1696	1/1	0.86	0.25	40,40,40,40	0
56	MG	YB	208	1/1	0.86	0.59	117,117,117,117	0
56	MG	QA	1680	1/1	0.86	0.10	48,48,48,48	0
56	MG	YA	3046	1/1	0.86	0.19	56,56,56,56	0
56	MG	RA	3903	1/1	0.86	0.27	51,51,51,51	0
56	MG	XA	1701	1/1	0.86	0.13	47,47,47,47	0
56	MG	RA	3654	1/1	0.86	0.26	72,72,72,72	0
56	MG	YA	3578	1/1	0.86	0.20	48,48,48,48	0
56	MG	YA	3257	1/1	0.86	0.23	59,59,59,59	0
56	MG	RA	3504	1/1	0.86	0.34	80,80,80,80	0
56	MG	RA	3208	1/1	0.86	0.23	67,67,67,67	0
56	MG	RA	3908	1/1	0.86	0.26	45,45,45,45	0
56	MG	YA	3436	1/1	0.86	0.18	37,37,37,37	0
56	MG	RA	3507	1/1	0.86	0.20	43,43,43,43	0
56	MG	YE	301	1/1	0.86	0.27	70,70,70,70	0
56	MG	RA	3989	1/1	0.86	0.30	87,87,87,87	0
56	MG	RA	3283	1/1	0.86	0.11	56,56,56,56	0
56	MG	YA	3596	1/1	0.86	0.26	45,45,45,45	0
56	MG	YA	3273	1/1	0.86	0.36	34,34,34,34	0
56	MG	YA	3059	1/1	0.86	0.12	42,42,42,42	0
56	MG	YA	3446	1/1	0.86	0.17	34,34,34,34	0
56	MG	RA	3912	1/1	0.86	0.26	64,64,64,64	0
56	MG	RA	3830	1/1	0.86	0.20	56,56,56,56	0
56	MG	RA	3210	1/1	0.86	0.31	90,90,90,90	0
56	MG	RA	3833	1/1	0.86	0.21	36,36,36,36	0
56	MG	RA	3421	1/1	0.86	0.38	34,34,34,34	0
56	MG	RA	3999	1/1	0.86	0.35	121,121,121,121	0
56	MG	YA	3176	1/1	0.86	0.19	58,58,58,58	0
56	MG	YA	3629	1/1	0.86	0.28	49,49,49,49	0
56	MG	RA	3610	1/1	0.86	0.18	81,81,81,81	0
56	MG	XA	1735	1/1	0.86	0.14	59,59,59,59	0
56	MG	RA	3612	1/1	0.86	0.25	67,67,67,67	0
56	MG	YA	3461	1/1	0.86	0.28	34,34,34,34	0
56	MG	RA	3925	1/1	0.86	0.19	50,50,50,50	0
56	MG	YA	3074	1/1	0.86	0.19	46,46,46,46	0
56	MG	RA	3093	1/1	0.86	0.42	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3382	1/1	0.86	0.13	34,34,34,34	0
56	MG	YA	3077	1/1	0.86	0.19	57,57,57,57	0
56	MG	RA	3720	1/1	0.86	0.09	47,47,47,47	0
56	MG	YA	3648	1/1	0.86	0.23	35,35,35,35	0
56	MG	RA	3513	1/1	0.86	0.27	46,46,46,46	0
56	MG	XA	1752	1/1	0.86	0.20	34,34,34,34	0
56	MG	RA	3153	1/1	0.86	0.19	60,60,60,60	0
56	MG	XA	1756	1/1	0.86	0.18	42,42,42,42	0
56	MG	YA	3083	1/1	0.86	0.33	76,76,76,76	0
56	MG	YA	3193	1/1	0.86	0.11	41,41,41,41	0
56	MG	RA	3515	1/1	0.86	0.25	76,76,76,76	0
56	MG	YA	3195	1/1	0.86	0.17	58,58,58,58	0
56	MG	YA	3317	1/1	0.86	0.45	34,34,34,34	0
56	MG	YA	3088	1/1	0.86	0.15	49,49,49,49	0
56	MG	RA	3845	1/1	0.86	0.77	97,97,97,97	0
56	MG	RA	3267	1/1	0.86	0.29	96,96,96,96	0
56	MG	RA	3386	1/1	0.86	0.21	50,50,50,50	0
56	MG	RA	3227	1/1	0.86	0.43	65,65,65,65	0
56	MG	XA	1772	1/1	0.86	0.10	50,50,50,50	0
56	MG	YA	3201	1/1	0.86	0.12	65,65,65,65	0
56	MG	RA	3348	1/1	0.86	0.13	57,57,57,57	0
56	MG	YA	3678	1/1	0.86	0.21	45,45,45,45	0
56	MG	RA	3245	1/1	0.86	0.23	50,50,50,50	0
56	MG	RA	3431	1/1	0.86	0.24	49,49,49,49	0
56	MG	RA	3791	1/1	0.86	0.09	38,38,38,38	0
56	MG	YA	3337	1/1	0.86	0.21	45,45,45,45	0
56	MG	RA	3480	1/1	0.86	0.24	64,64,64,64	0
56	MG	XA	1786	1/1	0.86	0.06	42,42,42,42	0
56	MG	RA	3627	1/1	0.86	0.11	62,62,62,62	0
56	MG	YA	3344	1/1	0.86	0.34	35,35,35,35	0
56	MG	RA	3678	1/1	0.86	0.18	40,40,40,40	0
56	MG	XF	202	1/1	0.86	0.10	82,82,82,82	0
56	MG	XA	1641	1/1	0.86	0.14	64,64,64,64	0
56	MG	QA	1803	1/1	0.86	0.06	61,61,61,61	0
56	MG	RA	3246	1/1	0.86	0.38	90,90,90,90	0
56	MG	RA	3018	1/1	0.86	0.32	95,95,95,95	0
56	MG	YA	3350	1/1	0.86	0.29	53,53,53,53	0
56	MG	RA	3044	1/1	0.86	0.40	74,74,74,74	0
56	MG	RA	3231	1/1	0.86	0.32	59,59,59,59	0
56	MG	RA	3530	1/1	0.86	0.21	43,43,43,43	0
56	MG	RA	3399	1/1	0.86	0.20	34,34,34,34	0
57	ZN	R6	101	1/1	0.86	0.34	170,170,170,170	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3362	1/1	0.86	0.23	35,35,35,35	0
56	MG	YA	3703	1/1	0.86	0.35	50,50,50,50	0
56	MG	RA	3216	1/1	0.86	0.43	81,81,81,81	0
56	MG	QA	1740	1/1	0.86	0.18	52,52,52,52	0
56	MG	YA	3125	1/1	0.87	0.09	35,35,35,35	0
56	MG	YA	3586	1/1	0.87	0.23	60,60,60,60	0
56	MG	R3	101	1/1	0.87	0.21	72,72,72,72	0
56	MG	RA	3157	1/1	0.87	0.43	89,89,89,89	0
56	MG	RA	4000	1/1	0.87	0.25	102,102,102,102	0
56	MG	YB	204	1/1	0.87	0.09	55,55,55,55	0
56	MG	YA	3592	1/1	0.87	0.33	34,34,34,34	0
56	MG	QA	1837	1/1	0.87	0.24	44,44,44,44	0
56	MG	YA	3131	1/1	0.87	0.30	74,74,74,74	0
56	MG	YA	3219	1/1	0.87	0.08	63,63,63,63	0
56	MG	YB	210	1/1	0.87	0.13	40,40,40,40	0
56	MG	RD	311	1/1	0.87	0.24	63,63,63,63	0
56	MG	RD	313	1/1	0.87	0.28	71,71,71,71	0
56	MG	YA	3605	1/1	0.87	0.26	34,34,34,34	0
56	MG	RA	3213	1/1	0.87	0.34	74,74,74,74	0
56	MG	YA	3472	1/1	0.87	0.27	35,35,35,35	0
56	MG	RA	3079	1/1	0.87	0.32	90,90,90,90	0
56	MG	YA	3339	1/1	0.87	0.21	38,38,38,38	0
56	MG	YA	3618	1/1	0.87	0.26	40,40,40,40	0
56	MG	YA	3479	1/1	0.87	0.36	69,69,69,69	0
56	MG	RA	3831	1/1	0.87	0.24	55,55,55,55	0
56	MG	YA	3624	1/1	0.87	0.17	54,54,54,54	0
56	MG	YA	3625	1/1	0.87	0.19	60,60,60,60	0
56	MG	YE	302	1/1	0.87	0.16	55,55,55,55	0
56	MG	RA	3521	1/1	0.87	0.14	58,58,58,58	0
56	MG	RA	3070	1/1	0.87	0.32	48,48,48,48	0
56	MG	RA	4010	1/1	0.87	0.34	108,108,108,108	0
56	MG	RA	3547	1/1	0.87	0.21	48,48,48,48	0
56	MG	YA	3632	1/1	0.87	0.33	34,34,34,34	0
56	MG	YA	3050	1/1	0.87	0.19	53,53,53,53	0
56	MG	RA	3548	1/1	0.87	0.15	53,53,53,53	0
56	MG	XA	1712	1/1	0.87	0.22	43,43,43,43	0
56	MG	RA	3625	1/1	0.87	0.16	38,38,38,38	0
56	MG	YP	201	1/1	0.87	0.27	73,73,73,73	0
56	MG	YA	3491	1/1	0.87	0.18	57,57,57,57	0
56	MG	RA	3379	1/1	0.87	0.17	34,34,34,34	0
56	MG	YA	3237	1/1	0.87	0.12	51,51,51,51	0
56	MG	QA	1729	1/1	0.87	0.12	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	3360	1/1	0.87	0.16	44,44,44,44	0
56	MG	YA	3361	1/1	0.87	0.34	34,34,34,34	0
56	MG	QA	1859	1/1	0.87	0.28	78,78,78,78	0
56	MG	RA	3248	1/1	0.87	0.22	71,71,71,71	0
56	MG	RA	3705	1/1	0.87	0.10	66,66,66,66	0
56	MG	YA	3504	1/1	0.87	0.28	34,34,34,34	0
56	MG	RA	3589	1/1	0.87	0.36	72,72,72,72	0
56	MG	RA	3360	1/1	0.87	0.31	55,55,55,55	0
56	MG	QA	1737	1/1	0.87	0.11	56,56,56,56	0
56	MG	XA	1728	1/1	0.87	0.10	58,58,58,58	0
56	MG	RA	3843	1/1	0.87	0.10	41,41,41,41	0
56	MG	RA	3476	1/1	0.87	0.24	34,34,34,34	0
56	MG	YA	3670	1/1	0.87	0.34	43,43,43,43	0
56	MG	RA	3125	1/1	0.87	0.20	48,48,48,48	0
56	MG	XA	1738	1/1	0.87	0.29	37,37,37,37	0
56	MG	RA	3846	1/1	0.87	0.28	41,41,41,41	0
56	MG	XA	1742	1/1	0.87	0.17	47,47,47,47	0
56	MG	RA	3479	1/1	0.87	0.21	61,61,61,61	0
56	MG	RA	3531	1/1	0.87	0.40	81,81,81,81	0
56	MG	RA	4032	1/1	0.87	0.34	94,94,94,94	0
56	MG	QA	1749	1/1	0.87	0.26	76,76,76,76	0
56	MG	RA	3407	1/1	0.87	0.14	55,55,55,55	0
56	MG	RA	3560	1/1	0.87	0.21	49,49,49,49	0
56	MG	RA	3716	1/1	0.87	0.09	48,48,48,48	0
56	MG	YA	3524	1/1	0.87	0.23	49,49,49,49	0
56	MG	QA	1685	1/1	0.87	0.17	92,92,92,92	0
56	MG	YA	3178	1/1	0.87	0.10	41,41,41,41	0
56	MG	RA	3533	1/1	0.87	0.15	61,61,61,61	0
56	MG	RA	3266	1/1	0.87	0.09	82,82,82,82	0
56	MG	YA	3269	1/1	0.87	0.19	40,40,40,40	0
56	MG	YA	3270	1/1	0.87	0.09	43,43,43,43	0
56	MG	XA	1630	1/1	0.87	0.18	57,57,57,57	0
56	MG	RA	3036	1/1	0.87	0.22	72,72,72,72	0
56	MG	RA	3643	1/1	0.87	0.30	64,64,64,64	0
56	MG	YA	3001	1/1	0.87	0.30	86,86,86,86	0
56	MG	YA	3420	1/1	0.87	0.18	44,44,44,44	0
56	MG	YA	3542	1/1	0.87	0.30	75,75,75,75	0
56	MG	YA	3002	1/1	0.87	0.12	35,35,35,35	0
56	MG	QA	1690	1/1	0.87	0.12	76,76,76,76	0
56	MG	YA	3095	1/1	0.87	0.15	41,41,41,41	0
56	MG	YA	3189	1/1	0.87	0.25	57,57,57,57	0
56	MG	XA	1777	1/1	0.87	0.18	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	3005	1/1	0.87	0.27	69,69,69,69	0
56	MG	RA	3229	1/1	0.87	0.21	71,71,71,71	0
56	MG	QA	1818	1/1	0.87	0.13	43,43,43,43	0
56	MG	YA	3008	1/1	0.87	0.14	42,42,42,42	0
56	MG	YA	3711	1/1	0.87	0.15	62,62,62,62	0
56	MG	XA	1784	1/1	0.87	0.09	88,88,88,88	0
56	MG	YA	3558	1/1	0.87	0.20	44,44,44,44	0
56	MG	RA	3681	1/1	0.87	0.10	41,41,41,41	0
56	MG	RA	3127	1/1	0.87	0.23	57,57,57,57	0
56	MG	RA	3054	1/1	0.87	0.38	100,100,100,100	0
56	MG	RA	3435	1/1	0.87	0.17	43,43,43,43	0
56	MG	RA	3417	1/1	0.87	0.22	55,55,55,55	0
56	MG	YA	3113	1/1	0.87	0.06	40,40,40,40	0
56	MG	RB	219	1/1	0.87	0.06	43,43,43,43	0
56	MG	RA	3873	1/1	0.87	0.18	58,58,58,58	0
56	MG	RA	3936	1/1	0.87	0.28	66,66,66,66	0
56	MG	RA	3688	1/1	0.87	0.22	45,45,45,45	0
56	MG	RA	3652	1/1	0.87	0.14	48,48,48,48	0
56	MG	YA	3027	1/1	0.87	0.18	38,38,38,38	0
56	MG	YA	3028	1/1	0.87	0.21	52,52,52,52	0
56	MG	YA	3581	1/1	0.87	0.25	34,34,34,34	0
56	MG	RA	3878	1/1	0.87	0.12	60,60,60,60	0
56	MG	RA	3440	1/1	0.87	0.17	37,37,37,37	0
56	MG	YA	3743	1/1	0.87	0.34	113,113,113,113	0
56	MG	YA	3745	1/1	0.87	0.23	64,64,64,64	0
56	MG	YA	3322	1/1	0.87	0.22	34,34,34,34	0
57	ZN	Y9	101	1/1	0.87	0.36	147,147,147,147	0
56	MG	YD	302	1/1	0.88	0.17	40,40,40,40	0
56	MG	YD	303	1/1	0.88	0.62	59,59,59,59	0
56	MG	RA	3590	1/1	0.88	0.24	68,68,68,68	0
56	MG	YA	3063	1/1	0.88	0.16	53,53,53,53	0
56	MG	YA	3649	1/1	0.88	0.22	39,39,39,39	0
56	MG	RA	3591	1/1	0.88	0.19	55,55,55,55	0
56	MG	YA	3654	1/1	0.88	0.28	34,34,34,34	0
56	MG	YA	3145	1/1	0.88	0.17	47,47,47,47	0
56	MG	RA	3385	1/1	0.88	0.40	34,34,34,34	0
56	MG	YA	3658	1/1	0.88	0.25	34,34,34,34	0
56	MG	YA	3303	1/1	0.88	0.13	50,50,50,50	0
56	MG	RD	301	1/1	0.88	0.27	57,57,57,57	0
56	MG	YF	302	1/1	0.88	0.47	91,91,91,91	0
56	MG	YA	3425	1/1	0.88	0.20	39,39,39,39	0
56	MG	YG	202	1/1	0.88	0.07	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	3665	1/1	0.88	0.40	60,60,60,60	0
56	MG	RA	3807	1/1	0.88	0.42	60,60,60,60	0
56	MG	YO	201	1/1	0.88	0.12	43,43,43,43	0
56	MG	YA	3309	1/1	0.88	0.22	36,36,36,36	0
56	MG	XA	1708	1/1	0.88	0.24	50,50,50,50	0
56	MG	RA	3062	1/1	0.88	0.12	42,42,42,42	0
56	MG	YA	3534	1/1	0.88	0.16	50,50,50,50	0
56	MG	YT	201	1/1	0.88	0.15	76,76,76,76	0
56	MG	YA	3430	1/1	0.88	0.20	34,34,34,34	0
56	MG	QA	1650	1/1	0.88	0.09	43,43,43,43	0
56	MG	RA	3069	1/1	0.88	0.20	48,48,48,48	0
56	MG	QV	104	1/1	0.88	0.30	63,63,63,63	0
56	MG	RA	3389	1/1	0.88	0.16	34,34,34,34	0
56	MG	YA	3321	1/1	0.88	0.46	34,34,34,34	0
56	MG	YA	3158	1/1	0.88	0.17	36,36,36,36	0
56	MG	RA	3710	1/1	0.88	0.15	41,41,41,41	0
56	MG	RA	3772	1/1	0.88	0.16	40,40,40,40	0
56	MG	RA	3282	1/1	0.88	0.14	46,46,46,46	0
56	MG	RA	4009	1/1	0.88	0.10	73,73,73,73	0
56	MG	RA	3432	1/1	0.88	0.16	37,37,37,37	0
56	MG	RA	3743	1/1	0.88	0.25	43,43,43,43	0
56	MG	YA	3556	1/1	0.88	0.20	35,35,35,35	0
56	MG	RA	3600	1/1	0.88	0.26	34,34,34,34	0
56	MG	RA	3858	1/1	0.88	0.10	50,50,50,50	0
56	MG	RA	3603	1/1	0.88	0.22	38,38,38,38	0
56	MG	YA	3015	1/1	0.88	0.31	84,84,84,84	0
56	MG	RA	3963	1/1	0.88	0.13	57,57,57,57	0
56	MG	RA	3685	1/1	0.88	0.12	53,53,53,53	0
56	MG	XA	1618	1/1	0.88	0.20	57,57,57,57	0
56	MG	RA	3091	1/1	0.88	0.29	101,101,101,101	0
56	MG	YA	3019	1/1	0.88	0.20	52,52,52,52	0
56	MG	RA	3335	1/1	0.88	0.29	34,34,34,34	0
56	MG	RA	3263	1/1	0.88	0.21	63,63,63,63	0
56	MG	RA	4025	1/1	0.88	0.16	68,68,68,68	0
56	MG	YA	3099	1/1	0.88	0.13	47,47,47,47	0
56	MG	RA	3458	1/1	0.88	0.15	39,39,39,39	0
56	MG	YA	3575	1/1	0.88	0.13	46,46,46,46	0
56	MG	RA	3866	1/1	0.88	0.33	47,47,47,47	0
56	MG	RA	3790	1/1	0.88	0.20	60,60,60,60	0
56	MG	YA	3579	1/1	0.88	0.17	40,40,40,40	0
56	MG	YA	3106	1/1	0.88	0.27	77,77,77,77	0
56	MG	YA	3107	1/1	0.88	0.14	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3474	1/1	0.88	0.26	43,43,43,43	0
56	MG	RA	3286	1/1	0.88	0.12	73,73,73,73	0
56	MG	YA	3478	1/1	0.88	0.23	35,35,35,35	0
56	MG	RA	3924	1/1	0.88	0.17	84,84,84,84	0
56	MG	RA	3692	1/1	0.88	0.42	96,96,96,96	0
56	MG	RA	3144	1/1	0.88	0.13	42,42,42,42	0
56	MG	RA	3167	1/1	0.88	0.14	62,62,62,62	0
56	MG	YA	3262	1/1	0.88	0.18	48,48,48,48	0
56	MG	YA	3485	1/1	0.88	0.29	34,34,34,34	0
56	MG	RA	3876	1/1	0.88	0.16	34,34,34,34	0
56	MG	RA	3198	1/1	0.88	0.16	45,45,45,45	0
56	MG	YA	3732	1/1	0.88	0.17	47,47,47,47	0
56	MG	YA	3599	1/1	0.88	0.14	34,34,34,34	0
56	MG	YA	3734	1/1	0.88	0.27	50,50,50,50	0
56	MG	QA	1739	1/1	0.88	0.24	37,37,37,37	0
56	MG	YA	3375	1/1	0.88	0.22	39,39,39,39	0
56	MG	YA	3739	1/1	0.88	0.23	34,34,34,34	0
56	MG	RA	3358	1/1	0.88	0.20	34,34,34,34	0
56	MG	XA	1656	1/1	0.88	0.08	52,52,52,52	0
56	MG	YA	3380	1/1	0.88	0.32	36,36,36,36	0
56	MG	YA	3744	1/1	0.88	0.43	54,54,54,54	0
56	MG	YA	3271	1/1	0.88	0.38	34,34,34,34	0
56	MG	RA	3882	1/1	0.88	0.25	34,34,34,34	0
56	MG	RA	3191	1/1	0.88	0.27	76,76,76,76	0
56	MG	QA	1629	1/1	0.88	0.07	39,39,39,39	0
56	MG	YA	3388	1/1	0.88	0.24	34,34,34,34	0
56	MG	YA	3277	1/1	0.88	0.10	42,42,42,42	0
56	MG	YA	3502	1/1	0.88	0.26	72,72,72,72	0
56	MG	QA	1862	1/1	0.88	0.16	82,82,82,82	0
56	MG	QA	1744	1/1	0.88	0.10	43,43,43,43	0
56	MG	YA	3627	1/1	0.88	0.24	67,67,67,67	0
56	MG	RB	210	1/1	0.88	0.17	46,46,46,46	0
56	MG	RA	3933	1/1	0.88	0.44	95,95,95,95	0
56	MG	RA	3884	1/1	0.88	0.21	34,34,34,34	0
56	MG	RA	3990	1/1	0.88	0.34	69,69,69,69	0
57	ZN	R4	101	1/1	0.88	0.16	177,177,177,177	0
56	MG	YA	3633	1/1	0.88	0.19	45,45,45,45	0
56	MG	RA	3885	1/1	0.88	0.29	79,79,79,79	0
56	MG	RA	3993	1/1	0.88	0.30	94,94,94,94	0
56	MG	RA	3470	1/1	0.88	0.35	34,34,34,34	0
56	MG	YA	3514	1/1	0.88	0.18	48,48,48,48	0
56	MG	RA	3112	1/1	0.88	0.31	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	QA	1643	1/1	0.88	0.18	103,103,103,103	0
56	MG	YA	3036	1/1	0.89	0.28	54,54,54,54	0
56	MG	YA	3184	1/1	0.89	0.34	101,101,101,101	0
56	MG	YA	3696	1/1	0.89	0.13	48,48,48,48	0
56	MG	RA	3465	1/1	0.89	0.22	34,34,34,34	0
56	MG	XA	1702	1/1	0.89	0.17	43,43,43,43	0
56	MG	Y5	102	1/1	0.89	0.15	75,75,75,75	0
56	MG	YA	3111	1/1	0.89	0.14	56,56,56,56	0
56	MG	YA	3699	1/1	0.89	0.18	34,34,34,34	0
56	MG	YA	3187	1/1	0.89	0.19	57,57,57,57	0
56	MG	RE	301	1/1	0.89	0.33	76,76,76,76	0
56	MG	YA	3477	1/1	0.89	0.16	57,57,57,57	0
56	MG	RA	3773	1/1	0.89	0.24	64,64,64,64	0
56	MG	RE	307	1/1	0.89	0.16	58,58,58,58	0
56	MG	YA	3265	1/1	0.89	0.34	58,58,58,58	0
56	MG	XA	1607	1/1	0.89	0.16	43,43,43,43	0
56	MG	QD	301	1/1	0.89	0.18	47,47,47,47	0
56	MG	YA	3371	1/1	0.89	0.26	34,34,34,34	0
56	MG	RA	3890	1/1	0.89	0.23	37,37,37,37	0
56	MG	R7	102	1/1	0.89	0.14	67,67,67,67	0
56	MG	RA	3356	1/1	0.89	0.30	55,55,55,55	0
56	MG	YA	3379	1/1	0.89	0.15	42,42,42,42	0
56	MG	RA	3225	1/1	0.89	0.60	91,91,91,91	0
56	MG	RA	3982	1/1	0.89	0.25	66,66,66,66	0
56	MG	RA	3937	1/1	0.89	0.13	62,62,62,62	0
56	MG	RA	3893	1/1	0.89	0.23	47,47,47,47	0
56	MG	QA	1760	1/1	0.89	0.22	41,41,41,41	0
56	MG	YA	3718	1/1	0.89	0.16	37,37,37,37	0
56	MG	YA	3387	1/1	0.89	0.30	56,56,56,56	0
56	MG	RA	3376	1/1	0.89	0.24	34,34,34,34	0
56	MG	YA	3392	1/1	0.89	0.30	37,37,37,37	0
56	MG	YA	3723	1/1	0.89	0.09	64,64,64,64	0
56	MG	XA	1732	1/1	0.89	0.12	43,43,43,43	0
56	MG	RA	3262	1/1	0.89	0.19	76,76,76,76	0
56	MG	YA	3726	1/1	0.89	0.20	50,50,50,50	0
56	MG	RA	3433	1/1	0.89	0.14	59,59,59,59	0
56	MG	RA	3687	1/1	0.89	0.23	64,64,64,64	0
56	MG	YA	3397	1/1	0.89	0.38	34,34,34,34	0
56	MG	RA	3122	1/1	0.89	0.10	45,45,45,45	0
56	MG	YA	3206	1/1	0.89	0.27	86,86,86,86	0
56	MG	YA	3289	1/1	0.89	0.24	34,34,34,34	0
56	MG	YA	3062	1/1	0.89	0.11	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	3291	1/1	0.89	0.16	38,38,38,38	0
56	MG	RA	3332	1/1	0.89	0.25	49,49,49,49	0
56	MG	RA	3611	1/1	0.89	0.23	63,63,63,63	0
56	MG	RA	3502	1/1	0.89	0.21	41,41,41,41	0
56	MG	RB	209	1/1	0.89	0.40	55,55,55,55	0
56	MG	RA	3825	1/1	0.89	0.11	50,50,50,50	0
56	MG	RP	202	1/1	0.89	0.33	63,63,63,63	0
56	MG	YA	3416	1/1	0.89	0.06	43,43,43,43	0
56	MG	QA	1619	1/1	0.89	0.09	77,77,77,77	0
56	MG	RA	3303	1/1	0.89	0.19	46,46,46,46	0
56	MG	YA	3639	1/1	0.89	0.23	46,46,46,46	0
56	MG	RA	3828	1/1	0.89	0.14	35,35,35,35	0
56	MG	QA	1775	1/1	0.89	0.22	56,56,56,56	0
56	MG	RA	3264	1/1	0.89	0.39	106,106,106,106	0
56	MG	XA	1766	1/1	0.89	0.26	38,38,38,38	0
56	MG	RA	3639	1/1	0.89	0.11	49,49,49,49	0
56	MG	RA	3209	1/1	0.89	0.09	37,37,37,37	0
56	MG	RA	3134	1/1	0.89	0.28	91,91,91,91	0
56	MG	YA	3529	1/1	0.89	0.16	34,34,34,34	0
56	MG	RA	3914	1/1	0.89	0.25	97,97,97,97	0
56	MG	YA	3081	1/1	0.89	0.17	75,75,75,75	0
56	MG	YA	3013	1/1	0.89	0.20	35,35,35,35	0
56	MG	RA	3564	1/1	0.89	0.15	49,49,49,49	0
56	MG	QA	1732	1/1	0.89	0.10	41,41,41,41	0
56	MG	YA	3659	1/1	0.89	0.23	34,34,34,34	0
56	MG	YA	3085	1/1	0.89	0.25	81,81,81,81	0
56	MG	RA	3592	1/1	0.89	0.31	74,74,74,74	0
56	MG	YA	3090	1/1	0.89	0.11	34,34,34,34	0
56	MG	RA	3800	1/1	0.89	0.19	34,34,34,34	0
56	MG	YA	3543	1/1	0.89	0.19	49,49,49,49	0
56	MG	RA	3008	1/1	0.89	0.20	78,78,78,78	0
56	MG	YA	3167	1/1	0.89	0.22	52,52,52,52	0
56	MG	RD	302	1/1	0.89	0.12	43,43,43,43	0
56	MG	RA	3701	1/1	0.89	0.21	47,47,47,47	0
56	MG	RA	3297	1/1	0.89	0.18	78,78,78,78	0
56	MG	QA	1847	1/1	0.89	0.15	45,45,45,45	0
56	MG	QA	1637	1/1	0.89	0.08	35,35,35,35	0
56	MG	XT	201	1/1	0.89	0.17	63,63,63,63	0
56	MG	QA	1793	1/1	0.89	0.09	50,50,50,50	0
56	MG	YA	3341	1/1	0.89	0.19	45,45,45,45	0
56	MG	RA	3647	1/1	0.89	0.14	55,55,55,55	0
56	MG	YA	3559	1/1	0.89	0.22	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	4014	1/1	0.89	0.13	40,40,40,40	0
56	MG	YA	3101	1/1	0.89	0.14	35,35,35,35	0
56	MG	RA	3445	1/1	0.89	0.10	67,67,67,67	0
56	MG	YA	3348	1/1	0.89	0.35	34,34,34,34	0
56	MG	RA	3105	1/1	0.89	0.21	66,66,66,66	0
56	MG	RA	3572	1/1	0.89	0.12	58,58,58,58	0
56	MG	RA	3653	1/1	0.89	0.21	41,41,41,41	0
56	MG	YR	201	1/1	0.89	0.12	42,42,42,42	0
56	MG	YA	3108	1/1	0.89	0.26	34,34,34,34	0
56	MG	YT	202	1/1	0.89	0.09	38,38,38,38	0
56	MG	XA	1619	1/1	0.90	0.12	68,68,68,68	0
56	MG	YA	3356	1/1	0.90	0.12	38,38,38,38	0
56	MG	YA	3445	1/1	0.90	0.26	61,61,61,61	0
56	MG	YA	3641	1/1	0.90	0.28	34,34,34,34	0
56	MG	RA	3481	1/1	0.90	0.26	46,46,46,46	0
56	MG	YA	3738	1/1	0.90	0.20	59,59,59,59	0
56	MG	QA	1607	1/1	0.90	0.18	56,56,56,56	0
56	MG	RA	3426	1/1	0.90	0.19	45,45,45,45	0
56	MG	RA	3759	1/1	0.90	0.43	79,79,79,79	0
56	MG	RA	3760	1/1	0.90	0.21	54,54,54,54	0
56	MG	RA	3569	1/1	0.90	0.09	62,62,62,62	0
56	MG	YA	3541	1/1	0.90	0.23	57,57,57,57	0
56	MG	RA	3410	1/1	0.90	0.18	41,41,41,41	0
56	MG	RA	3870	1/1	0.90	0.37	44,44,44,44	0
56	MG	RA	3871	1/1	0.90	0.21	49,49,49,49	0
56	MG	QA	1616	1/1	0.90	0.13	58,58,58,58	0
56	MG	RA	3571	1/1	0.90	0.25	63,63,63,63	0
56	MG	RA	3915	1/1	0.90	0.20	53,53,53,53	0
56	MG	YA	3042	1/1	0.90	0.11	62,62,62,62	0
56	MG	XA	1729	1/1	0.90	0.15	75,75,75,75	0
56	MG	YA	3376	1/1	0.90	0.29	34,34,34,34	0
56	MG	YA	3662	1/1	0.90	0.25	34,34,34,34	0
56	MG	RA	3334	1/1	0.90	0.25	47,47,47,47	0
56	MG	RA	3485	1/1	0.90	0.22	51,51,51,51	0
56	MG	RA	3071	1/1	0.90	0.20	84,84,84,84	0
56	MG	QH	201	1/1	0.90	0.16	71,71,71,71	0
56	MG	YA	3232	1/1	0.90	0.18	56,56,56,56	0
56	MG	XA	1740	1/1	0.90	0.24	38,38,38,38	0
56	MG	RA	3551	1/1	0.90	0.16	39,39,39,39	0
56	MG	RA	3880	1/1	0.90	0.09	35,35,35,35	0
56	MG	YA	3304	1/1	0.90	0.37	44,44,44,44	0
56	MG	YA	3305	1/1	0.90	0.22	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3709	1/1	0.90	0.10	41,41,41,41	0
56	MG	YA	3675	1/1	0.90	0.29	34,34,34,34	0
56	MG	YA	3393	1/1	0.90	0.26	54,54,54,54	0
56	MG	RA	3488	1/1	0.90	0.43	38,38,38,38	0
56	MG	YA	3114	1/1	0.90	0.16	81,81,81,81	0
56	MG	YA	3312	1/1	0.90	0.29	34,34,34,34	0
56	MG	YA	3483	1/1	0.90	0.28	38,38,38,38	0
56	MG	RA	3085	1/1	0.90	0.45	122,122,122,122	0
56	MG	RA	3151	1/1	0.90	0.09	39,39,39,39	0
56	MG	YA	3399	1/1	0.90	0.32	86,86,86,86	0
56	MG	YA	3577	1/1	0.90	0.23	37,37,37,37	0
56	MG	RA	3159	1/1	0.90	0.16	75,75,75,75	0
56	MG	RA	3313	1/1	0.90	0.18	34,34,34,34	0
56	MG	XA	1668	1/1	0.90	0.10	57,57,57,57	0
56	MG	YA	3319	1/1	0.90	0.28	34,34,34,34	0
56	MG	RA	3278	1/1	0.90	0.12	47,47,47,47	0
56	MG	QA	1726	1/1	0.90	0.14	53,53,53,53	0
56	MG	RA	3776	1/1	0.90	0.13	51,51,51,51	0
56	MG	RA	3889	1/1	0.90	0.26	42,42,42,42	0
56	MG	YA	3409	1/1	0.90	0.26	48,48,48,48	0
56	MG	RE	305	1/1	0.90	0.37	70,70,70,70	0
56	MG	YA	3411	1/1	0.90	0.28	46,46,46,46	0
56	MG	RA	3234	1/1	0.90	0.26	103,103,103,103	0
56	MG	RA	3849	1/1	0.90	0.27	34,34,34,34	0
56	MG	YA	3004	1/1	0.90	0.23	34,34,34,34	0
56	MG	YA	3417	1/1	0.90	0.17	44,44,44,44	0
56	MG	XA	1682	1/1	0.90	0.18	53,53,53,53	0
56	MG	QA	1735	1/1	0.90	0.30	45,45,45,45	0
56	MG	RA	3640	1/1	0.90	0.12	37,37,37,37	0
56	MG	XA	1685	1/1	0.90	0.14	76,76,76,76	0
56	MG	YA	3507	1/1	0.90	0.29	34,34,34,34	0
56	MG	YA	3602	1/1	0.90	0.28	34,34,34,34	0
56	MG	YA	3508	1/1	0.90	0.19	40,40,40,40	0
56	MG	QA	1783	1/1	0.90	0.24	47,47,47,47	0
56	MG	RA	3436	1/1	0.90	0.29	39,39,39,39	0
56	MG	XA	1691	1/1	0.90	0.23	41,41,41,41	0
56	MG	XF	204	1/1	0.90	0.07	60,60,60,60	0
56	MG	RA	3406	1/1	0.90	0.14	34,34,34,34	0
56	MG	QA	1642	1/1	0.90	0.11	55,55,55,55	0
56	MG	RA	3940	1/1	0.90	0.18	46,46,46,46	0
56	MG	RF	305	1/1	0.90	0.21	85,85,85,85	0
56	MG	RA	3055	1/1	0.90	0.19	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	3750	1/1	0.90	0.25	34,34,34,34	0
56	MG	RA	3721	1/1	0.90	0.15	58,58,58,58	0
56	MG	RA	3003	1/1	0.90	0.13	40,40,40,40	0
56	MG	YA	3147	1/1	0.90	0.24	36,36,36,36	0
56	MG	YA	3435	1/1	0.90	0.30	53,53,53,53	0
56	MG	RF	310	1/1	0.90	0.20	62,62,62,62	0
56	MG	QA	1796	1/1	0.90	0.16	60,60,60,60	0
56	MG	QA	1748	1/1	0.90	0.11	62,62,62,62	0
56	MG	RA	3522	1/1	0.90	0.22	58,58,58,58	0
56	MG	RA	3135	1/1	0.90	0.24	89,89,89,89	0
56	MG	YA	3441	1/1	0.90	0.09	41,41,41,41	0
56	MG	RA	4015	1/1	0.91	0.17	42,42,42,42	0
56	MG	YA	3266	1/1	0.91	0.23	42,42,42,42	0
56	MG	YA	3268	1/1	0.91	0.32	34,34,34,34	0
56	MG	RA	4016	1/1	0.91	0.37	101,101,101,101	0
56	MG	RD	310	1/1	0.91	0.11	40,40,40,40	0
56	MG	RA	3103	1/1	0.91	0.31	55,55,55,55	0
56	MG	YA	3634	1/1	0.91	0.25	59,59,59,59	0
56	MG	YA	3531	1/1	0.91	0.17	34,34,34,34	0
56	MG	QA	1790	1/1	0.91	0.12	68,68,68,68	0
56	MG	YA	3637	1/1	0.91	0.17	36,36,36,36	0
56	MG	QA	1845	1/1	0.91	0.30	52,52,52,52	0
56	MG	RD	312	1/1	0.91	0.35	91,91,91,91	0
56	MG	RA	3078	1/1	0.91	0.19	60,60,60,60	0
56	MG	YA	3278	1/1	0.91	0.32	34,34,34,34	0
56	MG	RA	4019	1/1	0.91	0.30	84,84,84,84	0
56	MG	YA	3022	1/1	0.91	0.47	95,95,95,95	0
56	MG	YA	3364	1/1	0.91	0.27	36,36,36,36	0
56	MG	RA	3819	1/1	0.91	0.17	60,60,60,60	0
56	MG	RA	3387	1/1	0.91	0.32	34,34,34,34	0
56	MG	YA	3650	1/1	0.91	0.16	44,44,44,44	0
56	MG	YA	3544	1/1	0.91	0.17	42,42,42,42	0
56	MG	YA	3652	1/1	0.91	0.28	37,37,37,37	0
56	MG	YA	3283	1/1	0.91	0.33	49,49,49,49	0
56	MG	XA	1640	1/1	0.91	0.13	52,52,52,52	0
56	MG	RA	3331	1/1	0.91	0.15	58,58,58,58	0
56	MG	YA	3547	1/1	0.91	0.23	45,45,45,45	0
56	MG	QA	1853	1/1	0.91	0.17	50,50,50,50	0
56	MG	RA	3367	1/1	0.91	0.19	40,40,40,40	0
56	MG	RA	3753	1/1	0.91	0.28	34,34,34,34	0
56	MG	RA	3237	1/1	0.91	0.11	47,47,47,47	0
56	MG	RA	3826	1/1	0.91	0.09	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	3438	1/1	0.91	0.09	36,36,36,36	0
56	MG	RA	3161	1/1	0.91	0.23	76,76,76,76	0
56	MG	RA	3301	1/1	0.91	0.23	34,34,34,34	0
56	MG	YB	217	1/1	0.91	0.23	55,55,55,55	0
56	MG	RA	3172	1/1	0.91	0.12	58,58,58,58	0
56	MG	YA	3296	1/1	0.91	0.10	34,34,34,34	0
56	MG	XA	1655	1/1	0.91	0.06	46,46,46,46	0
56	MG	RA	3217	1/1	0.91	0.08	55,55,55,55	0
56	MG	YA	3299	1/1	0.91	0.16	35,35,35,35	0
56	MG	RA	3492	1/1	0.91	0.07	40,40,40,40	0
56	MG	XA	1755	1/1	0.91	0.15	57,57,57,57	0
56	MG	RA	3992	1/1	0.91	0.22	87,87,87,87	0
56	MG	YA	3230	1/1	0.91	0.20	85,85,85,85	0
56	MG	RA	3909	1/1	0.91	0.19	48,48,48,48	0
56	MG	RA	3573	1/1	0.91	0.26	47,47,47,47	0
56	MG	RA	3190	1/1	0.91	0.24	89,89,89,89	0
56	MG	RA	3608	1/1	0.91	0.19	34,34,34,34	0
56	MG	RA	3072	1/1	0.91	0.28	54,54,54,54	0
56	MG	RA	3377	1/1	0.91	0.24	34,34,34,34	0
56	MG	XA	1667	1/1	0.91	0.14	58,58,58,58	0
56	MG	QA	1714	1/1	0.91	0.07	62,62,62,62	0
56	MG	YA	3238	1/1	0.91	0.36	85,85,85,85	0
56	MG	XA	1770	1/1	0.91	0.23	52,52,52,52	0
56	MG	RB	211	1/1	0.91	0.08	65,65,65,65	0
56	MG	RA	3956	1/1	0.91	0.11	44,44,44,44	0
56	MG	XA	1773	1/1	0.91	0.20	41,41,41,41	0
56	MG	YA	3051	1/1	0.91	0.19	52,52,52,52	0
56	MG	RA	3578	1/1	0.91	0.21	37,37,37,37	0
56	MG	XA	1776	1/1	0.91	0.22	47,47,47,47	0
56	MG	RA	4001	1/1	0.91	0.21	78,78,78,78	0
56	MG	YA	3495	1/1	0.91	0.10	38,38,38,38	0
56	MG	RQ	202	1/1	0.91	0.18	56,56,56,56	0
56	MG	RA	4002	1/1	0.91	0.26	36,36,36,36	0
56	MG	RA	3579	1/1	0.91	0.10	64,64,64,64	0
56	MG	RA	3840	1/1	0.91	0.17	61,61,61,61	0
56	MG	XA	1783	1/1	0.91	0.07	63,63,63,63	0
56	MG	YA	3060	1/1	0.91	0.12	35,35,35,35	0
56	MG	YA	3415	1/1	0.91	0.09	39,39,39,39	0
56	MG	RA	3021	1/1	0.91	0.17	53,53,53,53	0
56	MG	RA	3380	1/1	0.91	0.40	34,34,34,34	0
56	MG	YV	201	1/1	0.91	0.11	62,62,62,62	0
56	MG	YW	201	1/1	0.91	0.08	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	3473	1/1	0.91	0.19	47,47,47,47	0
56	MG	YA	3330	1/1	0.91	0.15	39,39,39,39	0
56	MG	YA	3126	1/1	0.91	0.25	46,46,46,46	0
56	MG	YA	3332	1/1	0.91	0.17	35,35,35,35	0
56	MG	RU	202	1/1	0.91	0.33	96,96,96,96	0
56	MG	RA	3474	1/1	0.91	0.29	34,34,34,34	0
56	MG	YA	3607	1/1	0.91	0.16	39,39,39,39	0
56	MG	YA	3336	1/1	0.91	0.35	34,34,34,34	0
56	MG	RA	3381	1/1	0.91	0.21	34,34,34,34	0
56	MG	RA	3164	1/1	0.91	0.14	36,36,36,36	0
56	MG	YA	3615	1/1	0.91	0.20	34,34,34,34	0
56	MG	YA	3259	1/1	0.91	0.15	63,63,63,63	0
56	MG	XA	1606	1/1	0.91	0.05	72,72,72,72	0
56	MG	RA	3477	1/1	0.91	0.10	41,41,41,41	0
56	MG	RA	3107	1/1	0.91	0.21	88,88,88,88	0
56	MG	YA	3433	1/1	0.91	0.28	34,34,34,34	0
56	MG	YA	3135	1/1	0.91	0.23	67,67,67,67	0
56	MG	QA	1633	1/1	0.91	0.05	51,51,51,51	0
56	MG	RA	3310	1/1	0.91	0.23	54,54,54,54	0
56	MG	RA	3755	1/1	0.92	0.20	48,48,48,48	0
56	MG	RA	3261	1/1	0.92	0.15	51,51,51,51	0
56	MG	QA	1856	1/1	0.92	0.07	55,55,55,55	0
56	MG	YA	3742	1/1	0.92	0.13	63,63,63,63	0
56	MG	YA	3137	1/1	0.92	0.23	34,34,34,34	0
56	MG	YA	3138	1/1	0.92	0.06	45,45,45,45	0
56	MG	YA	3401	1/1	0.92	0.10	47,47,47,47	0
56	MG	YA	3746	1/1	0.92	0.31	69,69,69,69	0
56	MG	RE	304	1/1	0.92	0.26	34,34,34,34	0
56	MG	R0	101	1/1	0.92	0.12	53,53,53,53	0
56	MG	RA	3354	1/1	0.92	0.11	74,74,74,74	0
56	MG	R0	104	1/1	0.92	0.14	73,73,73,73	0
56	MG	RA	3606	1/1	0.92	0.28	36,36,36,36	0
56	MG	YA	3329	1/1	0.92	0.37	34,34,34,34	0
56	MG	RA	3095	1/1	0.92	0.10	53,53,53,53	0
56	MG	RA	3630	1/1	0.92	0.27	71,71,71,71	0
56	MG	RA	3486	1/1	0.92	0.13	41,41,41,41	0
56	MG	YA	3089	1/1	0.92	0.06	53,53,53,53	0
56	MG	YA	3664	1/1	0.92	0.23	34,34,34,34	0
56	MG	YA	3413	1/1	0.92	0.15	34,34,34,34	0
56	MG	YA	3267	1/1	0.92	0.33	87,87,87,87	0
56	MG	XA	1644	1/1	0.92	0.08	46,46,46,46	0
56	MG	YB	213	1/1	0.92	0.20	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3853	1/1	0.92	0.18	34,34,34,34	0
56	MG	YA	3034	1/1	0.92	0.11	37,37,37,37	0
56	MG	RA	3920	1/1	0.92	0.34	34,34,34,34	0
56	MG	YA	3418	1/1	0.92	0.21	44,44,44,44	0
56	MG	QA	1727	1/1	0.92	0.23	44,44,44,44	0
56	MG	YA	3580	1/1	0.92	0.27	34,34,34,34	0
56	MG	RA	3565	1/1	0.92	0.18	34,34,34,34	0
56	MG	RA	3923	1/1	0.92	0.26	70,70,70,70	0
56	MG	YA	3039	1/1	0.92	0.06	39,39,39,39	0
56	MG	YA	3276	1/1	0.92	0.29	34,34,34,34	0
56	MG	YD	304	1/1	0.92	0.29	58,58,58,58	0
56	MG	QA	1731	1/1	0.92	0.15	59,59,59,59	0
56	MG	YA	3681	1/1	0.92	0.25	59,59,59,59	0
56	MG	RA	3962	1/1	0.92	0.15	48,48,48,48	0
56	MG	XA	1754	1/1	0.92	0.11	43,43,43,43	0
56	MG	RA	3081	1/1	0.92	0.37	68,68,68,68	0
56	MG	RA	3006	1/1	0.92	0.18	61,61,61,61	0
56	MG	YA	3429	1/1	0.92	0.14	41,41,41,41	0
56	MG	YA	3220	1/1	0.92	0.09	37,37,37,37	0
56	MG	YA	3593	1/1	0.92	0.23	37,37,37,37	0
56	MG	XA	1761	1/1	0.92	0.31	43,43,43,43	0
56	MG	RA	3635	1/1	0.92	0.22	44,44,44,44	0
56	MG	RA	3142	1/1	0.92	0.14	66,66,66,66	0
56	MG	RA	3405	1/1	0.92	0.31	34,34,34,34	0
56	MG	RA	3968	1/1	0.92	0.20	64,64,64,64	0
56	MG	YA	3600	1/1	0.92	0.10	34,34,34,34	0
56	MG	YA	3286	1/1	0.92	0.18	43,43,43,43	0
56	MG	RA	3969	1/1	0.92	0.22	34,34,34,34	0
56	MG	YA	3168	1/1	0.92	0.18	39,39,39,39	0
56	MG	RA	3284	1/1	0.92	0.14	56,56,56,56	0
56	MG	YQ	201	1/1	0.92	0.22	52,52,52,52	0
56	MG	RA	3109	1/1	0.92	0.12	35,35,35,35	0
56	MG	RA	3897	1/1	0.92	0.30	74,74,74,74	0
56	MG	YA	3053	1/1	0.92	0.14	41,41,41,41	0
56	MG	YA	3612	1/1	0.92	0.26	55,55,55,55	0
56	MG	RA	3493	1/1	0.92	0.13	34,34,34,34	0
56	MG	YA	3614	1/1	0.92	0.27	34,34,34,34	0
56	MG	RA	3456	1/1	0.92	0.19	40,40,40,40	0
56	MG	RQ	201	1/1	0.92	0.12	61,61,61,61	0
56	MG	YA	3617	1/1	0.92	0.10	43,43,43,43	0
56	MG	RA	3900	1/1	0.92	0.29	80,80,80,80	0
56	MG	YA	3450	1/1	0.92	0.13	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	Y5	101	1/1	0.92	0.11	43,43,43,43	0
56	MG	RA	3110	1/1	0.92	0.27	46,46,46,46	0
56	MG	QA	1792	1/1	0.92	0.17	37,37,37,37	0
56	MG	RA	3035	1/1	0.92	0.15	61,61,61,61	0
56	MG	RA	3019	1/1	0.92	0.34	85,85,85,85	0
56	MG	XA	1692	1/1	0.92	0.28	49,49,49,49	0
56	MG	XF	201	1/1	0.92	0.07	53,53,53,53	0
56	MG	RA	3411	1/1	0.92	0.27	89,89,89,89	0
56	MG	YA	3064	1/1	0.92	0.25	67,67,67,67	0
56	MG	RA	3325	1/1	0.92	0.10	52,52,52,52	0
56	MG	RA	3601	1/1	0.92	0.21	40,40,40,40	0
56	MG	YA	3460	1/1	0.92	0.19	55,55,55,55	0
56	MG	RA	3397	1/1	0.92	0.19	40,40,40,40	0
56	MG	YA	3384	1/1	0.92	0.31	34,34,34,34	0
56	MG	YA	3463	1/1	0.92	0.22	43,43,43,43	0
56	MG	RA	3725	1/1	0.92	0.14	34,34,34,34	0
56	MG	YA	3310	1/1	0.92	0.26	34,34,34,34	0
56	MG	QA	1849	1/1	0.92	0.15	42,42,42,42	0
56	MG	YA	3730	1/1	0.92	0.21	66,66,66,66	0
56	MG	YA	3640	1/1	0.92	0.40	34,34,34,34	0
56	MG	RA	3987	1/1	0.92	0.25	87,87,87,87	0
56	MG	XA	1707	1/1	0.92	0.16	53,53,53,53	0
56	MG	RA	3815	1/1	0.92	0.40	34,34,34,34	0
56	MG	RV	203	1/1	0.92	0.14	55,55,55,55	0
56	MG	RA	3700	1/1	0.92	0.10	41,41,41,41	0
56	MG	YA	3645	1/1	0.92	0.25	61,61,61,61	0
56	MG	RA	3934	1/1	0.93	0.15	50,50,50,50	0
56	MG	RS	201	1/1	0.93	0.15	41,41,41,41	0
56	MG	RT	201	1/1	0.93	0.08	46,46,46,46	0
56	MG	RA	3935	1/1	0.93	0.16	46,46,46,46	0
56	MG	RA	3015	1/1	0.93	0.41	97,97,97,97	0
56	MG	YA	3552	1/1	0.93	0.21	49,49,49,49	0
56	MG	XA	1734	1/1	0.93	0.17	39,39,39,39	0
56	MG	YA	3030	1/1	0.93	0.19	66,66,66,66	0
56	MG	YA	3079	1/1	0.93	0.20	37,37,37,37	0
56	MG	RA	3168	1/1	0.93	0.07	46,46,46,46	0
56	MG	YA	3132	1/1	0.93	0.12	39,39,39,39	0
56	MG	RE	303	1/1	0.93	0.25	68,68,68,68	0
56	MG	RA	3971	1/1	0.93	0.21	35,35,35,35	0
56	MG	RA	3182	1/1	0.93	0.15	59,59,59,59	0
56	MG	RA	3794	1/1	0.93	0.20	77,77,77,77	0
56	MG	RA	3416	1/1	0.93	0.24	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3357	1/1	0.93	0.05	36,36,36,36	0
56	MG	RA	3703	1/1	0.93	0.14	58,58,58,58	0
56	MG	QL	201	1/1	0.93	0.17	55,55,55,55	0
56	MG	YA	3724	1/1	0.93	0.35	48,48,48,48	0
56	MG	YA	3246	1/1	0.93	0.26	68,68,68,68	0
56	MG	YA	3141	1/1	0.93	0.08	41,41,41,41	0
56	MG	RA	3662	1/1	0.93	0.24	47,47,47,47	0
56	MG	QN	102	1/1	0.93	0.07	57,57,57,57	0
56	MG	RA	3799	1/1	0.93	0.12	34,34,34,34	0
56	MG	YA	3573	1/1	0.93	0.13	36,36,36,36	0
56	MG	RA	3529	1/1	0.93	0.17	40,40,40,40	0
56	MG	YA	3653	1/1	0.93	0.21	36,36,36,36	0
56	MG	QA	1663	1/1	0.93	0.15	64,64,64,64	0
56	MG	YA	3367	1/1	0.93	0.26	41,41,41,41	0
56	MG	RA	3461	1/1	0.93	0.11	34,34,34,34	0
56	MG	XA	1681	1/1	0.93	0.28	46,46,46,46	0
56	MG	XA	1764	1/1	0.93	0.23	50,50,50,50	0
56	MG	YA	3737	1/1	0.93	0.22	68,68,68,68	0
56	MG	RA	3390	1/1	0.93	0.14	65,65,65,65	0
56	MG	RA	3774	1/1	0.93	0.06	49,49,49,49	0
56	MG	RA	3403	1/1	0.93	0.14	35,35,35,35	0
56	MG	YA	3741	1/1	0.93	0.06	38,38,38,38	0
56	MG	YA	3153	1/1	0.93	0.06	42,42,42,42	0
56	MG	RA	3233	1/1	0.93	0.34	89,89,89,89	0
56	MG	YA	3377	1/1	0.93	0.27	46,46,46,46	0
56	MG	XA	1612	1/1	0.93	0.08	42,42,42,42	0
56	MG	RA	3344	1/1	0.93	0.09	34,34,34,34	0
56	MG	QA	1630	1/1	0.93	0.21	44,44,44,44	0
56	MG	YA	3316	1/1	0.93	0.34	34,34,34,34	0
56	MG	QA	1843	1/1	0.93	0.14	42,42,42,42	0
56	MG	XA	1617	1/1	0.93	0.14	34,34,34,34	0
56	MG	YA	3318	1/1	0.93	0.12	34,34,34,34	0
56	MG	YA	3447	1/1	0.93	0.22	39,39,39,39	0
56	MG	RA	3778	1/1	0.93	0.12	42,42,42,42	0
56	MG	YA	3449	1/1	0.93	0.14	35,35,35,35	0
56	MG	RA	3393	1/1	0.93	0.40	34,34,34,34	0
56	MG	RA	3895	1/1	0.93	0.35	55,55,55,55	0
56	MG	YA	3597	1/1	0.93	0.15	35,35,35,35	0
56	MG	QA	1718	1/1	0.93	0.33	37,37,37,37	0
56	MG	RA	3129	1/1	0.93	0.06	43,43,43,43	0
56	MG	YA	3389	1/1	0.93	0.21	35,35,35,35	0
56	MG	YA	3390	1/1	0.93	0.17	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	3649	1/1	0.93	0.12	39,39,39,39	0
56	MG	RA	3811	1/1	0.93	0.23	37,37,37,37	0
56	MG	YA	3528	1/1	0.93	0.21	34,34,34,34	0
56	MG	YA	3606	1/1	0.93	0.18	34,34,34,34	0
56	MG	RA	3469	1/1	0.93	0.21	34,34,34,34	0
56	MG	YA	3608	1/1	0.93	0.18	34,34,34,34	0
56	MG	RA	3084	1/1	0.93	0.09	45,45,45,45	0
56	MG	RA	3048	1/1	0.93	0.08	41,41,41,41	0
56	MG	RA	4028	1/1	0.93	0.17	89,89,89,89	0
56	MG	RD	309	1/1	0.93	0.08	47,47,47,47	0
56	MG	RQ	203	1/1	0.93	0.15	41,41,41,41	0
56	MG	QA	1728	1/1	0.93	0.24	54,54,54,54	0
56	MG	RA	3576	1/1	0.93	0.07	51,51,51,51	0
56	MG	RA	3306	1/1	0.93	0.20	34,34,34,34	0
56	MG	YD	308	1/1	0.93	0.13	49,49,49,49	0
56	MG	YA	3469	1/1	0.93	0.16	60,60,60,60	0
56	MG	YA	3403	1/1	0.93	0.21	34,34,34,34	0
56	MG	YA	3335	1/1	0.93	0.23	34,34,34,34	0
56	MG	RA	3043	1/1	0.93	0.17	34,34,34,34	0
56	MG	RR	202	1/1	0.93	0.14	71,71,71,71	0
56	MG	RA	3733	1/1	0.94	0.17	40,40,40,40	0
56	MG	RA	3171	1/1	0.94	0.17	46,46,46,46	0
56	MG	YA	3532	1/1	0.94	0.15	37,37,37,37	0
56	MG	RA	3347	1/1	0.94	0.20	35,35,35,35	0
56	MG	RA	3981	1/1	0.94	0.15	39,39,39,39	0
56	MG	RA	3250	1/1	0.94	0.44	91,91,91,91	0
56	MG	RA	4007	1/1	0.94	0.23	85,85,85,85	0
56	MG	YA	3537	1/1	0.94	0.18	36,36,36,36	0
56	MG	QA	1632	1/1	0.94	0.07	38,38,38,38	0
56	MG	YA	3391	1/1	0.94	0.24	34,34,34,34	0
56	MG	YA	3342	1/1	0.94	0.33	34,34,34,34	0
56	MG	RA	3651	1/1	0.94	0.17	53,53,53,53	0
56	MG	YA	3105	1/1	0.94	0.16	34,34,34,34	0
56	MG	YA	3603	1/1	0.94	0.39	34,34,34,34	0
56	MG	RA	3554	1/1	0.94	0.24	37,37,37,37	0
56	MG	YA	3490	1/1	0.94	0.11	36,36,36,36	0
56	MG	RA	3496	1/1	0.94	0.24	43,43,43,43	0
56	MG	YA	3443	1/1	0.94	0.41	41,41,41,41	0
56	MG	RA	3466	1/1	0.94	0.29	34,34,34,34	0
56	MG	YA	3609	1/1	0.94	0.17	38,38,38,38	0
56	MG	RA	3321	1/1	0.94	0.34	36,36,36,36	0
56	MG	QV	106	1/1	0.94	0.06	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3613	1/1	0.94	0.23	41,41,41,41	0
56	MG	YA	3674	1/1	0.94	0.22	34,34,34,34	0
56	MG	YA	3497	1/1	0.94	0.15	50,50,50,50	0
56	MG	RA	3375	1/1	0.94	0.17	41,41,41,41	0
56	MG	YW	202	1/1	0.94	0.19	62,62,62,62	0
56	MG	YA	3311	1/1	0.94	0.30	35,35,35,35	0
56	MG	RA	3220	1/1	0.94	0.20	69,69,69,69	0
56	MG	YA	3680	1/1	0.94	0.28	36,36,36,36	0
56	MG	YA	3501	1/1	0.94	0.19	45,45,45,45	0
56	MG	RA	3460	1/1	0.94	0.11	39,39,39,39	0
56	MG	QA	1613	1/1	0.94	0.30	48,48,48,48	0
56	MG	RA	3786	1/1	0.94	0.09	42,42,42,42	0
56	MG	QA	1704	1/1	0.94	0.20	40,40,40,40	0
56	MG	YA	3274	1/1	0.94	0.19	34,34,34,34	0
56	MG	QA	1829	1/1	0.94	0.22	34,34,34,34	0
56	MG	RA	3660	1/1	0.94	0.35	43,43,43,43	0
56	MG	RE	302	1/1	0.94	0.21	60,60,60,60	0
56	MG	YA	3459	1/1	0.94	0.12	44,44,44,44	0
56	MG	YA	3011	1/1	0.94	0.07	37,37,37,37	0
56	MG	RA	3312	1/1	0.94	0.25	34,34,34,34	0
56	MG	YA	3695	1/1	0.94	0.23	43,43,43,43	0
56	MG	YA	3571	1/1	0.94	0.17	34,34,34,34	0
56	MG	XJ	201	1/1	0.94	0.05	42,42,42,42	0
56	MG	RA	3729	1/1	0.94	0.11	40,40,40,40	0
56	MG	YA	3242	1/1	0.94	0.20	56,56,56,56	0
56	MG	YA	3370	1/1	0.94	0.27	34,34,34,34	0
56	MG	YA	3087	1/1	0.94	0.25	38,38,38,38	0
56	MG	YA	3373	1/1	0.94	0.08	47,47,47,47	0
56	MG	XA	1736	1/1	0.94	0.21	55,55,55,55	0
56	MG	RA	3879	1/1	0.94	0.15	41,41,41,41	0
56	MG	YA	3468	1/1	0.94	0.33	34,34,34,34	0
56	MG	RA	3854	1/1	0.94	0.30	62,62,62,62	0
56	MG	RA	3088	1/1	0.94	0.06	49,49,49,49	0
56	MG	RA	3550	1/1	0.94	0.21	35,35,35,35	0
56	MG	RR	203	1/1	0.94	0.08	46,46,46,46	0
56	MG	RA	3680	1/1	0.94	0.24	42,42,42,42	0
56	MG	R5	102	1/1	0.94	0.20	41,41,41,41	0
56	MG	YA	3058	1/1	0.94	0.12	42,42,42,42	0
56	MG	YA	3134	1/1	0.94	0.07	42,42,42,42	0
56	MG	YA	3515	1/1	0.95	0.24	34,34,34,34	0
56	MG	YB	209	1/1	0.95	0.10	55,55,55,55	0
56	MG	YA	3476	1/1	0.95	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3560	1/1	0.95	0.13	35,35,35,35	0
56	MG	YA	3124	1/1	0.95	0.12	34,34,34,34	0
56	MG	QA	1696	1/1	0.95	0.22	56,56,56,56	0
56	MG	QA	1834	1/1	0.95	0.33	37,37,37,37	0
56	MG	YA	3564	1/1	0.95	0.23	34,34,34,34	0
56	MG	RG	203	1/1	0.95	0.05	45,45,45,45	0
56	MG	RA	3582	1/1	0.95	0.12	35,35,35,35	0
56	MG	RA	3378	1/1	0.95	0.41	34,34,34,34	0
56	MG	YA	3295	1/1	0.95	0.10	38,38,38,38	0
56	MG	RA	3369	1/1	0.95	0.19	34,34,34,34	0
56	MG	YA	3297	1/1	0.95	0.25	34,34,34,34	0
56	MG	RA	3499	1/1	0.95	0.30	46,46,46,46	0
56	MG	YA	3372	1/1	0.95	0.11	37,37,37,37	0
56	MG	YA	3721	1/1	0.95	0.18	34,34,34,34	0
56	MG	YA	3071	1/1	0.95	0.13	70,70,70,70	0
56	MG	YA	3102	1/1	0.95	0.10	34,34,34,34	0
56	MG	QA	1605	1/1	0.95	0.22	34,34,34,34	0
56	MG	RA	3117	1/1	0.95	0.17	68,68,68,68	0
56	MG	QA	1705	1/1	0.95	0.20	34,34,34,34	0
56	MG	YA	3628	1/1	0.95	0.13	59,59,59,59	0
56	MG	YA	3677	1/1	0.95	0.23	42,42,42,42	0
56	MG	RA	3111	1/1	0.95	0.16	49,49,49,49	0
56	MG	RA	3787	1/1	0.95	0.08	46,46,46,46	0
56	MG	RA	3252	1/1	0.95	0.06	36,36,36,36	0
56	MG	RA	3864	1/1	0.95	0.30	34,34,34,34	0
56	MG	YA	3419	1/1	0.95	0.10	35,35,35,35	0
56	MG	YA	3343	1/1	0.95	0.24	34,34,34,34	0
56	MG	RA	3413	1/1	0.95	0.19	57,57,57,57	0
56	MG	RA	3155	1/1	0.95	0.11	47,47,47,47	0
56	MG	YA	3686	1/1	0.95	0.22	34,34,34,34	0
56	MG	YA	3385	1/1	0.95	0.27	34,34,34,34	0
56	MG	RA	3947	1/1	0.95	0.11	54,54,54,54	0
56	MG	YA	3588	1/1	0.95	0.34	45,45,45,45	0
56	MG	RA	3290	1/1	0.95	0.17	44,44,44,44	0
56	MG	RD	305	1/1	0.95	0.12	39,39,39,39	0
56	MG	RA	3366	1/1	0.95	0.32	41,41,41,41	0
56	MG	RA	3950	1/1	0.95	0.19	56,56,56,56	0
56	MG	YA	3548	1/1	0.95	0.36	34,34,34,34	0
56	MG	YA	3148	1/1	0.95	0.30	99,99,99,99	0
56	MG	YA	3550	1/1	0.95	0.17	53,53,53,53	0
56	MG	RA	3869	1/1	0.95	0.30	37,37,37,37	0
56	MG	QA	1745	1/1	0.95	0.22	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	3852	1/1	0.95	0.33	45,45,45,45	0
56	MG	RA	3042	1/1	0.95	0.10	41,41,41,41	0
56	MG	RA	3872	1/1	0.95	0.34	56,56,56,56	0
56	MG	RA	3292	1/1	0.95	0.29	55,55,55,55	0
57	ZN	Y4	101	1/1	0.95	0.11	133,133,133,133	0
56	MG	YA	3704	1/1	0.95	0.08	38,38,38,38	0
56	MG	RA	3824	1/1	0.95	0.19	37,37,37,37	0
56	MG	XA	1758	1/1	0.95	0.21	34,34,34,34	0
56	MG	RA	3128	1/1	0.96	0.08	40,40,40,40	0
56	MG	XA	1741	1/1	0.96	0.30	35,35,35,35	0
56	MG	RA	3330	1/1	0.96	0.14	38,38,38,38	0
56	MG	RB	214	1/1	0.96	0.09	46,46,46,46	0
56	MG	RA	3983	1/1	0.96	0.09	52,52,52,52	0
56	MG	R0	102	1/1	0.96	0.10	54,54,54,54	0
56	MG	RA	3595	1/1	0.96	0.08	53,53,53,53	0
56	MG	RA	3139	1/1	0.96	0.47	84,84,84,84	0
56	MG	QA	1700	1/1	0.96	0.20	41,41,41,41	0
56	MG	YA	3589	1/1	0.96	0.33	38,38,38,38	0
56	MG	YA	3211	1/1	0.96	0.19	34,34,34,34	0
56	MG	XA	1751	1/1	0.96	0.23	34,34,34,34	0
56	MG	YA	3621	1/1	0.96	0.15	49,49,49,49	0
56	MG	YA	3623	1/1	0.96	0.60	67,67,67,67	0
56	MG	RA	3040	1/1	0.96	0.07	47,47,47,47	0
56	MG	RA	3166	1/1	0.96	0.11	69,69,69,69	0
56	MG	RA	3904	1/1	0.96	0.14	40,40,40,40	0
56	MG	YA	3594	1/1	0.96	0.24	34,34,34,34	0
56	MG	RB	203	1/1	0.96	0.06	58,58,58,58	0
56	MG	YA	3728	1/1	0.96	0.53	56,56,56,56	0
56	MG	RA	3795	1/1	0.96	0.16	46,46,46,46	0
56	MG	RA	4020	1/1	0.96	0.12	52,52,52,52	0
56	MG	YA	3014	1/1	0.96	0.11	64,64,64,64	0
56	MG	RA	3946	1/1	0.96	0.10	42,42,42,42	0
56	MG	QA	1857	1/1	0.96	0.18	34,34,34,34	0
56	MG	QA	1708	1/1	0.96	0.04	38,38,38,38	0
56	MG	YA	3516	1/1	0.96	0.24	35,35,35,35	0
56	MG	RA	3437	1/1	0.96	0.24	34,34,34,34	0
56	MG	RA	3359	1/1	0.96	0.22	47,47,47,47	0
56	MG	YA	3020	1/1	0.96	0.15	40,40,40,40	0
56	MG	YA	3045	1/1	0.96	0.09	38,38,38,38	0
56	MG	RA	3741	1/1	0.96	0.26	34,34,34,34	0
56	MG	RA	3328	1/1	0.96	0.28	45,45,45,45	0
56	MG	RA	3602	1/1	0.96	0.05	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	YA	3442	1/1	0.96	0.12	45,45,45,45	0
56	MG	XA	1635	1/1	0.96	0.08	51,51,51,51	0
58	SF4	QD	302	8/8	0.96	0.06	50,73,103,107	0
56	MG	RA	3108	1/1	0.97	0.10	36,36,36,36	0
56	MG	RA	3877	1/1	0.97	0.21	34,34,34,34	0
56	MG	RA	3145	1/1	0.97	0.07	50,50,50,50	0
56	MG	QA	1820	1/1	0.97	0.15	41,41,41,41	0
56	MG	RA	3287	1/1	0.97	0.04	41,41,41,41	0
56	MG	YD	306	1/1	0.97	0.13	60,60,60,60	0
56	MG	XA	1731	1/1	0.97	0.04	44,44,44,44	0
56	MG	YA	3086	1/1	0.97	0.16	46,46,46,46	0
56	MG	RA	3365	1/1	0.97	0.27	35,35,35,35	0
56	MG	YA	3307	1/1	0.97	0.12	34,34,34,34	0
56	MG	RA	3921	1/1	0.97	0.08	38,38,38,38	0
56	MG	YB	211	1/1	0.97	0.21	40,40,40,40	0
56	MG	RT	202	1/1	0.97	0.04	43,43,43,43	0
56	MG	RA	3506	1/1	0.97	0.12	39,39,39,39	0
56	MG	YA	3012	1/1	0.97	0.08	67,67,67,67	0
56	MG	RA	3959	1/1	0.97	0.10	40,40,40,40	0
56	MG	RA	3783	1/1	0.97	0.23	87,87,87,87	0
56	MG	RA	3013	1/1	0.97	0.10	35,35,35,35	0
56	MG	XA	1637	1/1	0.97	0.08	64,64,64,64	0
56	MG	YA	3657	1/1	0.97	0.06	34,34,34,34	0
56	MG	YA	3622	1/1	0.97	0.32	34,34,34,34	0
56	MG	YA	3224	1/1	0.97	0.07	47,47,47,47	0
58	SF4	XD	301	8/8	0.97	0.05	59,70,92,92	0
56	MG	YA	3208	1/1	0.98	0.07	46,46,46,46	0
56	MG	YA	3355	1/1	0.98	0.24	38,38,38,38	0
57	ZN	QN	101	1/1	0.98	0.04	105,105,105,105	0
56	MG	YA	3693	1/1	0.98	0.15	34,34,34,34	0
56	MG	YA	3152	1/1	0.98	0.15	35,35,35,35	0
56	MG	QA	1838	1/1	0.98	0.31	34,34,34,34	0
56	MG	YA	3190	1/1	0.98	0.10	41,41,41,41	0
56	MG	RA	3336	1/1	0.98	0.13	34,34,34,34	0
56	MG	RA	3046	1/1	0.98	0.04	40,40,40,40	0
56	MG	YA	3353	1/1	0.98	0.43	34,34,34,34	0
57	ZN	XN	101	1/1	0.99	0.03	93,93,93,93	0
56	MG	YA	3352	1/1	0.99	0.32	34,34,34,34	0
56	MG	YA	3638	1/1	0.99	0.19	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.