



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 08:39 PM UTC

PDB ID : 6NTA / pdb_00006nta
Title : Modified ASL proline bound to Thermus thermophilus 70S (cognate)
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Deposited on : 2019-01-28
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (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

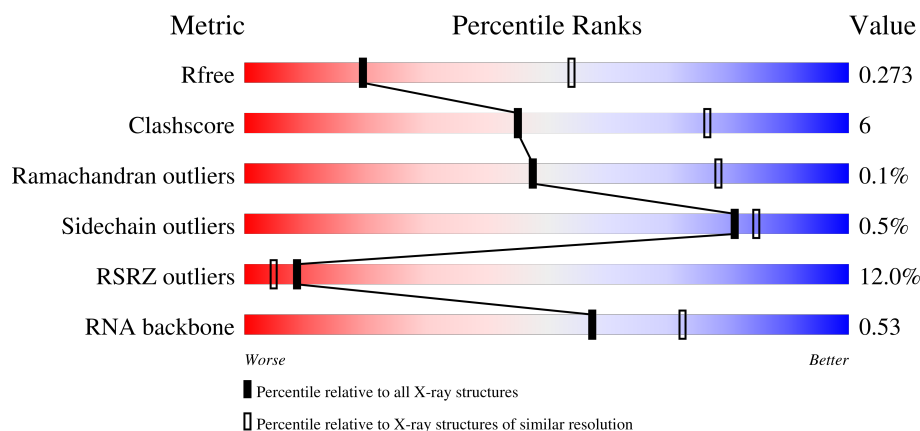
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	QA	1521	11% 58% 34% 7%
1	XA	1521	11% 56% 34% 8%
2	QB	256	15% 72% 17% 8%
2	XB	256	19% 67% 23% 8%

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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	

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Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	17	
22	XV	17	
23	QX	19	
23	XX	19	
24	RA	2915	
24	YA	2915	
25	RB	122	
25	YB	122	
26	RD	276	
26	YD	276	
27	RE	206	
27	YE	206	

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Mol	Chain	Length	Quality of chain
28	RF	210	
28	YF	210	
29	RG	182	
29	YG	182	
30	RH	180	
30	YH	180	
31	RI	148	
31	YI	148	
32	RN	140	
32	YN	140	
33	RO	122	
33	YO	122	
34	RP	150	
34	YP	150	
35	RQ	141	
35	YQ	141	
36	RR	118	
36	YR	118	
37	RS	112	
37	YS	112	
38	RT	146	
38	YT	146	
39	RU	118	
39	YU	118	
40	RV	101	

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Mol	Chain	Length	Quality of chain
40	YV	101	% 88% 12%
41	RW	113	4% 84% 16%
41	YW	113	% 90% 10%
42	RX	96	6% 83% 11% ..
42	YX	96	6% 84% 10% ..
43	RY	110	24% 83% 14% ..
43	YY	110	6% 81% 16% .
44	RZ	206	20% 77% 18% ..
44	YZ	206	9% 77% 18% ..
45	R0	85	9% 75% 14% 11%
45	Y0	85	4% 78% 11% 12%
46	R1	98	22% 81% 15% ..
46	Y1	98	13% 74% 17% . 5%
47	R2	72	8% 69% 25% ..
47	Y2	72	12% 72% 19% . 6%
48	R3	60	2% 70% 27% ..
48	Y3	60	8% 82% 17% .
49	R4	71	25% 70% 24% . ..
49	Y4	71	20% 62% 32% . ..
50	R5	60	15% 85% 13% .
50	Y5	60	2% 78% 20% .
51	R6	54	2% 81% 17% .
51	Y6	54	2% 80% 19% .
52	R7	49	12% 92% . .
52	Y7	49	6% 92% 6% .

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Mol	Chain	Length	Quality of chain
53	R8	65	
53	Y8	65	
54	R9	37	
54	Y9	37	

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
55	MG	YA	3201	-	-	-	X
55	MG	YD	301	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 289311 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 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1500	Total	C	N	O	P	0	0	0
			32247	14353	5981	10414	1499			
1	XA	1500	Total	C	N	O	P	0	0	0
			32249	14354	5984	10412	1499			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	235	Total	C	N	O	S	0	0	0
			1907	1217	342	343	5			
2	XB	236	Total	C	N	O	S	0	0	0
			1915	1223	343	344	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	QC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	XC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	QD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	XD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	XE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	QF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	XF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	QG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	XG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			
8	XH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	QI	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	XI	126	Total	C	N	O		0	0	0
			998	633	193	172				

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	QJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	XJ	96	Total	C	N	O	S	0	0	0
			777	487	153	136	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	XK	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	QL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	XL	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	120	Total	C	N	O	S	0	0	0
			955	591	197	165	2			
13	XM	119	Total	C	N	O	S	0	0	0
			946	585	195	164	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	XO	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	QP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	XP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	QQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	XQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	XR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	XS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	XT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	QU	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	XU	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called P-site ASLPro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	17	Total	C	N	O	P	0	0	0
			365	163	65	120	17			
22	XV	15	Total	C	N	O	P	0	0	0
			322	144	57	106	15			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	10	Total	C	N	O	P	0	0	0
			217	97	43	67	10			
23	XX	12	Total	C	N	O	P	0	0	0
			262	117	53	80	12			

- Molecule 24 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	RA	2881	Total	C	N	O	P	0	0	0
			62051	27618	11609	19944	2880			
24	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- Molecule 25 is a RNA chain called 5S rRNA.

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

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	YD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
27	YE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	RF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
28	YF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	RG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
29	YG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
30	YH	173	Total	C	N	O	S	0	0	0
			1330	845	250	234	1			

- Molecule 31 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	RI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
31	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	RN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
32	YN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 33 is a protein called 50S ribosomal protein L14.

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

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
34	YP	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 35 is a protein called 50S ribosomal protein L16.

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

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	RR	117	Total	C	N	O	0	0	0
			960	599	202	159			
36	YR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	RS	111	Total	C	N	O	0	0	0
			882	556	176	150			
37	YS	111	Total	C	N	O	0	0	0
			882	556	176	150			

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
38	YT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
39	YU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
40	YV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
41	YW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	RX	92	Total	C	N	O	0	0	0
			725	471	131	123			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	YX	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			
43	YY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RZ	203	Total	C	N	O	S	0	0	0
			1601	1020	283	295	3			
44	YZ	203	Total	C	N	O	S	0	0	0
			1601	1020	283	295	3			

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	R0	76	Total	C	N	O	S	0	0	0
			603	372	128	102	1			
45	Y0	75	Total	C	N	O	S	0	0	0
			599	370	127	101	1			

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
46	Y1	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
47	Y2	68	Total	C	N	O	S	0	0	0
			575	355	117	102	1			

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	R3	59	Total	C	N	O	0	0	0
			469	298	90	81			
48	Y3	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	R4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			
49	Y4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

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

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	R7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
52	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

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

- Molecule 54 is a protein called 50S ribosomal protein L36.

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

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	74	Total	Mg	0	0
			74	74		
55	QC	1	Total	Mg	0	0
			1	1		
55	QF	1	Total	Mg	0	0
			1	1		
55	QH	1	Total	Mg	0	0
			1	1		
55	QM	1	Total	Mg	0	0
			1	1		
55	RA	487	Total	Mg	0	0
			487	487		
55	RB	6	Total	Mg	0	0
			6	6		
55	RE	4	Total	Mg	0	0
			4	4		
55	RF	2	Total	Mg	0	0
			2	2		
55	RI	1	Total	Mg	0	0
			1	1		
55	RN	1	Total	Mg	0	0
			1	1		
55	RO	1	Total	Mg	0	0
			1	1		
55	RP	1	Total	Mg	0	0
			1	1		
55	RQ	2	Total	Mg	0	0
			2	2		

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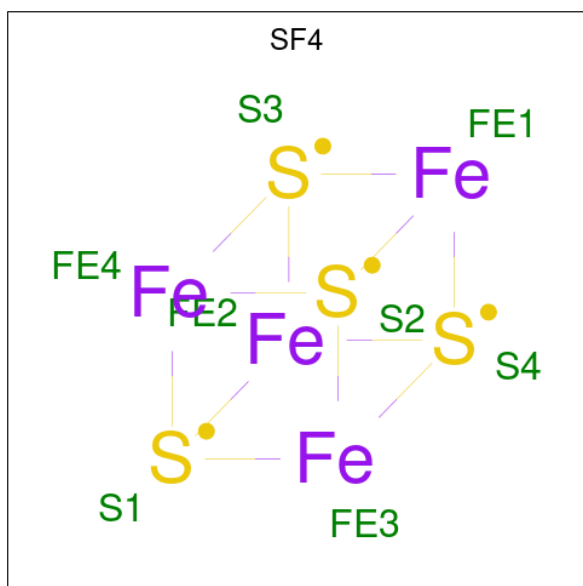
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	RR	2	Total 2	Mg 2	0	0
55	RT	1	Total 1	Mg 1	0	0
55	RX	1	Total 1	Mg 1	0	0
55	RY	1	Total 1	Mg 1	0	0
55	R0	1	Total 1	Mg 1	0	0
55	R1	2	Total 2	Mg 2	0	0
55	R8	1	Total 1	Mg 1	0	0
55	XA	92	Total 92	Mg 92	0	0
55	XE	1	Total 1	Mg 1	0	0
55	XK	1	Total 1	Mg 1	0	0
55	XL	2	Total 2	Mg 2	0	0
55	XM	2	Total 2	Mg 2	0	0
55	XN	1	Total 1	Mg 1	0	0
55	XQ	1	Total 1	Mg 1	0	0
55	XS	1	Total 1	Mg 1	0	0
55	YA	542	Total 542	Mg 542	0	0
55	YB	15	Total 15	Mg 15	0	0
55	YD	3	Total 3	Mg 3	0	0
55	YE	3	Total 3	Mg 3	0	0
55	YO	1	Total 1	Mg 1	0	0
55	YQ	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	YR	2	Total	Mg	0	0
			2	2		
55	YX	2	Total	Mg	0	0
			2	2		
55	Y0	2	Total	Mg	0	0
			2	2		
55	Y1	1	Total	Mg	0	0
			1	1		
55	Y5	1	Total	Mg	0	0
			1	1		
55	Y7	1	Total	Mg	0	0
			1	1		
55	Y8	2	Total	Mg	0	0
			2	2		

- Molecule 56 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

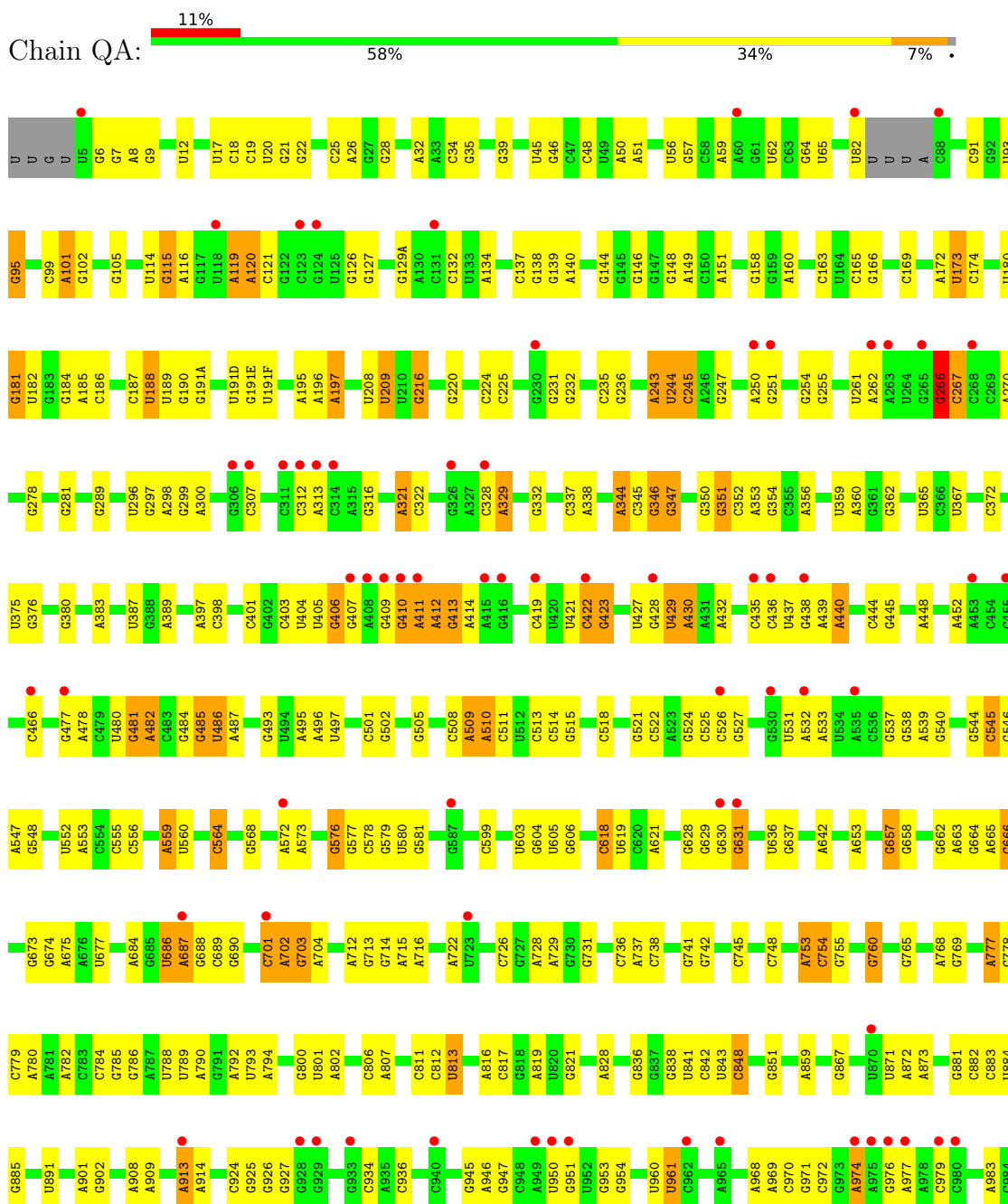
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

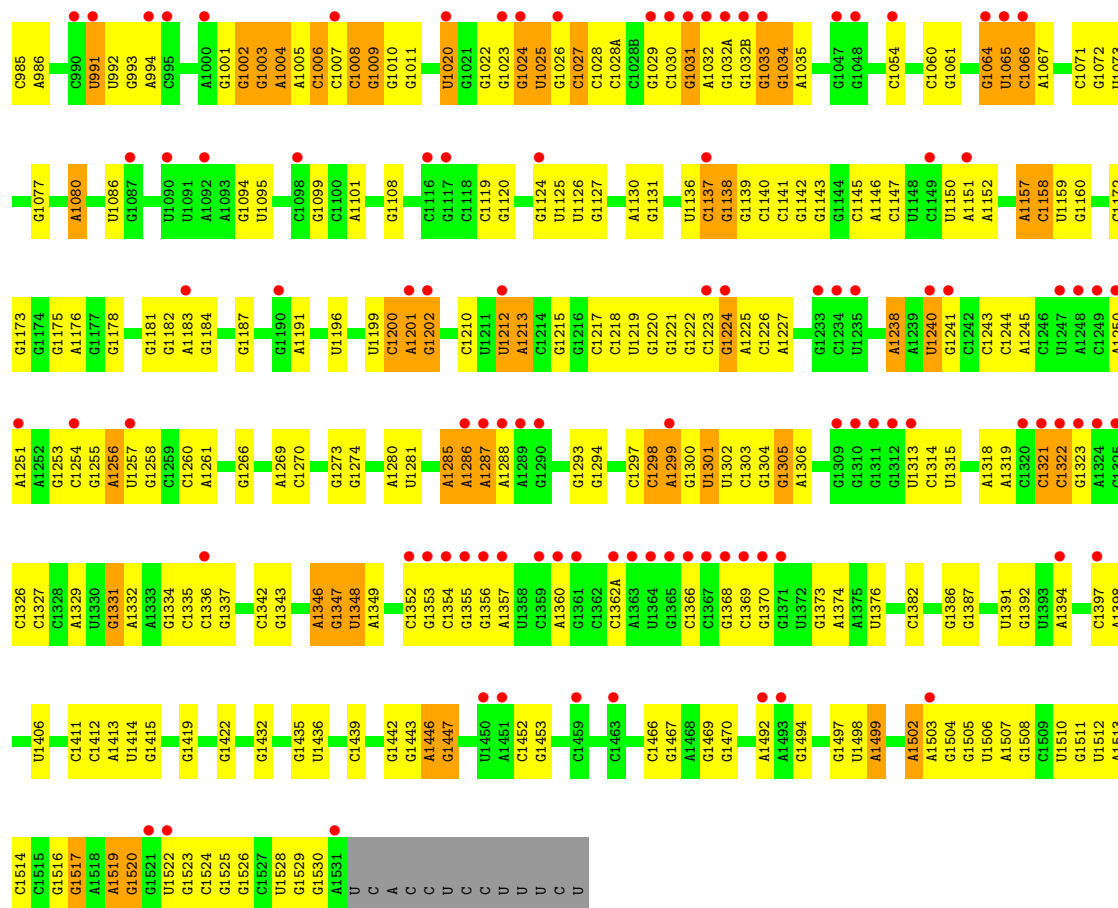
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QN	1	Total 1	Zn 1	0	0
57	RY	1	Total 1	Zn 1	0	0
57	R4	1	Total 1	Zn 1	0	0
57	R5	1	Total 1	Zn 1	0	0
57	R6	1	Total 1	Zn 1	0	0
57	R9	1	Total 1	Zn 1	0	0
57	XN	1	Total 1	Zn 1	0	0
57	YY	1	Total 1	Zn 1	0	0
57	Y4	1	Total 1	Zn 1	0	0
57	Y5	1	Total 1	Zn 1	0	0
57	Y6	1	Total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

3 Residue-property plots

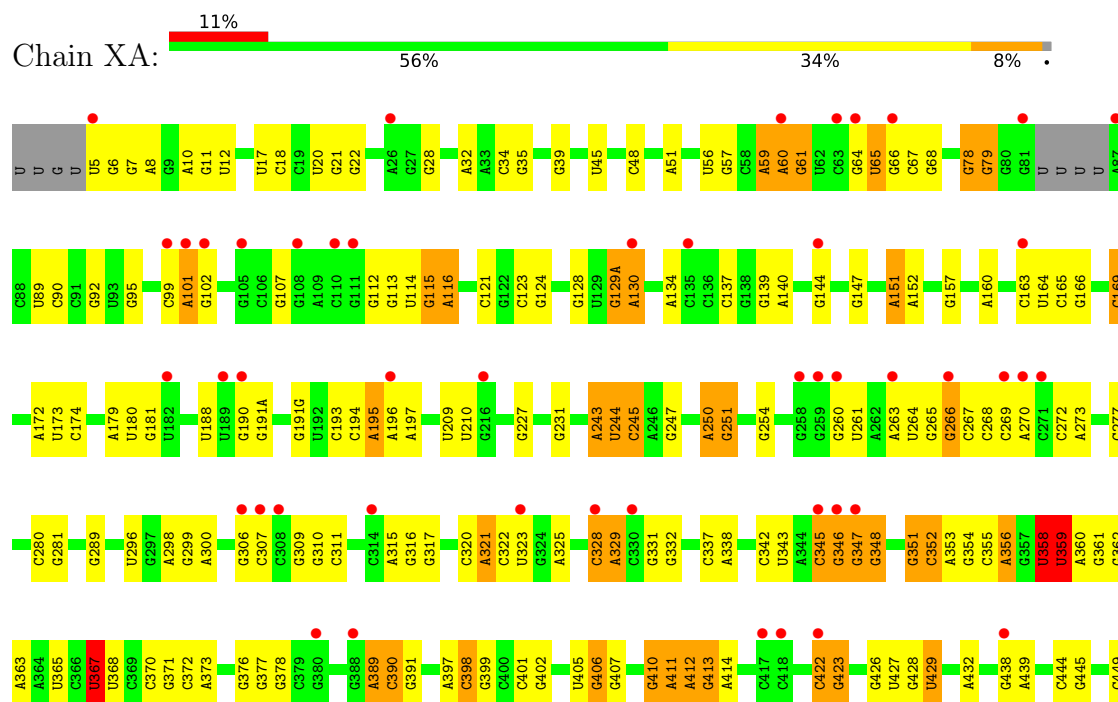
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

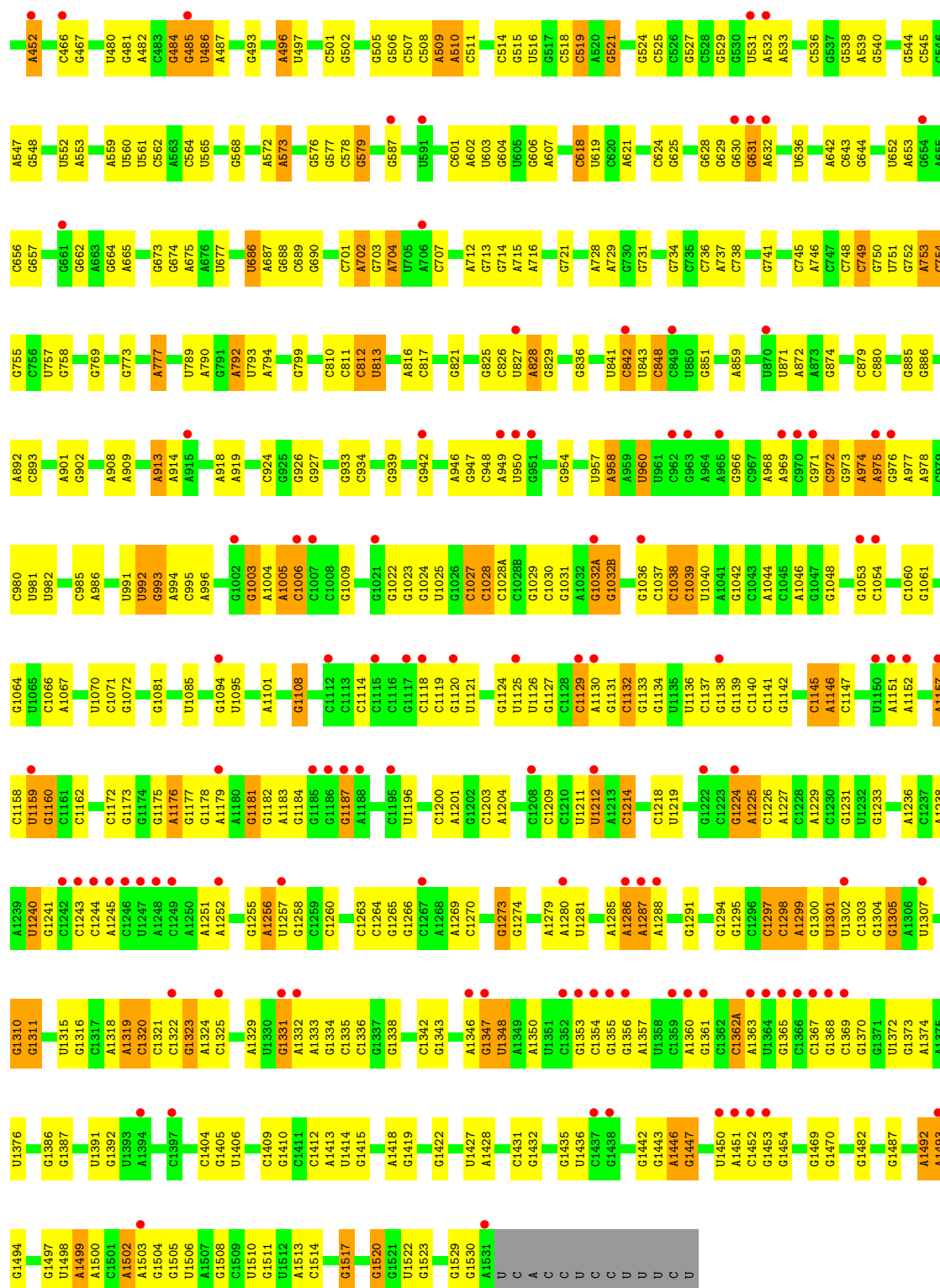
• Molecule 1: 16S rRNA



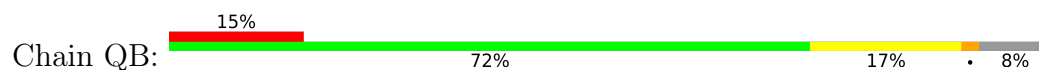


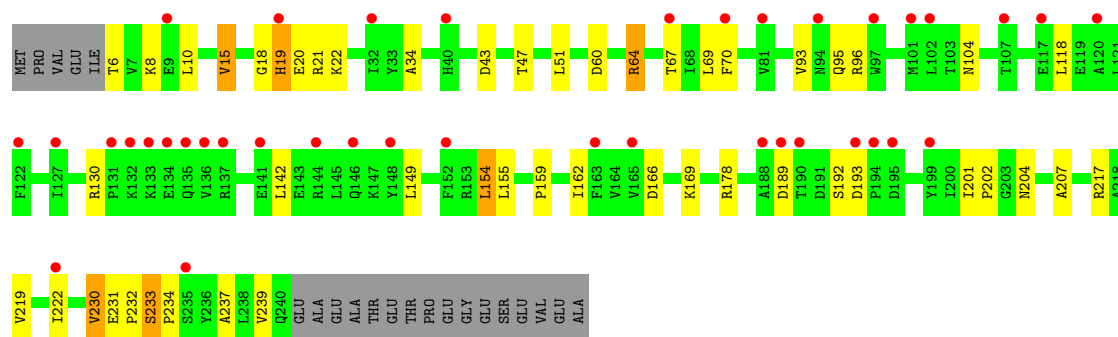
• Molecule 1: 16S rRNA



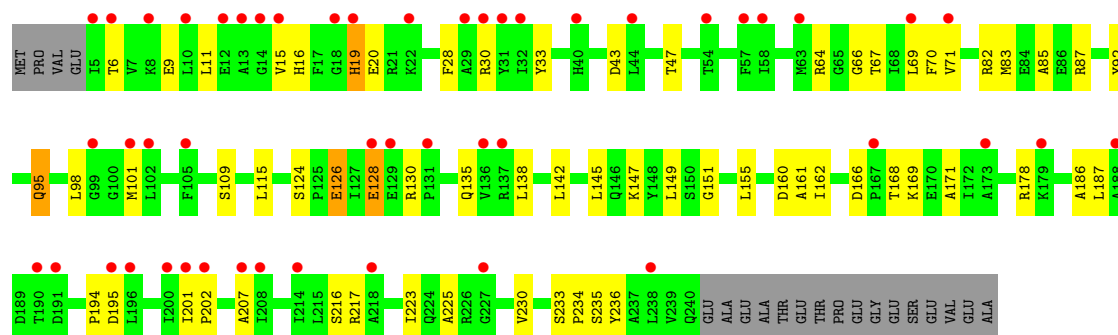


• Molecule 2: 30S ribosomal protein S2

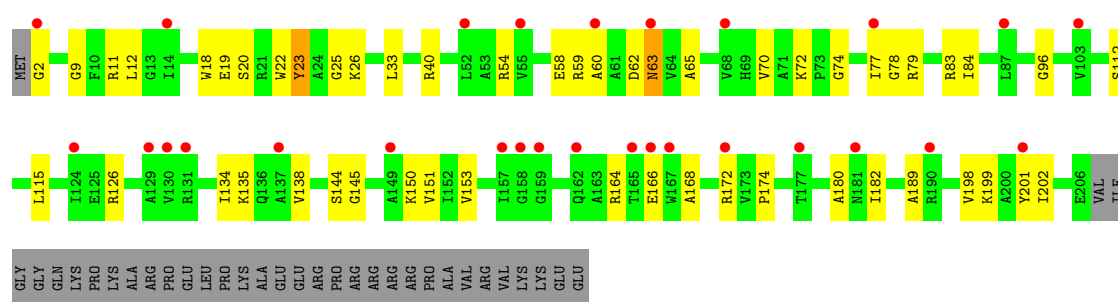




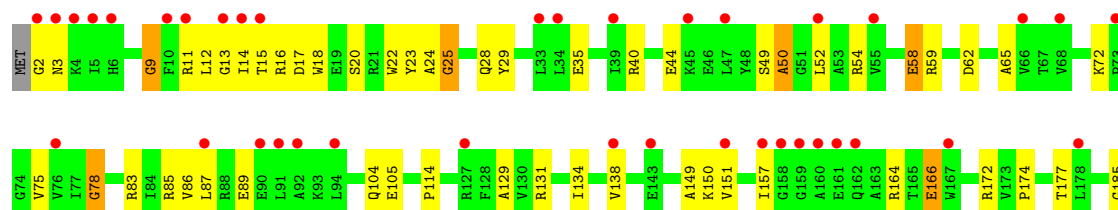
• Molecule 2: 30S ribosomal protein S2

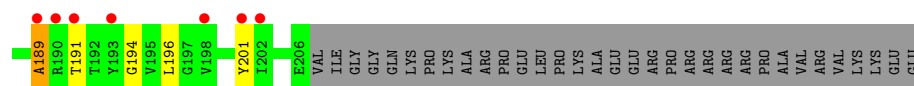


• Molecule 3: 30S ribosomal protein S3

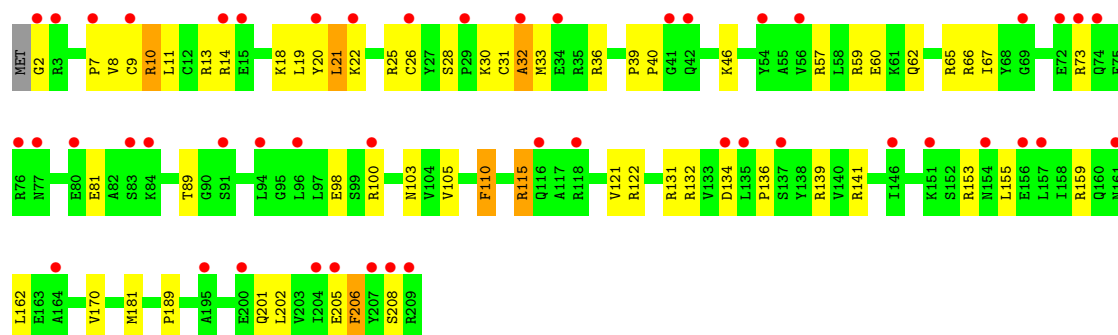
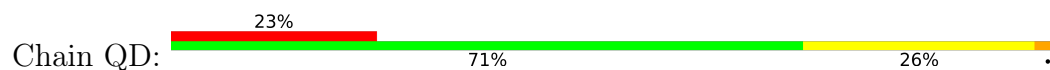


• Molecule 3: 30S ribosomal protein S3

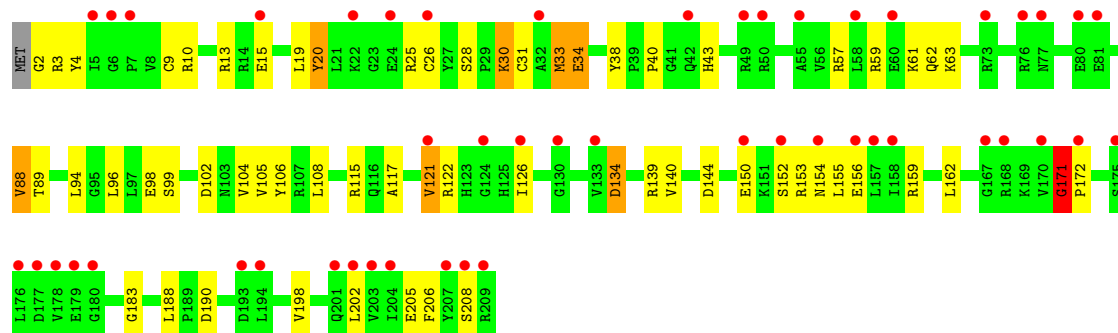
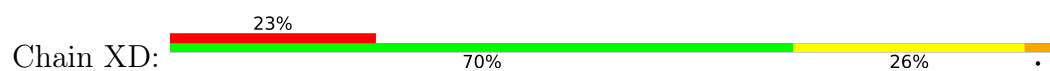




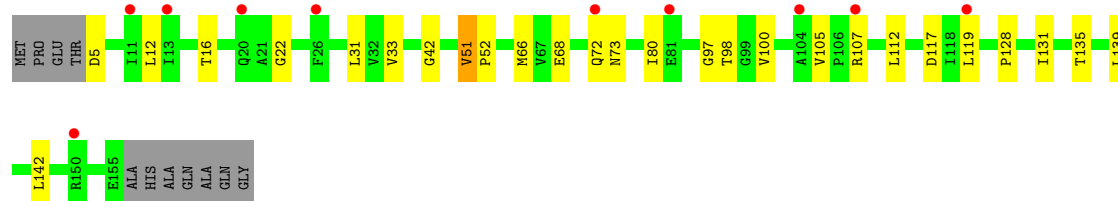
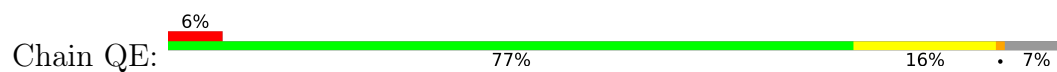
• Molecule 4: 30S ribosomal protein S4



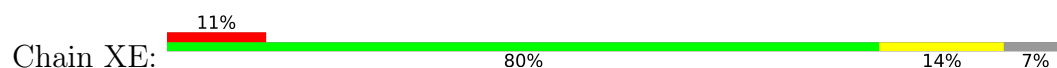
• Molecule 4: 30S ribosomal protein S4

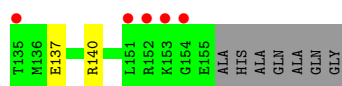


• Molecule 5: 30S ribosomal protein S5

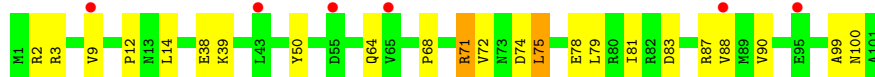
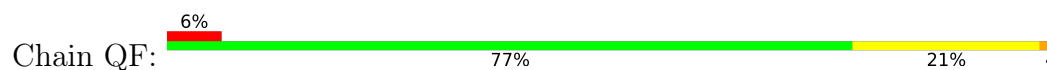


• Molecule 5: 30S ribosomal protein S5





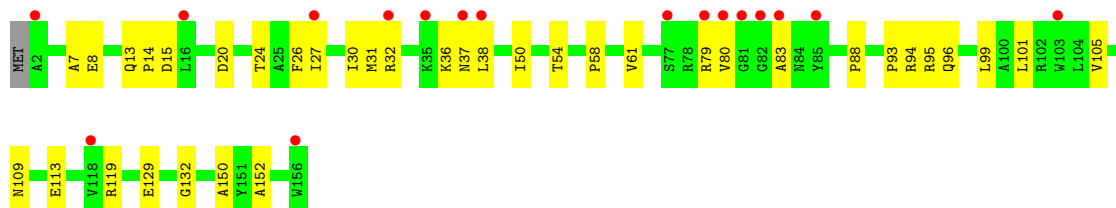
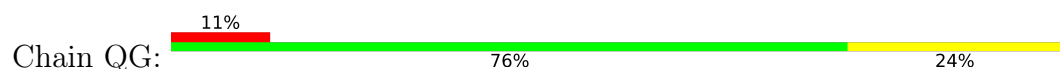
- Molecule 6: 30S ribosomal protein S6



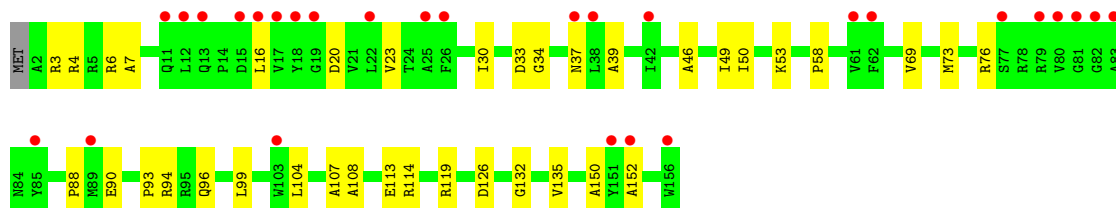
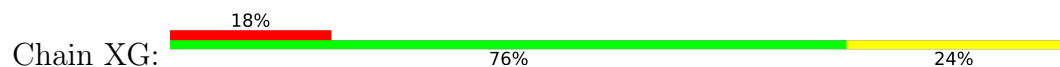
- Molecule 6: 30S ribosomal protein S6



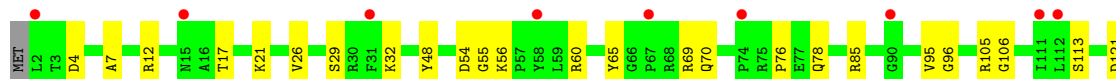
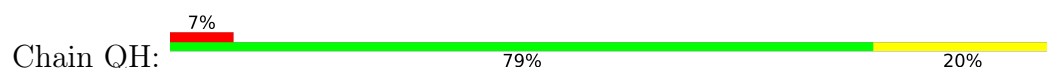
- Molecule 7: 30S ribosomal protein S7



- Molecule 7: 30S ribosomal protein S7



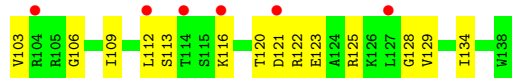
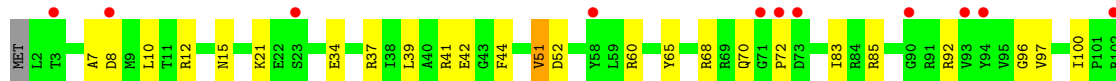
- Molecule 8: 30S ribosomal protein S8





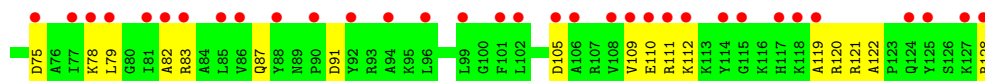
- Molecule 8: 30S ribosomal protein S8

Chain XH: 12% 71% 28% ..



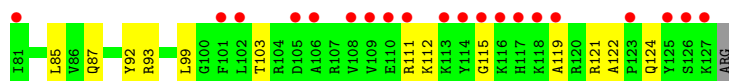
- Molecule 9: 30S ribosomal protein S9

Chain QI: 44% 65% 34% ..



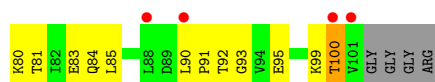
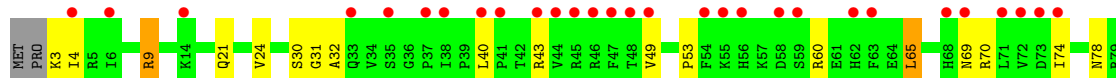
- Molecule 9: 30S ribosomal protein S9

Chain XI: 35% 64% 32% ..



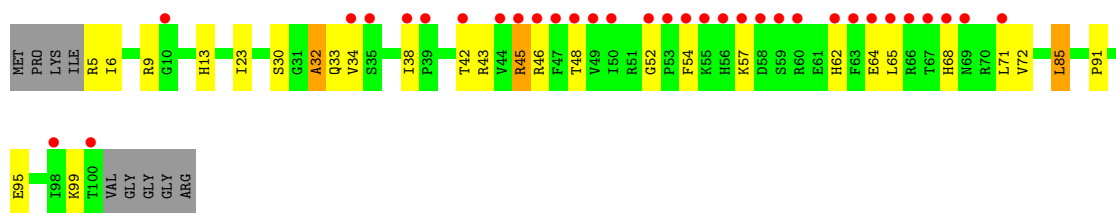
- Molecule 10: 30S ribosomal protein S10

Chain QJ: 31% 66% 26% 6%

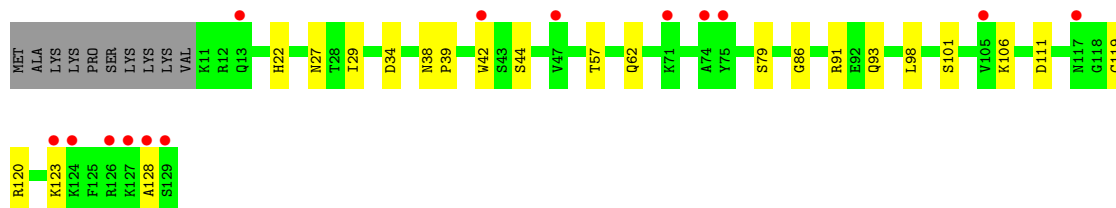
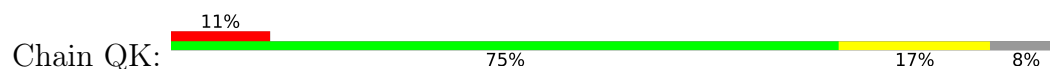


- Molecule 10: 30S ribosomal protein S10

Chain XJ: 31% 65% 24% 9%



- Molecule 11: 30S ribosomal protein S11



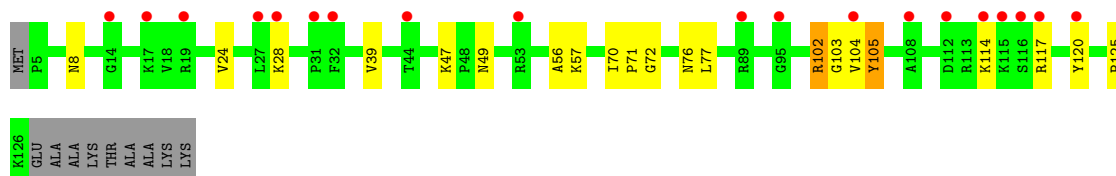
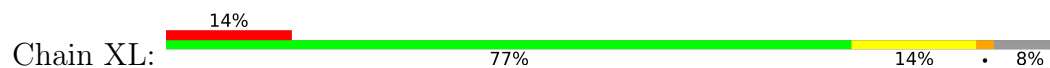
- Molecule 11: 30S ribosomal protein S11



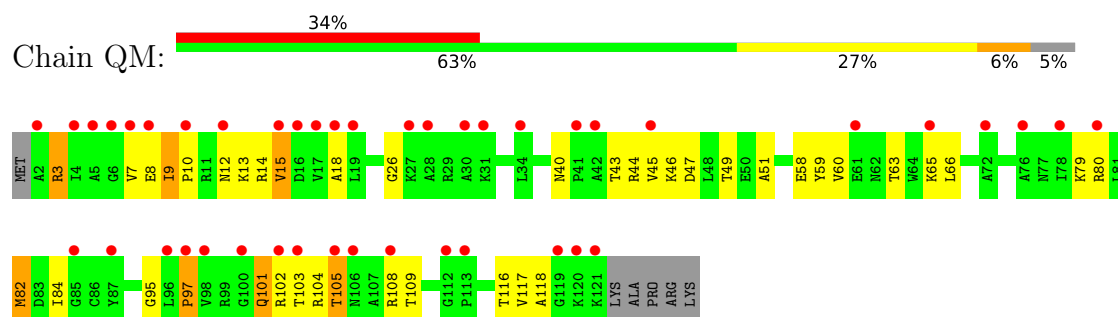
- Molecule 12: 30S ribosomal protein S12



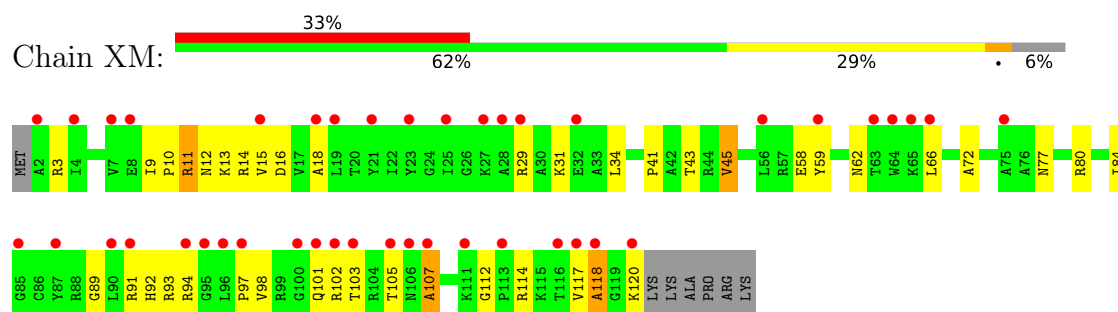
- Molecule 12: 30S ribosomal protein S12



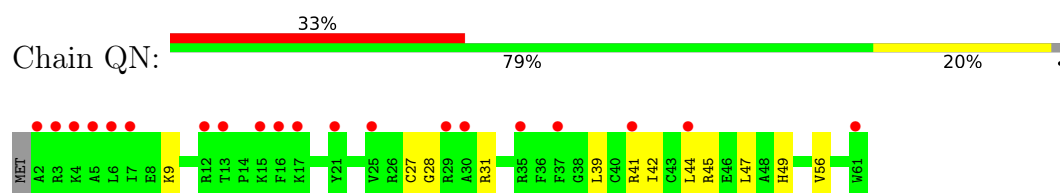
- Molecule 13: 30S ribosomal protein S13



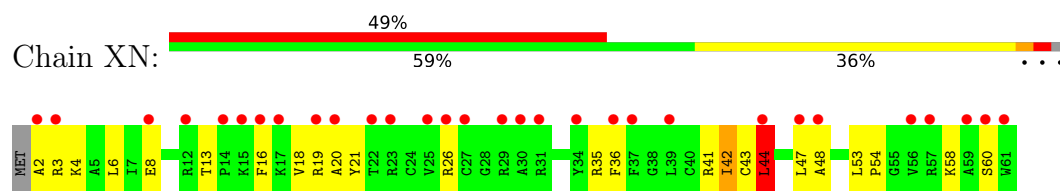
- Molecule 13: 30S ribosomal protein S13



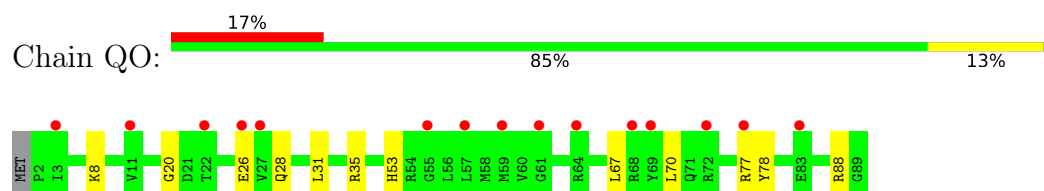
- Molecule 14: 30S ribosomal protein S14 type Z



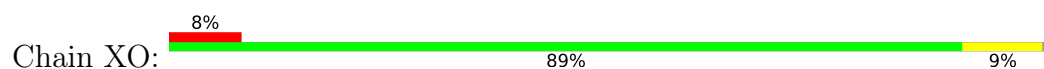
- Molecule 14: 30S ribosomal protein S14 type Z

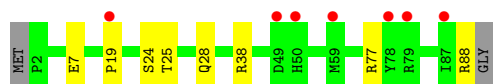


- Molecule 15: 30S ribosomal protein S15

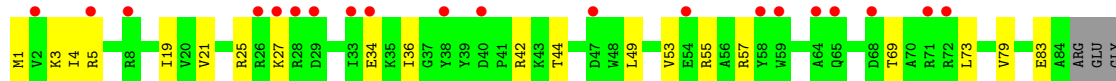
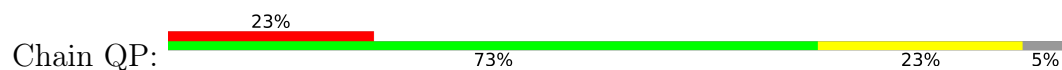


- Molecule 15: 30S ribosomal protein S15

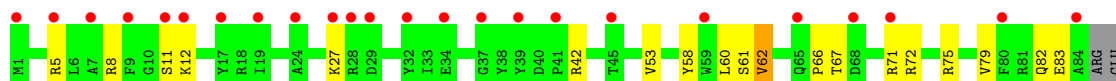
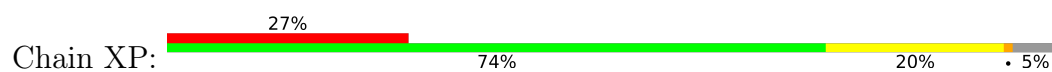




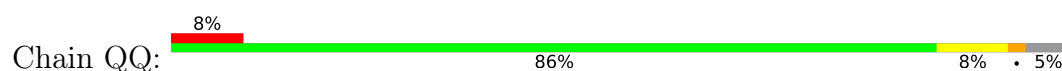
- Molecule 16: 30S ribosomal protein S16



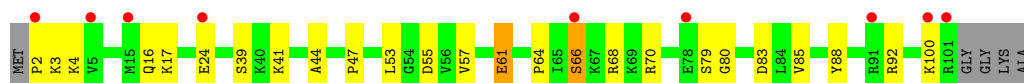
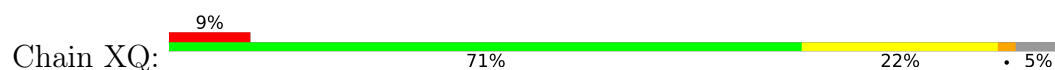
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

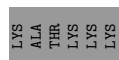
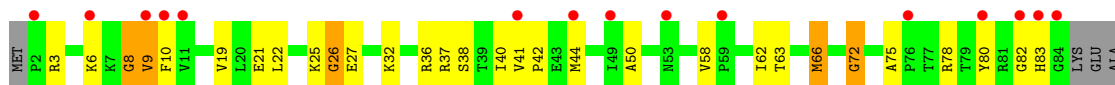


- Molecule 18: 30S ribosomal protein S18

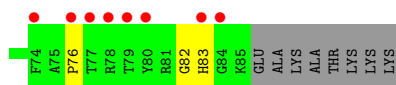
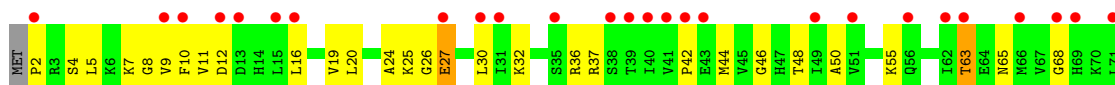
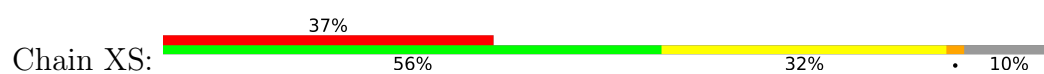




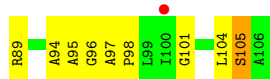
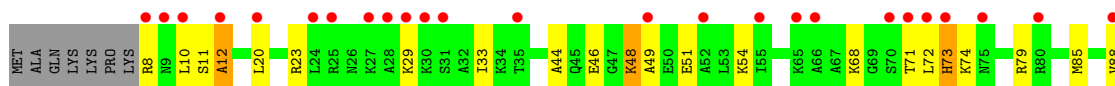
- Molecule 19: 30S ribosomal protein S19



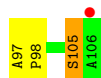
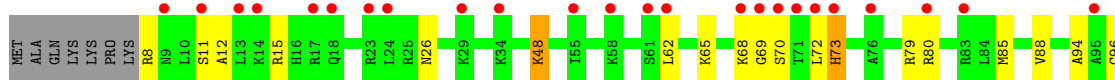
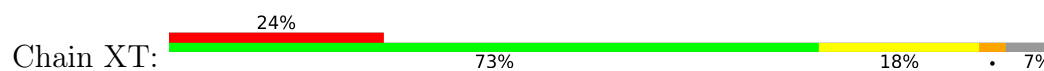
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20

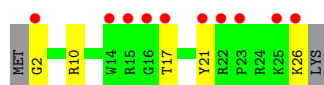
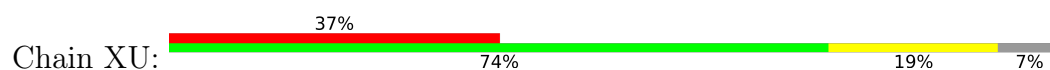


- Molecule 21: 30S ribosomal protein Thx

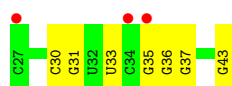




- Molecule 21: 30S ribosomal protein Thx



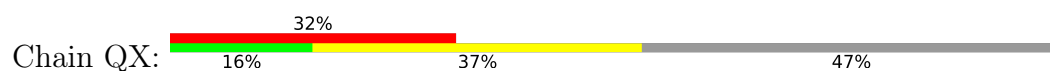
- Molecule 22: P-site ASLPro



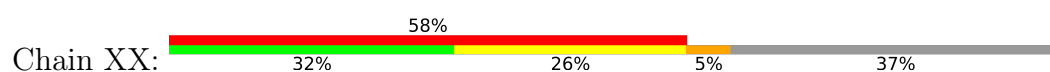
- Molecule 22: P-site ASLPro



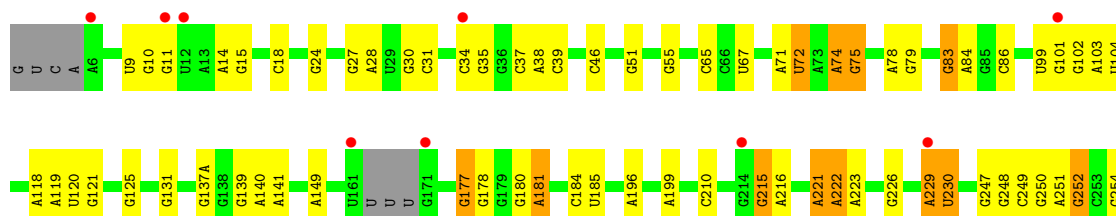
- Molecule 23: mRNA

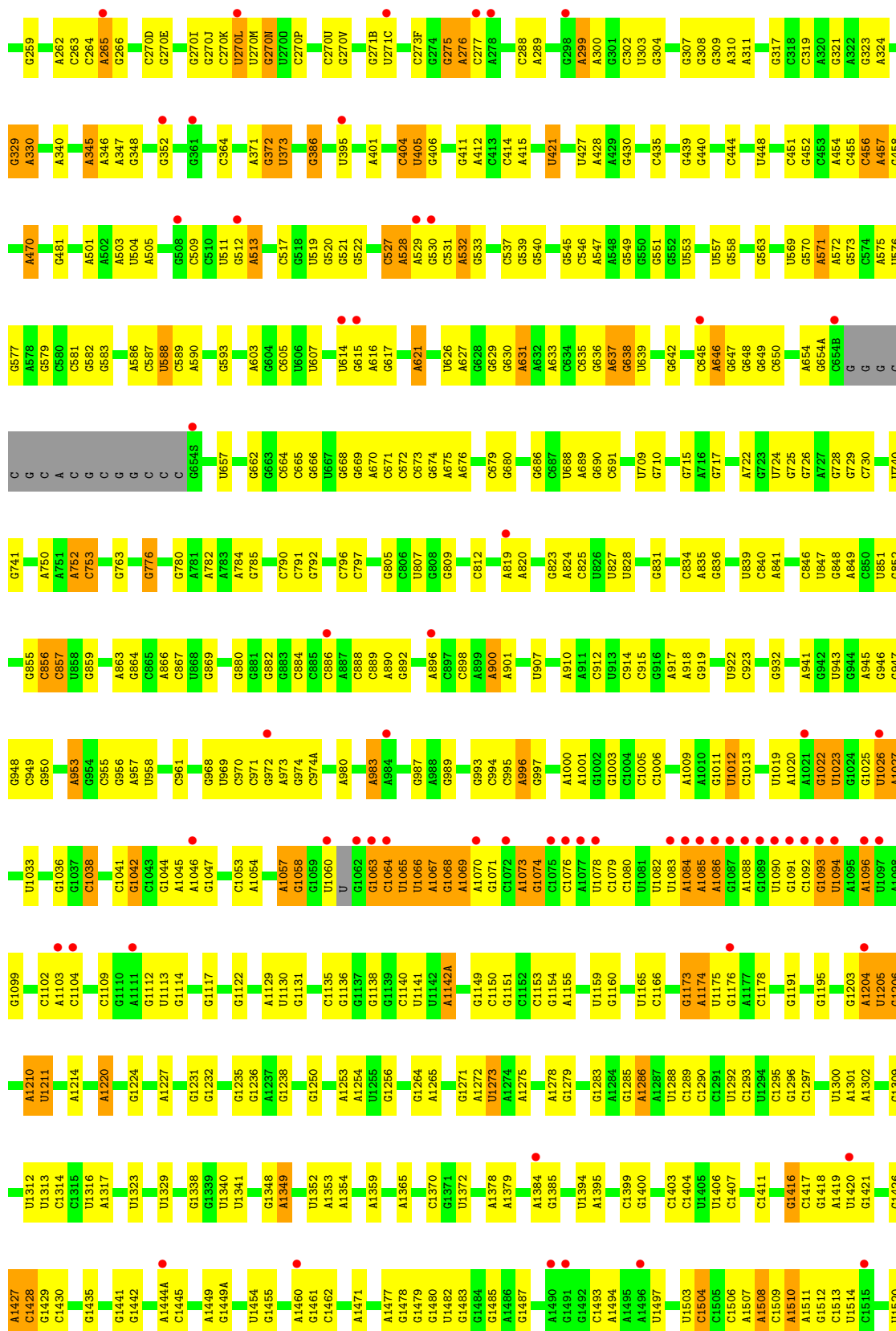


- Molecule 23: mRNA



- Molecule 24: 23S rRNA



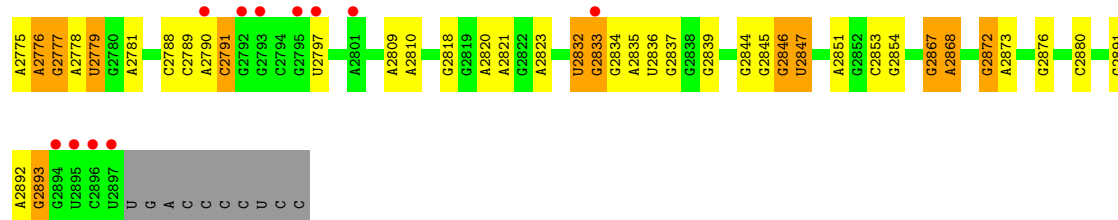




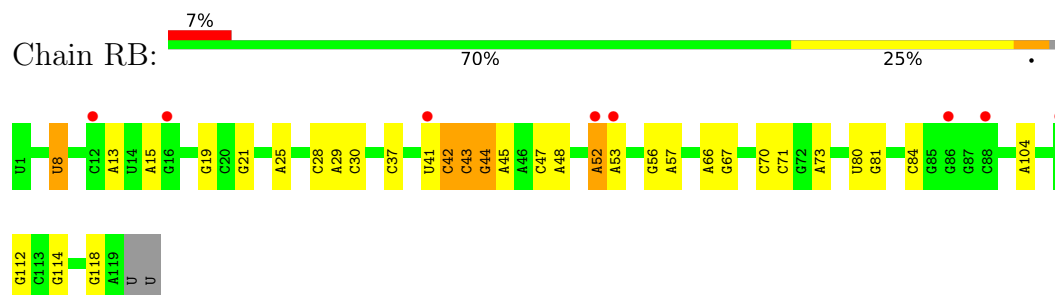
Chain YA:



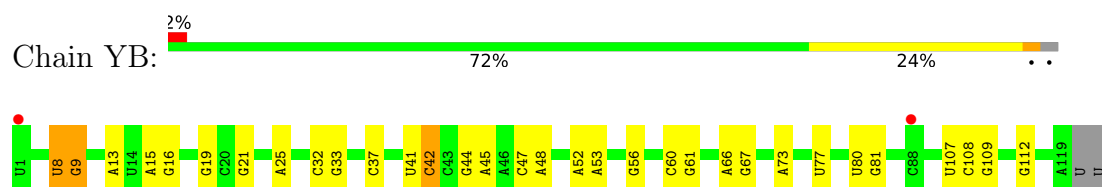




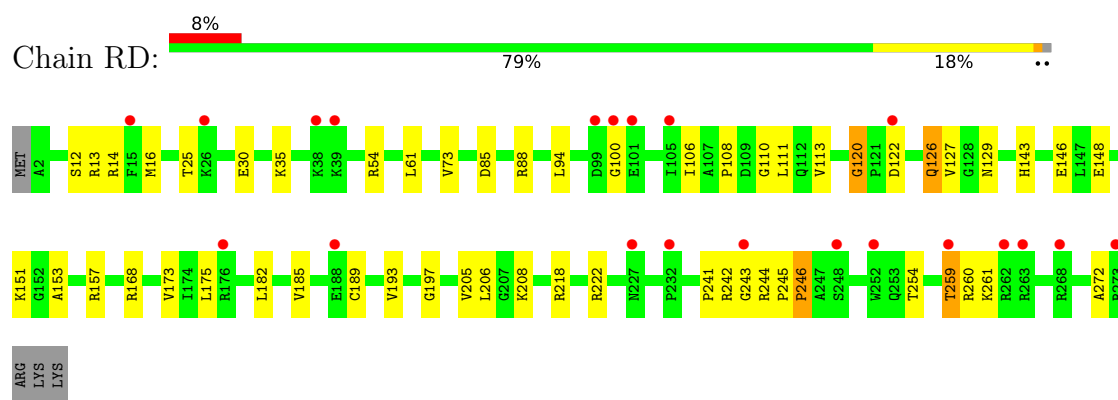
• Molecule 25: 5S rRNA



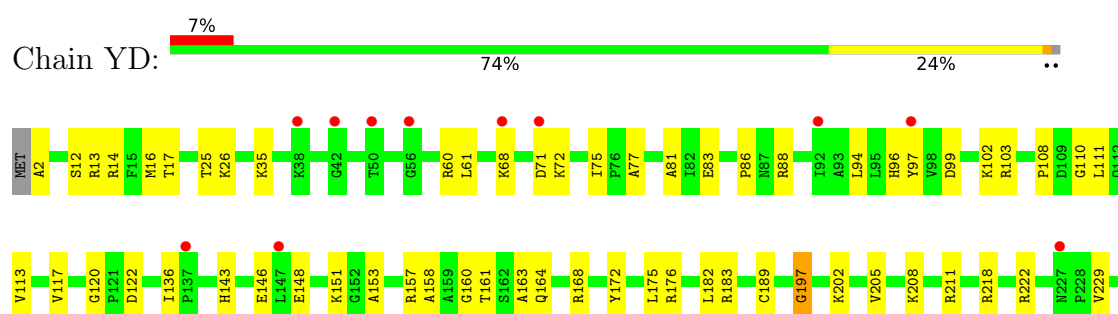
• Molecule 25: 5S rRNA

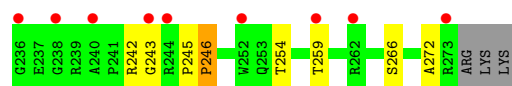


• Molecule 26: 50S ribosomal protein L2

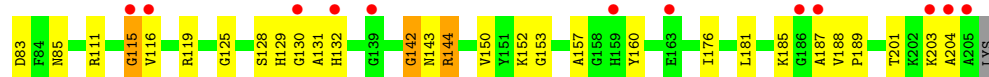
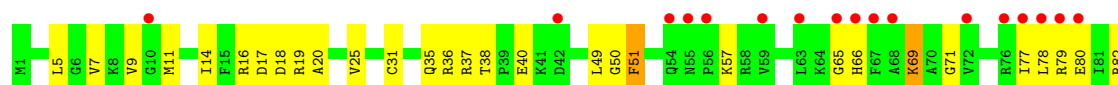
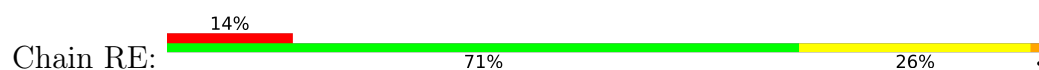


• Molecule 26: 50S ribosomal protein L2

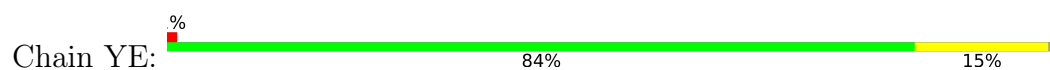




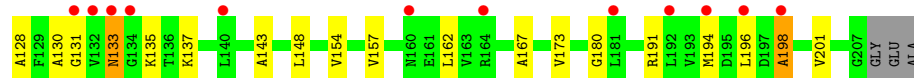
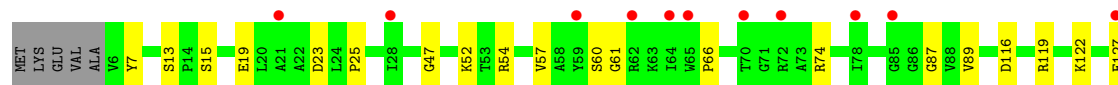
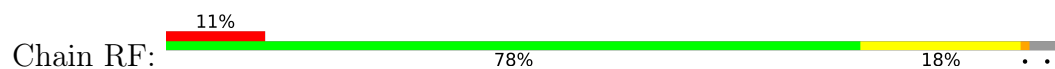
- Molecule 27: 50S ribosomal protein L3



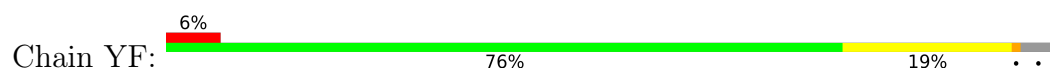
- Molecule 27: 50S ribosomal protein L3



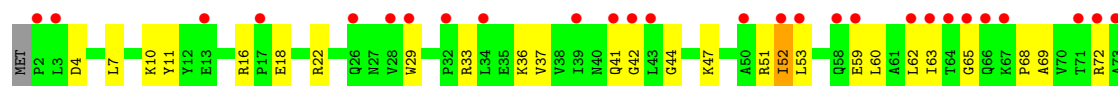
- Molecule 28: 50S ribosomal protein L4

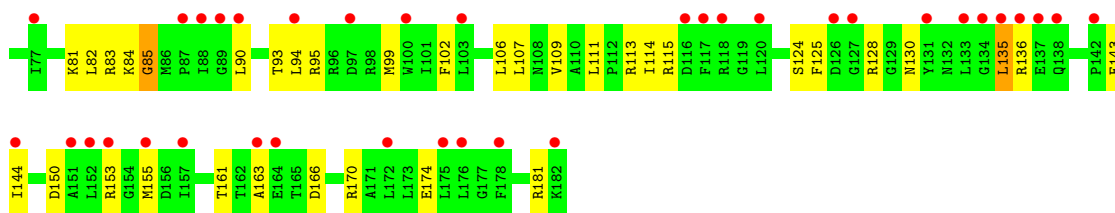


- Molecule 28: 50S ribosomal protein L4

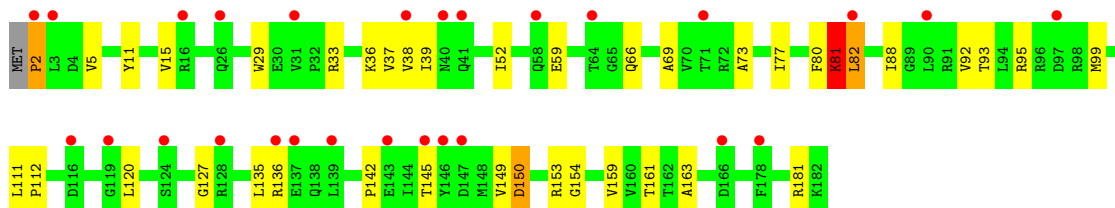
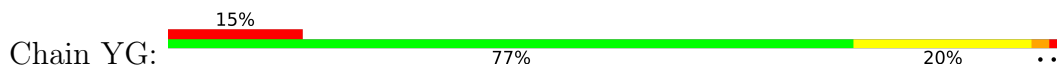


- Molecule 29: 50S ribosomal protein L5

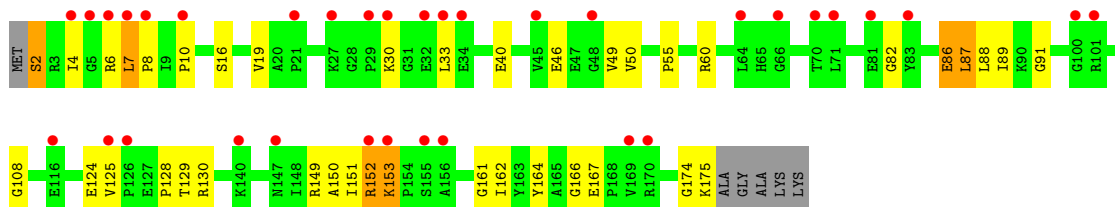
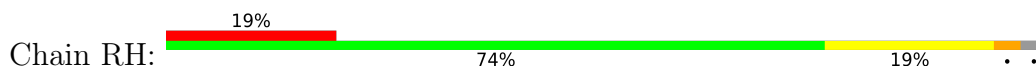




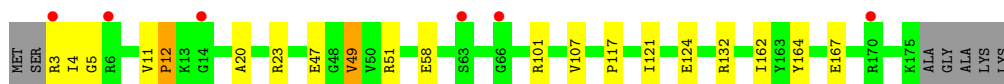
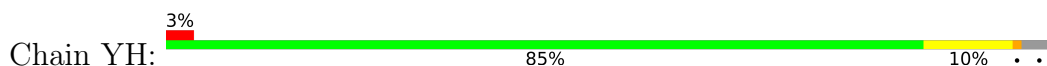
• Molecule 29: 50S ribosomal protein L5



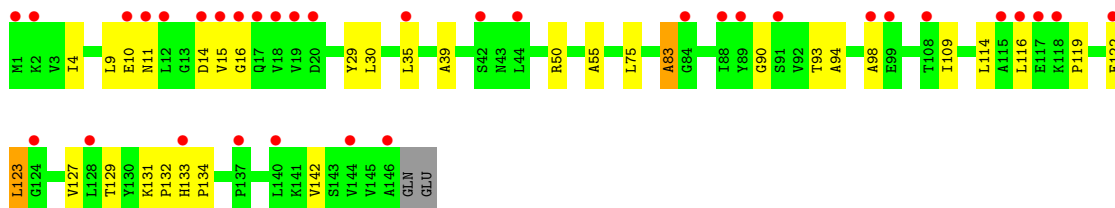
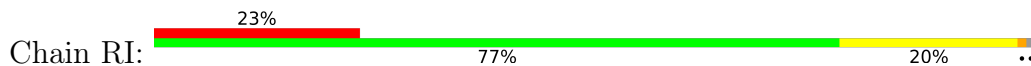
• Molecule 30: 50S ribosomal protein L6



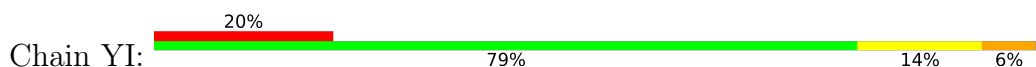
• Molecule 30: 50S ribosomal protein L6

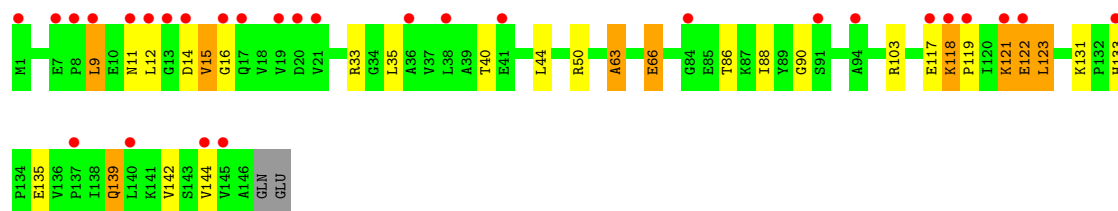


• Molecule 31: 50S ribosomal protein L9

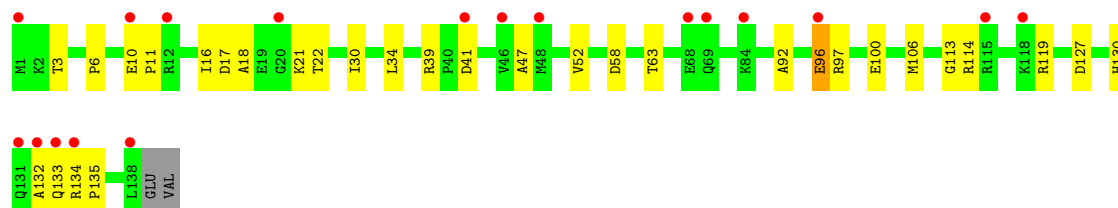
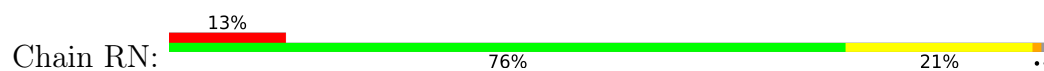


• Molecule 31: 50S ribosomal protein L9

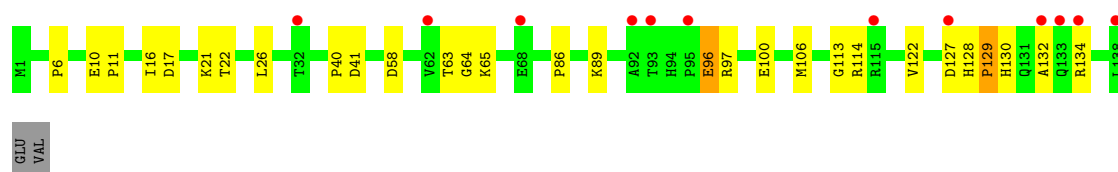
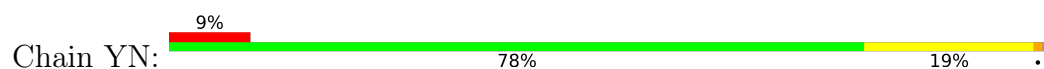




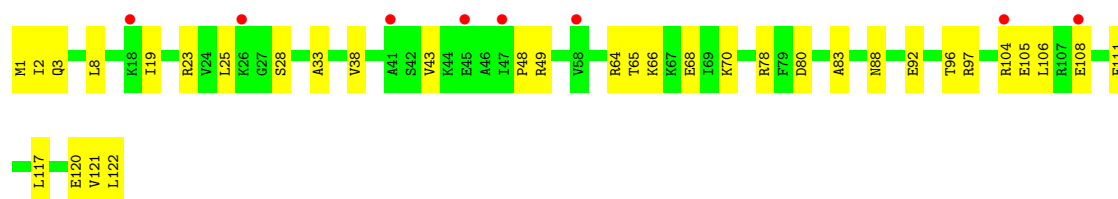
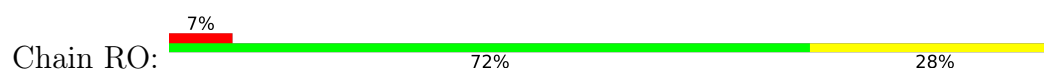
• Molecule 32: 50S ribosomal protein L13



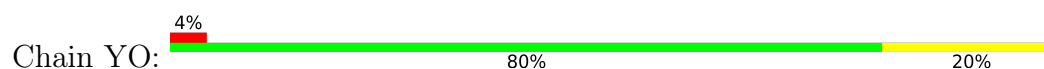
• Molecule 32: 50S ribosomal protein L13



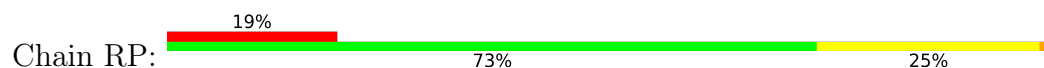
• Molecule 33: 50S ribosomal protein L14

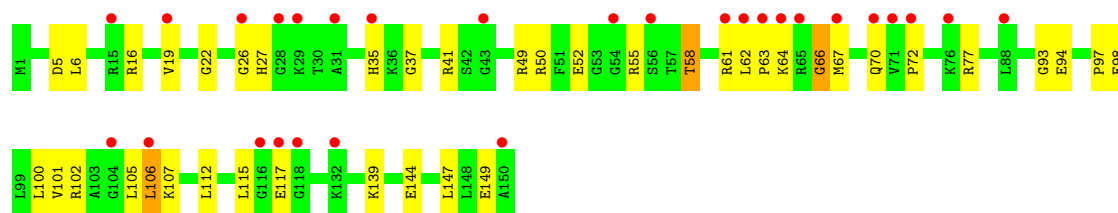


• Molecule 33: 50S ribosomal protein L14

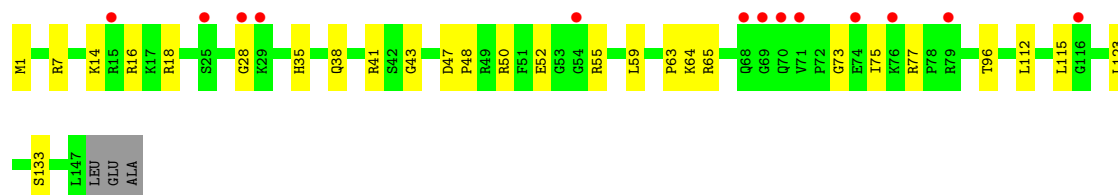
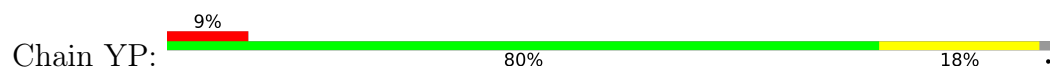


• Molecule 34: 50S ribosomal protein L15

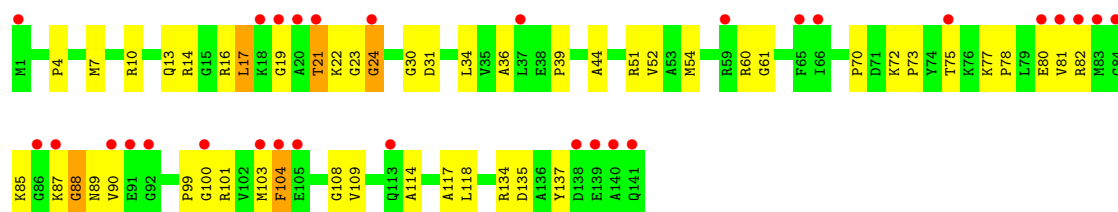




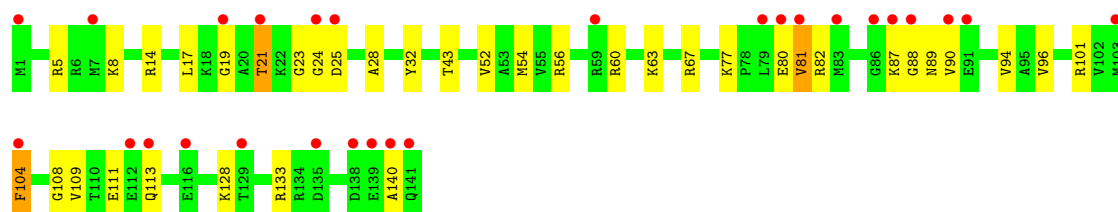
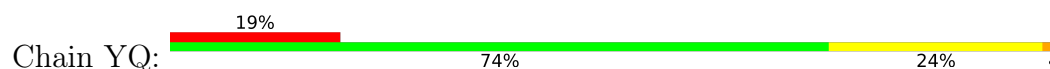
• Molecule 34: 50S ribosomal protein L15



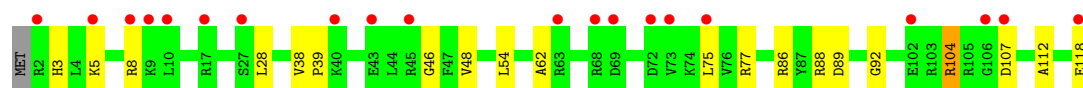
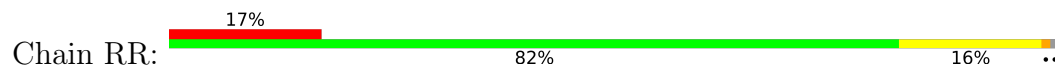
• Molecule 35: 50S ribosomal protein L16



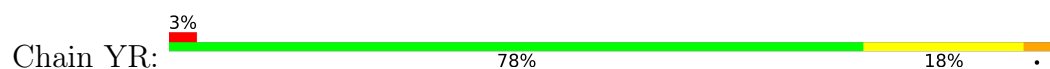
• Molecule 35: 50S ribosomal protein L16



• Molecule 36: 50S ribosomal protein L17

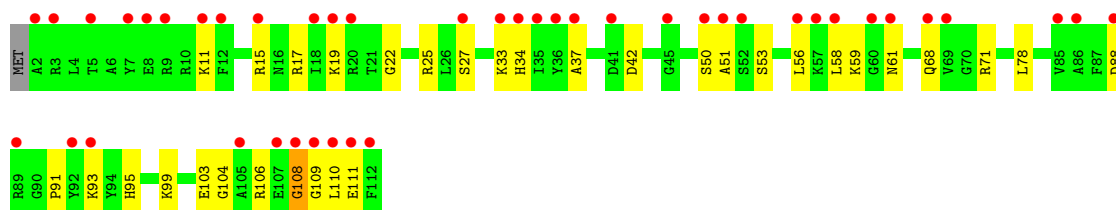
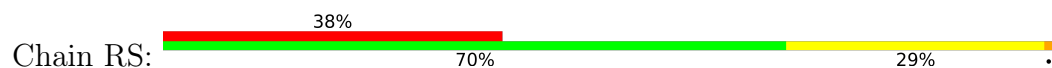


• Molecule 36: 50S ribosomal protein L17

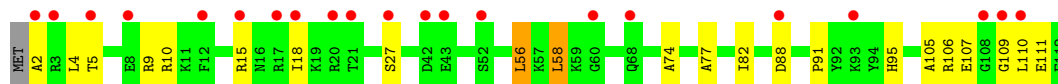
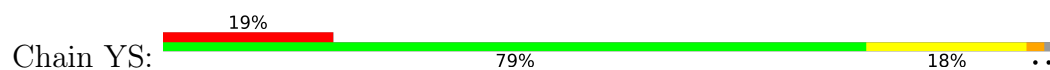




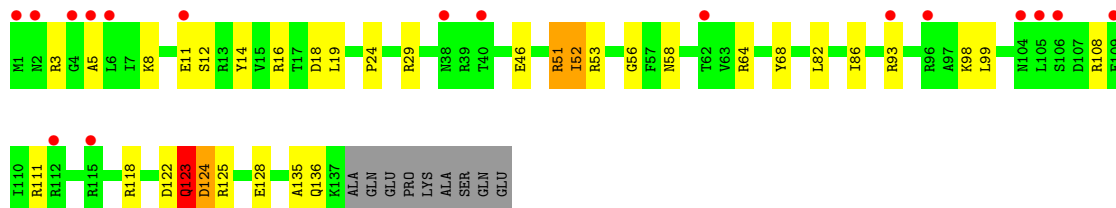
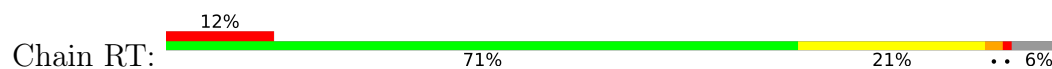
- Molecule 37: 50S ribosomal protein L18



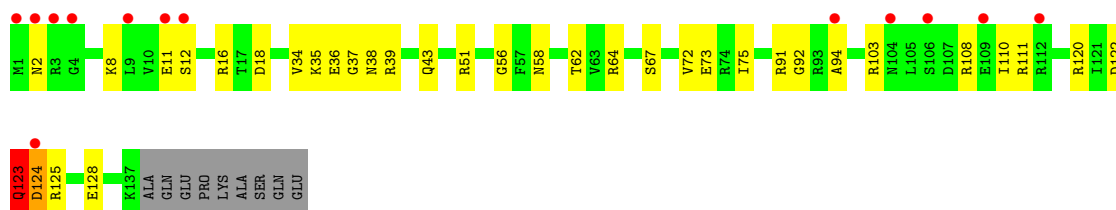
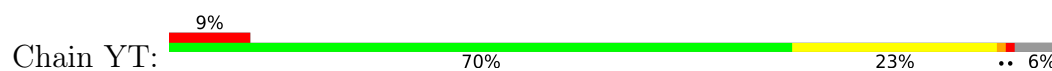
- Molecule 37: 50S ribosomal protein L18



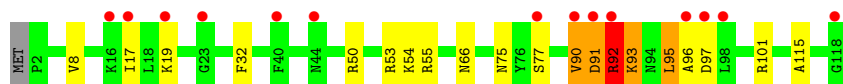
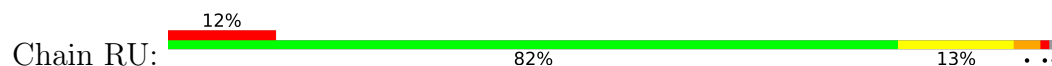
- Molecule 38: 50S ribosomal protein L19



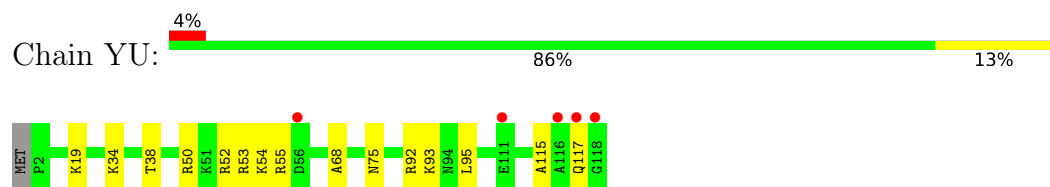
- Molecule 38: 50S ribosomal protein L19



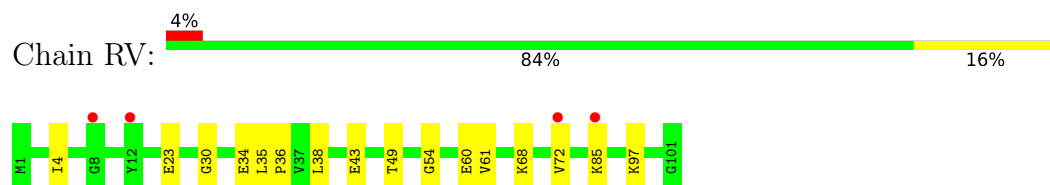
- Molecule 39: 50S ribosomal protein L20



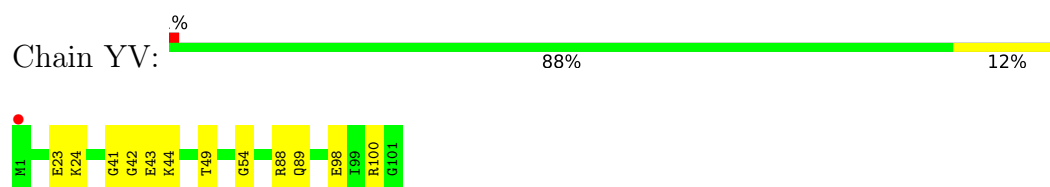
• Molecule 39: 50S ribosomal protein L20



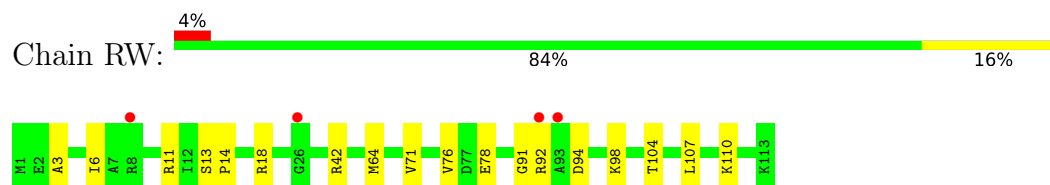
• Molecule 40: 50S ribosomal protein L21



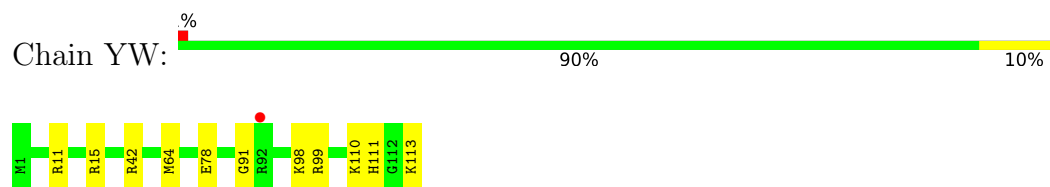
• Molecule 40: 50S ribosomal protein L21



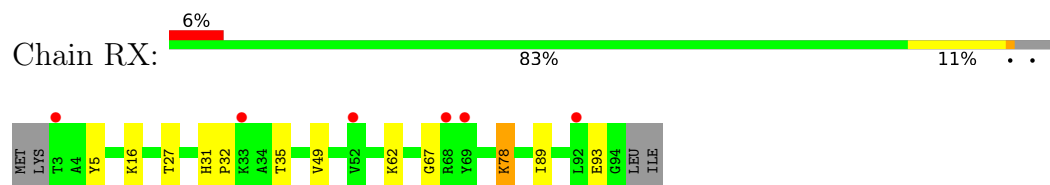
• Molecule 41: 50S ribosomal protein L22



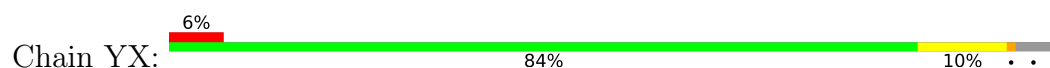
• Molecule 41: 50S ribosomal protein L22

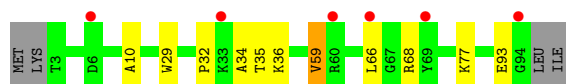


• Molecule 42: 50S ribosomal protein L23

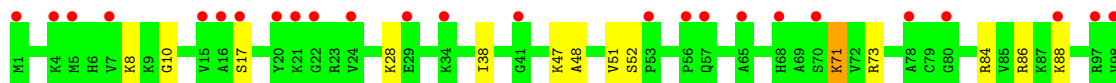
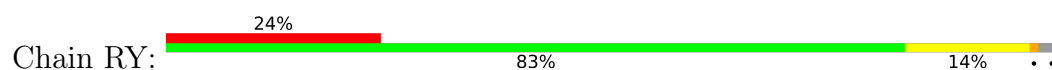


• Molecule 42: 50S ribosomal protein L23

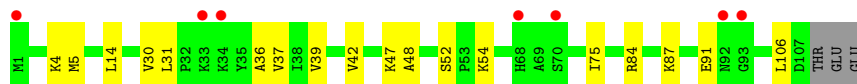
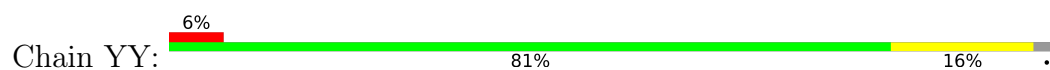




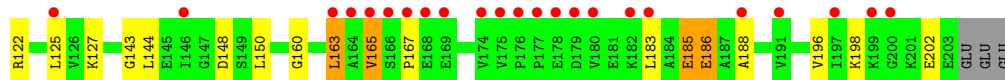
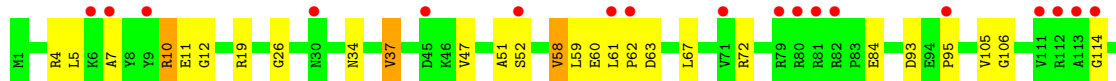
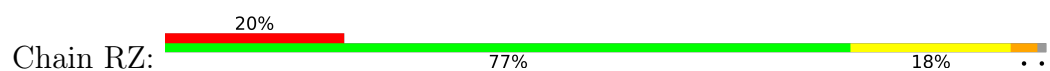
- Molecule 43: 50S ribosomal protein L24



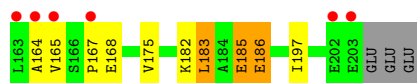
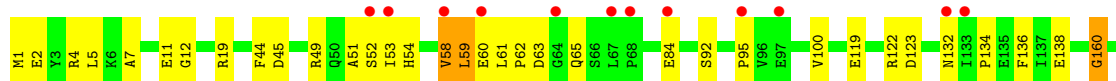
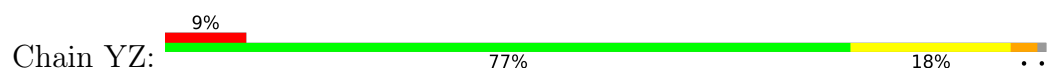
- Molecule 43: 50S ribosomal protein L24



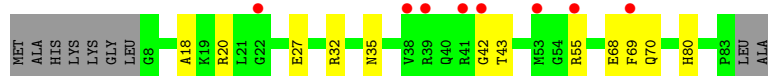
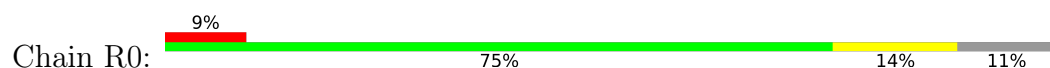
- Molecule 44: 50S ribosomal protein L25



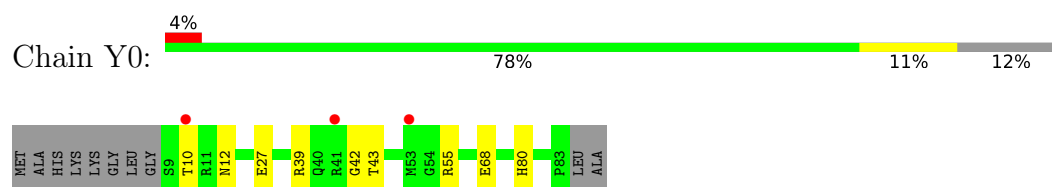
- Molecule 44: 50S ribosomal protein L25



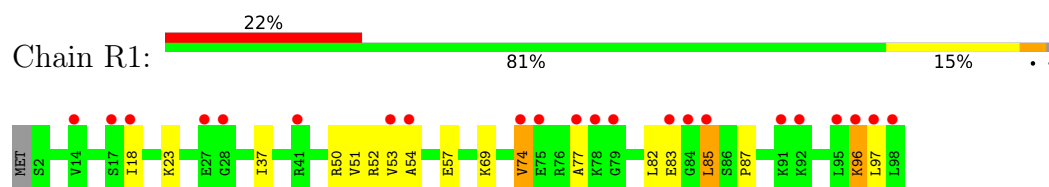
- Molecule 45: 50S ribosomal protein L27



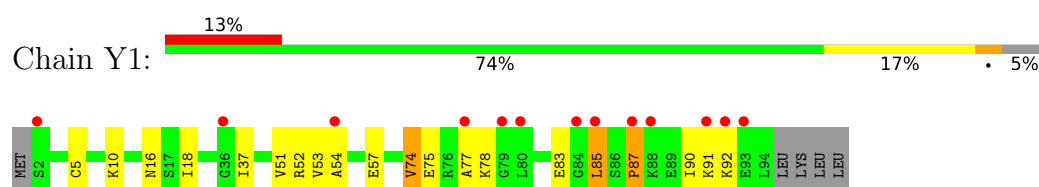
- Molecule 45: 50S ribosomal protein L27



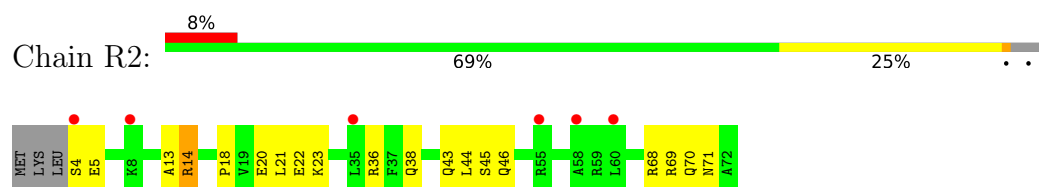
- Molecule 46: 50S ribosomal protein L28



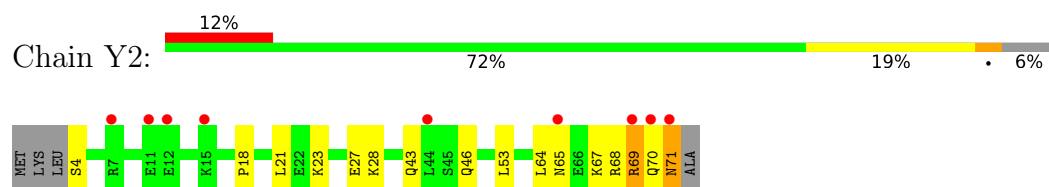
- Molecule 46: 50S ribosomal protein L28



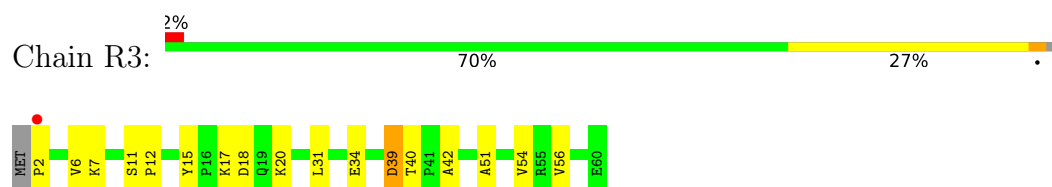
- Molecule 47: 50S ribosomal protein L29



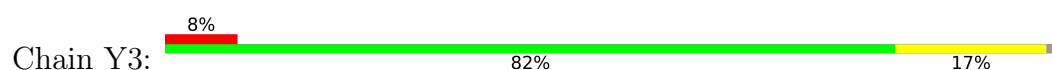
- Molecule 47: 50S ribosomal protein L29

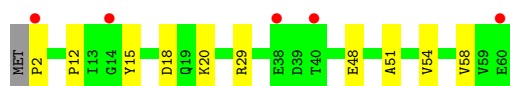


- Molecule 48: 50S ribosomal protein L30

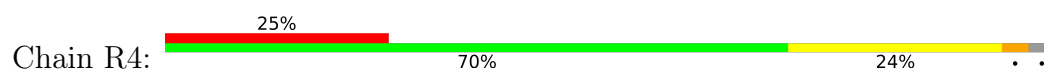


- Molecule 48: 50S ribosomal protein L30





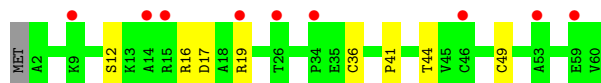
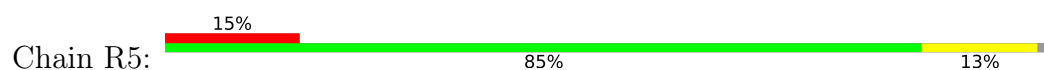
- Molecule 49: 50S ribosomal protein L31



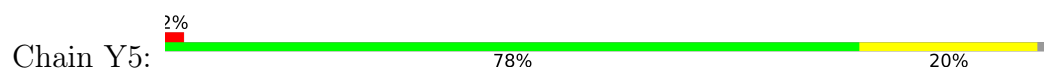
- Molecule 49: 50S ribosomal protein L31



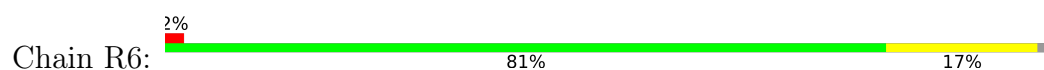
- Molecule 50: 50S ribosomal protein L32



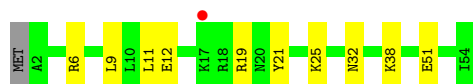
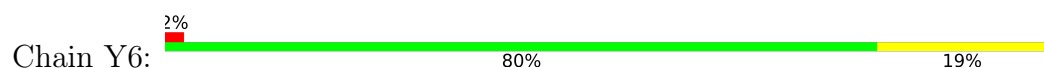
- Molecule 50: 50S ribosomal protein L32



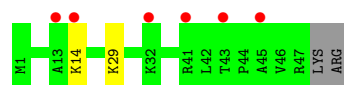
- Molecule 51: 50S ribosomal protein L33



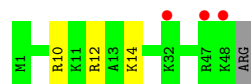
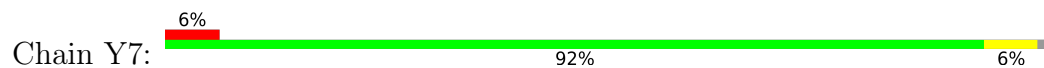
- Molecule 51: 50S ribosomal protein L33



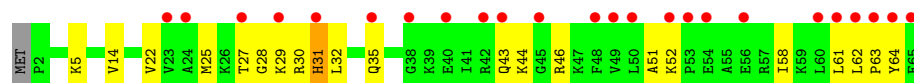
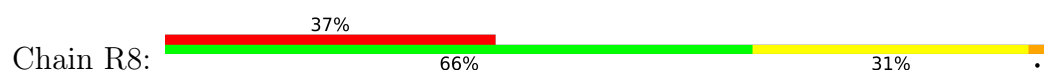
- Molecule 52: 50S ribosomal protein L34



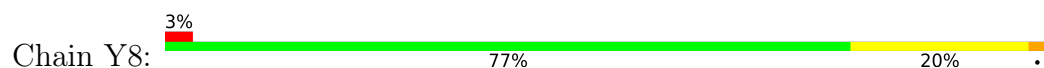
- Molecule 52: 50S ribosomal protein L34



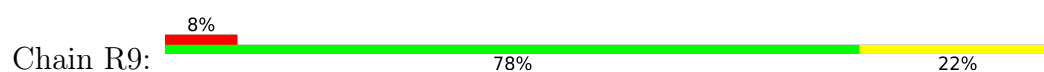
- Molecule 53: 50S ribosomal protein L35



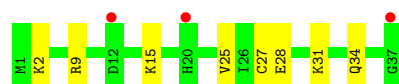
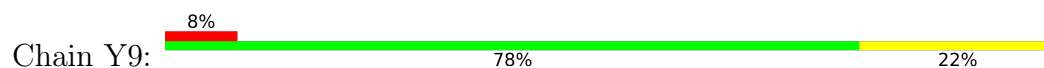
- Molecule 53: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L36



- Molecule 54: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.79Å 451.91Å 621.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.71 – 3.10 152.71 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (152.71-3.10) 98.0 (152.71-3.10)	Depositor EDS
R_{merge}	0.36	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.244 , 0.274 0.242 , 0.273	Depositor DCC
R_{free} test set	48505 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 76.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	289311	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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: SF4, 1MG, MG, ZN

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	QA	0.16	0/36098	0.34	1/56341 (0.0%)
1	XA	0.17	1/36101 (0.0%)	0.36	10/56346 (0.0%)
2	QB	0.21	0/1942	0.59	3/2619 (0.1%)
2	XB	0.19	0/1950	0.55	2/2630 (0.1%)
3	QC	0.21	0/1629	0.53	0/2195
3	XC	0.20	0/1629	0.54	1/2195 (0.0%)
4	QD	0.41	0/1733	1.05	11/2318 (0.5%)
4	XD	0.33	0/1733	1.17	19/2318 (0.8%)
5	QE	0.21	0/1171	0.53	0/1576
5	XE	0.22	0/1171	0.50	0/1576
6	QF	0.18	0/856	0.44	0/1154
6	XF	0.16	0/856	0.41	0/1154
7	QG	0.20	0/1276	0.52	0/1709
7	XG	0.19	0/1276	0.47	0/1709
8	QH	0.20	0/1128	0.46	0/1517
8	XH	0.20	0/1128	0.46	0/1517
9	QI	0.23	0/1029	0.58	0/1379
9	XI	0.22	0/1017	0.63	0/1365
10	QJ	0.22	0/814	0.59	0/1095
10	XJ	0.19	0/790	0.45	0/1063
11	QK	0.20	0/900	0.44	0/1213
11	XK	0.18	0/879	0.42	0/1187
12	QL	0.23	0/991	0.49	0/1327
12	XL	0.21	0/972	0.53	0/1301
13	QM	0.23	0/965	0.70	1/1292 (0.1%)
13	XM	0.22	0/956	0.68	3/1281 (0.2%)
14	QN	0.25	0/501	0.63	0/664
14	XN	0.22	0/501	0.56	0/664
15	QO	0.20	0/745	0.53	0/992
15	XO	0.15	0/740	0.38	0/987
16	QP	0.20	0/721	0.46	0/970
16	XP	0.19	0/721	0.48	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.19	0/847	0.44	0/1131
17	XQ	0.19	0/847	0.42	0/1131
18	QR	0.19	0/579	0.50	0/768
18	XR	0.17	0/579	0.45	0/768
19	QS	0.23	0/680	0.64	0/915
19	XS	0.20	0/689	0.56	1/926 (0.1%)
20	QT	0.23	0/765	0.56	0/1007
20	XT	0.18	0/765	0.54	0/1007
21	QU	0.21	0/221	0.45	0/288
21	XU	0.20	0/221	0.48	0/288
22	QV	0.28	0/380	0.24	0/590
22	XV	0.30	0/332	0.25	0/515
23	QX	0.22	0/243	0.36	0/377
23	XX	0.23	0/294	0.28	0/457
24	RA	0.19	0/69498	0.36	0/108491
24	YA	0.22	0/69543	0.38	1/108563 (0.0%)
25	RB	0.17	0/2878	0.34	0/4490
25	YB	0.20	0/2878	0.37	0/4490
26	RD	0.24	0/2165	0.46	0/2919
26	YD	0.27	0/2165	0.48	0/2919
27	RE	0.27	0/1601	0.62	0/2160
27	YE	0.27	0/1596	0.54	0/2153
28	RF	0.23	0/1620	0.46	0/2194
28	YF	0.25	0/1620	0.48	0/2194
29	RG	0.22	0/1499	0.60	0/2016
29	YG	0.23	0/1499	0.60	0/2016
30	RH	0.24	0/1362	0.55	0/1841
30	YH	0.28	0/1356	0.53	0/1833
31	RI	0.21	0/1151	0.63	2/1558 (0.1%)
31	YI	0.22	0/1151	0.63	1/1558 (0.1%)
32	RN	0.23	0/1131	0.49	0/1525
32	YN	0.27	0/1131	0.52	0/1525
33	RO	0.22	0/943	0.45	0/1269
33	YO	0.24	0/943	0.48	0/1269
34	RP	0.25	0/1162	0.63	0/1544
34	YP	0.27	0/1139	0.58	0/1514
35	RQ	0.23	0/1143	0.60	0/1527
35	YQ	0.26	0/1143	0.63	1/1527 (0.1%)
36	RR	0.26	0/974	0.54	0/1302
36	YR	0.28	0/974	0.56	0/1302
37	RS	0.23	0/892	0.62	0/1187
37	YS	0.27	0/892	0.64	0/1187
38	RT	0.25	0/1155	0.59	0/1542

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YT	0.27	0/1155	0.63	2/1542 (0.1%)
39	RU	0.23	0/982	0.56	3/1306 (0.2%)
39	YU	0.25	0/982	0.43	0/1306
40	RV	0.22	0/790	0.50	0/1057
40	YV	0.26	0/790	0.48	0/1057
41	RW	0.22	0/911	0.49	0/1220
41	YW	0.25	0/911	0.55	0/1220
42	RX	0.21	0/739	0.48	0/993
42	YX	0.26	0/739	0.52	0/993
43	RY	0.19	0/831	0.45	0/1108
43	YY	0.21	0/831	0.41	0/1108
44	RZ	0.33	1/1634 (0.1%)	0.74	2/2216 (0.1%)
44	YZ	0.30	0/1634	0.66	1/2216 (0.0%)
45	R0	0.23	0/611	0.47	0/814
45	Y0	0.25	0/607	0.45	0/809
46	R1	0.25	0/770	0.55	0/1022
46	Y1	0.26	0/736	0.55	0/978
47	R2	0.17	0/583	0.42	0/771
47	Y2	0.29	0/577	0.51	0/764
48	R3	0.19	0/474	0.43	0/635
48	Y3	0.22	0/474	0.49	0/635
49	R4	0.26	0/578	0.70	0/776
49	Y4	0.24	0/578	0.65	0/776
50	R5	0.25	0/473	0.47	0/639
50	Y5	0.28	0/473	0.51	0/639
51	R6	0.19	0/460	0.45	0/613
51	Y6	0.23	0/460	0.42	0/613
52	R7	0.23	0/417	0.45	0/550
52	Y7	0.26	0/426	0.48	0/561
53	R8	0.30	0/525	0.61	0/691
53	Y8	0.28	0/525	0.49	0/691
54	R9	0.18	0/310	0.37	0/407
54	Y9	0.22	0/310	0.38	0/407
All	All	0.21	2/312861 (0.0%)	0.43	65/467540 (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
1	XA	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	QB	0	17
2	XB	0	22
3	QC	0	16
3	XC	0	19
5	QE	0	5
5	XE	0	8
6	QF	0	5
7	QG	0	8
7	XG	0	8
8	QH	0	4
8	XH	0	5
9	QI	0	12
9	XI	0	11
10	QJ	0	12
10	XJ	0	9
11	QK	0	1
11	XK	0	4
12	QL	0	10
12	XL	0	10
13	QM	0	19
13	XM	0	15
14	QN	0	1
14	XN	0	7
15	QO	0	2
15	XO	0	2
16	QP	0	3
16	XP	0	4
17	QQ	0	3
17	XQ	0	4
18	QR	0	5
18	XR	0	3
19	QS	0	12
19	XS	0	21
20	QT	0	16
20	XT	0	12
21	QU	0	2
21	XU	0	2
26	RD	0	11
26	YD	0	8
27	RE	0	20
27	YE	0	7
28	RF	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
28	YF	0	14
29	RG	0	16
29	YG	0	13
30	RH	0	24
30	YH	0	2
31	RI	0	21
31	YI	0	22
32	RN	0	12
32	YN	0	10
33	RO	0	1
33	YO	0	1
34	RP	0	25
34	YP	0	8
35	RQ	0	14
35	YQ	0	13
36	RR	0	3
36	YR	0	5
37	RS	0	13
37	YS	0	9
38	RT	0	13
38	YT	0	11
39	RU	0	7
39	YU	0	2
40	RV	0	6
40	YV	0	6
41	RW	0	4
41	YW	0	3
42	RX	0	4
42	YX	0	2
43	RY	0	4
43	YY	0	4
44	RZ	0	20
44	YZ	0	16
45	R0	0	2
45	Y0	0	2
46	R1	0	7
46	Y1	0	8
47	R2	0	8
47	Y2	0	3
48	R3	0	1
48	Y3	0	2
49	R4	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
49	Y4	0	12
50	Y5	0	1
53	R8	0	12
53	Y8	0	1
54	R9	0	1
All	All	0	775

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	RZ	185	GLU	CA-C	5.52	1.60	1.52
1	XA	358	U	O4'-C1'	-5.45	1.33	1.41

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	XD	33	MET	N-CA-C	-13.14	93.72	114.09
44	RZ	186	GLU	N-CA-C	-12.42	97.24	111.03
4	XD	89	THR	N-CA-C	11.79	125.40	111.02
4	XD	34	GLU	N-CA-C	-10.54	100.55	113.41
1	XA	359	U	C6-N1-C1'	7.81	144.64	121.20

There are no chirality outliers.

5 of 775 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	15	VAL	Peptide
2	QB	19	HIS	Peptide
2	QB	21	ARG	Peptide
2	QB	22	LYS	Peptide
2	QB	34	ALA	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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16277	364	0
1	XA	32249	0	16278	390	0
2	QB	1907	0	1958	22	0
2	XB	1915	0	1969	25	0
3	QC	1605	0	1668	23	0
3	XC	1605	0	1668	28	0
4	QD	1703	0	1763	47	0
4	XD	1703	0	1763	38	0
5	QE	1155	0	1213	14	0
5	XE	1155	0	1213	9	0
6	QF	843	0	857	14	0
6	XF	843	0	857	9	0
7	QG	1257	0	1296	19	0
7	XG	1257	0	1296	20	0
8	QH	1108	0	1165	15	0
8	XH	1108	0	1165	21	0
9	QI	1010	0	1037	26	0
9	XI	998	0	1024	23	0
10	QJ	801	0	849	16	0
10	XJ	777	0	816	16	0
11	QK	885	0	904	15	0
11	XK	864	0	881	20	0
12	QL	975	0	1062	21	0
12	XL	956	0	1046	10	0
13	QM	955	0	1021	19	0
13	XM	946	0	1008	22	0
14	QN	492	0	529	10	0
14	XN	492	0	529	14	0
15	QO	734	0	771	8	0
15	XO	729	0	768	5	0
16	QP	705	0	725	13	0
16	XP	705	0	725	10	0
17	QQ	834	0	904	8	0
17	XQ	834	0	904	16	0
18	QR	574	0	644	8	0
18	XR	574	0	644	7	0
19	QS	665	0	686	17	0
19	XS	674	0	699	9	0
20	QT	763	0	861	15	0
20	XT	763	0	861	10	0
21	QU	217	0	234	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	XU	217	0	234	3	0
22	QV	365	0	186	4	0
22	XV	322	0	164	5	0
23	QX	217	0	110	4	0
23	XX	262	0	132	3	0
24	RA	62051	0	31280	492	0
24	YA	62091	0	31294	492	0
25	RB	2573	0	1306	19	0
25	YB	2573	0	1306	15	0
26	RD	2115	0	2195	37	0
26	YD	2115	0	2195	43	0
27	RE	1568	0	1634	31	0
27	YE	1563	0	1629	19	0
28	RF	1585	0	1632	19	0
28	YF	1585	0	1632	20	0
29	RG	1474	0	1535	32	0
29	YG	1474	0	1535	22	0
30	RH	1336	0	1418	12	0
30	YH	1330	0	1413	11	0
31	RI	1136	0	1223	7	0
31	YI	1136	0	1223	8	0
32	RN	1104	0	1180	13	0
32	YN	1104	0	1180	12	0
33	RO	933	0	996	22	0
33	YO	933	0	996	17	0
34	RP	1145	0	1227	15	0
34	YP	1122	0	1205	17	0
35	RQ	1122	0	1178	28	0
35	YQ	1122	0	1179	22	0
36	RR	960	0	1021	11	0
36	YR	960	0	1021	17	0
37	RS	882	0	943	17	0
37	YS	882	0	943	10	0
38	RT	1141	0	1202	19	0
38	YT	1141	0	1202	18	0
39	RU	964	0	1021	14	0
39	YU	964	0	1021	12	0
40	RV	779	0	852	6	0
40	YV	779	0	852	4	0
41	RW	900	0	964	9	0
41	YW	900	0	964	6	0
42	RX	725	0	778	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	YX	725	0	778	6	0
43	RY	818	0	909	11	0
43	YY	818	0	909	9	0
44	RZ	1601	0	1630	22	0
44	YZ	1601	0	1630	25	0
45	R0	603	0	620	7	0
45	Y0	599	0	617	5	0
46	R1	763	0	848	9	0
46	Y1	729	0	802	8	0
47	R2	581	0	629	7	0
47	Y2	575	0	624	9	0
48	R3	469	0	518	10	0
48	Y3	469	0	518	6	0
49	R4	565	0	557	9	0
49	Y4	565	0	557	11	0
50	R5	459	0	476	7	0
50	Y5	459	0	476	8	0
51	R6	453	0	473	6	0
51	Y6	453	0	473	7	0
52	R7	409	0	454	2	0
52	Y7	418	0	467	3	0
53	R8	517	0	582	12	0
53	Y8	517	0	582	9	0
54	R9	307	0	335	4	0
54	Y9	307	0	335	6	0
55	QA	74	0	0	0	0
55	QC	1	0	0	0	0
55	QF	1	0	0	0	0
55	QH	1	0	0	0	0
55	QM	1	0	0	0	0
55	R0	1	0	0	0	0
55	R1	2	0	0	0	0
55	R8	1	0	0	0	0
55	RA	487	0	0	0	0
55	RB	6	0	0	0	0
55	RE	4	0	0	0	0
55	RF	2	0	0	0	0
55	RI	1	0	0	0	0
55	RN	1	0	0	0	0
55	RO	1	0	0	0	0
55	RP	1	0	0	0	0
55	RQ	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	RR	2	0	0	0	0
55	RT	1	0	0	0	0
55	RX	1	0	0	0	0
55	RY	1	0	0	0	0
55	XA	92	0	0	0	0
55	XE	1	0	0	0	0
55	XK	1	0	0	0	0
55	XL	2	0	0	0	0
55	XM	2	0	0	0	0
55	XN	1	0	0	0	0
55	XQ	1	0	0	0	0
55	XS	1	0	0	0	0
55	Y0	2	0	0	0	0
55	Y1	1	0	0	0	0
55	Y5	1	0	0	0	0
55	Y7	1	0	0	0	0
55	Y8	2	0	0	0	0
55	YA	542	0	0	0	0
55	YB	15	0	0	0	0
55	YD	3	0	0	0	0
55	YE	3	0	0	0	0
55	YO	1	0	0	0	0
55	YQ	3	0	0	0	0
55	YR	2	0	0	0	0
55	YX	2	0	0	0	0
56	QD	8	0	0	0	0
56	XD	8	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
All	All	289311	0	196538	2739	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 2739 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)
35:RQ:51:ARG:NH2	44:RZ:186:GLU:OE1	1.59	1.34
24:RA:2135:A:N6	24:RA:2156:G:H21	1.54	1.05
47:Y2:65:ASN:O	47:Y2:69:ARG:HG3	1.55	1.05
35:YQ:52:VAL:HG13	44:YZ:183:LEU:CD1	1.88	1.03
24:RA:2135:A:H62	24:RA:2156:G:N2	1.57	1.02

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	211 (91%)	22 (9%)	0	100	100
2	XB	234/256 (91%)	213 (91%)	21 (9%)	0	100	100
3	QC	203/239 (85%)	185 (91%)	18 (9%)	0	100	100
3	XC	203/239 (85%)	191 (94%)	12 (6%)	0	100	100
4	QD	206/209 (99%)	185 (90%)	18 (9%)	3 (2%)	8	32
4	XD	206/209 (99%)	189 (92%)	15 (7%)	2 (1%)	12	41
5	QE	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
5	XE	149/162 (92%)	139 (93%)	10 (7%)	0	100	100
6	QF	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
7	QG	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
7	XG	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
8	QH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
8	XH	135/138 (98%)	130 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	QI	125/128 (98%)	117 (94%)	8 (6%)	0	100	100
9	XI	124/128 (97%)	112 (90%)	12 (10%)	0	100	100
10	QJ	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
10	XJ	94/105 (90%)	90 (96%)	4 (4%)	0	100	100
11	QK	117/129 (91%)	110 (94%)	7 (6%)	0	100	100
11	XK	114/129 (88%)	109 (96%)	5 (4%)	0	100	100
12	QL	123/132 (93%)	113 (92%)	10 (8%)	0	100	100
12	XL	120/132 (91%)	107 (89%)	13 (11%)	0	100	100
13	QM	118/126 (94%)	105 (89%)	12 (10%)	1 (1%)	16	47
13	XM	117/126 (93%)	103 (88%)	14 (12%)	0	100	100
14	QN	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
14	XN	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
15	QO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	XO	85/89 (96%)	85 (100%)	0	0	100	100
16	QP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
17	XQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
18	QR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
19	XS	82/93 (88%)	71 (87%)	11 (13%)	0	100	100
20	QT	97/106 (92%)	92 (95%)	5 (5%)	0	100	100
20	XT	97/106 (92%)	89 (92%)	8 (8%)	0	100	100
21	QU	23/27 (85%)	23 (100%)	0	0	100	100
21	XU	23/27 (85%)	23 (100%)	0	0	100	100
26	RD	270/276 (98%)	258 (96%)	12 (4%)	0	100	100
26	YD	270/276 (98%)	257 (95%)	13 (5%)	0	100	100
27	RE	203/206 (98%)	171 (84%)	32 (16%)	0	100	100
27	YE	202/206 (98%)	193 (96%)	9 (4%)	0	100	100
28	RF	200/210 (95%)	189 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	YF	200/210 (95%)	189 (94%)	11 (6%)	0	100	100
29	RG	179/182 (98%)	158 (88%)	21 (12%)	0	100	100
29	YG	179/182 (98%)	161 (90%)	17 (10%)	1 (1%)	21	52
30	RH	172/180 (96%)	153 (89%)	18 (10%)	1 (1%)	21	52
30	YH	171/180 (95%)	163 (95%)	8 (5%)	0	100	100
31	RI	144/148 (97%)	125 (87%)	19 (13%)	0	100	100
31	YI	144/148 (97%)	129 (90%)	15 (10%)	0	100	100
32	RN	136/140 (97%)	124 (91%)	12 (9%)	0	100	100
32	YN	136/140 (97%)	125 (92%)	11 (8%)	0	100	100
33	RO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
33	YO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
34	RP	148/150 (99%)	133 (90%)	15 (10%)	0	100	100
34	YP	145/150 (97%)	137 (94%)	7 (5%)	1 (1%)	18	49
35	RQ	139/141 (99%)	122 (88%)	16 (12%)	1 (1%)	18	49
35	YQ	139/141 (99%)	120 (86%)	19 (14%)	0	100	100
36	RR	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
36	YR	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
37	RS	109/112 (97%)	95 (87%)	14 (13%)	0	100	100
37	YS	109/112 (97%)	95 (87%)	14 (13%)	0	100	100
38	RT	135/146 (92%)	123 (91%)	10 (7%)	2 (2%)	8	32
38	YT	135/146 (92%)	118 (87%)	15 (11%)	2 (2%)	8	32
39	RU	115/118 (98%)	108 (94%)	6 (5%)	1 (1%)	14	44
39	YU	115/118 (98%)	112 (97%)	3 (3%)	0	100	100
40	RV	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
40	YV	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
41	RW	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
41	YW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
42	RX	90/96 (94%)	88 (98%)	2 (2%)	0	100	100
42	YX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
43	RY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
43	YY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	RZ	201/206 (98%)	182 (90%)	19 (10%)	0	100	100
44	YZ	201/206 (98%)	181 (90%)	20 (10%)	0	100	100
45	R0	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
45	Y0	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
46	R1	95/98 (97%)	84 (88%)	11 (12%)	0	100	100
46	Y1	91/98 (93%)	83 (91%)	8 (9%)	0	100	100
47	R2	67/72 (93%)	66 (98%)	1 (2%)	0	100	100
47	Y2	66/72 (92%)	63 (96%)	2 (3%)	1 (2%)	8	32
48	R3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
48	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
49	R4	67/71 (94%)	57 (85%)	10 (15%)	0	100	100
49	Y4	67/71 (94%)	54 (81%)	13 (19%)	0	100	100
50	R5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
50	Y5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
51	R6	51/54 (94%)	51 (100%)	0	0	100	100
51	Y6	51/54 (94%)	51 (100%)	0	0	100	100
52	R7	45/49 (92%)	45 (100%)	0	0	100	100
52	Y7	46/49 (94%)	46 (100%)	0	0	100	100
53	R8	62/65 (95%)	49 (79%)	13 (21%)	0	100	100
53	Y8	62/65 (95%)	62 (100%)	0	0	100	100
54	R9	35/37 (95%)	35 (100%)	0	0	100	100
54	Y9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11484/12128 (95%)	10666 (93%)	802 (7%)	16 (0%)	48	78

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	QD	155	LEU
38	RT	124	ASP
4	XD	155	LEU
4	XD	171	GLY
34	YP	63	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	
2	QB	203/220 (92%)	203 (100%)	0	100	100
2	XB	204/220 (93%)	203 (100%)	1 (0%)	81	85
3	QC	159/188 (85%)	158 (99%)	1 (1%)	78	83
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	180/181 (99%)	176 (98%)	4 (2%)	45	71
4	XD	180/181 (99%)	178 (99%)	2 (1%)	65	78
5	QE	116/123 (94%)	115 (99%)	1 (1%)	70	80
5	XE	116/123 (94%)	116 (100%)	0	100	100
6	QF	90/90 (100%)	89 (99%)	1 (1%)	65	78
6	XF	90/90 (100%)	89 (99%)	1 (1%)	65	78
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	118/119 (99%)	118 (100%)	0	100	100
8	XH	118/119 (99%)	116 (98%)	2 (2%)	53	74
9	QI	98/99 (99%)	98 (100%)	0	100	100
9	XI	97/99 (98%)	95 (98%)	2 (2%)	47	71
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	104 (100%)	0	100	100
12	XL	103/109 (94%)	103 (100%)	0	100	100
13	QM	96/101 (95%)	96 (100%)	0	100	100
13	XM	95/101 (94%)	95 (100%)	0	100	100
14	QN	49/50 (98%)	49 (100%)	0	100	100
14	XN	49/50 (98%)	48 (98%)	1 (2%)	48	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	95 (100%)	0	100	100
17	XQ	95/97 (98%)	94 (99%)	1 (1%)	65	78
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	72 (100%)	0	100	100
19	XS	73/80 (91%)	72 (99%)	1 (1%)	59	76
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
26	RD	214/218 (98%)	214 (100%)	0	100	100
26	YD	214/218 (98%)	214 (100%)	0	100	100
27	RE	165/166 (99%)	164 (99%)	1 (1%)	78	83
27	YE	165/166 (99%)	164 (99%)	1 (1%)	78	83
28	RF	161/166 (97%)	161 (100%)	0	100	100
28	YF	161/166 (97%)	161 (100%)	0	100	100
29	RG	155/156 (99%)	155 (100%)	0	100	100
29	YG	155/156 (99%)	154 (99%)	1 (1%)	78	83
30	RH	145/148 (98%)	142 (98%)	3 (2%)	47	71
30	YH	144/148 (97%)	142 (99%)	2 (1%)	59	76
31	RI	122/124 (98%)	121 (99%)	1 (1%)	73	81
31	YI	122/124 (98%)	120 (98%)	2 (2%)	55	75
32	RN	117/119 (98%)	116 (99%)	1 (1%)	70	80
32	YN	117/119 (98%)	116 (99%)	1 (1%)	70	80
33	RO	100/100 (100%)	100 (100%)	0	100	100
33	YO	100/100 (100%)	100 (100%)	0	100	100
34	RP	116/116 (100%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	YP	114/116 (98%)	114 (100%)	0	100	100
35	RQ	111/111 (100%)	110 (99%)	1 (1%)	70	80
35	YQ	111/111 (100%)	108 (97%)	3 (3%)	39	67
36	RR	100/101 (99%)	100 (100%)	0	100	100
36	YR	100/101 (99%)	100 (100%)	0	100	100
37	RS	87/88 (99%)	87 (100%)	0	100	100
37	YS	87/88 (99%)	87 (100%)	0	100	100
38	RT	120/127 (94%)	119 (99%)	1 (1%)	73	81
38	YT	120/127 (94%)	120 (100%)	0	100	100
39	RU	93/94 (99%)	93 (100%)	0	100	100
39	YU	93/94 (99%)	93 (100%)	0	100	100
40	RV	82/82 (100%)	82 (100%)	0	100	100
40	YV	82/82 (100%)	82 (100%)	0	100	100
41	RW	92/92 (100%)	92 (100%)	0	100	100
41	YW	92/92 (100%)	92 (100%)	0	100	100
42	RX	74/78 (95%)	74 (100%)	0	100	100
42	YX	74/78 (95%)	72 (97%)	2 (3%)	39	67
43	RY	88/91 (97%)	88 (100%)	0	100	100
43	YY	88/91 (97%)	88 (100%)	0	100	100
44	RZ	174/179 (97%)	172 (99%)	2 (1%)	65	78
44	YZ	174/179 (97%)	171 (98%)	3 (2%)	53	74
45	R0	61/67 (91%)	61 (100%)	0	100	100
45	Y0	61/67 (91%)	61 (100%)	0	100	100
46	R1	82/83 (99%)	82 (100%)	0	100	100
46	Y1	78/83 (94%)	78 (100%)	0	100	100
47	R2	64/67 (96%)	64 (100%)	0	100	100
47	Y2	64/67 (96%)	62 (97%)	2 (3%)	35	64
48	R3	51/52 (98%)	51 (100%)	0	100	100
48	Y3	51/52 (98%)	51 (100%)	0	100	100
49	R4	62/63 (98%)	62 (100%)	0	100	100
49	Y4	62/63 (98%)	62 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	R5	51/52 (98%)	51 (100%)	0	100	100
50	Y5	51/52 (98%)	50 (98%)	1 (2%)	48	72
51	R6	51/52 (98%)	51 (100%)	0	100	100
51	Y6	51/52 (98%)	51 (100%)	0	100	100
52	R7	40/42 (95%)	40 (100%)	0	100	100
52	Y7	41/42 (98%)	41 (100%)	0	100	100
53	R8	54/55 (98%)	54 (100%)	0	100	100
53	Y8	54/55 (98%)	53 (98%)	1 (2%)	50	73
54	R9	34/34 (100%)	34 (100%)	0	100	100
54	Y9	34/34 (100%)	34 (100%)	0	100	100
All	All	9706/10066 (96%)	9659 (100%)	47 (0%)	81	85

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	YE	75	VAL
35	YQ	21	THR
29	YG	112	PRO
31	YI	9	LEU
35	YQ	96	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
6	XF	16	GLN
38	YT	2	ASN
17	XQ	93	GLN
36	YR	71	GLN
33	YO	89	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1521 (98%)	275 (18%)	34 (2%)
1	XA	1499/1521 (98%)	278 (18%)	35 (2%)
22	QV	16/17 (94%)	1 (6%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	XV	14/17 (82%)	2 (14%)	0
23	QX	9/19 (47%)	4 (44%)	1 (11%)
23	XX	11/19 (57%)	5 (45%)	0
24	RA	2877/2915 (98%)	547 (19%)	37 (1%)
24	YA	2880/2915 (98%)	529 (18%)	41 (1%)
25	RB	119/122 (97%)	17 (14%)	1 (0%)
25	YB	119/122 (97%)	16 (13%)	1 (0%)
All	All	9042/9188 (98%)	1674 (18%)	150 (1%)

5 of 1674 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	32	A
1	QA	39	G
1	QA	48	C

5 of 150 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	YA	404	C
24	YA	2610	C
24	YA	827	U
24	YA	1210	A
24	RA	846	C

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

2 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	$\# Z > 2$
22	1MG	XV	37	22	23,26,27	1.21	3 (13%)	33,39,42	1.70	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	1MG	QV	37	22	23,26,27	1.21	3 (13%)	33,39,42	1.70	5 (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
22	1MG	XV	37	22	-	0/7/25/26	0/3/3/3
22	1MG	QV	37	22	-	1/7/25/26	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	XV	37	1MG	C5-C4	3.27	1.47	1.38
22	QV	37	1MG	C5-C4	3.26	1.47	1.38
22	XV	37	1MG	C2-N1	2.49	1.41	1.37
22	QV	37	1MG	C2-N1	2.42	1.41	1.37
22	QV	37	1MG	C5-N7	-2.28	1.34	1.39

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	XV	37	1MG	C5-C4-N3	-5.50	119.64	128.39
22	QV	37	1MG	C5-C4-N3	-5.44	119.73	128.39
22	XV	37	1MG	C2-N3-C4	4.43	121.94	111.98
22	QV	37	1MG	C2-N3-C4	4.33	121.70	111.98
22	QV	37	1MG	N9-C4-N3	4.26	134.47	125.95

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	QV	37	1MG	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1285 ligands modelled in this entry, 1283 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	$\# Z > 2$
56	SF4	QD	301	4	0,12,12	-	-	-		
56	SF4	XD	301	4	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
56	SF4	QD	301	4	-	-	0/6/5/5
56	SF4	XD	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1521 (98%)	0.92	169 (11%) 10 5	50, 97, 229, 320	0
1	XA	1500/1521 (98%)	0.89	160 (10%) 11 6	39, 106, 235, 312	0
2	QB	235/256 (91%)	1.25	39 (16%) 4 2	85, 129, 170, 195	0
2	XB	236/256 (92%)	1.28	49 (20%) 2 1	82, 131, 169, 192	0
3	QC	205/239 (85%)	1.07	28 (13%) 6 4	95, 138, 177, 204	0
3	XC	205/239 (85%)	1.35	45 (21%) 2 1	90, 138, 168, 190	0
4	QD	208/209 (99%)	1.49	48 (23%) 2 1	61, 98, 133, 193	0
4	XD	208/209 (99%)	1.41	49 (23%) 2 1	69, 106, 152, 176	0
5	QE	151/162 (93%)	0.76	10 (6%) 24 13	60, 92, 124, 151	0
5	XE	151/162 (93%)	0.94	18 (11%) 9 5	56, 98, 139, 156	0
6	QF	101/101 (100%)	0.97	6 (5%) 28 15	68, 97, 125, 161	0
6	XF	101/101 (100%)	1.00	8 (7%) 18 10	59, 94, 133, 164	0
7	QG	155/156 (99%)	1.10	17 (10%) 10 5	110, 139, 174, 189	0
7	XG	155/156 (99%)	1.31	28 (18%) 3 1	94, 128, 172, 184	0
8	QH	137/138 (99%)	0.73	9 (6%) 24 13	61, 96, 122, 154	0
8	XH	137/138 (99%)	1.12	17 (12%) 8 5	61, 98, 131, 159	0
9	QI	127/128 (99%)	2.05	56 (44%) 0 0	92, 159, 200, 238	0
9	XI	126/128 (98%)	1.72	45 (35%) 1 0	94, 146, 176, 192	0
10	QJ	99/105 (94%)	1.77	33 (33%) 1 0	124, 158, 194, 209	0
10	XJ	96/105 (91%)	1.70	33 (34%) 1 0	122, 157, 190, 205	0
11	QK	119/129 (92%)	1.15	14 (11%) 9 5	72, 98, 147, 173	0
11	XK	116/129 (89%)	1.00	15 (12%) 7 4	65, 96, 128, 163	0
12	QL	125/132 (94%)	1.04	21 (16%) 4 2	53, 80, 122, 157	0
12	XL	122/132 (92%)	1.04	19 (15%) 5 2	53, 85, 117, 146	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)		Q<0.9
13	QM	120/126 (95%)	1.72	43 (35%)	1	0	111, 161, 206, 235
13	XM	119/126 (94%)	1.80	42 (35%)	1	0	132, 169, 201, 218
14	QN	60/61 (98%)	1.89	20 (33%)	1	0	108, 134, 170, 201
14	XN	60/61 (98%)	2.13	30 (50%)	0	0	100, 145, 177, 197
15	QO	88/89 (98%)	1.12	15 (17%)	4	2	53, 94, 130, 159
15	XO	87/89 (97%)	0.99	7 (8%)	18	10	55, 88, 131, 170
16	QP	84/88 (95%)	1.47	20 (23%)	2	1	73, 91, 131, 156
16	XP	84/88 (95%)	1.67	24 (28%)	1	1	79, 105, 141, 161
17	QQ	100/105 (95%)	0.88	8 (8%)	18	10	57, 87, 113, 135
17	XQ	100/105 (95%)	0.86	9 (9%)	15	8	52, 90, 128, 152
18	QR	70/88 (79%)	0.76	6 (8%)	16	9	62, 91, 132, 144
18	XR	70/88 (79%)	0.70	5 (7%)	22	12	60, 96, 131, 149
19	QS	83/93 (89%)	1.29	15 (18%)	3	1	138, 170, 202, 219
19	XS	84/93 (90%)	1.72	34 (40%)	0	0	137, 180, 217, 231
20	QT	99/106 (93%)	1.40	26 (26%)	1	1	55, 93, 139, 151
20	XT	99/106 (93%)	1.46	25 (25%)	1	1	67, 103, 157, 177
21	QU	25/27 (92%)	3.33	18 (72%)	0	0	133, 146, 174, 182
21	XU	25/27 (92%)	1.88	10 (40%)	1	0	120, 142, 174, 181
22	QV	16/17 (94%)	1.12	3 (18%)	3	1	105, 127, 175, 197
22	XV	14/17 (82%)	1.29	3 (21%)	2	1	103, 121, 154, 155
23	QX	10/19 (52%)	2.95	6 (60%)	0	0	93, 176, 229, 247
23	XX	12/19 (63%)	3.27	11 (91%)	0	0	120, 193, 254, 256
24	RA	2881/2915 (98%)	0.45	170 (5%)	28	15	32, 65, 205, 394
24	YA	2883/2915 (98%)	0.21	141 (4%)	35	18	22, 44, 207, 343
25	RB	120/122 (98%)	0.95	9 (7%)	20	11	67, 107, 159, 188
25	YB	120/122 (98%)	0.33	2 (1%)	69	48	45, 66, 96, 138
26	RD	272/276 (98%)	0.83	21 (7%)	19	10	28, 58, 94, 126
26	YD	272/276 (98%)	0.63	20 (7%)	20	11	25, 45, 78, 96
27	RE	205/206 (99%)	0.98	29 (14%)	6	3	33, 66, 126, 185
27	YE	204/206 (99%)	0.32	2 (0%)	79	61	20, 47, 87, 112
28	RF	202/210 (96%)	0.95	23 (11%)	10	5	37, 73, 128, 160

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	YF	202/210 (96%)	0.67	13 (6%)	25	14	25, 51, 108, 157	0
29	RG	181/182 (99%)	1.86	63 (34%)	1	0	103, 153, 199, 220	0
29	YG	181/182 (99%)	1.19	27 (14%)	5	3	65, 110, 161, 181	0
30	RH	174/180 (96%)	1.37	34 (19%)	3	1	89, 120, 155, 214	0
30	YH	173/180 (96%)	0.45	6 (3%)	47	27	33, 61, 92, 139	0
31	RI	146/148 (98%)	1.38	34 (23%)	2	1	54, 108, 140, 171	0
31	YI	146/148 (98%)	0.97	29 (19%)	3	1	48, 99, 135, 173	0
32	RN	138/140 (98%)	1.04	18 (13%)	7	4	41, 74, 122, 137	0
32	YN	138/140 (98%)	0.71	12 (8%)	16	9	25, 50, 104, 145	0
33	RO	122/122 (100%)	0.71	8 (6%)	24	13	37, 66, 97, 141	0
33	YO	122/122 (100%)	0.37	5 (4%)	41	23	28, 50, 82, 125	0
34	RP	150/150 (100%)	1.20	28 (18%)	3	1	43, 84, 133, 195	0
34	YP	147/150 (98%)	0.77	13 (8%)	15	9	27, 56, 92, 119	0
35	RQ	141/141 (100%)	1.23	30 (21%)	2	1	45, 81, 129, 170	0
35	YQ	141/141 (100%)	1.08	27 (19%)	3	1	28, 54, 100, 192	0
36	RR	117/118 (99%)	1.20	20 (17%)	4	2	39, 64, 101, 131	0
36	YR	117/118 (99%)	0.59	4 (3%)	48	28	25, 45, 77, 100	0
37	RS	111/112 (99%)	1.92	43 (38%)	1	0	77, 108, 160, 176	0
37	YS	111/112 (99%)	1.02	21 (18%)	3	1	44, 66, 108, 147	0
38	RT	137/146 (93%)	0.89	17 (12%)	8	5	43, 73, 143, 181	0
38	YT	137/146 (93%)	0.69	13 (9%)	14	7	34, 58, 117, 154	0
39	RU	117/118 (99%)	0.85	14 (11%)	9	5	37, 67, 115, 148	0
39	YU	117/118 (99%)	0.37	5 (4%)	40	22	22, 40, 74, 173	0
40	RV	101/101 (100%)	0.51	4 (3%)	42	23	38, 80, 114, 142	0
40	YV	101/101 (100%)	0.15	1 (0%)	79	61	17, 47, 96, 120	0
41	RW	113/113 (100%)	0.43	4 (3%)	47	27	33, 58, 97, 185	0
41	YW	113/113 (100%)	0.21	1 (0%)	81	63	22, 37, 90, 167	0
42	RX	92/96 (95%)	0.53	6 (6%)	25	13	48, 64, 106, 121	0
42	YX	92/96 (95%)	0.58	6 (6%)	25	13	27, 46, 76, 114	0
43	RY	107/110 (97%)	1.29	26 (24%)	2	1	56, 88, 119, 160	0
43	YY	107/110 (97%)	0.51	7 (6%)	25	13	26, 60, 96, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RZ	203/206 (98%)	1.43	41 (20%) 3 1	71, 110, 144, 180	0
44	YZ	203/206 (98%)	0.76	18 (8%) 15 8	47, 78, 123, 141	0
45	R0	76/85 (89%)	0.92	8 (10%) 11 6	52, 77, 104, 126	0
45	Y0	75/85 (88%)	0.52	3 (4%) 42 23	29, 47, 75, 94	0
46	R1	97/98 (98%)	1.19	22 (22%) 2 1	35, 67, 124, 164	0
46	Y1	93/98 (94%)	0.75	13 (13%) 6 4	25, 50, 107, 161	0
47	R2	69/72 (95%)	0.77	6 (8%) 16 9	48, 90, 130, 169	0
47	Y2	68/72 (94%)	0.88	9 (13%) 7 4	34, 57, 112, 165	0
48	R3	59/60 (98%)	0.69	1 (1%) 69 48	42, 71, 123, 191	0
48	Y3	59/60 (98%)	0.39	5 (8%) 16 9	24, 43, 81, 131	0
49	R4	69/71 (97%)	1.47	18 (26%) 1 1	126, 182, 219, 233	0
49	Y4	69/71 (97%)	1.32	14 (20%) 3 1	110, 163, 226, 241	0
50	R5	59/60 (98%)	1.00	9 (15%) 5 3	35, 57, 105, 118	0
50	Y5	59/60 (98%)	0.24	1 (1%) 69 48	16, 43, 90, 117	0
51	R6	53/54 (98%)	0.35	1 (1%) 66 45	48, 70, 98, 116	0
51	Y6	53/54 (98%)	0.21	1 (1%) 66 45	36, 53, 79, 87	0
52	R7	47/49 (95%)	0.63	6 (12%) 7 4	32, 48, 84, 94	0
52	Y7	48/49 (97%)	0.42	3 (6%) 26 14	24, 36, 73, 130	0
53	R8	64/65 (98%)	1.81	24 (37%) 1 0	30, 66, 120, 167	0
53	Y8	64/65 (98%)	0.37	2 (3%) 51 30	27, 43, 63, 96	0
54	R9	37/37 (100%)	0.97	3 (8%) 18 10	53, 82, 103, 142	0
54	Y9	37/37 (100%)	0.48	3 (8%) 18 10	31, 48, 74, 76	0
All	All	20736/21316 (97%)	0.82	2483 (11%) 9 5	16, 80, 183, 394	0

The worst 5 of 2483 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	QK	128	ALA	10.2
4	XD	130	GLY	8.9
29	RG	135	LEU	8.4
14	QN	2	ALA	8.3
53	R8	62	LEU	8.2

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
22	1MG	XV	37	24/25	0.84	0.13	102,113,116,117	0
22	1MG	QV	37	24/25	0.89	0.11	62,93,101,103	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(Å ²)	Q<0.9
55	MG	XA	1651	1/1	0.17	0.33	103,103,103,103	0
55	MG	YA	3361	1/1	0.27	0.20	152,152,152,152	0
55	MG	YA	3346	1/1	0.45	0.25	74,74,74,74	0
55	MG	RA	3418	1/1	0.46	0.26	74,74,74,74	0
55	MG	RA	3179	1/1	0.46	0.23	85,85,85,85	0
55	MG	YD	301	1/1	0.46	0.43	74,74,74,74	0
55	MG	YB	210	1/1	0.48	0.35	94,94,94,94	0
55	MG	XA	1664	1/1	0.50	0.18	150,150,150,150	0
55	MG	XM	202	1/1	0.55	0.33	79,79,79,79	0
55	MG	RA	3186	1/1	0.59	0.18	71,71,71,71	0
55	MG	QA	1623	1/1	0.60	0.22	82,82,82,82	0
55	MG	YA	3486	1/1	0.60	0.26	84,84,84,84	0
55	MG	QA	1656	1/1	0.60	0.38	91,91,91,91	0
55	MG	XA	1656	1/1	0.60	0.33	134,134,134,134	0
55	MG	RA	3197	1/1	0.61	0.20	65,65,65,65	0
55	MG	YA	3362	1/1	0.62	0.29	104,104,104,104	0
55	MG	RA	3195	1/1	0.63	0.12	83,83,83,83	0
55	MG	XA	1668	1/1	0.64	0.32	74,74,74,74	0
55	MG	RA	3385	1/1	0.65	0.28	83,83,83,83	0
55	MG	YB	209	1/1	0.65	0.23	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3201	1/1	0.65	0.39	82,82,82,82	0
55	MG	YA	3397	1/1	0.65	0.15	83,83,83,83	0
55	MG	RA	3453	1/1	0.66	0.18	73,73,73,73	0
55	MG	QM	201	1/1	0.66	0.14	110,110,110,110	0
55	MG	RA	3083	1/1	0.67	0.22	50,50,50,50	0
55	MG	RA	3439	1/1	0.67	0.17	59,59,59,59	0
55	MG	QA	1645	1/1	0.68	0.12	61,61,61,61	0
55	MG	YA	3232	1/1	0.68	0.33	70,70,70,70	0
55	MG	YA	3245	1/1	0.69	0.24	82,82,82,82	0
55	MG	YO	201	1/1	0.69	0.19	90,90,90,90	0
55	MG	RA	3257	1/1	0.70	0.12	54,54,54,54	0
55	MG	RA	3417	1/1	0.70	0.24	72,72,72,72	0
55	MG	RA	3370	1/1	0.70	0.19	47,47,47,47	0
55	MG	RA	3208	1/1	0.71	0.21	81,81,81,81	0
55	MG	RA	3155	1/1	0.71	0.24	61,61,61,61	0
55	MG	RA	3442	1/1	0.71	0.24	77,77,77,77	0
55	MG	RA	3339	1/1	0.71	0.16	80,80,80,80	0
55	MG	YA	3394	1/1	0.72	0.18	57,57,57,57	0
55	MG	YA	3188	1/1	0.72	0.19	45,45,45,45	0
55	MG	RA	3298	1/1	0.72	0.31	69,69,69,69	0
55	MG	RA	3309	1/1	0.72	0.34	75,75,75,75	0
55	MG	RA	3327	1/1	0.72	0.09	76,76,76,76	0
55	MG	RA	3262	1/1	0.72	0.25	63,63,63,63	0
55	MG	YA	3187	1/1	0.72	0.22	59,59,59,59	0
57	ZN	Y4	101	1/1	0.72	0.10	284,284,284,284	0
55	MG	XA	1683	1/1	0.73	0.13	159,159,159,159	0
55	MG	YA	3210	1/1	0.73	0.14	43,43,43,43	0
55	MG	YA	3219	1/1	0.73	0.20	50,50,50,50	0
55	MG	QA	1641	1/1	0.73	0.23	67,67,67,67	0
55	MG	RA	3153	1/1	0.73	0.14	64,64,64,64	0
55	MG	YA	3412	1/1	0.73	0.40	55,55,55,55	0
55	MG	YA	3356	1/1	0.74	0.17	102,102,102,102	0
55	MG	YA	3511	1/1	0.74	0.28	59,59,59,59	0
55	MG	QA	1640	1/1	0.74	0.17	83,83,83,83	0
55	MG	RA	3386	1/1	0.74	0.23	60,60,60,60	0
55	MG	YB	212	1/1	0.74	0.17	27,27,27,27	0
55	MG	YA	3014	1/1	0.74	0.16	39,39,39,39	0
55	MG	RA	3407	1/1	0.74	0.20	60,60,60,60	0
55	MG	RA	3207	1/1	0.74	0.34	65,65,65,65	0
55	MG	QA	1667	1/1	0.75	0.22	80,80,80,80	0
55	MG	RA	3313	1/1	0.75	0.19	50,50,50,50	0
55	MG	RA	3411	1/1	0.75	0.11	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3527	1/1	0.76	0.25	53,53,53,53	0
55	MG	RA	3452	1/1	0.76	0.14	82,82,82,82	0
55	MG	RA	3123	1/1	0.76	0.16	44,44,44,44	0
55	MG	XA	1637	1/1	0.76	0.17	118,118,118,118	0
55	MG	RA	3152	1/1	0.76	0.12	19,19,19,19	0
55	MG	YE	303	1/1	0.76	0.27	92,92,92,92	0
55	MG	YA	3493	1/1	0.76	0.30	77,77,77,77	0
55	MG	RA	3055	1/1	0.76	0.09	64,64,64,64	0
55	MG	YA	3425	1/1	0.77	0.19	59,59,59,59	0
55	MG	YA	3481	1/1	0.77	0.08	56,56,56,56	0
55	MG	RA	3067	1/1	0.77	0.11	40,40,40,40	0
55	MG	XA	1680	1/1	0.77	0.13	62,62,62,62	0
55	MG	RA	3180	1/1	0.77	0.12	66,66,66,66	0
55	MG	RF	302	1/1	0.77	0.29	55,55,55,55	0
55	MG	YA	3528	1/1	0.77	0.25	44,44,44,44	0
55	MG	YB	206	1/1	0.77	0.18	72,72,72,72	0
55	MG	RQ	202	1/1	0.77	0.20	60,60,60,60	0
55	MG	RA	3140	1/1	0.77	0.20	48,48,48,48	0
55	MG	YA	3389	1/1	0.77	0.20	62,62,62,62	0
55	MG	QH	201	1/1	0.77	0.18	69,69,69,69	0
55	MG	RA	3115	1/1	0.77	0.18	53,53,53,53	0
55	MG	RA	3120	1/1	0.77	0.25	73,73,73,73	0
55	MG	YA	3423	1/1	0.77	0.23	55,55,55,55	0
55	MG	YA	3453	1/1	0.78	0.17	48,48,48,48	0
55	MG	YA	3472	1/1	0.78	0.12	51,51,51,51	0
55	MG	RA	3437	1/1	0.78	0.13	49,49,49,49	0
55	MG	QA	1666	1/1	0.78	0.21	58,58,58,58	0
55	MG	YA	3266	1/1	0.78	0.11	34,34,34,34	0
55	MG	YA	3305	1/1	0.78	0.30	71,71,71,71	0
55	MG	RA	3305	1/1	0.78	0.14	57,57,57,57	0
55	MG	RA	3364	1/1	0.78	0.13	62,62,62,62	0
55	MG	YA	3539	1/1	0.78	0.34	77,77,77,77	0
55	MG	RA	3416	1/1	0.78	0.17	57,57,57,57	0
55	MG	RA	3454	1/1	0.78	0.11	65,65,65,65	0
55	MG	RA	3455	1/1	0.78	0.24	74,74,74,74	0
55	MG	YA	3151	1/1	0.78	0.32	56,56,56,56	0
55	MG	RA	3191	1/1	0.78	0.34	43,43,43,43	0
55	MG	QA	1652	1/1	0.78	0.12	87,87,87,87	0
55	MG	RA	3421	1/1	0.78	0.22	53,53,53,53	0
55	MG	RA	3431	1/1	0.78	0.23	47,47,47,47	0
55	MG	YA	3204	1/1	0.79	0.15	60,60,60,60	0
55	MG	YA	3205	1/1	0.79	0.15	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3510	1/1	0.79	0.22	52,52,52,52	0
55	MG	YA	3380	1/1	0.79	0.17	67,67,67,67	0
55	MG	YA	3524	1/1	0.79	0.20	43,43,43,43	0
55	MG	YA	3381	1/1	0.79	0.12	83,83,83,83	0
55	MG	QA	1648	1/1	0.79	0.08	53,53,53,53	0
55	MG	YA	3008	1/1	0.79	0.11	42,42,42,42	0
55	MG	RA	3027	1/1	0.79	0.25	46,46,46,46	0
55	MG	RA	3333	1/1	0.79	0.13	61,61,61,61	0
55	MG	YA	3181	1/1	0.79	0.18	37,37,37,37	0
55	MG	RA	3127	1/1	0.79	0.37	88,88,88,88	0
55	MG	YA	3339	1/1	0.79	0.21	27,27,27,27	0
55	MG	RA	3438	1/1	0.79	0.15	57,57,57,57	0
55	MG	YA	3201	1/1	0.79	0.44	54,54,54,54	0
55	MG	YQ	202	1/1	0.79	0.21	97,97,97,97	0
55	MG	YA	3483	1/1	0.79	0.09	49,49,49,49	0
55	MG	YA	3379	1/1	0.80	0.10	17,17,17,17	0
55	MG	YA	3502	1/1	0.80	0.33	55,55,55,55	0
55	MG	YA	3504	1/1	0.80	0.19	53,53,53,53	0
55	MG	YA	3507	1/1	0.80	0.24	59,59,59,59	0
55	MG	RA	3350	1/1	0.80	0.19	76,76,76,76	0
55	MG	RA	3061	1/1	0.80	0.09	29,29,29,29	0
55	MG	YA	3011	1/1	0.80	0.16	31,31,31,31	0
55	MG	RA	3441	1/1	0.80	0.09	47,47,47,47	0
55	MG	YA	3260	1/1	0.80	0.21	61,61,61,61	0
55	MG	XA	1643	1/1	0.80	0.13	70,70,70,70	0
55	MG	RA	3157	1/1	0.80	0.19	30,30,30,30	0
55	MG	RA	3293	1/1	0.80	0.27	54,54,54,54	0
55	MG	YA	3450	1/1	0.80	0.13	71,71,71,71	0
55	MG	YA	3342	1/1	0.80	0.16	45,45,45,45	0
55	MG	RA	3199	1/1	0.80	0.11	46,46,46,46	0
55	MG	YA	3474	1/1	0.80	0.43	56,56,56,56	0
55	MG	RA	3392	1/1	0.80	0.13	46,46,46,46	0
55	MG	RA	3246	1/1	0.80	0.25	46,46,46,46	0
55	MG	RA	3486	1/1	0.80	0.17	51,51,51,51	0
55	MG	YA	3284	1/1	0.81	0.12	58,58,58,58	0
55	MG	YA	3475	1/1	0.81	0.27	44,44,44,44	0
55	MG	YA	3296	1/1	0.81	0.17	49,49,49,49	0
55	MG	RA	3429	1/1	0.81	0.14	71,71,71,71	0
55	MG	RA	3323	1/1	0.81	0.17	53,53,53,53	0
55	MG	YA	3058	1/1	0.81	0.19	32,32,32,32	0
55	MG	YA	3112	1/1	0.81	0.33	31,31,31,31	0
55	MG	YA	3348	1/1	0.81	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3506	1/1	0.81	0.27	84,84,84,84	0
55	MG	YA	3143	1/1	0.81	0.12	24,24,24,24	0
55	MG	YA	3150	1/1	0.81	0.34	58,58,58,58	0
55	MG	XA	1610	1/1	0.81	0.13	81,81,81,81	0
55	MG	YA	3377	1/1	0.81	0.07	62,62,62,62	0
55	MG	RA	3297	1/1	0.81	0.20	35,35,35,35	0
55	MG	QA	1633	1/1	0.81	0.12	44,44,44,44	0
55	MG	RA	3394	1/1	0.81	0.15	45,45,45,45	0
55	MG	RA	3396	1/1	0.81	0.17	48,48,48,48	0
55	MG	XA	1659	1/1	0.81	0.17	54,54,54,54	0
55	MG	RA	3135	1/1	0.81	0.15	35,35,35,35	0
55	MG	RA	3268	1/1	0.81	0.17	72,72,72,72	0
55	MG	RA	3363	1/1	0.81	0.14	62,62,62,62	0
55	MG	RA	3311	1/1	0.81	0.21	64,64,64,64	0
55	MG	XA	1690	1/1	0.81	0.12	102,102,102,102	0
55	MG	RA	3254	1/1	0.81	0.19	47,47,47,47	0
55	MG	Y1	101	1/1	0.81	0.16	45,45,45,45	0
55	MG	RA	3372	1/1	0.81	0.22	48,48,48,48	0
55	MG	RA	3475	1/1	0.82	0.24	40,40,40,40	0
55	MG	XA	1678	1/1	0.82	0.16	47,47,47,47	0
55	MG	RA	3352	1/1	0.82	0.34	80,80,80,80	0
55	MG	QA	1635	1/1	0.82	0.26	49,49,49,49	0
55	MG	RA	3286	1/1	0.82	0.28	55,55,55,55	0
55	MG	XA	1691	1/1	0.82	0.43	127,127,127,127	0
55	MG	XL	202	1/1	0.82	0.10	63,63,63,63	0
55	MG	QA	1626	1/1	0.82	0.19	59,59,59,59	0
55	MG	YA	3221	1/1	0.82	0.42	71,71,71,71	0
55	MG	QA	1668	1/1	0.82	0.14	31,31,31,31	0
55	MG	XA	1639	1/1	0.82	0.08	68,68,68,68	0
55	MG	QA	1625	1/1	0.82	0.16	60,60,60,60	0
55	MG	YA	3422	1/1	0.82	0.24	75,75,75,75	0
55	MG	XA	1650	1/1	0.82	0.09	108,108,108,108	0
55	MG	YA	3267	1/1	0.82	0.18	43,43,43,43	0
55	MG	QA	1643	1/1	0.82	0.09	43,43,43,43	0
55	MG	YA	3293	1/1	0.82	0.24	40,40,40,40	0
55	MG	YA	3113	1/1	0.82	0.14	41,41,41,41	0
55	MG	RA	3347	1/1	0.82	0.08	40,40,40,40	0
55	MG	RA	3092	1/1	0.82	0.12	34,34,34,34	0
55	MG	RA	3466	1/1	0.82	0.14	47,47,47,47	0
55	MG	YA	3163	1/1	0.82	0.11	32,32,32,32	0
55	MG	YA	3158	1/1	0.83	0.19	56,56,56,56	0
55	MG	YA	3390	1/1	0.83	0.13	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1689	1/1	0.83	0.19	74,74,74,74	0
55	MG	RA	3425	1/1	0.83	0.17	50,50,50,50	0
55	MG	RA	3401	1/1	0.83	0.16	43,43,43,43	0
55	MG	RA	3150	1/1	0.83	0.19	45,45,45,45	0
55	MG	RA	3410	1/1	0.83	0.10	32,32,32,32	0
55	MG	RA	3171	1/1	0.83	0.13	51,51,51,51	0
55	MG	YA	3434	1/1	0.83	0.31	56,56,56,56	0
55	MG	YA	3446	1/1	0.83	0.10	40,40,40,40	0
55	MG	XA	1655	1/1	0.83	0.27	113,113,113,113	0
55	MG	RA	3485	1/1	0.83	0.28	43,43,43,43	0
55	MG	YA	3465	1/1	0.83	0.13	48,48,48,48	0
55	MG	RA	3255	1/1	0.83	0.17	39,39,39,39	0
55	MG	RF	301	1/1	0.83	0.27	80,80,80,80	0
55	MG	RA	3229	1/1	0.83	0.23	40,40,40,40	0
55	MG	RA	3233	1/1	0.83	0.13	35,35,35,35	0
55	MG	RA	3240	1/1	0.83	0.20	53,53,53,53	0
55	MG	YA	3262	1/1	0.83	0.13	27,27,27,27	0
55	MG	Y7	101	1/1	0.83	0.29	47,47,47,47	0
55	MG	XA	1611	1/1	0.83	0.14	59,59,59,59	0
55	MG	RA	3348	1/1	0.84	0.11	46,46,46,46	0
55	MG	XA	1618	1/1	0.84	0.09	51,51,51,51	0
55	MG	XA	1625	1/1	0.84	0.19	47,47,47,47	0
55	MG	YA	3089	1/1	0.84	0.26	35,35,35,35	0
55	MG	YA	3307	1/1	0.84	0.20	69,69,69,69	0
55	MG	YA	3319	1/1	0.84	0.20	48,48,48,48	0
55	MG	RA	3399	1/1	0.84	0.22	40,40,40,40	0
55	MG	RA	3143	1/1	0.84	0.15	68,68,68,68	0
55	MG	YA	3489	1/1	0.84	0.13	48,48,48,48	0
55	MG	RA	3312	1/1	0.84	0.27	64,64,64,64	0
55	MG	RA	3451	1/1	0.84	0.10	58,58,58,58	0
55	MG	YA	3350	1/1	0.84	0.16	50,50,50,50	0
55	MG	RA	3294	1/1	0.84	0.23	36,36,36,36	0
55	MG	RA	3321	1/1	0.84	0.11	39,39,39,39	0
55	MG	RA	3172	1/1	0.84	0.14	37,37,37,37	0
55	MG	RA	3007	1/1	0.84	0.37	53,53,53,53	0
55	MG	RA	3375	1/1	0.84	0.15	39,39,39,39	0
55	MG	RA	3379	1/1	0.84	0.17	76,76,76,76	0
55	MG	XA	1671	1/1	0.84	0.11	47,47,47,47	0
55	MG	XA	1676	1/1	0.84	0.22	59,59,59,59	0
55	MG	RA	3423	1/1	0.84	0.15	53,53,53,53	0
55	MG	RA	3328	1/1	0.84	0.16	38,38,38,38	0
55	MG	XA	1681	1/1	0.84	0.37	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3158	1/1	0.84	0.15	52,52,52,52	0
55	MG	YA	3421	1/1	0.84	0.16	34,34,34,34	0
55	MG	RA	3225	1/1	0.84	0.21	24,24,24,24	0
55	MG	RQ	201	1/1	0.84	0.12	51,51,51,51	0
55	MG	RA	3432	1/1	0.84	0.14	49,49,49,49	0
55	MG	Y0	101	1/1	0.84	0.26	49,49,49,49	0
55	MG	R0	101	1/1	0.84	0.14	49,49,49,49	0
55	MG	XA	1601	1/1	0.84	0.19	50,50,50,50	0
55	MG	RA	3310	1/1	0.84	0.08	42,42,42,42	0
55	MG	XA	1652	1/1	0.85	0.12	44,44,44,44	0
55	MG	RA	3282	1/1	0.85	0.13	34,34,34,34	0
55	MG	RA	3100	1/1	0.85	0.24	75,75,75,75	0
55	MG	YA	3276	1/1	0.85	0.13	47,47,47,47	0
55	MG	QA	1655	1/1	0.85	0.19	61,61,61,61	0
55	MG	YA	3185	1/1	0.85	0.15	65,65,65,65	0
55	MG	RA	3474	1/1	0.85	0.29	45,45,45,45	0
55	MG	RA	3188	1/1	0.85	0.14	41,41,41,41	0
55	MG	RA	3365	1/1	0.85	0.11	40,40,40,40	0
55	MG	RA	3168	1/1	0.85	0.20	47,47,47,47	0
55	MG	YA	3325	1/1	0.85	0.09	30,30,30,30	0
55	MG	RA	3450	1/1	0.85	0.30	52,52,52,52	0
55	MG	YA	3207	1/1	0.85	0.28	41,41,41,41	0
55	MG	YA	3208	1/1	0.85	0.19	29,29,29,29	0
55	MG	XA	1642	1/1	0.85	0.18	34,34,34,34	0
55	MG	YA	3455	1/1	0.85	0.07	14,14,14,14	0
55	MG	YA	3460	1/1	0.85	0.11	52,52,52,52	0
55	MG	RA	3273	1/1	0.85	0.27	47,47,47,47	0
55	MG	YA	3354	1/1	0.85	0.23	55,55,55,55	0
55	MG	YA	3134	1/1	0.85	0.20	65,65,65,65	0
55	MG	YA	3222	1/1	0.85	0.12	50,50,50,50	0
55	MG	RA	3315	1/1	0.85	0.12	46,46,46,46	0
55	MG	YA	3147	1/1	0.85	0.14	46,46,46,46	0
57	ZN	R4	101	1/1	0.85	0.12	236,236,236,236	0
55	MG	RA	3316	1/1	0.85	0.13	48,48,48,48	0
55	MG	XA	1657	1/1	0.86	0.09	57,57,57,57	0
55	MG	RA	3247	1/1	0.86	0.22	46,46,46,46	0
55	MG	XA	1663	1/1	0.86	0.09	44,44,44,44	0
55	MG	RA	3073	1/1	0.86	0.18	31,31,31,31	0
55	MG	YA	3309	1/1	0.86	0.12	50,50,50,50	0
55	MG	YA	3471	1/1	0.86	0.15	32,32,32,32	0
55	MG	YA	3311	1/1	0.86	0.12	22,22,22,22	0
55	MG	YA	3315	1/1	0.86	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
55	MG	RT	201	1/1	0.86	0.12	83,83,83,83	0
55	MG	RX	101	1/1	0.86	0.09	38,38,38,38	0
55	MG	YA	3335	1/1	0.86	0.30	54,54,54,54	0
55	MG	YA	3167	1/1	0.86	0.21	45,45,45,45	0
55	MG	RA	3131	1/1	0.86	0.11	58,58,58,58	0
55	MG	QA	1632	1/1	0.86	0.12	29,29,29,29	0
55	MG	YA	3497	1/1	0.86	0.16	70,70,70,70	0
55	MG	XA	1607	1/1	0.86	0.14	45,45,45,45	0
55	MG	RA	3116	1/1	0.86	0.31	44,44,44,44	0
55	MG	XA	1682	1/1	0.86	0.18	67,67,67,67	0
55	MG	RA	3334	1/1	0.86	0.17	45,45,45,45	0
55	MG	XA	1612	1/1	0.86	0.08	42,42,42,42	0
55	MG	YA	3206	1/1	0.86	0.14	27,27,27,27	0
55	MG	YA	3375	1/1	0.86	0.14	57,57,57,57	0
55	MG	RA	3267	1/1	0.86	0.17	46,46,46,46	0
55	MG	XA	1623	1/1	0.86	0.18	59,59,59,59	0
55	MG	YA	3529	1/1	0.86	0.26	48,48,48,48	0
55	MG	YA	3534	1/1	0.86	0.13	20,20,20,20	0
55	MG	RA	3344	1/1	0.86	0.14	28,28,28,28	0
55	MG	RA	3119	1/1	0.86	0.19	53,53,53,53	0
55	MG	YB	208	1/1	0.86	0.25	64,64,64,64	0
55	MG	RA	3192	1/1	0.86	0.25	40,40,40,40	0
55	MG	RA	3193	1/1	0.86	0.12	64,64,64,64	0
55	MG	RA	3436	1/1	0.86	0.33	51,51,51,51	0
55	MG	RA	3085	1/1	0.86	0.13	21,21,21,21	0
55	MG	YA	3407	1/1	0.86	0.14	43,43,43,43	0
55	MG	YA	3246	1/1	0.86	0.17	25,25,25,25	0
55	MG	YA	3086	1/1	0.86	0.08	35,35,35,35	0
55	MG	RB	203	1/1	0.86	0.26	35,35,35,35	0
55	MG	RB	205	1/1	0.86	0.15	45,45,45,45	0
55	MG	RA	3357	1/1	0.86	0.14	63,63,63,63	0
55	MG	QA	1646	1/1	0.86	0.15	77,77,77,77	0
55	MG	YA	3135	1/1	0.86	0.22	15,15,15,15	0
55	MG	YA	3399	1/1	0.87	0.17	52,52,52,52	0
55	MG	YA	3401	1/1	0.87	0.09	50,50,50,50	0
55	MG	YA	3495	1/1	0.87	0.08	38,38,38,38	0
55	MG	XK	201	1/1	0.87	0.13	46,46,46,46	0
55	MG	QA	1620	1/1	0.87	0.09	51,51,51,51	0
55	MG	YA	3419	1/1	0.87	0.20	33,33,33,33	0
55	MG	RI	201	1/1	0.87	0.82	93,93,93,93	0
55	MG	XA	1665	1/1	0.87	0.09	43,43,43,43	0
55	MG	QA	1649	1/1	0.87	0.20	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3460	1/1	0.87	0.13	40,40,40,40	0
55	MG	YA	3518	1/1	0.87	0.26	12,12,12,12	0
55	MG	YA	3427	1/1	0.87	0.11	41,41,41,41	0
55	MG	RA	3049	1/1	0.87	0.10	24,24,24,24	0
55	MG	YA	3072	1/1	0.87	0.24	36,36,36,36	0
55	MG	YA	3084	1/1	0.87	0.22	29,29,29,29	0
55	MG	YA	3198	1/1	0.87	0.19	40,40,40,40	0
55	MG	YA	3368	1/1	0.87	0.31	55,55,55,55	0
55	MG	YB	201	1/1	0.87	0.15	30,30,30,30	0
55	MG	YA	3456	1/1	0.87	0.09	60,60,60,60	0
55	MG	RA	3471	1/1	0.87	0.21	71,71,71,71	0
55	MG	RA	3111	1/1	0.87	0.19	45,45,45,45	0
55	MG	YA	3470	1/1	0.87	0.31	68,68,68,68	0
55	MG	RA	3275	1/1	0.87	0.23	58,58,58,58	0
55	MG	RA	3449	1/1	0.87	0.27	49,49,49,49	0
55	MG	YA	3129	1/1	0.87	0.25	46,46,46,46	0
55	MG	RA	3006	1/1	0.87	0.12	39,39,39,39	0
55	MG	YA	3476	1/1	0.87	0.15	57,57,57,57	0
55	MG	YR	201	1/1	0.87	0.15	18,18,18,18	0
55	MG	YA	3477	1/1	0.87	0.22	50,50,50,50	0
55	MG	RA	3388	1/1	0.87	0.08	40,40,40,40	0
55	MG	RA	3412	1/1	0.87	0.15	39,39,39,39	0
55	MG	RA	3259	1/1	0.87	0.16	56,56,56,56	0
55	MG	YA	3488	1/1	0.87	0.16	57,57,57,57	0
55	MG	YA	3118	1/1	0.88	0.33	26,26,26,26	0
55	MG	YA	3367	1/1	0.88	0.11	50,50,50,50	0
55	MG	YA	3479	1/1	0.88	0.21	49,49,49,49	0
55	MG	YA	3223	1/1	0.88	0.15	25,25,25,25	0
55	MG	RA	3381	1/1	0.88	0.14	49,49,49,49	0
55	MG	RA	3337	1/1	0.88	0.08	43,43,43,43	0
55	MG	RA	3424	1/1	0.88	0.22	63,63,63,63	0
55	MG	YA	3249	1/1	0.88	0.14	45,45,45,45	0
55	MG	YA	3250	1/1	0.88	0.32	63,63,63,63	0
55	MG	YA	3136	1/1	0.88	0.12	17,17,17,17	0
55	MG	RA	3040	1/1	0.88	0.11	22,22,22,22	0
55	MG	RA	3139	1/1	0.88	0.16	22,22,22,22	0
55	MG	YA	3149	1/1	0.88	0.13	41,41,41,41	0
55	MG	RA	3166	1/1	0.88	0.16	24,24,24,24	0
55	MG	YA	3280	1/1	0.88	0.10	24,24,24,24	0
55	MG	YA	3403	1/1	0.88	0.17	43,43,43,43	0
55	MG	RA	3480	1/1	0.88	0.09	30,30,30,30	0
55	MG	RA	3393	1/1	0.88	0.32	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3415	1/1	0.88	0.15	45,45,45,45	0
55	MG	RA	3167	1/1	0.88	0.10	31,31,31,31	0
55	MG	RA	3243	1/1	0.88	0.21	34,34,34,34	0
55	MG	YA	3179	1/1	0.88	0.18	27,27,27,27	0
55	MG	RA	3398	1/1	0.88	0.16	70,70,70,70	0
55	MG	RA	3279	1/1	0.88	0.26	55,55,55,55	0
55	MG	YA	3002	1/1	0.88	0.15	30,30,30,30	0
55	MG	RA	3081	1/1	0.88	0.08	27,27,27,27	0
55	MG	YA	3443	1/1	0.88	0.17	35,35,35,35	0
55	MG	QA	1650	1/1	0.88	0.09	54,54,54,54	0
55	MG	YA	3331	1/1	0.88	0.10	23,23,23,23	0
55	MG	RA	3445	1/1	0.88	0.09	45,45,45,45	0
55	MG	YA	3454	1/1	0.88	0.11	59,59,59,59	0
55	MG	YA	3034	1/1	0.88	0.15	22,22,22,22	0
55	MG	YA	3340	1/1	0.88	0.29	44,44,44,44	0
55	MG	RA	3250	1/1	0.88	0.13	36,36,36,36	0
55	MG	RA	3050	1/1	0.88	0.18	14,14,14,14	0
55	MG	QA	1611	1/1	0.88	0.19	25,25,25,25	0
55	MG	RA	3332	1/1	0.88	0.17	48,48,48,48	0
55	MG	QA	1669	1/1	0.88	0.09	47,47,47,47	0
55	MG	QA	1653	1/1	0.88	0.09	72,72,72,72	0
55	MG	XA	1608	1/1	0.88	0.12	67,67,67,67	0
55	MG	RA	3204	1/1	0.89	0.19	30,30,30,30	0
55	MG	XA	1645	1/1	0.89	0.15	42,42,42,42	0
55	MG	YA	3016	1/1	0.89	0.15	50,50,50,50	0
55	MG	XA	1648	1/1	0.89	0.08	47,47,47,47	0
55	MG	RA	3156	1/1	0.89	0.24	38,38,38,38	0
55	MG	YA	3355	1/1	0.89	0.14	35,35,35,35	0
55	MG	RA	3303	1/1	0.89	0.07	32,32,32,32	0
55	MG	YA	3217	1/1	0.89	0.07	22,22,22,22	0
55	MG	RA	3341	1/1	0.89	0.08	18,18,18,18	0
55	MG	YA	3366	1/1	0.89	0.19	57,57,57,57	0
55	MG	RA	3031	1/1	0.89	0.22	24,24,24,24	0
55	MG	RA	3346	1/1	0.89	0.17	45,45,45,45	0
55	MG	YA	3106	1/1	0.89	0.11	32,32,32,32	0
55	MG	RA	3306	1/1	0.89	0.20	44,44,44,44	0
55	MG	YA	3240	1/1	0.89	0.20	43,43,43,43	0
55	MG	RA	3274	1/1	0.89	0.11	34,34,34,34	0
55	MG	YA	3116	1/1	0.89	0.14	12,12,12,12	0
55	MG	YA	3382	1/1	0.89	0.14	35,35,35,35	0
55	MG	YA	3498	1/1	0.89	0.26	39,39,39,39	0
55	MG	YA	3387	1/1	0.89	0.13	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1660	1/1	0.89	0.10	32,32,32,32	0
55	MG	RA	3443	1/1	0.89	0.13	38,38,38,38	0
55	MG	YA	3132	1/1	0.89	0.17	5,5,5,5	0
55	MG	RA	3147	1/1	0.89	0.13	33,33,33,33	0
55	MG	RA	3278	1/1	0.89	0.18	54,54,54,54	0
55	MG	RA	3163	1/1	0.89	0.10	29,29,29,29	0
55	MG	RA	3200	1/1	0.89	0.18	34,34,34,34	0
55	MG	XA	1605	1/1	0.89	0.20	41,41,41,41	0
55	MG	RA	3284	1/1	0.89	0.20	51,51,51,51	0
55	MG	QA	1661	1/1	0.89	0.09	65,65,65,65	0
55	MG	RA	3368	1/1	0.89	0.08	19,19,19,19	0
55	MG	YA	3535	1/1	0.89	0.15	36,36,36,36	0
55	MG	YA	3537	1/1	0.89	0.15	17,17,17,17	0
55	MG	YA	3304	1/1	0.89	0.19	46,46,46,46	0
55	MG	RA	3288	1/1	0.89	0.19	49,49,49,49	0
55	MG	RA	3290	1/1	0.89	0.15	31,31,31,31	0
55	MG	XA	1615	1/1	0.89	0.23	57,57,57,57	0
55	MG	RA	3291	1/1	0.89	0.07	37,37,37,37	0
55	MG	RA	3470	1/1	0.89	0.23	34,34,34,34	0
55	MG	YA	3435	1/1	0.89	0.11	31,31,31,31	0
55	MG	RA	3260	1/1	0.89	0.16	59,59,59,59	0
55	MG	YA	3323	1/1	0.89	0.09	18,18,18,18	0
55	MG	YA	3447	1/1	0.89	0.16	59,59,59,59	0
55	MG	YA	3449	1/1	0.89	0.17	39,39,39,39	0
55	MG	YA	3186	1/1	0.89	0.14	29,29,29,29	0
55	MG	YA	3451	1/1	0.89	0.08	34,34,34,34	0
55	MG	Y0	102	1/1	0.89	0.13	32,32,32,32	0
55	MG	XA	1635	1/1	0.89	0.14	23,23,23,23	0
55	MG	RA	3203	1/1	0.89	0.15	24,24,24,24	0
55	MG	Y8	101	1/1	0.89	0.30	34,34,34,34	0
55	MG	RA	3427	1/1	0.89	0.07	23,23,23,23	0
55	MG	RA	3295	1/1	0.89	0.08	32,32,32,32	0
55	MG	XA	1677	1/1	0.90	0.14	52,52,52,52	0
55	MG	RA	3253	1/1	0.90	0.12	34,34,34,34	0
55	MG	RA	3128	1/1	0.90	0.16	28,28,28,28	0
55	MG	RA	3113	1/1	0.90	0.20	33,33,33,33	0
55	MG	YA	3313	1/1	0.90	0.30	42,42,42,42	0
55	MG	RA	3413	1/1	0.90	0.10	59,59,59,59	0
55	MG	YA	3317	1/1	0.90	0.10	37,37,37,37	0
55	MG	RA	3209	1/1	0.90	0.16	30,30,30,30	0
55	MG	YA	3321	1/1	0.90	0.47	76,76,76,76	0
55	MG	YA	3463	1/1	0.90	0.23	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3458	1/1	0.90	0.17	56,56,56,56	0
55	MG	YA	3469	1/1	0.90	0.28	52,52,52,52	0
55	MG	RA	3292	1/1	0.90	0.09	45,45,45,45	0
55	MG	YA	3330	1/1	0.90	0.07	18,18,18,18	0
55	MG	XA	1622	1/1	0.90	0.23	42,42,42,42	0
55	MG	XA	1692	1/1	0.90	0.17	60,60,60,60	0
55	MG	RA	3210	1/1	0.90	0.17	57,57,57,57	0
55	MG	RA	3329	1/1	0.90	0.12	40,40,40,40	0
55	MG	RA	3214	1/1	0.90	0.16	60,60,60,60	0
55	MG	YA	3200	1/1	0.90	0.08	20,20,20,20	0
55	MG	YA	3347	1/1	0.90	0.12	53,53,53,53	0
55	MG	QA	1637	1/1	0.90	0.12	35,35,35,35	0
55	MG	YA	3006	1/1	0.90	0.13	39,39,39,39	0
55	MG	RA	3380	1/1	0.90	0.10	76,76,76,76	0
55	MG	RA	3426	1/1	0.90	0.11	49,49,49,49	0
55	MG	YA	3491	1/1	0.90	0.14	41,41,41,41	0
55	MG	RA	3264	1/1	0.90	0.21	24,24,24,24	0
55	MG	YA	3358	1/1	0.90	0.11	30,30,30,30	0
55	MG	XA	1644	1/1	0.90	0.16	42,42,42,42	0
55	MG	YA	3017	1/1	0.90	0.14	54,54,54,54	0
55	MG	YA	3216	1/1	0.90	0.07	27,27,27,27	0
55	MG	RA	3005	1/1	0.90	0.16	40,40,40,40	0
55	MG	YA	3041	1/1	0.90	0.23	6,6,6,6	0
55	MG	YA	3049	1/1	0.90	0.12	16,16,16,16	0
55	MG	YA	3508	1/1	0.90	0.15	29,29,29,29	0
55	MG	YA	3376	1/1	0.90	0.18	44,44,44,44	0
55	MG	RA	3230	1/1	0.90	0.19	49,49,49,49	0
55	MG	XA	1649	1/1	0.90	0.14	51,51,51,51	0
55	MG	RA	3198	1/1	0.90	0.08	56,56,56,56	0
55	MG	YA	3235	1/1	0.90	0.15	44,44,44,44	0
55	MG	YA	3236	1/1	0.90	0.19	26,26,26,26	0
55	MG	RE	301	1/1	0.90	0.19	27,27,27,27	0
55	MG	RA	3018	1/1	0.90	0.21	26,26,26,26	0
55	MG	RA	3079	1/1	0.90	0.12	36,36,36,36	0
55	MG	RA	3057	1/1	0.90	0.13	4,4,4,4	0
55	MG	RA	3165	1/1	0.90	0.12	37,37,37,37	0
55	MG	RA	3112	1/1	0.90	0.18	36,36,36,36	0
55	MG	RA	3351	1/1	0.90	0.09	36,36,36,36	0
55	MG	YA	3126	1/1	0.90	0.07	1,1,1,1	0
55	MG	YA	3404	1/1	0.90	0.14	44,44,44,44	0
55	MG	RA	3400	1/1	0.90	0.19	61,61,61,61	0
55	MG	YA	3268	1/1	0.90	0.30	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3270	1/1	0.90	0.18	58,58,58,58	0
55	MG	RY	201	1/1	0.90	0.30	175,175,175,175	0
55	MG	YA	3279	1/1	0.90	0.10	32,32,32,32	0
55	MG	RA	3252	1/1	0.90	0.17	46,46,46,46	0
55	MG	YA	3281	1/1	0.90	0.29	37,37,37,37	0
55	MG	RA	3404	1/1	0.90	0.19	48,48,48,48	0
55	MG	XA	1604	1/1	0.90	0.08	61,61,61,61	0
55	MG	YA	3432	1/1	0.90	0.18	37,37,37,37	0
55	MG	XA	1673	1/1	0.90	0.12	39,39,39,39	0
55	MG	YA	3297	1/1	0.90	0.35	57,57,57,57	0
55	MG	YA	3298	1/1	0.90	0.12	25,25,25,25	0
55	MG	RA	3356	1/1	0.90	0.20	35,35,35,35	0
55	MG	YA	3115	1/1	0.91	0.08	10,10,10,10	0
55	MG	RA	3095	1/1	0.91	0.14	35,35,35,35	0
55	MG	RA	3280	1/1	0.91	0.14	54,54,54,54	0
55	MG	YA	3124	1/1	0.91	0.11	27,27,27,27	0
55	MG	YA	3239	1/1	0.91	0.08	28,28,28,28	0
55	MG	YA	3466	1/1	0.91	0.57	71,71,71,71	0
55	MG	XA	1609	1/1	0.91	0.21	44,44,44,44	0
55	MG	RA	3281	1/1	0.91	0.19	57,57,57,57	0
55	MG	YA	3357	1/1	0.91	0.15	53,53,53,53	0
55	MG	RA	3249	1/1	0.91	0.11	27,27,27,27	0
55	MG	YA	3248	1/1	0.91	0.22	20,20,20,20	0
55	MG	XA	1679	1/1	0.91	0.05	52,52,52,52	0
55	MG	YA	3365	1/1	0.91	0.09	34,34,34,34	0
55	MG	RA	3456	1/1	0.91	0.15	46,46,46,46	0
55	MG	XA	1614	1/1	0.91	0.06	23,23,23,23	0
55	MG	RA	3185	1/1	0.91	0.14	59,59,59,59	0
55	MG	XA	1616	1/1	0.91	0.17	40,40,40,40	0
55	MG	RA	3369	1/1	0.91	0.10	36,36,36,36	0
55	MG	RA	3162	1/1	0.91	0.15	45,45,45,45	0
55	MG	QA	1624	1/1	0.91	0.06	41,41,41,41	0
55	MG	YA	3156	1/1	0.91	0.22	43,43,43,43	0
55	MG	RA	3026	1/1	0.91	0.19	34,34,34,34	0
55	MG	RA	3376	1/1	0.91	0.13	65,65,65,65	0
55	MG	YA	3385	1/1	0.91	0.13	53,53,53,53	0
55	MG	YA	3386	1/1	0.91	0.06	38,38,38,38	0
55	MG	RA	3330	1/1	0.91	0.20	34,34,34,34	0
55	MG	YA	3170	1/1	0.91	0.27	42,42,42,42	0
55	MG	YA	3286	1/1	0.91	0.21	38,38,38,38	0
55	MG	YA	3291	1/1	0.91	0.17	33,33,33,33	0
55	MG	YA	3396	1/1	0.91	0.20	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3126	1/1	0.91	0.20	24,24,24,24	0
55	MG	QA	1670	1/1	0.91	0.28	30,30,30,30	0
55	MG	YA	3183	1/1	0.91	0.20	44,44,44,44	0
55	MG	RA	3218	1/1	0.91	0.21	58,58,58,58	0
55	MG	YA	3299	1/1	0.91	0.06	58,58,58,58	0
55	MG	RB	201	1/1	0.91	0.06	38,38,38,38	0
55	MG	YA	3409	1/1	0.91	0.19	41,41,41,41	0
55	MG	YA	3532	1/1	0.91	0.14	23,23,23,23	0
55	MG	RA	3430	1/1	0.91	0.20	52,52,52,52	0
55	MG	RA	3219	1/1	0.91	0.11	20,20,20,20	0
55	MG	YA	3417	1/1	0.91	0.17	36,36,36,36	0
55	MG	YA	3192	1/1	0.91	0.07	24,24,24,24	0
55	MG	RA	3029	1/1	0.91	0.21	15,15,15,15	0
55	MG	RA	3435	1/1	0.91	0.07	48,48,48,48	0
55	MG	RA	3169	1/1	0.91	0.17	62,62,62,62	0
55	MG	YA	3424	1/1	0.91	0.14	33,33,33,33	0
55	MG	RA	3266	1/1	0.91	0.10	33,33,33,33	0
55	MG	YB	211	1/1	0.91	0.28	38,38,38,38	0
55	MG	YA	3318	1/1	0.91	0.07	42,42,42,42	0
55	MG	RA	3114	1/1	0.91	0.14	31,31,31,31	0
55	MG	RA	3231	1/1	0.91	0.27	45,45,45,45	0
55	MG	RA	3270	1/1	0.91	0.10	48,48,48,48	0
55	MG	YA	3437	1/1	0.91	0.08	39,39,39,39	0
55	MG	QC	301	1/1	0.91	0.09	91,91,91,91	0
55	MG	RA	3178	1/1	0.91	0.12	42,42,42,42	0
55	MG	QA	1631	1/1	0.91	0.11	68,68,68,68	0
55	MG	RA	3402	1/1	0.91	0.11	46,46,46,46	0
55	MG	YA	3336	1/1	0.91	0.09	40,40,40,40	0
55	MG	YA	3108	1/1	0.91	0.14	18,18,18,18	0
55	MG	RA	3353	1/1	0.91	0.12	47,47,47,47	0
55	MG	RA	3202	1/1	0.91	0.12	30,30,30,30	0
55	MG	XA	1640	1/1	0.92	0.15	66,66,66,66	0
55	MG	YA	3010	1/1	0.92	0.12	50,50,50,50	0
55	MG	YA	3189	1/1	0.92	0.07	26,26,26,26	0
55	MG	RA	3019	1/1	0.92	0.18	14,14,14,14	0
55	MG	QA	1654	1/1	0.92	0.07	77,77,77,77	0
55	MG	RA	3487	1/1	0.92	0.13	40,40,40,40	0
55	MG	RA	3002	1/1	0.92	0.14	35,35,35,35	0
55	MG	RA	3106	1/1	0.92	0.11	24,24,24,24	0
55	MG	YA	3322	1/1	0.92	0.12	67,67,67,67	0
55	MG	QA	1662	1/1	0.92	0.07	63,63,63,63	0
55	MG	YA	3042	1/1	0.92	0.18	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RB	206	1/1	0.92	0.23	27,27,27,27	0
55	MG	RA	3184	1/1	0.92	0.11	23,23,23,23	0
55	MG	YA	3332	1/1	0.92	0.12	30,30,30,30	0
55	MG	RE	302	1/1	0.92	0.14	18,18,18,18	0
55	MG	YA	3457	1/1	0.92	0.21	57,57,57,57	0
55	MG	RA	3251	1/1	0.92	0.10	58,58,58,58	0
55	MG	YA	3337	1/1	0.92	0.09	44,44,44,44	0
55	MG	QA	1665	1/1	0.92	0.08	43,43,43,43	0
55	MG	RA	3391	1/1	0.92	0.10	24,24,24,24	0
55	MG	YA	3467	1/1	0.92	0.11	42,42,42,42	0
55	MG	YA	3468	1/1	0.92	0.09	49,49,49,49	0
55	MG	YA	3090	1/1	0.92	0.10	15,15,15,15	0
55	MG	YA	3344	1/1	0.92	0.11	18,18,18,18	0
55	MG	YA	3101	1/1	0.92	0.18	36,36,36,36	0
55	MG	RA	3134	1/1	0.92	0.17	40,40,40,40	0
55	MG	YA	3225	1/1	0.92	0.08	26,26,26,26	0
55	MG	YA	3227	1/1	0.92	0.10	8,8,8,8	0
55	MG	YA	3352	1/1	0.92	0.11	30,30,30,30	0
55	MG	QA	1605	1/1	0.92	0.11	30,30,30,30	0
55	MG	YA	3233	1/1	0.92	0.12	29,29,29,29	0
55	MG	RA	3213	1/1	0.92	0.11	37,37,37,37	0
55	MG	RA	3190	1/1	0.92	0.07	48,48,48,48	0
55	MG	YA	3484	1/1	0.92	0.08	49,49,49,49	0
55	MG	YA	3238	1/1	0.92	0.18	35,35,35,35	0
55	MG	YA	3487	1/1	0.92	0.05	37,37,37,37	0
55	MG	RA	3215	1/1	0.92	0.14	22,22,22,22	0
55	MG	RA	3137	1/1	0.92	0.20	66,66,66,66	0
55	MG	YA	3363	1/1	0.92	0.12	23,23,23,23	0
55	MG	YA	3364	1/1	0.92	0.16	61,61,61,61	0
55	MG	YA	3494	1/1	0.92	0.06	22,22,22,22	0
55	MG	YA	3243	1/1	0.92	0.15	39,39,39,39	0
55	MG	YA	3244	1/1	0.92	0.14	34,34,34,34	0
55	MG	RA	3446	1/1	0.92	0.12	43,43,43,43	0
55	MG	YA	3499	1/1	0.92	0.04	15,15,15,15	0
55	MG	RA	3013	1/1	0.92	0.12	19,19,19,19	0
55	MG	YA	3503	1/1	0.92	0.07	43,43,43,43	0
55	MG	RA	3221	1/1	0.92	0.19	30,30,30,30	0
55	MG	YA	3505	1/1	0.92	0.12	43,43,43,43	0
55	MG	QA	1618	1/1	0.92	0.06	41,41,41,41	0
55	MG	RA	3226	1/1	0.92	0.13	50,50,50,50	0
55	MG	YA	3251	1/1	0.92	0.17	16,16,16,16	0
55	MG	YA	3256	1/1	0.92	0.06	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3355	1/1	0.92	0.23	53,53,53,53	0
55	MG	YA	3513	1/1	0.92	0.12	33,33,33,33	0
55	MG	RA	3053	1/1	0.92	0.14	15,15,15,15	0
55	MG	YA	3519	1/1	0.92	0.13	1,1,1,1	0
55	MG	YA	3383	1/1	0.92	0.16	45,45,45,45	0
55	MG	YA	3265	1/1	0.92	0.05	23,23,23,23	0
55	MG	RA	3146	1/1	0.92	0.22	46,46,46,46	0
55	MG	RA	3271	1/1	0.92	0.25	53,53,53,53	0
55	MG	RA	3272	1/1	0.92	0.11	41,41,41,41	0
55	MG	XA	1686	1/1	0.92	0.13	31,31,31,31	0
55	MG	YA	3393	1/1	0.92	0.12	56,56,56,56	0
55	MG	RA	3088	1/1	0.92	0.09	20,20,20,20	0
55	MG	YA	3277	1/1	0.92	0.20	36,36,36,36	0
55	MG	RA	3170	1/1	0.92	0.08	32,32,32,32	0
55	MG	RA	3234	1/1	0.92	0.06	21,21,21,21	0
55	MG	YB	207	1/1	0.92	0.13	64,64,64,64	0
55	MG	RA	3277	1/1	0.92	0.17	29,29,29,29	0
55	MG	YA	3402	1/1	0.92	0.06	40,40,40,40	0
55	MG	RA	3472	1/1	0.92	0.09	31,31,31,31	0
55	MG	YA	3166	1/1	0.92	0.18	26,26,26,26	0
55	MG	YA	3289	1/1	0.92	0.13	46,46,46,46	0
55	MG	YB	213	1/1	0.92	0.25	34,34,34,34	0
55	MG	YB	215	1/1	0.92	0.07	34,34,34,34	0
55	MG	XL	201	1/1	0.92	0.10	59,59,59,59	0
55	MG	YD	302	1/1	0.92	0.08	14,14,14,14	0
55	MG	RA	3371	1/1	0.92	0.07	53,53,53,53	0
55	MG	YA	3414	1/1	0.92	0.09	38,38,38,38	0
55	MG	YA	3173	1/1	0.92	0.18	22,22,22,22	0
55	MG	YA	3178	1/1	0.92	0.11	34,34,34,34	0
55	MG	RA	3238	1/1	0.92	0.10	32,32,32,32	0
55	MG	YA	3420	1/1	0.92	0.11	22,22,22,22	0
55	MG	XS	101	1/1	0.92	0.04	70,70,70,70	0
55	MG	Y5	102	1/1	0.92	0.08	24,24,24,24	0
55	MG	YA	3300	1/1	0.92	0.10	40,40,40,40	0
55	MG	RA	3374	1/1	0.92	0.05	47,47,47,47	0
55	MG	YA	3003	1/1	0.92	0.09	27,27,27,27	0
55	MG	RA	3482	1/1	0.92	0.17	27,27,27,27	0
55	MG	RA	3101	1/1	0.93	0.07	62,62,62,62	0
55	MG	YA	3428	1/1	0.93	0.25	69,69,69,69	0
55	MG	XA	1672	1/1	0.93	0.10	56,56,56,56	0
55	MG	RA	3011	1/1	0.93	0.18	13,13,13,13	0
55	MG	YA	3161	1/1	0.93	0.17	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3107	1/1	0.93	0.14	25,25,25,25	0
55	MG	RA	3414	1/1	0.93	0.09	38,38,38,38	0
55	MG	RA	3415	1/1	0.93	0.13	46,46,46,46	0
55	MG	YA	3310	1/1	0.93	0.09	17,17,17,17	0
55	MG	RA	3138	1/1	0.93	0.10	38,38,38,38	0
55	MG	YA	3312	1/1	0.93	0.31	63,63,63,63	0
55	MG	QA	1614	1/1	0.93	0.06	60,60,60,60	0
55	MG	YA	3174	1/1	0.93	0.16	44,44,44,44	0
55	MG	RE	304	1/1	0.93	0.15	70,70,70,70	0
55	MG	RA	3014	1/1	0.93	0.12	23,23,23,23	0
55	MG	RA	3419	1/1	0.93	0.26	33,33,33,33	0
55	MG	QA	1616	1/1	0.93	0.14	49,49,49,49	0
55	MG	RA	3174	1/1	0.93	0.10	52,52,52,52	0
55	MG	YA	3461	1/1	0.93	0.16	47,47,47,47	0
55	MG	RA	3256	1/1	0.93	0.12	20,20,20,20	0
55	MG	RA	3299	1/1	0.93	0.24	46,46,46,46	0
55	MG	YA	3327	1/1	0.93	0.13	31,31,31,31	0
55	MG	YA	3329	1/1	0.93	0.10	26,26,26,26	0
55	MG	RA	3362	1/1	0.93	0.11	26,26,26,26	0
55	MG	RA	3175	1/1	0.93	0.09	50,50,50,50	0
55	MG	RA	3176	1/1	0.93	0.08	47,47,47,47	0
55	MG	YA	3333	1/1	0.93	0.11	39,39,39,39	0
55	MG	RA	3177	1/1	0.93	0.15	30,30,30,30	0
55	MG	RA	3307	1/1	0.93	0.19	55,55,55,55	0
55	MG	QA	1673	1/1	0.93	0.14	37,37,37,37	0
55	MG	YA	3338	1/1	0.93	0.17	9,9,9,9	0
55	MG	YA	3203	1/1	0.93	0.11	33,33,33,33	0
55	MG	RA	3263	1/1	0.93	0.11	29,29,29,29	0
55	MG	QA	1660	1/1	0.93	0.07	36,36,36,36	0
55	MG	RA	3216	1/1	0.93	0.23	32,32,32,32	0
55	MG	RA	3149	1/1	0.93	0.08	34,34,34,34	0
55	MG	YA	3485	1/1	0.93	0.16	46,46,46,46	0
55	MG	RA	3314	1/1	0.93	0.10	35,35,35,35	0
55	MG	QA	1617	1/1	0.93	0.09	64,64,64,64	0
55	MG	YA	3212	1/1	0.93	0.07	30,30,30,30	0
55	MG	YA	3351	1/1	0.93	0.16	35,35,35,35	0
55	MG	YA	3013	1/1	0.93	0.15	25,25,25,25	0
55	MG	RA	3378	1/1	0.93	0.07	36,36,36,36	0
55	MG	RA	3151	1/1	0.93	0.05	38,38,38,38	0
55	MG	YA	3220	1/1	0.93	0.09	47,47,47,47	0
55	MG	RA	3444	1/1	0.93	0.26	46,46,46,46	0
55	MG	YA	3018	1/1	0.93	0.11	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3021	1/1	0.93	0.09	7,7,7,7	0
55	MG	YA	3501	1/1	0.93	0.10	44,44,44,44	0
55	MG	YA	3027	1/1	0.93	0.15	21,21,21,21	0
55	MG	YA	3226	1/1	0.93	0.07	6,6,6,6	0
55	MG	YA	3031	1/1	0.93	0.17	15,15,15,15	0
55	MG	YA	3228	1/1	0.93	0.06	28,28,28,28	0
55	MG	RA	3317	1/1	0.93	0.16	38,38,38,38	0
55	MG	RA	3319	1/1	0.93	0.16	38,38,38,38	0
55	MG	RA	3448	1/1	0.93	0.10	43,43,43,43	0
55	MG	YA	3371	1/1	0.93	0.25	48,48,48,48	0
55	MG	YA	3044	1/1	0.93	0.11	43,43,43,43	0
55	MG	QA	1604	1/1	0.93	0.17	26,26,26,26	0
55	MG	YA	3515	1/1	0.93	0.42	52,52,52,52	0
55	MG	YA	3051	1/1	0.93	0.25	36,36,36,36	0
55	MG	YA	3057	1/1	0.93	0.15	24,24,24,24	0
55	MG	YA	3522	1/1	0.93	0.21	12,12,12,12	0
55	MG	YA	3242	1/1	0.93	0.14	24,24,24,24	0
55	MG	XA	1634	1/1	0.93	0.11	37,37,37,37	0
55	MG	YA	3059	1/1	0.93	0.15	17,17,17,17	0
55	MG	RA	3030	1/1	0.93	0.19	14,14,14,14	0
55	MG	RA	3189	1/1	0.93	0.08	22,22,22,22	0
55	MG	XA	1638	1/1	0.93	0.07	39,39,39,39	0
55	MG	RA	3390	1/1	0.93	0.06	38,38,38,38	0
55	MG	RA	3121	1/1	0.93	0.15	32,32,32,32	0
55	MG	YA	3091	1/1	0.93	0.15	5,5,5,5	0
55	MG	YA	3541	1/1	0.93	0.21	19,19,19,19	0
55	MG	YA	3542	1/1	0.93	0.28	42,42,42,42	0
55	MG	RA	3122	1/1	0.93	0.16	38,38,38,38	0
55	MG	QA	1651	1/1	0.93	0.10	46,46,46,46	0
55	MG	YA	3395	1/1	0.93	0.10	39,39,39,39	0
55	MG	QA	1630	1/1	0.93	0.10	37,37,37,37	0
55	MG	RA	3236	1/1	0.93	0.21	48,48,48,48	0
55	MG	RA	3459	1/1	0.93	0.15	34,34,34,34	0
55	MG	RA	3194	1/1	0.93	0.15	49,49,49,49	0
55	MG	RA	3335	1/1	0.93	0.05	23,23,23,23	0
55	MG	RA	3467	1/1	0.93	0.13	69,69,69,69	0
55	MG	YA	3274	1/1	0.93	0.16	27,27,27,27	0
55	MG	YA	3405	1/1	0.93	0.08	26,26,26,26	0
55	MG	QA	1619	1/1	0.93	0.12	52,52,52,52	0
55	MG	RA	3338	1/1	0.93	0.11	39,39,39,39	0
55	MG	RA	3241	1/1	0.93	0.16	29,29,29,29	0
55	MG	RA	3340	1/1	0.93	0.13	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3406	1/1	0.93	0.12	50,50,50,50	0
55	MG	RA	3478	1/1	0.93	0.17	46,46,46,46	0
55	MG	XA	1661	1/1	0.93	0.10	71,71,71,71	0
55	MG	YA	3288	1/1	0.93	0.14	37,37,37,37	0
55	MG	YA	3142	1/1	0.93	0.09	40,40,40,40	0
55	MG	QA	1613	1/1	0.93	0.18	40,40,40,40	0
55	MG	RA	3408	1/1	0.93	0.24	38,38,38,38	0
55	MG	Y8	102	1/1	0.93	0.06	13,13,13,13	0
56	SF4	QD	301	8/8	0.93	0.15	151,161,177,182	0
55	MG	RA	3409	1/1	0.93	0.07	55,55,55,55	0
55	MG	RA	3052	1/1	0.93	0.10	27,27,27,27	0
55	MG	XA	1687	1/1	0.94	0.12	74,74,74,74	0
55	MG	YA	3458	1/1	0.94	0.10	24,24,24,24	0
55	MG	YA	3345	1/1	0.94	0.20	58,58,58,58	0
55	MG	YA	3237	1/1	0.94	0.06	40,40,40,40	0
55	MG	YA	3462	1/1	0.94	0.11	36,36,36,36	0
55	MG	RA	3004	1/1	0.94	0.23	31,31,31,31	0
55	MG	RA	3397	1/1	0.94	0.13	46,46,46,46	0
55	MG	RA	3433	1/1	0.94	0.17	37,37,37,37	0
55	MG	YA	3241	1/1	0.94	0.08	20,20,20,20	0
55	MG	RA	3484	1/1	0.94	0.06	30,30,30,30	0
55	MG	RA	3322	1/1	0.94	0.07	42,42,42,42	0
55	MG	RA	3075	1/1	0.94	0.13	24,24,24,24	0
55	MG	YA	3137	1/1	0.94	0.13	32,32,32,32	0
55	MG	RA	3324	1/1	0.94	0.19	42,42,42,42	0
55	MG	RA	3326	1/1	0.94	0.15	35,35,35,35	0
55	MG	XQ	201	1/1	0.94	0.08	50,50,50,50	0
55	MG	RA	3154	1/1	0.94	0.12	29,29,29,29	0
55	MG	RA	3403	1/1	0.94	0.11	42,42,42,42	0
55	MG	YA	3252	1/1	0.94	0.14	11,11,11,11	0
55	MG	XA	1641	1/1	0.94	0.11	31,31,31,31	0
55	MG	YA	3152	1/1	0.94	0.05	30,30,30,30	0
55	MG	QA	1636	1/1	0.94	0.13	46,46,46,46	0
55	MG	RA	3217	1/1	0.94	0.08	16,16,16,16	0
55	MG	QA	1671	1/1	0.94	0.05	17,17,17,17	0
55	MG	YA	3372	1/1	0.94	0.13	30,30,30,30	0
55	MG	QA	1659	1/1	0.94	0.12	30,30,30,30	0
55	MG	RA	3302	1/1	0.94	0.20	39,39,39,39	0
55	MG	YA	3490	1/1	0.94	0.09	35,35,35,35	0
55	MG	RA	3021	1/1	0.94	0.08	5,5,5,5	0
55	MG	YA	3378	1/1	0.94	0.11	26,26,26,26	0
55	MG	YA	3168	1/1	0.94	0.08	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3169	1/1	0.94	0.18	17,17,17,17	0
55	MG	YA	3015	1/1	0.94	0.19	12,12,12,12	0
55	MG	YA	3171	1/1	0.94	0.06	27,27,27,27	0
55	MG	RA	3159	1/1	0.94	0.09	47,47,47,47	0
55	MG	RP	201	1/1	0.94	0.10	47,47,47,47	0
55	MG	YA	3176	1/1	0.94	0.14	42,42,42,42	0
55	MG	YA	3177	1/1	0.94	0.06	19,19,19,19	0
55	MG	YA	3388	1/1	0.94	0.20	32,32,32,32	0
55	MG	RA	3336	1/1	0.94	0.10	44,44,44,44	0
55	MG	XA	1653	1/1	0.94	0.23	43,43,43,43	0
55	MG	YA	3391	1/1	0.94	0.12	30,30,30,30	0
55	MG	YA	3392	1/1	0.94	0.16	56,56,56,56	0
55	MG	YA	3024	1/1	0.94	0.08	6,6,6,6	0
55	MG	RA	3160	1/1	0.94	0.08	22,22,22,22	0
55	MG	RR	202	1/1	0.94	0.09	18,18,18,18	0
55	MG	YA	3032	1/1	0.94	0.18	15,15,15,15	0
55	MG	RA	3161	1/1	0.94	0.08	21,21,21,21	0
55	MG	XA	1658	1/1	0.94	0.07	51,51,51,51	0
55	MG	RA	3047	1/1	0.94	0.18	9,9,9,9	0
55	MG	YA	3301	1/1	0.94	0.14	6,6,6,6	0
55	MG	YA	3303	1/1	0.94	0.16	28,28,28,28	0
55	MG	RA	3090	1/1	0.94	0.16	18,18,18,18	0
55	MG	YA	3195	1/1	0.94	0.18	22,22,22,22	0
55	MG	YA	3530	1/1	0.94	0.15	10,10,10,10	0
55	MG	YA	3306	1/1	0.94	0.09	53,53,53,53	0
55	MG	YA	3045	1/1	0.94	0.16	15,15,15,15	0
55	MG	RA	3258	1/1	0.94	0.12	25,25,25,25	0
55	MG	YA	3050	1/1	0.94	0.23	9,9,9,9	0
55	MG	YA	3202	1/1	0.94	0.15	37,37,37,37	0
55	MG	YA	3540	1/1	0.94	0.08	26,26,26,26	0
55	MG	R1	101	1/1	0.94	0.18	32,32,32,32	0
55	MG	R8	101	1/1	0.94	0.12	23,23,23,23	0
55	MG	RA	3384	1/1	0.94	0.12	35,35,35,35	0
55	MG	XA	1603	1/1	0.94	0.10	26,26,26,26	0
55	MG	XA	1669	1/1	0.94	0.14	30,30,30,30	0
55	MG	RA	3164	1/1	0.94	0.07	25,25,25,25	0
55	MG	YA	3085	1/1	0.94	0.15	20,20,20,20	0
55	MG	RA	3148	1/1	0.94	0.12	40,40,40,40	0
55	MG	XA	1606	1/1	0.94	0.11	27,27,27,27	0
55	MG	RA	3422	1/1	0.94	0.22	37,37,37,37	0
55	MG	YA	3429	1/1	0.94	0.07	23,23,23,23	0
55	MG	YB	214	1/1	0.94	0.08	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3326	1/1	0.94	0.14	35,35,35,35	0
55	MG	RA	3462	1/1	0.94	0.13	34,34,34,34	0
55	MG	YA	3094	1/1	0.94	0.25	31,31,31,31	0
55	MG	YE	302	1/1	0.94	0.17	41,41,41,41	0
55	MG	YA	3436	1/1	0.94	0.18	40,40,40,40	0
55	MG	RA	3387	1/1	0.94	0.10	47,47,47,47	0
55	MG	YQ	201	1/1	0.94	0.17	37,37,37,37	0
55	MG	YA	3438	1/1	0.94	0.08	29,29,29,29	0
55	MG	YA	3102	1/1	0.94	0.13	21,21,21,21	0
55	MG	YX	101	1/1	0.94	0.09	61,61,61,61	0
55	MG	YX	102	1/1	0.94	0.09	53,53,53,53	0
55	MG	YA	3444	1/1	0.94	0.07	32,32,32,32	0
55	MG	RA	3130	1/1	0.94	0.07	53,53,53,53	0
55	MG	YA	3224	1/1	0.94	0.08	57,57,57,57	0
55	MG	RA	3287	1/1	0.94	0.19	50,50,50,50	0
55	MG	YA	3110	1/1	0.94	0.16	12,12,12,12	0
55	MG	QA	1674	1/1	0.94	0.21	43,43,43,43	0
55	MG	RA	3070	1/1	0.94	0.14	11,11,11,11	0
55	MG	RA	3265	1/1	0.94	0.10	20,20,20,20	0
55	MG	XA	1685	1/1	0.94	0.07	40,40,40,40	0
55	MG	RA	3320	1/1	0.94	0.18	29,29,29,29	0
55	MG	YA	3139	1/1	0.95	0.09	18,18,18,18	0
55	MG	QA	1628	1/1	0.95	0.07	39,39,39,39	0
55	MG	RA	3068	1/1	0.95	0.15	25,25,25,25	0
55	MG	YA	3144	1/1	0.95	0.11	20,20,20,20	0
55	MG	YA	3146	1/1	0.95	0.07	13,13,13,13	0
55	MG	RA	3440	1/1	0.95	0.14	21,21,21,21	0
55	MG	YA	3360	1/1	0.95	0.33	65,65,65,65	0
55	MG	YA	3009	1/1	0.95	0.14	36,36,36,36	0
55	MG	RA	3129	1/1	0.95	0.12	35,35,35,35	0
55	MG	RA	3196	1/1	0.95	0.09	34,34,34,34	0
55	MG	YA	3473	1/1	0.95	0.18	54,54,54,54	0
55	MG	XA	1647	1/1	0.95	0.10	58,58,58,58	0
55	MG	YA	3259	1/1	0.95	0.18	10,10,10,10	0
55	MG	RA	3358	1/1	0.95	0.18	50,50,50,50	0
55	MG	RA	3223	1/1	0.95	0.15	30,30,30,30	0
55	MG	YA	3478	1/1	0.95	0.06	37,37,37,37	0
55	MG	YA	3263	1/1	0.95	0.23	11,11,11,11	0
55	MG	RA	3016	1/1	0.95	0.14	21,21,21,21	0
55	MG	RO	201	1/1	0.95	0.08	45,45,45,45	0
55	MG	RA	3289	1/1	0.95	0.10	27,27,27,27	0
55	MG	RA	3036	1/1	0.95	0.18	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3023	1/1	0.95	0.09	13,13,13,13	0
55	MG	YA	3272	1/1	0.95	0.14	31,31,31,31	0
55	MG	XA	1654	1/1	0.95	0.17	25,25,25,25	0
55	MG	RA	3228	1/1	0.95	0.21	27,27,27,27	0
55	MG	RA	3261	1/1	0.95	0.25	41,41,41,41	0
55	MG	YA	3278	1/1	0.95	0.16	47,47,47,47	0
55	MG	YA	3172	1/1	0.95	0.10	20,20,20,20	0
55	MG	YA	3384	1/1	0.95	0.25	35,35,35,35	0
55	MG	QA	1629	1/1	0.95	0.11	33,33,33,33	0
55	MG	RA	3076	1/1	0.95	0.10	24,24,24,24	0
55	MG	YA	3036	1/1	0.95	0.16	6,6,6,6	0
55	MG	RA	3078	1/1	0.95	0.07	16,16,16,16	0
55	MG	QA	1642	1/1	0.95	0.06	48,48,48,48	0
55	MG	YA	3043	1/1	0.95	0.13	1,1,1,1	0
55	MG	YA	3290	1/1	0.95	0.09	11,11,11,11	0
55	MG	RA	3020	1/1	0.95	0.05	22,22,22,22	0
55	MG	RA	3182	1/1	0.95	0.15	40,40,40,40	0
55	MG	RA	3377	1/1	0.95	0.12	45,45,45,45	0
55	MG	RA	3206	1/1	0.95	0.19	36,36,36,36	0
55	MG	RA	3269	1/1	0.95	0.17	28,28,28,28	0
55	MG	RA	3304	1/1	0.95	0.15	22,22,22,22	0
55	MG	RA	3464	1/1	0.95	0.23	28,28,28,28	0
55	MG	YA	3512	1/1	0.95	0.13	50,50,50,50	0
55	MG	RA	3239	1/1	0.95	0.09	28,28,28,28	0
55	MG	YA	3193	1/1	0.95	0.07	31,31,31,31	0
55	MG	YA	3062	1/1	0.95	0.14	0,0,0,0	0
55	MG	YA	3197	1/1	0.95	0.06	24,24,24,24	0
55	MG	YA	3521	1/1	0.95	0.16	16,16,16,16	0
55	MG	RA	3383	1/1	0.95	0.06	29,29,29,29	0
55	MG	YA	3078	1/1	0.95	0.21	25,25,25,25	0
55	MG	YA	3308	1/1	0.95	0.09	39,39,39,39	0
55	MG	YA	3081	1/1	0.95	0.16	18,18,18,18	0
55	MG	YA	3083	1/1	0.95	0.11	8,8,8,8	0
55	MG	XA	1674	1/1	0.95	0.12	40,40,40,40	0
55	MG	YA	3531	1/1	0.95	0.06	40,40,40,40	0
55	MG	YA	3416	1/1	0.95	0.09	25,25,25,25	0
55	MG	RA	3469	1/1	0.95	0.05	31,31,31,31	0
55	MG	QA	1606	1/1	0.95	0.05	36,36,36,36	0
55	MG	YA	3088	1/1	0.95	0.12	6,6,6,6	0
55	MG	YA	3538	1/1	0.95	0.12	31,31,31,31	0
55	MG	RA	3117	1/1	0.95	0.20	28,28,28,28	0
55	MG	RA	3308	1/1	0.95	0.04	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1613	1/1	0.95	0.09	29,29,29,29	0
55	MG	YA	3211	1/1	0.95	0.09	8,8,8,8	0
55	MG	RA	3473	1/1	0.95	0.12	29,29,29,29	0
55	MG	YA	3426	1/1	0.95	0.09	24,24,24,24	0
55	MG	YA	3214	1/1	0.95	0.06	21,21,21,21	0
55	MG	YA	3098	1/1	0.95	0.10	27,27,27,27	0
55	MG	RA	3343	1/1	0.95	0.06	24,24,24,24	0
55	MG	YA	3430	1/1	0.95	0.07	29,29,29,29	0
55	MG	YA	3431	1/1	0.95	0.07	27,27,27,27	0
55	MG	RA	3022	1/1	0.95	0.12	15,15,15,15	0
55	MG	XA	1617	1/1	0.95	0.14	14,14,14,14	0
55	MG	RA	3476	1/1	0.95	0.11	45,45,45,45	0
55	MG	XA	1619	1/1	0.95	0.23	25,25,25,25	0
55	MG	XA	1621	1/1	0.95	0.11	35,35,35,35	0
55	MG	RA	3008	1/1	0.95	0.20	31,31,31,31	0
55	MG	YA	3440	1/1	0.95	0.09	27,27,27,27	0
55	MG	RA	3211	1/1	0.95	0.10	42,42,42,42	0
55	MG	QA	1663	1/1	0.95	0.23	22,22,22,22	0
55	MG	YA	3445	1/1	0.95	0.11	37,37,37,37	0
55	MG	XA	1626	1/1	0.95	0.05	33,33,33,33	0
55	MG	YA	3120	1/1	0.95	0.09	33,33,33,33	0
55	MG	YR	202	1/1	0.95	0.23	36,36,36,36	0
55	MG	YA	3448	1/1	0.95	0.05	31,31,31,31	0
55	MG	RA	3349	1/1	0.95	0.04	31,31,31,31	0
55	MG	YA	3125	1/1	0.95	0.07	40,40,40,40	0
55	MG	YA	3341	1/1	0.95	0.12	31,31,31,31	0
55	MG	RA	3091	1/1	0.95	0.05	13,13,13,13	0
55	MG	XM	201	1/1	0.95	0.12	77,77,77,77	0
55	MG	RA	3434	1/1	0.95	0.10	22,22,22,22	0
55	MG	YA	3133	1/1	0.95	0.08	5,5,5,5	0
55	MG	XN	101	1/1	0.95	0.05	52,52,52,52	0
55	MG	RA	3395	1/1	0.95	0.05	35,35,35,35	0
56	SF4	XD	301	8/8	0.95	0.10	127,140,142,159	0
55	MG	RA	3028	1/1	0.95	0.24	33,33,33,33	0
55	MG	QA	1639	1/1	0.95	0.14	28,28,28,28	0
57	ZN	Y9	101	1/1	0.95	0.06	44,44,44,44	0
55	MG	QA	1622	1/1	0.96	0.15	31,31,31,31	0
55	MG	RA	3015	1/1	0.96	0.07	7,7,7,7	0
55	MG	YA	3287	1/1	0.96	0.05	28,28,28,28	0
55	MG	RA	3093	1/1	0.96	0.12	16,16,16,16	0
55	MG	RA	3142	1/1	0.96	0.10	30,30,30,30	0
55	MG	YA	3153	1/1	0.96	0.06	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3154	1/1	0.96	0.11	6,6,6,6	0
55	MG	RA	3283	1/1	0.96	0.23	40,40,40,40	0
55	MG	YA	3295	1/1	0.96	0.09	29,29,29,29	0
55	MG	YA	3439	1/1	0.96	0.21	11,11,11,11	0
55	MG	YA	3157	1/1	0.96	0.09	9,9,9,9	0
55	MG	RA	3232	1/1	0.96	0.05	24,24,24,24	0
55	MG	YA	3159	1/1	0.96	0.04	10,10,10,10	0
55	MG	RA	3465	1/1	0.96	0.16	16,16,16,16	0
55	MG	YA	3162	1/1	0.96	0.13	36,36,36,36	0
55	MG	RA	3285	1/1	0.96	0.07	24,24,24,24	0
55	MG	YA	3164	1/1	0.96	0.07	9,9,9,9	0
55	MG	XA	1627	1/1	0.96	0.07	30,30,30,30	0
55	MG	XA	1628	1/1	0.96	0.05	29,29,29,29	0
55	MG	XA	1630	1/1	0.96	0.19	18,18,18,18	0
55	MG	XA	1631	1/1	0.96	0.08	29,29,29,29	0
55	MG	XA	1633	1/1	0.96	0.05	20,20,20,20	0
55	MG	YA	3020	1/1	0.96	0.11	12,12,12,12	0
55	MG	RA	3094	1/1	0.96	0.05	23,23,23,23	0
55	MG	RA	3468	1/1	0.96	0.07	30,30,30,30	0
55	MG	RA	3342	1/1	0.96	0.04	33,33,33,33	0
55	MG	YA	3459	1/1	0.96	0.06	26,26,26,26	0
55	MG	YA	3175	1/1	0.96	0.21	19,19,19,19	0
55	MG	RA	3405	1/1	0.96	0.15	15,15,15,15	0
55	MG	YA	3316	1/1	0.96	0.07	23,23,23,23	0
55	MG	QA	1603	1/1	0.96	0.20	18,18,18,18	0
55	MG	YA	3464	1/1	0.96	0.17	25,25,25,25	0
55	MG	RA	3235	1/1	0.96	0.17	39,39,39,39	0
55	MG	RA	3096	1/1	0.96	0.07	12,12,12,12	0
55	MG	YA	3180	1/1	0.96	0.08	5,5,5,5	0
55	MG	RA	3098	1/1	0.96	0.15	18,18,18,18	0
55	MG	RA	3051	1/1	0.96	0.13	25,25,25,25	0
55	MG	YA	3324	1/1	0.96	0.14	19,19,19,19	0
55	MG	RA	3017	1/1	0.96	0.16	9,9,9,9	0
55	MG	RA	3102	1/1	0.96	0.19	34,34,34,34	0
55	MG	RA	3479	1/1	0.96	0.10	26,26,26,26	0
55	MG	RA	3104	1/1	0.96	0.14	28,28,28,28	0
55	MG	YA	3046	1/1	0.96	0.12	4,4,4,4	0
55	MG	YA	3190	1/1	0.96	0.10	32,32,32,32	0
55	MG	YA	3191	1/1	0.96	0.09	20,20,20,20	0
55	MG	YA	3047	1/1	0.96	0.11	3,3,3,3	0
55	MG	RA	3481	1/1	0.96	0.12	37,37,37,37	0
55	MG	YA	3194	1/1	0.96	0.14	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3244	1/1	0.96	0.04	18,18,18,18	0
55	MG	RA	3296	1/1	0.96	0.12	33,33,33,33	0
55	MG	QF	201	1/1	0.96	0.08	30,30,30,30	0
55	MG	QA	1612	1/1	0.96	0.09	30,30,30,30	0
55	MG	RA	3110	1/1	0.96	0.06	28,28,28,28	0
55	MG	YA	3060	1/1	0.96	0.11	17,17,17,17	0
55	MG	QA	1602	1/1	0.96	0.16	33,33,33,33	0
55	MG	YA	3068	1/1	0.96	0.07	4,4,4,4	0
55	MG	YA	3070	1/1	0.96	0.07	17,17,17,17	0
55	MG	YA	3492	1/1	0.96	0.11	57,57,57,57	0
55	MG	RA	3420	1/1	0.96	0.08	43,43,43,43	0
55	MG	YA	3076	1/1	0.96	0.11	17,17,17,17	0
55	MG	RB	204	1/1	0.96	0.17	15,15,15,15	0
55	MG	YA	3079	1/1	0.96	0.07	18,18,18,18	0
55	MG	YA	3080	1/1	0.96	0.16	1,1,1,1	0
55	MG	RA	3359	1/1	0.96	0.16	41,41,41,41	0
55	MG	YA	3500	1/1	0.96	0.22	27,27,27,27	0
55	MG	YA	3213	1/1	0.96	0.05	17,17,17,17	0
55	MG	RA	3360	1/1	0.96	0.07	40,40,40,40	0
55	MG	YA	3215	1/1	0.96	0.10	32,32,32,32	0
55	MG	RA	3361	1/1	0.96	0.04	32,32,32,32	0
55	MG	RA	3001	1/1	0.96	0.12	17,17,17,17	0
55	MG	YA	3218	1/1	0.96	0.18	30,30,30,30	0
55	MG	RA	3065	1/1	0.96	0.12	28,28,28,28	0
55	MG	YA	3087	1/1	0.96	0.12	13,13,13,13	0
55	MG	RA	3066	1/1	0.96	0.10	18,18,18,18	0
55	MG	QA	1607	1/1	0.96	0.10	52,52,52,52	0
55	MG	RA	3428	1/1	0.96	0.04	18,18,18,18	0
55	MG	RN	201	1/1	0.96	0.06	34,34,34,34	0
55	MG	YA	3514	1/1	0.96	0.11	11,11,11,11	0
55	MG	YA	3092	1/1	0.96	0.12	10,10,10,10	0
55	MG	YA	3370	1/1	0.96	0.10	20,20,20,20	0
55	MG	YA	3093	1/1	0.96	0.11	9,9,9,9	0
55	MG	YA	3520	1/1	0.96	0.18	6,6,6,6	0
55	MG	XA	1670	1/1	0.96	0.09	42,42,42,42	0
55	MG	RA	3003	1/1	0.96	0.19	31,31,31,31	0
55	MG	YA	3231	1/1	0.96	0.13	38,38,38,38	0
55	MG	YA	3525	1/1	0.96	0.23	1,1,1,1	0
55	MG	YA	3100	1/1	0.96	0.14	19,19,19,19	0
55	MG	QA	1634	1/1	0.96	0.10	28,28,28,28	0
55	MG	RA	3205	1/1	0.96	0.15	36,36,36,36	0
55	MG	YA	3103	1/1	0.96	0.13	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	QA	1644	1/1	0.96	0.15	45,45,45,45	0
55	MG	XA	1675	1/1	0.96	0.11	48,48,48,48	0
55	MG	YA	3109	1/1	0.96	0.14	19,19,19,19	0
55	MG	QA	1627	1/1	0.96	0.07	39,39,39,39	0
55	MG	YA	3536	1/1	0.96	0.07	10,10,10,10	0
55	MG	QA	1615	1/1	0.96	0.15	44,44,44,44	0
55	MG	RA	3077	1/1	0.96	0.11	17,17,17,17	0
55	MG	QA	1657	1/1	0.96	0.18	56,56,56,56	0
55	MG	QA	1658	1/1	0.96	0.07	32,32,32,32	0
55	MG	RA	3080	1/1	0.96	0.18	26,26,26,26	0
55	MG	R1	102	1/1	0.96	0.11	45,45,45,45	0
55	MG	YA	3247	1/1	0.96	0.13	36,36,36,36	0
55	MG	YB	202	1/1	0.96	0.12	10,10,10,10	0
55	MG	YA	3122	1/1	0.96	0.14	37,37,37,37	0
55	MG	RA	3038	1/1	0.96	0.06	14,14,14,14	0
55	MG	RA	3318	1/1	0.96	0.06	18,18,18,18	0
55	MG	QA	1647	1/1	0.96	0.11	21,21,21,21	0
55	MG	YA	3127	1/1	0.96	0.17	7,7,7,7	0
55	MG	YA	3253	1/1	0.96	0.14	7,7,7,7	0
55	MG	YA	3398	1/1	0.96	0.12	28,28,28,28	0
55	MG	YA	3128	1/1	0.96	0.29	35,35,35,35	0
55	MG	YA	3257	1/1	0.96	0.13	15,15,15,15	0
55	MG	RA	3382	1/1	0.96	0.14	42,42,42,42	0
55	MG	YA	3130	1/1	0.96	0.11	22,22,22,22	0
55	MG	YA	3131	1/1	0.96	0.09	22,22,22,22	0
55	MG	RA	3041	1/1	0.96	0.10	16,16,16,16	0
55	MG	YA	3406	1/1	0.96	0.09	13,13,13,13	0
55	MG	YA	3264	1/1	0.96	0.12	13,13,13,13	0
55	MG	YA	3408	1/1	0.96	0.16	30,30,30,30	0
55	MG	RA	3173	1/1	0.96	0.09	25,25,25,25	0
55	MG	RA	3086	1/1	0.96	0.16	16,16,16,16	0
55	MG	RA	3133	1/1	0.96	0.12	26,26,26,26	0
55	MG	RA	3220	1/1	0.96	0.14	18,18,18,18	0
55	MG	RA	3042	1/1	0.96	0.20	27,27,27,27	0
55	MG	YA	3138	1/1	0.96	0.07	28,28,28,28	0
55	MG	YA	3418	1/1	0.96	0.13	32,32,32,32	0
55	MG	YA	3273	1/1	0.96	0.19	35,35,35,35	0
55	MG	RA	3222	1/1	0.96	0.16	16,16,16,16	0
55	MG	YA	3275	1/1	0.96	0.16	5,5,5,5	0
55	MG	RA	3089	1/1	0.96	0.15	9,9,9,9	0
55	MG	RA	3224	1/1	0.96	0.09	19,19,19,19	0
55	MG	RA	3276	1/1	0.96	0.06	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3145	1/1	0.96	0.07	6,6,6,6	0
55	MG	RA	3136	1/1	0.96	0.12	30,30,30,30	0
55	MG	RA	3045	1/1	0.96	0.24	32,32,32,32	0
55	MG	YA	3283	1/1	0.96	0.20	9,9,9,9	0
55	MG	RA	3237	1/1	0.97	0.18	27,27,27,27	0
55	MG	XE	201	1/1	0.97	0.12	64,64,64,64	0
55	MG	QA	1672	1/1	0.97	0.14	45,45,45,45	0
55	MG	RA	3010	1/1	0.97	0.06	20,20,20,20	0
55	MG	RA	3105	1/1	0.97	0.12	50,50,50,50	0
55	MG	QA	1610	1/1	0.97	0.14	12,12,12,12	0
55	MG	RA	3242	1/1	0.97	0.13	19,19,19,19	0
55	MG	RA	3033	1/1	0.97	0.07	9,9,9,9	0
55	MG	YA	3373	1/1	0.97	0.05	18,18,18,18	0
55	MG	YA	3374	1/1	0.97	0.06	18,18,18,18	0
55	MG	YA	3480	1/1	0.97	0.12	34,34,34,34	0
55	MG	RA	3108	1/1	0.97	0.04	20,20,20,20	0
55	MG	RA	3245	1/1	0.97	0.12	28,28,28,28	0
55	MG	YA	3182	1/1	0.97	0.24	25,25,25,25	0
55	MG	YA	3001	1/1	0.97	0.13	26,26,26,26	0
55	MG	YA	3184	1/1	0.97	0.07	20,20,20,20	0
55	MG	RR	201	1/1	0.97	0.11	22,22,22,22	0
55	MG	YA	3097	1/1	0.97	0.16	1,1,1,1	0
55	MG	XA	1646	1/1	0.97	0.16	27,27,27,27	0
55	MG	YA	3099	1/1	0.97	0.07	14,14,14,14	0
55	MG	YA	3282	1/1	0.97	0.14	16,16,16,16	0
55	MG	YA	3004	1/1	0.97	0.05	16,16,16,16	0
55	MG	RA	3109	1/1	0.97	0.05	35,35,35,35	0
55	MG	YA	3285	1/1	0.97	0.13	21,21,21,21	0
55	MG	YA	3007	1/1	0.97	0.10	39,39,39,39	0
55	MG	YA	3496	1/1	0.97	0.11	26,26,26,26	0
55	MG	RA	3457	1/1	0.97	0.09	18,18,18,18	0
55	MG	YA	3105	1/1	0.97	0.12	2,2,2,2	0
55	MG	RA	3035	1/1	0.97	0.12	24,24,24,24	0
55	MG	YA	3107	1/1	0.97	0.08	10,10,10,10	0
55	MG	YA	3196	1/1	0.97	0.14	27,27,27,27	0
55	MG	RA	3248	1/1	0.97	0.18	38,38,38,38	0
55	MG	YA	3294	1/1	0.97	0.04	42,42,42,42	0
55	MG	RA	3145	1/1	0.97	0.17	21,21,21,21	0
55	MG	RA	3373	1/1	0.97	0.05	16,16,16,16	0
55	MG	RA	3463	1/1	0.97	0.11	12,12,12,12	0
55	MG	QA	1601	1/1	0.97	0.14	37,37,37,37	0
55	MG	YA	3114	1/1	0.97	0.08	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3509	1/1	0.97	0.05	15,15,15,15	0
55	MG	RA	3037	1/1	0.97	0.14	12,12,12,12	0
55	MG	XA	1602	1/1	0.97	0.04	22,22,22,22	0
55	MG	YA	3302	1/1	0.97	0.09	4,4,4,4	0
55	MG	YA	3117	1/1	0.97	0.14	13,13,13,13	0
55	MG	RA	3082	1/1	0.97	0.16	8,8,8,8	0
55	MG	YA	3019	1/1	0.97	0.15	1,1,1,1	0
55	MG	YA	3209	1/1	0.97	0.06	10,10,10,10	0
55	MG	QA	1621	1/1	0.97	0.20	24,24,24,24	0
55	MG	RA	3181	1/1	0.97	0.07	52,52,52,52	0
55	MG	YA	3022	1/1	0.97	0.14	4,4,4,4	0
55	MG	RA	3058	1/1	0.97	0.13	11,11,11,11	0
55	MG	RA	3183	1/1	0.97	0.14	23,23,23,23	0
55	MG	YA	3026	1/1	0.97	0.17	13,13,13,13	0
55	MG	YA	3526	1/1	0.97	0.29	32,32,32,32	0
55	MG	XA	1662	1/1	0.97	0.14	33,33,33,33	0
55	MG	YA	3314	1/1	0.97	0.08	28,28,28,28	0
55	MG	YA	3030	1/1	0.97	0.10	1,1,1,1	0
55	MG	RA	3039	1/1	0.97	0.11	21,21,21,21	0
55	MG	RA	3087	1/1	0.97	0.20	21,21,21,21	0
55	MG	RA	3062	1/1	0.97	0.12	16,16,16,16	0
55	MG	YA	3533	1/1	0.97	0.06	1,1,1,1	0
55	MG	YA	3035	1/1	0.97	0.13	15,15,15,15	0
55	MG	YA	3320	1/1	0.97	0.06	18,18,18,18	0
55	MG	XA	1666	1/1	0.97	0.05	30,30,30,30	0
55	MG	RA	3063	1/1	0.97	0.16	23,23,23,23	0
55	MG	RA	3064	1/1	0.97	0.12	32,32,32,32	0
55	MG	RA	3300	1/1	0.97	0.14	15,15,15,15	0
55	MG	RA	3023	1/1	0.97	0.11	9,9,9,9	0
55	MG	YA	3141	1/1	0.97	0.11	5,5,5,5	0
55	MG	QA	1638	1/1	0.97	0.06	26,26,26,26	0
55	MG	YA	3328	1/1	0.97	0.08	19,19,19,19	0
55	MG	RA	3389	1/1	0.97	0.07	24,24,24,24	0
55	MG	YB	203	1/1	0.97	0.12	40,40,40,40	0
55	MG	YB	204	1/1	0.97	0.15	20,20,20,20	0
55	MG	RA	3345	1/1	0.97	0.17	25,25,25,25	0
55	MG	RA	3124	1/1	0.97	0.05	25,25,25,25	0
55	MG	YA	3234	1/1	0.97	0.07	26,26,26,26	0
55	MG	RA	3483	1/1	0.97	0.06	19,19,19,19	0
55	MG	XA	1620	1/1	0.97	0.22	32,32,32,32	0
55	MG	YA	3441	1/1	0.97	0.10	4,4,4,4	0
55	MG	YA	3442	1/1	0.97	0.17	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3052	1/1	0.97	0.14	15,15,15,15	0
55	MG	RA	3227	1/1	0.97	0.16	28,28,28,28	0
55	MG	QA	1664	1/1	0.97	0.19	12,12,12,12	0
55	MG	RA	3044	1/1	0.97	0.11	20,20,20,20	0
55	MG	XA	1624	1/1	0.97	0.15	19,19,19,19	0
55	MG	RA	3069	1/1	0.97	0.08	11,11,11,11	0
55	MG	YA	3066	1/1	0.97	0.17	10,10,10,10	0
55	MG	YA	3067	1/1	0.97	0.12	32,32,32,32	0
55	MG	QA	1609	1/1	0.97	0.14	16,16,16,16	0
55	MG	YA	3069	1/1	0.97	0.17	13,13,13,13	0
55	MG	YQ	203	1/1	0.97	0.11	34,34,34,34	0
55	MG	YA	3160	1/1	0.97	0.13	23,23,23,23	0
55	MG	RA	3097	1/1	0.97	0.07	13,13,13,13	0
55	MG	RA	3071	1/1	0.97	0.10	20,20,20,20	0
55	MG	YA	3073	1/1	0.97	0.08	11,11,11,11	0
55	MG	YA	3074	1/1	0.97	0.07	4,4,4,4	0
55	MG	YA	3353	1/1	0.97	0.11	3,3,3,3	0
55	MG	YA	3165	1/1	0.97	0.07	22,22,22,22	0
55	MG	YA	3075	1/1	0.97	0.11	13,13,13,13	0
55	MG	RA	3354	1/1	0.97	0.18	36,36,36,36	0
55	MG	XA	1688	1/1	0.97	0.12	15,15,15,15	0
55	MG	YA	3258	1/1	0.97	0.12	15,15,15,15	0
55	MG	YA	3359	1/1	0.97	0.05	11,11,11,11	0
55	MG	RA	3132	1/1	0.97	0.18	19,19,19,19	0
55	MG	RA	3046	1/1	0.97	0.05	23,23,23,23	0
55	MG	YA	3261	1/1	0.97	0.17	6,6,6,6	0
55	MG	RA	3074	1/1	0.97	0.05	20,20,20,20	0
55	MG	YA	3516	1/1	0.98	0.16	4,4,4,4	0
55	MG	RA	3048	1/1	0.98	0.18	6,6,6,6	0
55	MG	RA	3056	1/1	0.98	0.23	6,6,6,6	0
55	MG	YA	3071	1/1	0.98	0.13	20,20,20,20	0
55	MG	YA	3334	1/1	0.98	0.12	16,16,16,16	0
55	MG	YA	3123	1/1	0.98	0.11	15,15,15,15	0
55	MG	YA	3523	1/1	0.98	0.09	1,1,1,1	0
55	MG	RA	3103	1/1	0.98	0.09	12,12,12,12	0
55	MG	XA	1629	1/1	0.98	0.11	8,8,8,8	0
55	MG	RA	3118	1/1	0.98	0.10	23,23,23,23	0
55	MG	YA	3025	1/1	0.98	0.11	6,6,6,6	0
55	MG	RA	3043	1/1	0.98	0.06	4,4,4,4	0
55	MG	YA	3230	1/1	0.98	0.05	8,8,8,8	0
55	MG	RA	3461	1/1	0.98	0.10	3,3,3,3	0
55	MG	YA	3343	1/1	0.98	0.13	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3028	1/1	0.98	0.10	8,8,8,8	0
55	MG	YA	3029	1/1	0.98	0.14	13,13,13,13	0
55	MG	RB	202	1/1	0.98	0.04	56,56,56,56	0
55	MG	RA	3187	1/1	0.98	0.23	30,30,30,30	0
55	MG	RA	3301	1/1	0.98	0.15	22,22,22,22	0
55	MG	YA	3349	1/1	0.98	0.12	34,34,34,34	0
55	MG	YA	3292	1/1	0.98	0.17	23,23,23,23	0
55	MG	YA	3413	1/1	0.98	0.06	9,9,9,9	0
55	MG	XA	1667	1/1	0.98	0.24	27,27,27,27	0
55	MG	RA	3366	1/1	0.98	0.05	27,27,27,27	0
55	MG	RA	3367	1/1	0.98	0.04	19,19,19,19	0
55	MG	YA	3037	1/1	0.98	0.17	4,4,4,4	0
55	MG	YA	3039	1/1	0.98	0.06	1,1,1,1	0
55	MG	YA	3140	1/1	0.98	0.07	26,26,26,26	0
55	MG	YA	3040	1/1	0.98	0.14	7,7,7,7	0
55	MG	YB	205	1/1	0.98	0.15	18,18,18,18	0
55	MG	YA	3482	1/1	0.98	0.11	47,47,47,47	0
55	MG	QA	1608	1/1	0.98	0.05	21,21,21,21	0
55	MG	RA	3059	1/1	0.98	0.07	6,6,6,6	0
55	MG	RA	3060	1/1	0.98	0.04	21,21,21,21	0
55	MG	RA	3325	1/1	0.98	0.06	23,23,23,23	0
55	MG	YA	3095	1/1	0.98	0.04	1,1,1,1	0
55	MG	YA	3096	1/1	0.98	0.17	20,20,20,20	0
55	MG	YA	3148	1/1	0.98	0.06	4,4,4,4	0
55	MG	YA	3199	1/1	0.98	0.07	31,31,31,31	0
55	MG	RA	3009	1/1	0.98	0.17	24,24,24,24	0
55	MG	RA	3072	1/1	0.98	0.11	10,10,10,10	0
55	MG	YA	3254	1/1	0.98	0.14	2,2,2,2	0
55	MG	YD	303	1/1	0.98	0.06	10,10,10,10	0
55	MG	YE	301	1/1	0.98	0.17	1,1,1,1	0
55	MG	RA	3141	1/1	0.98	0.17	22,22,22,22	0
55	MG	YA	3433	1/1	0.98	0.11	30,30,30,30	0
55	MG	RA	3447	1/1	0.98	0.13	19,19,19,19	0
55	MG	RA	3212	1/1	0.98	0.07	14,14,14,14	0
55	MG	RA	3084	1/1	0.98	0.14	10,10,10,10	0
55	MG	RA	3331	1/1	0.98	0.05	26,26,26,26	0
55	MG	YA	3104	1/1	0.98	0.05	13,13,13,13	0
55	MG	YA	3055	1/1	0.98	0.15	11,11,11,11	0
55	MG	YA	3056	1/1	0.98	0.09	15,15,15,15	0
55	MG	YA	3012	1/1	0.98	0.08	18,18,18,18	0
55	MG	RA	3477	1/1	0.98	0.13	14,14,14,14	0
55	MG	RA	3032	1/1	0.98	0.08	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3144	1/1	0.98	0.14	21,21,21,21	0
55	MG	YA	3061	1/1	0.98	0.07	1,1,1,1	0
55	MG	YA	3269	1/1	0.98	0.21	16,16,16,16	0
55	MG	XA	1684	1/1	0.98	0.26	46,46,46,46	0
55	MG	YA	3271	1/1	0.98	0.18	7,7,7,7	0
55	MG	YA	3064	1/1	0.98	0.14	9,9,9,9	0
55	MG	RA	3012	1/1	0.98	0.11	17,17,17,17	0
57	ZN	QN	101	1/1	0.98	0.05	161,161,161,161	0
55	MG	RA	3099	1/1	0.98	0.12	14,14,14,14	0
57	ZN	R5	101	1/1	0.98	0.07	120,120,120,120	0
57	ZN	R6	101	1/1	0.98	0.04	66,66,66,66	0
57	ZN	R9	101	1/1	0.98	0.06	68,68,68,68	0
57	ZN	XN	102	1/1	0.98	0.05	120,120,120,120	0
55	MG	YA	3452	1/1	0.98	0.19	33,33,33,33	0
55	MG	RA	3054	1/1	0.98	0.15	11,11,11,11	0
55	MG	YA	3119	1/1	0.99	0.05	10,10,10,10	0
55	MG	RE	303	1/1	0.99	0.11	19,19,19,19	0
55	MG	YA	3121	1/1	0.99	0.05	4,4,4,4	0
55	MG	YA	3517	1/1	0.99	0.18	10,10,10,10	0
55	MG	YA	3255	1/1	0.99	0.16	11,11,11,11	0
55	MG	RA	3034	1/1	0.99	0.03	1,1,1,1	0
55	MG	RA	3125	1/1	0.99	0.11	2,2,2,2	0
55	MG	YA	3400	1/1	0.99	0.04	10,10,10,10	0
55	MG	YA	3063	1/1	0.99	0.04	4,4,4,4	0
55	MG	YA	3077	1/1	0.99	0.03	9,9,9,9	0
55	MG	XA	1636	1/1	0.99	0.03	28,28,28,28	0
55	MG	YA	3065	1/1	0.99	0.03	13,13,13,13	0
55	MG	YA	3053	1/1	0.99	0.09	15,15,15,15	0
55	MG	YA	3111	1/1	0.99	0.09	1,1,1,1	0
55	MG	YA	3054	1/1	0.99	0.11	1,1,1,1	0
55	MG	YA	3082	1/1	0.99	0.04	1,1,1,1	0
55	MG	RA	3024	1/1	0.99	0.07	21,21,21,21	0
55	MG	YA	3410	1/1	0.99	0.07	2,2,2,2	0
57	ZN	RY	202	1/1	0.99	0.04	102,102,102,102	0
55	MG	YA	3411	1/1	0.99	0.10	10,10,10,10	0
55	MG	RA	3025	1/1	0.99	0.10	1,1,1,1	0
55	MG	YA	3038	1/1	0.99	0.08	1,1,1,1	0
55	MG	YA	3369	1/1	0.99	0.08	13,13,13,13	0
55	MG	XA	1632	1/1	0.99	0.08	13,13,13,13	0
55	MG	YA	3048	1/1	0.99	0.12	14,14,14,14	0
57	ZN	Y5	101	1/1	0.99	0.03	66,66,66,66	0
55	MG	YA	3155	1/1	0.99	0.09	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	ZN	YY	201	1/1	1.00	0.01	60,60,60,60	0
55	MG	YA	3005	1/1	1.00	0.03	8,8,8,8	0
55	MG	YA	3229	1/1	1.00	0.02	2,2,2,2	0
57	ZN	Y6	101	1/1	1.00	0.12	70,70,70,70	0
55	MG	YA	3033	1/1	1.00	0.02	1,1,1,1	0

6.5 Other polymers [i](#)

There are no such residues in this entry.