wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2026 – 04:15 AM EDT

PDB ID	:	6OXA / pdb_00006oxa
Title	:	Dimeric E.coli YoeB bound to Thermus thermophilus 70S pre-cleavage (AAU)
Authors	:	Pavelich, I.J.; Hoffer, E.D.; Maehigashi, T.; Dunham, C.M.
Deposited on	:	2019-05-13
Resolution	:	3.25 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 (i) 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 (i)) were used in the production of this report:

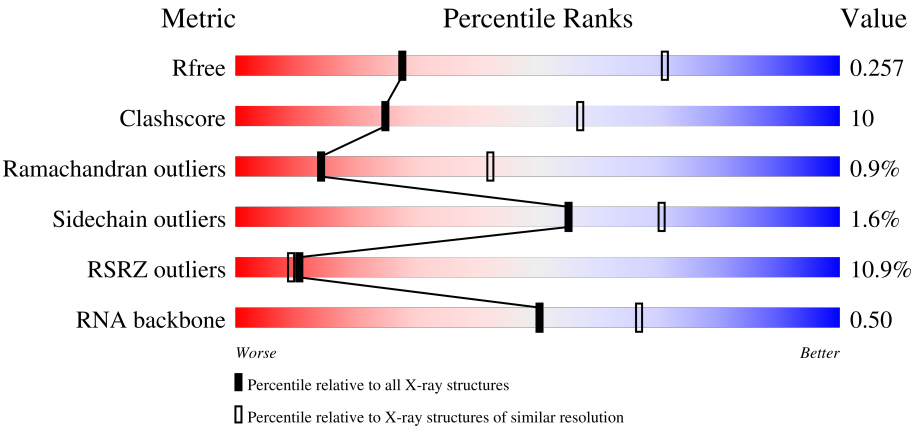
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)
RNA backbone	3983	1006 (3.54-2.98)

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 <=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	3% 57% 34% 8%
1	XA	1521	3% 59% 31% 8%
2	QB	256	8% 32% 51% 7% 8%
2	XB	256	12% 78% 14% 8%

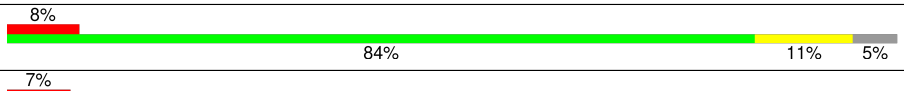
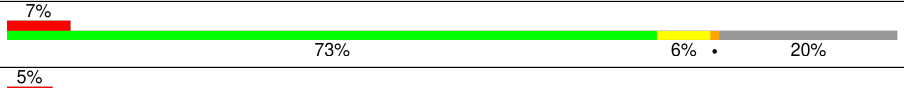
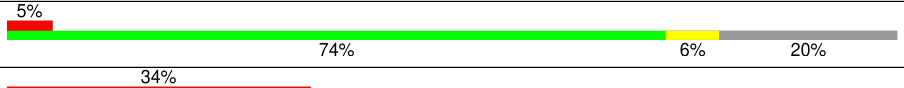
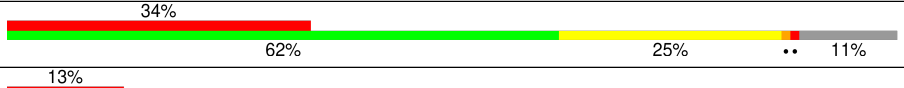
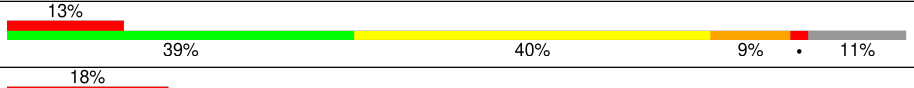
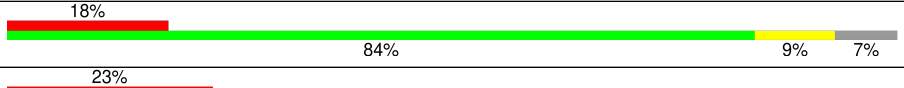
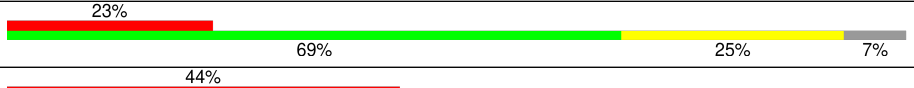
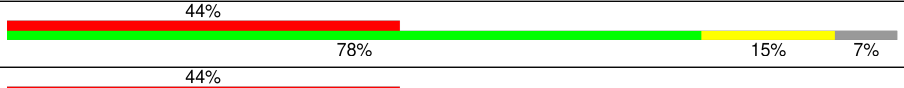
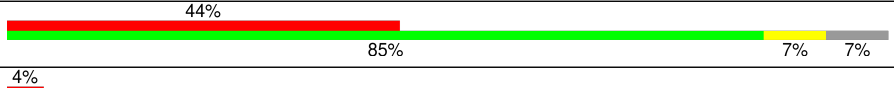
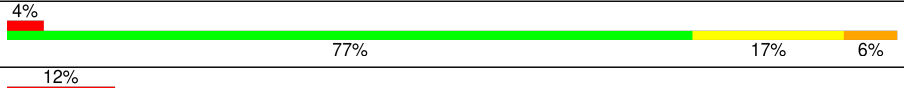
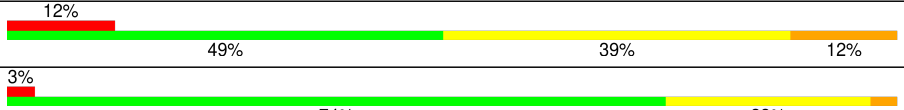
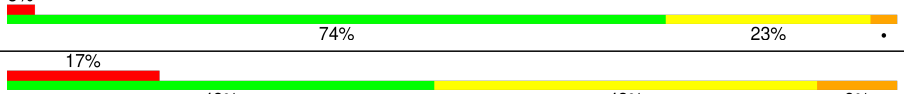
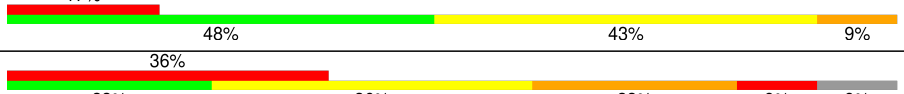
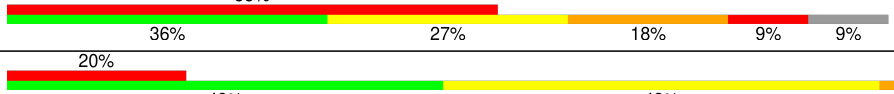
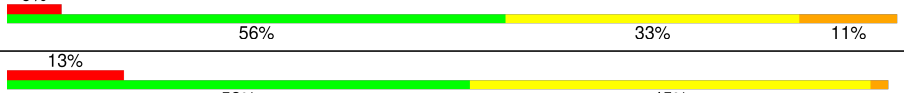
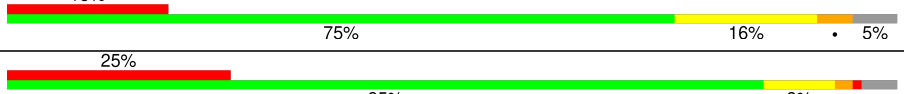
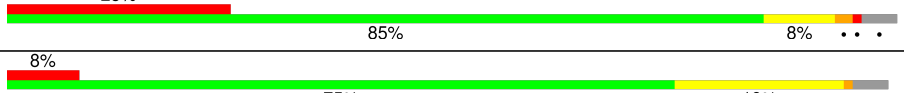
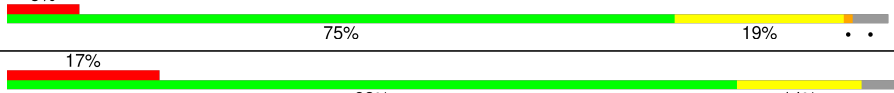
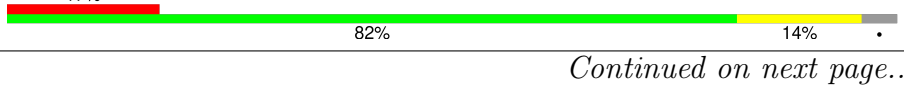
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Mol	Chain	Length	Quality of chain
3	QC	239	8% 70% 15% 14%
3	XC	239	3% 76% 10% 14%
4	QD	209	14% 79% 20%
4	XD	209	17% 78% 21%
5	QE	162	12% 83% 10% 7%
5	XE	162	7% 81% 12% 7%
6	QF	101	4% 89% 11%
6	XF	101	12% 82% 18%
7	QG	156	17% 90% 8%
7	XG	156	22% 88% 11%
8	QH	138	16% 79% 18%
8	XH	138	9% 81% 17%
9	QI	128	22% 72% 27%
9	XI	128	23% 78% 20%
10	QJ	105	35% 80% 14% 6%
10	XJ	105	20% 63% 29% 9%
11	QK	129	20% 80% 12% 8%
11	XK	129	12% 78% 12% 10%
12	QM	126	23% 70% 22% 5%
12	XM	126	22% 79% 13% 6%
13	QN	61	39% 74% 25%
13	XN	61	28% 87% 11%
14	QO	89	11% 88% 11%
14	XO	89	3% 84% 13%
15	QP	88	8% 88% 8% 5%

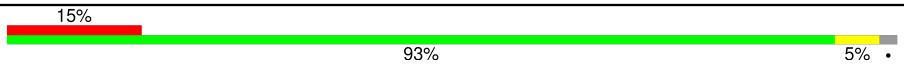
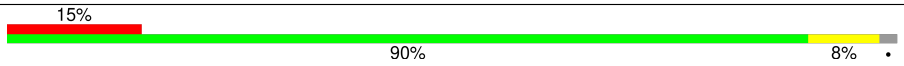
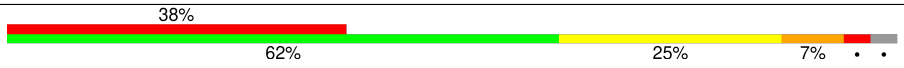
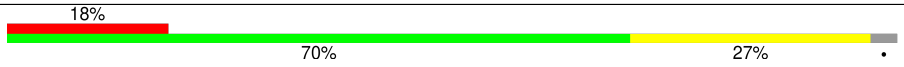
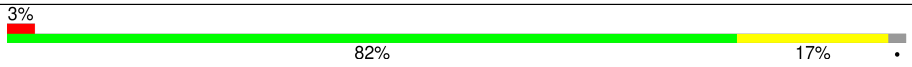
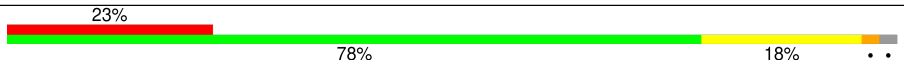
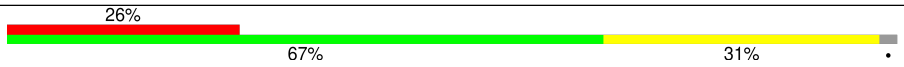
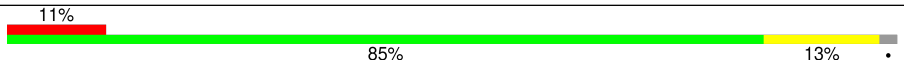
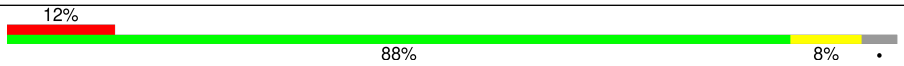
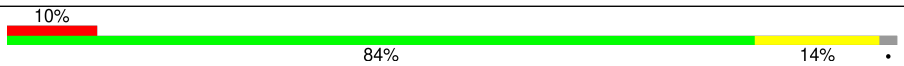
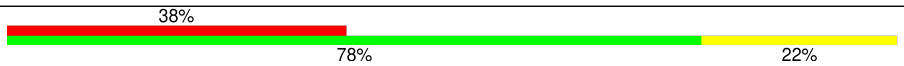
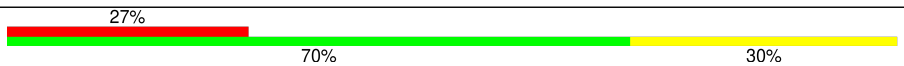
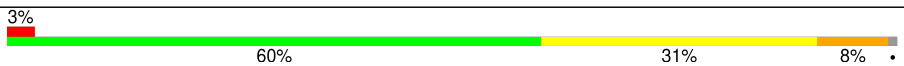
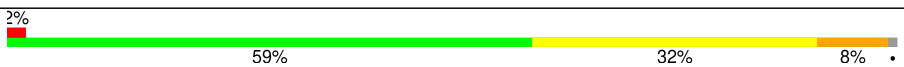
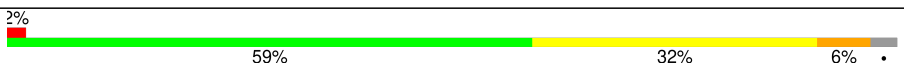
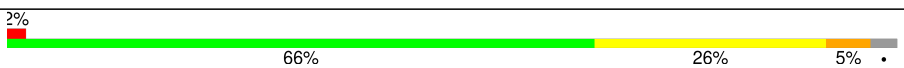
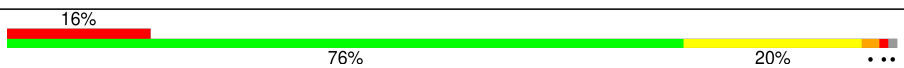
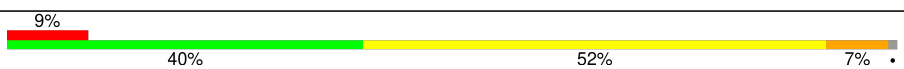
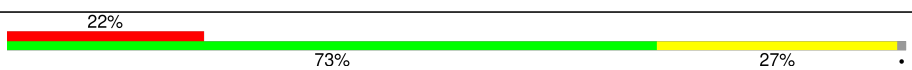
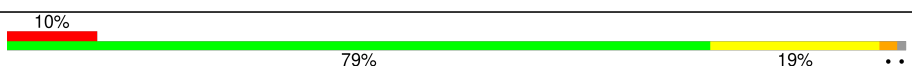
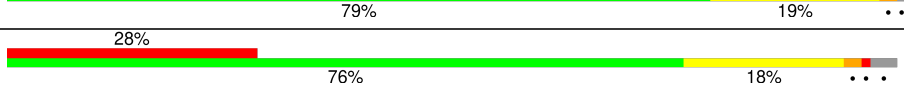
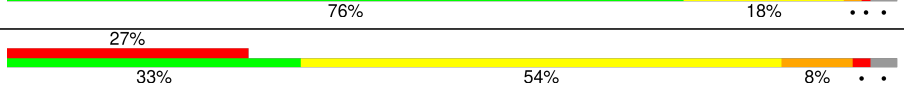
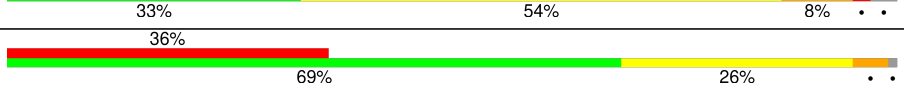
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Mol	Chain	Length	Quality of chain
15	XP	88	
16	QQ	105	
16	XQ	105	
17	QR	88	
17	XR	88	
18	QS	93	
18	XS	93	
19	QT	106	
19	XT	106	
20	QU	27	
20	XU	27	
21	QV	77	
21	QW	77	
21	XV	77	
21	XW	77	
22	QX	22	
22	XX	22	
23	QY	84	
23	QZ	84	
23	XY	84	
23	XZ	84	
24	R0	85	
24	Y0	85	
25	R2	72	
25	Y2	72	

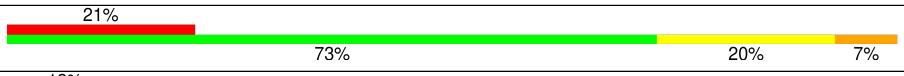
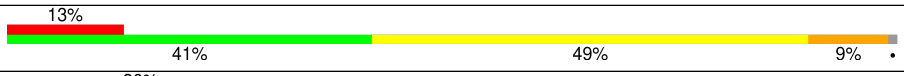
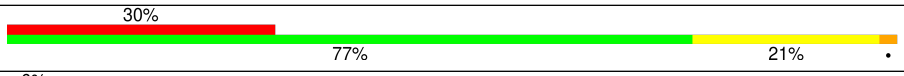
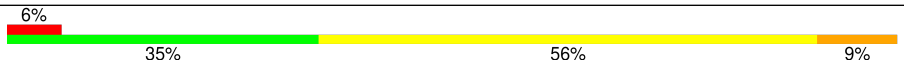
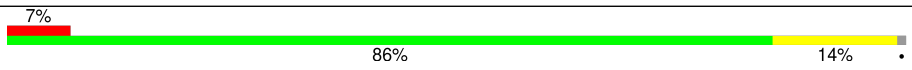
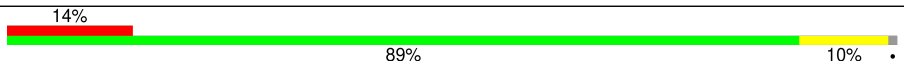
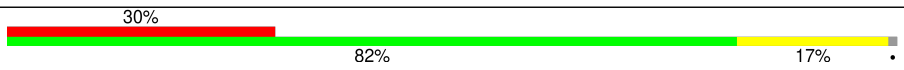
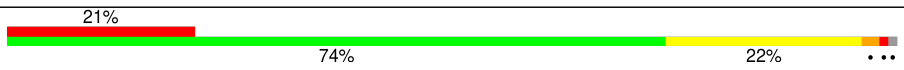
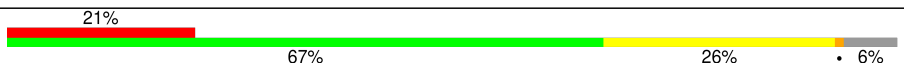
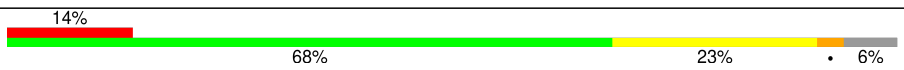
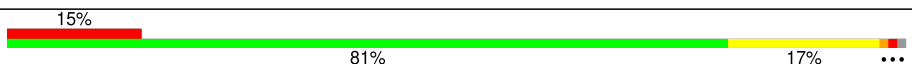
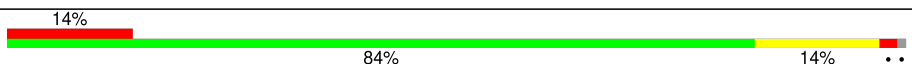
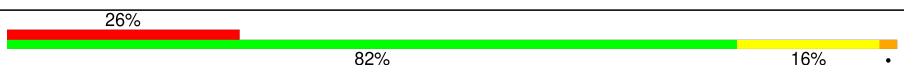
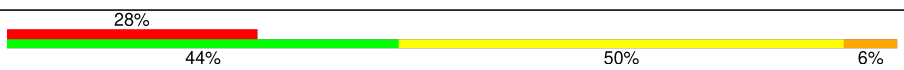
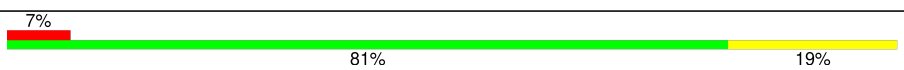
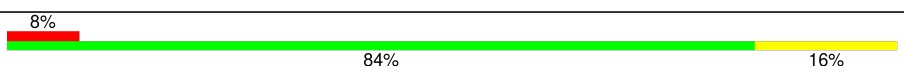
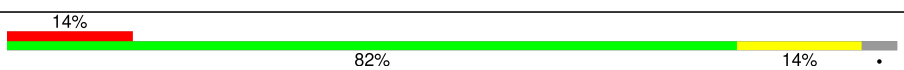
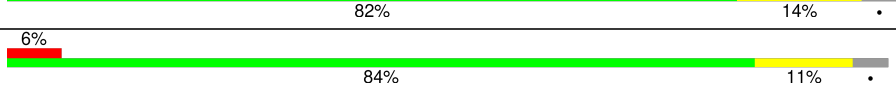
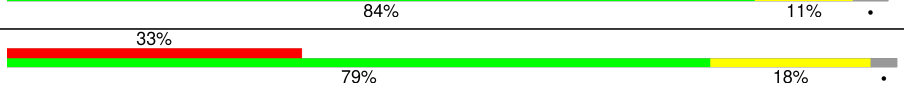
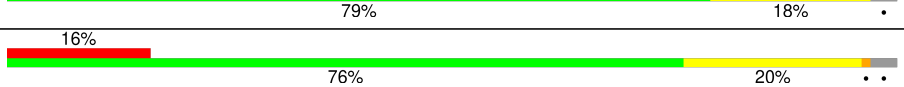
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Mol	Chain	Length	Quality of chain
26	R3	60	
26	Y3	60	
27	R4	71	
27	Y4	71	
28	R5	60	
28	Y5	60	
29	R6	54	
29	Y6	54	
30	R7	49	
30	Y7	49	
31	R9	37	
31	Y9	37	
32	RA	2915	
32	YA	2915	
33	RB	124	
33	YB	124	
34	RD	276	
34	YD	276	
35	RE	206	
35	YE	206	
36	RG	182	
36	YG	182	
37	RH	180	
37	YH	180	
38	RI	148	

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Mol	Chain	Length	Quality of chain
38	YI	148	
39	RN	140	
39	YN	140	
40	RO	122	
40	YO	122	
41	RP	150	
41	YP	150	
42	RQ	141	
42	YQ	141	
43	RR	118	
43	YR	118	
44	RS	112	
44	YS	112	
45	RT	146	
45	YT	146	
46	RU	118	
46	YU	118	
47	RV	101	
47	YV	101	
48	RW	113	
48	YW	113	
49	RX	96	
49	YX	96	
50	RY	110	
50	YY	110	

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Mol	Chain	Length	Quality of chain
51	QL	132	19% 67% 25% 5%
51	XL	132	14% 77% 14% 8%
52	R1	98	42% 57% 38%
52	Y1	98	26% 81% 12% 5%
53	R8	65	17% 57% 40%
53	Y8	65	38% 72% 20% 6%
54	RF	210	9% 61% 33%
54	YF	210	8% 80% 16%
55	RZ	206	13% 44% 41% 11%
55	YZ	206	10% 58% 30% 11%
56	ZA	3	33% 67%
56	ZB	3	67% 33%

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
57	MG	QA	1637	-	-	-	X
57	MG	RA	3001	-	-	-	X
57	MG	RA	3126	-	-	-	X
57	MG	RQ	201	-	-	-	X
57	MG	XA	1710	-	-	-	X
57	MG	XD	302	-	-	-	X
57	MG	YA	3096	-	-	-	X
57	MG	YD	302	-	-	-	X

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 298432 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	1510	Total	C	N	O	P	0	0	0
			32452	14444	6009	10489	1510			
1	XA	1507	Total	C	N	O	P	0	0	0
			32389	14416	5999	10467	1507			

- 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 S13.

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

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

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

- Molecule 16 is a protein called 30S ribosomal protein S17.

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

- Molecule 17 is a protein called 30S ribosomal protein S18.

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

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
18	XS	83	Total	C	N	O	S	0	0	0
			656	418	123	113	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

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

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

- Molecule 21 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	QV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
21	QW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
21	XV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
21	XW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QX	20	Total	C	N	O	P	0	0	0
			435	198	87	131	19			
22	XX	20	Total	C	N	O	P	0	0	0
			435	198	87	131	19			

- Molecule 23 is a protein called Addiction module toxin, Txe/YoeB family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QY	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
23	QZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
23	XY	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
23	XZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			
24	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 26 is a protein called 50S ribosomal protein L30.

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

- Molecule 27 is a protein called 50S ribosomal protein L31.

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

- Molecule 28 is a protein called 50S ribosomal protein L32.

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

- Molecule 29 is a protein called 50S ribosomal protein L33.

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

- Molecule 30 is a protein called 50S ribosomal protein L34.

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

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

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

- Molecule 32 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	RA	2891	Total	C	N	O	P	0	0	0
			62266	27713	11649	20014	2890			
32	YA	2875	Total	C	N	O	P	0	0	0
			61921	27560	11583	19904	2874			

- Molecule 33 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	RB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			
33	YB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			

- Molecule 34 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
34	YD	274	Total	C	N	O	S	0	0	0
			2135	1347	426	359	3			

- Molecule 35 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
35	YE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 36 is a protein called 50S ribosomal protein L5.

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

- Molecule 37 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
37	YH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 38 is a protein called 50S ribosomal protein L9.

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

- Molecule 39 is a protein called 50S ribosomal protein L13.

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

- Molecule 40 is a protein called 50S ribosomal protein L14.

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

- Molecule 41 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

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

- Molecule 42 is a protein called 50S ribosomal protein L16.

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

- Molecule 43 is a protein called 50S ribosomal protein L17.

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

- Molecule 44 is a protein called 50S ribosomal protein L18.

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

- Molecule 45 is a protein called 50S ribosomal protein L19.

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

- Molecule 46 is a protein called 50S ribosomal protein L20.

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

- Molecule 47 is a protein called 50S ribosomal protein L21.

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

- Molecule 48 is a protein called 50S ribosomal protein L22.

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

- Molecule 49 is a protein called 50S ribosomal protein L23.

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

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

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

- Molecule 51 is a protein called 30S ribosomal protein S12.

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

- Molecule 52 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	Y1	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			
52	R1	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			

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

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

- Molecule 54 is a protein called 50S ribosomal protein L4.

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

- Molecule 55 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			
55	YZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

- Molecule 56 is a RNA chain called CCPuro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	ZA	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
56	ZB	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	94	Total	Mg	0	0
			94	94		

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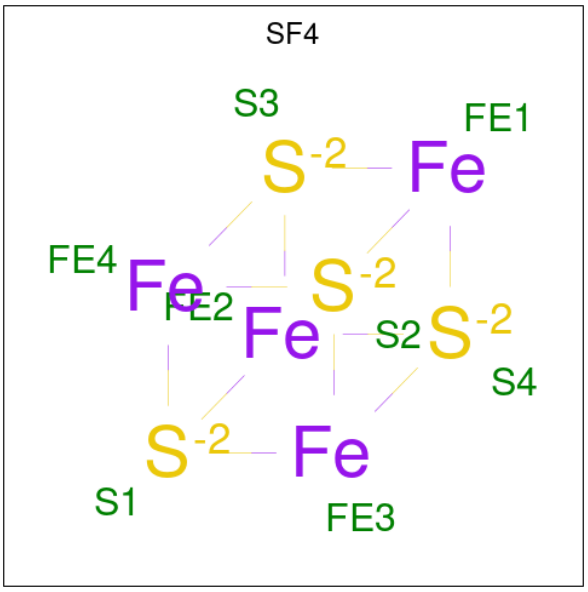
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	QD	2	Total Mg 2 2	0	0
57	QE	1	Total Mg 1 1	0	0
57	QF	1	Total Mg 1 1	0	0
57	QV	3	Total Mg 3 3	0	0
57	QX	1	Total Mg 1 1	0	0
57	R0	1	Total Mg 1 1	0	0
57	RA	302	Total Mg 302 302	0	0
57	RB	3	Total Mg 3 3	0	0
57	RD	1	Total Mg 1 1	0	0
57	RE	1	Total Mg 1 1	0	0
57	RN	1	Total Mg 1 1	0	0
57	RO	1	Total Mg 1 1	0	0
57	RP	2	Total Mg 2 2	0	0
57	RQ	2	Total Mg 2 2	0	0
57	RR	2	Total Mg 2 2	0	0
57	RY	1	Total Mg 1 1	0	0
57	XA	116	Total Mg 116 116	0	0
57	XD	1	Total Mg 1 1	0	0
57	XE	1	Total Mg 1 1	0	0
57	XF	1	Total Mg 1 1	0	0
57	XL	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	XM	1	Total Mg 1 1	0	0
57	XV	3	Total Mg 3 3	0	0
57	Y0	2	Total Mg 2 2	0	0
57	Y3	1	Total Mg 1 1	0	0
57	Y9	1	Total Mg 1 1	0	0
57	YA	326	Total Mg 326 326	0	0
57	YB	5	Total Mg 5 5	0	0
57	YF	1	Total Mg 1 1	0	0
57	YG	1	Total Mg 1 1	0	0
57	YO	1	Total Mg 1 1	0	0
57	YD	5	Total Mg 5 5	0	0
57	YQ	3	Total Mg 3 3	0	0
57	YV	1	Total Mg 1 1	0	0
57	YE	5	Total Mg 5 5	0	0
57	R8	1	Total Mg 1 1	0	0

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



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

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

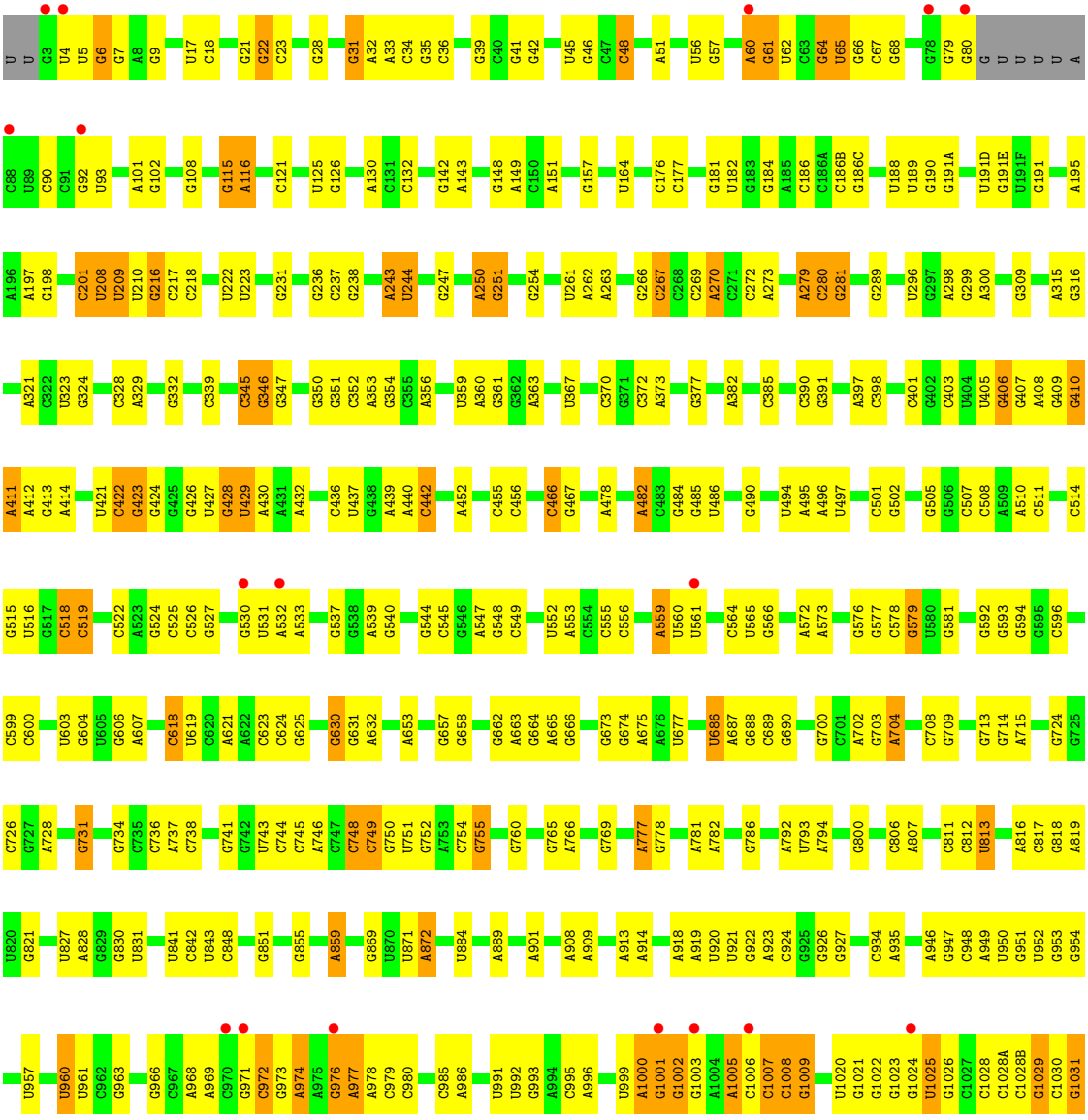
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	QN	1	Total Zn 1 1	0	0
59	R4	1	Total Zn 1 1	0	0
59	R5	1	Total Zn 1 1	0	0
59	R6	1	Total Zn 1 1	0	0
59	R9	1	Total Zn 1 1	0	0
59	XN	1	Total Zn 1 1	0	0
59	Y4	1	Total Zn 1 1	0	0
59	Y6	1	Total Zn 1 1	0	0

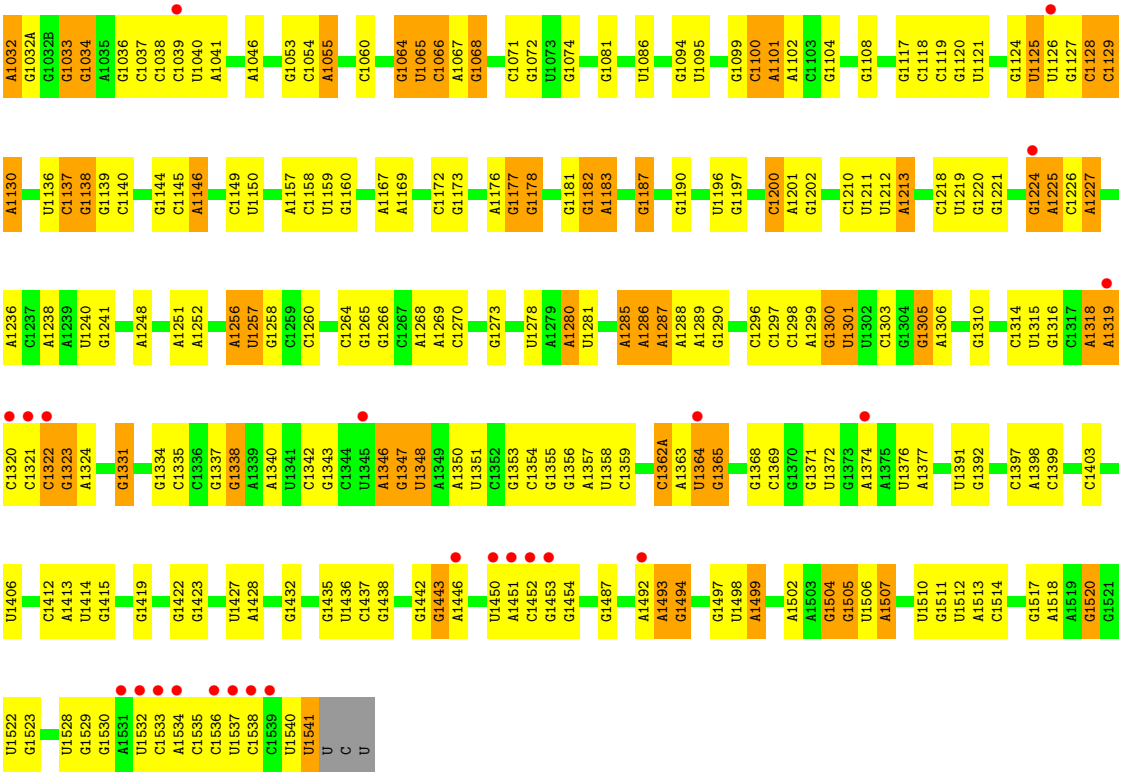
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

Chain QA: 

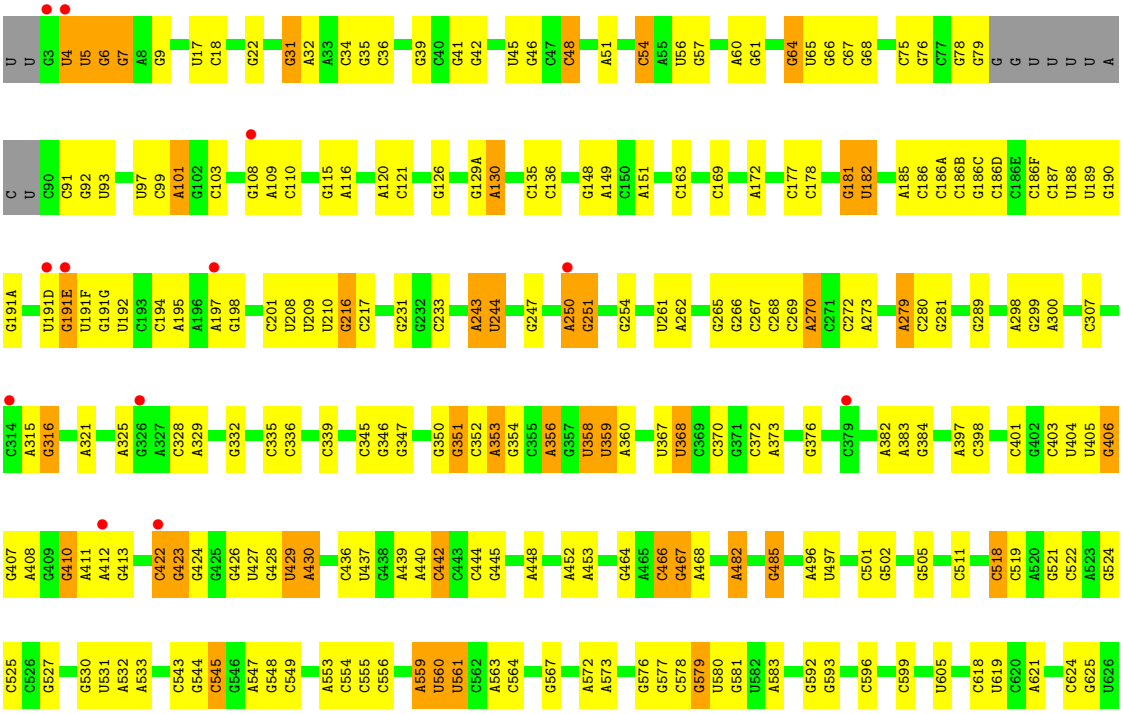


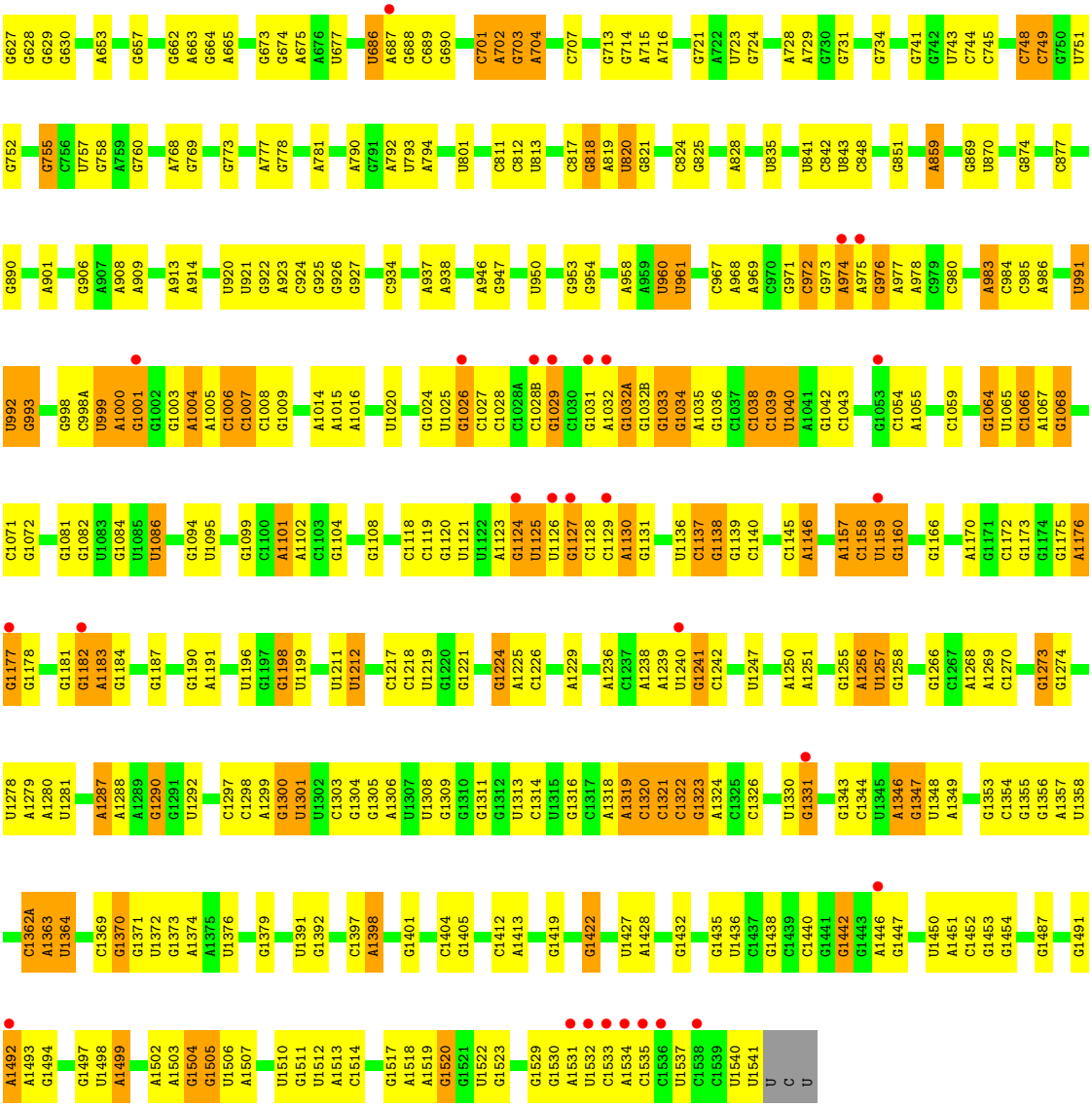


• Molecule 1: 16S rRNA

Chain XA:



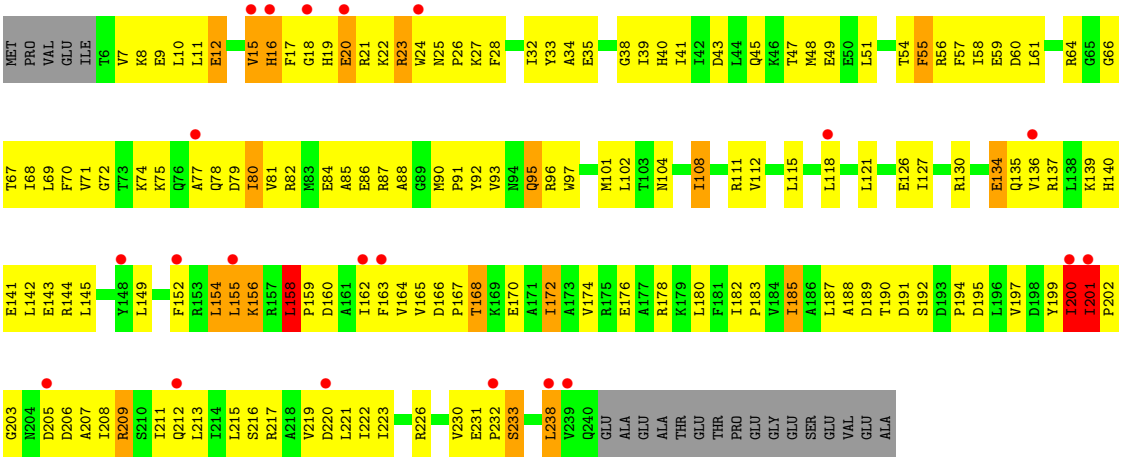




• Molecule 2: 30S ribosomal protein S2

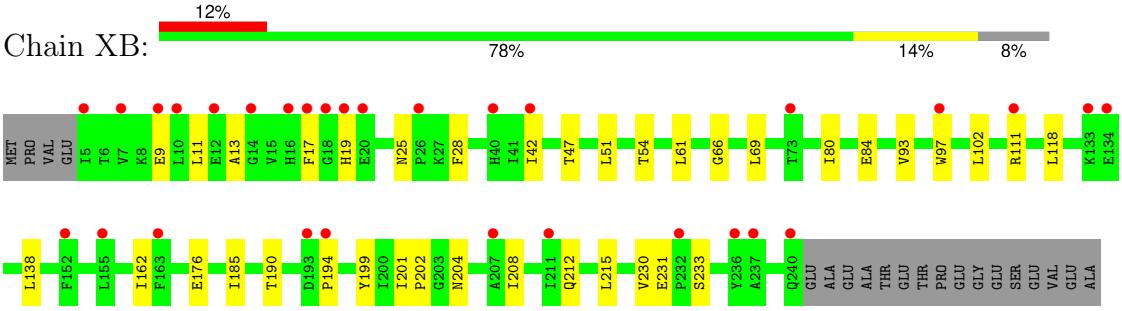
Chain QB:





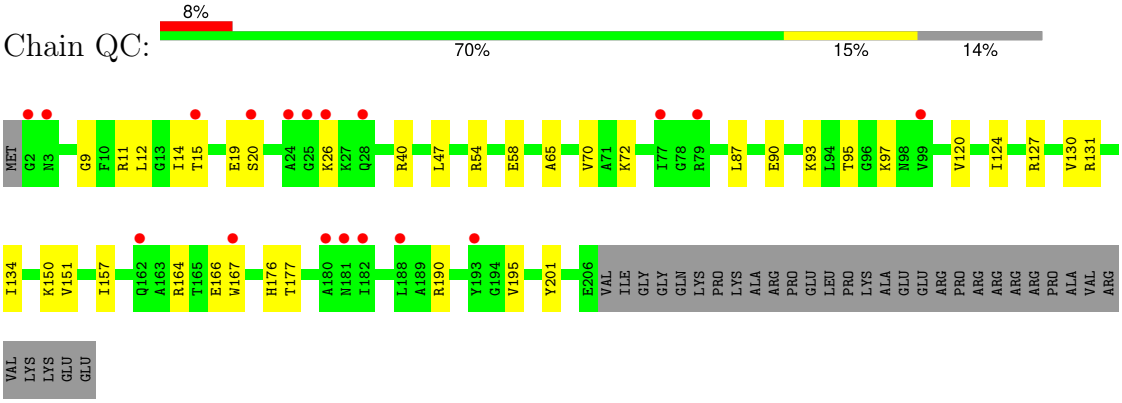
• Molecule 2: 30S ribosomal protein S2

Chain XB:



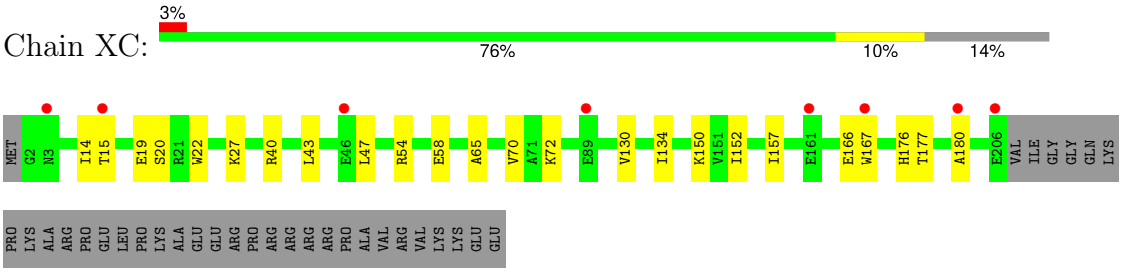
• Molecule 3: 30S ribosomal protein S3

Chain QC:



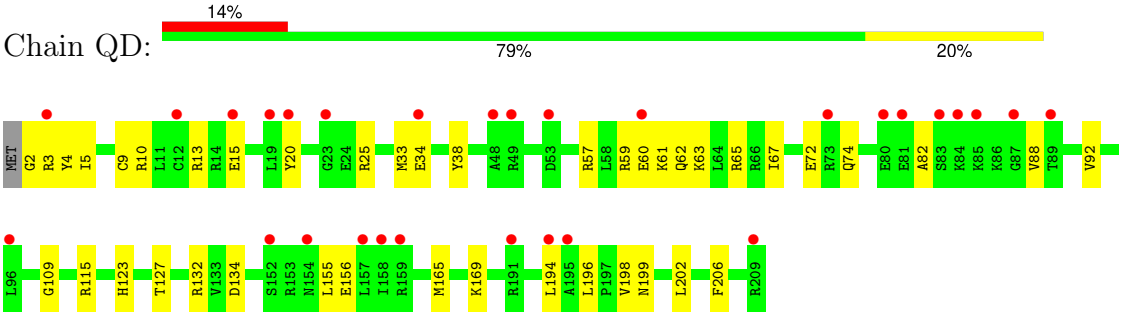
• Molecule 3: 30S ribosomal protein S3

Chain XC:



• Molecule 4: 30S ribosomal protein S4

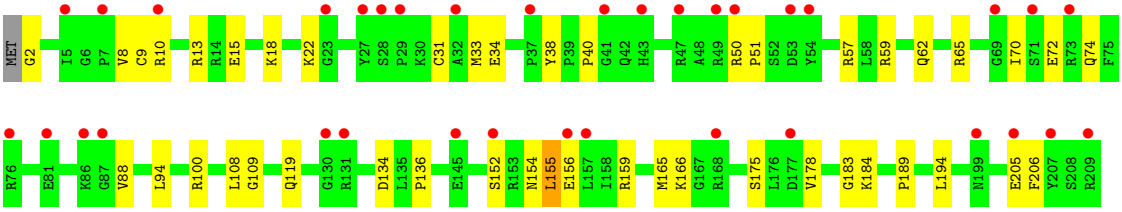
Chain QD:



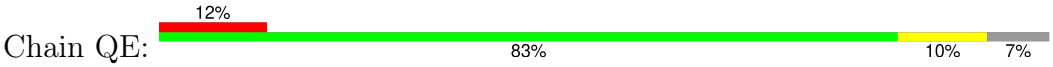
• Molecule 4: 30S ribosomal protein S4

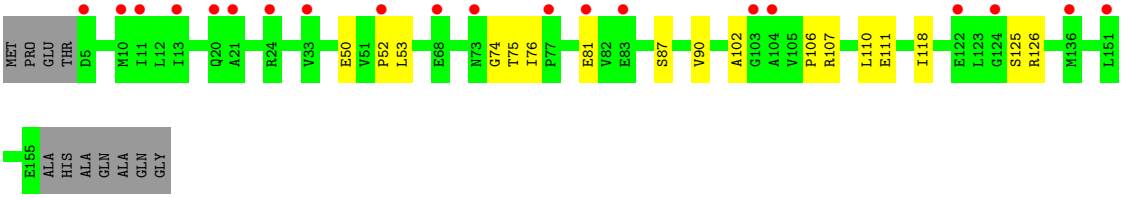
Chain XD:



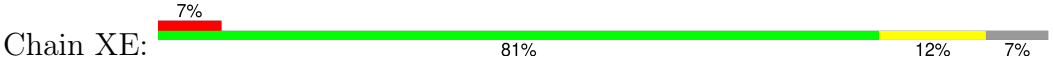


• Molecule 5: 30S ribosomal protein S5



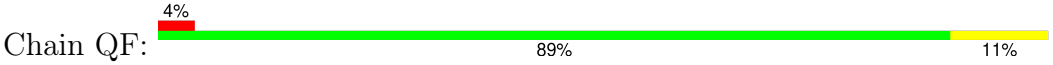


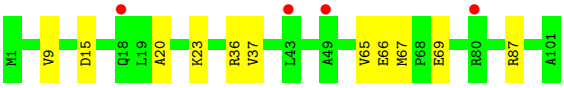
• Molecule 5: 30S ribosomal protein S5



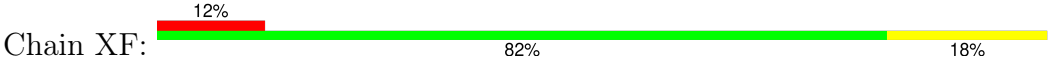


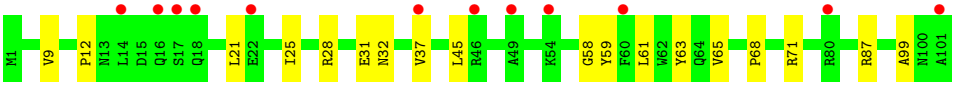
• Molecule 6: 30S ribosomal protein S6



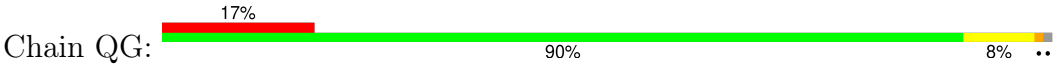


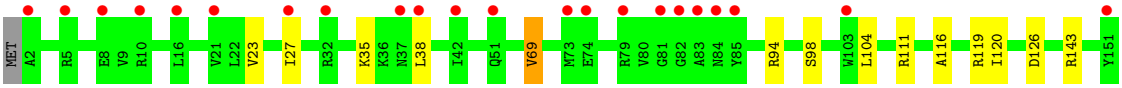
• Molecule 6: 30S ribosomal protein S6





• Molecule 7: 30S ribosomal protein S7



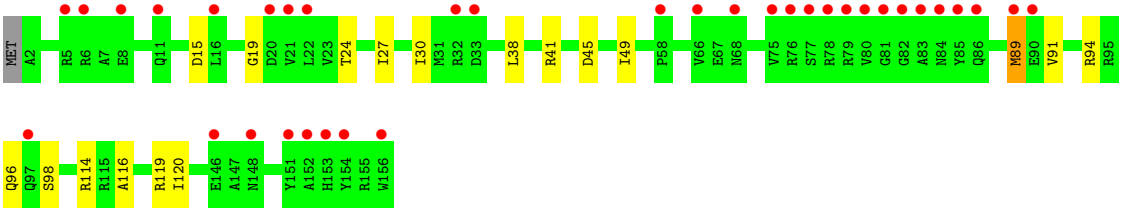




• Molecule 7: 30S ribosomal protein S7

Chain XG:

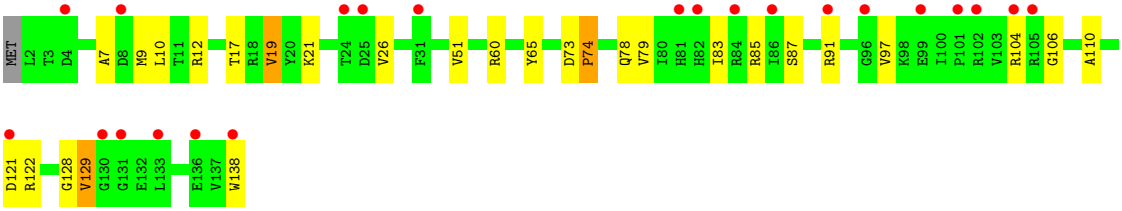




• Molecule 8: 30S ribosomal protein S8

Chain QH:

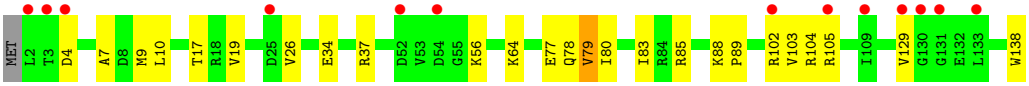




• Molecule 8: 30S ribosomal protein S8

Chain XH:

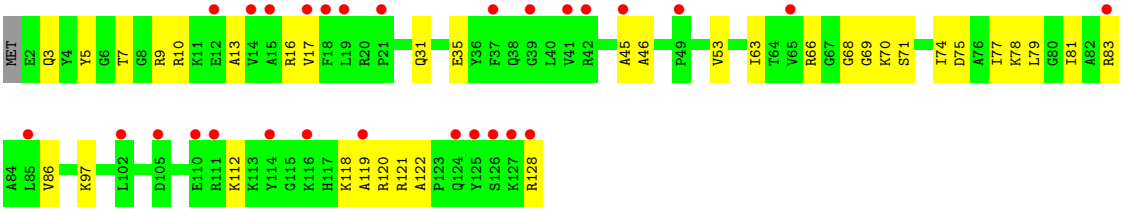




• Molecule 9: 30S ribosomal protein S9

Chain QI:

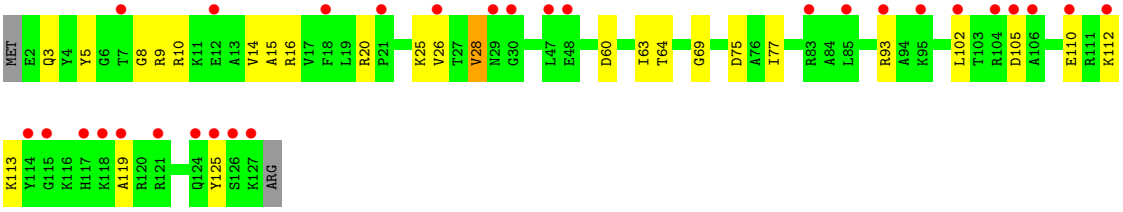




• Molecule 9: 30S ribosomal protein S9

Chain XI:

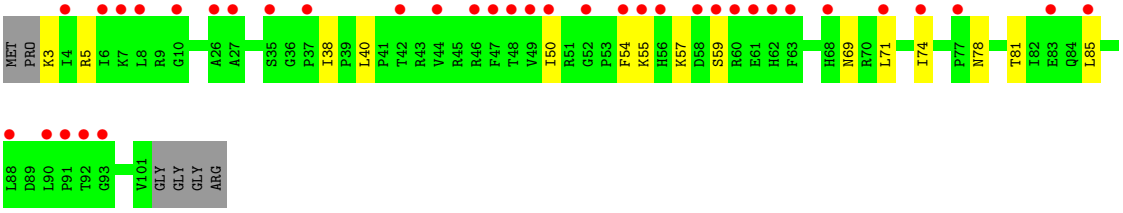




• Molecule 10: 30S ribosomal protein S10

Chain QJ:

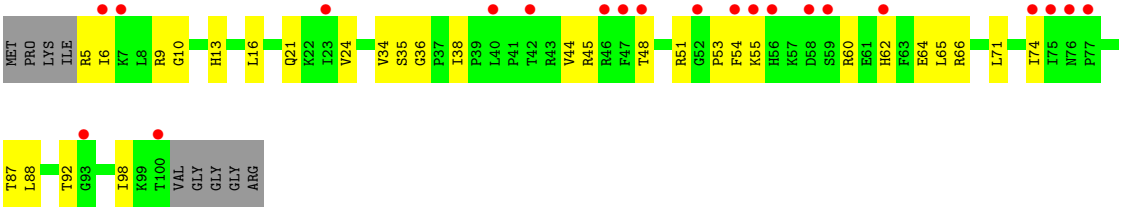




• Molecule 10: 30S ribosomal protein S10

Chain XJ:

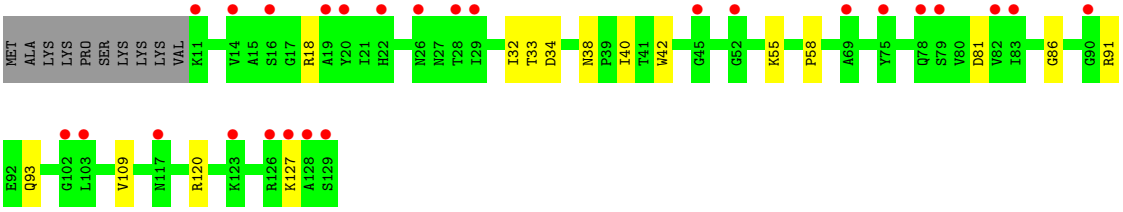




• Molecule 11: 30S ribosomal protein S11

Chain QK:

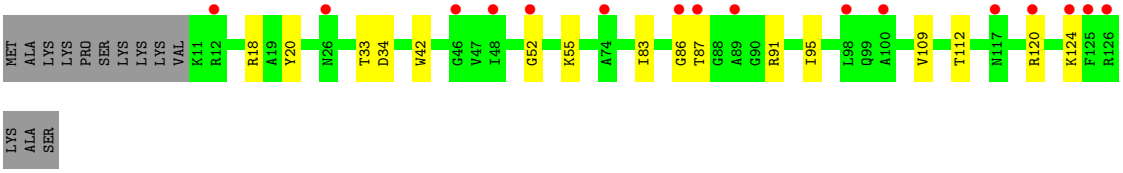




• Molecule 11: 30S ribosomal protein S11

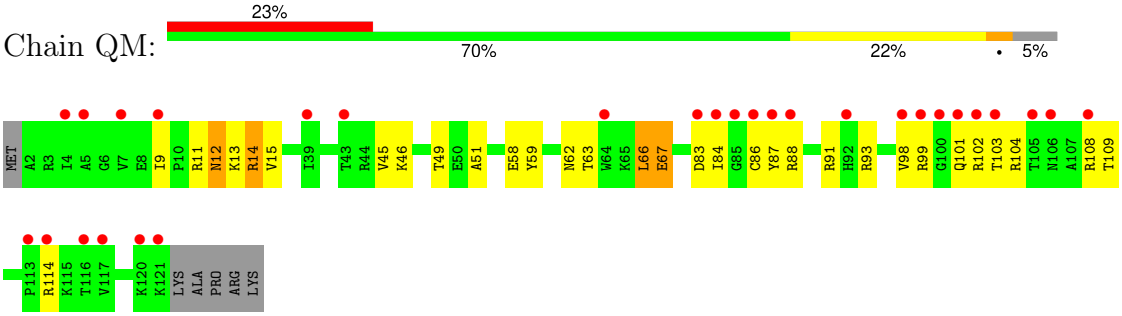
Chain XK:





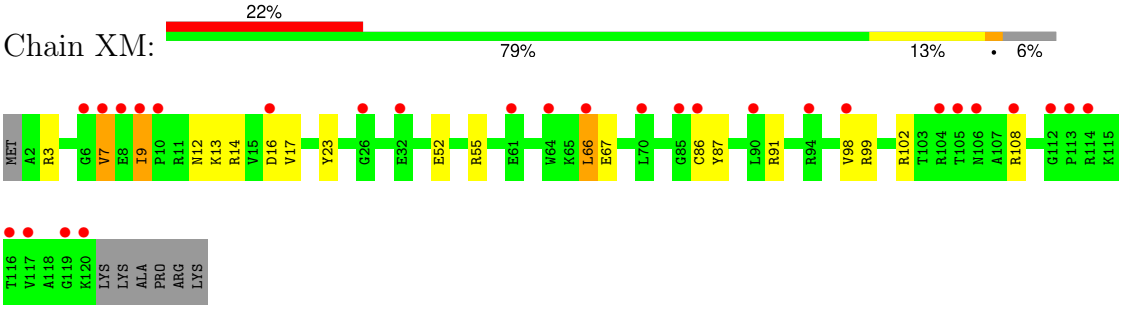
• Molecule 12: 30S ribosomal protein S13

Chain QM:



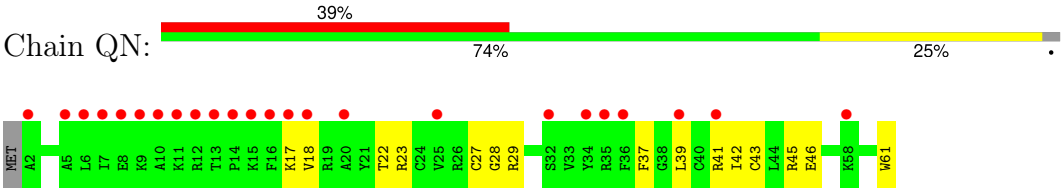
• Molecule 12: 30S ribosomal protein S13

Chain XM:



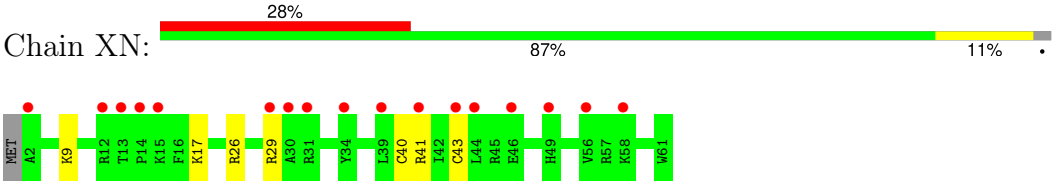
• Molecule 13: 30S ribosomal protein S14 type Z

Chain QN:



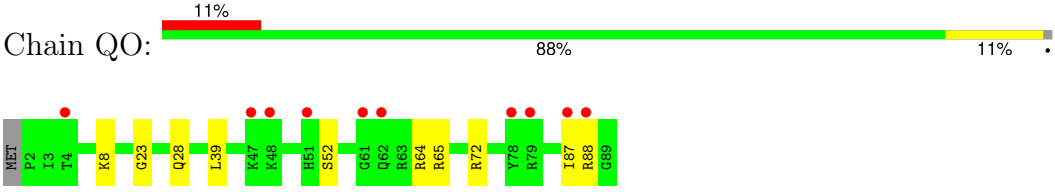
• Molecule 13: 30S ribosomal protein S14 type Z

Chain XN:



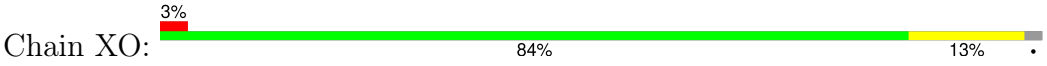
• Molecule 14: 30S ribosomal protein S15

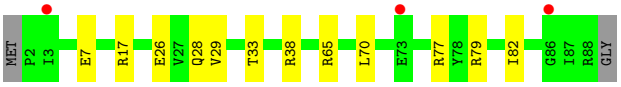
Chain QO:



• Molecule 14: 30S ribosomal protein S15

Chain XO:

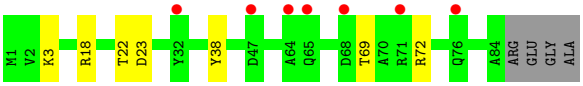




• Molecule 15: 30S ribosomal protein S16

Chain QP:

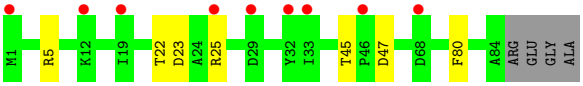




• Molecule 15: 30S ribosomal protein S16

Chain XP:

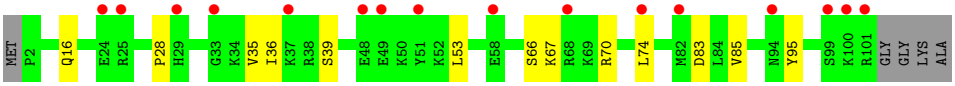




• Molecule 16: 30S ribosomal protein S17

Chain QQ:

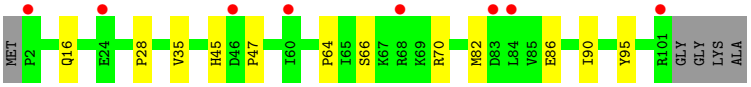




• Molecule 16: 30S ribosomal protein S17

Chain XQ:

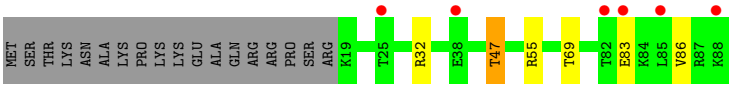




• Molecule 17: 30S ribosomal protein S18

Chain QR:

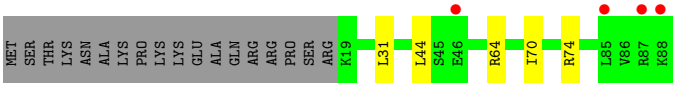




• Molecule 17: 30S ribosomal protein S18

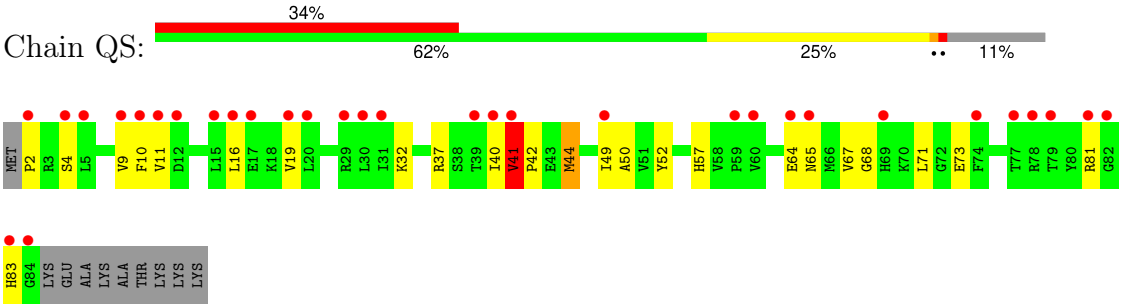
Chain XR:





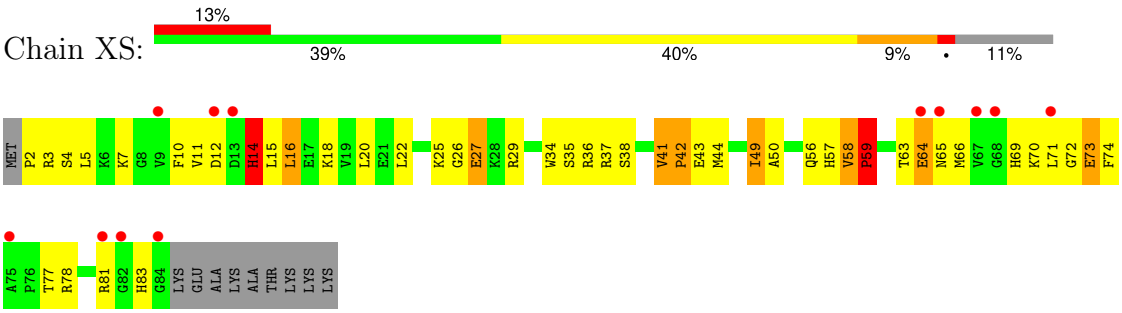
• Molecule 18: 30S ribosomal protein S19

Chain QS:



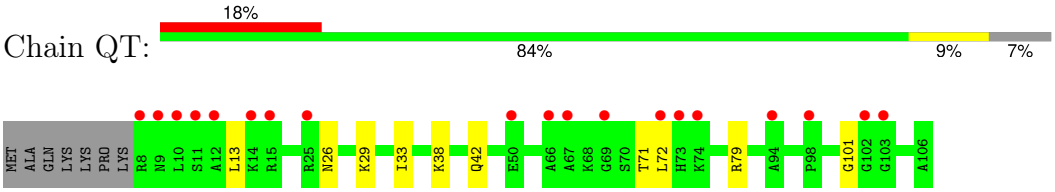
• Molecule 18: 30S ribosomal protein S19

Chain XS:



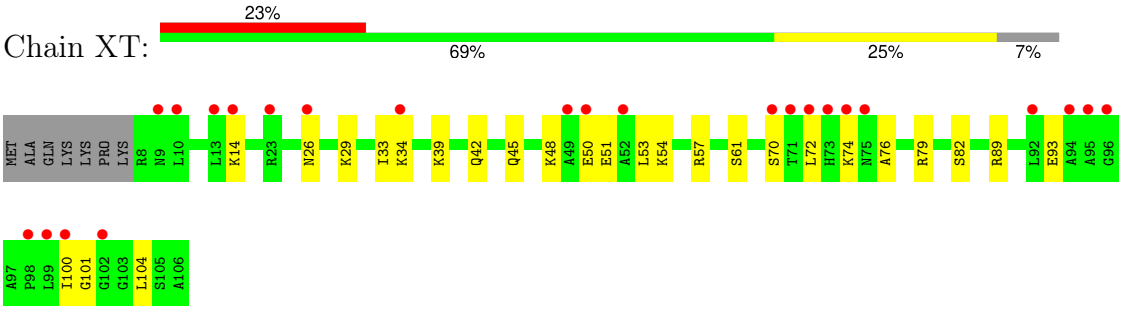
• Molecule 19: 30S ribosomal protein S20

Chain QT:



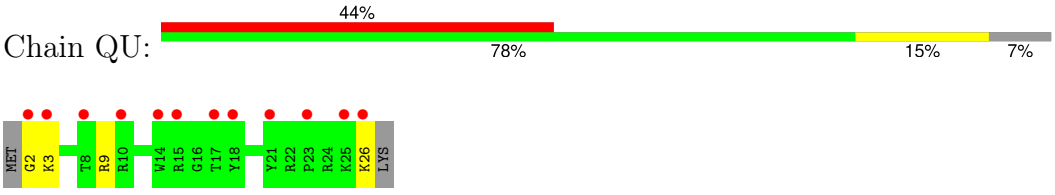
• Molecule 19: 30S ribosomal protein S20

Chain XT:



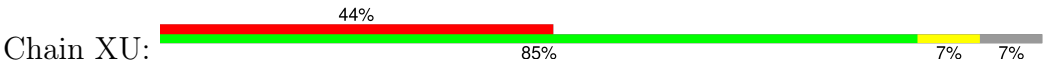
• Molecule 20: 30S ribosomal protein Thx

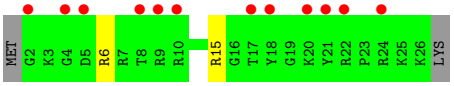
Chain QU:



• Molecule 20: 30S ribosomal protein Thx

Chain XU:

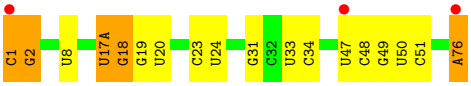




• Molecule 21: P-site tRNA-fMet

Chain QV:

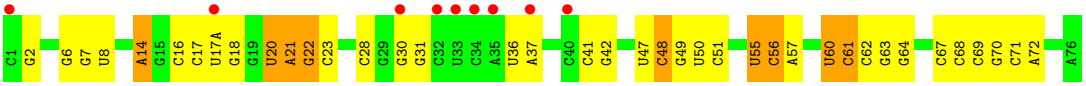




• Molecule 21: P-site tRNA-fMet

Chain QW:

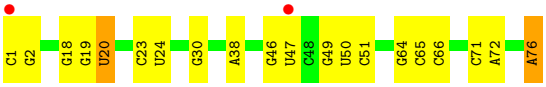




• Molecule 21: P-site tRNA-fMet

Chain XV:

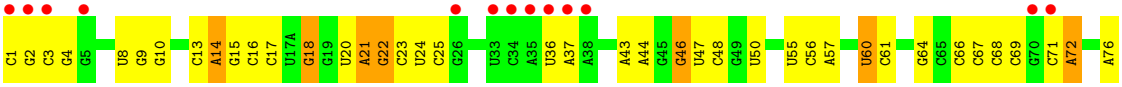




• Molecule 21: P-site tRNA-fMet

Chain XW:

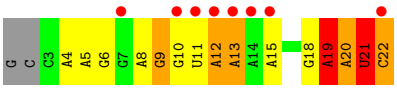




• Molecule 22: mRNA

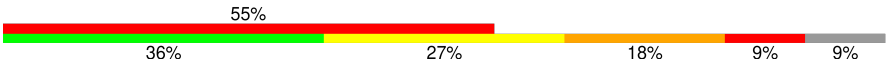
Chain QX:

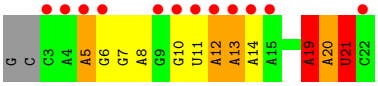




• Molecule 22: mRNA

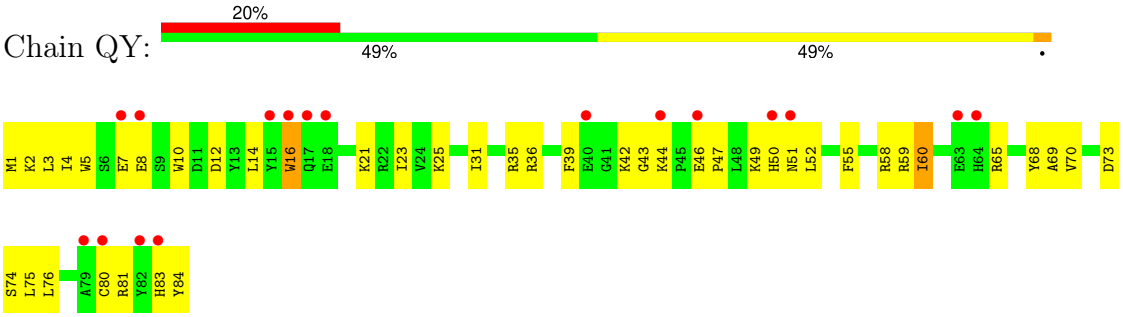
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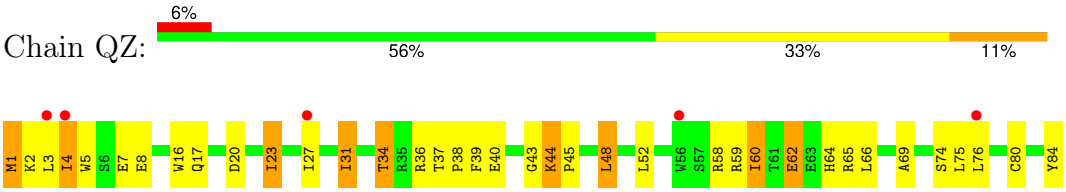
• Molecule 23: Addiction module toxin, Txe/YoeB family

Chain QY:



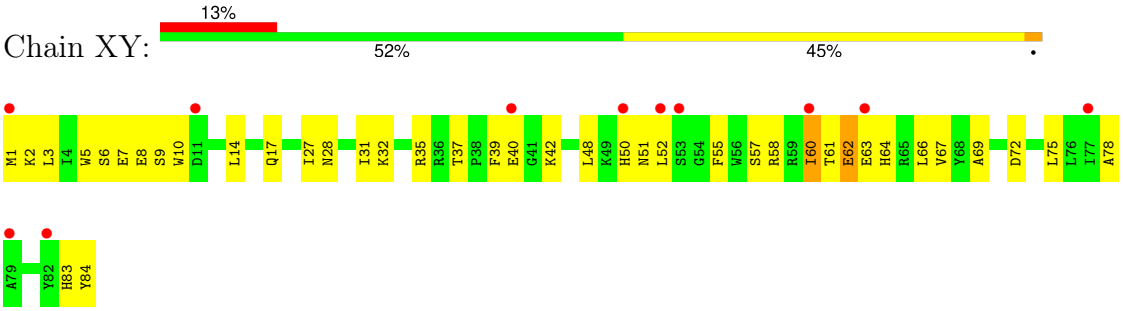
• Molecule 23: Addiction module toxin, Txe/YoeB family

Chain QZ:



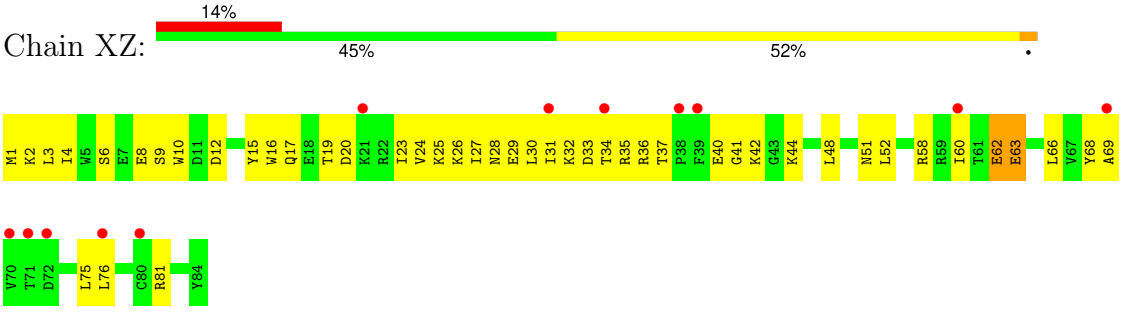
• Molecule 23: Addiction module toxin, Txe/YoeB family

Chain XY:



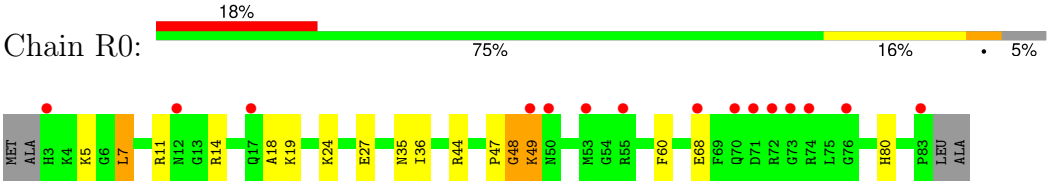
• Molecule 23: Addiction module toxin, Txe/YoeB family

Chain XZ:



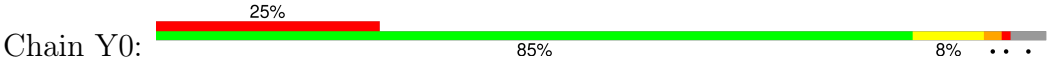
• Molecule 24: 50S ribosomal protein L27

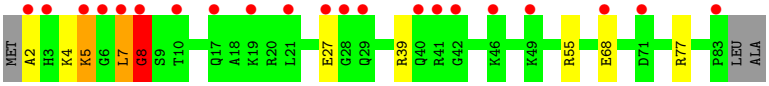
Chain R0:



• Molecule 24: 50S ribosomal protein L27

Chain Y0:

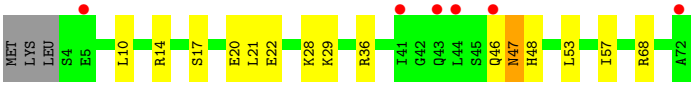




• Molecule 25: 50S ribosomal protein L29

Chain R2:

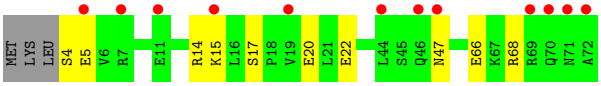




• Molecule 25: 50S ribosomal protein L29

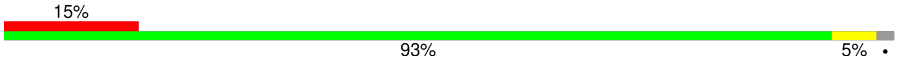
Chain Y2:

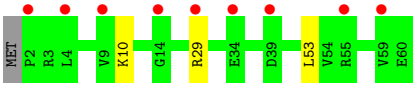




• Molecule 26: 50S ribosomal protein L30

Chain R3:

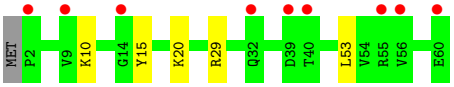




• Molecule 26: 50S ribosomal protein L30

Chain Y3:

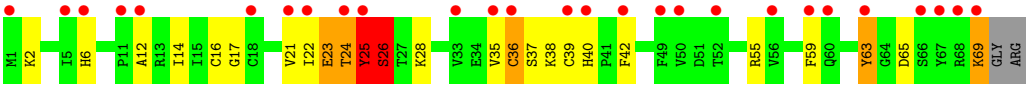




• Molecule 27: 50S ribosomal protein L31

Chain R4:

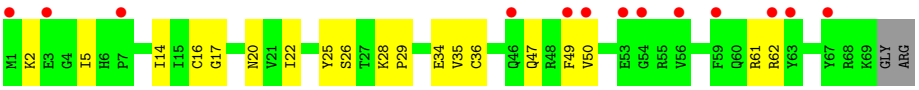




• Molecule 27: 50S ribosomal protein L31

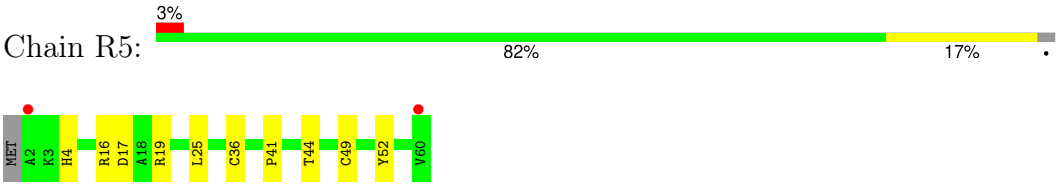
Chain Y4:





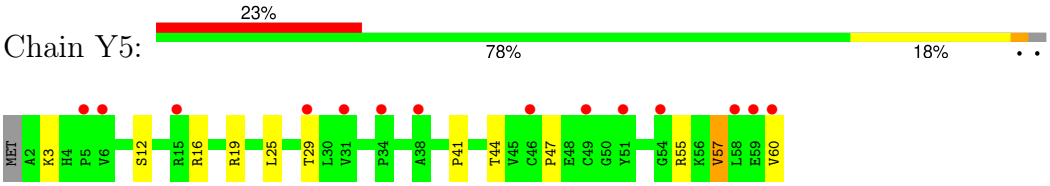
• Molecule 28: 50S ribosomal protein L32

Chain R5:



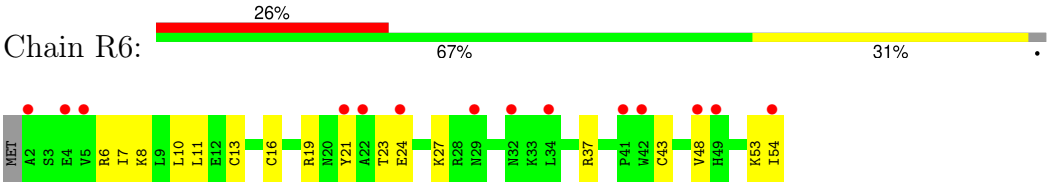
• Molecule 28: 50S ribosomal protein L32

Chain Y5:



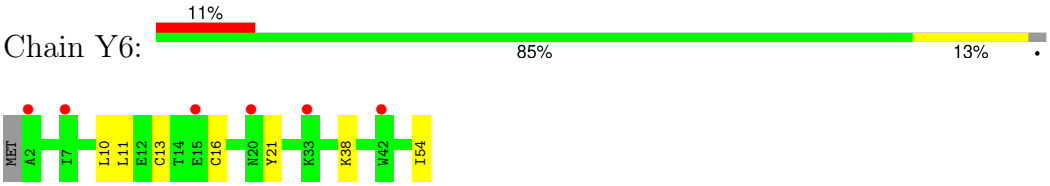
• Molecule 29: 50S ribosomal protein L33

Chain R6:



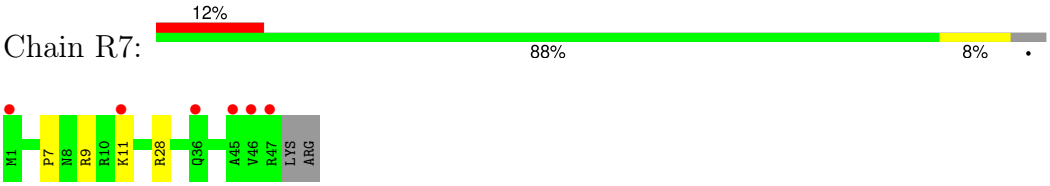
• Molecule 29: 50S ribosomal protein L33

Chain Y6:



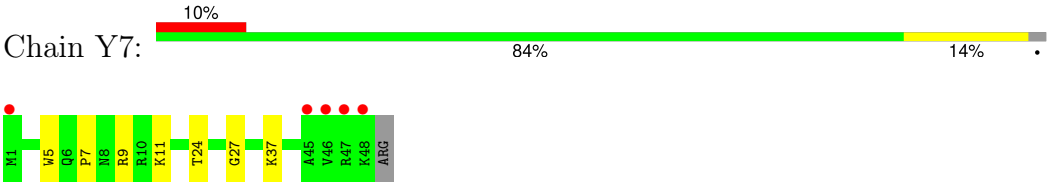
• Molecule 30: 50S ribosomal protein L34

Chain R7:



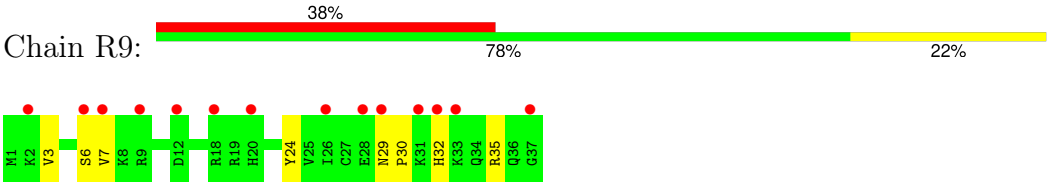
• Molecule 30: 50S ribosomal protein L34

Chain Y7:



• Molecule 31: 50S ribosomal protein L36

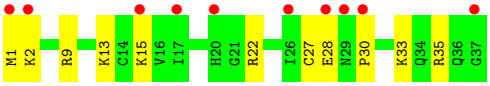
Chain R9:



• Molecule 31: 50S ribosomal protein L36

Chain Y9:

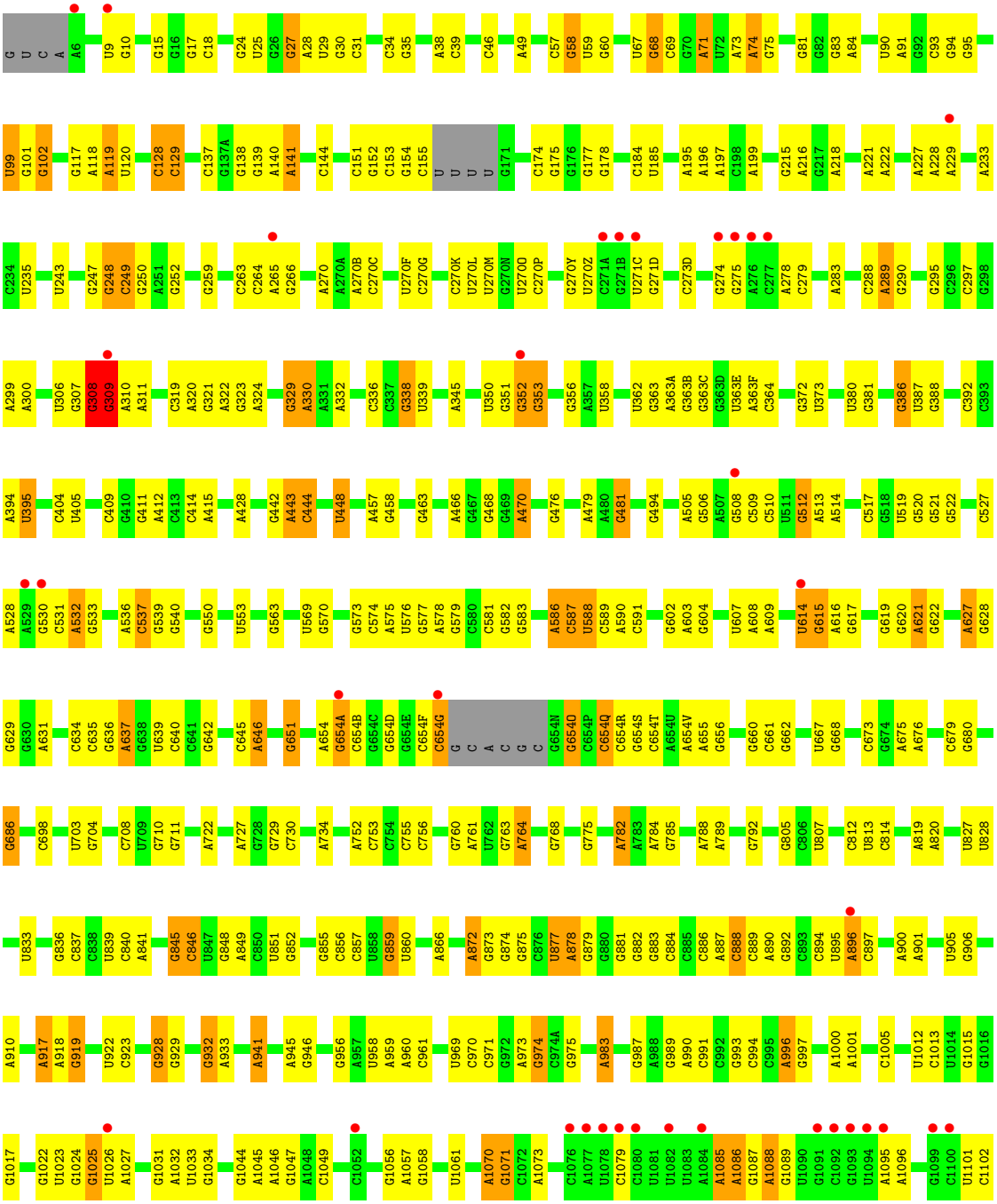


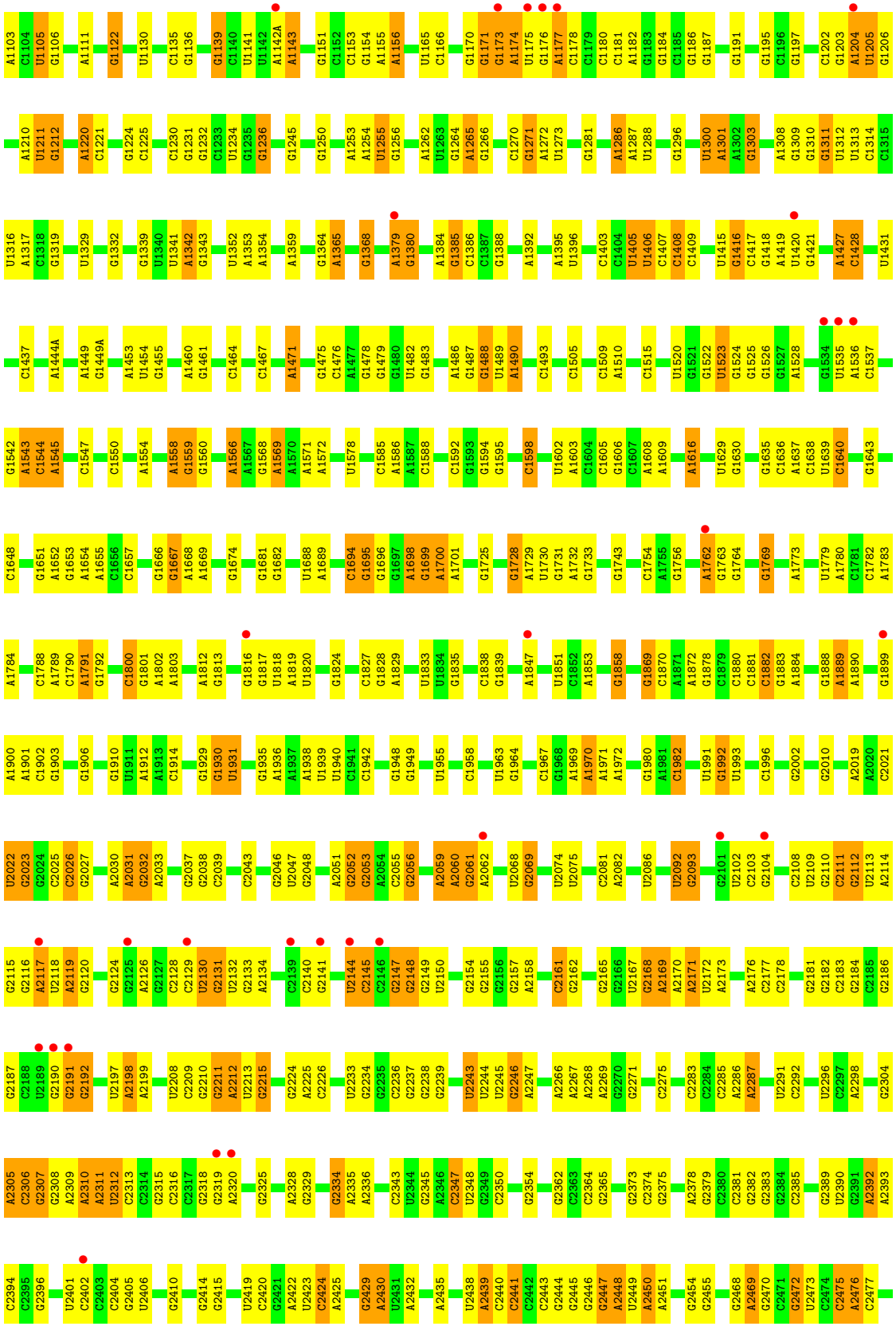


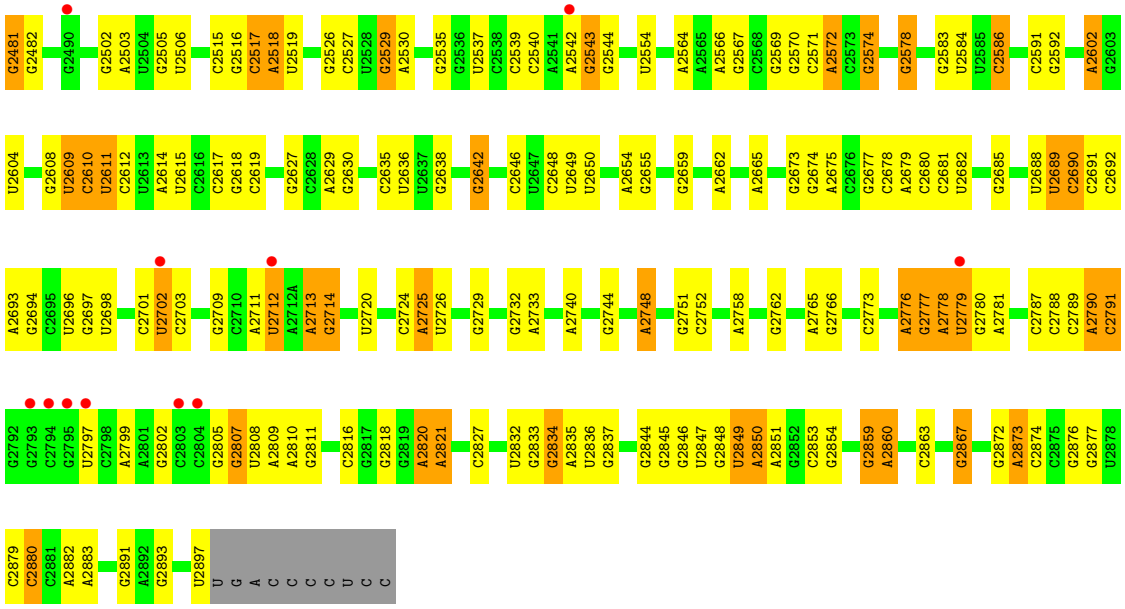
• Molecule 32: 23S rRNA

Chain RA:





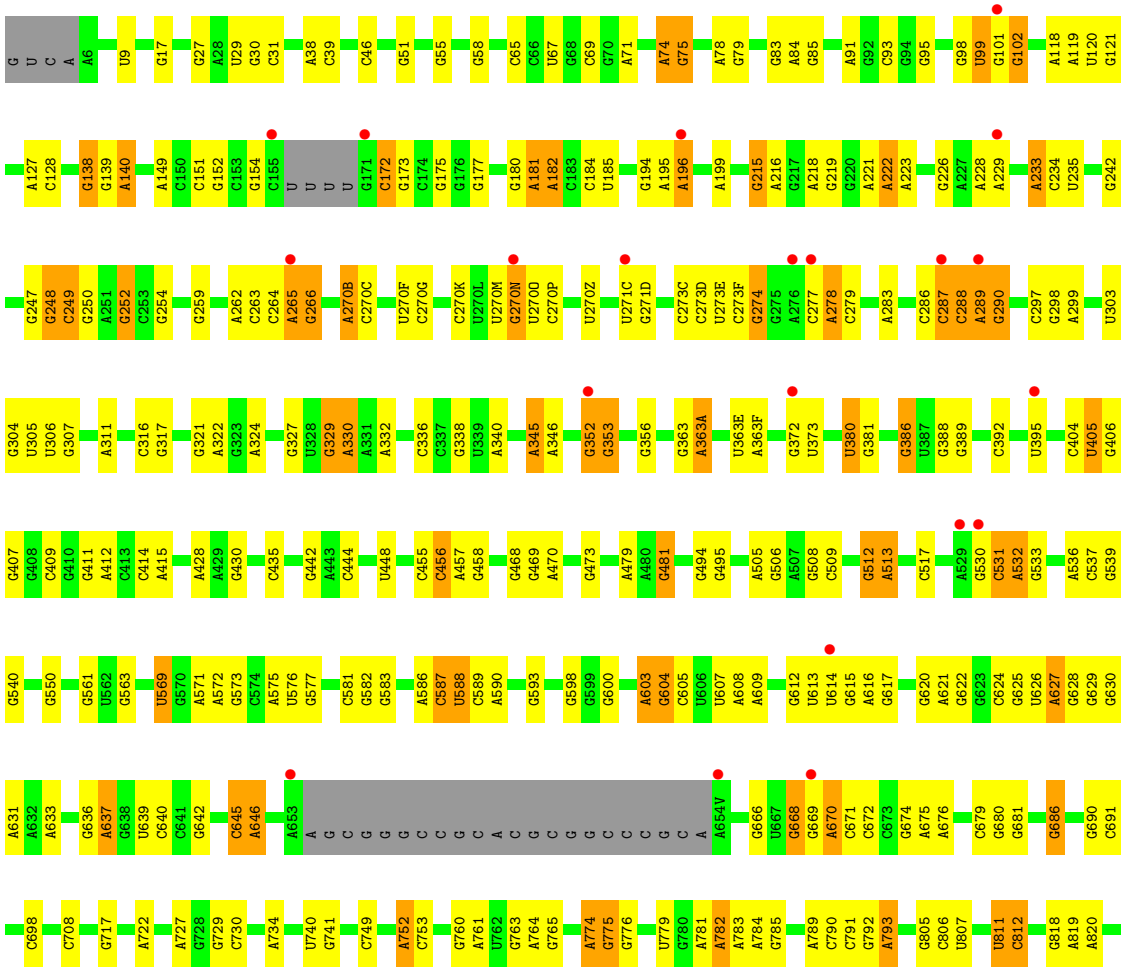

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A1210 U1211 G1212 A1220 C1221 G1224 C1225 C1230 G1231 G1232 G1233 U1234 G1235 G1236 G1245 G1250 A1253 A1254 U1255 G1256 A1262 U1263 G1264 A1265 G1266 C1270 G1271 A1272 U1273 G1281 A1286 A1287 U1288 G1296 U1300 A1301 A1302 G1303 A1308 G1309 G1310 G1311 U1312 U1313 C1314 C1315
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C1648 G1651 A1652 G1653 A1654 A1655 C1656 C1657 G1666 G1667 A1668 A1669 G1674 G1681 G1682 U1688 A1689 C1694 G1695 G1696 G1697 A1698 G1699 A1700 A1701 G1725 G1728 A1729 U1730 G1731 A1732 G1733 G1743 C1754 A1755 G1756 A1762 G1763 G1764 G1769 A1773 U1779 A1780 C1781 C1782 A1783
A1784 C1788 A1789 C1790 A1791 G1792 C1800 G1801 A1802 A1803 A1812 G1813 G1816 G1817 U1818 A1819 U1820 G1824 C1827 G1828 A1829 U1833 U1834 G1835 C1838 G1839 A1847 U1851 C1852 A1853 G1858 G1869 C1870 A1871 A1872 G1878 C1879 C1880 C1881 C1882 G1883 A1884 G1888 A1889 A1890 G1899
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C2394 C2395 G2396 U2401 C2402 C2403 C2404 G2405 U2406 G2410 G2414 G2415 U2419 C2420 G2421 A2422 U2423 C2424 A2425 G2429 A2430 U2431 A2432 A2435 U2438 A2439 C2440 C2441 C2442 C2443 G2444 G2445 G2446 G2447 A2448 U2449 A2450 A2451 G2454 G2455 G2468 A2469 G2470 C2471 G2472 U2473 C2474 C2475 A2476 C2477

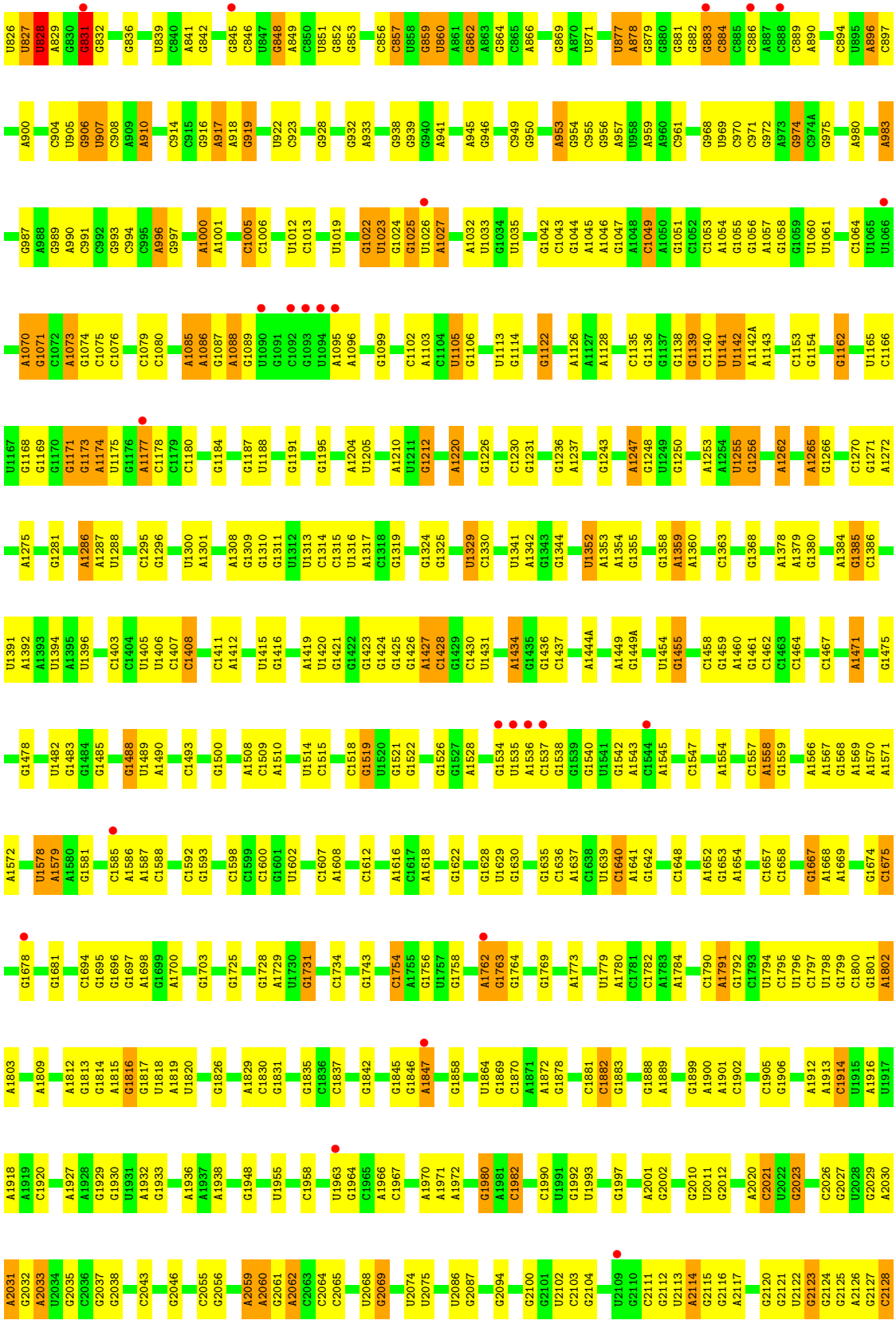


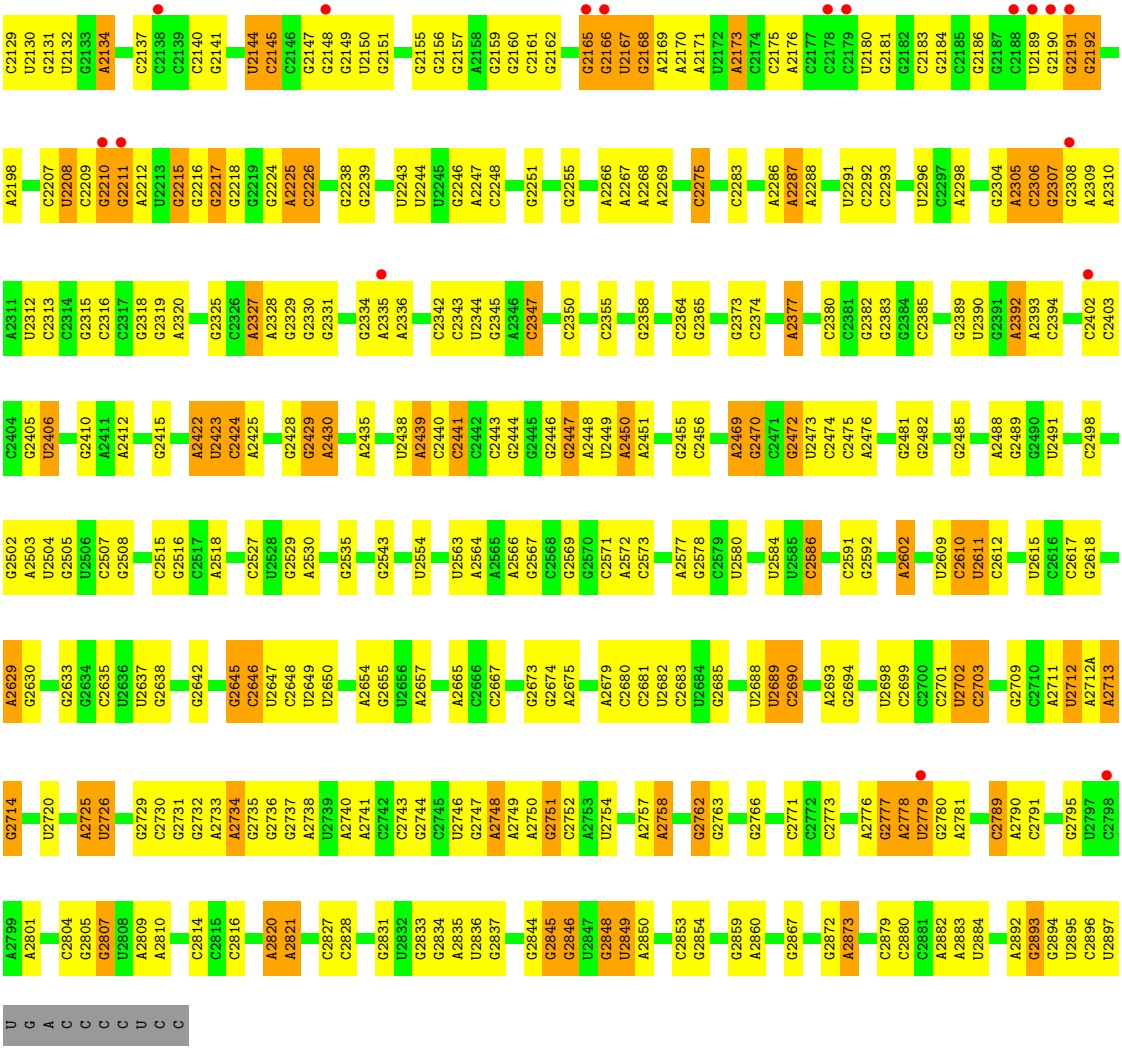
• Molecule 32: 23S rRNA

Chain YA:





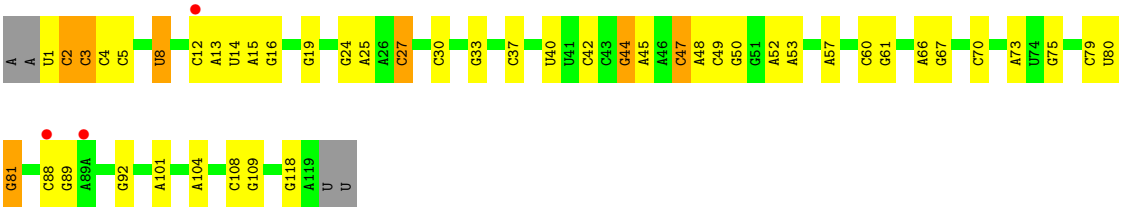

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A900 C904 U905 G906 U907 C908 A909 A910 C914 C915 G916 A917 A918 G919 U922 C923 G928 G932 A933 G938 G939 G940 A941 A945 G946 C949 G950 A953 G954 C955 G956 A957 U958 A959 A960 C961 G968 U969 C970 C971 G972 A973 G974 C974A G975 A980 A983
G987 A988 G989 A990 C991 C992 Q993 C994 C995 A996 G997 A1000 A1001 C1005 C1006 U1012 C1013 U1019 G1022 U1023 G1024 G1025 U1026 A1027 A1032 U1033 G1034 U1035 G1042 C1043 G1044 A1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 C1053 A1054 G1055 G1056 A1057 G1058 G1059 U1060 U1061 C1064 U1065 U1066
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U1391 A1392 A1393 U1394 A1395 U1396 C1403 C1404 U1405 U1406 C1407 C1408 C1411 A1412 U1415 G1416 A1419 U1420 G1421 G1422 G1423 G1424 G1425 G1426 A1427 C1428 G1429 C1430 U1431 A1434 G1435 G1436 C1437 A1444A A1449 G1449A U1454 G1455 C1458 G1459 A1460 G1461 C1462 C1463 C1464 C1467 A1471 G1475
G1478 U1482 G1483 G1484 G1485 G1488 U1489 A1490 C1493 G1500 A1508 C1509 A1510 U1514 C1515 C1518 G1519 U1520 G1521 G1522 G1526 G1527 A1528 G1534 U1535 A1536 C1537 G1538 G1539 G1540 U1541 G1542 A1543 C1544 A1545 C1547 A1554 C1557 A1558 G1559 A1566 A1567 G1568 A1569 A1570 A1571
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A1918 A1919 C1920 A1927 A1928 G1929 G1930 U1931 A1932 G1933 A1936 A1937 A1938 G1948 U1955 C1958 U1963 G1964 C1965 A1966 C1967 A1970 A1971 A1972 G1980 A1981 C1982 C1990 U1991 G1992 U1993 G1997 A2001 G2002 G2010 U2011 G2012 A2020 C2021 U2022 G2023 C2026 G2027 U2028 G2029 A2030
A2031 G2032 A2033 U2034 G2035 C2036 G2037 G2038 C2043 G2046 C2055 G2056 A2059 A2060 G2061 A2062 C2063 C2064 C2065 U2068 G2069 U2074 U2075 U2086 G2087 G2094 G2100 G2101 U2102 C2103 G2104 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128



• Molecule 33: 5S rRNA

Chain RB:

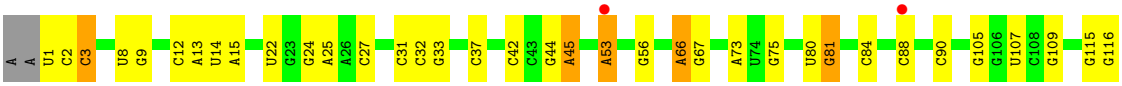




• Molecule 33: 5S rRNA

Chain YB:

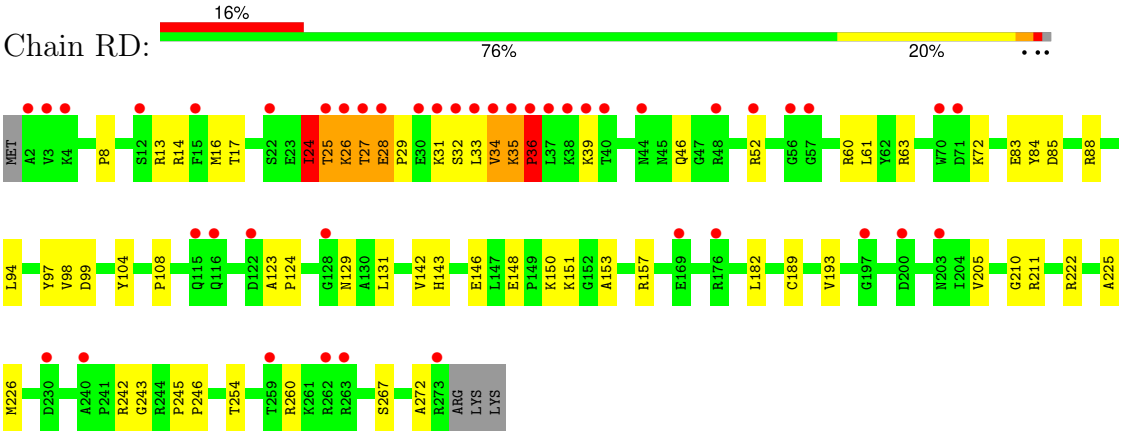






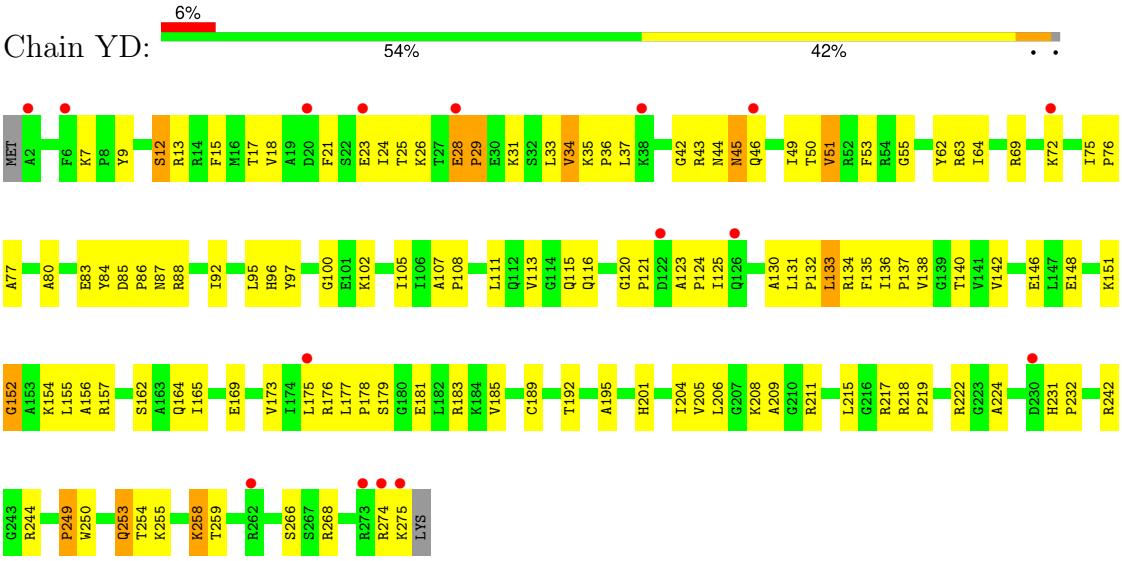
• Molecule 34: 50S ribosomal protein L2

Chain RD:



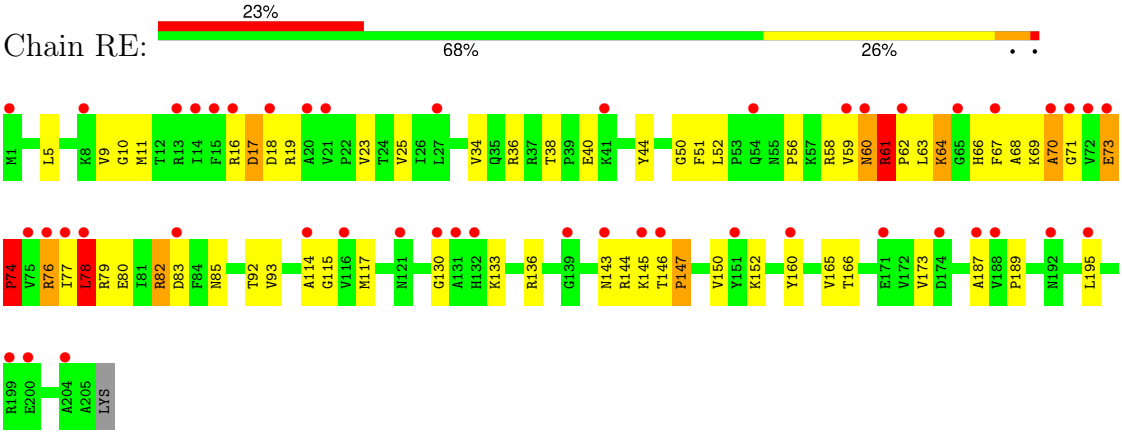
• Molecule 34: 50S ribosomal protein L2

Chain YD:



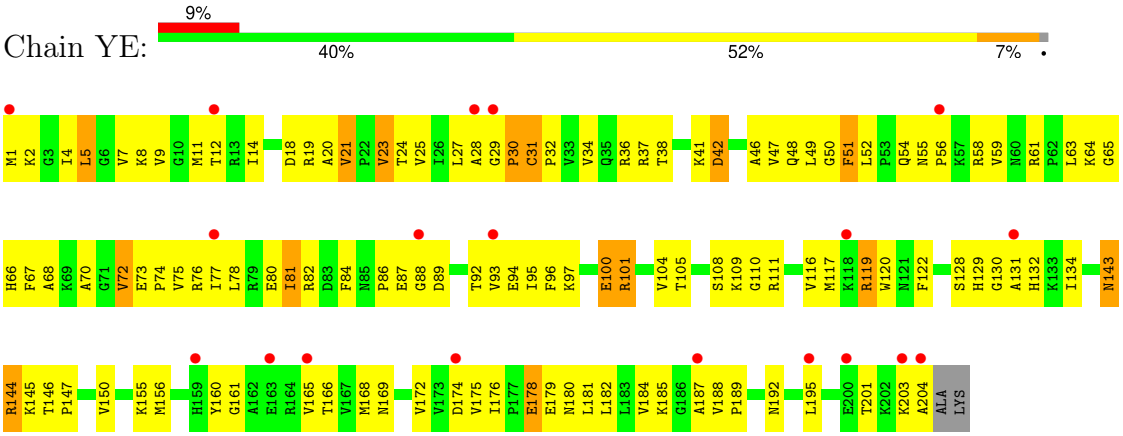
• Molecule 35: 50S ribosomal protein L3

Chain RE:



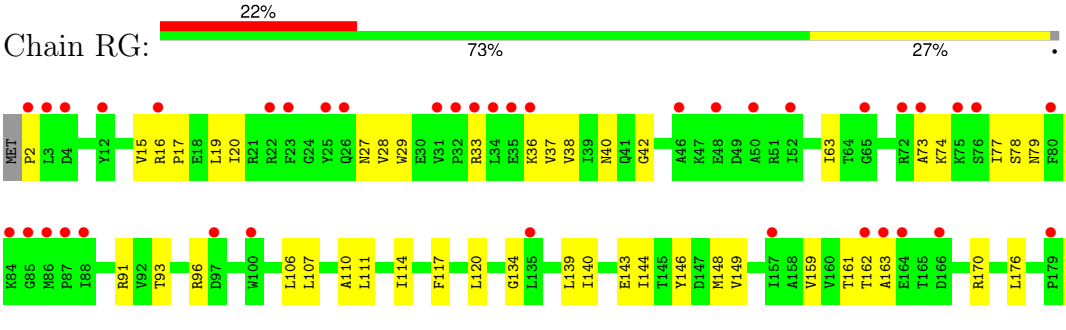
• Molecule 35: 50S ribosomal protein L3

Chain YE:



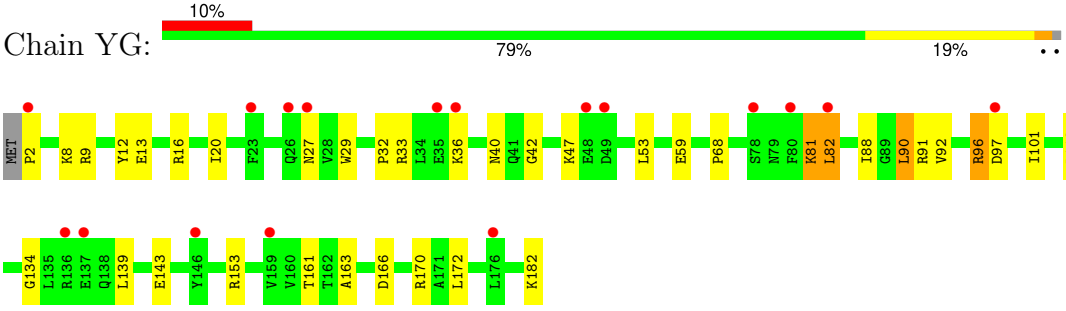
• Molecule 36: 50S ribosomal protein L5

Chain RG:



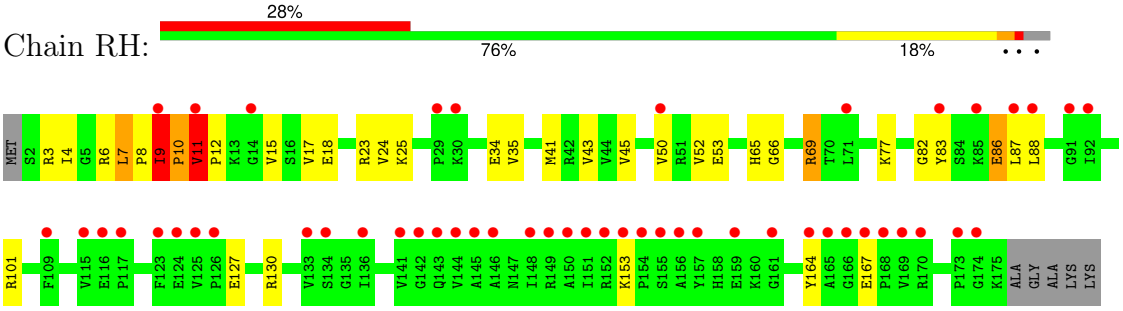
• Molecule 36: 50S ribosomal protein L5

Chain YG:



• Molecule 37: 50S ribosomal protein L6

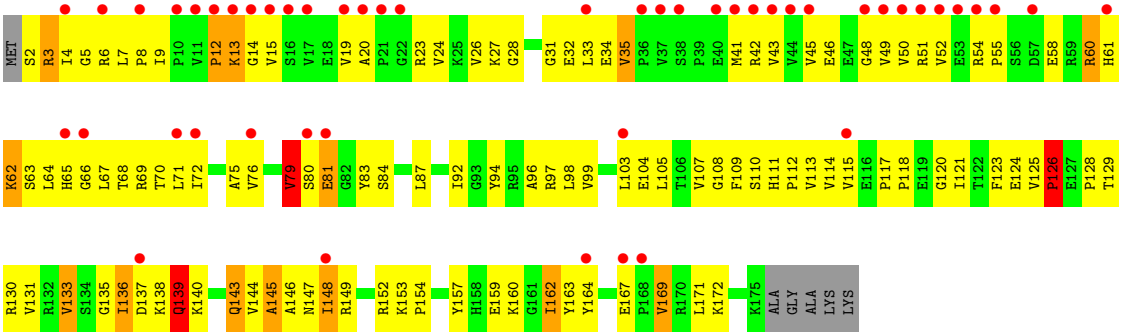
Chain RH:



• Molecule 37: 50S ribosomal protein L6

Chain YH:

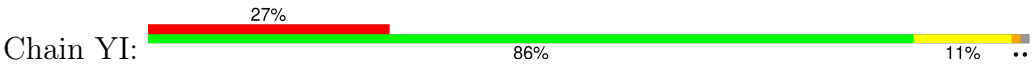




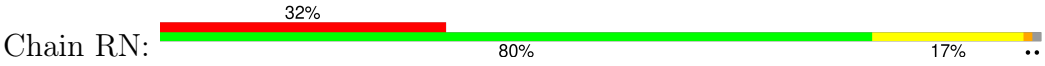
• Molecule 38: 50S ribosomal protein L9



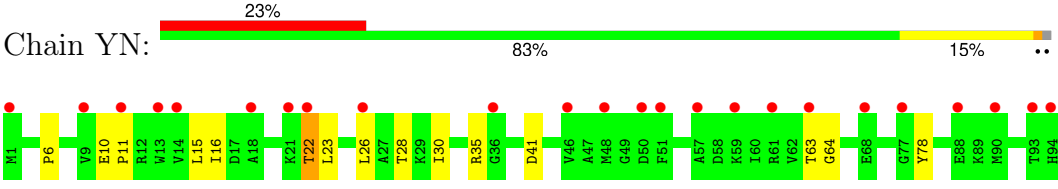
• Molecule 38: 50S ribosomal protein L9

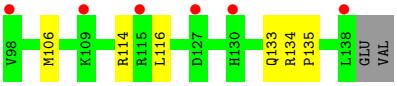


• Molecule 39: 50S ribosomal protein L13



• Molecule 39: 50S ribosomal protein L13

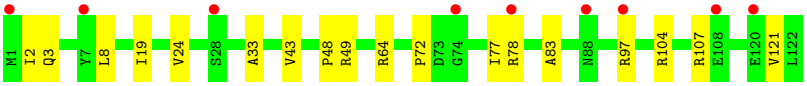




• Molecule 40: 50S ribosomal protein L14

Chain RO:

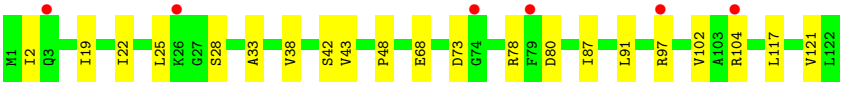




• Molecule 40: 50S ribosomal protein L14

Chain YO:

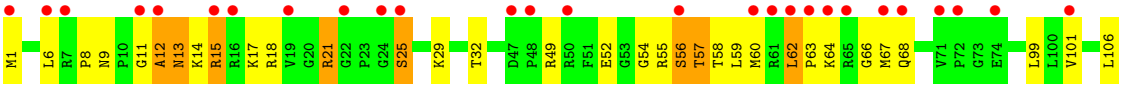




• Molecule 41: 50S ribosomal protein L15

Chain RP:



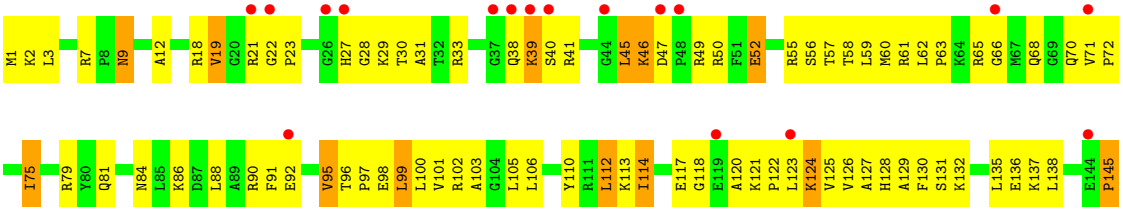




• Molecule 41: 50S ribosomal protein L15

Chain YP:

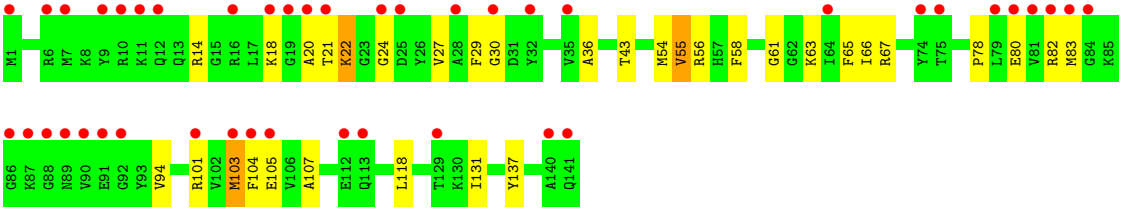




• Molecule 42: 50S ribosomal protein L16

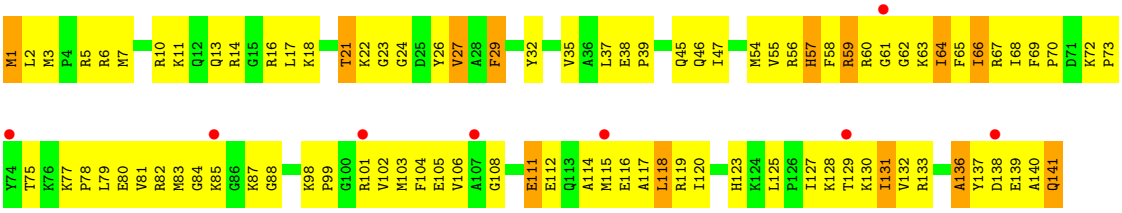
Chain RQ:



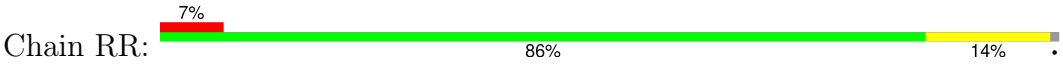


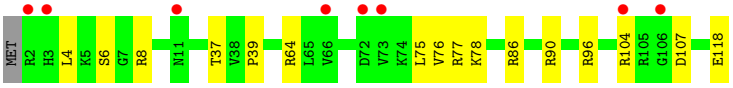
• Molecule 42: 50S ribosomal protein L16





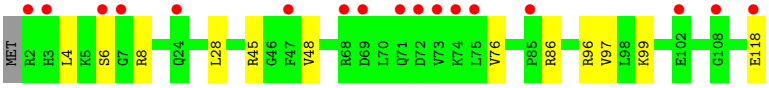
• Molecule 43: 50S ribosomal protein L17



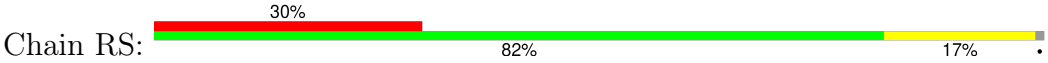


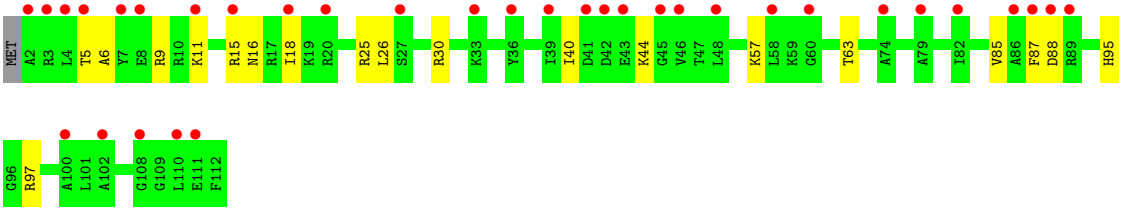
• Molecule 43: 50S ribosomal protein L17



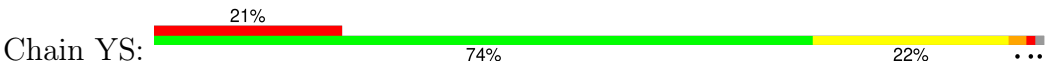


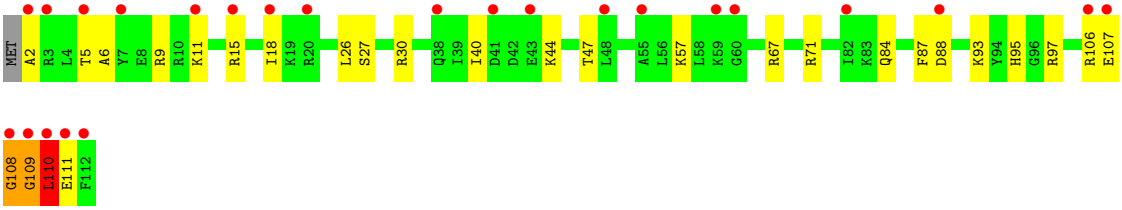
• Molecule 44: 50S ribosomal protein L18





• Molecule 44: 50S ribosomal protein L18

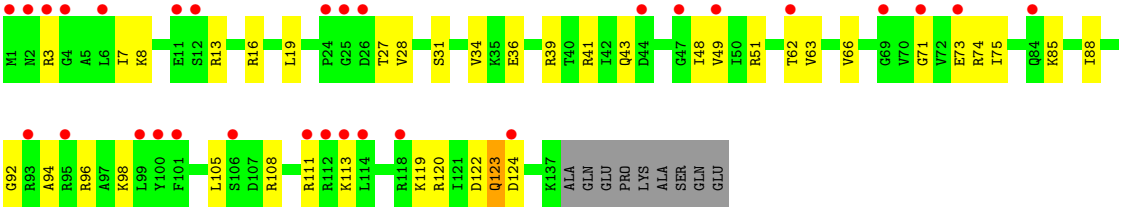




• Molecule 45: 50S ribosomal protein L19

Chain RT:

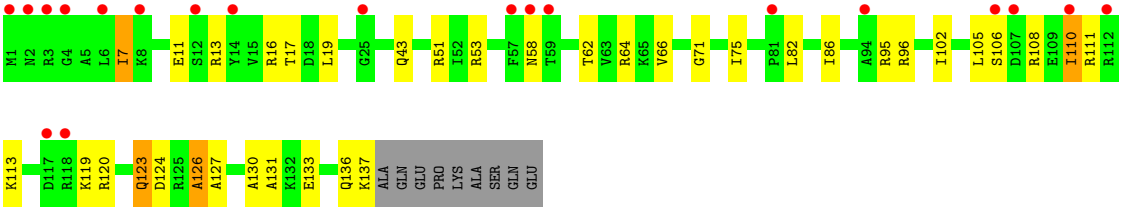




• Molecule 45: 50S ribosomal protein L19

Chain YT:

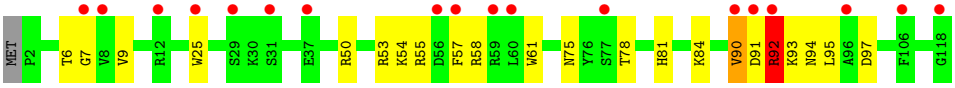




• Molecule 46: 50S ribosomal protein L20

Chain RU:

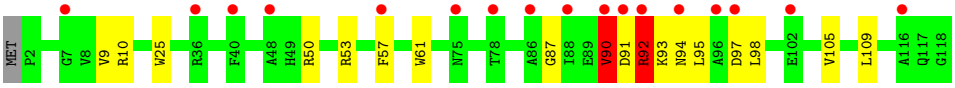




• Molecule 46: 50S ribosomal protein L20

Chain YU:

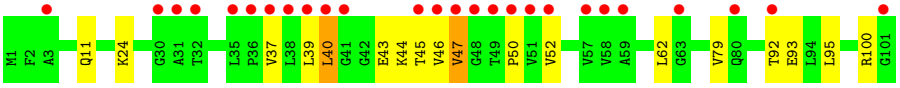




• Molecule 47: 50S ribosomal protein L21

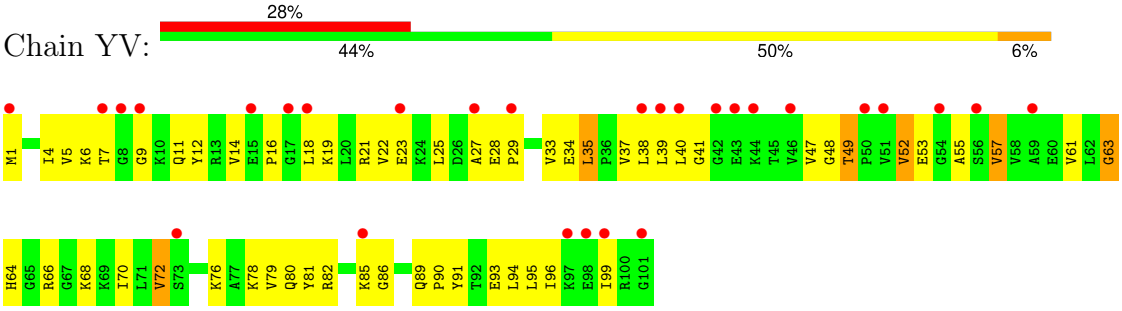
Chain RV:





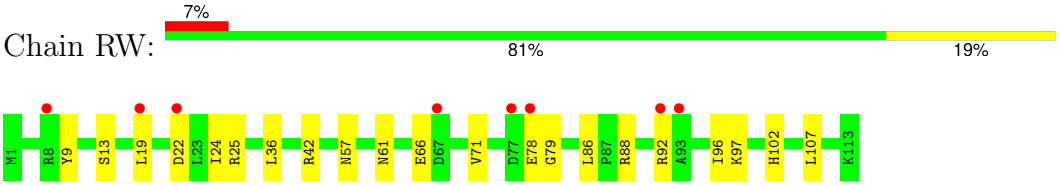
• Molecule 47: 50S ribosomal protein L21

Chain YV:



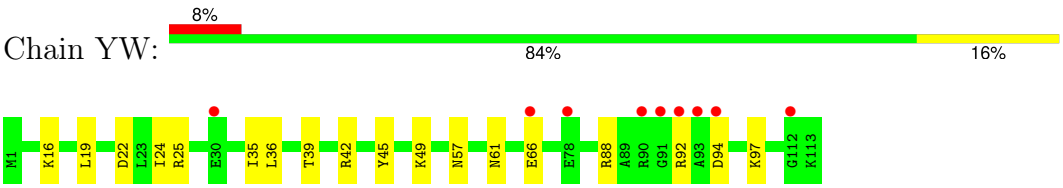
• Molecule 48: 50S ribosomal protein L22

Chain RW:



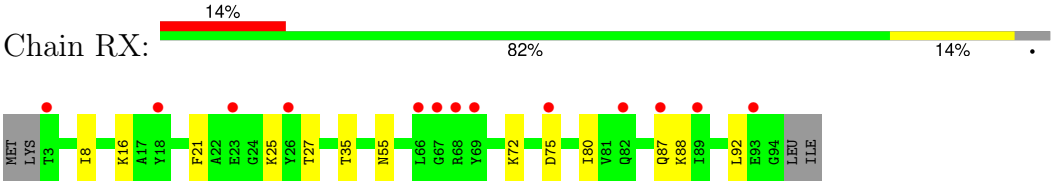
• Molecule 48: 50S ribosomal protein L22

Chain YW:



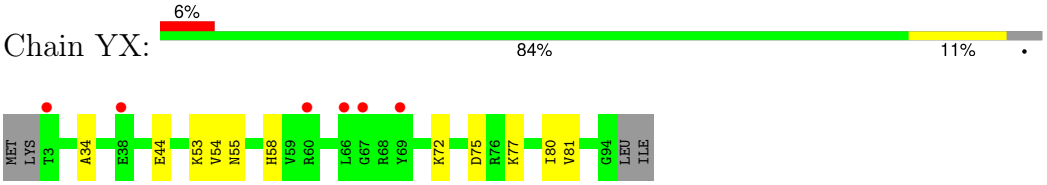
• Molecule 49: 50S ribosomal protein L23

Chain RX:



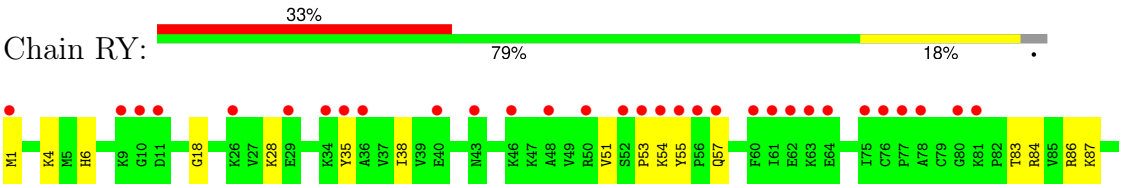
• Molecule 49: 50S ribosomal protein L23

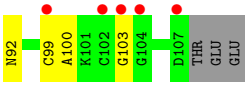
Chain YX:



• Molecule 50: 50S ribosomal protein L24

Chain RY:

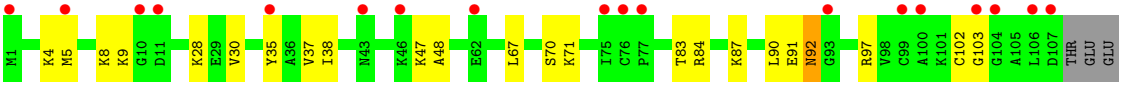




• Molecule 50: 50S ribosomal protein L24

Chain YY:

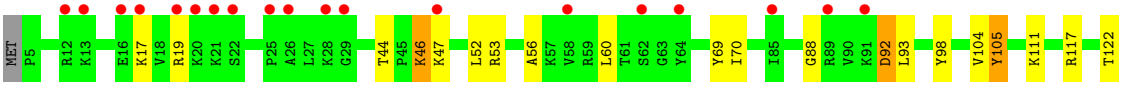


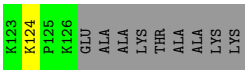


• Molecule 51: 30S ribosomal protein S12

Chain XL:



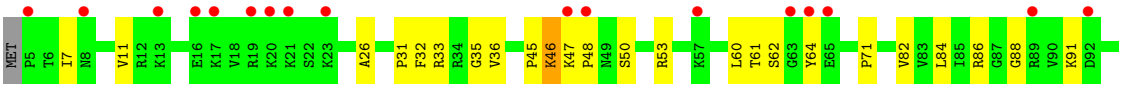


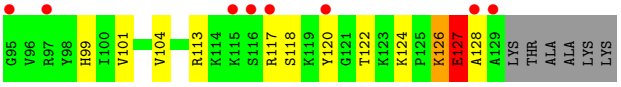


• Molecule 51: 30S ribosomal protein S12

Chain QL:



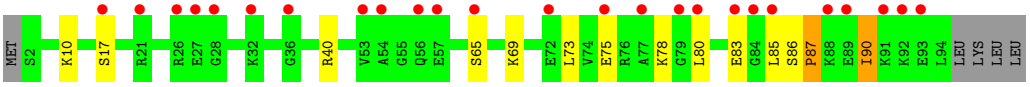




• Molecule 52: 50S ribosomal protein L28

Chain Y1:

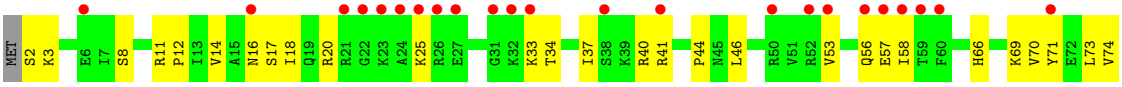




• Molecule 52: 50S ribosomal protein L28

Chain R1:

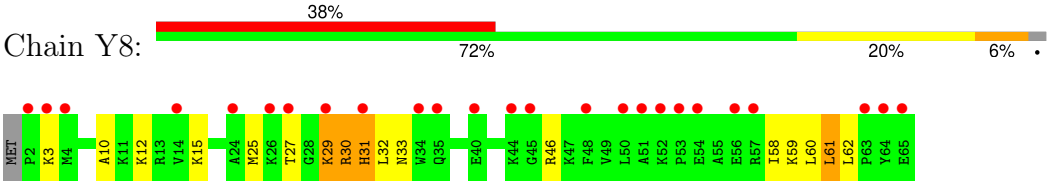






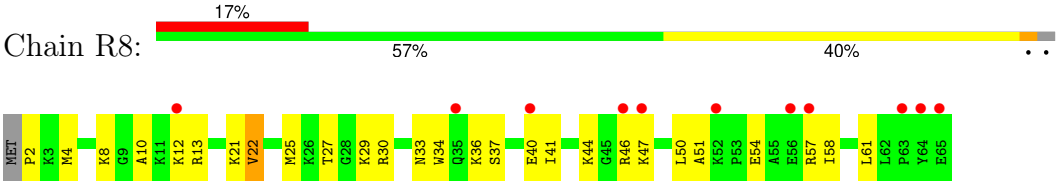
• Molecule 53: 50S ribosomal protein L35

Chain Y8:



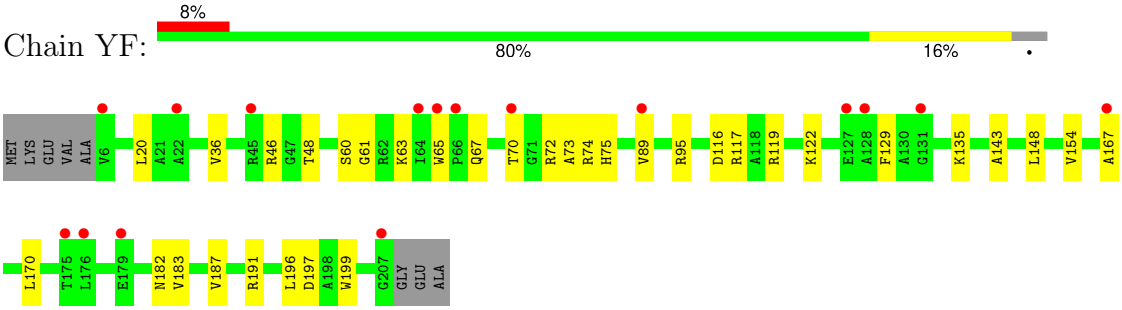
• Molecule 53: 50S ribosomal protein L35

Chain R8:



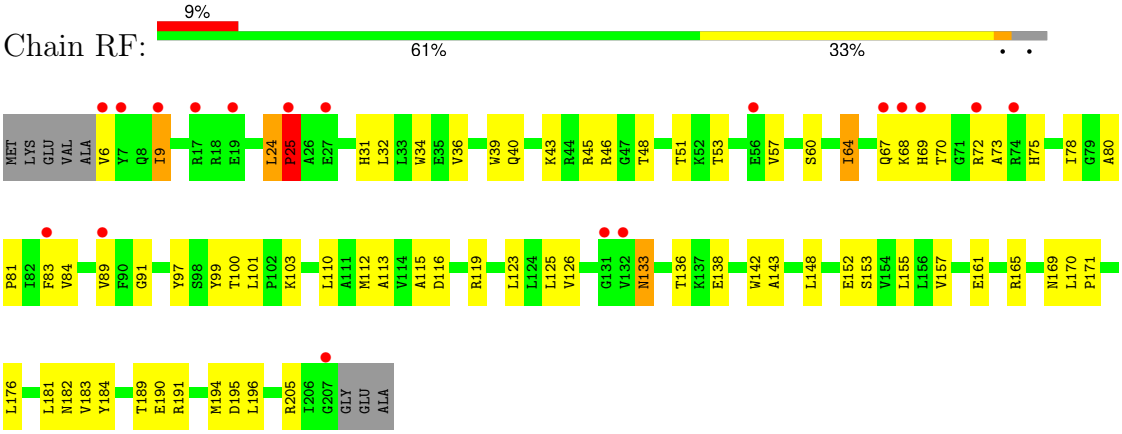
• Molecule 54: 50S ribosomal protein L4

Chain YF:



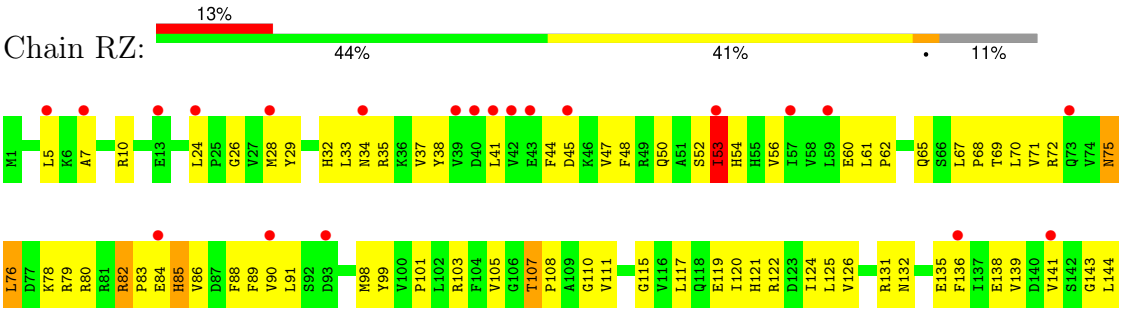
• Molecule 54: 50S ribosomal protein L4

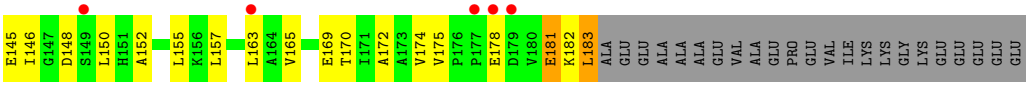
Chain RF:



• Molecule 55: 50S ribosomal protein L25

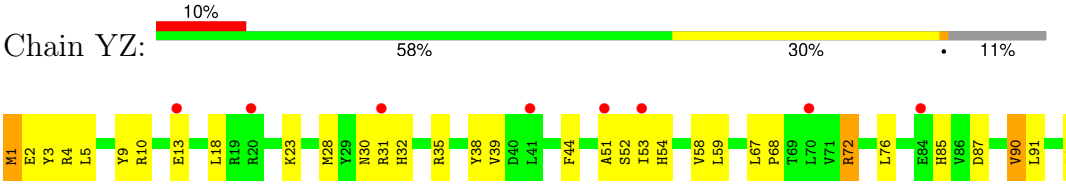
Chain RZ:





• Molecule 55: 50S ribosomal protein L25

Chain YZ:



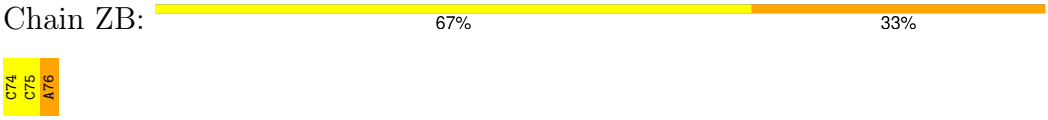
• Molecule 56: CCPuro

Chain ZA:



• Molecule 56: CCPuro

Chain ZB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	212.79Å 453.08Å 608.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.59 – 3.25 146.59 – 3.25	Depositor EDS
% Data completeness (in resolution range)	93.4 (146.59-3.25) 93.4 (146.59-3.25)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.229 , 0.256 0.230 , 0.257	Depositor DCC
R_{free} test set	41088 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å^2)	60.8	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 75.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	298432	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PPU, SF4, OMU, A2M, 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	0.20	0/36324	0.40	0/56690
1	XA	0.22	2/36254 (0.0%)	0.41	1/56581 (0.0%)
2	QB	1.06	4/1942 (0.2%)	1.52	11/2619 (0.4%)
2	XB	0.31	0/1950	0.85	5/2630 (0.2%)
3	QC	0.25	0/1629	0.70	0/2195
3	XC	0.25	0/1629	0.71	1/2195 (0.0%)
4	QD	0.28	0/1733	0.76	3/2318 (0.1%)
4	XD	0.30	0/1733	0.75	2/2318 (0.1%)
5	QE	0.25	0/1171	0.72	0/1576
5	XE	0.28	0/1171	0.76	2/1576 (0.1%)
6	QF	0.28	0/856	0.66	0/1154
6	XF	0.23	0/856	0.67	0/1154
7	QG	0.25	0/1276	0.70	1/1709 (0.1%)
7	XG	0.36	0/1276	0.70	0/1709
8	QH	0.61	2/1128 (0.2%)	0.97	6/1517 (0.4%)
8	XH	0.28	0/1128	0.67	2/1517 (0.1%)
9	QI	0.32	0/1029	0.97	3/1379 (0.2%)
9	XI	0.30	0/1017	0.80	0/1365
10	QJ	0.31	0/814	0.81	0/1095
10	XJ	0.33	0/790	0.91	3/1063 (0.3%)
11	QK	0.28	0/900	0.71	0/1213
11	XK	0.28	0/879	0.74	0/1187
12	QM	0.36	0/965	0.98	2/1292 (0.2%)
12	XM	0.29	0/956	0.93	5/1281 (0.4%)
13	QN	0.32	0/501	0.78	0/664
13	XN	0.31	0/501	0.78	0/664
14	QO	0.23	0/745	0.68	0/992
14	XO	0.24	0/740	0.63	0/987
15	QP	0.26	0/721	0.72	0/970
15	XP	0.27	0/721	0.74	0/970
16	QQ	0.23	0/847	0.67	0/1131
16	XQ	0.27	0/847	0.72	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	QR	0.26	0/579	0.73	1/768 (0.1%)
17	XR	0.26	0/579	0.73	0/768
18	QS	0.43	0/680	0.95	1/915 (0.1%)
18	XS	1.41	4/671 (0.6%)	1.69	7/904 (0.8%)
19	QT	0.27	0/765	0.83	1/1007 (0.1%)
19	XT	0.29	0/765	0.85	3/1007 (0.3%)
20	QU	0.20	0/221	0.59	0/288
20	XU	0.27	0/221	0.71	0/288
21	QV	0.17	0/1832	0.35	0/2855
21	QW	0.15	0/1832	0.31	0/2855
21	XV	0.19	0/1832	0.38	0/2855
21	XW	0.15	0/1832	0.31	0/2855
22	QX	0.18	0/414	0.34	0/645
22	XX	0.29	0/414	0.39	0/645
23	QY	0.92	0/743	1.20	1/1002 (0.1%)
23	QZ	0.94	0/743	1.26	2/1002 (0.2%)
23	XY	0.93	0/743	1.23	4/1002 (0.4%)
23	XZ	0.92	0/743	1.13	0/1002
24	R0	0.41	0/652	0.88	3/867 (0.3%)
24	Y0	0.44	0/657	0.94	6/874 (0.7%)
25	R2	0.27	0/583	0.86	1/771 (0.1%)
25	Y2	0.35	0/583	0.91	1/771 (0.1%)
26	R3	0.27	0/474	0.77	0/635
26	Y3	0.27	0/474	0.78	0/635
27	R4	0.50	0/578	1.47	16/776 (2.1%)
27	Y4	0.35	0/578	0.99	2/776 (0.3%)
28	R5	0.27	0/473	0.69	0/639
28	Y5	0.44	0/473	0.74	0/639
29	R6	0.23	0/460	0.71	0/613
29	Y6	0.27	0/460	0.72	0/613
30	R7	0.26	0/417	0.61	0/550
30	Y7	0.27	0/426	0.66	0/561
31	R9	0.26	0/310	0.73	0/407
31	Y9	0.22	0/310	0.69	0/407
32	RA	0.23	0/69739	0.41	6/108870 (0.0%)
32	YA	0.24	0/69353	0.42	5/108267 (0.0%)
33	RB	0.26	0/2881	0.43	0/4494
33	YB	0.30	1/2881 (0.0%)	0.45	0/4494
34	RD	0.36	0/2165	0.99	11/2919 (0.4%)
34	YD	1.04	2/2185 (0.1%)	1.40	13/2944 (0.4%)
35	RE	0.42	0/1601	1.15	17/2160 (0.8%)
35	YE	1.00	2/1592 (0.1%)	1.49	11/2149 (0.5%)
36	RG	0.38	0/1499	0.89	1/2016 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
36	YG	0.29	0/1499	0.84	4/2016 (0.2%)
37	RH	0.48	1/1362 (0.1%)	1.12	13/1841 (0.7%)
37	YH	1.02	0/1356	1.42	19/1834 (1.0%)
38	RI	0.83	1/1151 (0.1%)	1.31	13/1558 (0.8%)
38	YI	0.32	0/1151	0.97	6/1558 (0.4%)
39	RN	0.30	0/1131	0.94	7/1525 (0.5%)
39	YN	0.29	0/1131	0.92	5/1525 (0.3%)
40	RO	0.28	0/943	0.69	0/1269
40	YO	0.27	0/943	0.71	0/1269
41	RP	0.40	0/1162	1.10	8/1544 (0.5%)
41	YP	0.96	0/1152	1.34	2/1533 (0.1%)
42	RQ	0.37	0/1143	0.98	6/1527 (0.4%)
42	YQ	0.96	0/1143	1.36	9/1527 (0.6%)
43	RR	0.29	0/974	0.92	4/1302 (0.3%)
43	YR	0.28	0/974	0.86	1/1302 (0.1%)
44	RS	0.34	0/892	0.91	1/1187 (0.1%)
44	YS	0.36	0/892	1.01	6/1187 (0.5%)
45	RT	0.29	0/1155	0.93	7/1542 (0.5%)
45	YT	0.35	0/1155	0.99	7/1542 (0.5%)
46	RU	0.30	0/982	0.85	7/1306 (0.5%)
46	YU	0.30	0/982	0.88	7/1306 (0.5%)
47	RV	0.36	0/790	1.00	7/1057 (0.7%)
47	YV	1.00	0/790	1.47	9/1057 (0.9%)
48	RW	0.25	0/911	0.72	0/1220
48	YW	0.28	0/911	0.73	0/1220
49	RX	0.28	0/739	0.70	0/993
49	YX	0.26	0/739	0.72	0/993
50	RY	0.40	1/831 (0.1%)	0.89	5/1108 (0.5%)
50	YY	0.28	0/831	0.75	0/1108
51	QL	0.23	0/991	0.54	0/1327
51	XL	0.32	0/972	0.88	4/1301 (0.3%)
52	R1	0.46	0/744	0.65	0/989
52	Y1	0.44	0/736	0.83	0/978
53	R8	0.54	0/525	0.67	0/691
53	Y8	0.42	0/525	1.13	4/691 (0.6%)
54	RF	0.56	2/1620 (0.1%)	0.69	3/2194 (0.1%)
54	YF	0.32	0/1620	0.82	2/2194 (0.1%)
55	RZ	0.69	2/1493 (0.1%)	1.05	4/2026 (0.2%)
55	YZ	0.47	0/1493	0.65	0/2026
56	ZA	1.23	1/40 (2.5%)	1.30	0/60
56	ZB	0.40	0/40	0.81	0/60
All	All	0.34	25/323056 (0.0%)	0.61	330/482845 (0.1%)

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
2	QB	0	1
24	Y0	0	1
32	YA	0	1
37	YH	0	1
41	RP	0	1
51	QL	0	1
53	R8	0	1
All	All	0	7

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	RI	142	VAL	N-CA	-22.69	1.20	1.46
34	YD	29	PRO	N-CA	19.39	1.70	1.47
18	XS	59	PRO	N-CA	17.90	1.70	1.47
54	RF	25	PRO	N-CA	17.43	1.69	1.47
18	XS	42	PRO	N-CA	17.00	1.70	1.47

The worst 5 of 330 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	RI	142	VAL	N-CA-C	25.75	145.56	108.48
34	YD	28	GLU	CA-C-N	17.32	138.54	119.83
34	YD	28	GLU	C-N-CA	17.32	138.54	119.83
35	YE	21	VAL	CA-C-N	16.84	136.60	119.76
35	YE	21	VAL	C-N-CA	16.84	136.60	119.76

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	12	GLU	Mainchain
41	RP	11	GLY	Mainchain
24	Y0	8	GLY	Mainchain
32	YA	1162	G	Sidechain
37	YH	13	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32452	0	16381	375	0
1	XA	32389	0	16350	350	0
2	QB	1907	0	1958	288	0
2	XB	1915	0	1969	18	0
3	QC	1605	0	1668	23	0
3	XC	1605	0	1668	14	0
4	QD	1703	0	1763	29	0
4	XD	1703	0	1763	37	0
5	QE	1155	0	1213	9	0
5	XE	1155	0	1213	10	0
6	QF	843	0	857	7	0
6	XF	843	0	857	12	0
7	QG	1257	0	1296	9	0
7	XG	1257	0	1296	14	0
8	QH	1108	0	1165	17	0
8	XH	1108	0	1165	15	0
9	QI	1010	0	1037	24	0
9	XI	998	0	1024	20	0
10	QJ	801	0	849	12	0
10	XJ	777	0	816	21	0
11	QK	885	0	904	11	0
11	XK	864	0	881	11	0
12	QM	955	0	1021	22	0
12	XM	946	0	1008	14	0
13	QN	492	0	529	11	0
13	XN	492	0	529	4	0
14	QO	734	0	771	9	0
14	XO	729	0	768	7	0
15	QP	705	0	725	4	0
15	XP	705	0	725	5	0
16	QQ	834	0	904	10	0
16	XQ	834	0	904	8	0
17	QR	574	0	644	4	0
17	XR	574	0	644	4	0
18	QS	665	0	686	45	0
18	XS	656	0	666	74	0
19	QT	763	0	861	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XT	763	0	861	19	0
20	QU	217	0	234	4	0
20	XU	217	0	234	1	0
21	QV	1640	0	837	11	0
21	QW	1640	0	837	28	0
21	XV	1640	0	837	15	0
21	XW	1640	0	837	21	0
22	QX	435	0	225	18	0
22	XX	435	0	225	12	0
23	QY	723	0	713	93	0
23	QZ	723	0	713	105	0
23	XY	723	0	713	60	0
23	XZ	723	0	713	89	0
24	R0	643	0	667	9	0
24	Y0	648	0	672	15	0
25	R2	581	0	629	11	0
25	Y2	581	0	629	5	0
26	R3	469	0	518	2	0
26	Y3	469	0	518	5	0
27	R4	565	0	559	15	0
27	Y4	565	0	557	10	0
28	R5	459	0	476	9	0
28	Y5	459	0	480	11	0
29	R6	453	0	473	17	0
29	Y6	453	0	473	5	0
30	R7	409	0	454	4	0
30	Y7	418	0	467	6	0
31	R9	307	0	335	6	0
31	Y9	307	0	335	9	0
32	RA	62266	0	31390	624	0
32	YA	61921	0	31212	697	0
33	RB	2576	0	1305	32	0
33	YB	2576	0	1305	22	0
34	RD	2115	0	2195	47	0
34	YD	2135	0	2220	170	0
35	RE	1568	0	1634	52	0
35	YE	1559	0	1618	229	0
36	RG	1474	0	1535	30	0
36	YG	1474	0	1535	23	0
37	RH	1336	0	1418	41	0
37	YH	1330	0	1407	195	0
38	RI	1136	0	1223	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	YI	1136	0	1223	7	0
39	RN	1104	0	1180	14	0
39	YN	1104	0	1180	11	0
40	RO	933	0	996	17	0
40	YO	933	0	996	14	0
41	RP	1145	0	1228	79	0
41	YP	1135	0	1212	197	0
42	RQ	1122	0	1179	32	0
42	YQ	1122	0	1179	176	0
43	RR	960	0	1021	10	0
43	YR	960	0	1021	8	0
44	RS	882	0	943	13	0
44	YS	882	0	943	18	0
45	RT	1141	0	1202	23	0
45	YT	1141	0	1202	41	0
46	RU	964	0	1022	22	0
46	YU	964	0	1021	30	0
47	RV	779	0	852	9	0
47	YV	779	0	852	93	0
48	RW	900	0	964	13	0
48	YW	900	0	964	12	0
49	RX	725	0	778	9	0
49	YX	725	0	778	7	0
50	RY	818	0	913	14	0
50	YY	818	0	913	17	0
51	QL	975	0	1062	41	0
51	XL	956	0	1046	16	0
52	R1	737	0	813	38	0
52	Y1	729	0	802	7	0
53	R8	517	0	582	67	0
53	Y8	517	0	582	31	0
54	RF	1585	0	1632	82	0
54	YF	1585	0	1632	24	0
55	RZ	1461	0	1493	111	0
55	YZ	1461	0	1493	106	0
56	ZA	74	0	51	15	0
56	ZB	74	0	51	14	0
57	QA	94	0	0	0	0
57	QD	2	0	0	0	0
57	QE	1	0	0	0	0
57	QF	1	0	0	0	0
57	QV	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	QX	1	0	0	0	0
57	R0	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	302	0	0	0	0
57	RB	3	0	0	0	0
57	RD	1	0	0	0	0
57	RE	1	0	0	0	0
57	RN	1	0	0	0	0
57	RO	1	0	0	0	0
57	RP	2	0	0	0	0
57	RQ	2	0	0	0	0
57	RR	2	0	0	0	0
57	RY	1	0	0	0	0
57	XA	116	0	0	0	0
57	XD	1	0	0	0	0
57	XE	1	0	0	0	0
57	XF	1	0	0	0	0
57	XL	1	0	0	0	0
57	XM	1	0	0	0	0
57	XV	3	0	0	0	0
57	Y0	2	0	0	0	0
57	Y3	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YA	326	0	0	0	0
57	YB	5	0	0	0	0
57	YD	5	0	0	0	0
57	YE	5	0	0	0	0
57	YF	1	0	0	0	0
57	YG	1	0	0	0	0
57	YO	1	0	0	0	0
57	YQ	3	0	0	0	0
57	YV	1	0	0	0	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
59	QN	1	0	0	0	0
59	R4	1	0	0	0	0
59	R5	1	0	0	0	0
59	R6	1	0	0	0	0
59	R9	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y4	1	0	0	0	0
59	Y6	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	298432	0	202697	4794	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 10.

The worst 5 of 4794 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)
42:YQ:64:ILE:CD1	55:YZ:178:GLU:HG3	1.19	1.65
37:YH:123:PHE:CE1	37:YH:133:VAL:HG12	1.26	1.62
37:YH:5:GLY:HA3	37:YH:65:HIS:CE1	1.22	1.59
41:YP:100:LEU:CD1	41:YP:112:LEU:HD11	1.37	1.55
54:RF:9:ILE:HD11	54:RF:125:LEU:CD1	1.39	1.51

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%)	212 (91%)	18 (8%)	3 (1%)	9 34
2	XB	234/256 (91%)	208 (89%)	25 (11%)	1 (0%)	30 59
3	QC	203/239 (85%)	190 (94%)	13 (6%)	0	100 100
3	XC	203/239 (85%)	193 (95%)	10 (5%)	0	100 100
4	QD	206/209 (99%)	191 (93%)	13 (6%)	2 (1%)	12 40
4	XD	206/209 (99%)	191 (93%)	13 (6%)	2 (1%)	12 40
5	QE	149/162 (92%)	139 (93%)	9 (6%)	1 (1%)	18 48
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	18 48
6	QF	99/101 (98%)	99 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	143 (94%)	10 (6%)	0	100	100
8	QH	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
8	XH	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
9	QI	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	16	44
9	XI	124/128 (97%)	114 (92%)	10 (8%)	0	100	100
10	QJ	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
10	XJ	94/105 (90%)	85 (90%)	8 (8%)	1 (1%)	11	38
11	QK	117/129 (91%)	109 (93%)	8 (7%)	0	100	100
11	XK	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
12	QM	118/126 (94%)	101 (86%)	13 (11%)	4 (3%)	3	17
12	XM	117/126 (93%)	99 (85%)	17 (14%)	1 (1%)	14	42
13	QN	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	7	29
13	XN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	29
14	QO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
14	XO	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
15	QP	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
15	XP	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
16	QQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
16	XQ	98/105 (93%)	94 (96%)	4 (4%)	0	100	100
17	QR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
17	XR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
18	QS	81/93 (87%)	68 (84%)	12 (15%)	1 (1%)	10	36
18	XS	81/93 (87%)	73 (90%)	6 (7%)	2 (2%)	4	22
19	QT	97/106 (92%)	87 (90%)	10 (10%)	0	100	100
19	XT	97/106 (92%)	88 (91%)	9 (9%)	0	100	100
20	QU	23/27 (85%)	23 (100%)	0	0	100	100
20	XU	23/27 (85%)	23 (100%)	0	0	100	100
23	QY	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
23	QZ	82/84 (98%)	76 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
23	XY	82/84 (98%)	78 (95%)	4 (5%)	0	100 100
23	XZ	82/84 (98%)	79 (96%)	3 (4%)	0	100 100
24	R0	79/85 (93%)	73 (92%)	4 (5%)	2 (2%)	4 22
24	Y0	80/85 (94%)	77 (96%)	3 (4%)	0	100 100
25	R2	67/72 (93%)	61 (91%)	5 (8%)	1 (2%)	8 32
25	Y2	67/72 (93%)	64 (96%)	3 (4%)	0	100 100
26	R3	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
26	Y3	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
27	R4	67/71 (94%)	46 (69%)	17 (25%)	4 (6%)	1 8
27	Y4	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	8 32
28	R5	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
28	Y5	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
29	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
29	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
30	R7	45/49 (92%)	45 (100%)	0	0	100 100
30	Y7	46/49 (94%)	46 (100%)	0	0	100 100
31	R9	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
31	Y9	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
34	RD	270/276 (98%)	237 (88%)	26 (10%)	7 (3%)	4 21
34	YD	272/276 (99%)	261 (96%)	11 (4%)	0	100 100
35	RE	203/206 (98%)	159 (78%)	34 (17%)	10 (5%)	1 11
35	YE	202/206 (98%)	190 (94%)	9 (4%)	3 (2%)	8 32
36	RG	179/182 (98%)	153 (86%)	24 (13%)	2 (1%)	11 38
36	YG	179/182 (98%)	149 (83%)	29 (16%)	1 (1%)	21 51
37	RH	172/180 (96%)	145 (84%)	20 (12%)	7 (4%)	2 13
37	YH	172/180 (96%)	163 (95%)	7 (4%)	2 (1%)	10 36
38	RI	144/148 (97%)	115 (80%)	24 (17%)	5 (4%)	3 17
38	YI	144/148 (97%)	119 (83%)	21 (15%)	4 (3%)	4 20
39	RN	136/140 (97%)	115 (85%)	18 (13%)	3 (2%)	5 25
39	YN	136/140 (97%)	119 (88%)	15 (11%)	2 (2%)	8 32
40	RO	120/122 (98%)	112 (93%)	8 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	YO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
41	RP	148/150 (99%)	112 (76%)	32 (22%)	4 (3%)	4	21
41	YP	147/150 (98%)	137 (93%)	8 (5%)	2 (1%)	9	33
42	RQ	139/141 (99%)	115 (83%)	22 (16%)	2 (1%)	9	33
42	YQ	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	18	48
43	RR	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	14	42
43	YR	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	42
44	RS	109/112 (97%)	91 (84%)	18 (16%)	0	100	100
44	YS	109/112 (97%)	91 (84%)	17 (16%)	1 (1%)	14	42
45	RT	135/146 (92%)	118 (87%)	15 (11%)	2 (2%)	8	32
45	YT	135/146 (92%)	114 (84%)	19 (14%)	2 (2%)	8	32
46	RU	115/118 (98%)	108 (94%)	6 (5%)	1 (1%)	14	42
46	YU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	42
47	RV	99/101 (98%)	82 (83%)	16 (16%)	1 (1%)	12	40
47	YV	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
48	RW	111/113 (98%)	105 (95%)	5 (4%)	1 (1%)	14	42
48	YW	111/113 (98%)	102 (92%)	8 (7%)	1 (1%)	14	42
49	RX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
49	YX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
50	RY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
50	YY	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
51	QL	123/132 (93%)	109 (89%)	13 (11%)	1 (1%)	16	44
51	XL	120/132 (91%)	100 (83%)	19 (16%)	1 (1%)	16	44
52	R1	92/98 (94%)	86 (94%)	4 (4%)	2 (2%)	5	25
52	Y1	91/98 (93%)	81 (89%)	10 (11%)	0	100	100
53	R8	62/65 (95%)	55 (89%)	7 (11%)	0	100	100
53	Y8	62/65 (95%)	47 (76%)	12 (19%)	3 (5%)	2	11
54	RF	200/210 (95%)	196 (98%)	3 (2%)	1 (0%)	24	55
54	YF	200/210 (95%)	185 (92%)	13 (6%)	2 (1%)	12	40
55	RZ	181/206 (88%)	171 (94%)	9 (5%)	1 (1%)	21	51
55	YZ	181/206 (88%)	175 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11786/12464 (95%)	10743 (91%)	935 (8%)	108 (1%)	14 42

5 of 108 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	QM	12	ASN
18	QS	41	VAL
27	R4	24	THR
27	R4	25	TYR
34	RD	25	THR

5.3.2 Protein sidechains (i)

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%)	178 (88%)	25 (12%)	4 19
2	XB	204/220 (93%)	203 (100%)	1 (0%)	81 82
3	QC	159/188 (85%)	159 (100%)	0	100 100
3	XC	159/188 (85%)	159 (100%)	0	100 100
4	QD	180/181 (99%)	179 (99%)	1 (1%)	78 81
4	XD	180/181 (99%)	180 (100%)	0	100 100
5	QE	116/123 (94%)	116 (100%)	0	100 100
5	XE	116/123 (94%)	115 (99%)	1 (1%)	70 76
6	QF	90/90 (100%)	90 (100%)	0	100 100
6	XF	90/90 (100%)	90 (100%)	0	100 100
7	QG	126/127 (99%)	126 (100%)	0	100 100
7	XG	126/127 (99%)	124 (98%)	2 (2%)	55 70
8	QH	118/119 (99%)	118 (100%)	0	100 100
8	XH	118/119 (99%)	117 (99%)	1 (1%)	73 78
9	QI	98/99 (99%)	98 (100%)	0	100 100
9	XI	97/99 (98%)	95 (98%)	2 (2%)	47 66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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	QM	96/101 (95%)	95 (99%)	1 (1%)	68 75
12	XM	95/101 (94%)	94 (99%)	1 (1%)	65 75
13	QN	49/50 (98%)	49 (100%)	0	100 100
13	XN	49/50 (98%)	49 (100%)	0	100 100
14	QO	79/80 (99%)	79 (100%)	0	100 100
14	XO	79/80 (99%)	79 (100%)	0	100 100
15	QP	72/74 (97%)	72 (100%)	0	100 100
15	XP	72/74 (97%)	72 (100%)	0	100 100
16	QQ	95/97 (98%)	95 (100%)	0	100 100
16	XQ	95/97 (98%)	95 (100%)	0	100 100
17	QR	61/77 (79%)	61 (100%)	0	100 100
17	XR	61/77 (79%)	61 (100%)	0	100 100
18	QS	72/80 (90%)	69 (96%)	3 (4%)	26 53
18	XS	69/80 (86%)	60 (87%)	9 (13%)	4 17
19	QT	76/82 (93%)	76 (100%)	0	100 100
19	XT	76/82 (93%)	75 (99%)	1 (1%)	61 73
20	QU	20/22 (91%)	20 (100%)	0	100 100
20	XU	20/22 (91%)	20 (100%)	0	100 100
23	QY	78/78 (100%)	77 (99%)	1 (1%)	61 73
23	QZ	78/78 (100%)	70 (90%)	8 (10%)	7 25
23	XY	78/78 (100%)	78 (100%)	0	100 100
23	XZ	78/78 (100%)	76 (97%)	2 (3%)	40 62
24	R0	65/67 (97%)	63 (97%)	2 (3%)	35 59
24	Y0	65/67 (97%)	65 (100%)	0	100 100
25	R2	64/67 (96%)	64 (100%)	0	100 100
25	Y2	64/67 (96%)	64 (100%)	0	100 100
26	R3	51/52 (98%)	51 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	Y3	51/52 (98%)	51 (100%)	0	100 100
27	R4	62/63 (98%)	60 (97%)	2 (3%)	34 58
27	Y4	62/63 (98%)	62 (100%)	0	100 100
28	R5	51/52 (98%)	51 (100%)	0	100 100
28	Y5	51/52 (98%)	50 (98%)	1 (2%)	48 66
29	R6	51/52 (98%)	51 (100%)	0	100 100
29	Y6	51/52 (98%)	51 (100%)	0	100 100
30	R7	40/42 (95%)	40 (100%)	0	100 100
30	Y7	41/42 (98%)	41 (100%)	0	100 100
31	R9	34/34 (100%)	34 (100%)	0	100 100
31	Y9	34/34 (100%)	34 (100%)	0	100 100
34	RD	214/218 (98%)	213 (100%)	1 (0%)	81 82
34	YD	216/218 (99%)	210 (97%)	6 (3%)	38 60
35	RE	165/166 (99%)	162 (98%)	3 (2%)	51 69
35	YE	164/166 (99%)	154 (94%)	10 (6%)	17 44
36	RG	155/156 (99%)	155 (100%)	0	100 100
36	YG	155/156 (99%)	154 (99%)	1 (1%)	78 81
37	RH	145/148 (98%)	140 (97%)	5 (3%)	32 57
37	YH	144/148 (97%)	134 (93%)	10 (7%)	14 41
38	RI	122/124 (98%)	120 (98%)	2 (2%)	55 70
38	YI	122/124 (98%)	122 (100%)	0	100 100
39	RN	117/119 (98%)	117 (100%)	0	100 100
39	YN	117/119 (98%)	116 (99%)	1 (1%)	70 76
40	RO	100/100 (100%)	100 (100%)	0	100 100
40	YO	100/100 (100%)	100 (100%)	0	100 100
41	RP	116/116 (100%)	113 (97%)	3 (3%)	40 62
41	YP	115/116 (99%)	101 (88%)	14 (12%)	5 20
42	RQ	111/111 (100%)	110 (99%)	1 (1%)	70 76
42	YQ	111/111 (100%)	104 (94%)	7 (6%)	16 43
43	RR	100/101 (99%)	100 (100%)	0	100 100
43	YR	100/101 (99%)	100 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
44	RS	87/88 (99%)	86 (99%)	1 (1%)	65 75
44	YS	87/88 (99%)	87 (100%)	0	100 100
45	RT	120/127 (94%)	119 (99%)	1 (1%)	73 78
45	YT	120/127 (94%)	119 (99%)	1 (1%)	73 78
46	RU	93/94 (99%)	93 (100%)	0	100 100
46	YU	93/94 (99%)	92 (99%)	1 (1%)	65 75
47	RV	82/82 (100%)	80 (98%)	2 (2%)	43 64
47	YV	82/82 (100%)	80 (98%)	2 (2%)	43 64
48	RW	92/92 (100%)	92 (100%)	0	100 100
48	YW	92/92 (100%)	92 (100%)	0	100 100
49	RX	74/78 (95%)	74 (100%)	0	100 100
49	YX	74/78 (95%)	74 (100%)	0	100 100
50	RY	88/91 (97%)	87 (99%)	1 (1%)	65 75
50	YY	88/91 (97%)	86 (98%)	2 (2%)	44 65
51	QL	104/109 (95%)	102 (98%)	2 (2%)	50 67
51	XL	103/109 (94%)	103 (100%)	0	100 100
52	R1	79/83 (95%)	79 (100%)	0	100 100
52	Y1	78/83 (94%)	73 (94%)	5 (6%)	16 42
53	R8	54/55 (98%)	53 (98%)	1 (2%)	50 67
53	Y8	54/55 (98%)	54 (100%)	0	100 100
54	RF	161/166 (97%)	158 (98%)	3 (2%)	50 67
54	YF	161/166 (97%)	160 (99%)	1 (1%)	78 81
55	RZ	162/179 (90%)	155 (96%)	7 (4%)	26 52
55	YZ	162/179 (90%)	158 (98%)	4 (2%)	42 63
All	All	9997/10378 (96%)	9835 (98%)	162 (2%)	55 70

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
37	YH	24	VAL
18	XS	77	THR
37	YH	79	VAL
35	YE	42	ASP
55	RZ	76	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
40	YO	3	GLN
47	YV	89	GLN
44	YS	38	GLN
34	YD	87	ASN
35	YE	135	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1508/1521 (99%)	309 (20%)	50 (3%)
1	XA	1505/1521 (98%)	301 (20%)	48 (3%)
21	QV	77/77 (100%)	7 (9%)	2 (2%)
21	QW	76/77 (98%)	14 (18%)	1 (1%)
21	XV	77/77 (100%)	7 (9%)	1 (1%)
21	XW	76/77 (98%)	15 (19%)	1 (1%)
22	QX	19/22 (86%)	9 (47%)	1 (5%)
22	XX	19/22 (86%)	7 (36%)	2 (10%)
32	RA	2888/2915 (99%)	599 (20%)	47 (1%)
32	YA	2872/2915 (98%)	580 (20%)	42 (1%)
33	RB	119/124 (95%)	26 (21%)	1 (0%)
33	YB	119/124 (95%)	21 (17%)	1 (0%)
56	ZA	1/3 (33%)	1 (100%)	0
56	ZB	1/3 (33%)	0	0
All	All	9357/9478 (98%)	1896 (20%)	197 (2%)

5 of 1896 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	4	U
1	QA	5	U
1	QA	6	G
1	QA	9	G
1	QA	22	G

5 of 197 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	358	U
1	XA	1190	G
1	XA	547	A

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Mol	Chain	Res	Type
1	XA	1004	A
21	XV	1	C

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

8 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	A2M	QX	19	22	22,25,26	1.54	4 (18%)	30,36,39	2.12	10 (33%)
22	A2M	QX	20	22	22,25,26	1.55	4 (18%)	30,36,39	2.06	6 (20%)
22	OMU	QX	21	22,1	19,22,23	1.81	4 (21%)	25,31,34	2.19	9 (36%)
22	A2M	XX	20	22	22,25,26	1.48	5 (22%)	30,36,39	2.10	8 (26%)
22	OMU	XX	21	22,1	19,22,23	1.23	3 (15%)	25,31,34	1.80	5 (20%)
56	PPU	ZB	76	32,56	37,40,41	1.20	5 (13%)	47,57,60	2.08	13 (27%)
56	PPU	ZA	76	32,56	37,40,41	1.61	7 (18%)	47,57,60	2.23	16 (34%)
22	A2M	XX	19	22	22,25,26	1.47	5 (22%)	30,36,39	2.10	10 (33%)

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	A2M	QX	19	22	-	0/9/27/28	0/3/3/3
22	A2M	QX	20	22	-	1/9/27/28	0/3/3/3
22	OMU	QX	21	22,1	-	2/9/27/28	0/2/2/2
22	A2M	XX	20	22	-	2/9/27/28	0/3/3/3
22	OMU	XX	21	22,1	-	2/9/27/28	0/2/2/2
56	PPU	ZB	76	32,56	-	6/25/43/44	0/4/4/4
56	PPU	ZA	76	32,56	-	4/25/43/44	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	A2M	XX	19	22	-	2/9/27/28	0/3/3/3

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QX	20	A2M	C5-C4	4.86	1.47	1.39
22	QX	19	A2M	C5-C4	4.82	1.47	1.39
22	XX	20	A2M	C5-C4	4.40	1.46	1.39
22	XX	19	A2M	C5-C4	4.35	1.46	1.39
56	ZB	76	PPU	C5-C4	4.33	1.46	1.39

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	QX	20	A2M	C5-C4-N3	-6.40	117.91	126.72
22	XX	20	A2M	C5-C4-N3	-6.08	118.34	126.72
22	QX	19	A2M	C5-C4-N3	-5.90	118.60	126.72
56	ZB	76	PPU	C5-C4-N3	-5.83	118.69	126.72
22	XX	19	A2M	C5-C4-N3	-5.57	119.05	126.72

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	XX	21	OMU	C3'-C4'-C5'-O5'
22	XX	21	OMU	O4'-C4'-C5'-O5'
56	ZA	76	PPU	C4'-C3'-N3'-C
56	ZB	76	PPU	C5-C6-N6-C10
22	QX	21	OMU	O4'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	QX	19	A2M	3	0
22	QX	20	A2M	2	0
22	QX	21	OMU	3	0
22	XX	20	A2M	3	0
22	XX	21	OMU	2	0
56	ZB	76	PPU	12	0
56	ZA	76	PPU	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	XX	19	A2M	5	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 906 ligands modelled in this entry, 904 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	SF4	XD	301	4	0,12,12	-	-	-		
58	SF4	QD	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
58	SF4	XD	301	4	-	-	0/6/5/5
58	SF4	QD	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 (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	1510/1521 (99%)	0.23	41 (2%) 56 38	44, 86, 196, 383	0
1	XA	1507/1521 (99%)	0.09	40 (2%) 56 38	34, 75, 177, 475	0
2	QB	235/256 (91%)	0.84	21 (8%) 15 12	58, 118, 181, 243	0
2	XB	236/256 (92%)	0.98	30 (12%) 8 6	53, 108, 176, 224	0
3	QC	205/239 (85%)	1.00	18 (8%) 15 12	67, 114, 167, 195	0
3	XC	205/239 (85%)	0.70	8 (3%) 43 29	51, 88, 139, 192	0
4	QD	208/209 (99%)	1.02	29 (13%) 6 5	44, 79, 119, 165	0
4	XD	208/209 (99%)	1.09	35 (16%) 4 4	42, 78, 119, 205	0
5	QE	151/162 (93%)	1.09	20 (13%) 7 6	45, 79, 122, 166	0
5	XE	151/162 (93%)	0.79	12 (7%) 18 14	39, 70, 119, 208	0
6	QF	101/101 (100%)	0.79	4 (3%) 42 28	53, 90, 121, 159	0
6	XF	101/101 (100%)	0.87	12 (11%) 9 8	44, 82, 116, 238	0
7	QG	155/156 (99%)	1.18	27 (17%) 4 4	76, 113, 152, 223	0
7	XG	155/156 (99%)	1.29	35 (22%) 2 2	58, 98, 152, 174	0
8	QH	137/138 (99%)	1.14	22 (16%) 4 4	48, 83, 119, 136	0
8	XH	137/138 (99%)	0.83	13 (9%) 14 11	40, 79, 119, 154	0
9	QI	127/128 (99%)	1.34	28 (22%) 2 2	80, 133, 168, 206	0
9	XI	126/128 (98%)	1.55	29 (23%) 2 2	60, 110, 158, 181	0
10	QJ	99/105 (94%)	1.88	37 (37%) 1 1	88, 136, 195, 218	0
10	XJ	96/105 (91%)	1.41	21 (21%) 2 2	62, 122, 189, 238	0
11	QK	119/129 (92%)	1.31	26 (21%) 2 2	41, 93, 148, 208	0
11	XK	116/129 (89%)	1.07	16 (13%) 6 5	46, 80, 122, 180	0
12	QM	120/126 (95%)	1.49	29 (24%) 2 2	67, 119, 180, 215	0
12	XM	119/126 (94%)	1.30	28 (23%) 2 2	55, 99, 146, 265	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	QN	60/61 (98%)	2.09	24 (40%) 1 1	66, 114, 161, 194	0
13	XN	60/61 (98%)	1.42	17 (28%) 1 1	57, 91, 132, 201	0
14	QO	88/89 (98%)	0.99	10 (11%) 10 9	49, 87, 131, 146	0
14	XO	87/89 (97%)	0.64	3 (3%) 48 32	47, 75, 122, 143	0
15	QP	84/88 (95%)	0.98	7 (8%) 17 13	50, 79, 125, 202	0
15	XP	84/88 (95%)	1.02	9 (10%) 11 9	51, 80, 121, 198	0
16	QQ	100/105 (95%)	1.13	16 (16%) 5 4	51, 78, 118, 144	0
16	XQ	100/105 (95%)	0.74	8 (8%) 18 14	49, 81, 109, 143	0
17	QR	70/88 (79%)	0.84	6 (8%) 16 13	56, 95, 138, 180	0
17	XR	70/88 (79%)	0.68	4 (5%) 29 20	39, 76, 125, 148	0
18	QS	83/93 (89%)	1.85	32 (38%) 1 1	87, 133, 189, 224	0
18	XS	83/93 (89%)	1.03	12 (14%) 6 5	64, 96, 157, 174	0
19	QT	99/106 (93%)	1.32	19 (19%) 3 3	61, 96, 160, 220	0
19	XT	99/106 (93%)	1.41	24 (24%) 2 2	55, 93, 163, 203	0
20	QU	25/27 (92%)	2.41	12 (48%) 0 0	86, 117, 154, 187	0
20	XU	25/27 (92%)	2.55	12 (48%) 0 0	73, 104, 134, 150	0
21	QV	77/77 (100%)	0.15	3 (3%) 43 29	49, 95, 154, 202	0
21	QW	77/77 (100%)	1.20	9 (11%) 9 8	68, 198, 300, 360	0
21	XV	77/77 (100%)	0.06	2 (2%) 57 38	40, 81, 134, 208	0
21	XW	77/77 (100%)	1.10	13 (16%) 4 4	78, 237, 321, 383	0
22	QX	17/22 (77%)	1.97	8 (47%) 0 0	55, 210, 302, 312	0
22	XX	17/22 (77%)	2.67	12 (70%) 0 0	47, 206, 295, 330	0
23	QY	84/84 (100%)	1.27	17 (20%) 3 2	49, 83, 128, 162	0
23	QZ	84/84 (100%)	0.68	5 (5%) 27 19	73, 122, 172, 216	0
23	XY	84/84 (100%)	1.03	11 (13%) 7 6	36, 70, 108, 121	0
23	XZ	84/84 (100%)	1.07	12 (14%) 6 5	69, 108, 153, 213	0
24	R0	81/85 (95%)	1.26	15 (18%) 3 3	45, 66, 98, 144	0
24	Y0	82/85 (96%)	1.34	21 (25%) 1 2	38, 63, 105, 111	0
25	R2	69/72 (95%)	0.84	6 (8%) 16 12	38, 89, 166, 200	0
25	Y2	69/72 (95%)	1.08	12 (17%) 4 4	39, 71, 125, 264	0
26	R3	59/60 (98%)	1.13	9 (15%) 5 5	44, 72, 125, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
26	Y3	59/60 (98%)	1.08	9 (15%) 5 5	44, 74, 122, 162	0
27	R4	69/71 (97%)	1.90	27 (39%) 1 1	106, 159, 243, 324	0
27	Y4	69/71 (97%)	1.07	13 (18%) 3 3	82, 133, 191, 238	0
28	R5	59/60 (98%)	0.75	2 (3%) 48 32	35, 66, 139, 176	0
28	Y5	59/60 (98%)	1.44	14 (23%) 2 2	28, 76, 152, 166	0
29	R6	53/54 (98%)	1.40	14 (26%) 1 1	74, 109, 153, 159	0
29	Y6	53/54 (98%)	0.96	6 (11%) 10 9	71, 97, 153, 195	0
30	R7	47/49 (95%)	0.73	6 (12%) 7 6	27, 46, 79, 139	0
30	Y7	48/49 (97%)	0.87	5 (10%) 11 9	25, 43, 112, 140	0
31	R9	37/37 (100%)	1.88	14 (37%) 1 1	87, 124, 155, 209	0
31	Y9	37/37 (100%)	1.56	10 (27%) 1 1	75, 116, 153, 158	0
32	RA	2891/2915 (99%)	0.01	78 (2%) 56 38	24, 63, 207, 475	0
32	YA	2875/2915 (98%)	-0.06	62 (2%) 62 43	19, 58, 247, 435	0
33	RB	120/124 (96%)	0.39	3 (2%) 58 39	58, 103, 141, 194	0
33	YB	120/124 (96%)	0.14	2 (1%) 69 50	57, 83, 120, 191	0
34	RD	272/276 (98%)	1.11	43 (15%) 5 4	26, 62, 110, 239	0
34	YD	274/276 (99%)	0.57	16 (5%) 29 19	13, 44, 80, 120	0
35	RE	205/206 (99%)	1.33	47 (22%) 2 2	31, 79, 154, 219	0
35	YE	204/206 (99%)	0.90	19 (9%) 14 11	31, 67, 122, 155	0
36	RG	181/182 (99%)	1.35	40 (22%) 2 2	72, 113, 153, 188	0
36	YG	181/182 (99%)	0.99	18 (9%) 13 10	53, 98, 147, 195	0
37	RH	174/180 (96%)	1.62	51 (29%) 1 1	94, 147, 219, 276	0
37	YH	174/180 (96%)	1.63	49 (28%) 1 1	60, 124, 195, 262	0
38	RI	146/148 (98%)	1.83	54 (36%) 1 1	59, 115, 160, 186	0
38	YI	146/148 (98%)	1.53	40 (27%) 1 1	44, 98, 151, 201	0
39	RN	138/140 (98%)	1.71	45 (32%) 1 1	46, 80, 138, 218	0
39	YN	138/140 (98%)	1.39	32 (23%) 2 2	47, 81, 138, 181	0
40	RO	122/122 (100%)	0.87	9 (7%) 20 15	35, 72, 107, 130	0
40	YO	122/122 (100%)	0.64	6 (4%) 35 23	34, 61, 91, 120	0
41	RP	150/150 (100%)	1.25	32 (21%) 2 2	30, 77, 140, 258	0
41	YP	149/150 (99%)	0.94	19 (12%) 7 6	33, 61, 103, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
42	RQ	141/141 (100%)	1.64	43 (30%) 1 1	37, 80, 141, 230	0
42	YQ	141/141 (100%)	0.73	8 (5%) 29 20	37, 69, 110, 233	0
43	RR	117/118 (99%)	0.80	8 (6%) 23 16	38, 68, 106, 164	0
43	YR	117/118 (99%)	1.29	17 (14%) 6 5	41, 65, 107, 161	0
44	RS	111/112 (99%)	1.54	34 (30%) 1 1	64, 107, 160, 226	0
44	YS	111/112 (99%)	1.32	24 (21%) 2 2	46, 78, 123, 204	0
45	RT	137/146 (93%)	1.35	30 (21%) 2 2	53, 85, 141, 206	0
45	YT	137/146 (93%)	1.02	20 (14%) 6 5	40, 79, 148, 229	0
46	RU	117/118 (99%)	1.02	18 (15%) 5 5	30, 62, 123, 192	0
46	YU	117/118 (99%)	1.10	17 (14%) 6 5	36, 69, 117, 168	0
47	RV	101/101 (100%)	1.28	26 (25%) 1 1	37, 79, 138, 251	0
47	YV	101/101 (100%)	1.50	28 (27%) 1 1	33, 86, 143, 218	0
48	RW	113/113 (100%)	0.59	8 (7%) 22 16	31, 58, 112, 209	0
48	YW	113/113 (100%)	0.65	9 (7%) 18 14	34, 62, 122, 209	0
49	RX	92/96 (95%)	1.06	13 (14%) 6 5	37, 72, 114, 146	0
49	YX	92/96 (95%)	0.63	6 (6%) 25 17	31, 62, 99, 125	0
50	RY	107/110 (97%)	1.72	36 (33%) 1 1	39, 84, 133, 166	0
50	YY	107/110 (97%)	1.19	18 (16%) 4 4	35, 92, 141, 173	0
51	QL	125/132 (94%)	1.20	25 (20%) 3 2	44, 74, 124, 180	0
51	XL	122/132 (92%)	0.85	19 (15%) 5 4	32, 64, 102, 125	0
52	R1	94/98 (95%)	1.86	41 (43%) 0 1	32, 76, 156, 196	0
52	Y1	93/98 (94%)	1.50	25 (26%) 1 1	29, 57, 118, 129	0
53	R8	64/65 (98%)	1.12	11 (17%) 4 4	35, 58, 105, 158	0
53	Y8	64/65 (98%)	1.71	25 (39%) 1 1	35, 63, 100, 210	0
54	RF	202/210 (96%)	0.69	18 (8%) 15 12	24, 57, 114, 193	0
54	YF	202/210 (96%)	0.76	16 (7%) 18 14	25, 64, 135, 185	0
55	RZ	183/206 (88%)	1.15	26 (14%) 6 5	65, 111, 154, 191	0
55	YZ	183/206 (88%)	1.08	21 (11%) 9 8	59, 102, 146, 177	0
56	ZA	2/3 (66%)	-0.06	0 100 100	47, 47, 47, 49	0
56	ZB	2/3 (66%)	0.38	0 100 100	54, 54, 54, 63	0
All	All	21359/21942 (97%)	0.67	2326 (10%) 10 9	13, 79, 174, 475	0

The worst 5 of 2326 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	QK	129	SER	10.4
34	RD	34	VAL	9.4
38	YI	15	VAL	8.8
27	R4	24	THR	8.7
37	YH	17	VAL	8.5

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, 95^{th} 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	OMU	QX	21	21/22	0.91	0.15	41,76,85,86	0
22	A2M	XX	19	23/24	0.92	0.14	65,85,93,95	0
22	A2M	QX	20	23/24	0.92	0.12	71,74,83,87	0
22	A2M	QX	19	23/24	0.92	0.16	55,86,89,89	0
56	PPU	ZA	76	37/38	0.94	0.14	38,63,68,70	0
56	PPU	ZB	76	37/38	0.94	0.12	42,50,59,64	0
22	A2M	XX	20	23/24	0.95	0.10	60,66,73,77	0
22	OMU	XX	21	21/22	0.95	0.11	66,73,83,96	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, 95^{th} 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
57	MG	RQ	201	1/1	-0.29	0.50	181,181,181,181	0
57	MG	QA	1617	1/1	-0.09	0.27	71,71,71,71	0
57	MG	YA	3180	1/1	-0.06	0.37	105,105,105,105	0
57	MG	YA	3108	1/1	0.10	0.24	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3058	1/1	0.10	0.23	98,98,98,98	0
57	MG	YA	3164	1/1	0.12	0.22	64,64,64,64	0
57	MG	YA	3184	1/1	0.15	0.30	84,84,84,84	0
57	MG	RA	3074	1/1	0.16	0.31	55,55,55,55	0
57	MG	RA	3126	1/1	0.25	0.41	57,57,57,57	0
57	MG	XA	1634	1/1	0.27	0.22	51,51,51,51	0
57	MG	RA	3174	1/1	0.30	0.39	88,88,88,88	0
57	MG	YA	3170	1/1	0.30	0.22	50,50,50,50	0
57	MG	YA	3096	1/1	0.32	0.41	94,94,94,94	0
57	MG	QA	1604	1/1	0.36	0.28	97,97,97,97	0
57	MG	YA	3154	1/1	0.37	0.15	80,80,80,80	0
57	MG	YA	3159	1/1	0.37	0.32	91,91,91,91	0
57	MG	XA	1603	1/1	0.38	0.31	51,51,51,51	0
57	MG	XA	1614	1/1	0.38	0.27	36,36,36,36	0
57	MG	RA	3111	1/1	0.42	0.18	70,70,70,70	0
57	MG	QA	1637	1/1	0.43	0.48	104,104,104,104	0
57	MG	RA	3170	1/1	0.44	0.19	38,38,38,38	0
57	MG	R0	101	1/1	0.45	0.31	58,58,58,58	0
57	MG	RA	3050	1/1	0.45	0.26	30,30,30,30	0
57	MG	RY	201	1/1	0.48	0.38	59,59,59,59	0
57	MG	YA	3080	1/1	0.48	0.22	38,38,38,38	0
57	MG	YA	3112	1/1	0.48	0.28	39,39,39,39	0
57	MG	RA	3129	1/1	0.49	0.20	56,56,56,56	0
57	MG	RA	3133	1/1	0.50	0.28	63,63,63,63	0
57	MG	YA	3125	1/1	0.50	0.13	58,58,58,58	0
57	MG	RA	3178	1/1	0.51	0.17	50,50,50,50	0
57	MG	RA	3165	1/1	0.51	0.21	75,75,75,75	0
57	MG	YE	304	1/1	0.51	0.36	95,95,95,95	0
57	MG	YA	3172	1/1	0.52	0.18	56,56,56,56	0
57	MG	QA	1622	1/1	0.52	0.17	47,47,47,47	0
57	MG	RA	3097	1/1	0.52	0.22	32,32,32,32	0
57	MG	RA	3180	1/1	0.52	0.21	54,54,54,54	0
57	MG	RA	3188	1/1	0.53	0.25	59,59,59,59	0
57	MG	YA	3142	1/1	0.53	0.32	40,40,40,40	0
57	MG	RA	3160	1/1	0.54	0.21	56,56,56,56	0
57	MG	XA	1605	1/1	0.54	0.17	52,52,52,52	0
57	MG	XA	1710	1/1	0.54	0.41	70,70,70,70	0
57	MG	RA	3190	1/1	0.55	0.32	56,56,56,56	0
57	MG	QA	1692	1/1	0.56	0.16	72,72,72,72	0
57	MG	YA	3115	1/1	0.56	0.32	56,56,56,56	0
57	MG	RA	3293	1/1	0.56	0.26	82,82,82,82	0
57	MG	RA	3150	1/1	0.56	0.21	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QA	1625	1/1	0.56	0.20	52,52,52,52	0
57	MG	XA	1636	1/1	0.56	0.28	53,53,53,53	0
57	MG	RA	3161	1/1	0.57	0.12	70,70,70,70	0
57	MG	QA	1638	1/1	0.57	0.25	65,65,65,65	0
57	MG	RA	3136	1/1	0.57	0.16	58,58,58,58	0
57	MG	QA	1610	1/1	0.58	0.16	68,68,68,68	0
57	MG	YA	3312	1/1	0.58	0.24	62,62,62,62	0
57	MG	YO	201	1/1	0.58	0.26	65,65,65,65	0
57	MG	RN	201	1/1	0.58	0.16	42,42,42,42	0
57	MG	XA	1626	1/1	0.59	0.16	64,64,64,64	0
57	MG	RA	3166	1/1	0.59	0.26	61,61,61,61	0
57	MG	RA	3153	1/1	0.60	0.21	13,13,13,13	0
57	MG	YA	3051	1/1	0.61	0.25	47,47,47,47	0
57	MG	QA	1647	1/1	0.62	0.15	68,68,68,68	0
57	MG	QA	1691	1/1	0.62	0.19	61,61,61,61	0
57	MG	RA	3298	1/1	0.62	0.16	26,26,26,26	0
57	MG	YA	3243	1/1	0.62	0.26	47,47,47,47	0
57	MG	YA	3289	1/1	0.62	0.15	53,53,53,53	0
57	MG	XA	1638	1/1	0.62	0.25	56,56,56,56	0
57	MG	RA	3300	1/1	0.62	0.21	21,21,21,21	0
57	MG	RA	3156	1/1	0.62	0.26	32,32,32,32	0
59	ZN	R4	101	1/1	0.62	0.14	193,193,193,193	0
57	MG	XD	302	1/1	0.63	0.55	92,92,92,92	0
57	MG	YA	3004	1/1	0.63	0.24	27,27,27,27	0
57	MG	YA	3144	1/1	0.63	0.18	48,48,48,48	0
57	MG	RA	3059	1/1	0.63	0.20	21,21,21,21	0
57	MG	QA	1632	1/1	0.64	0.18	67,67,67,67	0
57	MG	YA	3088	1/1	0.64	0.17	51,51,51,51	0
57	MG	YA	3185	1/1	0.64	0.19	44,44,44,44	0
57	MG	RA	3268	1/1	0.65	0.16	48,48,48,48	0
57	MG	RA	3141	1/1	0.65	0.26	29,29,29,29	0
57	MG	RA	3098	1/1	0.66	0.22	35,35,35,35	0
57	MG	XL	201	1/1	0.66	0.18	60,60,60,60	0
57	MG	QA	1680	1/1	0.66	0.24	86,86,86,86	0
57	MG	YA	3295	1/1	0.66	0.17	55,55,55,55	0
57	MG	RA	3186	1/1	0.66	0.25	70,70,70,70	0
57	MG	QA	1603	1/1	0.66	0.16	72,72,72,72	0
57	MG	YE	302	1/1	0.66	0.34	90,90,90,90	0
57	MG	XA	1694	1/1	0.66	0.27	49,49,49,49	0
57	MG	RA	3162	1/1	0.66	0.30	70,70,70,70	0
57	MG	YV	201	1/1	0.67	0.23	84,84,84,84	0
57	MG	YA	3186	1/1	0.67	0.15	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3001	1/1	0.67	0.48	66,66,66,66	0
57	MG	RA	3157	1/1	0.67	0.13	36,36,36,36	0
57	MG	YA	3315	1/1	0.68	0.21	42,42,42,42	0
57	MG	RA	3094	1/1	0.68	0.17	49,49,49,49	0
57	MG	RA	3125	1/1	0.68	0.21	41,41,41,41	0
57	MG	YA	3174	1/1	0.69	0.28	59,59,59,59	0
57	MG	RA	3151	1/1	0.69	0.20	83,83,83,83	0
57	MG	RA	3026	1/1	0.69	0.31	74,74,74,74	0
57	MG	YA	3100	1/1	0.69	0.24	42,42,42,42	0
57	MG	YA	3124	1/1	0.69	0.26	51,51,51,51	0
57	MG	RA	3209	1/1	0.70	0.22	39,39,39,39	0
57	MG	RA	3155	1/1	0.70	0.19	56,56,56,56	0
57	MG	XA	1610	1/1	0.70	0.23	50,50,50,50	0
57	MG	XA	1693	1/1	0.70	0.09	44,44,44,44	0
57	MG	RA	3128	1/1	0.70	0.23	47,47,47,47	0
57	MG	RA	3104	1/1	0.70	0.22	50,50,50,50	0
57	MG	YA	3131	1/1	0.71	0.26	45,45,45,45	0
57	MG	RA	3137	1/1	0.71	0.25	35,35,35,35	0
57	MG	YA	3248	1/1	0.71	0.14	27,27,27,27	0
57	MG	YA	3001	1/1	0.71	0.20	52,52,52,52	0
59	ZN	R5	101	1/1	0.71	0.33	137,137,137,137	0
57	MG	XA	1615	1/1	0.72	0.12	44,44,44,44	0
57	MG	YA	3138	1/1	0.72	0.11	49,49,49,49	0
57	MG	QA	1646	1/1	0.72	0.36	64,64,64,64	0
57	MG	YA	3297	1/1	0.72	0.11	65,65,65,65	0
57	MG	XA	1632	1/1	0.72	0.15	65,65,65,65	0
57	MG	RA	3131	1/1	0.72	0.25	47,47,47,47	0
57	MG	RA	3118	1/1	0.73	0.31	59,59,59,59	0
57	MG	YA	3122	1/1	0.73	0.15	40,40,40,40	0
57	MG	YA	3017	1/1	0.73	0.18	27,27,27,27	0
57	MG	QA	1693	1/1	0.73	0.18	50,50,50,50	0
57	MG	YA	3128	1/1	0.73	0.18	38,38,38,38	0
57	MG	RR	202	1/1	0.73	0.26	47,47,47,47	0
57	MG	YE	303	1/1	0.73	0.22	24,24,24,24	0
57	MG	QA	1689	1/1	0.73	0.14	42,42,42,42	0
57	MG	YA	3140	1/1	0.73	0.20	85,85,85,85	0
57	MG	YA	3296	1/1	0.73	0.24	54,54,54,54	0
57	MG	RA	3084	1/1	0.74	0.16	56,56,56,56	0
57	MG	XA	1705	1/1	0.74	0.23	54,54,54,54	0
57	MG	XA	1709	1/1	0.74	0.22	48,48,48,48	0
57	MG	YA	3105	1/1	0.74	0.33	53,53,53,53	0
57	MG	YA	3279	1/1	0.74	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QA	1677	1/1	0.74	0.08	39,39,39,39	0
57	MG	XA	1639	1/1	0.74	0.18	44,44,44,44	0
57	MG	YA	3063	1/1	0.74	0.19	32,32,32,32	0
57	MG	QA	1667	1/1	0.74	0.10	52,52,52,52	0
57	MG	YA	3145	1/1	0.75	0.10	48,48,48,48	0
57	MG	YA	3319	1/1	0.75	0.20	13,13,13,13	0
57	MG	YA	3173	1/1	0.75	0.24	40,40,40,40	0
57	MG	RA	3093	1/1	0.75	0.22	48,48,48,48	0
57	MG	QA	1608	1/1	0.75	0.22	30,30,30,30	0
57	MG	YA	3160	1/1	0.75	0.21	43,43,43,43	0
57	MG	RA	3068	1/1	0.75	0.23	22,22,22,22	0
57	MG	RA	3090	1/1	0.75	0.24	64,64,64,64	0
57	MG	YA	3224	1/1	0.75	0.23	56,56,56,56	0
57	MG	RA	3051	1/1	0.76	0.32	45,45,45,45	0
57	MG	RA	3032	1/1	0.76	0.10	17,17,17,17	0
57	MG	YA	3110	1/1	0.76	0.10	20,20,20,20	0
57	MG	QA	1682	1/1	0.76	0.17	72,72,72,72	0
57	MG	RA	3139	1/1	0.76	0.16	53,53,53,53	0
57	MG	RA	3176	1/1	0.77	0.13	47,47,47,47	0
57	MG	RA	3121	1/1	0.77	0.17	47,47,47,47	0
57	MG	XA	1618	1/1	0.77	0.16	40,40,40,40	0
57	MG	YA	3150	1/1	0.77	0.11	13,13,13,13	0
57	MG	RA	3232	1/1	0.77	0.13	50,50,50,50	0
57	MG	RA	3245	1/1	0.77	0.17	48,48,48,48	0
57	MG	YQ	3001	1/1	0.77	0.23	59,59,59,59	0
57	MG	QA	1628	1/1	0.77	0.21	35,35,35,35	0
57	MG	RA	3278	1/1	0.77	0.15	45,45,45,45	0
57	MG	YA	3268	1/1	0.77	0.23	42,42,42,42	0
57	MG	RA	3067	1/1	0.77	0.22	23,23,23,23	0
57	MG	YA	3002	1/1	0.77	0.12	47,47,47,47	0
57	MG	RA	3078	1/1	0.77	0.28	32,32,32,32	0
57	MG	XA	1643	1/1	0.78	0.14	61,61,61,61	0
57	MG	YD	302	1/1	0.78	0.50	126,126,126,126	0
57	MG	XA	1625	1/1	0.78	0.09	37,37,37,37	0
57	MG	RA	3106	1/1	0.78	0.27	43,43,43,43	0
57	MG	YA	3162	1/1	0.78	0.18	55,55,55,55	0
57	MG	YA	3308	1/1	0.78	0.10	57,57,57,57	0
57	MG	RA	3244	1/1	0.78	0.18	60,60,60,60	0
57	MG	XA	1633	1/1	0.78	0.16	33,33,33,33	0
57	MG	YA	3284	1/1	0.78	0.21	48,48,48,48	0
57	MG	RA	3189	1/1	0.79	0.18	84,84,84,84	0
57	MG	YA	3177	1/1	0.79	0.14	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QA	1627	1/1	0.79	0.10	69,69,69,69	0
57	MG	YE	301	1/1	0.79	0.27	82,82,82,82	0
57	MG	RA	3142	1/1	0.79	0.13	42,42,42,42	0
57	MG	RA	3053	1/1	0.79	0.18	56,56,56,56	0
57	MG	YA	3317	1/1	0.79	0.19	24,24,24,24	0
57	MG	QA	1630	1/1	0.79	0.17	44,44,44,44	0
57	MG	RA	3064	1/1	0.79	0.21	19,19,19,19	0
57	MG	YA	3301	1/1	0.80	0.21	53,53,53,53	0
57	MG	QA	1612	1/1	0.80	0.11	41,41,41,41	0
57	MG	RA	3246	1/1	0.80	0.28	36,36,36,36	0
57	MG	RA	3182	1/1	0.80	0.18	46,46,46,46	0
57	MG	RA	3109	1/1	0.80	0.18	31,31,31,31	0
57	MG	YA	3015	1/1	0.80	0.22	22,22,22,22	0
57	MG	RA	3290	1/1	0.80	0.11	61,61,61,61	0
57	MG	XA	1647	1/1	0.80	0.30	69,69,69,69	0
57	MG	QA	1635	1/1	0.80	0.09	33,33,33,33	0
57	MG	RA	3112	1/1	0.80	0.26	49,49,49,49	0
57	MG	QA	1679	1/1	0.80	0.22	74,74,74,74	0
57	MG	YA	3286	1/1	0.80	0.16	40,40,40,40	0
57	MG	RA	3018	1/1	0.80	0.15	18,18,18,18	0
57	MG	QA	1623	1/1	0.80	0.12	39,39,39,39	0
57	MG	YA	3176	1/1	0.80	0.19	45,45,45,45	0
57	MG	RA	3060	1/1	0.80	0.24	39,39,39,39	0
57	MG	RA	3004	1/1	0.81	0.12	17,17,17,17	0
57	MG	RA	3005	1/1	0.81	0.15	41,41,41,41	0
57	MG	RA	3107	1/1	0.81	0.24	37,37,37,37	0
57	MG	YA	3179	1/1	0.81	0.20	41,41,41,41	0
57	MG	YA	3309	1/1	0.81	0.26	49,49,49,49	0
57	MG	RA	3058	1/1	0.81	0.11	21,21,21,21	0
57	MG	RA	3088	1/1	0.81	0.13	27,27,27,27	0
57	MG	QA	1666	1/1	0.81	0.20	36,36,36,36	0
57	MG	RA	3019	1/1	0.81	0.20	18,18,18,18	0
57	MG	YB	201	1/1	0.81	0.19	29,29,29,29	0
57	MG	QA	1694	1/1	0.81	0.10	55,55,55,55	0
57	MG	YA	3155	1/1	0.81	0.30	75,75,75,75	0
57	MG	RA	3301	1/1	0.81	0.13	49,49,49,49	0
57	MG	RA	3191	1/1	0.81	0.30	68,68,68,68	0
57	MG	YA	3003	1/1	0.81	0.17	41,41,41,41	0
57	MG	RA	3122	1/1	0.81	0.13	47,47,47,47	0
57	MG	RA	3228	1/1	0.81	0.20	38,38,38,38	0
57	MG	QA	1629	1/1	0.81	0.19	55,55,55,55	0
57	MG	YA	3292	1/1	0.81	0.19	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QA	1636	1/1	0.81	0.21	44,44,44,44	0
57	MG	YA	3183	1/1	0.82	0.13	73,73,73,73	0
57	MG	YA	3303	1/1	0.82	0.19	60,60,60,60	0
57	MG	RA	3140	1/1	0.82	0.13	42,42,42,42	0
57	MG	RA	3163	1/1	0.82	0.19	53,53,53,53	0
57	MG	YA	3006	1/1	0.82	0.22	40,40,40,40	0
57	MG	RA	3082	1/1	0.82	0.15	47,47,47,47	0
57	MG	RA	3252	1/1	0.82	0.18	46,46,46,46	0
57	MG	YA	3246	1/1	0.82	0.12	29,29,29,29	0
57	MG	YA	3021	1/1	0.82	0.19	41,41,41,41	0
57	MG	RA	3179	1/1	0.82	0.17	52,52,52,52	0
57	MG	RQ	202	1/1	0.82	0.35	75,75,75,75	0
57	MG	QF	301	1/1	0.82	0.10	37,37,37,37	0
57	MG	XA	1714	1/1	0.82	0.17	57,57,57,57	0
57	MG	RA	3285	1/1	0.82	0.26	50,50,50,50	0
57	MG	YA	3141	1/1	0.82	0.31	53,53,53,53	0
57	MG	RA	3286	1/1	0.82	0.32	55,55,55,55	0
57	MG	RA	3146	1/1	0.82	0.20	38,38,38,38	0
57	MG	RA	3173	1/1	0.82	0.18	50,50,50,50	0
57	MG	YA	3298	1/1	0.82	0.20	51,51,51,51	0
57	MG	YG	201	1/1	0.83	0.12	41,41,41,41	0
57	MG	YA	3163	1/1	0.83	0.25	53,53,53,53	0
57	MG	XA	1689	1/1	0.83	0.10	37,37,37,37	0
57	MG	RA	3103	1/1	0.83	0.13	22,22,22,22	0
57	MG	YA	3153	1/1	0.83	0.25	52,52,52,52	0
57	MG	RA	3263	1/1	0.83	0.19	45,45,45,45	0
57	MG	RA	3144	1/1	0.83	0.11	58,58,58,58	0
57	MG	YA	3294	1/1	0.83	0.20	40,40,40,40	0
57	MG	XA	1646	1/1	0.83	0.07	30,30,30,30	0
57	MG	YA	3039	1/1	0.83	0.19	43,43,43,43	0
57	MG	RA	3193	1/1	0.83	0.24	19,19,19,19	0
59	ZN	Y4	101	1/1	0.83	0.17	276,276,276,276	0
57	MG	XA	1669	1/1	0.84	0.14	31,31,31,31	0
57	MG	RA	3080	1/1	0.84	0.24	18,18,18,18	0
57	MG	XA	1629	1/1	0.84	0.13	25,25,25,25	0
57	MG	RA	3226	1/1	0.84	0.26	51,51,51,51	0
57	MG	XA	1696	1/1	0.84	0.17	44,44,44,44	0
57	MG	XA	1699	1/1	0.84	0.10	44,44,44,44	0
57	MG	YA	3137	1/1	0.84	0.18	26,26,26,26	0
57	MG	RA	3102	1/1	0.84	0.20	46,46,46,46	0
57	MG	XA	1706	1/1	0.84	0.15	66,66,66,66	0
57	MG	RA	3138	1/1	0.84	0.21	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3313	1/1	0.84	0.08	40,40,40,40	0
57	MG	YA	3065	1/1	0.84	0.21	23,23,23,23	0
57	MG	YA	3316	1/1	0.84	0.14	75,75,75,75	0
57	MG	YA	3078	1/1	0.84	0.26	16,16,16,16	0
57	MG	YA	3189	1/1	0.84	0.22	26,26,26,26	0
57	MG	YA	3199	1/1	0.84	0.24	21,21,21,21	0
57	MG	YB	205	1/1	0.84	0.18	53,53,53,53	0
57	MG	YA	3215	1/1	0.84	0.19	28,28,28,28	0
57	MG	RA	3092	1/1	0.84	0.14	28,28,28,28	0
57	MG	YA	3237	1/1	0.84	0.12	28,28,28,28	0
57	MG	XA	1712	1/1	0.84	0.20	56,56,56,56	0
57	MG	RA	3044	1/1	0.84	0.23	40,40,40,40	0
57	MG	YA	3099	1/1	0.84	0.20	13,13,13,13	0
57	MG	QA	1620	1/1	0.84	0.08	31,31,31,31	0
57	MG	QA	1641	1/1	0.84	0.12	54,54,54,54	0
57	MG	XA	1645	1/1	0.84	0.19	43,43,43,43	0
57	MG	R8	101	1/1	0.84	0.18	55,55,55,55	0
57	MG	RA	3134	1/1	0.84	0.15	36,36,36,36	0
57	MG	RA	3145	1/1	0.84	0.24	51,51,51,51	0
57	MG	YA	3114	1/1	0.84	0.21	25,25,25,25	0
57	MG	XA	1688	1/1	0.85	0.17	41,41,41,41	0
57	MG	Y0	101	1/1	0.85	0.09	15,15,15,15	0
57	MG	Y3	101	1/1	0.85	0.17	33,33,33,33	0
57	MG	RA	3003	1/1	0.85	0.21	60,60,60,60	0
57	MG	RA	3192	1/1	0.85	0.23	54,54,54,54	0
57	MG	YA	3311	1/1	0.85	0.29	62,62,62,62	0
57	MG	YA	3146	1/1	0.85	0.12	73,73,73,73	0
57	MG	RP	202	1/1	0.85	0.22	49,49,49,49	0
57	MG	YA	3314	1/1	0.85	0.13	31,31,31,31	0
57	MG	RA	3248	1/1	0.85	0.19	56,56,56,56	0
57	MG	XA	1642	1/1	0.85	0.10	61,61,61,61	0
57	MG	YA	3109	1/1	0.85	0.13	22,22,22,22	0
57	MG	XA	1704	1/1	0.85	0.13	40,40,40,40	0
57	MG	YA	3244	1/1	0.85	0.11	24,24,24,24	0
57	MG	RA	3100	1/1	0.85	0.31	50,50,50,50	0
57	MG	RA	3233	1/1	0.85	0.22	45,45,45,45	0
57	MG	YA	3024	1/1	0.85	0.16	75,75,75,75	0
57	MG	YD	301	1/1	0.85	0.26	90,90,90,90	0
57	MG	YA	3277	1/1	0.85	0.17	32,32,32,32	0
57	MG	YD	305	1/1	0.85	0.57	50,50,50,50	0
57	MG	YA	3030	1/1	0.85	0.14	25,25,25,25	0
57	MG	YA	3166	1/1	0.85	0.20	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3297	1/1	0.85	0.19	31,31,31,31	0
57	MG	QA	1658	1/1	0.85	0.15	42,42,42,42	0
57	MG	YA	3290	1/1	0.85	0.12	53,53,53,53	0
57	MG	YA	3057	1/1	0.85	0.10	65,65,65,65	0
57	MG	XA	1661	1/1	0.85	0.20	39,39,39,39	0
57	MG	YA	3136	1/1	0.85	0.17	25,25,25,25	0
57	MG	RA	3270	1/1	0.85	0.10	56,56,56,56	0
57	MG	XA	1675	1/1	0.85	0.03	11,11,11,11	0
57	MG	QA	1684	1/1	0.86	0.13	52,52,52,52	0
57	MG	YA	3066	1/1	0.86	0.17	19,19,19,19	0
57	MG	YA	3182	1/1	0.86	0.15	39,39,39,39	0
57	MG	RA	3281	1/1	0.86	0.21	50,50,50,50	0
57	MG	RA	3065	1/1	0.86	0.13	37,37,37,37	0
57	MG	XA	1613	1/1	0.86	0.20	37,37,37,37	0
57	MG	YA	3143	1/1	0.86	0.10	54,54,54,54	0
57	MG	YA	3093	1/1	0.86	0.17	60,60,60,60	0
57	MG	YA	3198	1/1	0.86	0.19	39,39,39,39	0
57	MG	RA	3213	1/1	0.86	0.19	39,39,39,39	0
57	MG	YA	3203	1/1	0.86	0.16	38,38,38,38	0
57	MG	QA	1640	1/1	0.86	0.23	45,45,45,45	0
57	MG	YA	3148	1/1	0.86	0.07	41,41,41,41	0
57	MG	RA	3007	1/1	0.86	0.12	22,22,22,22	0
57	MG	YA	3104	1/1	0.86	0.28	46,46,46,46	0
57	MG	XA	1621	1/1	0.86	0.08	32,32,32,32	0
57	MG	QV	102	1/1	0.86	0.10	20,20,20,20	0
57	MG	YA	3157	1/1	0.86	0.15	31,31,31,31	0
57	MG	QA	1626	1/1	0.86	0.21	39,39,39,39	0
57	MG	RA	3184	1/1	0.86	0.18	59,59,59,59	0
57	MG	RA	3108	1/1	0.86	0.21	25,25,25,25	0
57	MG	YQ	3003	1/1	0.86	0.31	105,105,105,105	0
57	MG	XA	1698	1/1	0.86	0.16	51,51,51,51	0
57	MG	RA	3187	1/1	0.86	0.29	150,150,150,150	0
57	MG	RA	3096	1/1	0.86	0.32	53,53,53,53	0
57	MG	QA	1645	1/1	0.86	0.11	35,35,35,35	0
57	MG	XA	1637	1/1	0.86	0.14	25,25,25,25	0
57	MG	YA	3127	1/1	0.86	0.18	40,40,40,40	0
57	MG	RA	3149	1/1	0.86	0.11	12,12,12,12	0
57	MG	QA	1621	1/1	0.86	0.17	34,34,34,34	0
57	MG	RA	3113	1/1	0.86	0.26	58,58,58,58	0
57	MG	QA	1663	1/1	0.87	0.19	61,61,61,61	0
57	MG	RA	3071	1/1	0.87	0.17	59,59,59,59	0
57	MG	XA	1654	1/1	0.87	0.16	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3185	1/1	0.87	0.42	127,127,127,127	0
57	MG	RA	3072	1/1	0.87	0.20	14,14,14,14	0
57	MG	RA	3021	1/1	0.87	0.26	21,21,21,21	0
57	MG	RA	3243	1/1	0.87	0.23	48,48,48,48	0
57	MG	RA	3294	1/1	0.87	0.09	36,36,36,36	0
57	MG	YA	3018	1/1	0.87	0.12	19,19,19,19	0
57	MG	RA	3296	1/1	0.87	0.22	48,48,48,48	0
57	MG	QA	1616	1/1	0.87	0.09	28,28,28,28	0
57	MG	RA	3154	1/1	0.87	0.07	37,37,37,37	0
57	MG	RA	3127	1/1	0.87	0.15	28,28,28,28	0
57	MG	YA	3049	1/1	0.87	0.26	15,15,15,15	0
57	MG	YA	3050	1/1	0.87	0.20	44,44,44,44	0
57	MG	XA	1631	1/1	0.87	0.14	46,46,46,46	0
57	MG	YA	3134	1/1	0.87	0.12	64,64,64,64	0
57	MG	RA	3006	1/1	0.87	0.21	22,22,22,22	0
57	MG	RD	301	1/1	0.87	0.13	1,1,1,1	0
57	MG	YA	3059	1/1	0.87	0.26	26,26,26,26	0
57	MG	YA	3060	1/1	0.87	0.18	15,15,15,15	0
57	MG	YA	3323	1/1	0.87	0.24	34,34,34,34	0
57	MG	QD	302	1/1	0.87	0.21	64,64,64,64	0
57	MG	RO	201	1/1	0.87	0.17	51,51,51,51	0
57	MG	YA	3210	1/1	0.87	0.19	36,36,36,36	0
57	MG	RA	3011	1/1	0.87	0.25	24,24,24,24	0
57	MG	YA	3219	1/1	0.87	0.21	34,34,34,34	0
57	MG	YA	3072	1/1	0.87	0.25	29,29,29,29	0
57	MG	RA	3267	1/1	0.87	0.19	50,50,50,50	0
57	MG	RA	3202	1/1	0.87	0.22	34,34,34,34	0
57	MG	RR	201	1/1	0.87	0.13	25,25,25,25	0
57	MG	YA	3089	1/1	0.87	0.10	41,41,41,41	0
57	MG	YA	3090	1/1	0.87	0.14	29,29,29,29	0
57	MG	YA	3250	1/1	0.87	0.21	36,36,36,36	0
57	MG	YA	3253	1/1	0.87	0.18	32,32,32,32	0
57	MG	YA	3266	1/1	0.87	0.26	44,44,44,44	0
57	MG	QA	1687	1/1	0.87	0.26	70,70,70,70	0
57	MG	YA	3094	1/1	0.87	0.38	108,108,108,108	0
57	MG	RA	3274	1/1	0.87	0.21	48,48,48,48	0
57	MG	YA	3158	1/1	0.87	0.16	49,49,49,49	0
57	MG	QA	1676	1/1	0.88	0.09	47,47,47,47	0
57	MG	YA	3107	1/1	0.88	0.23	24,24,24,24	0
57	MG	YA	3306	1/1	0.88	0.29	67,67,67,67	0
57	MG	XA	1648	1/1	0.88	0.08	77,77,77,77	0
57	MG	RA	3110	1/1	0.88	0.32	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3214	1/1	0.88	0.17	33,33,33,33	0
57	MG	QA	1686	1/1	0.88	0.16	33,33,33,33	0
57	MG	YA	3111	1/1	0.88	0.21	39,39,39,39	0
57	MG	YA	3221	1/1	0.88	0.22	25,25,25,25	0
57	MG	QA	1643	1/1	0.88	0.17	27,27,27,27	0
57	MG	RA	3283	1/1	0.88	0.19	54,54,54,54	0
57	MG	QA	1619	1/1	0.88	0.09	25,25,25,25	0
57	MG	YA	3121	1/1	0.88	0.10	10,10,10,10	0
57	MG	RA	3114	1/1	0.88	0.17	33,33,33,33	0
57	MG	QA	1606	1/1	0.88	0.18	20,20,20,20	0
57	MG	QA	1633	1/1	0.88	0.10	48,48,48,48	0
57	MG	YA	3077	1/1	0.88	0.20	37,37,37,37	0
57	MG	YA	3257	1/1	0.88	0.16	43,43,43,43	0
57	MG	RA	3194	1/1	0.88	0.15	8,8,8,8	0
57	MG	YA	3129	1/1	0.88	0.19	48,48,48,48	0
57	MG	XA	1604	1/1	0.88	0.19	28,28,28,28	0
57	MG	YA	3133	1/1	0.88	0.19	37,37,37,37	0
57	MG	YQ	3002	1/1	0.88	0.42	96,96,96,96	0
57	MG	YA	3016	1/1	0.88	0.14	10,10,10,10	0
57	MG	RA	3042	1/1	0.88	0.21	23,23,23,23	0
57	MG	XA	1703	1/1	0.88	0.09	54,54,54,54	0
57	MG	YA	3092	1/1	0.88	0.20	31,31,31,31	0
57	MG	RA	3259	1/1	0.88	0.19	59,59,59,59	0
57	MG	RA	3164	1/1	0.88	0.08	30,30,30,30	0
57	MG	RA	3212	1/1	0.88	0.18	33,33,33,33	0
57	MG	YA	3035	1/1	0.88	0.20	21,21,21,21	0
57	MG	RA	3008	1/1	0.88	0.24	24,24,24,24	0
59	ZN	R9	101	1/1	0.88	0.26	110,110,110,110	0
57	MG	XA	1616	1/1	0.88	0.15	25,25,25,25	0
59	ZN	Y6	101	1/1	0.88	0.21	209,209,209,209	0
57	MG	RA	3196	1/1	0.89	0.18	17,17,17,17	0
57	MG	RA	3200	1/1	0.89	0.15	23,23,23,23	0
57	MG	YA	3299	1/1	0.89	0.22	50,50,50,50	0
57	MG	RA	3201	1/1	0.89	0.26	35,35,35,35	0
57	MG	RA	3183	1/1	0.89	0.20	21,21,21,21	0
57	MG	RA	3266	1/1	0.89	0.11	44,44,44,44	0
57	MG	YA	3307	1/1	0.89	0.14	43,43,43,43	0
57	MG	RA	3204	1/1	0.89	0.22	26,26,26,26	0
57	MG	YA	3103	1/1	0.89	0.15	55,55,55,55	0
57	MG	RA	3083	1/1	0.89	0.18	25,25,25,25	0
57	MG	YA	3031	1/1	0.89	0.23	9,9,9,9	0
57	MG	QV	101	1/1	0.89	0.20	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3220	1/1	0.89	0.21	35,35,35,35	0
57	MG	YA	3038	1/1	0.89	0.29	37,37,37,37	0
57	MG	QA	1609	1/1	0.89	0.20	45,45,45,45	0
57	MG	YA	3156	1/1	0.89	0.30	31,31,31,31	0
57	MG	YA	3240	1/1	0.89	0.09	31,31,31,31	0
57	MG	YA	3322	1/1	0.89	0.20	4,4,4,4	0
57	MG	YA	3046	1/1	0.89	0.16	19,19,19,19	0
57	MG	RA	3217	1/1	0.89	0.22	28,28,28,28	0
57	MG	YB	203	1/1	0.89	0.18	29,29,29,29	0
57	MG	RA	3171	1/1	0.89	0.16	38,38,38,38	0
57	MG	YA	3113	1/1	0.89	0.11	30,30,30,30	0
57	MG	QA	1642	1/1	0.89	0.08	45,45,45,45	0
57	MG	YA	3251	1/1	0.89	0.17	52,52,52,52	0
57	MG	RA	3158	1/1	0.89	0.13	29,29,29,29	0
57	MG	RA	3147	1/1	0.89	0.24	30,30,30,30	0
57	MG	RA	3287	1/1	0.89	0.11	45,45,45,45	0
57	MG	YA	3267	1/1	0.89	0.15	36,36,36,36	0
57	MG	RA	3237	1/1	0.89	0.22	26,26,26,26	0
57	MG	YA	3272	1/1	0.89	0.23	38,38,38,38	0
57	MG	XF	301	1/1	0.89	0.11	47,47,47,47	0
57	MG	RA	3238	1/1	0.89	0.15	32,32,32,32	0
57	MG	QA	1670	1/1	0.89	0.15	34,34,34,34	0
57	MG	XA	1658	1/1	0.89	0.17	27,27,27,27	0
57	MG	RA	3116	1/1	0.89	0.18	44,44,44,44	0
57	MG	RA	3061	1/1	0.89	0.19	28,28,28,28	0
57	MG	XA	1670	1/1	0.89	0.24	40,40,40,40	0
57	MG	XA	1674	1/1	0.89	0.23	41,41,41,41	0
57	MG	RA	3119	1/1	0.89	0.17	33,33,33,33	0
57	MG	YA	3010	1/1	0.89	0.30	38,38,38,38	0
57	MG	YA	3288	1/1	0.90	0.18	44,44,44,44	0
57	MG	RA	3284	1/1	0.90	0.28	54,54,54,54	0
57	MG	QA	1665	1/1	0.90	0.12	44,44,44,44	0
57	MG	RA	3239	1/1	0.90	0.28	44,44,44,44	0
57	MG	YA	3293	1/1	0.90	0.17	47,47,47,47	0
57	MG	RA	3159	1/1	0.90	0.14	26,26,26,26	0
57	MG	XA	1607	1/1	0.90	0.18	21,21,21,21	0
57	MG	QA	1671	1/1	0.90	0.07	38,38,38,38	0
57	MG	RA	3132	1/1	0.90	0.10	36,36,36,36	0
57	MG	XE	201	1/1	0.90	0.09	47,47,47,47	0
57	MG	YA	3132	1/1	0.90	0.14	27,27,27,27	0
57	MG	XA	1650	1/1	0.90	0.15	24,24,24,24	0
57	MG	XA	1653	1/1	0.90	0.18	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3305	1/1	0.90	0.19	42,42,42,42	0
57	MG	RA	3047	1/1	0.90	0.13	11,11,11,11	0
57	MG	YA	3190	1/1	0.90	0.20	23,23,23,23	0
57	MG	QA	1672	1/1	0.90	0.21	40,40,40,40	0
57	MG	YA	3087	1/1	0.90	0.21	10,10,10,10	0
57	MG	YA	3139	1/1	0.90	0.27	40,40,40,40	0
57	MG	RA	3207	1/1	0.90	0.23	30,30,30,30	0
57	MG	YA	3212	1/1	0.90	0.19	34,34,34,34	0
57	MG	XA	1667	1/1	0.90	0.24	43,43,43,43	0
57	MG	XA	1617	1/1	0.90	0.15	21,21,21,21	0
57	MG	YA	3216	1/1	0.90	0.19	44,44,44,44	0
57	MG	YA	3217	1/1	0.90	0.18	27,27,27,27	0
57	MG	YA	3091	1/1	0.90	0.26	39,39,39,39	0
57	MG	RA	3208	1/1	0.90	0.14	29,29,29,29	0
57	MG	XA	1673	1/1	0.90	0.17	41,41,41,41	0
57	MG	QA	1639	1/1	0.90	0.19	52,52,52,52	0
57	MG	YA	3225	1/1	0.90	0.07	19,19,19,19	0
57	MG	RA	3264	1/1	0.90	0.33	55,55,55,55	0
57	MG	YF	301	1/1	0.90	0.09	45,45,45,45	0
57	MG	XA	1683	1/1	0.90	0.14	45,45,45,45	0
57	MG	XA	1684	1/1	0.90	0.23	42,42,42,42	0
57	MG	RB	203	1/1	0.90	0.23	46,46,46,46	0
57	MG	QA	1685	1/1	0.90	0.11	42,42,42,42	0
57	MG	XA	1691	1/1	0.90	0.24	43,43,43,43	0
57	MG	RA	3152	1/1	0.90	0.17	24,24,24,24	0
57	MG	RA	3169	1/1	0.90	0.15	38,38,38,38	0
57	MG	RA	3055	1/1	0.90	0.21	4,4,4,4	0
57	MG	XA	1697	1/1	0.90	0.15	56,56,56,56	0
57	MG	YA	3262	1/1	0.90	0.39	36,36,36,36	0
57	MG	RA	3031	1/1	0.90	0.18	16,16,16,16	0
57	MG	YA	3042	1/1	0.90	0.11	27,27,27,27	0
57	MG	QA	1602	1/1	0.90	0.18	27,27,27,27	0
57	MG	YA	3270	1/1	0.90	0.36	45,45,45,45	0
57	MG	RA	3079	1/1	0.90	0.15	26,26,26,26	0
57	MG	YA	3167	1/1	0.90	0.15	49,49,49,49	0
57	MG	YA	3169	1/1	0.90	0.25	51,51,51,51	0
57	MG	RA	3035	1/1	0.90	0.16	17,17,17,17	0
57	MG	YA	3120	1/1	0.90	0.15	32,32,32,32	0
57	MG	QA	1675	1/1	0.91	0.14	24,24,24,24	0
57	MG	YA	3023	1/1	0.91	0.20	21,21,21,21	0
57	MG	QA	1690	1/1	0.91	0.30	57,57,57,57	0
57	MG	RA	3115	1/1	0.91	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3203	1/1	0.91	0.27	61,61,61,61	0
57	MG	QA	1601	1/1	0.91	0.19	17,17,17,17	0
57	MG	YA	3102	1/1	0.91	0.22	15,15,15,15	0
57	MG	RA	3168	1/1	0.91	0.13	54,54,54,54	0
57	MG	RA	3117	1/1	0.91	0.19	20,20,20,20	0
57	MG	XA	1649	1/1	0.91	0.23	59,59,59,59	0
57	MG	RA	3250	1/1	0.91	0.10	45,45,45,45	0
57	MG	YA	3274	1/1	0.91	0.18	37,37,37,37	0
57	MG	XA	1651	1/1	0.91	0.24	22,22,22,22	0
57	MG	QA	1650	1/1	0.91	0.12	21,21,21,21	0
57	MG	YA	3281	1/1	0.91	0.22	37,37,37,37	0
57	MG	RA	3254	1/1	0.91	0.16	43,43,43,43	0
57	MG	YA	3285	1/1	0.91	0.17	38,38,38,38	0
57	MG	RA	3255	1/1	0.91	0.13	42,42,42,42	0
57	MG	RA	3257	1/1	0.91	0.09	25,25,25,25	0
57	MG	RA	3025	1/1	0.91	0.32	30,30,30,30	0
57	MG	RA	3172	1/1	0.91	0.14	45,45,45,45	0
57	MG	QA	1651	1/1	0.91	0.15	26,26,26,26	0
57	MG	YA	3119	1/1	0.91	0.29	22,22,22,22	0
57	MG	XA	1628	1/1	0.91	0.07	54,54,54,54	0
57	MG	RA	3225	1/1	0.91	0.22	13,13,13,13	0
57	MG	XA	1630	1/1	0.91	0.15	32,32,32,32	0
57	MG	XA	1682	1/1	0.91	0.20	36,36,36,36	0
57	MG	RA	3135	1/1	0.91	0.13	31,31,31,31	0
57	MG	RA	3175	1/1	0.91	0.28	61,61,61,61	0
57	MG	YE	305	1/1	0.91	0.20	27,27,27,27	0
57	MG	RA	3148	1/1	0.91	0.09	46,46,46,46	0
57	MG	YA	3302	1/1	0.91	0.16	50,50,50,50	0
57	MG	RA	3273	1/1	0.91	0.12	54,54,54,54	0
57	MG	RA	3076	1/1	0.91	0.11	28,28,28,28	0
57	MG	RA	3275	1/1	0.91	0.11	34,34,34,34	0
57	MG	QA	1656	1/1	0.91	0.12	28,28,28,28	0
57	MG	XA	1692	1/1	0.92	0.16	51,51,51,51	0
57	MG	YA	3037	1/1	0.92	0.18	7,7,7,7	0
57	MG	QA	1652	1/1	0.92	0.19	43,43,43,43	0
57	MG	QA	1668	1/1	0.92	0.07	37,37,37,37	0
57	MG	RA	3242	1/1	0.92	0.20	42,42,42,42	0
57	MG	RA	3027	1/1	0.92	0.16	3,3,3,3	0
57	MG	XA	1641	1/1	0.92	0.16	22,22,22,22	0
57	MG	RA	3054	1/1	0.92	0.14	22,22,22,22	0
57	MG	RA	3028	1/1	0.92	0.16	45,45,45,45	0
57	MG	XA	1606	1/1	0.92	0.17	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QA	1655	1/1	0.92	0.17	30,30,30,30	0
57	MG	YA	3195	1/1	0.92	0.17	21,21,21,21	0
57	MG	YA	3130	1/1	0.92	0.16	29,29,29,29	0
57	MG	QA	1624	1/1	0.92	0.07	45,45,45,45	0
57	MG	XA	1708	1/1	0.92	0.13	36,36,36,36	0
57	MG	YA	3062	1/1	0.92	0.10	31,31,31,31	0
57	MG	RA	3249	1/1	0.92	0.22	42,42,42,42	0
57	MG	RA	3292	1/1	0.92	0.18	44,44,44,44	0
57	MG	XA	1711	1/1	0.92	0.10	29,29,29,29	0
57	MG	RA	3210	1/1	0.92	0.22	33,33,33,33	0
57	MG	YA	3076	1/1	0.92	0.14	5,5,5,5	0
57	MG	RA	3014	1/1	0.92	0.15	17,17,17,17	0
57	MG	XA	1652	1/1	0.92	0.19	23,23,23,23	0
57	MG	RA	3036	1/1	0.92	0.15	19,19,19,19	0
57	MG	YA	3085	1/1	0.92	0.17	24,24,24,24	0
57	MG	RA	3215	1/1	0.92	0.18	30,30,30,30	0
57	MG	YA	3230	1/1	0.92	0.12	28,28,28,28	0
57	MG	XA	1655	1/1	0.92	0.17	15,15,15,15	0
57	MG	XV	102	1/1	0.92	0.18	33,33,33,33	0
57	MG	YA	3325	1/1	0.92	0.14	49,49,49,49	0
57	MG	XA	1620	1/1	0.92	0.21	34,34,34,34	0
57	MG	RA	3216	1/1	0.92	0.24	28,28,28,28	0
57	MG	YA	3152	1/1	0.92	0.12	20,20,20,20	0
57	MG	XA	1666	1/1	0.92	0.21	32,32,32,32	0
57	MG	YA	3249	1/1	0.92	0.20	51,51,51,51	0
57	MG	XA	1622	1/1	0.92	0.20	36,36,36,36	0
57	MG	XA	1623	1/1	0.92	0.15	23,23,23,23	0
57	MG	RA	3063	1/1	0.92	0.10	25,25,25,25	0
57	MG	YD	304	1/1	0.92	0.29	117,117,117,117	0
57	MG	RA	3218	1/1	0.92	0.19	28,28,28,28	0
57	MG	XA	1627	1/1	0.92	0.22	25,25,25,25	0
57	MG	YA	3101	1/1	0.92	0.17	30,30,30,30	0
57	MG	YA	3013	1/1	0.92	0.21	21,21,21,21	0
57	MG	RA	3037	1/1	0.92	0.16	22,22,22,22	0
57	MG	QA	1657	1/1	0.92	0.27	41,41,41,41	0
57	MG	YA	3271	1/1	0.92	0.30	52,52,52,52	0
57	MG	RA	3066	1/1	0.92	0.12	49,49,49,49	0
57	MG	QA	1688	1/1	0.92	0.15	48,48,48,48	0
57	MG	XA	1685	1/1	0.92	0.12	52,52,52,52	0
57	MG	XA	1686	1/1	0.92	0.14	44,44,44,44	0
57	MG	RA	3199	1/1	0.92	0.26	26,26,26,26	0
57	MG	YA	3283	1/1	0.92	0.25	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3025	1/1	0.92	0.19	9,9,9,9	0
57	MG	RA	3236	1/1	0.92	0.16	27,27,27,27	0
57	MG	QA	1681	1/1	0.92	0.15	36,36,36,36	0
57	MG	YA	3048	1/1	0.93	0.20	17,17,17,17	0
57	MG	XA	1668	1/1	0.93	0.08	23,23,23,23	0
57	MG	RA	3279	1/1	0.93	0.12	48,48,48,48	0
57	MG	YA	3181	1/1	0.93	0.19	102,102,102,102	0
57	MG	XA	1716	1/1	0.93	0.20	39,39,39,39	0
57	MG	YA	3123	1/1	0.93	0.21	20,20,20,20	0
57	MG	RA	3280	1/1	0.93	0.24	51,51,51,51	0
57	MG	RA	3081	1/1	0.93	0.12	22,22,22,22	0
57	MG	RA	3039	1/1	0.93	0.17	15,15,15,15	0
57	MG	XA	1602	1/1	0.93	0.25	28,28,28,28	0
57	MG	XA	1678	1/1	0.93	0.08	33,33,33,33	0
57	MG	XA	1635	1/1	0.93	0.17	30,30,30,30	0
57	MG	QA	1669	1/1	0.93	0.10	26,26,26,26	0
57	MG	RA	3123	1/1	0.93	0.17	12,12,12,12	0
57	MG	YA	3300	1/1	0.93	0.18	46,46,46,46	0
57	MG	YA	3068	1/1	0.93	0.20	4,4,4,4	0
57	MG	RA	3002	1/1	0.93	0.14	15,15,15,15	0
57	MG	RA	3143	1/1	0.93	0.12	23,23,23,23	0
57	MG	QA	1613	1/1	0.93	0.08	43,43,43,43	0
57	MG	YA	3005	1/1	0.93	0.21	91,91,91,91	0
57	MG	RA	3013	1/1	0.93	0.16	19,19,19,19	0
57	MG	YA	3008	1/1	0.93	0.18	4,4,4,4	0
57	MG	YA	3086	1/1	0.93	0.17	23,23,23,23	0
57	MG	YA	3310	1/1	0.93	0.25	52,52,52,52	0
57	MG	YA	3009	1/1	0.93	0.20	25,25,25,25	0
57	MG	XA	1690	1/1	0.93	0.16	41,41,41,41	0
57	MG	XA	1612	1/1	0.93	0.16	28,28,28,28	0
57	MG	RA	3091	1/1	0.93	0.11	42,42,42,42	0
57	MG	YA	3226	1/1	0.93	0.23	34,34,34,34	0
57	MG	QA	1644	1/1	0.93	0.06	44,44,44,44	0
57	MG	YA	3235	1/1	0.93	0.14	24,24,24,24	0
57	MG	RA	3015	1/1	0.93	0.22	3,3,3,3	0
57	MG	YA	3149	1/1	0.93	0.17	46,46,46,46	0
57	MG	YA	3242	1/1	0.93	0.18	40,40,40,40	0
57	MG	XA	1695	1/1	0.93	0.08	29,29,29,29	0
57	MG	RA	3016	1/1	0.93	0.20	17,17,17,17	0
57	MG	YA	3022	1/1	0.93	0.18	22,22,22,22	0
57	MG	YA	3098	1/1	0.93	0.24	47,47,47,47	0
57	MG	RA	3241	1/1	0.93	0.15	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3033	1/1	0.93	0.10	29,29,29,29	0
57	MG	RA	3271	1/1	0.93	0.07	41,41,41,41	0
57	MG	YA	3029	1/1	0.93	0.13	21,21,21,21	0
57	MG	YA	3254	1/1	0.93	0.16	27,27,27,27	0
57	MG	YA	3256	1/1	0.93	0.17	40,40,40,40	0
57	MG	RB	202	1/1	0.93	0.25	42,42,42,42	0
57	MG	YA	3258	1/1	0.93	0.16	36,36,36,36	0
57	MG	RA	3272	1/1	0.93	0.11	66,66,66,66	0
57	MG	YA	3034	1/1	0.93	0.13	17,17,17,17	0
57	MG	RA	3017	1/1	0.93	0.20	1,1,1,1	0
57	MG	YA	3036	1/1	0.93	0.14	30,30,30,30	0
57	MG	QA	1683	1/1	0.93	0.05	40,40,40,40	0
57	MG	QA	1653	1/1	0.93	0.14	33,33,33,33	0
57	MG	RP	201	1/1	0.93	0.08	15,15,15,15	0
57	MG	RA	3276	1/1	0.93	0.25	56,56,56,56	0
57	MG	YA	3043	1/1	0.93	0.18	20,20,20,20	0
57	MG	RA	3038	1/1	0.93	0.15	27,27,27,27	0
57	MG	YA	3280	1/1	0.93	0.45	69,69,69,69	0
59	ZN	R6	101	1/1	0.93	0.11	223,223,223,223	0
57	MG	YA	3047	1/1	0.93	0.18	12,12,12,12	0
57	MG	YA	3282	1/1	0.93	0.17	48,48,48,48	0
57	MG	YA	3117	1/1	0.93	0.20	27,27,27,27	0
57	MG	YA	3207	1/1	0.94	0.12	19,19,19,19	0
57	MG	RA	3214	1/1	0.94	0.21	19,19,19,19	0
57	MG	XA	1660	1/1	0.94	0.15	45,45,45,45	0
57	MG	RA	3052	1/1	0.94	0.16	5,5,5,5	0
57	MG	QA	1660	1/1	0.94	0.24	37,37,37,37	0
57	MG	RA	3130	1/1	0.94	0.13	19,19,19,19	0
57	MG	YA	3007	1/1	0.94	0.14	1,1,1,1	0
57	MG	YA	3052	1/1	0.94	0.16	3,3,3,3	0
57	MG	QA	1662	1/1	0.94	0.23	41,41,41,41	0
57	MG	XA	1702	1/1	0.94	0.12	29,29,29,29	0
57	MG	RA	3221	1/1	0.94	0.17	42,42,42,42	0
57	MG	YA	3012	1/1	0.94	0.12	12,12,12,12	0
57	MG	YA	3061	1/1	0.94	0.07	13,13,13,13	0
57	MG	XA	1640	1/1	0.94	0.07	40,40,40,40	0
57	MG	RA	3022	1/1	0.94	0.16	25,25,25,25	0
57	MG	RA	3069	1/1	0.94	0.24	23,23,23,23	0
57	MG	XA	1707	1/1	0.94	0.07	49,49,49,49	0
57	MG	YA	3118	1/1	0.94	0.11	23,23,23,23	0
57	MG	RA	3086	1/1	0.94	0.14	27,27,27,27	0
57	MG	YA	3165	1/1	0.94	0.16	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3071	1/1	0.94	0.14	35,35,35,35	0
57	MG	YA	3247	1/1	0.94	0.12	48,48,48,48	0
57	MG	XA	1677	1/1	0.94	0.24	41,41,41,41	0
57	MG	YA	3168	1/1	0.94	0.21	53,53,53,53	0
57	MG	YA	3073	1/1	0.94	0.23	19,19,19,19	0
57	MG	YA	3075	1/1	0.94	0.17	21,21,21,21	0
57	MG	XA	1644	1/1	0.94	0.12	29,29,29,29	0
57	MG	XA	1680	1/1	0.94	0.10	42,42,42,42	0
57	MG	RA	3070	1/1	0.94	0.18	16,16,16,16	0
57	MG	RA	3261	1/1	0.94	0.10	37,37,37,37	0
57	MG	YA	3027	1/1	0.94	0.23	21,21,21,21	0
57	MG	YA	3260	1/1	0.94	0.13	32,32,32,32	0
57	MG	RA	3023	1/1	0.94	0.21	40,40,40,40	0
57	MG	RA	3167	1/1	0.94	0.15	38,38,38,38	0
57	MG	RA	3045	1/1	0.94	0.15	16,16,16,16	0
57	MG	RA	3046	1/1	0.94	0.15	11,11,11,11	0
57	MG	YA	3269	1/1	0.94	0.33	49,49,49,49	0
57	MG	RA	3124	1/1	0.94	0.19	28,28,28,28	0
57	MG	YA	3135	1/1	0.94	0.17	38,38,38,38	0
57	MG	XV	101	1/1	0.94	0.23	30,30,30,30	0
57	MG	QA	1631	1/1	0.94	0.22	62,62,62,62	0
57	MG	YA	3275	1/1	0.94	0.10	36,36,36,36	0
57	MG	RA	3211	1/1	0.94	0.23	38,38,38,38	0
57	MG	QV	103	1/1	0.94	0.07	2,2,2,2	0
57	MG	YA	3193	1/1	0.94	0.16	16,16,16,16	0
57	MG	YA	3194	1/1	0.94	0.15	27,27,27,27	0
57	MG	Y9	101	1/1	0.94	0.11	73,73,73,73	0
57	MG	YA	3097	1/1	0.94	0.17	31,31,31,31	0
57	MG	QA	1664	1/1	0.94	0.14	44,44,44,44	0
57	MG	YA	3200	1/1	0.94	0.11	28,28,28,28	0
57	MG	YA	3201	1/1	0.94	0.11	36,36,36,36	0
57	MG	YA	3287	1/1	0.94	0.18	39,39,39,39	0
57	MG	YA	3202	1/1	0.94	0.10	26,26,26,26	0
57	MG	YA	3045	1/1	0.94	0.22	17,17,17,17	0
57	MG	YA	3206	1/1	0.94	0.22	27,27,27,27	0
57	MG	RA	3195	1/1	0.95	0.22	14,14,14,14	0
57	MG	RA	3043	1/1	0.95	0.17	15,15,15,15	0
57	MG	YA	3178	1/1	0.95	0.12	41,41,41,41	0
57	MG	YA	3245	1/1	0.95	0.15	30,30,30,30	0
57	MG	RA	3260	1/1	0.95	0.05	29,29,29,29	0
57	MG	YA	3014	1/1	0.95	0.16	1,1,1,1	0
57	MG	YA	3053	1/1	0.95	0.16	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3054	1/1	0.95	0.19	15,15,15,15	0
57	MG	YA	3055	1/1	0.95	0.20	13,13,13,13	0
57	MG	XA	1624	1/1	0.95	0.11	28,28,28,28	0
57	MG	RA	3197	1/1	0.95	0.21	15,15,15,15	0
57	MG	XA	1713	1/1	0.95	0.15	24,24,24,24	0
57	MG	QA	1674	1/1	0.95	0.09	40,40,40,40	0
57	MG	XA	1687	1/1	0.95	0.16	25,25,25,25	0
57	MG	RA	3095	1/1	0.95	0.11	35,35,35,35	0
57	MG	YA	3147	1/1	0.95	0.12	16,16,16,16	0
57	MG	YA	3261	1/1	0.95	0.18	20,20,20,20	0
57	MG	RA	3062	1/1	0.95	0.12	7,7,7,7	0
57	MG	YA	3263	1/1	0.95	0.41	52,52,52,52	0
57	MG	YA	3320	1/1	0.95	0.21	10,10,10,10	0
57	MG	YA	3321	1/1	0.95	0.12	19,19,19,19	0
57	MG	YA	3064	1/1	0.95	0.13	12,12,12,12	0
57	MG	XA	1601	1/1	0.95	0.13	13,13,13,13	0
57	MG	YA	3324	1/1	0.95	0.19	6,6,6,6	0
57	MG	RA	3120	1/1	0.95	0.10	4,4,4,4	0
57	MG	YA	3026	1/1	0.95	0.14	15,15,15,15	0
57	MG	XM	201	1/1	0.95	0.08	49,49,49,49	0
57	MG	QX	101	1/1	0.95	0.21	31,31,31,31	0
57	MG	YA	3205	1/1	0.95	0.23	25,25,25,25	0
57	MG	YA	3116	1/1	0.95	0.09	26,26,26,26	0
57	MG	QA	1634	1/1	0.95	0.20	44,44,44,44	0
57	MG	YA	3209	1/1	0.95	0.11	31,31,31,31	0
57	MG	XV	103	1/1	0.95	0.09	25,25,25,25	0
57	MG	YA	3032	1/1	0.95	0.18	16,16,16,16	0
57	MG	RA	3223	1/1	0.95	0.10	26,26,26,26	0
57	MG	YA	3161	1/1	0.95	0.13	35,35,35,35	0
57	MG	RA	3205	1/1	0.95	0.17	21,21,21,21	0
57	MG	QA	1654	1/1	0.95	0.12	28,28,28,28	0
57	MG	YA	3082	1/1	0.95	0.12	25,25,25,25	0
57	MG	RA	3056	1/1	0.95	0.13	21,21,21,21	0
57	MG	RA	3251	1/1	0.95	0.20	44,44,44,44	0
57	MG	RA	3302	1/1	0.95	0.06	38,38,38,38	0
57	MG	RB	201	1/1	0.95	0.16	29,29,29,29	0
57	MG	RA	3230	1/1	0.95	0.17	22,22,22,22	0
57	MG	YA	3228	1/1	0.95	0.24	24,24,24,24	0
57	MG	RA	3277	1/1	0.95	0.08	59,59,59,59	0
57	MG	YA	3231	1/1	0.95	0.09	24,24,24,24	0
57	MG	RA	3253	1/1	0.95	0.10	29,29,29,29	0
57	MG	RA	3048	1/1	0.95	0.09	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	ZN	XN	101	1/1	0.95	0.10	64,64,64,64	0
57	MG	YA	3238	1/1	0.95	0.09	16,16,16,16	0
57	MG	QA	1673	1/1	0.95	0.13	48,48,48,48	0
57	MG	QA	1648	1/1	0.96	0.14	28,28,28,28	0
57	MG	QA	1659	1/1	0.96	0.20	37,37,37,37	0
57	MG	XA	1662	1/1	0.96	0.12	58,58,58,58	0
57	MG	YA	3291	1/1	0.96	0.17	37,37,37,37	0
57	MG	YA	3222	1/1	0.96	0.19	23,23,23,23	0
57	MG	YA	3020	1/1	0.96	0.16	26,26,26,26	0
57	MG	YA	3067	1/1	0.96	0.14	22,22,22,22	0
57	MG	RE	301	1/1	0.96	0.18	15,15,15,15	0
57	MG	YA	3227	1/1	0.96	0.23	37,37,37,37	0
57	MG	YA	3070	1/1	0.96	0.12	26,26,26,26	0
57	MG	YA	3229	1/1	0.96	0.10	17,17,17,17	0
57	MG	RA	3075	1/1	0.96	0.12	7,7,7,7	0
57	MG	RA	3219	1/1	0.96	0.05	20,20,20,20	0
57	MG	YA	3234	1/1	0.96	0.18	24,24,24,24	0
57	MG	RA	3247	1/1	0.96	0.25	41,41,41,41	0
57	MG	YA	3236	1/1	0.96	0.22	31,31,31,31	0
57	MG	RA	3034	1/1	0.96	0.19	14,14,14,14	0
57	MG	YA	3171	1/1	0.96	0.46	35,35,35,35	0
57	MG	YA	3239	1/1	0.96	0.17	36,36,36,36	0
57	MG	XA	1672	1/1	0.96	0.17	21,21,21,21	0
57	MG	YA	3126	1/1	0.96	0.06	30,30,30,30	0
57	MG	RA	3222	1/1	0.96	0.15	22,22,22,22	0
57	MG	RA	3077	1/1	0.96	0.16	15,15,15,15	0
57	MG	QA	1618	1/1	0.96	0.23	24,24,24,24	0
57	MG	RA	3282	1/1	0.96	0.14	37,37,37,37	0
57	MG	YA	3084	1/1	0.96	0.10	24,24,24,24	0
57	MG	RA	3049	1/1	0.96	0.19	6,6,6,6	0
57	MG	YA	3033	1/1	0.96	0.18	15,15,15,15	0
57	MG	RA	3227	1/1	0.96	0.16	29,29,29,29	0
57	MG	YA	3318	1/1	0.96	0.17	9,9,9,9	0
57	MG	RA	3024	1/1	0.96	0.18	16,16,16,16	0
57	MG	YA	3252	1/1	0.96	0.18	33,33,33,33	0
57	MG	QA	1611	1/1	0.96	0.14	39,39,39,39	0
57	MG	RA	3231	1/1	0.96	0.20	27,27,27,27	0
57	MG	RA	3289	1/1	0.96	0.18	42,42,42,42	0
57	MG	RA	3101	1/1	0.96	0.19	10,10,10,10	0
57	MG	RA	3291	1/1	0.96	0.24	50,50,50,50	0
57	MG	Y0	102	1/1	0.96	0.17	13,13,13,13	0
57	MG	YB	202	1/1	0.96	0.14	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1608	1/1	0.96	0.21	18,18,18,18	0
57	MG	YB	204	1/1	0.96	0.04	41,41,41,41	0
57	MG	XA	1609	1/1	0.96	0.12	15,15,15,15	0
57	MG	YA	3197	1/1	0.96	0.10	21,21,21,21	0
57	MG	YA	3264	1/1	0.96	0.23	39,39,39,39	0
57	MG	RA	3010	1/1	0.96	0.14	12,12,12,12	0
57	MG	RA	3234	1/1	0.96	0.06	34,34,34,34	0
57	MG	RA	3235	1/1	0.96	0.24	36,36,36,36	0
57	MG	QD	303	1/1	0.96	0.06	58,58,58,58	0
57	MG	RA	3265	1/1	0.96	0.13	26,26,26,26	0
57	MG	RA	3041	1/1	0.96	0.15	3,3,3,3	0
57	MG	YA	3204	1/1	0.96	0.16	16,16,16,16	0
57	MG	YA	3273	1/1	0.96	0.04	39,39,39,39	0
57	MG	RA	3299	1/1	0.96	0.08	22,22,22,22	0
57	MG	YA	3151	1/1	0.96	0.14	28,28,28,28	0
57	MG	YA	3276	1/1	0.96	0.24	46,46,46,46	0
57	MG	RA	3012	1/1	0.96	0.10	25,25,25,25	0
57	MG	YA	3278	1/1	0.96	0.10	45,45,45,45	0
57	MG	YA	3208	1/1	0.96	0.15	20,20,20,20	0
57	MG	RA	3029	1/1	0.96	0.21	16,16,16,16	0
59	ZN	QN	101	1/1	0.96	0.13	59,59,59,59	0
57	MG	RA	3240	1/1	0.96	0.11	35,35,35,35	0
57	MG	YA	3211	1/1	0.96	0.24	36,36,36,36	0
57	MG	YA	3011	1/1	0.96	0.09	20,20,20,20	0
57	MG	XA	1700	1/1	0.96	0.19	36,36,36,36	0
57	MG	XA	1701	1/1	0.96	0.09	40,40,40,40	0
57	MG	RA	3089	1/1	0.96	0.16	4,4,4,4	0
57	MG	RA	3020	1/1	0.96	0.06	12,12,12,12	0
57	MG	YA	3265	1/1	0.97	0.30	62,62,62,62	0
57	MG	YA	3218	1/1	0.97	0.14	30,30,30,30	0
57	MG	QA	1649	1/1	0.97	0.06	26,26,26,26	0
57	MG	RA	3288	1/1	0.97	0.17	38,38,38,38	0
57	MG	YA	3079	1/1	0.97	0.13	1,1,1,1	0
57	MG	YA	3019	1/1	0.97	0.15	6,6,6,6	0
57	MG	YA	3081	1/1	0.97	0.14	27,27,27,27	0
57	MG	RA	3256	1/1	0.97	0.32	49,49,49,49	0
57	MG	YA	3083	1/1	0.97	0.13	17,17,17,17	0
57	MG	QA	1678	1/1	0.97	0.06	39,39,39,39	0
57	MG	RA	3258	1/1	0.97	0.26	51,51,51,51	0
57	MG	YA	3187	1/1	0.97	0.17	12,12,12,12	0
57	MG	YA	3188	1/1	0.97	0.18	5,5,5,5	0
57	MG	RA	3220	1/1	0.97	0.09	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3232	1/1	0.97	0.09	17,17,17,17	0
57	MG	YA	3326	1/1	0.97	0.16	21,21,21,21	0
57	MG	YA	3233	1/1	0.97	0.16	26,26,26,26	0
57	MG	RA	3105	1/1	0.97	0.13	37,37,37,37	0
57	MG	YA	3191	1/1	0.97	0.17	5,5,5,5	0
57	MG	YA	3192	1/1	0.97	0.24	13,13,13,13	0
57	MG	QA	1605	1/1	0.97	0.10	29,29,29,29	0
57	MG	YA	3056	1/1	0.97	0.09	15,15,15,15	0
57	MG	XA	1679	1/1	0.97	0.12	28,28,28,28	0
57	MG	YA	3196	1/1	0.97	0.24	26,26,26,26	0
57	MG	RA	3295	1/1	0.97	0.22	22,22,22,22	0
57	MG	XA	1681	1/1	0.97	0.19	32,32,32,32	0
57	MG	YD	303	1/1	0.97	0.08	31,31,31,31	0
57	MG	RA	3262	1/1	0.97	0.22	37,37,37,37	0
57	MG	RA	3040	1/1	0.97	0.16	23,23,23,23	0
57	MG	XA	1656	1/1	0.97	0.10	29,29,29,29	0
57	MG	RA	3224	1/1	0.97	0.12	19,19,19,19	0
57	MG	XA	1659	1/1	0.97	0.22	31,31,31,31	0
57	MG	RA	3181	1/1	0.97	0.13	26,26,26,26	0
57	MG	QA	1614	1/1	0.97	0.07	43,43,43,43	0
57	MG	QA	1615	1/1	0.97	0.14	46,46,46,46	0
57	MG	XA	1663	1/1	0.97	0.22	24,24,24,24	0
57	MG	XA	1715	1/1	0.97	0.21	45,45,45,45	0
57	MG	YA	3040	1/1	0.97	0.15	6,6,6,6	0
57	MG	XA	1665	1/1	0.97	0.26	24,24,24,24	0
57	MG	YA	3106	1/1	0.97	0.10	13,13,13,13	0
57	MG	RA	3057	1/1	0.97	0.16	16,16,16,16	0
57	MG	YA	3259	1/1	0.97	0.12	36,36,36,36	0
57	MG	YA	3213	1/1	0.97	0.18	17,17,17,17	0
57	MG	YA	3074	1/1	0.97	0.12	20,20,20,20	0
57	MG	YA	3175	1/1	0.97	0.10	15,15,15,15	0
57	MG	RA	3269	1/1	0.97	0.14	31,31,31,31	0
57	MG	QA	1661	1/1	0.97	0.09	16,16,16,16	0
57	MG	QE	201	1/1	0.98	0.13	31,31,31,31	0
57	MG	XA	1664	1/1	0.98	0.08	34,34,34,34	0
57	MG	XA	1611	1/1	0.98	0.04	35,35,35,35	0
57	MG	YA	3041	1/1	0.98	0.09	1,1,1,1	0
57	MG	RA	3198	1/1	0.98	0.19	15,15,15,15	0
57	MG	RA	3229	1/1	0.98	0.06	21,21,21,21	0
57	MG	YA	3044	1/1	0.98	0.07	5,5,5,5	0
57	MG	YA	3241	1/1	0.98	0.19	25,25,25,25	0
57	MG	RA	3085	1/1	0.98	0.07	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3073	1/1	0.98	0.10	33,33,33,33	0
57	MG	RA	3099	1/1	0.98	0.15	4,4,4,4	0
57	MG	YA	3028	1/1	0.98	0.13	18,18,18,18	0
57	MG	YA	3069	1/1	0.98	0.20	17,17,17,17	0
57	MG	YA	3223	1/1	0.98	0.10	14,14,14,14	0
57	MG	XA	1671	1/1	0.98	0.24	26,26,26,26	0
57	MG	RA	3177	1/1	0.98	0.15	1,1,1,1	0
57	MG	XA	1657	1/1	0.98	0.06	8,8,8,8	0
57	MG	RA	3087	1/1	0.98	0.11	15,15,15,15	0
57	MG	YA	3095	1/1	0.98	0.14	25,25,25,25	0
57	MG	XA	1619	1/1	0.98	0.24	23,23,23,23	0
57	MG	XA	1676	1/1	0.98	0.20	26,26,26,26	0
57	MG	YA	3304	1/1	0.98	0.16	33,33,33,33	0
57	MG	RA	3009	1/1	0.98	0.17	7,7,7,7	0
57	MG	QA	1607	1/1	0.98	0.16	19,19,19,19	0
57	MG	RA	3206	1/1	0.98	0.19	30,30,30,30	0
57	MG	RA	3030	1/1	0.99	0.09	8,8,8,8	0
57	MG	YA	3255	1/1	0.99	0.19	30,30,30,30	0
58	SF4	QD	301	8/8	0.99	0.04	47,50,57,83	0
58	SF4	XD	301	8/8	0.99	0.06	29,44,75,86	0

6.5 Other polymers (i)

There are no such residues in this entry.