wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2026 – 09:07 AM EDT

PDB ID	:	6OXI / pdb_00006oxi
Title	:	Dimeric E.coli YoeB bound to Thermus thermophilus 70S post-cleavage (UAA)
Authors	:	Pavelich, I.J.; Hoffer, E.D.; Maehigashi, T.; Dunham, C.M.
Deposited on	:	2019-05-13
Resolution	:	3.50 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:

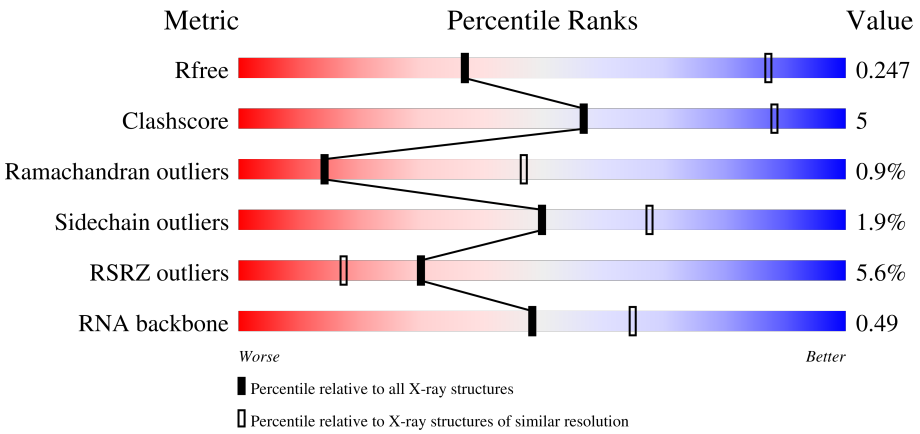
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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	2%, 62%, 32%, 5% •
1	XA	1521	2%, 64%, 30%, 5% •
2	QB	256	2%, 67%, 18%, 5% •, 8%
2	XB	256	5%, 72%, 16%, •, 8%

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Mol	Chain	Length	Quality of chain
3	QC	239	5% 71% 14% 14%
3	XC	239	4% 72% 13% • 14%
4	QD	209	3% 70% 28% •
4	XD	209	8% 76% 22% •
5	QE	162	6% 79% 14% • 7%
5	XE	162	5% 77% 15% • 7%
6	QF	101	3% 79% 21%
6	XF	101	83% 16% •
7	QG	156	5% 81% 17% • •
7	XG	156	10% 81% 16% • • •
8	QH	138	4% 76% 22% • •
8	XH	138	4% 81% 17% • •
9	QI	128	12% 76% 21% • •
9	XI	128	14% 70% 27% • •
10	QJ	105	21% 72% 18% • • 6%
10	XJ	105	10% 61% 28% • 9%
11	QK	129	7% 76% 16% 8%
11	XK	129	2% 78% 10% • • 10%
12	QL	132	13% 75% 18% • • 5%
12	XL	132	5% 70% 19% • 8%
13	QM	126	14% 67% 22% 5% • 5%
13	XM	126	13% 69% 22% • 6%
14	QN	61	38% 82% 16% •
14	XN	61	8% 74% 25% •
15	QO	89	3% 92% 7% •

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Mol	Chain	Length	Quality of chain
15	XO	89	3% 90% 8%
16	QP	88	7% 76% 19% 5%
16	XP	88	9% 82% 11% 5%
17	QQ	105	8% 81% 13% 5%
17	XQ	105	8% 76% 19% 5%
18	QR	88	57% 20% 20%
18	XR	88	% 60% 15% 5% 20%
19	QS	93	10% 62% 19% 6% 11%
19	XS	93	5% 69% 19% 11%
20	QT	106	16% 73% 21% 7%
20	XT	106	12% 66% 25% 7%
21	QU	27	44% 67% 19% 7% 7%
21	XU	27	19% 70% 15% 7% 7%
22	QV	77	3% 81% 19%
22	XV	77	3% 83% 16%
23	QX	20	35% 35% 50% 5% 10%
23	XX	20	30% 35% 45% 10% 10%
24	QY	84	14% 77% 19%
24	QZ	84	% 68% 27% 5%
24	XY	84	7% 75% 25%
24	XZ	84	12% 79% 18%
25	R0	85	9% 72% 22% 5%
25	Y0	85	7% 75% 20%
26	R1	98	16% 81% 13%
26	Y1	98	3% 73% 26%

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Mol	Chain	Length	Quality of chain
27	R2	72	7% 67% 25%
27	Y2	72	6% 83% 12%
28	R3	60	2% 78% 20%
28	Y3	60	2% 82% 17%
29	R4	71	6% 49% 38% 7%
29	Y4	71	14% 73% 20%
30	R5	60	5% 72% 27%
30	Y5	60	5% 87% 10%
31	R6	54	24% 65% 28% 6%
31	Y6	54	31% 83% 15%
32	R7	49	8% 86% 10%
32	Y7	49	12% 80% 18%
33	R8	65	15% 69% 22% 6%
33	Y8	65	17% 68% 25%
34	R9	37	38% 65% 30% 5%
34	Y9	37	35% 78% 19%
35	RA	2915	2% 64% 31%
35	YA	2915	2% 66% 28%
36	RB	124	4% 58% 34% 5%
36	YB	124	2% 66% 26% 5%
37	RD	276	12% 72% 24%
37	YD	276	2% 87% 12%
38	RE	206	6% 69% 25% 5%
38	YE	206	3% 77% 21%
39	RF	210	4% 83% 12%

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Mol	Chain	Length	Quality of chain
39	YF	210	4% 75% 20%
40	RG	182	5% 75% 21%
40	YG	182	8% 75% 23%
41	RH	180	17% 73% 18%
41	YH	180	12% 81% 15%
42	RI	148	15% 68% 22% 5%
42	YI	148	6% 81% 14%
43	RN	140	16% 76% 19%
43	YN	140	8% 79% 17%
44	RO	122	% 74% 26%
44	YO	122	3% 79% 21%
45	RP	150	11% 69% 27%
45	YP	150	7% 77% 22%
46	RQ	141	9% 70% 26%
46	YQ	141	4% 79% 21%
47	RR	118	3% 79% 19%
47	YR	118	9% 77% 20%
48	RS	112	14% 74% 24%
48	YS	112	12% 76% 21%
49	RT	146	8% 66% 25% 6%
49	YT	146	8% 71% 19% 6%
50	RU	118	5% 77% 19%
50	YU	118	11% 81% 15%
51	RV	101	3% 69% 25%
51	YV	101	16% 70% 25% 5%

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Mol	Chain	Length	Quality of chain
52	RW	113	6% 88% 12%
52	YW	113	6% 78% 21%
53	RX	96	10% 79% 17%
53	YX	96	% 80% 15%
54	RY	110	23% 75% 18% 5%
54	YY	110	8% 82% 14%
55	RZ	206	% 73% 13% 11%
55	YZ	206	2% 63% 24% 11%
56	ZA	3	67% 33%
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	QY	101	-	-	-	X
57	MG	RA	3302	-	-	-	X
57	MG	XA	1651	-	-	-	X

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 295153 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
			Total	C	N	O	P			
1	QA	1510	32452	14444	6009	10489	1510	0	0	0
1	XA	1507	32389	14416	5999	10467	1507	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called P-site tRNA-fMet.

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

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	QX	18	394	176	79	121	18	0	0	0
23	XX	18	394	176	79	121	18	0	0	0

- Molecule 24 is a protein called Addiction module toxin, Txe/YoeB family.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	R1	94	737	463	146	127	1	0	0	0
26	Y1	97	763	481	150	131	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	R2	69	581	358	118	104	1	0	0	0
27	Y2	69	581	358	118	104	1	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
35	RA	2891	62266	27713	11649	20014	2890	0	0	0
35	YA	2878	61981	27587	11589	19928	2877	0	0	0

- Molecule 36 is a RNA chain called 5S rRNA.

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

- Molecule 37 is a protein called 50S ribosomal protein L2.

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

- Molecule 38 is a protein called 50S ribosomal protein L3.

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

- Molecule 39 is a protein called 50S ribosomal protein L4.

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

- Molecule 40 is a protein called 50S ribosomal protein L5.

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

- Molecule 41 is a protein called 50S ribosomal protein L6.

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

- Molecule 42 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	RI	145	1131	723	200	207	1	0	0	0
42	YI	146	1136	726	201	208	1	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L13.

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

- Molecule 44 is a protein called 50S ribosomal protein L14.

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

- Molecule 45 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	RP	150	1145	712	232	198	3	0	0	0
45	YP	149	1135	706	230	196	3	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L16.

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

- Molecule 47 is a protein called 50S ribosomal protein L17.

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

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

- Molecule 48 is a protein called 50S ribosomal protein L18.

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

- Molecule 49 is a protein called 50S ribosomal protein L19.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L21.

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

- Molecule 52 is a protein called 50S ribosomal protein L22.

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

- Molecule 53 is a protein called 50S ribosomal protein L23.

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

- Molecule 54 is a protein called 50S ribosomal protein L24.

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

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

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

- Molecule 56 is a RNA chain called CCPuro.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	QA	93	93	93	0	0
57	QD	1	1	1	0	0
57	QE	1	1	1	0	0
57	QV	3	3	3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	QY	1	1	1	0	0
57	R0	2	2	2	0	0
57	R3	1	1	1	0	0
57	RA	302	302	302	0	0
57	RB	3	3	3	0	0
57	RD	2	2	2	0	0
57	RE	1	1	1	0	0
57	RN	1	1	1	0	0
57	RO	1	1	1	0	0
57	RP	1	1	1	0	0
57	RQ	4	4	4	0	0
57	RR	1	1	1	0	0
57	RY	1	1	1	0	0
57	XA	99	99	99	0	0
57	XE	1	1	1	0	0
57	XF	1	1	1	0	0
57	XL	1	1	1	0	0
57	XM	1	1	1	0	0
57	XV	4	4	4	0	0
57	Y0	2	2	2	0	0
57	Y1	1	1	1	0	0

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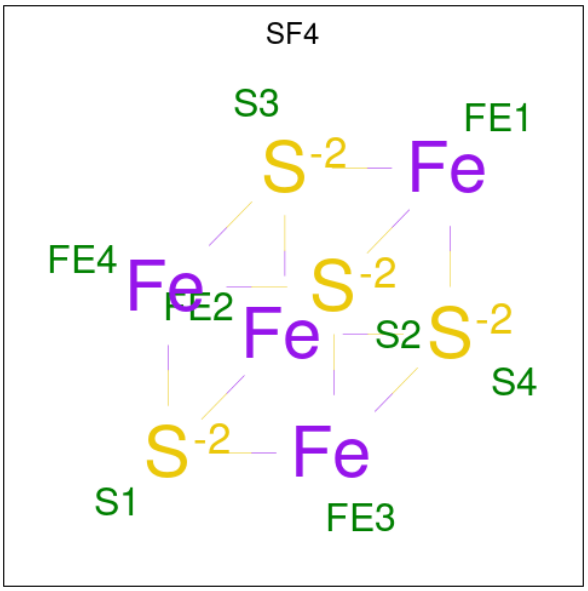
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	Y3	1	1	1	0	0
57	Y5	1	1	1	0	0
57	Y9	1	1	1	0	0
57	YA	335	335	335	0	0
57	YB	3	3	3	0	0
57	YD	4	4	4	0	0
57	YE	5	5	5	0	0
57	YF	1	1	1	0	0
57	YG	1	1	1	0	0
57	YO	1	1	1	0	0
57	YP	1	1	1	0	0
57	YQ	5	5	5	0	0
57	YR	1	1	1	0	0
57	YV	1	1	1	0	0

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



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

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

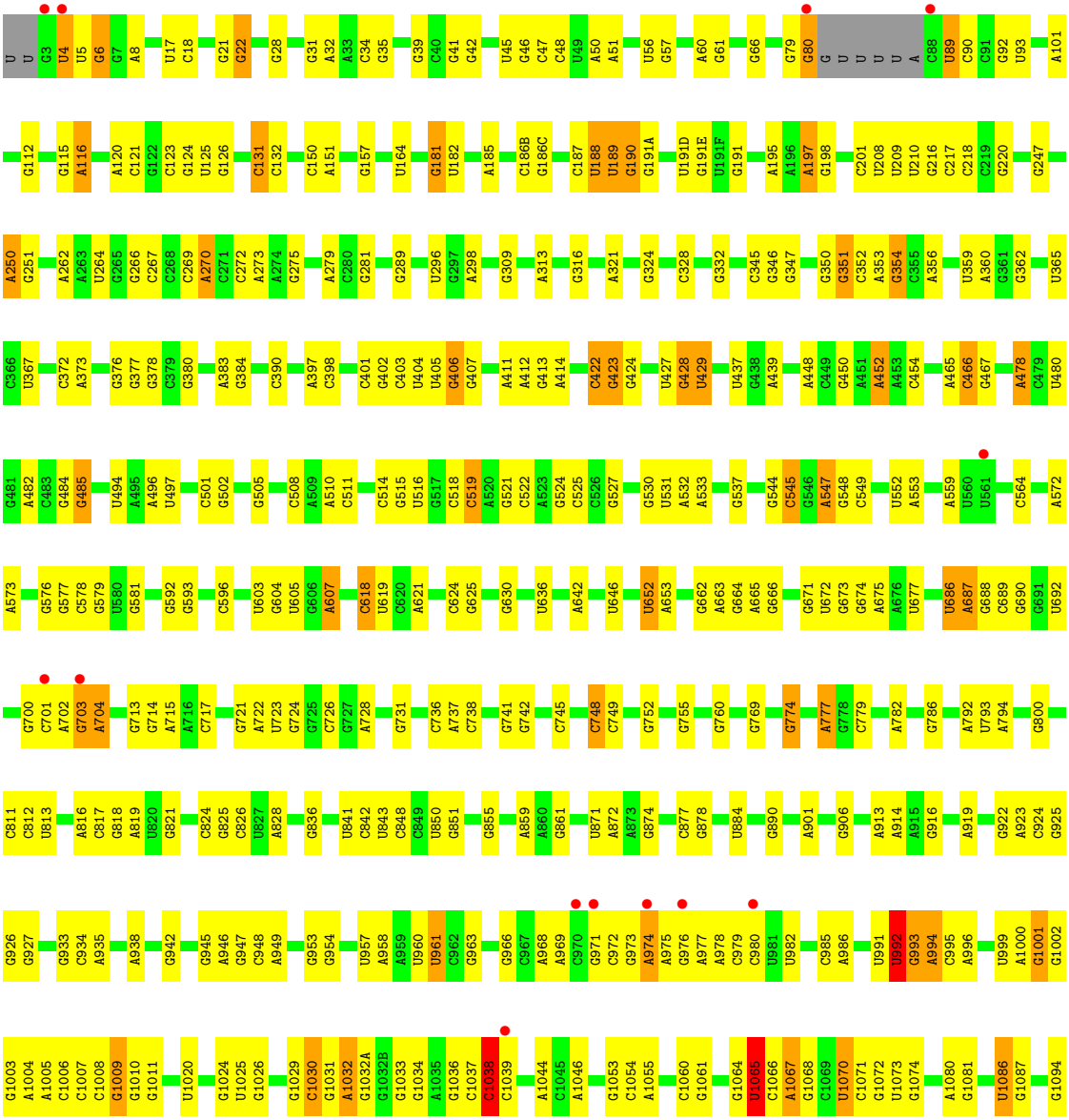
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
59	QN	1	1	1	0	0
			Total	Zn		
59	R4	1	1	1	0	0
			Total	Zn		
59	R5	1	1	1	0	0
			Total	Zn		
59	R6	1	1	1	0	0
			Total	Zn		
59	R9	1	1	1	0	0
			Total	Zn		
59	XN	1	1	1	0	0
			Total	Zn		
59	Y4	1	1	1	0	0
			Total	Zn		
59	Y6	1	1	1	0	0

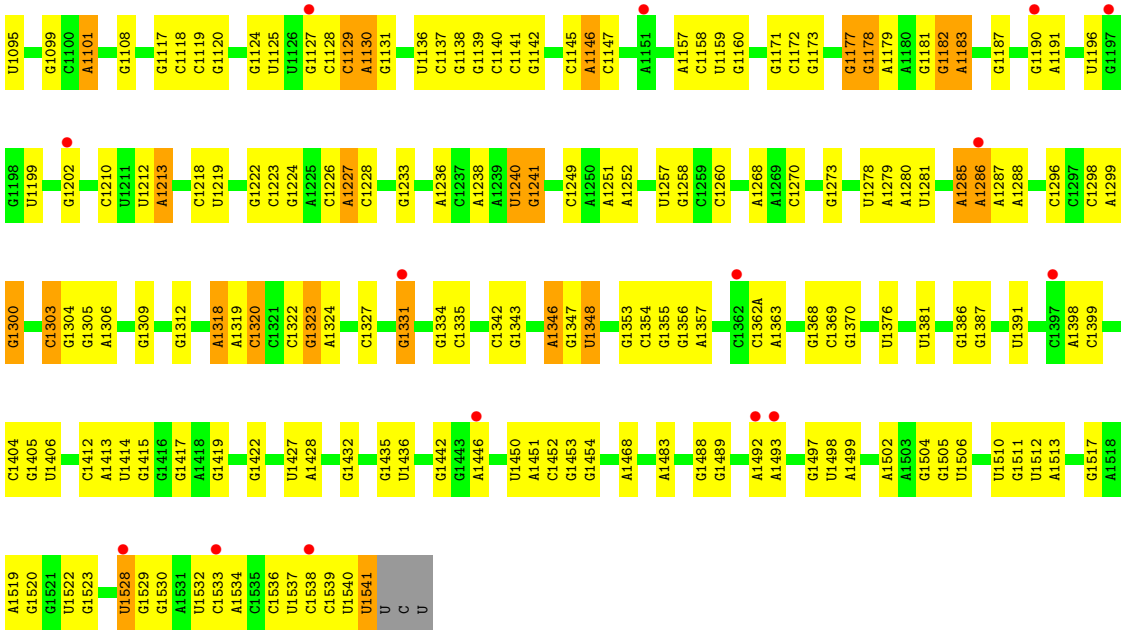
3 Residue-property plots (i)

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

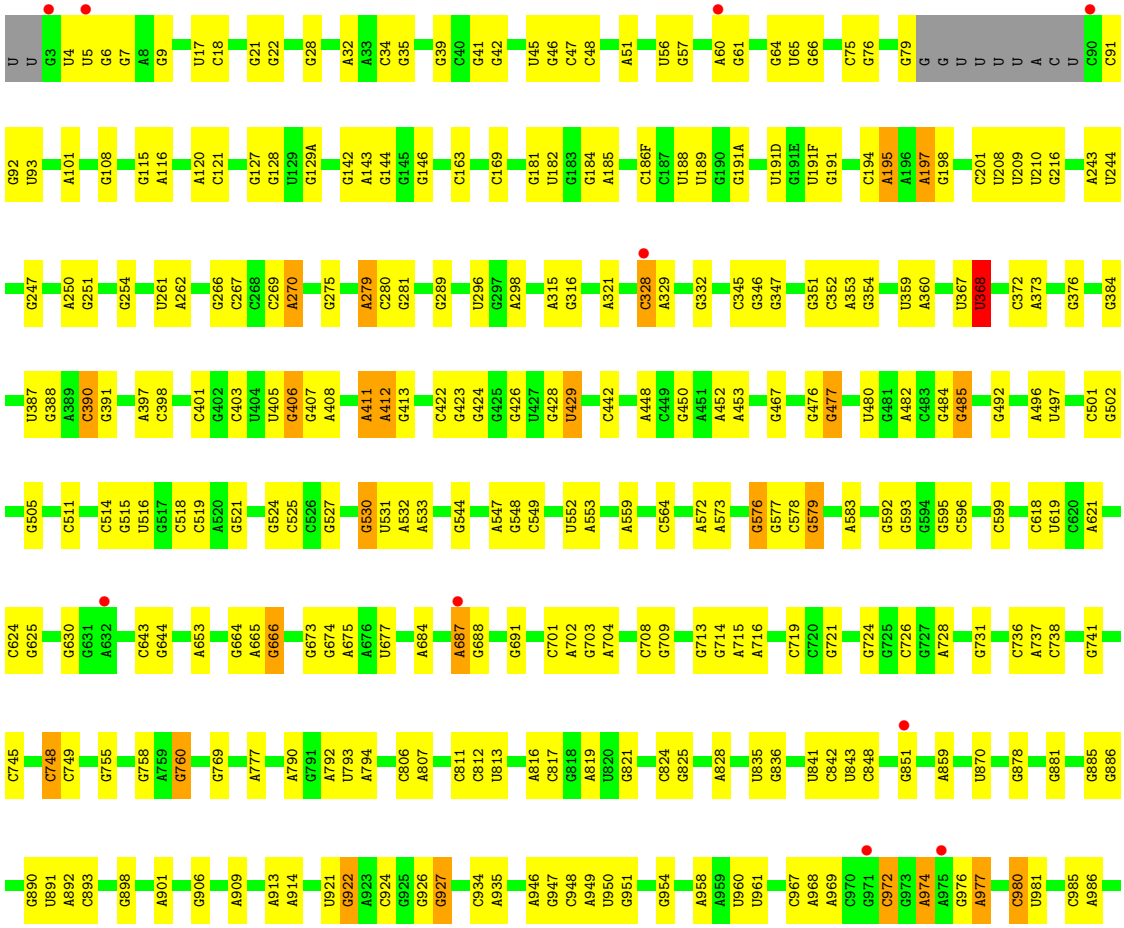
Chain QA:

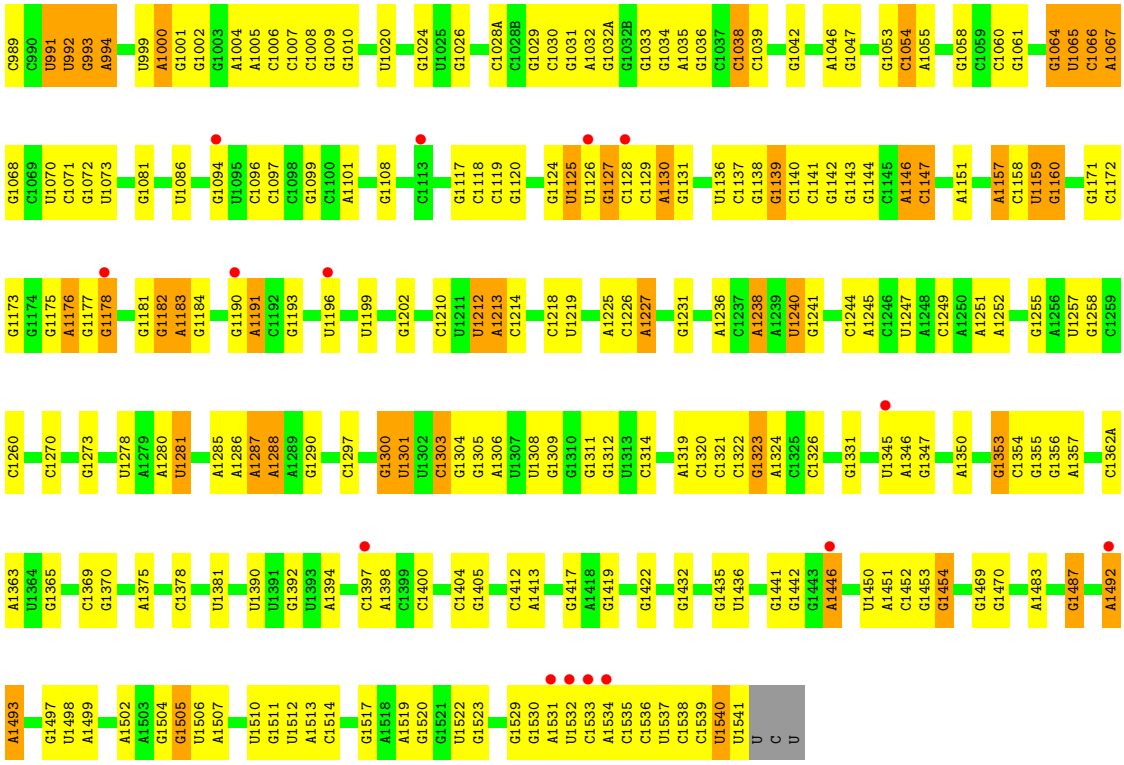




- Molecule 1: 16S rRNA

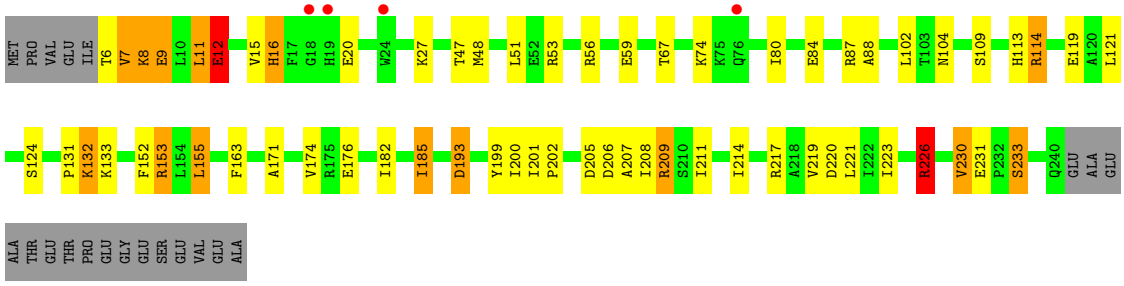
Chain XA:





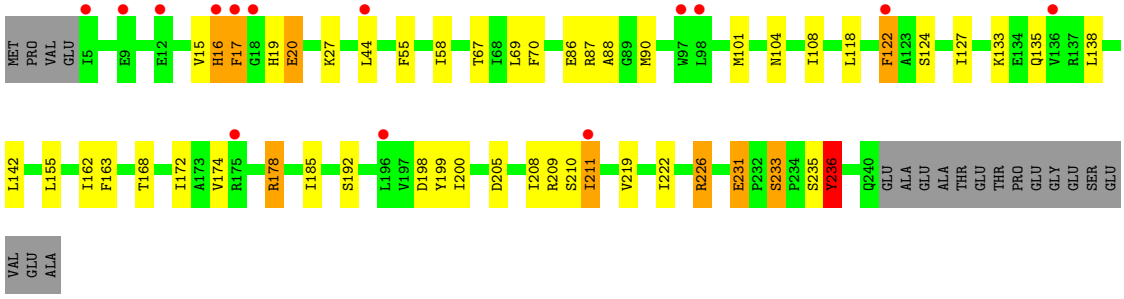
- Molecule 2: 30S ribosomal protein S2

Chain QB:



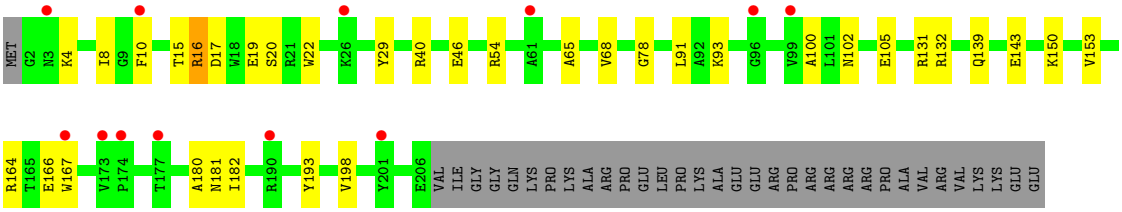
- Molecule 2: 30S ribosomal protein S2

Chain XB:



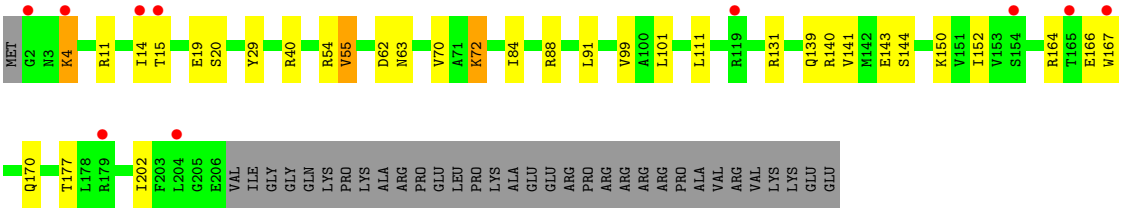
- Molecule 3: 30S ribosomal protein S3

Chain QC:



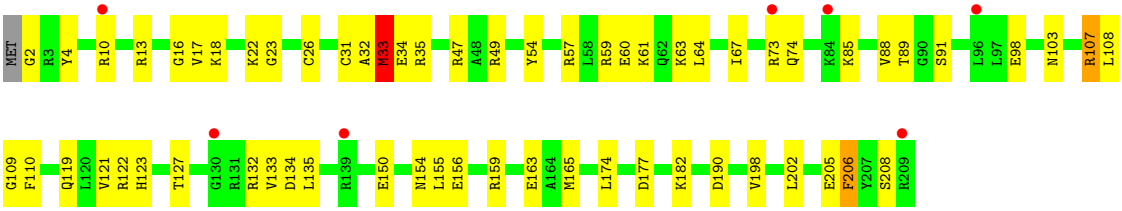
- Molecule 3: 30S ribosomal protein S3

Chain XC:



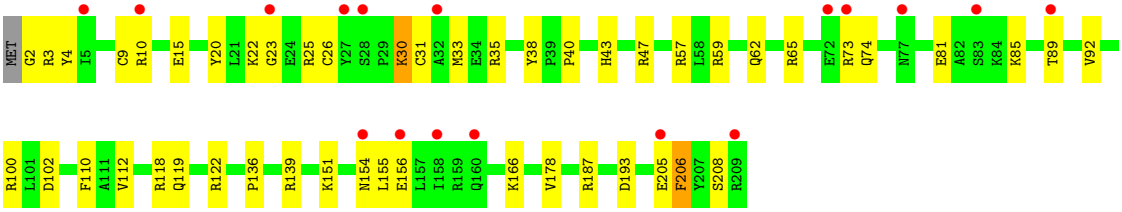
- Molecule 4: 30S ribosomal protein S4

Chain QD:



- Molecule 4: 30S ribosomal protein S4

Chain XD:



- Molecule 5: 30S ribosomal protein S5

Chain QE:

ALA GLN GLY

• Molecule 5: 30S ribosomal protein S5

Chain XE:

MET PRO GLU THR D5 M10 I11 M19 Q20 A21 G22 G23 R24 R25 F26 V51 P52 L53 Q56 R63 M66 V69 I80 E81 G85 V90 L91 A102 V105 P106 R107 E111 T120 G124 P128 T135 G154 E155 ALA HIS ALA GLN

ALA GLN GLY

• Molecule 6: 30S ribosomal protein S6

Chain QF:

M1 R2 R3 V6 V9 L10 N13 L14 D15 Q16 S17 R46 K54 Y59 F60 L61 W62 Y63 Q64 V65 E66 E69 A76 L79 R80 R87 V88 M89 V90 S93 A101

• Molecule 6: 30S ribosomal protein S6

Chain XF:

M1 R2 V9 L10 E22 L30 V37 L45 R46 Y59 F60 L61 V65 V72 L75 R82 R87 E95 N100 A101

• Molecule 7: 30S ribosomal protein S7

Chain QG:

MET A2 R3 R4 E8 V9 R10 D15 L16 V17 Y18 G19 D20 V23 N28 K29 I30 M31 D45 L59 K60 V61 F62 V75 R78 R79 V80 Y85 Q86 V87 P88 R94 R119 L124 A150 Y151 A152 H153 Y154 R155 W156

• Molecule 7: 30S ribosomal protein S7

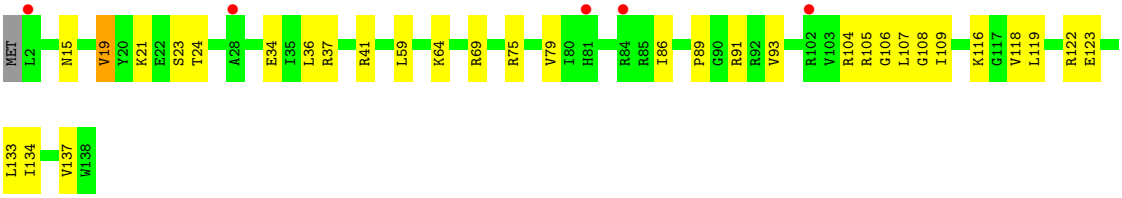
Chain XG:

MET A2 R3 R4 Q13 P14 D15 L16 G19 D20 V23 F26 K29 R32 D33 N37 I42 F43 Y44 E57 R76 S77 R78 R79 V80 G81 G82 A83 N84 V87 R94 S98 L101 R111 R114 R119 M125 D126 A150 Y151 A152

H153 Y154 R155 W156

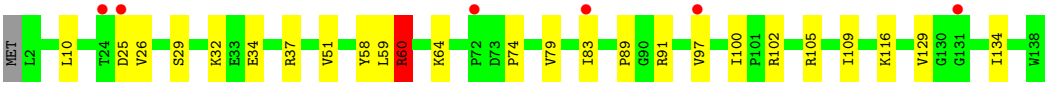
• Molecule 8: 30S ribosomal protein S8

Chain QH:



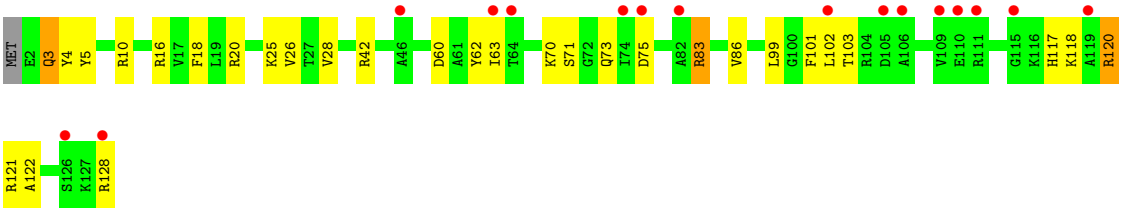
• Molecule 8: 30S ribosomal protein S8

Chain XH:



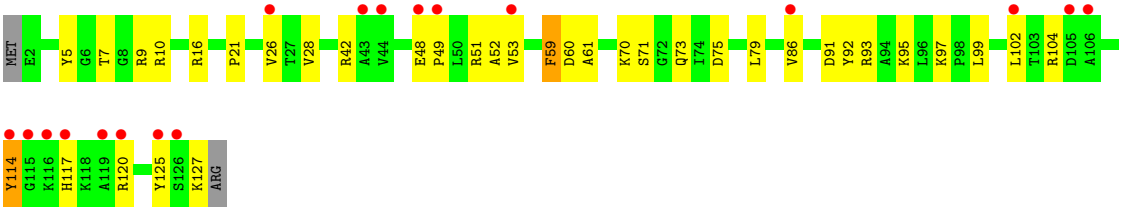
• Molecule 9: 30S ribosomal protein S9

Chain QI:



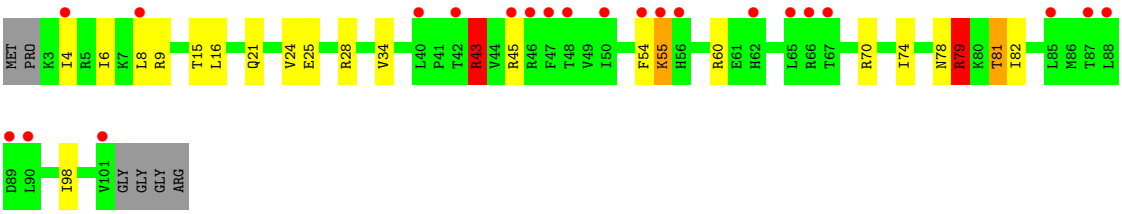
• Molecule 9: 30S ribosomal protein S9

Chain XI:



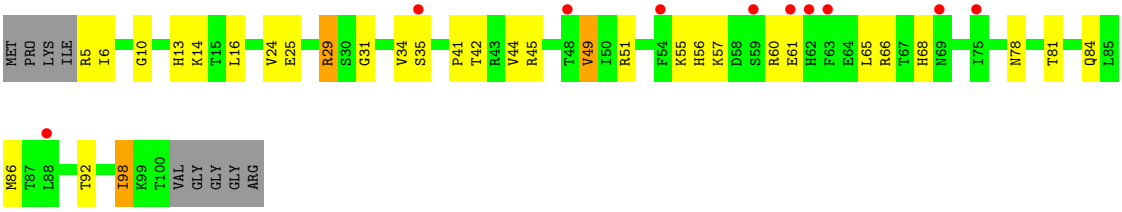
• Molecule 10: 30S ribosomal protein S10

Chain QJ:



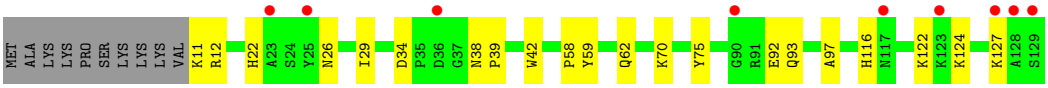
• Molecule 10: 30S ribosomal protein S10

Chain XJ:



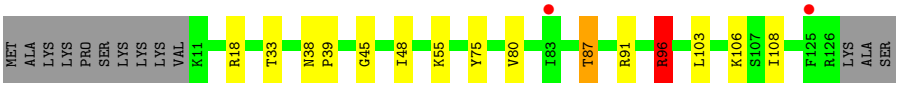
- Molecule 11: 30S ribosomal protein S11

Chain QK:



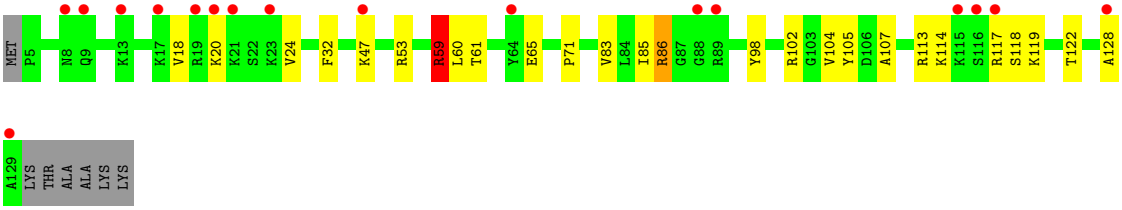
- Molecule 11: 30S ribosomal protein S11

Chain XK:



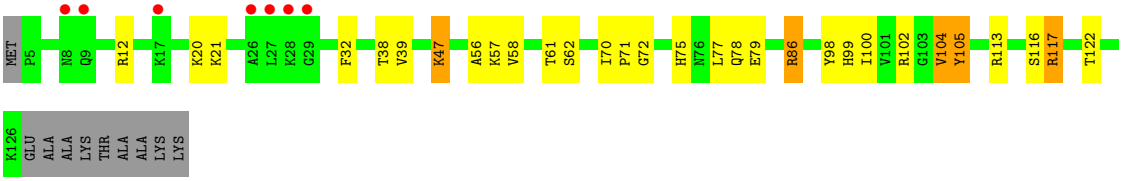
- Molecule 12: 30S ribosomal protein S12

Chain QL:



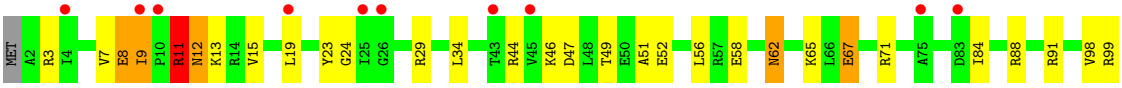
- Molecule 12: 30S ribosomal protein S12

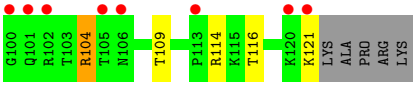
Chain XL:



- Molecule 13: 30S ribosomal protein S13

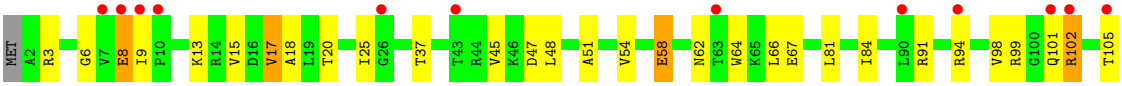
Chain QM:

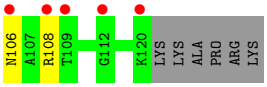




• Molecule 13: 30S ribosomal protein S13

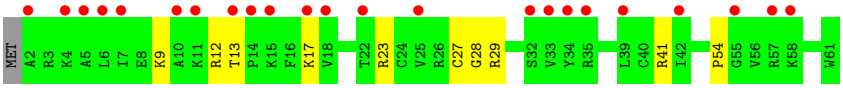
Chain XM:





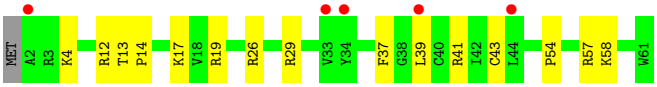
• Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:



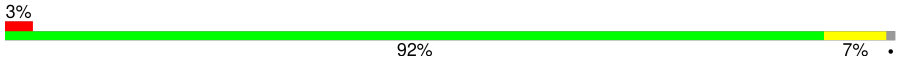
• Molecule 14: 30S ribosomal protein S14 type Z

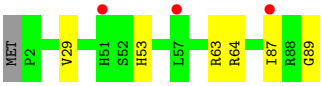
Chain XN:



• Molecule 15: 30S ribosomal protein S15

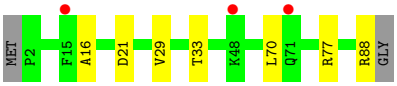
Chain QO:





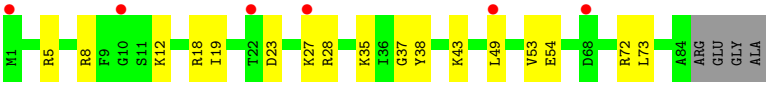
• Molecule 15: 30S ribosomal protein S15

Chain XO:



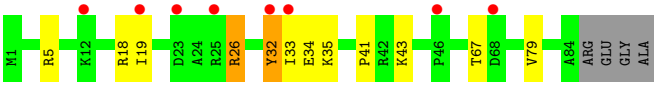
• Molecule 16: 30S ribosomal protein S16

Chain QP:



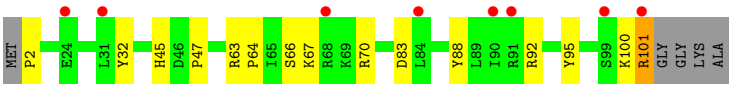
• Molecule 16: 30S ribosomal protein S16

Chain XP:



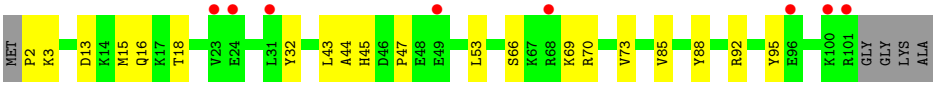
• Molecule 17: 30S ribosomal protein S17

Chain QQ:



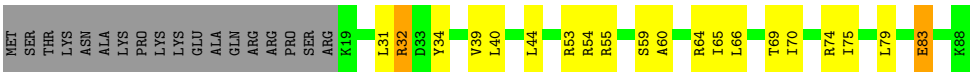
• Molecule 17: 30S ribosomal protein S17

Chain XQ:



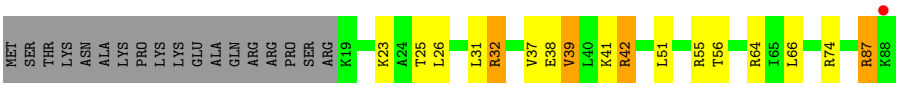
• Molecule 18: 30S ribosomal protein S18

Chain QR:



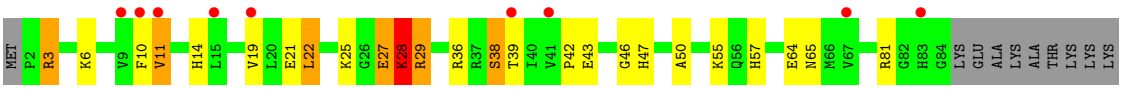
• Molecule 18: 30S ribosomal protein S18

Chain XR:



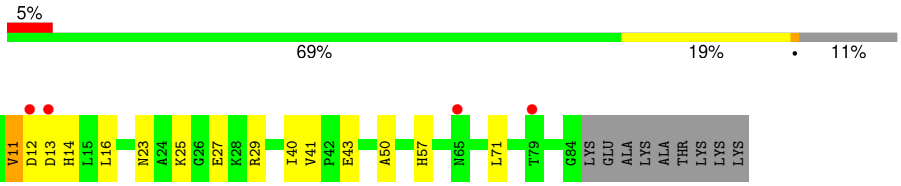
• Molecule 19: 30S ribosomal protein S19

Chain QS:



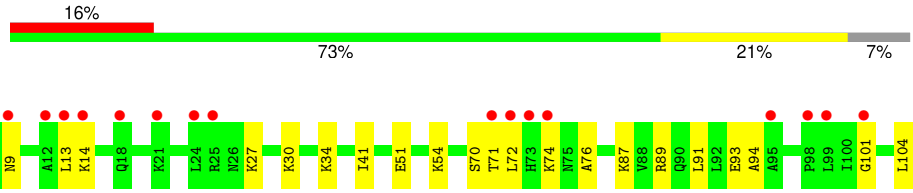
• Molecule 19: 30S ribosomal protein S19

Chain XS:



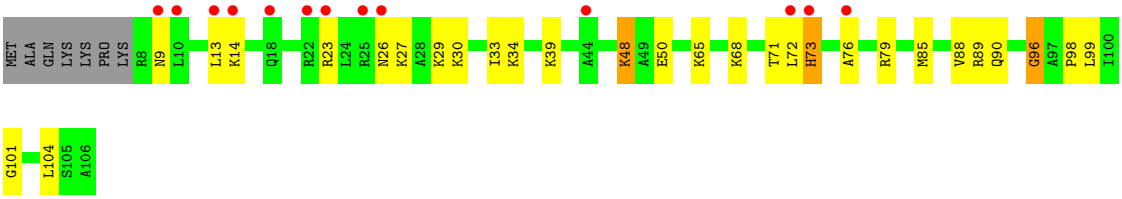
• Molecule 20: 30S ribosomal protein S20

Chain QT:



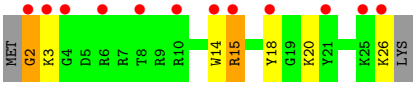
• Molecule 20: 30S ribosomal protein S20

Chain XT:



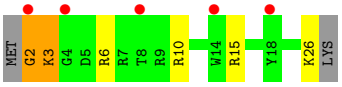
• Molecule 21: 30S ribosomal protein Thx

Chain QU:



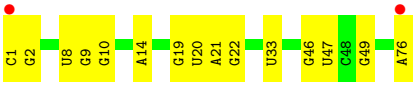
• Molecule 21: 30S ribosomal protein Thx

Chain XU:



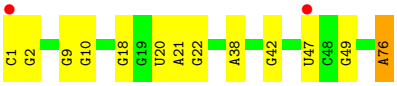
• Molecule 22: P-site tRNA-fMet

Chain QV:



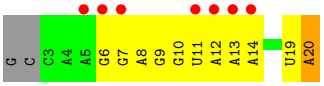
• Molecule 22: P-site tRNA-fMet

Chain XV:



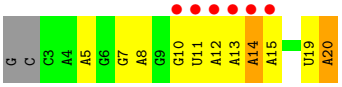
• Molecule 23: mRNA

Chain QX:



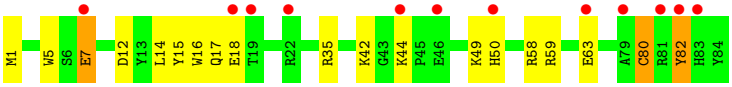
• Molecule 23: mRNA

Chain XX:



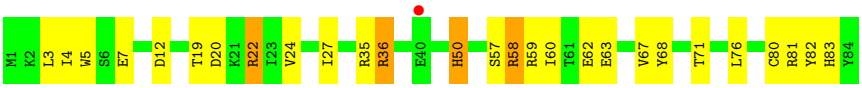
• Molecule 24: Addiction module toxin, Txe/YoeB family

Chain QY:



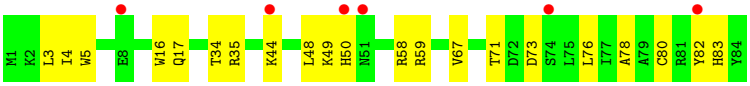
• Molecule 24: Addiction module toxin, Txe/YoeB family

Chain QZ:



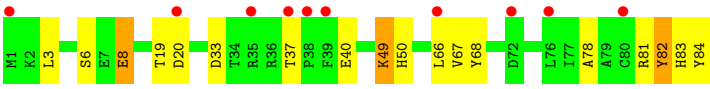
• Molecule 24: Addiction module toxin, Txe/YoeB family

Chain XY:



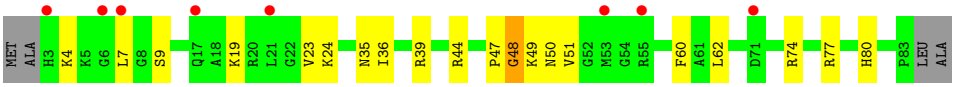
• Molecule 24: Addiction module toxin, Txe/YoeB family

Chain XZ:



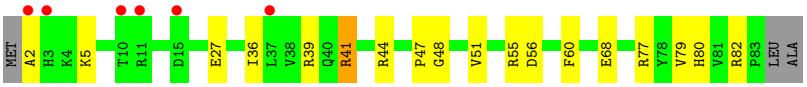
• Molecule 25: 50S ribosomal protein L27

Chain R0:



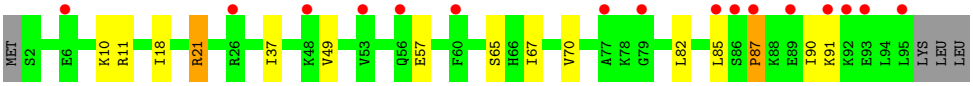
- Molecule 25: 50S ribosomal protein L27

Chain Y0:



- Molecule 26: 50S ribosomal protein L28

Chain R1:

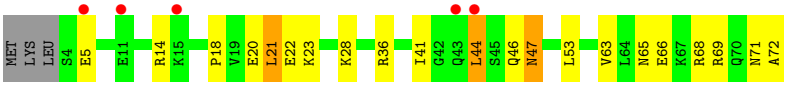


- Molecule 26: 50S ribosomal protein L28

Chain Y1:

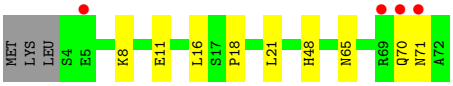
- Molecule 27: 50S ribosomal protein L29

Chain R2:



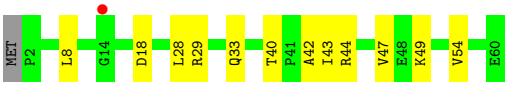
- Molecule 27: 50S ribosomal protein L29

Chain Y2:



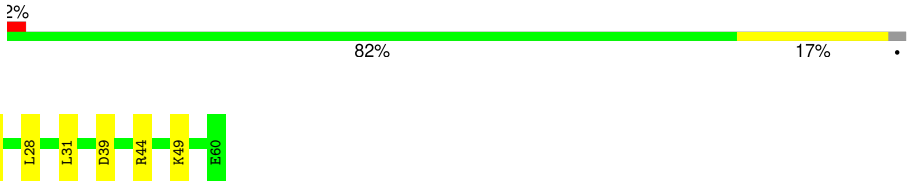
- Molecule 28: 50S ribosomal protein L30

Chain R3:



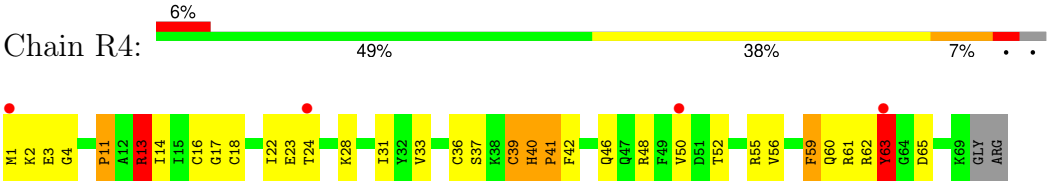
• Molecule 28: 50S ribosomal protein L30

Chain Y3:



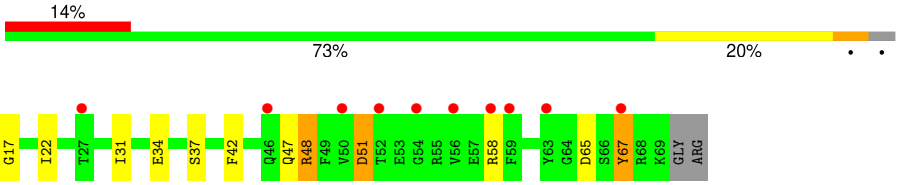
• Molecule 29: 50S ribosomal protein L31

Chain R4:



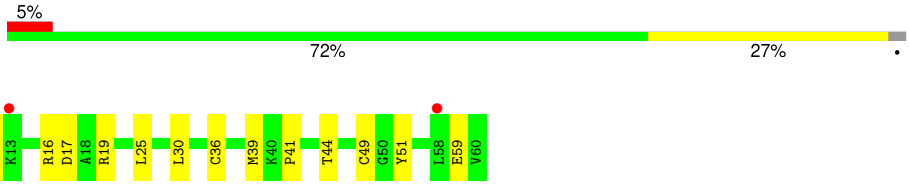
• Molecule 29: 50S ribosomal protein L31

Chain Y4:



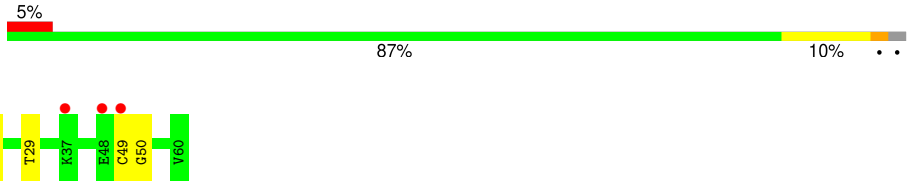
• Molecule 30: 50S ribosomal protein L32

Chain R5:



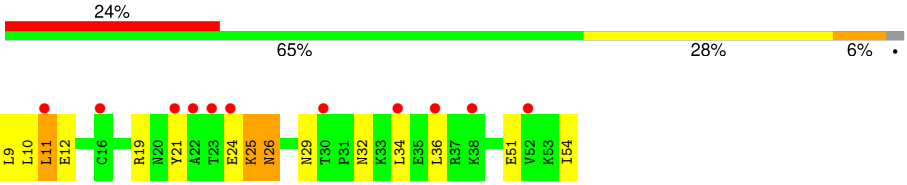
• Molecule 30: 50S ribosomal protein L32

Chain Y5:



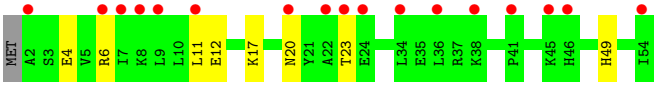
• Molecule 31: 50S ribosomal protein L33

Chain R6:



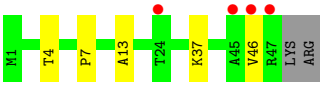
• Molecule 31: 50S ribosomal protein L33

Chain Y6:



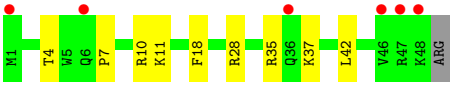
• Molecule 32: 50S ribosomal protein L34

Chain R7:



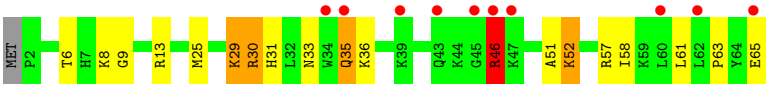
• Molecule 32: 50S ribosomal protein L34

Chain Y7:



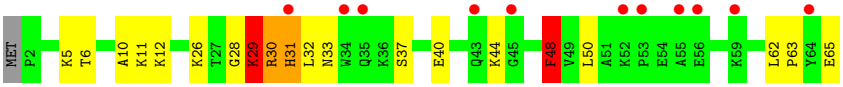
• Molecule 33: 50S ribosomal protein L35

Chain R8:



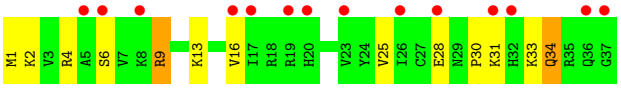
• Molecule 33: 50S ribosomal protein L35

Chain Y8:



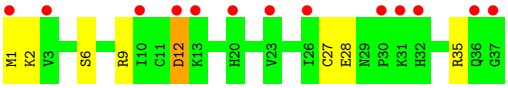
• Molecule 34: 50S ribosomal protein L36

Chain R9:



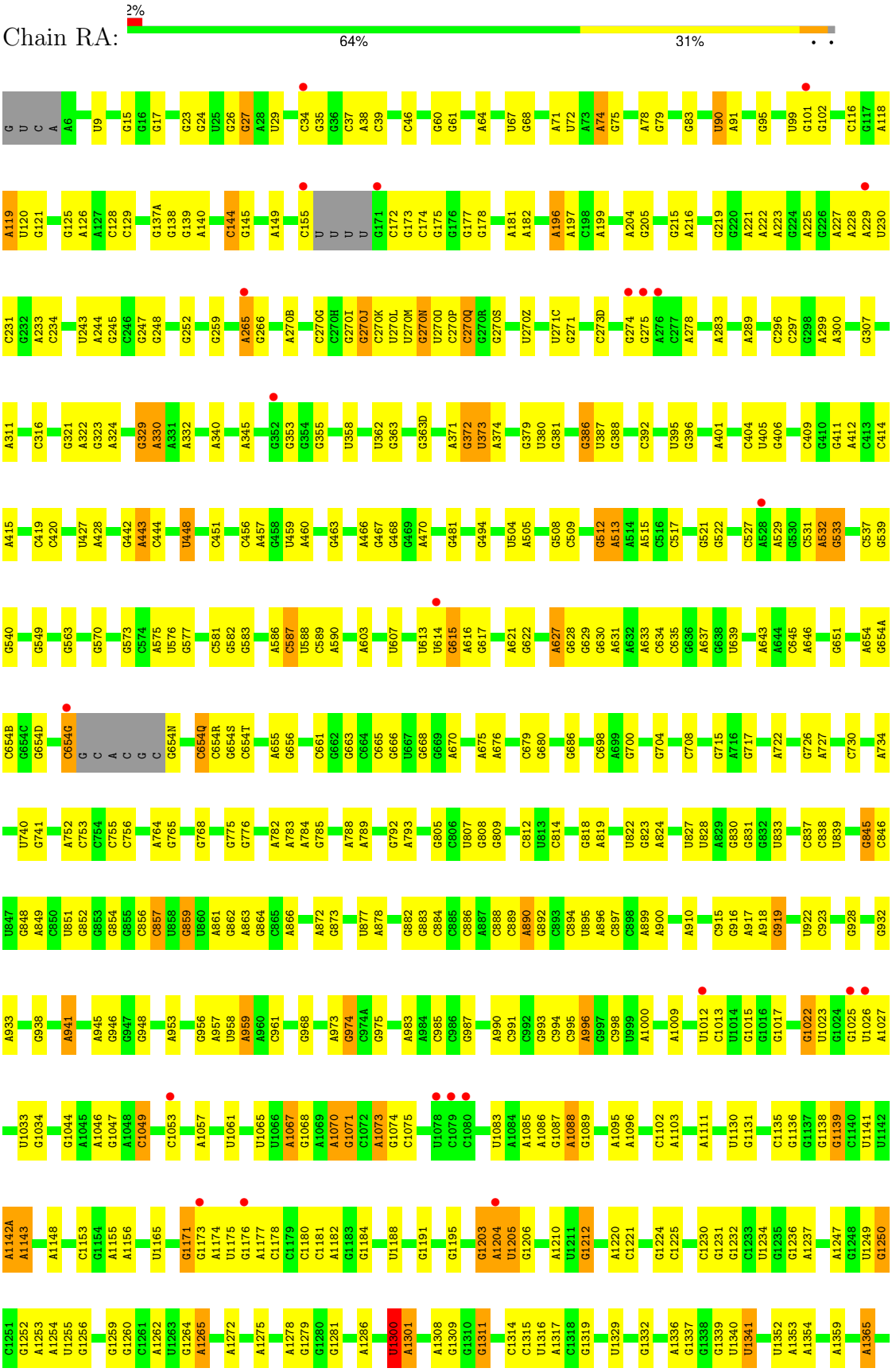
• Molecule 34: 50S ribosomal protein L36

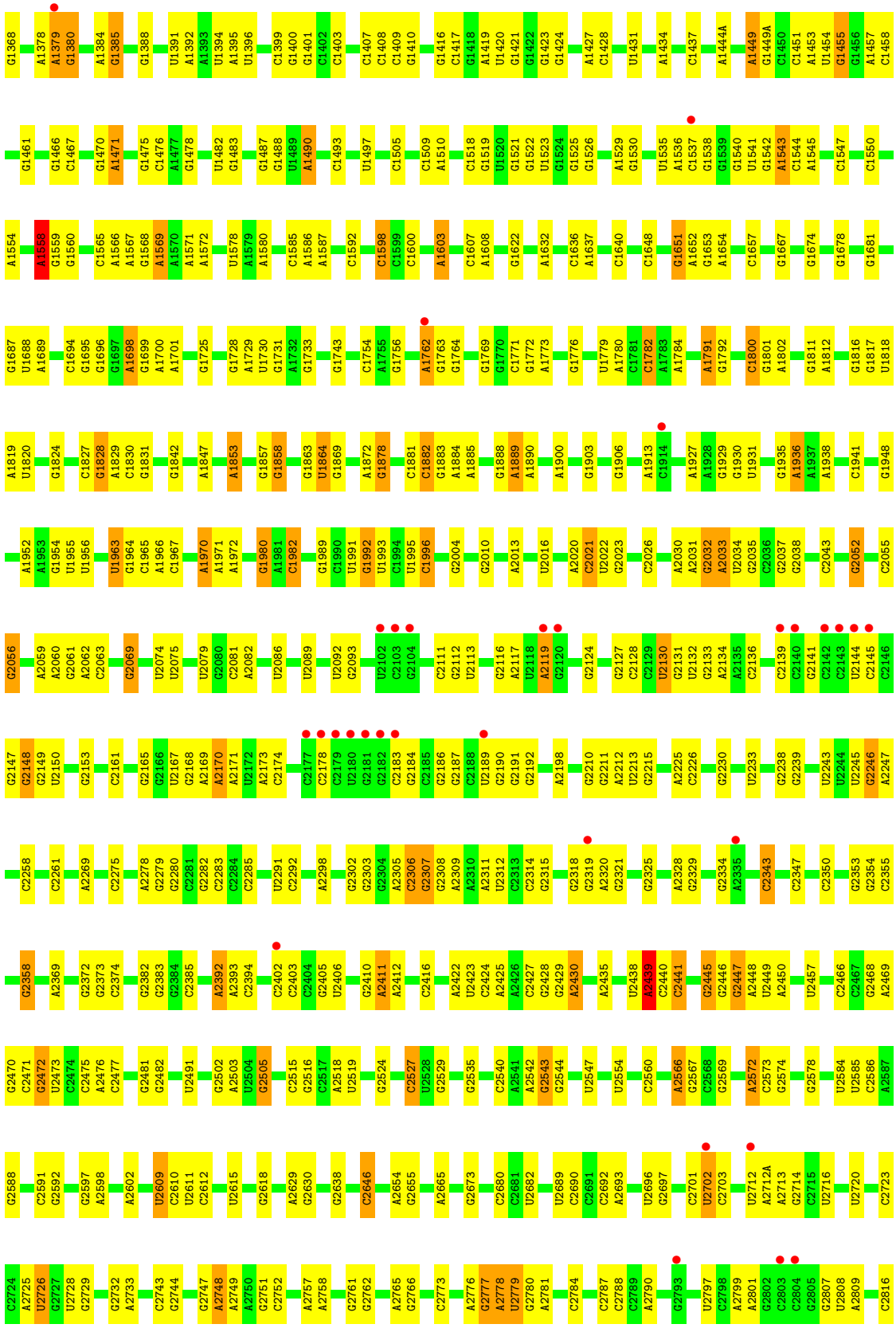
Chain Y9:



• Molecule 35: 23S rRNA

Chain RA:




G1368 A1378 A1379 G1380 A1384 G1385 G1388 U1391 A1392 A1393 U1394 A1395 U1396 C1399 G1400 G1401 C1402 C1403 C1407 C1408 C1409 G1410 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1423 G1424 A1427 C1428 U1431 A1434 C1437 A1444A A1449 G1449A C1450 C1451 A1453 U1454 G1455 G1456 A1457 C1458
G1461 G1466 C1467 G1470 A1471 G1475 C1476 A1477 G1478 U1482 G1483 G1487 G1488 U1489 A1490 C1493 U1497 C1505 C1509 A1510 C1518 G1519 U1520 G1521 G1522 U1523 G1524 G1525 G1526 A1529 G1530 U1535 A1536 C1537 G1538 G1539 G1540 U1541 G1542 A1543 C1544 A1545 C1547 C1550
A1554 A1558 G1559 G1560 C1565 A1566 A1567 G1568 A1569 A1570 A1571 A1572 U1578 A1579 A1580 C1585 A1586 A1587 C1592 C1598 C1599 C1600 A1603 C1607 A1608 G1622 A1632 C1636 A1637 C1640 C1648 G1651 A1652 G1653 A1654 C1657 G1667 G1674 G1678 G1681
G1687 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 G1770 C1771 G1772 A1773 G1776 U1779 A1780 C1781 C1782 A1783 A1784 A1791 G1792 C1800 G1801 A1802 G1811 A1812 G1816 G1817 U1818
A1819 U1820 G1824 C1827 G1828 A1829 C1830 G1831 G1842 A1847 A1853 G1857 G1858 G1863 U1864 G1869 A1872 G1878 C1881 C1882 G1883 A1884 A1885 G1888 A1889 A1890 A1900 G1903 G1906 A1913 C1914 A1927 A1928 G1929 G1930 U1931 G1935 A1936 A1937 A1938 C1941 G1948
A1952 A1953 G1954 U1955 U1956 U1963 G1964 C1965 A1966 C1967 A1970 A1971 A1972 G1980 A1981 C1982 G1989 C1990 U1991 G1992 U1993 C1994 U1995 C1996 G2004 G2010 A2013 U2016 A2020 C2021 U2022 G2023 C2026 A2030 A2031 G2032 A2033 U2034 G2035 C2036 G2037 G2038 C2043 G2052 C2055
G2056 A2059 A2060 G2061 A2062 C2063 G2069 U2074 U2075 U2079 G2080 C2081 A2082 U2086 U2089 U2092 G2093 U2102 C2103 G2104 C2111 G2112 U2113 G2116 A2117 U2118 A2119 G2120 G2124 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146
G2147 G2148 G2149 U2150 G2153 C2161 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2177 C2178 C2179 U2180 G2181 G2182 C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2190 G2191 G2192 A2198 G2210 G2211 A2212 U2213 G2215 A2225 C2226 G2230 U2233 G2238 G2239 U2243 U2244 U2245 G2246 A2247
C2258 C2261 A2269 C2275 A2278 G2279 G2280 C2281 G2282 C2283 C2284 C2285 U2291 C2292 A2298 G2302 G2303 G2304 A2305 C2306 G2307 G2308 A2309 A2310 A2311 U2312 C2313 C2314 G2315 G2318 G2319 A2320 G2321 G2325 A2328 G2329 G2334 A2335 C2343 C2347 C2350 G2353 G2354 C2355
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G2470 C2471 G2472 U2473 C2474 C2475 A2476 C2477 G2481 G2482 U2491 G2502 A2503 U2504 G2505 C2515 G2516 C2517 A2518 U2519 G2524 C2527 U2528 G2529 G2535 C2540 A2541 A2542 G2543 G2544 U2547 U2554 C2560 A2566 G2567 C2568 G2569 A2572 C2573 G2574 G2578 U2584 C2585 C2586 A2587
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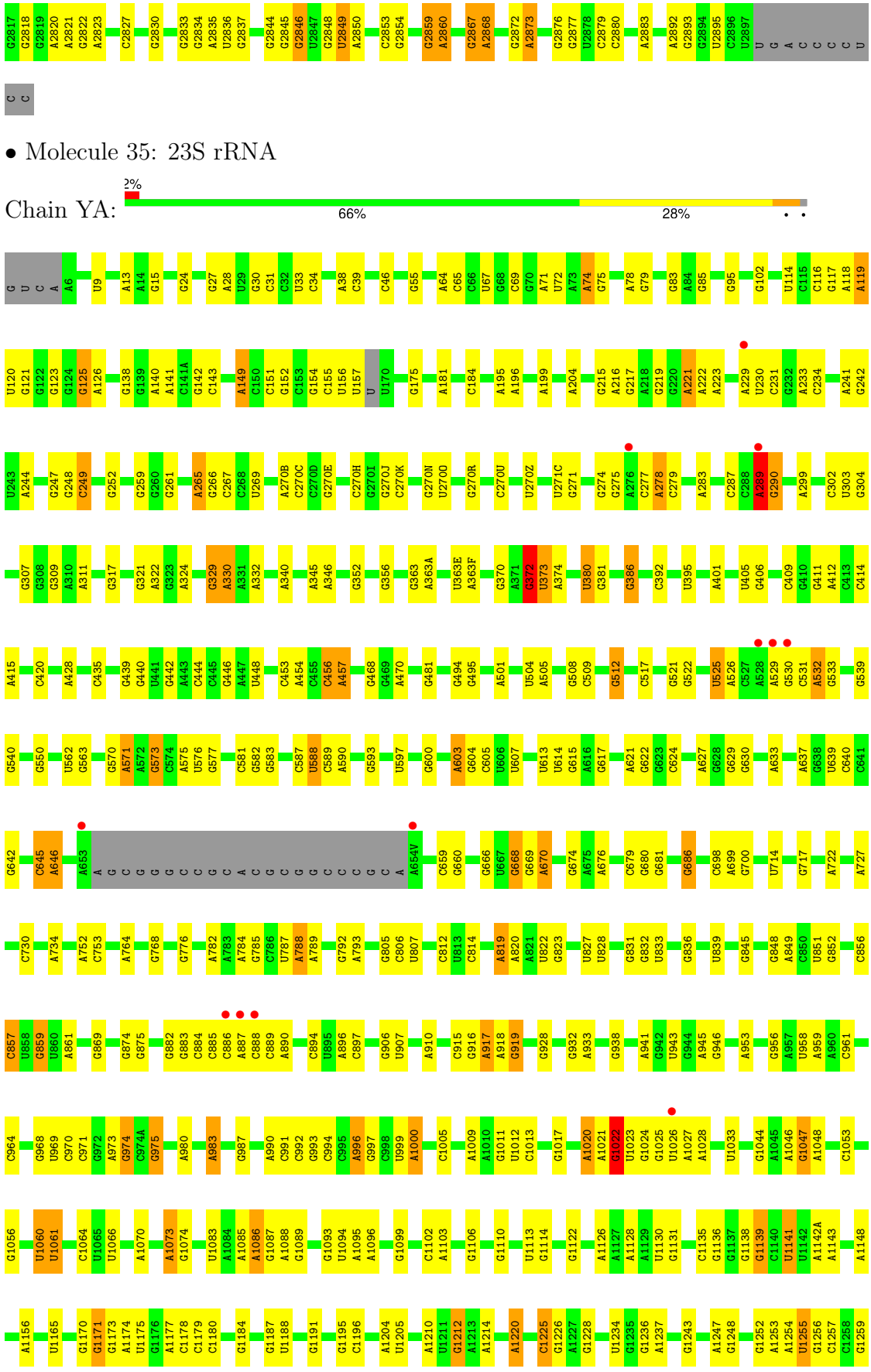
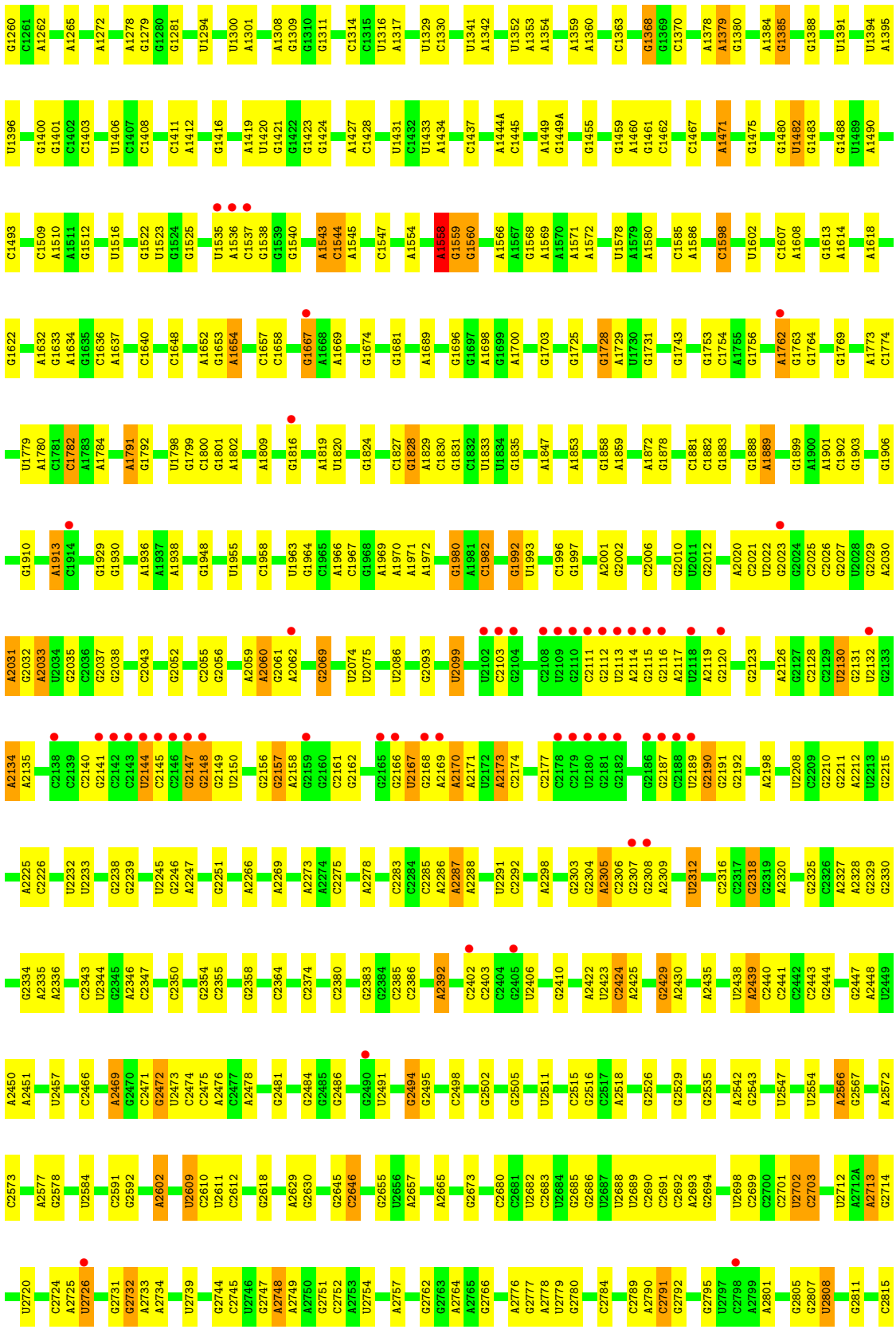
C2724 A2725 U2726 G2727 U2728 G2729 G2732 A2733 C2743 G2744 G2747 A2748 A2749 A2750 G2751 C2752 A2757 A2758 G2761 G2762 A2765 G2766 C2773 A2776 G2777 A2778 U2779 G2780 A2781 C2784 C2787 C2788 C2789 A2790 G2793 U2797 C2798 A2799 A2801 G2802 C2803 C2804 G2805 G2807 U2808 A2809 C2816



• Molecule 35: 23S rRNA

Chain YA: 2% 66% 28%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U1396 G1400 G1401 C1402 C1403 U1406 C1407 C1408 C1411 A1412 G1416 A1419 U1420 G1421 G1422 G1423 G1424 A1427 C1428 U1431 C1432 U1433 A1434 C1437 A1444A C1445 A1449 G1449A G1455 G1459 A1460 G1461 C1462 C1467 A1471 G1475 G1480 U1482 G1483 G1488 U1489 A1490
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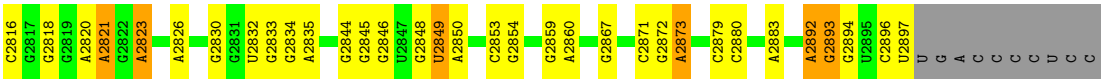
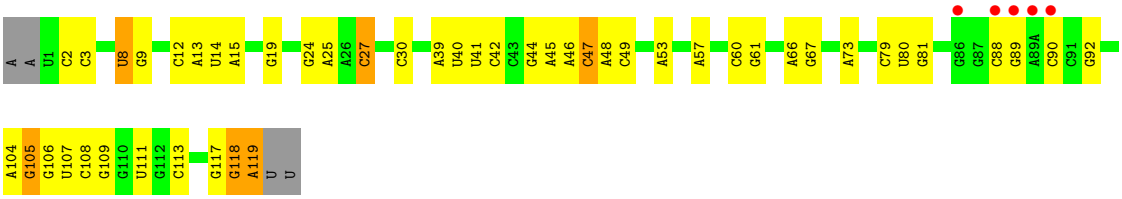


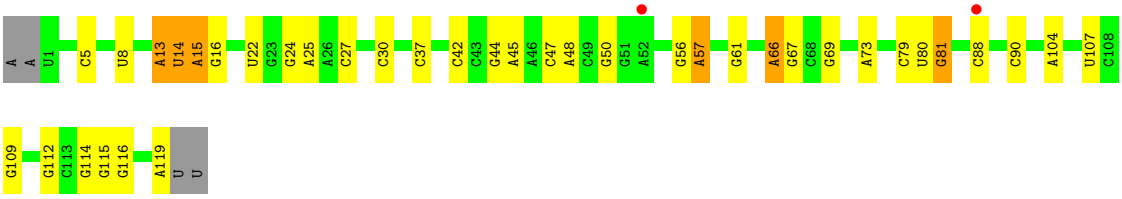
- Molecule 36: 5S rRNA

Chain RB:



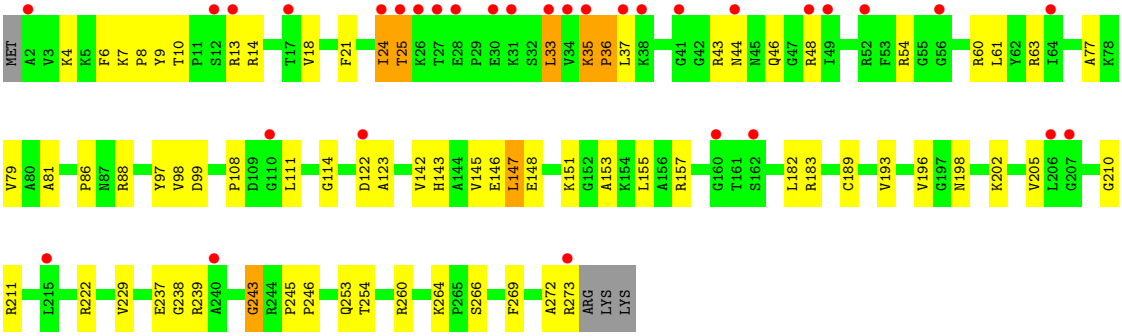
- Molecule 36: 5S rRNA

Chain YB:



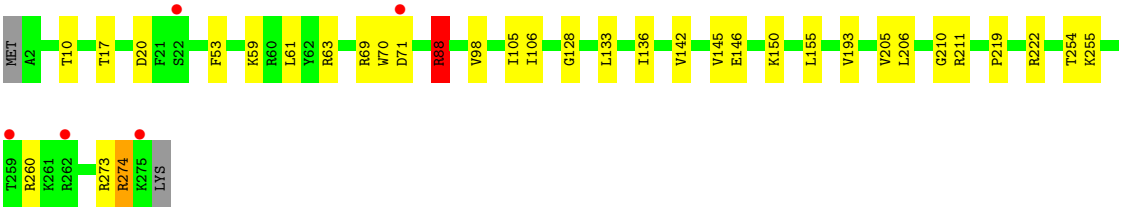
- Molecule 37: 50S ribosomal protein L2

Chain RD:



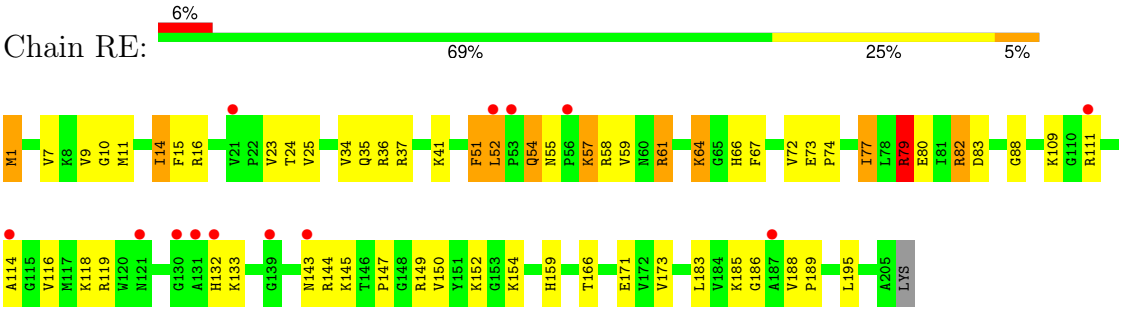
- Molecule 37: 50S ribosomal protein L2

Chain YD:



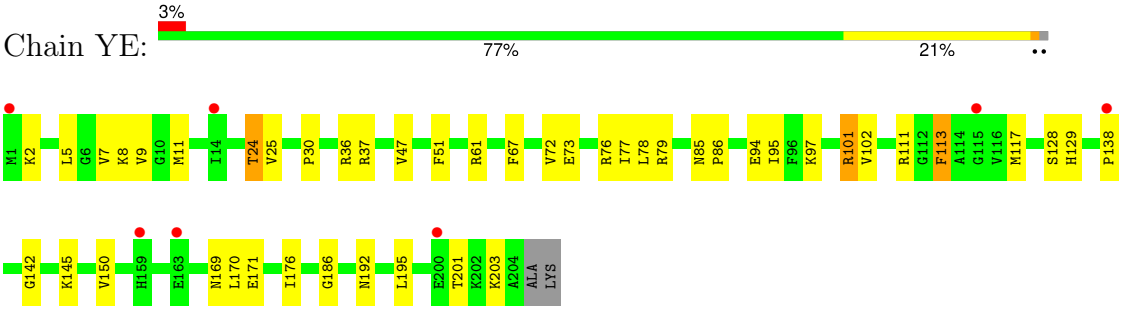
- Molecule 38: 50S ribosomal protein L3

Chain RE:



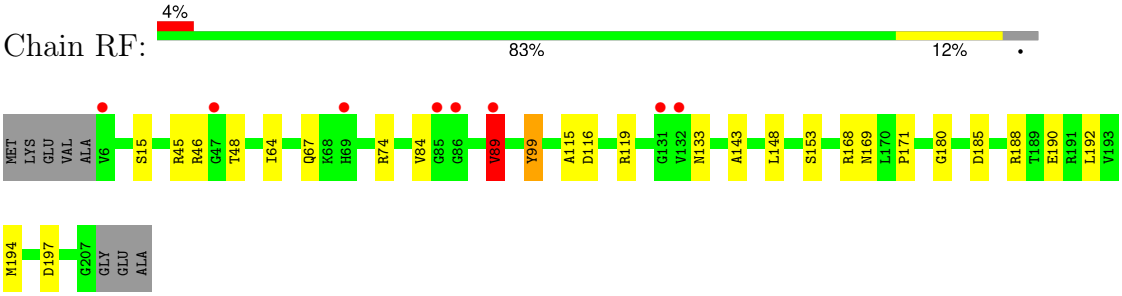
- Molecule 38: 50S ribosomal protein L3

Chain YE:



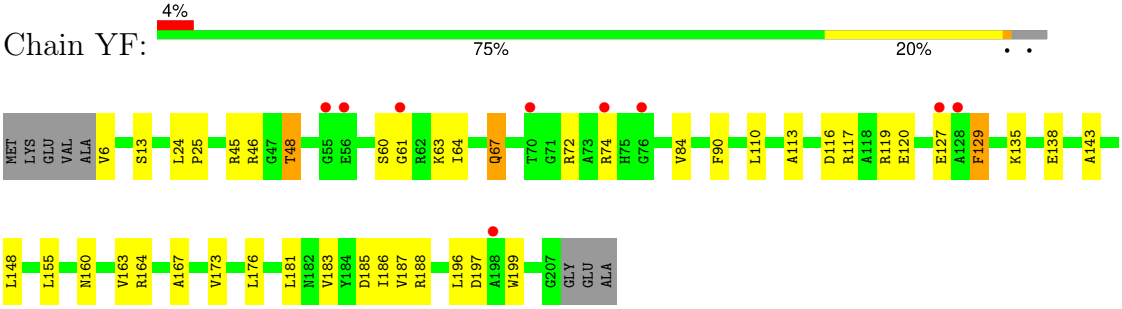
- Molecule 39: 50S ribosomal protein L4

Chain RF:



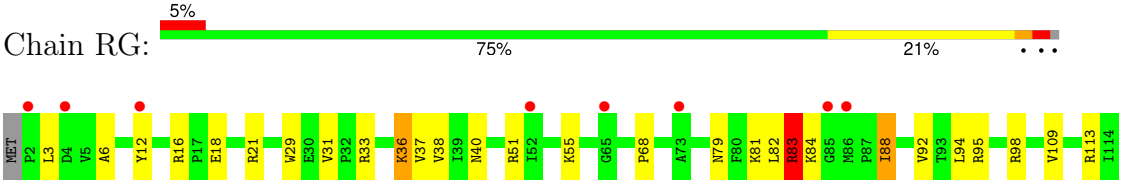
- Molecule 39: 50S ribosomal protein L4

Chain YF:



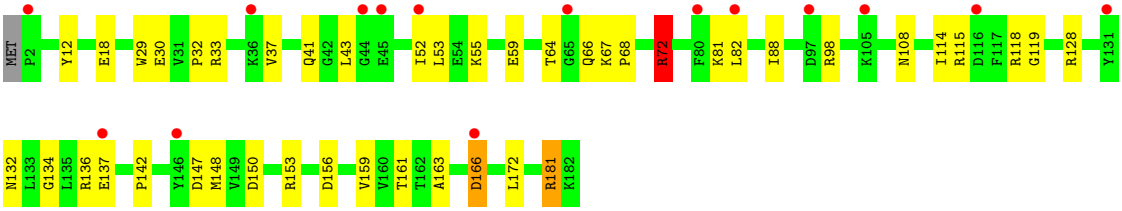
- Molecule 40: 50S ribosomal protein L5

Chain RG:



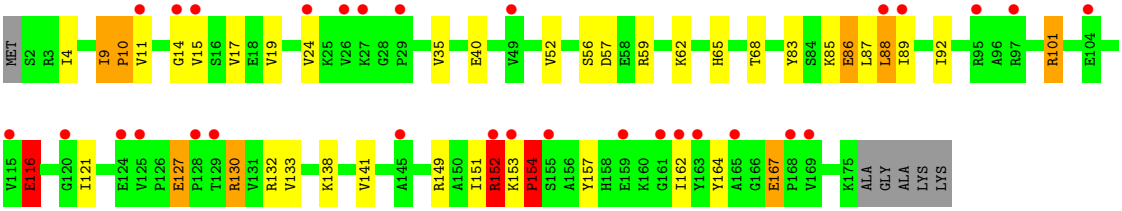
• Molecule 40: 50S ribosomal protein L5

Chain YG:



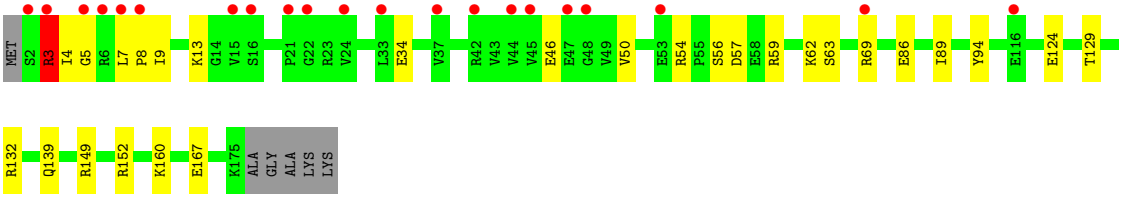
• Molecule 41: 50S ribosomal protein L6

Chain RH:



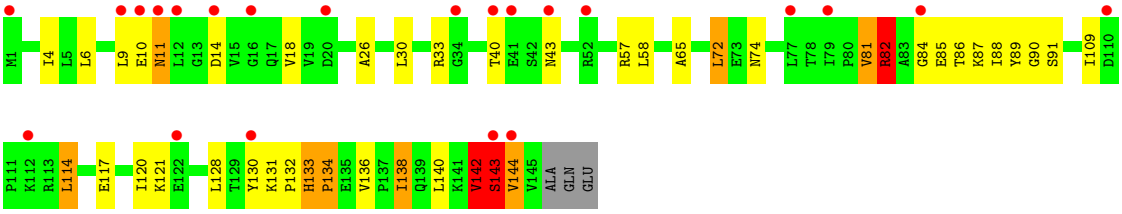
• Molecule 41: 50S ribosomal protein L6

Chain YH:



• Molecule 42: 50S ribosomal protein L9

Chain RI:

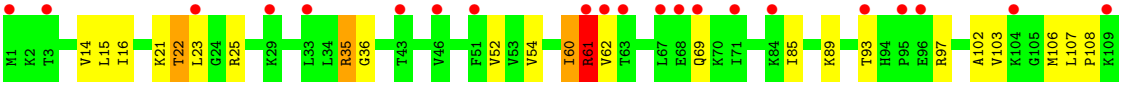


• Molecule 42: 50S ribosomal protein L9

Chain YI:

• Molecule 43: 50S ribosomal protein L13

Chain RN:

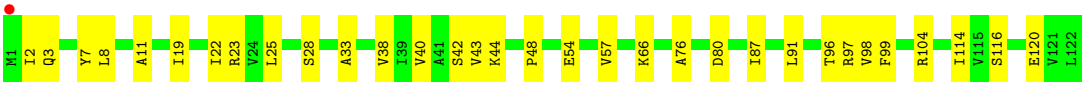


• Molecule 43: 50S ribosomal protein L13

Chain YN:

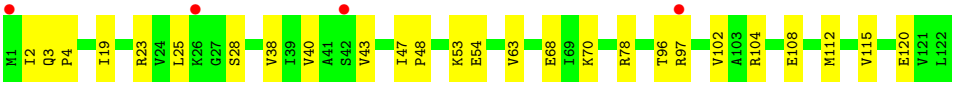
• Molecule 44: 50S ribosomal protein L14

Chain RO:



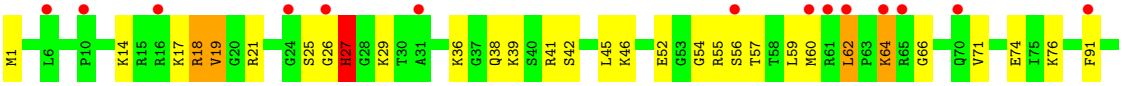
• Molecule 44: 50S ribosomal protein L14

Chain YO:



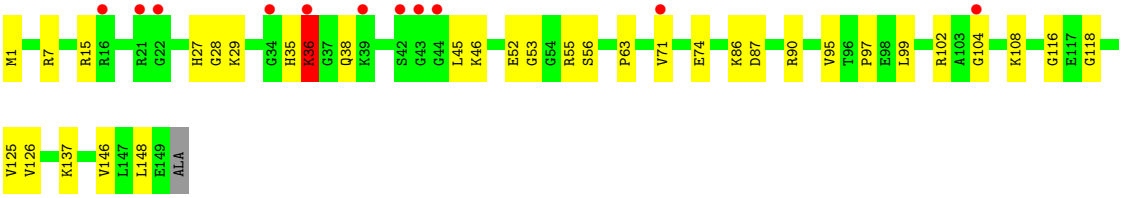
• Molecule 45: 50S ribosomal protein L15

Chain RP:



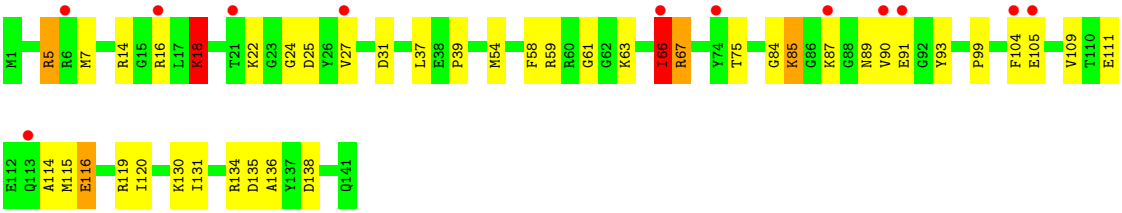
• Molecule 45: 50S ribosomal protein L15

Chain YP:



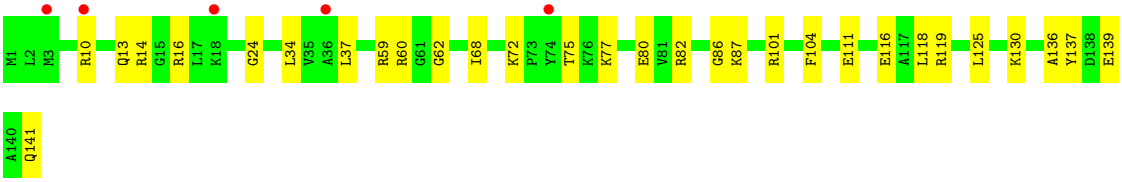
• Molecule 46: 50S ribosomal protein L16

Chain RQ:



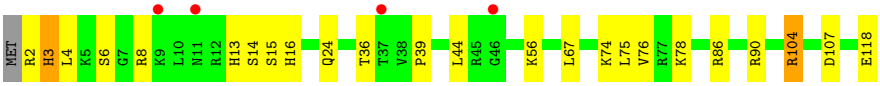
• Molecule 46: 50S ribosomal protein L16

Chain YQ:



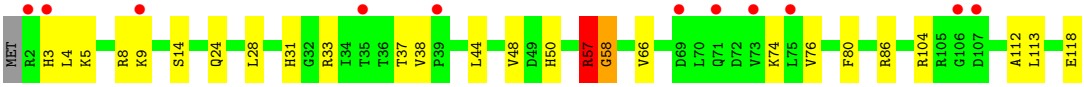
• Molecule 47: 50S ribosomal protein L17

Chain RR:



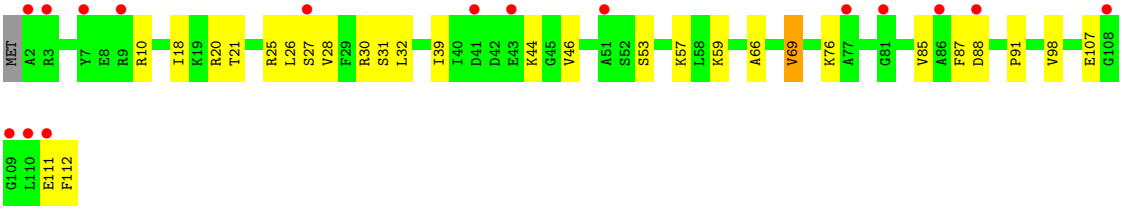
• Molecule 47: 50S ribosomal protein L17

Chain YR:



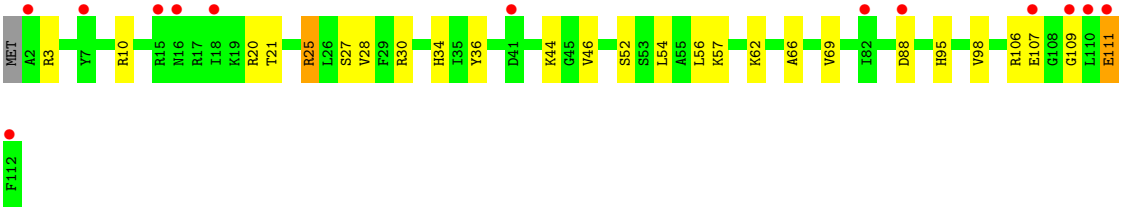
• Molecule 48: 50S ribosomal protein L18

Chain RS:



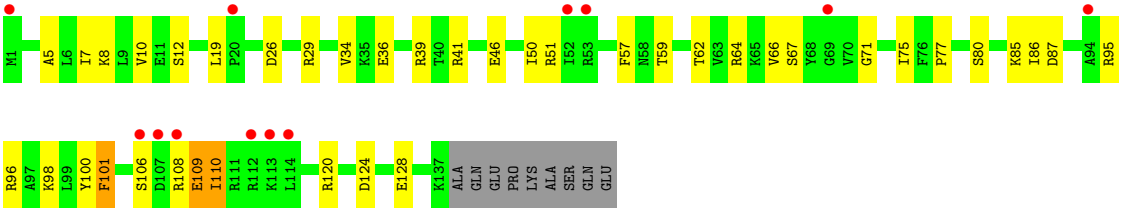
• Molecule 48: 50S ribosomal protein L18

Chain YS:



• Molecule 49: 50S ribosomal protein L19

Chain RT:

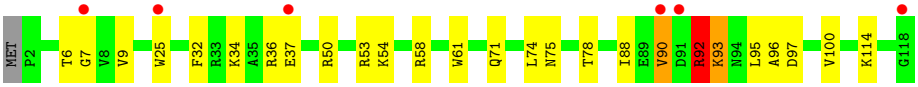


• Molecule 49: 50S ribosomal protein L19

Chain YT:

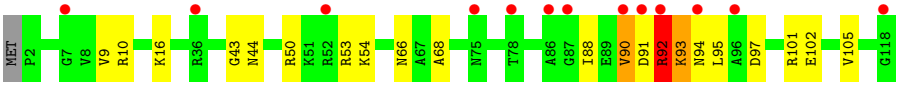
• Molecule 50: 50S ribosomal protein L20

Chain RU:



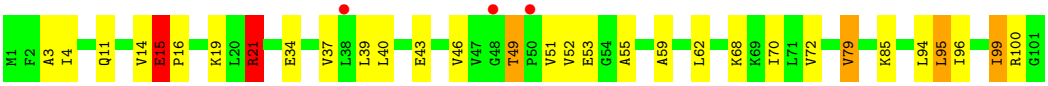
• Molecule 50: 50S ribosomal protein L20

Chain YU:



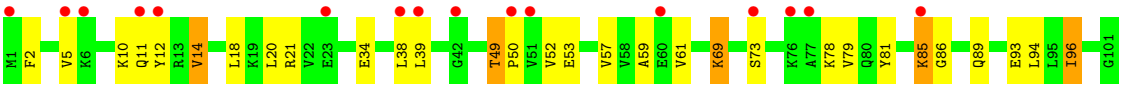
• Molecule 51: 50S ribosomal protein L21

Chain RV:



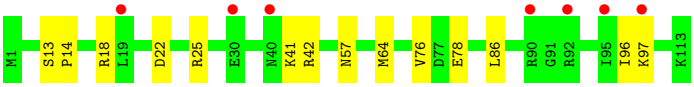
• Molecule 51: 50S ribosomal protein L21

Chain YV:



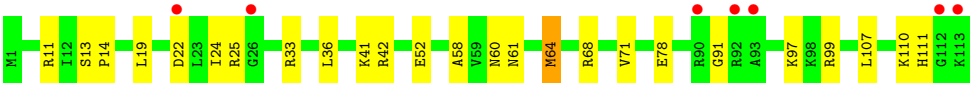
• Molecule 52: 50S ribosomal protein L22

Chain RW:



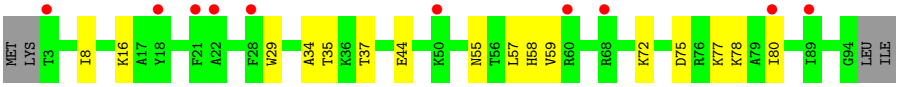
• Molecule 52: 50S ribosomal protein L22

Chain YW:



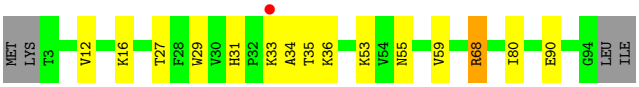
• Molecule 53: 50S ribosomal protein L23

Chain RX:



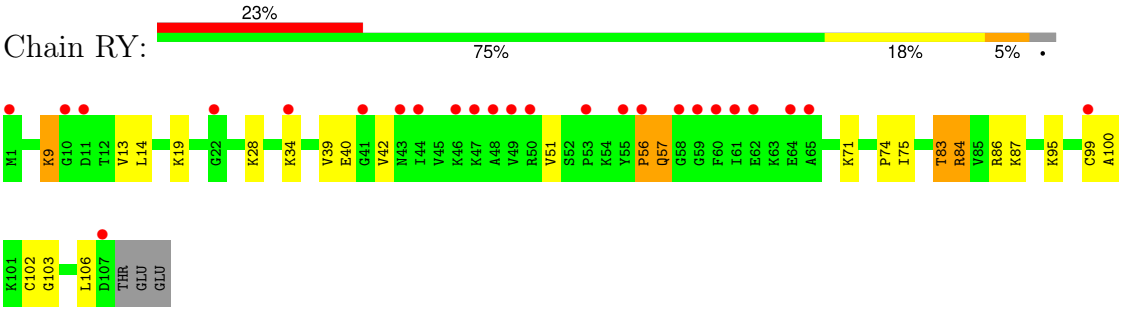
• Molecule 53: 50S ribosomal protein L23

Chain YX:



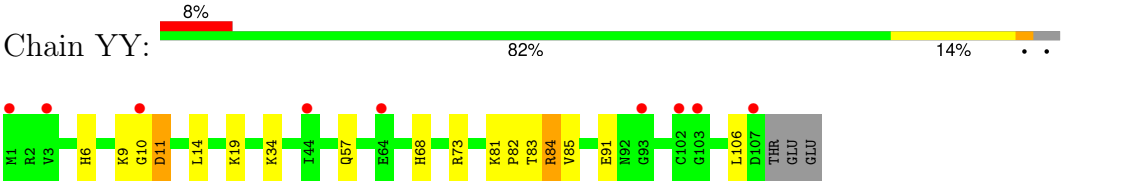
• Molecule 54: 50S ribosomal protein L24

Chain RY:



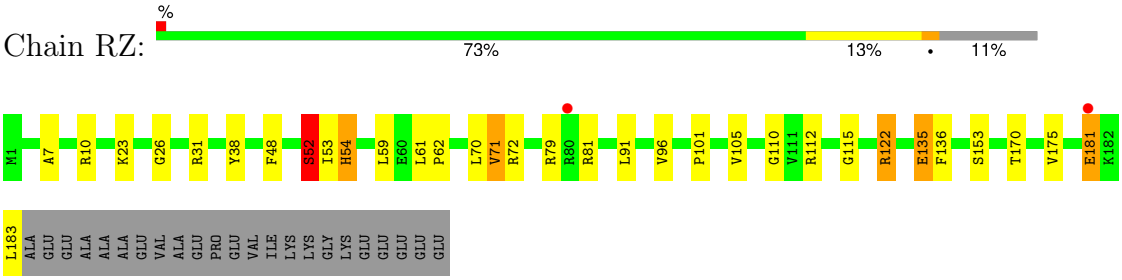
- Molecule 54: 50S ribosomal protein L24

Chain YY:



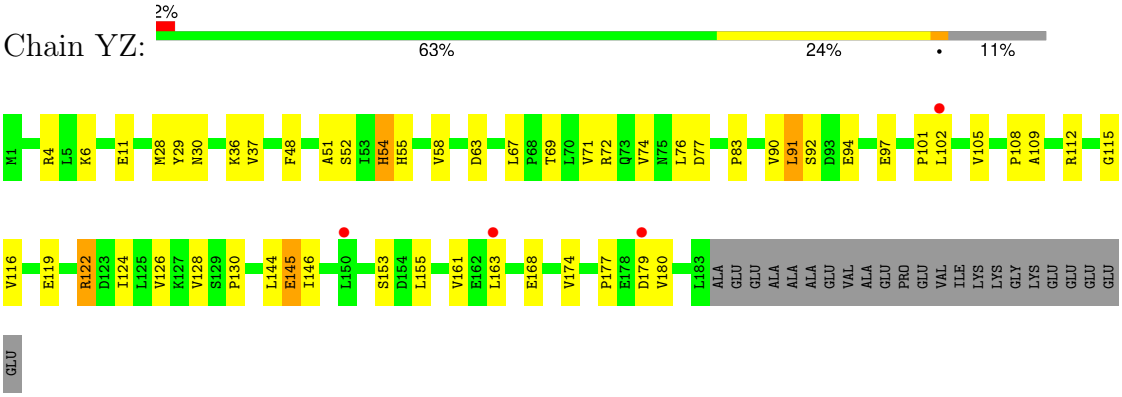
- Molecule 55: 50S ribosomal protein L25

Chain RZ:



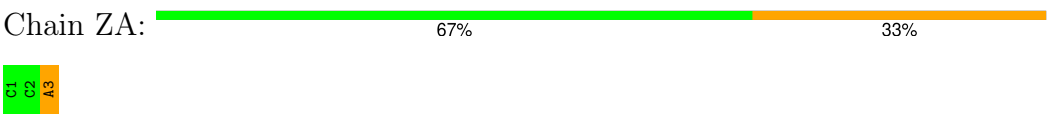
- Molecule 55: 50S ribosomal protein L25

Chain YZ:



- Molecule 56: CCPuro

Chain ZA:



- Molecule 56: CCPuro

Chain ZB:

C1 C2 A3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	214.68Å 453.51Å 609.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.72 – 3.50 146.72 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (146.72-3.50) 98.0 (146.72-3.50)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.216 , 0.246 0.218 , 0.247	Depositor DCC
R_{free} test set	33274 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å^2)	89.9	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 86.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	295153	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: A3P, MG, PPU, SF4, 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	0.43	11/56690 (0.0%)
1	XA	0.57	6/36254 (0.0%)	0.44	11/56581 (0.0%)
2	QB	0.63	6/1942 (0.3%)	1.15	21/2619 (0.8%)
2	XB	0.34	0/1950	1.07	18/2630 (0.7%)
3	QC	0.33	0/1629	1.05	12/2195 (0.5%)
3	XC	0.33	0/1629	0.97	5/2195 (0.2%)
4	QD	0.32	0/1733	1.03	13/2318 (0.6%)
4	XD	0.33	0/1733	1.12	19/2318 (0.8%)
5	QE	0.33	0/1171	0.94	3/1576 (0.2%)
5	XE	0.27	0/1171	0.88	3/1576 (0.2%)
6	QF	0.25	0/856	0.83	1/1154 (0.1%)
6	XF	0.27	0/856	0.87	2/1154 (0.2%)
7	QG	0.36	0/1276	1.10	12/1709 (0.7%)
7	XG	0.33	0/1276	0.93	5/1709 (0.3%)
8	QH	0.27	0/1128	0.99	4/1517 (0.3%)
8	XH	0.25	0/1128	0.92	6/1517 (0.4%)
9	QI	0.45	0/1029	1.20	9/1379 (0.7%)
9	XI	0.32	0/1017	1.11	12/1365 (0.9%)
10	QJ	0.42	0/814	1.12	8/1095 (0.7%)
10	XJ	0.35	0/790	1.13	9/1063 (0.8%)
11	QK	0.32	0/900	0.97	4/1213 (0.3%)
11	XK	0.32	0/879	0.98	4/1187 (0.3%)
12	QL	0.30	0/991	1.15	11/1327 (0.8%)
12	XL	0.37	0/972	1.18	15/1301 (1.2%)
13	QM	0.41	0/965	1.29	10/1292 (0.8%)
13	XM	0.35	0/956	1.17	11/1281 (0.9%)
14	QN	0.35	0/501	1.19	3/664 (0.5%)
14	XN	0.26	0/501	0.91	1/664 (0.2%)
15	QO	0.28	0/745	0.85	1/992 (0.1%)
15	XO	0.25	0/740	0.72	0/987
16	QP	0.31	0/721	1.09	6/970 (0.6%)
16	XP	0.28	0/721	1.00	4/970 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	QQ	0.30	0/847	1.04	5/1131 (0.4%)
17	XQ	0.28	0/847	0.84	1/1131 (0.1%)
18	QR	0.34	0/579	1.16	4/768 (0.5%)
18	XR	0.34	0/579	1.08	6/768 (0.8%)
19	QS	0.42	0/680	1.27	15/915 (1.6%)
19	XS	0.30	0/671	1.19	7/904 (0.8%)
20	QT	0.36	0/765	1.27	9/1007 (0.9%)
20	XT	0.35	0/765	1.16	8/1007 (0.8%)
21	QU	0.39	0/221	1.11	3/288 (1.0%)
21	XU	0.26	0/221	1.04	2/288 (0.7%)
22	QV	0.19	0/1832	0.40	0/2855
22	XV	0.19	0/1832	0.39	0/2855
23	QX	0.22	0/414	0.58	0/645
23	XX	0.19	0/414	0.48	0/645
24	QY	0.41	0/743	1.09	7/1002 (0.7%)
24	QZ	0.60	2/743 (0.3%)	1.39	11/1002 (1.1%)
24	XY	0.31	0/743	1.07	5/1002 (0.5%)
24	XZ	0.38	0/743	1.25	11/1002 (1.1%)
25	R0	0.37	0/652	1.17	5/867 (0.6%)
25	Y0	0.28	0/657	0.99	1/874 (0.1%)
26	R1	0.40	0/744	1.07	8/989 (0.8%)
26	Y1	0.36	0/770	1.01	2/1022 (0.2%)
27	R2	0.41	0/583	1.33	11/771 (1.4%)
27	Y2	0.30	0/583	0.93	0/771
28	R3	0.28	0/474	0.96	2/635 (0.3%)
28	Y3	0.31	0/474	1.02	3/635 (0.5%)
29	R4	0.59	0/578	1.59	15/776 (1.9%)
29	Y4	0.37	0/578	1.29	6/776 (0.8%)
30	R5	0.32	0/473	0.92	2/639 (0.3%)
30	Y5	0.39	0/473	1.02	1/639 (0.2%)
31	R6	0.32	0/460	1.18	5/613 (0.8%)
31	Y6	0.33	0/460	0.99	1/613 (0.2%)
32	R7	0.27	0/417	0.84	1/550 (0.2%)
32	Y7	0.29	0/426	0.88	2/561 (0.4%)
33	R8	0.48	0/525	1.28	8/691 (1.2%)
33	Y8	0.50	0/525	1.11	6/691 (0.9%)
34	R9	0.41	0/310	1.10	3/407 (0.7%)
34	Y9	0.32	0/310	1.15	2/407 (0.5%)
35	RA	0.21	0/69739	0.44	8/108870 (0.0%)
35	YA	0.21	0/69419	0.44	9/108369 (0.0%)
36	RB	0.23	0/2881	0.45	1/4494 (0.0%)
36	YB	0.28	0/2881	0.47	1/4494 (0.0%)
37	RD	0.35	0/2165	1.27	25/2919 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
37	YD	0.29	0/2185	1.01	11/2944 (0.4%)
38	RE	0.45	0/1601	1.24	20/2160 (0.9%)
38	YE	0.35	0/1592	1.16	14/2149 (0.7%)
39	RF	0.27	0/1620	0.94	9/2194 (0.4%)
39	YF	0.31	0/1620	1.06	9/2194 (0.4%)
40	RG	0.35	0/1499	1.21	21/2016 (1.0%)
40	YG	0.48	3/1499 (0.2%)	1.13	13/2016 (0.6%)
41	RH	0.44	0/1362	1.48	40/1841 (2.2%)
41	YH	0.35	0/1356	0.96	5/1834 (0.3%)
42	RI	2.65	3/1146 (0.3%)	1.65	31/1551 (2.0%)
42	YI	0.44	0/1151	1.26	20/1558 (1.3%)
43	RN	0.41	0/1131	1.17	10/1525 (0.7%)
43	YN	0.28	0/1131	1.05	10/1525 (0.7%)
44	RO	0.26	0/943	0.96	6/1269 (0.5%)
44	YO	0.29	0/943	0.96	3/1269 (0.2%)
45	RP	0.43	0/1162	1.34	20/1544 (1.3%)
45	YP	0.31	0/1152	1.13	12/1533 (0.8%)
46	RQ	0.46	0/1143	1.19	11/1527 (0.7%)
46	YQ	0.27	0/1143	1.04	6/1527 (0.4%)
47	RR	0.30	0/974	1.20	6/1302 (0.5%)
47	YR	0.35	0/974	1.09	13/1302 (1.0%)
48	RS	0.36	0/892	1.21	7/1187 (0.6%)
48	YS	0.40	0/892	1.21	9/1187 (0.8%)
49	RT	0.41	0/1155	1.16	6/1542 (0.4%)
49	YT	0.41	0/1155	1.16	14/1542 (0.9%)
50	RU	0.34	0/982	1.08	9/1306 (0.7%)
50	YU	0.33	0/982	0.96	5/1306 (0.4%)
51	RV	0.59	1/790 (0.1%)	1.24	6/1057 (0.6%)
51	YV	1.29	6/790 (0.8%)	1.34	10/1057 (0.9%)
52	RW	0.28	0/911	0.96	2/1220 (0.2%)
52	YW	0.28	0/911	0.91	2/1220 (0.2%)
53	RX	0.27	0/739	0.94	2/993 (0.2%)
53	YX	0.31	0/739	0.92	2/993 (0.2%)
54	RY	0.33	0/831	1.10	11/1108 (1.0%)
54	YY	0.29	0/831	1.11	12/1108 (1.1%)
55	RZ	0.37	0/1493	1.15	17/2026 (0.8%)
55	YZ	0.30	0/1493	1.08	13/2026 (0.6%)
56	ZA	0.28	0/40	0.52	0/60
56	ZB	0.27	0/40	0.47	0/60
All	All	0.36	27/319487 (0.0%)	0.69	893/477274 (0.2%)

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
7	XG	0	1
8	XH	0	1
10	QJ	0	1
11	XK	0	1
24	QZ	0	1
37	RD	0	2
37	YD	0	1
38	RE	0	1
40	RG	0	2
40	YG	0	1
41	RH	0	2
41	YH	0	1
42	RI	0	4
47	RR	0	1
47	YR	0	1
51	RV	0	1
All	All	0	23

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	RI	82	ARG	CZ-NH1	87.21	2.54	1.32
1	XA	368	U	N3-C4	47.56	2.33	1.38
1	XA	368	U	C2-N3	46.00	2.29	1.37
1	XA	368	U	N1-C2	41.62	2.21	1.38
1	XA	368	U	N1-C6	40.83	2.19	1.38

The worst 5 of 893 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	RR	76	VAL	N-CA-C	-19.67	93.29	112.96
37	RD	35	LYS	N-CA-C	-17.68	92.31	108.22
42	RI	11	ASN	CA-C-N	15.29	149.12	122.67
42	RI	11	ASN	C-N-CA	15.29	149.12	122.67
48	RS	107	GLU	N-CA-C	-15.26	92.38	112.68

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	12	GLU	Sidechain
10	QJ	79	ARG	Sidechain
24	QZ	50	HIS	Peptide
37	RD	33	LEU	Peptide
37	RD	35	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	16383	245	0
1	XA	32389	0	16350	221	0
2	QB	1907	0	1958	31	0
2	XB	1915	0	1969	27	0
3	QC	1605	0	1668	13	0
3	XC	1605	0	1668	17	0
4	QD	1703	0	1767	32	0
4	XD	1703	0	1767	24	0
5	QE	1155	0	1213	12	0
5	XE	1155	0	1213	15	0
6	QF	843	0	857	13	0
6	XF	843	0	857	10	0
7	QG	1257	0	1296	10	0
7	XG	1257	0	1296	17	0
8	QH	1108	0	1165	21	0
8	XH	1108	0	1165	13	0
9	QI	1010	0	1037	17	0
9	XI	998	0	1024	20	0
10	QJ	801	0	849	11	0
10	XJ	777	0	816	18	0
11	QK	885	0	904	12	0
11	XK	864	0	881	9	0
12	QL	975	0	1062	11	0
12	XL	956	0	1046	13	0
13	QM	955	0	1021	27	0
13	XM	946	0	1008	16	0
14	QN	492	0	529	5	0
14	XN	492	0	529	12	0
15	QO	734	0	771	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	XO	729	0	768	4	0
16	QP	705	0	725	12	0
16	XP	705	0	725	6	0
17	QQ	834	0	904	9	0
17	XQ	834	0	904	12	0
18	QR	574	0	644	9	0
18	XR	574	0	644	12	0
19	QS	665	0	686	15	0
19	XS	656	0	666	9	0
20	QT	763	0	861	9	0
20	XT	763	0	861	15	0
21	QU	217	0	234	5	0
21	XU	217	0	234	7	0
22	QV	1640	0	837	4	0
22	XV	1640	0	837	3	0
23	QX	394	0	196	2	0
23	XX	394	0	196	4	0
24	QY	723	0	713	11	0
24	QZ	723	0	713	11	0
24	XY	723	0	713	9	0
24	XZ	723	0	713	7	0
25	R0	643	0	667	13	0
25	Y0	648	0	672	15	0
26	R1	737	0	813	6	0
26	Y1	763	0	848	18	0
27	R2	581	0	629	8	0
27	Y2	581	0	629	4	0
28	R3	469	0	518	5	0
28	Y3	469	0	518	5	0
29	R4	565	0	561	26	0
29	Y4	565	0	559	10	0
30	R5	459	0	476	11	0
30	Y5	459	0	480	6	0
31	R6	453	0	474	10	0
31	Y6	453	0	474	4	0
32	R7	409	0	454	3	0
32	Y7	418	0	467	6	0
33	R8	517	0	582	11	0
33	Y8	517	0	582	12	0
34	R9	307	0	337	10	0
34	Y9	307	0	336	5	0
35	RA	62266	0	31392	354	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	YA	61981	0	31243	341	0
36	RB	2576	0	1303	28	0
36	YB	2576	0	1305	19	0
37	RD	2115	0	2195	39	0
37	YD	2135	0	2221	19	0
38	RE	1568	0	1634	38	0
38	YE	1559	0	1617	25	0
39	RF	1585	0	1632	15	0
39	YF	1585	0	1632	25	0
40	RG	1474	0	1535	23	0
40	YG	1474	0	1535	20	0
41	RH	1336	0	1418	12	0
41	YH	1330	0	1407	18	0
42	RI	1131	0	1218	16	0
42	YI	1136	0	1223	9	0
43	RN	1104	0	1180	17	0
43	YN	1104	0	1180	15	0
44	RO	933	0	996	17	0
44	YO	933	0	996	16	0
45	RP	1145	0	1228	29	0
45	YP	1135	0	1212	17	0
46	RQ	1122	0	1179	27	0
46	YQ	1122	0	1179	20	0
47	RR	960	0	1021	12	0
47	YR	960	0	1021	11	0
48	RS	882	0	943	14	0
48	YS	882	0	943	15	0
49	RT	1141	0	1202	21	0
49	YT	1141	0	1202	14	0
50	RU	964	0	1022	19	0
50	YU	964	0	1022	22	0
51	RV	779	0	852	16	0
51	YV	779	0	852	26	0
52	RW	900	0	964	8	0
52	YW	900	0	964	16	0
53	RX	725	0	778	11	0
53	YX	725	0	778	8	0
54	RY	818	0	913	12	0
54	YY	818	0	913	5	0
55	RZ	1461	0	1493	17	0
55	YZ	1461	0	1493	27	0
56	ZA	74	0	51	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	ZB	74	0	51	7	0
57	QA	93	0	0	0	0
57	QD	1	0	0	0	0
57	QE	1	0	0	0	0
57	QV	3	0	0	0	0
57	QY	1	0	0	0	0
57	R0	2	0	0	0	0
57	R3	1	0	0	0	0
57	RA	302	0	0	0	0
57	RB	3	0	0	0	0
57	RD	2	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	1	0	0	0	0
57	RQ	4	0	0	0	0
57	RR	1	0	0	0	0
57	RY	1	0	0	0	0
57	XA	99	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	4	0	0	0	0
57	Y0	2	0	0	0	0
57	Y1	1	0	0	0	0
57	Y3	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YA	335	0	0	0	0
57	YB	3	0	0	0	0
57	YD	4	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	YP	1	0	0	0	0
57	YQ	5	0	0	0	0
57	YR	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
All	All	295153	0	201057	2224	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 5.

The worst 5 of 2224 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)
51:YV:85:LYS:CG	51:YV:85:LYS:CD	1.86	1.53
51:YV:85:LYS:CG	51:YV:85:LYS:CB	1.82	1.50
1:XA:368:U:C5	1:XA:368:U:C6	2.05	1.45
51:YV:85:LYS:NZ	51:YV:85:LYS:CE	1.87	1.36
51:YV:85:LYS:CD	51:YV:85:LYS:CE	2.10	1.30

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%)	202 (87%)	27 (12%)	4 (2%)	7 35
2	XB	234/256 (91%)	211 (90%)	21 (9%)	2 (1%)	14 47
3	QC	203/239 (85%)	186 (92%)	17 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	XC	203/239 (85%)	188 (93%)	14 (7%)	1 (0%)	24	57
4	QD	206/209 (99%)	193 (94%)	11 (5%)	2 (1%)	12	44
4	XD	206/209 (99%)	187 (91%)	17 (8%)	2 (1%)	12	44
5	QE	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
5	XE	149/162 (92%)	142 (95%)	7 (5%)	0	100	100
6	QF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
6	XF	99/101 (98%)	99 (100%)	0	0	100	100
7	QG	153/156 (98%)	144 (94%)	8 (5%)	1 (1%)	18	51
7	XG	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
8	QH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
8	XH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
9	QI	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
9	XI	124/128 (97%)	113 (91%)	11 (9%)	0	100	100
10	QJ	97/105 (92%)	85 (88%)	12 (12%)	0	100	100
10	XJ	94/105 (90%)	80 (85%)	13 (14%)	1 (1%)	11	43
11	QK	117/129 (91%)	107 (92%)	10 (8%)	0	100	100
11	XK	114/129 (88%)	105 (92%)	9 (8%)	0	100	100
12	QL	123/132 (93%)	110 (89%)	11 (9%)	2 (2%)	7	36
12	XL	120/132 (91%)	103 (86%)	16 (13%)	1 (1%)	16	49
13	QM	118/126 (94%)	102 (86%)	13 (11%)	3 (2%)	4	28
13	XM	117/126 (93%)	96 (82%)	21 (18%)	0	100	100
14	QN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	35
14	XN	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7	35
15	QO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	XO	85/89 (96%)	84 (99%)	1 (1%)	0	100	100
16	QP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
17	XQ	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	QR	68/88 (77%)	64 (94%)	4 (6%)	0	100	100
18	XR	68/88 (77%)	64 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	QS	81/93 (87%)	69 (85%)	11 (14%)	1 (1%)	10	41
19	XS	81/93 (87%)	75 (93%)	6 (7%)	0	100	100
20	QT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
20	XT	97/106 (92%)	88 (91%)	6 (6%)	3 (3%)	3	25
21	QU	23/27 (85%)	20 (87%)	2 (9%)	1 (4%)	2	18
21	XU	23/27 (85%)	22 (96%)	0	1 (4%)	2	18
24	QY	82/84 (98%)	70 (85%)	10 (12%)	2 (2%)	4	29
24	QZ	82/84 (98%)	72 (88%)	10 (12%)	0	100	100
24	XY	82/84 (98%)	71 (87%)	8 (10%)	3 (4%)	2	21
24	XZ	82/84 (98%)	70 (85%)	11 (13%)	1 (1%)	10	41
25	R0	79/85 (93%)	72 (91%)	6 (8%)	1 (1%)	9	39
25	Y0	80/85 (94%)	72 (90%)	8 (10%)	0	100	100
26	R1	92/98 (94%)	82 (89%)	10 (11%)	0	100	100
26	Y1	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11	43
27	R2	67/72 (93%)	61 (91%)	5 (8%)	1 (2%)	8	37
27	Y2	67/72 (93%)	63 (94%)	2 (3%)	2 (3%)	3	25
28	R3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
28	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
29	R4	67/71 (94%)	46 (69%)	17 (25%)	4 (6%)	1	12
29	Y4	67/71 (94%)	54 (81%)	12 (18%)	1 (2%)	8	37
30	R5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
30	Y5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
31	R6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
31	Y6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
32	R7	45/49 (92%)	45 (100%)	0	0	100	100
32	Y7	46/49 (94%)	46 (100%)	0	0	100	100
33	R8	62/65 (95%)	54 (87%)	6 (10%)	2 (3%)	3	24
33	Y8	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	3	24
34	R9	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
34	Y9	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
37	RD	270/276 (98%)	244 (90%)	22 (8%)	4 (2%)	8	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	YD	272/276 (99%)	263 (97%)	9 (3%)	0	100	100
38	RE	203/206 (98%)	179 (88%)	20 (10%)	4 (2%)	6	32
38	YE	202/206 (98%)	191 (95%)	9 (4%)	2 (1%)	12	44
39	RF	200/210 (95%)	195 (98%)	5 (2%)	0	100	100
39	YF	200/210 (95%)	184 (92%)	14 (7%)	2 (1%)	12	44
40	RG	179/182 (98%)	152 (85%)	24 (13%)	3 (2%)	7	35
40	YG	179/182 (98%)	151 (84%)	26 (14%)	2 (1%)	11	43
41	RH	172/180 (96%)	137 (80%)	29 (17%)	6 (4%)	3	23
41	YH	172/180 (96%)	164 (95%)	8 (5%)	0	100	100
42	RI	143/148 (97%)	117 (82%)	20 (14%)	6 (4%)	2	19
42	YI	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	9	38
43	RN	136/140 (97%)	117 (86%)	17 (12%)	2 (2%)	8	37
43	YN	136/140 (97%)	118 (87%)	16 (12%)	2 (2%)	8	37
44	RO	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
44	YO	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	16	49
45	RP	148/150 (99%)	125 (84%)	19 (13%)	4 (3%)	4	27
45	YP	147/150 (98%)	138 (94%)	7 (5%)	2 (1%)	9	38
46	RQ	139/141 (99%)	121 (87%)	13 (9%)	5 (4%)	2	22
46	YQ	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
47	RR	115/118 (98%)	108 (94%)	6 (5%)	1 (1%)	14	47
47	YR	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	14	47
48	RS	109/112 (97%)	93 (85%)	15 (14%)	1 (1%)	14	47
48	YS	109/112 (97%)	93 (85%)	16 (15%)	0	100	100
49	RT	135/146 (92%)	119 (88%)	15 (11%)	1 (1%)	18	51
49	YT	135/146 (92%)	119 (88%)	16 (12%)	0	100	100
50	RU	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	14	47
50	YU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	47
51	RV	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
51	YV	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	12	44
52	RW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
52	YW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	RX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
53	YX	90/96 (94%)	86 (96%)	3 (3%)	1 (1%)	11	43
54	RY	105/110 (96%)	94 (90%)	11 (10%)	0	100	100
54	YY	105/110 (96%)	101 (96%)	3 (3%)	1 (1%)	12	44
55	RZ	181/206 (88%)	166 (92%)	13 (7%)	2 (1%)	11	43
55	YZ	181/206 (88%)	168 (93%)	13 (7%)	0	100	100
All	All	11789/12464 (95%)	10734 (91%)	950 (8%)	105 (1%)	14	47

5 of 105 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	208	ILE
14	QN	17	LYS
21	QU	3	LYS
24	QY	82	TYR
27	R2	47	ASN

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%)	196 (97%)	7 (3%)	32	57
2	XB	204/220 (93%)	201 (98%)	3 (2%)	57	71
3	QC	159/188 (85%)	155 (98%)	4 (2%)	42	63
3	XC	159/188 (85%)	156 (98%)	3 (2%)	50	68
4	QD	180/181 (99%)	175 (97%)	5 (3%)	38	61
4	XD	180/181 (99%)	180 (100%)	0	100	100
5	QE	116/123 (94%)	115 (99%)	1 (1%)	70	76
5	XE	116/123 (94%)	115 (99%)	1 (1%)	70	76
6	QF	90/90 (100%)	89 (99%)	1 (1%)	65	74
6	XF	90/90 (100%)	89 (99%)	1 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	QG	126/127 (99%)	123 (98%)	3 (2%)	43	64
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	77
9	QI	98/99 (99%)	93 (95%)	5 (5%)	21	48
9	XI	97/99 (98%)	95 (98%)	2 (2%)	47	66
10	QJ	89/92 (97%)	84 (94%)	5 (6%)	19	46
10	XJ	86/92 (94%)	85 (99%)	1 (1%)	63	73
11	QK	90/99 (91%)	88 (98%)	2 (2%)	45	65
11	XK	88/99 (89%)	87 (99%)	1 (1%)	65	74
12	QL	104/109 (95%)	103 (99%)	1 (1%)	68	75
12	XL	103/109 (94%)	102 (99%)	1 (1%)	68	75
13	QM	96/101 (95%)	95 (99%)	1 (1%)	68	75
13	XM	95/101 (94%)	93 (98%)	2 (2%)	47	66
14	QN	49/50 (98%)	48 (98%)	1 (2%)	48	67
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	70 (97%)	2 (3%)	38	61
17	QQ	95/97 (98%)	94 (99%)	1 (1%)	65	74
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	58 (95%)	3 (5%)	22	48
18	XR	61/77 (79%)	60 (98%)	1 (2%)	55	70
19	QS	72/80 (90%)	70 (97%)	2 (3%)	38	61
19	XS	69/80 (86%)	69 (100%)	0	100	100
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	74 (97%)	2 (3%)	40	62
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
24	QY	78/78 (100%)	76 (97%)	2 (3%)	40	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	QZ	78/78 (100%)	74 (95%)	4 (5%)	21	48
24	XY	78/78 (100%)	78 (100%)	0	100	100
24	XZ	78/78 (100%)	76 (97%)	2 (3%)	40	62
25	R0	65/67 (97%)	65 (100%)	0	100	100
25	Y0	65/67 (97%)	63 (97%)	2 (3%)	35	59
26	R1	79/83 (95%)	77 (98%)	2 (2%)	42	63
26	Y1	82/83 (99%)	81 (99%)	1 (1%)	63	73
27	R2	64/67 (96%)	62 (97%)	2 (3%)	35	59
27	Y2	64/67 (96%)	63 (98%)	1 (2%)	55	70
28	R3	51/52 (98%)	50 (98%)	1 (2%)	48	67
28	Y3	51/52 (98%)	51 (100%)	0	100	100
29	R4	62/63 (98%)	54 (87%)	8 (13%)	4	21
29	Y4	62/63 (98%)	60 (97%)	2 (3%)	34	59
30	R5	51/52 (98%)	51 (100%)	0	100	100
30	Y5	51/52 (98%)	51 (100%)	0	100	100
31	R6	51/52 (98%)	48 (94%)	3 (6%)	18	44
31	Y6	51/52 (98%)	49 (96%)	2 (4%)	28	54
32	R7	40/42 (95%)	40 (100%)	0	100	100
32	Y7	41/42 (98%)	41 (100%)	0	100	100
33	R8	54/55 (98%)	50 (93%)	4 (7%)	13	37
33	Y8	54/55 (98%)	52 (96%)	2 (4%)	30	56
34	R9	34/34 (100%)	33 (97%)	1 (3%)	37	60
34	Y9	34/34 (100%)	34 (100%)	0	100	100
37	RD	214/218 (98%)	210 (98%)	4 (2%)	50	68
37	YD	216/218 (99%)	215 (100%)	1 (0%)	81	80
38	RE	165/166 (99%)	157 (95%)	8 (5%)	23	49
38	YE	164/166 (99%)	163 (99%)	1 (1%)	78	79
39	RF	161/166 (97%)	159 (99%)	2 (1%)	63	73
39	YF	161/166 (97%)	160 (99%)	1 (1%)	78	79
40	RG	155/156 (99%)	151 (97%)	4 (3%)	40	62
40	YG	155/156 (99%)	153 (99%)	2 (1%)	61	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	RH	145/148 (98%)	142 (98%)	3 (2%)	47	66
41	YH	144/148 (97%)	141 (98%)	3 (2%)	47	66
42	RI	122/124 (98%)	116 (95%)	6 (5%)	22	48
42	YI	122/124 (98%)	119 (98%)	3 (2%)	42	63
43	RN	117/119 (98%)	116 (99%)	1 (1%)	70	76
43	YN	117/119 (98%)	116 (99%)	1 (1%)	70	76
44	RO	100/100 (100%)	100 (100%)	0	100	100
44	YO	100/100 (100%)	99 (99%)	1 (1%)	68	75
45	RP	116/116 (100%)	114 (98%)	2 (2%)	53	70
45	YP	115/116 (99%)	113 (98%)	2 (2%)	53	70
46	RQ	111/111 (100%)	106 (96%)	5 (4%)	24	50
46	YQ	111/111 (100%)	111 (100%)	0	100	100
47	RR	100/101 (99%)	99 (99%)	1 (1%)	68	75
47	YR	100/101 (99%)	99 (99%)	1 (1%)	68	75
48	RS	87/88 (99%)	84 (97%)	3 (3%)	32	57
48	YS	87/88 (99%)	86 (99%)	1 (1%)	65	74
49	RT	120/127 (94%)	115 (96%)	5 (4%)	26	52
49	YT	120/127 (94%)	117 (98%)	3 (2%)	42	63
50	RU	93/94 (99%)	92 (99%)	1 (1%)	65	74
50	YU	93/94 (99%)	91 (98%)	2 (2%)	45	65
51	RV	82/82 (100%)	73 (89%)	9 (11%)	6	26
51	YV	82/82 (100%)	80 (98%)	2 (2%)	43	64
52	RW	92/92 (100%)	92 (100%)	0	100	100
52	YW	92/92 (100%)	90 (98%)	2 (2%)	45	65
53	RX	74/78 (95%)	74 (100%)	0	100	100
53	YX	74/78 (95%)	73 (99%)	1 (1%)	59	71
54	RY	88/91 (97%)	88 (100%)	0	100	100
54	YY	88/91 (97%)	88 (100%)	0	100	100
55	RZ	162/179 (90%)	161 (99%)	1 (1%)	78	79
55	YZ	162/179 (90%)	159 (98%)	3 (2%)	50	68
All	All	10001/10378 (96%)	9812 (98%)	189 (2%)	50	68

5 of 189 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
51	RV	21	ARG
16	XP	32	TYR
51	RV	72	VAL
5	XE	155	GLU
25	Y0	82	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
48	RS	61	ASN
7	XG	109	ASN
46	YQ	57	HIS
49	RT	90	GLN
53	RX	55	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1508/1521 (99%)	293 (19%)	33 (2%)
1	XA	1505/1521 (98%)	302 (20%)	40 (2%)
22	QV	77/77 (100%)	8 (10%)	1 (1%)
22	XV	77/77 (100%)	9 (11%)	1 (1%)
23	QX	16/20 (80%)	7 (43%)	2 (12%)
23	XX	16/20 (80%)	8 (50%)	0
35	RA	2888/2915 (99%)	623 (21%)	37 (1%)
35	YA	2875/2915 (98%)	579 (20%)	28 (0%)
36	RB	119/124 (95%)	24 (20%)	1 (0%)
36	YB	119/124 (95%)	17 (14%)	1 (0%)
56	ZA	1/3 (33%)	0	0
56	ZB	1/3 (33%)	0	0
All	All	9202/9320 (98%)	1870 (20%)	144 (1%)

5 of 1870 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	4	U
1	QA	5	U
1	QA	6	G
1	QA	22	G
1	QA	32	A

5 of 144 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	YA	119	A
36	YB	66	A
35	YA	752	A
35	YA	2144	U
35	RA	1022	G

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

4 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	$\#\|Z\| > 2$
56	PPU	ZB	3	56,35	37,40,41	1.24	5 (13%)	47,57,60	2.40	19 (40%)
23	A3P	XX	20	23	25,28,29	3.32	8 (32%)	37,42,45	2.12	9 (24%)
23	A3P	QX	20	23	25,28,29	3.31	9 (36%)	37,42,45	2.18	11 (29%)
56	PPU	ZA	3	56,35	37,40,41	1.25	6 (16%)	47,57,60	2.29	14 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PPU	ZB	3	56,35	-	13/25/43/44	0/4/4/4
23	A3P	XX	20	23	-	1/12/30/31	0/3/3/3
23	A3P	QX	20	23	-	3/12/30/31	0/3/3/3
56	PPU	ZA	3	56,35	-	6/25/43/44	0/4/4/4

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	QX	20	A3P	O4'-C1'	11.03	1.67	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	XX	20	A3P	O4'-C1'	10.74	1.66	1.42
23	XX	20	A3P	C2'-C1'	-6.54	1.32	1.53
23	QX	20	A3P	C2'-C1'	-6.40	1.33	1.53
23	XX	20	A3P	O4'-C4'	-5.95	1.31	1.45

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	QX	20	A3P	C5-C4-N3	-6.47	117.81	126.72
56	ZB	3	PPU	C5-C4-N3	-6.28	118.07	126.72
23	XX	20	A3P	C5-C4-N3	-6.07	118.35	126.72
56	ZA	3	PPU	C5-C4-N3	-6.05	118.39	126.72
23	XX	20	A3P	N3-C2-N1	-5.02	120.98	128.58

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	ZA	3	PPU	N-CA-CB-CG
56	ZA	3	PPU	C-CA-CB-CG
56	ZB	3	PPU	N3'-C-CA-N
56	ZB	3	PPU	O-C-CA-CB
56	ZB	3	PPU	N3'-C-CA-CB

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	ZB	3	PPU	7	0
23	XX	20	A3P	2	0
23	QX	20	A3P	1	0
56	ZA	3	PPU	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 900 ligands modelled in this entry, 898 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	302	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	302	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	QA	1510/1521 (99%)	0.21	28 (1%)	66	41	49, 98, 212, 355	0
1	XA	1507/1521 (99%)	0.08	25 (1%)	69	43	45, 94, 192, 357	0
2	QB	235/256 (91%)	0.30	4 (1%)	69	43	74, 129, 195, 233	0
2	XB	236/256 (92%)	0.65	14 (5%)	28	16	70, 117, 191, 215	0
3	QC	205/239 (85%)	0.58	12 (5%)	28	16	78, 124, 163, 185	0
3	XC	205/239 (85%)	0.51	10 (4%)	35	19	66, 105, 158, 211	0
4	QD	208/209 (99%)	0.56	7 (3%)	48	27	56, 89, 122, 140	0
4	XD	208/209 (99%)	0.70	17 (8%)	17	11	54, 94, 137, 176	0
5	QE	151/162 (93%)	0.66	10 (6%)	24	15	51, 89, 126, 167	0
5	XE	151/162 (93%)	0.55	8 (5%)	32	18	59, 85, 129, 186	0
6	QF	101/101 (100%)	0.38	3 (2%)	52	30	75, 108, 147, 204	0
6	XF	101/101 (100%)	0.20	0	100	100	52, 85, 118, 164	0
7	QG	155/156 (99%)	0.49	8 (5%)	33	19	88, 127, 172, 241	0
7	XG	155/156 (99%)	0.67	15 (9%)	13	9	75, 113, 160, 233	0
8	QH	137/138 (99%)	0.45	5 (3%)	46	25	58, 91, 125, 158	0
8	XH	137/138 (99%)	0.61	6 (4%)	39	21	60, 90, 128, 156	0
9	QI	127/128 (99%)	1.04	16 (12%)	8	6	86, 142, 179, 263	0
9	XI	126/128 (98%)	0.98	18 (14%)	6	5	66, 121, 162, 174	0
10	QJ	99/105 (94%)	1.21	22 (22%)	2	2	95, 143, 201, 251	0
10	XJ	96/105 (91%)	0.87	10 (10%)	11	8	87, 133, 196, 223	0
11	QK	119/129 (92%)	0.84	9 (7%)	20	13	61, 109, 164, 270	0
11	XK	116/129 (89%)	0.44	2 (1%)	69	43	48, 93, 136, 182	0
12	QL	125/132 (94%)	0.73	17 (13%)	7	5	49, 80, 121, 230	0
12	XL	122/132 (92%)	0.62	7 (5%)	29	17	46, 78, 112, 193	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	QM	120/126 (95%)	0.91	18 (15%)	5	5	74, 129, 179, 206	0
13	XM	119/126 (94%)	0.92	17 (14%)	6	5	75, 113, 158, 172	0
14	QN	60/61 (98%)	1.72	23 (38%)	1	1	81, 121, 159, 212	0
14	XN	60/61 (98%)	0.83	5 (8%)	17	11	75, 102, 144, 214	0
15	QO	88/89 (98%)	0.74	3 (3%)	48	27	59, 96, 131, 139	0
15	XO	87/89 (97%)	0.70	3 (3%)	48	27	52, 88, 118, 147	0
16	QP	84/88 (95%)	0.78	6 (7%)	22	14	58, 87, 127, 181	0
16	XP	84/88 (95%)	0.87	8 (9%)	14	9	64, 100, 143, 184	0
17	QQ	100/105 (95%)	0.70	8 (8%)	18	12	60, 92, 126, 153	0
17	XQ	100/105 (95%)	0.72	8 (8%)	18	12	62, 93, 118, 175	0
18	QR	70/88 (79%)	0.45	0	100	100	70, 110, 153, 155	0
18	XR	70/88 (79%)	0.09	1 (1%)	73	48	48, 85, 130, 156	0
19	QS	83/93 (89%)	0.80	9 (10%)	11	8	91, 135, 185, 224	0
19	XS	83/93 (89%)	0.63	5 (6%)	27	16	84, 116, 169, 214	0
20	QT	99/106 (93%)	0.97	17 (17%)	4	4	68, 104, 173, 248	0
20	XT	99/106 (93%)	0.95	13 (13%)	7	6	72, 115, 173, 205	0
21	QU	25/27 (92%)	1.64	12 (48%)	0	1	97, 124, 152, 161	0
21	XU	25/27 (92%)	1.27	5 (20%)	3	3	92, 120, 141, 153	0
22	QV	77/77 (100%)	-0.05	2 (2%)	57	33	51, 103, 134, 192	0
22	XV	77/77 (100%)	-0.13	2 (2%)	57	33	56, 88, 122, 191	0
23	QX	17/20 (85%)	1.83	7 (41%)	0	1	76, 258, 314, 321	0
23	XX	17/20 (85%)	1.68	6 (35%)	1	1	57, 237, 321, 369	0
24	QY	84/84 (100%)	0.85	12 (14%)	6	5	65, 97, 131, 170	0
24	QZ	84/84 (100%)	0.31	1 (1%)	76	52	94, 149, 209, 227	0
24	XY	84/84 (100%)	0.65	6 (7%)	22	14	58, 91, 129, 154	0
24	XZ	84/84 (100%)	0.97	10 (11%)	9	6	88, 145, 204, 270	0
25	R0	81/85 (95%)	0.81	8 (9%)	13	8	52, 80, 104, 153	0
25	Y0	82/85 (96%)	0.93	6 (7%)	21	13	48, 83, 110, 131	0
26	R1	94/98 (95%)	1.21	16 (17%)	4	4	39, 83, 137, 200	0
26	Y1	97/98 (98%)	0.60	3 (3%)	51	29	34, 72, 113, 185	0
27	R2	69/72 (95%)	0.82	5 (7%)	21	14	54, 95, 135, 193	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
27	Y2	69/72 (95%)	0.57	4 (5%) 29 17	49, 83, 118, 238	0
28	R3	59/60 (98%)	0.45	1 (1%) 69 43	50, 82, 140, 155	0
28	Y3	59/60 (98%)	0.44	1 (1%) 69 43	52, 83, 125, 170	0
29	R4	69/71 (97%)	0.71	4 (5%) 29 17	105, 164, 223, 306	0
29	Y4	69/71 (97%)	0.97	10 (14%) 6 5	95, 131, 211, 285	0
30	R5	59/60 (98%)	0.74	3 (5%) 33 19	46, 81, 150, 183	0
30	Y5	59/60 (98%)	0.76	3 (5%) 33 19	42, 87, 154, 179	0
31	R6	53/54 (98%)	1.44	13 (24%) 2 2	147, 191, 254, 315	0
31	Y6	53/54 (98%)	1.53	17 (32%) 1 1	153, 180, 229, 243	0
32	R7	47/49 (95%)	0.60	4 (8%) 16 11	37, 57, 98, 138	0
32	Y7	48/49 (97%)	0.93	6 (12%) 8 6	38, 57, 88, 136	0
33	R8	64/65 (98%)	1.10	10 (15%) 5 5	42, 75, 121, 168	0
33	Y8	64/65 (98%)	1.02	11 (17%) 4 4	48, 75, 112, 154	0
34	R9	37/37 (100%)	1.61	14 (37%) 1 1	122, 162, 209, 225	0
34	Y9	37/37 (100%)	1.64	13 (35%) 1 1	135, 156, 195, 222	0
35	RA	2891/2915 (99%)	0.02	54 (1%) 66 41	39, 76, 264, 453	0
35	YA	2878/2915 (98%)	-0.06	66 (2%) 61 37	34, 73, 271, 478	0
36	RB	120/124 (96%)	0.18	5 (4%) 40 22	74, 122, 167, 189	0
36	YB	120/124 (96%)	0.11	2 (1%) 69 43	74, 109, 162, 192	0
37	RD	272/276 (98%)	0.91	32 (11%) 9 6	33, 74, 112, 258	0
37	YD	274/276 (99%)	0.32	5 (1%) 67 42	31, 57, 86, 130	0
38	RE	205/206 (99%)	0.74	13 (6%) 26 15	48, 88, 136, 200	0
38	YE	204/206 (99%)	0.60	7 (3%) 48 27	44, 83, 122, 169	0
39	RF	202/210 (96%)	0.42	8 (3%) 42 23	29, 67, 117, 227	0
39	YF	202/210 (96%)	0.56	9 (4%) 38 20	38, 76, 135, 191	0
40	RG	181/182 (99%)	0.61	9 (4%) 34 19	80, 123, 166, 244	0
40	YG	181/182 (99%)	0.86	15 (8%) 17 11	64, 111, 158, 189	0
41	RH	174/180 (96%)	1.15	30 (17%) 4 4	91, 141, 215, 280	0
41	YH	174/180 (96%)	0.69	21 (12%) 8 6	77, 128, 184, 219	0
42	RI	145/148 (97%)	1.03	22 (15%) 5 5	72, 115, 152, 209	0
42	YI	146/148 (98%)	0.58	9 (6%) 26 16	61, 103, 147, 217	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
43	RN	138/140 (98%)	1.07	23 (16%) 4 4	58, 96, 143, 175	0
43	YN	138/140 (98%)	0.90	11 (7%) 18 12	50, 88, 135, 171	0
44	RO	122/122 (100%)	0.48	1 (0%) 82 60	37, 73, 103, 126	0
44	YO	122/122 (100%)	0.64	4 (3%) 49 28	36, 68, 97, 137	0
45	RP	150/150 (100%)	0.91	16 (10%) 11 8	44, 85, 129, 206	0
45	YP	149/150 (99%)	0.60	11 (7%) 20 13	40, 78, 107, 144	0
46	RQ	141/141 (100%)	0.94	12 (8%) 16 11	45, 87, 131, 190	0
46	YQ	141/141 (100%)	0.43	5 (3%) 47 26	53, 82, 113, 137	0
47	RR	117/118 (99%)	0.57	4 (3%) 48 27	50, 79, 110, 218	0
47	YR	117/118 (99%)	0.68	11 (9%) 14 9	47, 77, 114, 162	0
48	RS	111/112 (99%)	1.04	16 (14%) 6 5	79, 116, 157, 259	0
48	YS	111/112 (99%)	0.87	13 (11%) 9 6	72, 100, 145, 293	0
49	RT	137/146 (93%)	0.71	12 (8%) 15 10	57, 89, 152, 199	0
49	YT	137/146 (93%)	0.66	11 (8%) 18 12	52, 86, 169, 273	0
50	RU	117/118 (99%)	0.72	6 (5%) 33 19	41, 74, 125, 172	0
50	YU	117/118 (99%)	0.93	13 (11%) 10 7	51, 82, 124, 170	0
51	RV	101/101 (100%)	0.44	3 (2%) 52 30	46, 87, 139, 175	0
51	YV	101/101 (100%)	1.05	16 (15%) 5 4	53, 96, 137, 220	0
52	RW	113/113 (100%)	0.71	7 (6%) 26 16	47, 71, 121, 195	0
52	YW	113/113 (100%)	0.57	7 (6%) 26 16	44, 73, 126, 229	0
53	RX	92/96 (95%)	0.70	10 (10%) 10 7	54, 84, 118, 167	0
53	YX	92/96 (95%)	0.37	1 (1%) 78 54	39, 72, 106, 140	0
54	RY	107/110 (97%)	1.21	25 (23%) 2 2	54, 93, 163, 279	0
54	YY	107/110 (97%)	0.80	9 (8%) 17 11	57, 98, 152, 179	0
55	RZ	183/206 (88%)	0.49	2 (1%) 78 54	79, 118, 157, 207	0
55	YZ	183/206 (88%)	0.47	4 (2%) 62 37	70, 113, 152, 166	0
56	ZA	2/3 (66%)	-0.43	0 100 100	49, 49, 49, 58	0
56	ZB	2/3 (66%)	-0.30	0 100 100	53, 53, 53, 62	0
All	All	21211/21784 (97%)	0.43	1192 (5%) 30 17	29, 91, 181, 478	0

The worst 5 of 1192 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	QK	129	SER	9.6
12	XL	28	LYS	9.4
14	QN	13	THR	8.2
14	QN	2	ALA	7.6
49	RT	106	SER	7.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	A3P	QX	20	26/27	0.91	0.13	82,85,97,100	0
23	A3P	XX	20	26/27	0.91	0.11	71,76,82,84	0
56	PPU	ZA	3	37/38	0.91	0.15	41,59,68,71	0
56	PPU	ZB	3	37/38	0.94	0.13	38,56,67,69	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	Y9	101	1/1	0.33	0.27	122,122,122,122	0
59	ZN	Y6	101	1/1	0.36	0.25	229,229,229,229	0
57	MG	RA	3174	1/1	0.49	0.21	51,51,51,51	0
57	MG	QA	1673	1/1	0.51	0.26	69,69,69,69	0
57	MG	YA	3081	1/1	0.54	0.29	38,38,38,38	0
57	MG	QA	1645	1/1	0.57	0.17	81,81,81,81	0
57	MG	RA	3155	1/1	0.57	0.21	89,89,89,89	0
57	MG	XA	1651	1/1	0.58	0.69	81,81,81,81	0
57	MG	RA	3295	1/1	0.63	0.20	51,51,51,51	0
57	MG	XA	1636	1/1	0.63	0.22	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3235	1/1	0.65	0.19	208,208,208,208	0
59	ZN	R5	101	1/1	0.66	0.20	244,244,244,244	0
57	MG	XA	1676	1/1	0.67	0.32	53,53,53,53	0
57	MG	XA	1699	1/1	0.67	0.19	49,49,49,49	0
57	MG	RA	3164	1/1	0.67	0.24	57,57,57,57	0
57	MG	YA	3060	1/1	0.67	0.34	40,40,40,40	0
57	MG	RA	3012	1/1	0.67	0.17	48,48,48,48	0
57	MG	RA	3081	1/1	0.67	0.34	55,55,55,55	0
57	MG	RA	3112	1/1	0.67	0.23	41,41,41,41	0
57	MG	QA	1646	1/1	0.67	0.13	67,67,67,67	0
57	MG	XA	1644	1/1	0.68	0.11	76,76,76,76	0
57	MG	RQ	202	1/1	0.68	0.18	58,58,58,58	0
57	MG	RA	3058	1/1	0.69	0.35	46,46,46,46	0
57	MG	YA	3103	1/1	0.69	0.31	81,81,81,81	0
57	MG	RA	3190	1/1	0.69	0.11	55,55,55,55	0
57	MG	YA	3321	1/1	0.69	0.12	69,69,69,69	0
57	MG	RA	3242	1/1	0.69	0.26	47,47,47,47	0
57	MG	RA	3134	1/1	0.69	0.16	52,52,52,52	0
57	MG	XA	1674	1/1	0.70	0.12	28,28,28,28	0
57	MG	RA	3086	1/1	0.70	0.21	26,26,26,26	0
57	MG	XA	1685	1/1	0.70	0.20	62,62,62,62	0
57	MG	QA	1657	1/1	0.71	0.32	74,74,74,74	0
57	MG	QY	101	1/1	0.71	0.41	77,77,77,77	0
57	MG	YA	3175	1/1	0.72	0.19	57,57,57,57	0
57	MG	RA	3167	1/1	0.72	0.14	59,59,59,59	0
57	MG	XA	1603	1/1	0.72	0.20	48,48,48,48	0
57	MG	YA	3057	1/1	0.72	0.17	38,38,38,38	0
57	MG	YA	3149	1/1	0.72	0.19	76,76,76,76	0
57	MG	RA	3177	1/1	0.73	0.17	46,46,46,46	0
57	MG	RA	3296	1/1	0.73	0.22	40,40,40,40	0
57	MG	XA	1693	1/1	0.73	0.23	48,48,48,48	0
57	MG	YA	3194	1/1	0.74	0.13	61,61,61,61	0
57	MG	RA	3271	1/1	0.74	0.11	53,53,53,53	0
57	MG	YA	3305	1/1	0.74	0.20	50,50,50,50	0
57	MG	XA	1687	1/1	0.75	0.17	50,50,50,50	0
57	MG	RA	3189	1/1	0.75	0.21	58,58,58,58	0
57	MG	RA	3294	1/1	0.75	0.28	54,54,54,54	0
57	MG	RA	3248	1/1	0.75	0.18	28,28,28,28	0
57	MG	YA	3287	1/1	0.76	0.13	44,44,44,44	0
57	MG	YA	3168	1/1	0.76	0.15	62,62,62,62	0
57	MG	YA	3222	1/1	0.76	0.18	29,29,29,29	0
57	MG	RA	3301	1/1	0.76	0.24	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3246	1/1	0.76	0.14	61,61,61,61	0
57	MG	RA	3302	1/1	0.77	0.49	80,80,80,80	0
57	MG	RA	3143	1/1	0.77	0.22	59,59,59,59	0
57	MG	YA	3265	1/1	0.77	0.11	44,44,44,44	0
57	MG	RA	3133	1/1	0.77	0.20	51,51,51,51	0
57	MG	YA	3011	1/1	0.77	0.33	43,43,43,43	0
57	MG	YA	3019	1/1	0.77	0.29	32,32,32,32	0
57	MG	RA	3061	1/1	0.77	0.22	67,67,67,67	0
57	MG	RA	3165	1/1	0.77	0.12	47,47,47,47	0
57	MG	YA	3257	1/1	0.78	0.18	50,50,50,50	0
57	MG	QA	1628	1/1	0.78	0.08	74,74,74,74	0
57	MG	YA	3279	1/1	0.78	0.17	50,50,50,50	0
57	MG	RA	3283	1/1	0.78	0.32	61,61,61,61	0
57	MG	RA	3147	1/1	0.79	0.14	56,56,56,56	0
57	MG	YA	3066	1/1	0.79	0.12	38,38,38,38	0
57	MG	RA	3014	1/1	0.79	0.23	58,58,58,58	0
57	MG	YA	3091	1/1	0.79	0.17	36,36,36,36	0
57	MG	YA	3055	1/1	0.79	0.14	7,7,7,7	0
59	ZN	R4	101	1/1	0.79	0.20	176,176,176,176	0
57	MG	RA	3107	1/1	0.79	0.20	41,41,41,41	0
59	ZN	R6	101	1/1	0.79	0.28	227,227,227,227	0
57	MG	YA	3161	1/1	0.79	0.10	44,44,44,44	0
57	MG	YA	3273	1/1	0.80	0.12	58,58,58,58	0
57	MG	YA	3277	1/1	0.80	0.10	52,52,52,52	0
57	MG	RA	3182	1/1	0.80	0.15	44,44,44,44	0
57	MG	YA	3107	1/1	0.80	0.24	71,71,71,71	0
57	MG	YA	3288	1/1	0.80	0.10	28,28,28,28	0
57	MG	YA	3110	1/1	0.80	0.20	41,41,41,41	0
57	MG	YA	3117	1/1	0.80	0.11	55,55,55,55	0
57	MG	YE	303	1/1	0.80	0.18	69,69,69,69	0
57	MG	YA	3236	1/1	0.80	0.17	38,38,38,38	0
57	MG	YA	3034	1/1	0.80	0.18	75,75,75,75	0
57	MG	XA	1641	1/1	0.80	0.20	51,51,51,51	0
57	MG	RA	3072	1/1	0.80	0.24	14,14,14,14	0
57	MG	YA	3184	1/1	0.81	0.19	37,37,37,37	0
57	MG	YA	3143	1/1	0.81	0.09	60,60,60,60	0
57	MG	YA	3219	1/1	0.81	0.25	37,37,37,37	0
57	MG	YG	201	1/1	0.81	0.14	59,59,59,59	0
57	MG	YA	3084	1/1	0.81	0.24	24,24,24,24	0
57	MG	YA	3049	1/1	0.81	0.19	42,42,42,42	0
57	MG	YA	3002	1/1	0.81	0.21	32,32,32,32	0
57	MG	YA	3138	1/1	0.81	0.16	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	RA	3056	1/1	0.82	0.11	54,54,54,54	0
57	MG	RA	3237	1/1	0.82	0.20	40,40,40,40	0
57	MG	RA	3276	1/1	0.82	0.18	48,48,48,48	0
57	MG	YA	3311	1/1	0.82	0.17	45,45,45,45	0
57	MG	RA	3277	1/1	0.82	0.14	45,45,45,45	0
57	MG	RB	202	1/1	0.82	0.19	27,27,27,27	0
57	MG	YE	305	1/1	0.82	0.11	66,66,66,66	0
57	MG	YA	3261	1/1	0.82	0.15	35,35,35,35	0
57	MG	RA	3241	1/1	0.82	0.12	36,36,36,36	0
57	MG	QA	1617	1/1	0.82	0.13	57,57,57,57	0
57	MG	YA	3141	1/1	0.82	0.16	41,41,41,41	0
57	MG	YA	3220	1/1	0.82	0.14	22,22,22,22	0
57	MG	XA	1677	1/1	0.83	0.18	46,46,46,46	0
57	MG	YA	3281	1/1	0.83	0.18	37,37,37,37	0
57	MG	YA	3183	1/1	0.83	0.14	44,44,44,44	0
57	MG	YB	202	1/1	0.83	0.32	47,47,47,47	0
57	MG	YD	301	1/1	0.83	0.20	24,24,24,24	0
57	MG	RA	3020	1/1	0.83	0.23	39,39,39,39	0
57	MG	YA	3223	1/1	0.84	0.15	31,31,31,31	0
57	MG	RA	3035	1/1	0.84	0.12	34,34,34,34	0
57	MG	RA	3268	1/1	0.84	0.23	56,56,56,56	0
57	MG	QA	1693	1/1	0.84	0.12	50,50,50,50	0
57	MG	YA	3251	1/1	0.84	0.19	68,68,68,68	0
57	MG	RA	3108	1/1	0.84	0.12	43,43,43,43	0
57	MG	XA	1667	1/1	0.84	0.20	26,26,26,26	0
57	MG	XA	1670	1/1	0.84	0.13	46,46,46,46	0
57	MG	YA	3270	1/1	0.84	0.17	44,44,44,44	0
57	MG	XA	1672	1/1	0.84	0.14	30,30,30,30	0
57	MG	QA	1618	1/1	0.84	0.15	55,55,55,55	0
57	MG	XA	1675	1/1	0.84	0.20	35,35,35,35	0
57	MG	YA	3280	1/1	0.84	0.24	42,42,42,42	0
57	MG	RA	3126	1/1	0.84	0.15	60,60,60,60	0
57	MG	YA	3133	1/1	0.84	0.14	32,32,32,32	0
57	MG	RA	3059	1/1	0.84	0.19	27,27,27,27	0
57	MG	RA	3183	1/1	0.84	0.19	56,56,56,56	0
57	MG	QA	1642	1/1	0.84	0.10	64,64,64,64	0
57	MG	YA	3314	1/1	0.84	0.14	50,50,50,50	0
57	MG	YA	3319	1/1	0.84	0.18	57,57,57,57	0
57	MG	QA	1620	1/1	0.84	0.15	75,75,75,75	0
57	MG	RA	3236	1/1	0.84	0.25	47,47,47,47	0
57	MG	RA	3074	1/1	0.84	0.26	23,23,23,23	0
57	MG	RD	301	1/1	0.84	0.13	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YE	304	1/1	0.84	0.25	60,60,60,60	0
57	MG	YA	3010	1/1	0.84	0.11	35,35,35,35	0
57	MG	RN	201	1/1	0.84	0.31	72,72,72,72	0
57	MG	YQ	202	1/1	0.84	0.34	70,70,70,70	0
57	MG	RO	201	1/1	0.84	0.24	60,60,60,60	0
57	MG	QA	1682	1/1	0.84	0.08	33,33,33,33	0
57	MG	RQ	204	1/1	0.84	0.14	53,53,53,53	0
57	MG	RA	3160	1/1	0.84	0.26	33,33,33,33	0
57	MG	YA	3097	1/1	0.85	0.10	52,52,52,52	0
57	MG	QA	1649	1/1	0.85	0.11	53,53,53,53	0
57	MG	RA	3258	1/1	0.85	0.27	44,44,44,44	0
57	MG	QA	1664	1/1	0.85	0.24	46,46,46,46	0
57	MG	RA	3270	1/1	0.85	0.14	41,41,41,41	0
57	MG	YA	3127	1/1	0.85	0.26	66,66,66,66	0
57	MG	RA	3090	1/1	0.85	0.13	34,34,34,34	0
57	MG	YA	3135	1/1	0.85	0.12	34,34,34,34	0
57	MG	RA	3106	1/1	0.85	0.18	18,18,18,18	0
57	MG	XA	1613	1/1	0.85	0.33	52,52,52,52	0
57	MG	YA	3283	1/1	0.85	0.20	32,32,32,32	0
57	MG	XA	1617	1/1	0.85	0.10	30,30,30,30	0
57	MG	XA	1619	1/1	0.85	0.14	48,48,48,48	0
57	MG	YA	3290	1/1	0.85	0.19	57,57,57,57	0
57	MG	XA	1635	1/1	0.85	0.15	36,36,36,36	0
57	MG	YA	3309	1/1	0.85	0.16	52,52,52,52	0
57	MG	YA	3012	1/1	0.85	0.14	68,68,68,68	0
57	MG	YA	3312	1/1	0.85	0.09	43,43,43,43	0
57	MG	YA	3171	1/1	0.85	0.13	45,45,45,45	0
57	MG	RA	3188	1/1	0.85	0.15	57,57,57,57	0
57	MG	R0	102	1/1	0.85	0.14	31,31,31,31	0
57	MG	YA	3328	1/1	0.85	0.44	77,77,77,77	0
57	MG	YA	3046	1/1	0.85	0.24	31,31,31,31	0
57	MG	RA	3158	1/1	0.85	0.08	40,40,40,40	0
57	MG	YA	3210	1/1	0.85	0.18	34,34,34,34	0
57	MG	YA	3215	1/1	0.85	0.24	35,35,35,35	0
57	MG	RA	3191	1/1	0.85	0.18	118,118,118,118	0
57	MG	RA	3024	1/1	0.85	0.25	13,13,13,13	0
57	MG	RA	3298	1/1	0.85	0.12	57,57,57,57	0
57	MG	XA	1671	1/1	0.85	0.18	39,39,39,39	0
57	MG	RA	3009	1/1	0.85	0.19	41,41,41,41	0
57	MG	RA	3120	1/1	0.85	0.12	45,45,45,45	0
57	MG	RA	3047	1/1	0.85	0.20	19,19,19,19	0
57	MG	RA	3032	1/1	0.86	0.23	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	3109	1/1	0.86	0.24	35,35,35,35	0
57	MG	QA	1679	1/1	0.86	0.14	35,35,35,35	0
57	MG	YA	3297	1/1	0.86	0.13	31,31,31,31	0
57	MG	YA	3115	1/1	0.86	0.17	18,18,18,18	0
57	MG	RA	3013	1/1	0.86	0.22	43,43,43,43	0
57	MG	XA	1618	1/1	0.86	0.11	42,42,42,42	0
57	MG	YA	3231	1/1	0.86	0.16	26,26,26,26	0
57	MG	YA	3042	1/1	0.86	0.21	9,9,9,9	0
57	MG	RA	3076	1/1	0.86	0.24	31,31,31,31	0
57	MG	XA	1630	1/1	0.86	0.09	66,66,66,66	0
57	MG	YA	3325	1/1	0.86	0.08	61,61,61,61	0
57	MG	XA	1632	1/1	0.86	0.12	47,47,47,47	0
57	MG	XA	1634	1/1	0.86	0.07	77,77,77,77	0
57	MG	R0	101	1/1	0.86	0.07	9,9,9,9	0
57	MG	QD	301	1/1	0.86	0.09	81,81,81,81	0
57	MG	QV	102	1/1	0.86	0.15	55,55,55,55	0
57	MG	XE	201	1/1	0.86	0.11	32,32,32,32	0
57	MG	RA	3170	1/1	0.86	0.17	74,74,74,74	0
57	MG	RA	3092	1/1	0.86	0.11	38,38,38,38	0
57	MG	YQ	203	1/1	0.86	0.20	64,64,64,64	0
57	MG	YA	3102	1/1	0.86	0.09	52,52,52,52	0
57	MG	RA	3100	1/1	0.86	0.14	39,39,39,39	0
57	MG	YA	3195	1/1	0.86	0.10	38,38,38,38	0
57	MG	YA	3284	1/1	0.86	0.15	36,36,36,36	0
57	MG	YA	3276	1/1	0.87	0.21	49,49,49,49	0
57	MG	QA	1612	1/1	0.87	0.26	33,33,33,33	0
57	MG	XA	1656	1/1	0.87	0.18	34,34,34,34	0
57	MG	YA	3152	1/1	0.87	0.10	44,44,44,44	0
57	MG	QA	1639	1/1	0.87	0.09	59,59,59,59	0
57	MG	RA	3178	1/1	0.87	0.25	63,63,63,63	0
57	MG	RA	3007	1/1	0.87	0.12	25,25,25,25	0
57	MG	RA	3097	1/1	0.87	0.09	36,36,36,36	0
57	MG	YA	3177	1/1	0.87	0.27	68,68,68,68	0
57	MG	RA	3261	1/1	0.87	0.18	44,44,44,44	0
57	MG	YA	3291	1/1	0.87	0.10	39,39,39,39	0
57	MG	RA	3186	1/1	0.87	0.13	36,36,36,36	0
57	MG	YA	3190	1/1	0.87	0.09	44,44,44,44	0
57	MG	QA	1665	1/1	0.87	0.19	31,31,31,31	0
57	MG	QA	1692	1/1	0.87	0.20	42,42,42,42	0
57	MG	YA	3087	1/1	0.87	0.28	22,22,22,22	0
57	MG	YA	3211	1/1	0.87	0.13	26,26,26,26	0
57	MG	RA	3274	1/1	0.87	0.22	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3142	1/1	0.87	0.25	28,28,28,28	0
57	MG	RA	3169	1/1	0.87	0.09	63,63,63,63	0
57	MG	RA	3193	1/1	0.87	0.15	57,57,57,57	0
57	MG	RA	3286	1/1	0.87	0.16	51,51,51,51	0
57	MG	XL	201	1/1	0.87	0.08	66,66,66,66	0
57	MG	RA	3207	1/1	0.87	0.17	17,17,17,17	0
57	MG	YA	3112	1/1	0.87	0.17	65,65,65,65	0
57	MG	YA	3239	1/1	0.87	0.09	39,39,39,39	0
57	MG	RA	3210	1/1	0.87	0.14	19,19,19,19	0
57	MG	YA	3006	1/1	0.87	0.12	33,33,33,33	0
57	MG	YA	3009	1/1	0.87	0.15	41,41,41,41	0
57	MG	RA	3211	1/1	0.87	0.22	27,27,27,27	0
57	MG	XA	1638	1/1	0.87	0.12	41,41,41,41	0
57	MG	RA	3232	1/1	0.87	0.31	57,57,57,57	0
59	ZN	R9	101	1/1	0.87	0.34	127,127,127,127	0
57	MG	RA	3082	1/1	0.87	0.17	33,33,33,33	0
57	MG	RA	3041	1/1	0.88	0.19	18,18,18,18	0
57	MG	RA	3029	1/1	0.88	0.10	35,35,35,35	0
57	MG	XA	1673	1/1	0.88	0.17	45,45,45,45	0
57	MG	RA	3166	1/1	0.88	0.24	54,54,54,54	0
57	MG	XA	1606	1/1	0.88	0.21	29,29,29,29	0
57	MG	YA	3286	1/1	0.88	0.10	33,33,33,33	0
57	MG	XA	1609	1/1	0.88	0.22	19,19,19,19	0
57	MG	YA	3185	1/1	0.88	0.17	68,68,68,68	0
57	MG	RA	3131	1/1	0.88	0.14	61,61,61,61	0
57	MG	YA	3191	1/1	0.88	0.10	56,56,56,56	0
57	MG	YA	3294	1/1	0.88	0.16	57,57,57,57	0
57	MG	YA	3085	1/1	0.88	0.15	14,14,14,14	0
57	MG	YA	3301	1/1	0.88	0.14	33,33,33,33	0
57	MG	XA	1679	1/1	0.88	0.14	36,36,36,36	0
57	MG	RA	3208	1/1	0.88	0.11	37,37,37,37	0
57	MG	RA	3066	1/1	0.88	0.15	36,36,36,36	0
57	MG	RA	3103	1/1	0.88	0.12	24,24,24,24	0
57	MG	XA	1620	1/1	0.88	0.12	42,42,42,42	0
57	MG	YA	3316	1/1	0.88	0.16	66,66,66,66	0
57	MG	RA	3136	1/1	0.88	0.18	52,52,52,52	0
57	MG	RA	3289	1/1	0.88	0.27	56,56,56,56	0
57	MG	RA	3141	1/1	0.88	0.15	32,32,32,32	0
57	MG	RA	3085	1/1	0.88	0.14	15,15,15,15	0
57	MG	YA	3003	1/1	0.88	0.15	36,36,36,36	0
57	MG	YA	3005	1/1	0.88	0.17	34,34,34,34	0
57	MG	R3	101	1/1	0.88	0.22	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	3088	1/1	0.88	0.14	33,33,33,33	0
57	MG	RA	3245	1/1	0.88	0.23	48,48,48,48	0
57	MG	RA	3111	1/1	0.88	0.17	41,41,41,41	0
57	MG	XA	1648	1/1	0.88	0.07	34,34,34,34	0
57	MG	QA	1689	1/1	0.88	0.16	70,70,70,70	0
57	MG	YV	301	1/1	0.88	0.08	68,68,68,68	0
57	MG	YA	3266	1/1	0.88	0.23	47,47,47,47	0
57	MG	RA	3115	1/1	0.88	0.23	25,25,25,25	0
57	MG	RA	3263	1/1	0.88	0.16	51,51,51,51	0
57	MG	RA	3264	1/1	0.88	0.16	41,41,41,41	0
57	MG	YA	3164	1/1	0.88	0.16	39,39,39,39	0
57	MG	YA	3165	1/1	0.89	0.07	49,49,49,49	0
57	MG	RA	3139	1/1	0.89	0.12	32,32,32,32	0
57	MG	YA	3169	1/1	0.89	0.17	44,44,44,44	0
57	MG	YA	3063	1/1	0.89	0.23	31,31,31,31	0
57	MG	RA	3096	1/1	0.89	0.12	38,38,38,38	0
57	MG	QA	1605	1/1	0.89	0.22	30,30,30,30	0
57	MG	RA	3045	1/1	0.89	0.18	40,40,40,40	0
57	MG	RA	3195	1/1	0.89	0.18	44,44,44,44	0
57	MG	RA	3205	1/1	0.89	0.26	16,16,16,16	0
57	MG	XA	1642	1/1	0.89	0.13	55,55,55,55	0
57	MG	XV	102	1/1	0.89	0.15	32,32,32,32	0
57	MG	YA	3193	1/1	0.89	0.17	38,38,38,38	0
57	MG	XV	103	1/1	0.89	0.18	57,57,57,57	0
57	MG	Y5	101	1/1	0.89	0.14	71,71,71,71	0
57	MG	YA	3302	1/1	0.89	0.22	50,50,50,50	0
57	MG	YA	3205	1/1	0.89	0.15	17,17,17,17	0
57	MG	RA	3173	1/1	0.89	0.13	29,29,29,29	0
57	MG	XA	1645	1/1	0.89	0.09	60,60,60,60	0
57	MG	RA	3025	1/1	0.89	0.18	15,15,15,15	0
57	MG	YA	3313	1/1	0.89	0.14	51,51,51,51	0
57	MG	RA	3209	1/1	0.89	0.20	26,26,26,26	0
57	MG	RA	3154	1/1	0.89	0.13	53,53,53,53	0
57	MG	YA	3221	1/1	0.89	0.20	27,27,27,27	0
57	MG	XA	1666	1/1	0.89	0.18	40,40,40,40	0
57	MG	YA	3322	1/1	0.89	0.12	71,71,71,71	0
57	MG	YA	3121	1/1	0.89	0.13	34,34,34,34	0
57	MG	YA	3228	1/1	0.89	0.14	34,34,34,34	0
57	MG	YA	3329	1/1	0.89	0.19	36,36,36,36	0
57	MG	XA	1604	1/1	0.89	0.18	21,21,21,21	0
57	MG	RA	3130	1/1	0.89	0.20	38,38,38,38	0
57	MG	RA	3223	1/1	0.89	0.16	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	1671	1/1	0.89	0.21	34,34,34,34	0
57	MG	YA	3240	1/1	0.89	0.18	36,36,36,36	0
57	MG	YA	3140	1/1	0.89	0.14	27,27,27,27	0
57	MG	RA	3089	1/1	0.89	0.21	25,25,25,25	0
57	MG	RA	3185	1/1	0.89	0.14	33,33,33,33	0
57	MG	RA	3239	1/1	0.89	0.24	57,57,57,57	0
57	MG	YA	3150	1/1	0.89	0.15	58,58,58,58	0
57	MG	QA	1662	1/1	0.89	0.18	63,63,63,63	0
57	MG	YA	3154	1/1	0.89	0.09	56,56,56,56	0
57	MG	QA	1641	1/1	0.89	0.23	55,55,55,55	0
57	MG	XA	1678	1/1	0.89	0.19	35,35,35,35	0
57	MG	RY	201	1/1	0.90	0.13	51,51,51,51	0
57	MG	YA	3014	1/1	0.90	0.17	38,38,38,38	0
57	MG	QA	1651	1/1	0.90	0.09	81,81,81,81	0
57	MG	YA	3030	1/1	0.90	0.10	27,27,27,27	0
57	MG	YA	3275	1/1	0.90	0.19	53,53,53,53	0
57	MG	RA	3280	1/1	0.90	0.11	37,37,37,37	0
57	MG	RA	3282	1/1	0.90	0.29	28,28,28,28	0
57	MG	YA	3163	1/1	0.90	0.14	41,41,41,41	0
57	MG	RA	3161	1/1	0.90	0.10	34,34,34,34	0
57	MG	XA	1612	1/1	0.90	0.15	27,27,27,27	0
57	MG	YA	3052	1/1	0.90	0.09	40,40,40,40	0
57	MG	RA	3033	1/1	0.90	0.19	55,55,55,55	0
57	MG	QA	1684	1/1	0.90	0.26	51,51,51,51	0
57	MG	YA	3059	1/1	0.90	0.22	8,8,8,8	0
57	MG	RA	3293	1/1	0.90	0.21	26,26,26,26	0
57	MG	RA	3037	1/1	0.90	0.14	18,18,18,18	0
57	MG	XA	1680	1/1	0.90	0.10	45,45,45,45	0
57	MG	YA	3071	1/1	0.90	0.18	16,16,16,16	0
57	MG	YA	3187	1/1	0.90	0.11	33,33,33,33	0
57	MG	RA	3039	1/1	0.90	0.13	31,31,31,31	0
57	MG	XA	1686	1/1	0.90	0.13	47,47,47,47	0
57	MG	RA	3110	1/1	0.90	0.15	54,54,54,54	0
57	MG	XA	1689	1/1	0.90	0.06	27,27,27,27	0
57	MG	QA	1602	1/1	0.90	0.18	33,33,33,33	0
57	MG	YA	3203	1/1	0.90	0.18	15,15,15,15	0
57	MG	RA	3299	1/1	0.90	0.21	47,47,47,47	0
57	MG	YA	3207	1/1	0.90	0.20	36,36,36,36	0
57	MG	YA	3100	1/1	0.90	0.39	67,67,67,67	0
57	MG	QA	1630	1/1	0.90	0.24	36,36,36,36	0
57	MG	YA	3320	1/1	0.90	0.14	57,57,57,57	0
57	MG	XF	301	1/1	0.90	0.05	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	3104	1/1	0.90	0.18	22,22,22,22	0
57	MG	YA	3324	1/1	0.90	0.19	47,47,47,47	0
57	MG	QA	1635	1/1	0.90	0.17	57,57,57,57	0
57	MG	YA	3327	1/1	0.90	0.36	71,71,71,71	0
57	MG	RB	201	1/1	0.90	0.08	41,41,41,41	0
57	MG	RA	3116	1/1	0.90	0.15	40,40,40,40	0
57	MG	YA	3331	1/1	0.90	0.11	30,30,30,30	0
57	MG	YA	3334	1/1	0.90	0.10	42,42,42,42	0
57	MG	YA	3335	1/1	0.90	0.28	44,44,44,44	0
57	MG	RB	203	1/1	0.90	0.13	21,21,21,21	0
57	MG	RA	3148	1/1	0.90	0.14	25,25,25,25	0
57	MG	YE	301	1/1	0.90	0.16	25,25,25,25	0
57	MG	YA	3230	1/1	0.90	0.15	34,34,34,34	0
57	MG	RA	3055	1/1	0.90	0.12	24,24,24,24	0
57	MG	RA	3099	1/1	0.90	0.15	37,37,37,37	0
57	MG	YA	3004	1/1	0.90	0.13	52,52,52,52	0
57	MG	XA	1649	1/1	0.90	0.24	55,55,55,55	0
57	MG	RQ	201	1/1	0.90	0.15	42,42,42,42	0
57	MG	YQ	204	1/1	0.90	0.18	86,86,86,86	0
57	MG	YA	3136	1/1	0.90	0.10	41,41,41,41	0
57	MG	RA	3227	1/1	0.90	0.12	31,31,31,31	0
57	MG	YA	3256	1/1	0.90	0.17	34,34,34,34	0
57	MG	RQ	203	1/1	0.90	0.14	32,32,32,32	0
57	MG	RA	3127	1/1	0.90	0.10	35,35,35,35	0
57	MG	YA	3262	1/1	0.90	0.11	55,55,55,55	0
57	MG	YA	3036	1/1	0.91	0.17	19,19,19,19	0
57	MG	XA	1607	1/1	0.91	0.10	51,51,51,51	0
57	MG	RA	3231	1/1	0.91	0.12	26,26,26,26	0
57	MG	YA	3048	1/1	0.91	0.19	9,9,9,9	0
57	MG	QA	1637	1/1	0.91	0.17	43,43,43,43	0
57	MG	YA	3162	1/1	0.91	0.18	42,42,42,42	0
57	MG	RA	3285	1/1	0.91	0.23	18,18,18,18	0
57	MG	RA	3031	1/1	0.91	0.16	29,29,29,29	0
57	MG	RA	3137	1/1	0.91	0.11	41,41,41,41	0
57	MG	YA	3282	1/1	0.91	0.10	24,24,24,24	0
57	MG	YA	3167	1/1	0.91	0.25	25,25,25,25	0
57	MG	RA	3138	1/1	0.91	0.15	46,46,46,46	0
57	MG	RA	3240	1/1	0.91	0.22	41,41,41,41	0
57	MG	YA	3061	1/1	0.91	0.16	23,23,23,23	0
57	MG	XA	1629	1/1	0.91	0.17	26,26,26,26	0
57	MG	QA	1619	1/1	0.91	0.14	55,55,55,55	0
57	MG	YA	3178	1/1	0.91	0.15	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QA	1621	1/1	0.91	0.17	41,41,41,41	0
57	MG	XA	1696	1/1	0.91	0.08	55,55,55,55	0
57	MG	YA	3298	1/1	0.91	0.15	36,36,36,36	0
57	MG	YA	3082	1/1	0.91	0.21	21,21,21,21	0
57	MG	XA	1698	1/1	0.91	0.26	49,49,49,49	0
57	MG	RA	3297	1/1	0.91	0.16	45,45,45,45	0
57	MG	RA	3101	1/1	0.91	0.17	40,40,40,40	0
57	MG	YA	3310	1/1	0.91	0.14	27,27,27,27	0
57	MG	RA	3246	1/1	0.91	0.16	43,43,43,43	0
57	MG	YA	3095	1/1	0.91	0.14	22,22,22,22	0
57	MG	YA	3096	1/1	0.91	0.23	23,23,23,23	0
57	MG	RA	3247	1/1	0.91	0.15	31,31,31,31	0
57	MG	XA	1640	1/1	0.91	0.24	59,59,59,59	0
57	MG	RA	3069	1/1	0.91	0.22	20,20,20,20	0
57	MG	YA	3209	1/1	0.91	0.16	30,30,30,30	0
57	MG	RA	3201	1/1	0.91	0.18	14,14,14,14	0
57	MG	RA	3172	1/1	0.91	0.14	60,60,60,60	0
57	MG	QA	1623	1/1	0.91	0.09	41,41,41,41	0
57	MG	RA	3128	1/1	0.91	0.19	16,16,16,16	0
57	MG	RA	3266	1/1	0.91	0.16	37,37,37,37	0
57	MG	YA	3111	1/1	0.91	0.17	33,33,33,33	0
57	MG	RA	3176	1/1	0.91	0.12	26,26,26,26	0
57	MG	RA	3152	1/1	0.91	0.10	75,75,75,75	0
57	MG	YA	3224	1/1	0.91	0.14	24,24,24,24	0
57	MG	XA	1657	1/1	0.91	0.21	28,28,28,28	0
57	MG	YA	3119	1/1	0.91	0.17	50,50,50,50	0
57	MG	QA	1643	1/1	0.91	0.30	69,69,69,69	0
57	MG	YA	3124	1/1	0.91	0.18	40,40,40,40	0
57	MG	RA	3272	1/1	0.91	0.07	38,38,38,38	0
57	MG	RA	3057	1/1	0.91	0.20	15,15,15,15	0
57	MG	YA	3134	1/1	0.91	0.13	54,54,54,54	0
57	MG	RA	3226	1/1	0.91	0.12	32,32,32,32	0
57	MG	YA	3248	1/1	0.91	0.09	39,39,39,39	0
57	MG	RA	3094	1/1	0.91	0.15	24,24,24,24	0
57	MG	YA	3254	1/1	0.91	0.19	39,39,39,39	0
57	MG	YA	3024	1/1	0.91	0.21	23,23,23,23	0
57	MG	YA	3139	1/1	0.91	0.19	32,32,32,32	0
57	MG	YA	3260	1/1	0.91	0.13	28,28,28,28	0
57	MG	RA	3279	1/1	0.91	0.15	44,44,44,44	0
57	MG	YA	3033	1/1	0.91	0.22	25,25,25,25	0
59	ZN	Y4	101	1/1	0.91	0.09	230,230,230,230	0
57	MG	RA	3228	1/1	0.91	0.19	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3091	1/1	0.92	0.12	32,32,32,32	0
57	MG	YA	3269	1/1	0.92	0.11	24,24,24,24	0
57	MG	RA	3038	1/1	0.92	0.22	26,26,26,26	0
57	MG	YA	3054	1/1	0.92	0.16	14,14,14,14	0
57	MG	YA	3274	1/1	0.92	0.10	43,43,43,43	0
57	MG	RA	3149	1/1	0.92	0.07	69,69,69,69	0
57	MG	RA	3150	1/1	0.92	0.11	58,58,58,58	0
57	MG	RA	3288	1/1	0.92	0.19	38,38,38,38	0
57	MG	RA	3117	1/1	0.92	0.25	44,44,44,44	0
57	MG	XA	1624	1/1	0.92	0.14	30,30,30,30	0
57	MG	XA	1690	1/1	0.92	0.20	54,54,54,54	0
57	MG	RA	3093	1/1	0.92	0.16	30,30,30,30	0
57	MG	YA	3174	1/1	0.92	0.20	45,45,45,45	0
57	MG	XA	1695	1/1	0.92	0.18	61,61,61,61	0
57	MG	YA	3073	1/1	0.92	0.08	46,46,46,46	0
57	MG	QA	1650	1/1	0.92	0.27	53,53,53,53	0
57	MG	YA	3179	1/1	0.92	0.24	49,49,49,49	0
57	MG	YA	3289	1/1	0.92	0.19	42,42,42,42	0
57	MG	YA	3180	1/1	0.92	0.19	50,50,50,50	0
57	MG	XA	1631	1/1	0.92	0.22	45,45,45,45	0
57	MG	YA	3292	1/1	0.92	0.16	49,49,49,49	0
57	MG	QA	1675	1/1	0.92	0.08	33,33,33,33	0
57	MG	RA	3243	1/1	0.92	0.10	22,22,22,22	0
57	MG	RA	3244	1/1	0.92	0.19	34,34,34,34	0
57	MG	YA	3299	1/1	0.92	0.16	31,31,31,31	0
57	MG	YA	3089	1/1	0.92	0.09	45,45,45,45	0
57	MG	RA	3043	1/1	0.92	0.26	16,16,16,16	0
57	MG	YA	3303	1/1	0.92	0.08	38,38,38,38	0
57	MG	YA	3192	1/1	0.92	0.15	70,70,70,70	0
57	MG	XV	101	1/1	0.92	0.16	8,8,8,8	0
57	MG	QA	1677	1/1	0.92	0.07	22,22,22,22	0
57	MG	XA	1639	1/1	0.92	0.14	33,33,33,33	0
57	MG	XV	104	1/1	0.92	0.10	18,18,18,18	0
57	MG	YA	3101	1/1	0.92	0.12	28,28,28,28	0
57	MG	RA	3077	1/1	0.92	0.17	6,6,6,6	0
57	MG	RA	3197	1/1	0.92	0.23	13,13,13,13	0
57	MG	YA	3317	1/1	0.92	0.10	32,32,32,32	0
57	MG	RA	3250	1/1	0.92	0.11	36,36,36,36	0
57	MG	RA	3255	1/1	0.92	0.10	29,29,29,29	0
57	MG	RA	3198	1/1	0.92	0.21	22,22,22,22	0
57	MG	RA	3079	1/1	0.92	0.16	32,32,32,32	0
57	MG	QA	1626	1/1	0.92	0.23	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	XA	1650	1/1	0.92	0.07	76,76,76,76	0
57	MG	RA	3105	1/1	0.92	0.16	47,47,47,47	0
57	MG	QA	1613	1/1	0.92	0.18	44,44,44,44	0
57	MG	QA	1614	1/1	0.92	0.06	53,53,53,53	0
57	MG	QA	1686	1/1	0.92	0.21	55,55,55,55	0
57	MG	YA	3229	1/1	0.92	0.12	38,38,38,38	0
57	MG	YA	3015	1/1	0.92	0.24	13,13,13,13	0
57	MG	YA	3018	1/1	0.92	0.13	28,28,28,28	0
57	MG	YA	3232	1/1	0.92	0.10	34,34,34,34	0
57	MG	QA	1611	1/1	0.92	0.18	21,21,21,21	0
57	MG	YA	3020	1/1	0.92	0.09	29,29,29,29	0
57	MG	RA	3212	1/1	0.92	0.17	26,26,26,26	0
57	MG	RA	3219	1/1	0.92	0.13	35,35,35,35	0
57	MG	YA	3137	1/1	0.92	0.12	42,42,42,42	0
57	MG	QA	1610	1/1	0.92	0.13	23,23,23,23	0
57	MG	XA	1605	1/1	0.92	0.18	18,18,18,18	0
57	MG	RA	3175	1/1	0.92	0.14	47,47,47,47	0
57	MG	YA	3037	1/1	0.92	0.21	29,29,29,29	0
57	MG	YA	3142	1/1	0.92	0.28	41,41,41,41	0
57	MG	YA	3258	1/1	0.92	0.10	19,19,19,19	0
57	MG	QA	1625	1/1	0.92	0.12	40,40,40,40	0
57	MG	YA	3044	1/1	0.92	0.22	23,23,23,23	0
57	MG	RA	3146	1/1	0.92	0.15	17,17,17,17	0
57	MG	XA	1610	1/1	0.92	0.24	33,33,33,33	0
57	MG	YA	3072	1/1	0.93	0.09	47,47,47,47	0
57	MG	XA	1602	1/1	0.93	0.10	47,47,47,47	0
57	MG	YA	3272	1/1	0.93	0.23	35,35,35,35	0
57	MG	YA	3077	1/1	0.93	0.25	20,20,20,20	0
57	MG	XA	1652	1/1	0.93	0.18	24,24,24,24	0
57	MG	YA	3001	1/1	0.93	0.15	31,31,31,31	0
57	MG	RA	3050	1/1	0.93	0.16	22,22,22,22	0
57	MG	YA	3173	1/1	0.93	0.07	59,59,59,59	0
57	MG	RA	3053	1/1	0.93	0.14	19,19,19,19	0
57	MG	XA	1661	1/1	0.93	0.23	38,38,38,38	0
57	MG	YA	3088	1/1	0.93	0.12	20,20,20,20	0
57	MG	RA	3023	1/1	0.93	0.14	25,25,25,25	0
57	MG	QV	101	1/1	0.93	0.20	20,20,20,20	0
57	MG	YA	3092	1/1	0.93	0.14	26,26,26,26	0
57	MG	YA	3008	1/1	0.93	0.20	46,46,46,46	0
57	MG	QA	1634	1/1	0.93	0.16	42,42,42,42	0
57	MG	RA	3179	1/1	0.93	0.12	30,30,30,30	0
57	MG	RA	3234	1/1	0.93	0.19	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3189	1/1	0.93	0.16	34,34,34,34	0
57	MG	QA	1652	1/1	0.93	0.14	54,54,54,54	0
57	MG	QA	1656	1/1	0.93	0.17	37,37,37,37	0
57	MG	RA	3119	1/1	0.93	0.12	33,33,33,33	0
57	MG	YA	3295	1/1	0.93	0.13	41,41,41,41	0
57	MG	QA	1615	1/1	0.93	0.12	46,46,46,46	0
57	MG	YA	3105	1/1	0.93	0.20	90,90,90,90	0
57	MG	RA	3124	1/1	0.93	0.15	37,37,37,37	0
57	MG	YA	3196	1/1	0.93	0.21	48,48,48,48	0
57	MG	YA	3198	1/1	0.93	0.19	19,19,19,19	0
57	MG	YA	3108	1/1	0.93	0.15	10,10,10,10	0
57	MG	YA	3304	1/1	0.93	0.08	47,47,47,47	0
57	MG	QA	1624	1/1	0.93	0.08	40,40,40,40	0
57	MG	YA	3021	1/1	0.93	0.17	16,16,16,16	0
57	MG	YA	3023	1/1	0.93	0.16	10,10,10,10	0
57	MG	RA	3156	1/1	0.93	0.14	20,20,20,20	0
57	MG	YA	3113	1/1	0.93	0.15	75,75,75,75	0
57	MG	YA	3114	1/1	0.93	0.21	33,33,33,33	0
57	MG	YA	3029	1/1	0.93	0.18	10,10,10,10	0
57	MG	YA	3315	1/1	0.93	0.09	40,40,40,40	0
57	MG	QA	1607	1/1	0.93	0.05	44,44,44,44	0
57	MG	YA	3031	1/1	0.93	0.20	35,35,35,35	0
57	MG	XA	1683	1/1	0.93	0.07	63,63,63,63	0
57	MG	RA	3192	1/1	0.93	0.10	31,31,31,31	0
57	MG	RA	3071	1/1	0.93	0.11	30,30,30,30	0
57	MG	QA	1688	1/1	0.93	0.09	57,57,57,57	0
57	MG	YA	3323	1/1	0.93	0.18	39,39,39,39	0
57	MG	RA	3162	1/1	0.93	0.13	33,33,33,33	0
57	MG	QA	1648	1/1	0.93	0.10	73,73,73,73	0
57	MG	XA	1692	1/1	0.93	0.12	42,42,42,42	0
57	MG	RA	3254	1/1	0.93	0.15	39,39,39,39	0
57	MG	YA	3233	1/1	0.93	0.21	34,34,34,34	0
57	MG	RA	3132	1/1	0.93	0.17	34,34,34,34	0
57	MG	YA	3332	1/1	0.93	0.14	28,28,28,28	0
57	MG	YA	3051	1/1	0.93	0.11	11,11,11,11	0
57	MG	YA	3237	1/1	0.93	0.12	45,45,45,45	0
57	MG	RA	3203	1/1	0.93	0.16	11,11,11,11	0
57	MG	QA	1640	1/1	0.93	0.18	51,51,51,51	0
57	MG	YD	304	1/1	0.93	0.23	56,56,56,56	0
57	MG	YA	3241	1/1	0.93	0.05	6,6,6,6	0
57	MG	RA	3102	1/1	0.93	0.18	22,22,22,22	0
57	MG	RA	3168	1/1	0.93	0.11	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QA	1672	1/1	0.93	0.12	52,52,52,52	0
57	MG	RA	3017	1/1	0.93	0.26	25,25,25,25	0
57	MG	YP	201	1/1	0.93	0.12	9,9,9,9	0
57	MG	YA	3151	1/1	0.93	0.20	25,25,25,25	0
57	MG	XA	1647	1/1	0.93	0.10	42,42,42,42	0
57	MG	RA	3171	1/1	0.93	0.11	45,45,45,45	0
57	MG	YQ	205	1/1	0.93	0.16	59,59,59,59	0
57	MG	YA	3156	1/1	0.93	0.13	36,36,36,36	0
57	MG	YA	3160	1/1	0.93	0.25	24,24,24,24	0
57	MG	QA	1633	1/1	0.93	0.15	49,49,49,49	0
57	MG	YA	3264	1/1	0.93	0.14	34,34,34,34	0
57	MG	YA	3068	1/1	0.93	0.19	16,16,16,16	0
57	MG	RA	3022	1/1	0.93	0.17	17,17,17,17	0
57	MG	YA	3267	1/1	0.93	0.13	51,51,51,51	0
57	MG	RR	201	1/1	0.94	0.20	33,33,33,33	0
57	MG	XA	1659	1/1	0.94	0.11	10,10,10,10	0
57	MG	RA	3224	1/1	0.94	0.16	26,26,26,26	0
57	MG	YA	3093	1/1	0.94	0.10	30,30,30,30	0
57	MG	RA	3028	1/1	0.94	0.13	20,20,20,20	0
57	MG	RA	3157	1/1	0.94	0.23	11,11,11,11	0
57	MG	XA	1668	1/1	0.94	0.18	24,24,24,24	0
57	MG	RA	3273	1/1	0.94	0.25	47,47,47,47	0
57	MG	RA	3129	1/1	0.94	0.17	37,37,37,37	0
57	MG	RA	3052	1/1	0.94	0.13	23,23,23,23	0
57	MG	QA	1608	1/1	0.94	0.12	45,45,45,45	0
57	MG	QA	1622	1/1	0.94	0.20	28,28,28,28	0
57	MG	RA	3235	1/1	0.94	0.05	22,22,22,22	0
57	MG	YA	3022	1/1	0.94	0.16	39,39,39,39	0
57	MG	QA	1616	1/1	0.94	0.12	43,43,43,43	0
57	MG	RA	3084	1/1	0.94	0.15	19,19,19,19	0
57	MG	YA	3025	1/1	0.94	0.09	2,2,2,2	0
57	MG	QA	1681	1/1	0.94	0.10	53,53,53,53	0
57	MG	RA	3194	1/1	0.94	0.23	46,46,46,46	0
57	MG	QA	1606	1/1	0.94	0.28	40,40,40,40	0
57	MG	YA	3032	1/1	0.94	0.15	21,21,21,21	0
57	MG	XA	1682	1/1	0.94	0.11	41,41,41,41	0
57	MG	YA	3116	1/1	0.94	0.31	28,28,28,28	0
57	MG	YA	3212	1/1	0.94	0.17	27,27,27,27	0
57	MG	RA	3015	1/1	0.94	0.24	29,29,29,29	0
57	MG	YA	3118	1/1	0.94	0.18	42,42,42,42	0
57	MG	XA	1622	1/1	0.94	0.17	15,15,15,15	0
57	MG	RA	3291	1/1	0.94	0.05	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3122	1/1	0.94	0.15	44,44,44,44	0
57	MG	YA	3039	1/1	0.94	0.19	13,13,13,13	0
57	MG	XA	1628	1/1	0.94	0.06	47,47,47,47	0
57	MG	YA	3130	1/1	0.94	0.11	31,31,31,31	0
57	MG	YA	3131	1/1	0.94	0.10	36,36,36,36	0
57	MG	RA	3060	1/1	0.94	0.16	10,10,10,10	0
57	MG	QA	1667	1/1	0.94	0.13	64,64,64,64	0
57	MG	YA	3047	1/1	0.94	0.15	33,33,33,33	0
57	MG	XA	1691	1/1	0.94	0.13	49,49,49,49	0
57	MG	RA	3202	1/1	0.94	0.24	20,20,20,20	0
57	MG	RA	3062	1/1	0.94	0.12	36,36,36,36	0
57	MG	XA	1694	1/1	0.94	0.13	20,20,20,20	0
57	MG	XA	1633	1/1	0.94	0.12	49,49,49,49	0
57	MG	RA	3204	1/1	0.94	0.14	26,26,26,26	0
57	MG	YA	3330	1/1	0.94	0.08	38,38,38,38	0
57	MG	QA	1638	1/1	0.94	0.11	32,32,32,32	0
57	MG	RA	3067	1/1	0.94	0.07	21,21,21,21	0
57	MG	RA	3300	1/1	0.94	0.12	38,38,38,38	0
57	MG	RA	3251	1/1	0.94	0.09	14,14,14,14	0
57	MG	RA	3118	1/1	0.94	0.16	33,33,33,33	0
57	MG	YA	3064	1/1	0.94	0.21	14,14,14,14	0
57	MG	YD	303	1/1	0.94	0.16	25,25,25,25	0
57	MG	QA	1653	1/1	0.94	0.14	38,38,38,38	0
57	MG	YA	3067	1/1	0.94	0.18	31,31,31,31	0
57	MG	YA	3157	1/1	0.94	0.23	4,4,4,4	0
57	MG	QA	1632	1/1	0.94	0.13	40,40,40,40	0
57	MG	RA	3260	1/1	0.94	0.27	46,46,46,46	0
57	MG	RA	3123	1/1	0.94	0.21	50,50,50,50	0
57	MG	Y1	101	1/1	0.94	0.12	44,44,44,44	0
57	MG	YA	3074	1/1	0.94	0.23	22,22,22,22	0
57	MG	RD	302	1/1	0.94	0.06	27,27,27,27	0
57	MG	YA	3166	1/1	0.94	0.13	42,42,42,42	0
57	MG	RA	3262	1/1	0.94	0.12	39,39,39,39	0
57	MG	YR	201	1/1	0.94	0.06	34,34,34,34	0
57	MG	RA	3003	1/1	0.94	0.13	30,30,30,30	0
57	MG	RA	3218	1/1	0.94	0.16	33,33,33,33	0
57	MG	RA	3265	1/1	0.94	0.12	41,41,41,41	0
57	MG	YA	3086	1/1	0.94	0.22	34,34,34,34	0
57	MG	RA	3098	1/1	0.94	0.20	49,49,49,49	0
57	MG	RA	3005	1/1	0.94	0.20	36,36,36,36	0
57	MG	YA	3278	1/1	0.94	0.10	37,37,37,37	0
57	MG	YA	3075	1/1	0.95	0.13	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QA	1691	1/1	0.95	0.15	44,44,44,44	0
57	MG	YA	3079	1/1	0.95	0.11	12,12,12,12	0
57	MG	RA	3083	1/1	0.95	0.14	36,36,36,36	0
57	MG	YA	3271	1/1	0.95	0.11	26,26,26,26	0
57	MG	RA	3049	1/1	0.95	0.17	10,10,10,10	0
57	MG	RA	3200	1/1	0.95	0.18	10,10,10,10	0
57	MG	QA	1680	1/1	0.95	0.17	35,35,35,35	0
57	MG	RA	3006	1/1	0.95	0.11	35,35,35,35	0
57	MG	YA	3007	1/1	0.95	0.15	37,37,37,37	0
57	MG	XA	1655	1/1	0.95	0.16	24,24,24,24	0
57	MG	RA	3122	1/1	0.95	0.19	21,21,21,21	0
57	MG	YA	3090	1/1	0.95	0.14	21,21,21,21	0
57	MG	RA	3087	1/1	0.95	0.14	10,10,10,10	0
57	MG	YA	3176	1/1	0.95	0.16	30,30,30,30	0
57	MG	RA	3163	1/1	0.95	0.08	27,27,27,27	0
57	MG	RA	3026	1/1	0.95	0.27	12,12,12,12	0
57	MG	XA	1664	1/1	0.95	0.12	40,40,40,40	0
57	MG	XA	1601	1/1	0.95	0.09	17,17,17,17	0
57	MG	YA	3181	1/1	0.95	0.06	61,61,61,61	0
57	MG	YA	3016	1/1	0.95	0.20	4,4,4,4	0
57	MG	YA	3098	1/1	0.95	0.10	56,56,56,56	0
57	MG	YA	3017	1/1	0.95	0.11	1,1,1,1	0
57	MG	YA	3186	1/1	0.95	0.07	33,33,33,33	0
57	MG	QA	1654	1/1	0.95	0.16	22,22,22,22	0
57	MG	YA	3293	1/1	0.95	0.06	46,46,46,46	0
57	MG	RA	3008	1/1	0.95	0.11	31,31,31,31	0
57	MG	XA	1669	1/1	0.95	0.11	34,34,34,34	0
57	MG	YA	3296	1/1	0.95	0.15	40,40,40,40	0
57	MG	RA	3030	1/1	0.95	0.16	36,36,36,36	0
57	MG	QA	1636	1/1	0.95	0.11	33,33,33,33	0
57	MG	RA	3010	1/1	0.95	0.21	42,42,42,42	0
57	MG	RA	3213	1/1	0.95	0.10	25,25,25,25	0
57	MG	RA	3216	1/1	0.95	0.24	29,29,29,29	0
57	MG	QA	1683	1/1	0.95	0.25	51,51,51,51	0
57	MG	XA	1611	1/1	0.95	0.24	31,31,31,31	0
57	MG	YA	3199	1/1	0.95	0.18	10,10,10,10	0
57	MG	YA	3201	1/1	0.95	0.21	21,21,21,21	0
57	MG	YA	3202	1/1	0.95	0.24	22,22,22,22	0
57	MG	RA	3034	1/1	0.95	0.13	1,1,1,1	0
57	MG	QA	1603	1/1	0.95	0.05	33,33,33,33	0
57	MG	RA	3065	1/1	0.95	0.13	7,7,7,7	0
57	MG	RA	3225	1/1	0.95	0.13	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3135	1/1	0.95	0.08	34,34,34,34	0
57	MG	RA	3036	1/1	0.95	0.21	35,35,35,35	0
57	MG	XA	1621	1/1	0.95	0.12	10,10,10,10	0
57	MG	QA	1676	1/1	0.95	0.08	27,27,27,27	0
57	MG	YA	3120	1/1	0.95	0.11	24,24,24,24	0
57	MG	XA	1623	1/1	0.95	0.06	40,40,40,40	0
57	MG	YA	3045	1/1	0.95	0.09	11,11,11,11	0
57	MG	RA	3229	1/1	0.95	0.20	45,45,45,45	0
57	MG	XA	1626	1/1	0.95	0.07	38,38,38,38	0
57	MG	YA	3128	1/1	0.95	0.20	4,4,4,4	0
57	MG	YA	3326	1/1	0.95	0.15	22,22,22,22	0
57	MG	YA	3225	1/1	0.95	0.10	31,31,31,31	0
57	MG	QA	1687	1/1	0.95	0.06	46,46,46,46	0
57	MG	RA	3016	1/1	0.95	0.10	24,24,24,24	0
57	MG	RA	3140	1/1	0.95	0.10	23,23,23,23	0
57	MG	RA	3181	1/1	0.95	0.19	7,7,7,7	0
57	MG	QA	1660	1/1	0.95	0.10	25,25,25,25	0
57	MG	RA	3073	1/1	0.95	0.06	50,50,50,50	0
57	MG	RA	3184	1/1	0.95	0.16	45,45,45,45	0
57	MG	YA	3058	1/1	0.95	0.23	28,28,28,28	0
57	MG	RA	3042	1/1	0.95	0.12	24,24,24,24	0
57	MG	YD	302	1/1	0.95	0.18	1,1,1,1	0
57	MG	RA	3075	1/1	0.95	0.15	11,11,11,11	0
57	MG	XA	1637	1/1	0.95	0.14	43,43,43,43	0
57	MG	YA	3062	1/1	0.95	0.16	23,23,23,23	0
57	MG	QA	1661	1/1	0.95	0.14	26,26,26,26	0
57	MG	YA	3147	1/1	0.95	0.04	37,37,37,37	0
57	MG	RA	3044	1/1	0.95	0.12	5,5,5,5	0
57	MG	YA	3252	1/1	0.95	0.12	23,23,23,23	0
57	MG	YO	201	1/1	0.95	0.23	57,57,57,57	0
57	MG	YA	3253	1/1	0.95	0.10	23,23,23,23	0
57	MG	RA	3078	1/1	0.95	0.12	52,52,52,52	0
57	MG	YA	3255	1/1	0.95	0.05	35,35,35,35	0
57	MG	RA	3002	1/1	0.95	0.07	23,23,23,23	0
57	MG	RA	3151	1/1	0.95	0.20	36,36,36,36	0
57	MG	XA	1643	1/1	0.95	0.09	29,29,29,29	0
57	MG	YA	3259	1/1	0.95	0.06	19,19,19,19	0
57	MG	YA	3155	1/1	0.95	0.05	61,61,61,61	0
57	MG	Y3	101	1/1	0.95	0.15	11,11,11,11	0
57	MG	RA	3113	1/1	0.95	0.16	19,19,19,19	0
57	MG	YA	3263	1/1	0.95	0.13	28,28,28,28	0
57	MG	YA	3158	1/1	0.95	0.06	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	RA	3046	1/1	0.95	0.14	31,31,31,31	0
57	MG	RA	3217	1/1	0.96	0.11	21,21,21,21	0
57	MG	XA	1681	1/1	0.96	0.11	35,35,35,35	0
57	MG	YA	3053	1/1	0.96	0.16	25,25,25,25	0
57	MG	RA	3196	1/1	0.96	0.06	33,33,33,33	0
57	MG	RA	3104	1/1	0.96	0.18	12,12,12,12	0
57	MG	XA	1646	1/1	0.96	0.11	30,30,30,30	0
57	MG	YA	3300	1/1	0.96	0.19	56,56,56,56	0
57	MG	YA	3234	1/1	0.96	0.25	47,47,47,47	0
57	MG	XA	1614	1/1	0.96	0.06	66,66,66,66	0
57	MG	RA	3180	1/1	0.96	0.08	24,24,24,24	0
57	MG	XA	1688	1/1	0.96	0.14	49,49,49,49	0
57	MG	YA	3013	1/1	0.96	0.16	38,38,38,38	0
57	MG	QA	1669	1/1	0.96	0.09	38,38,38,38	0
57	MG	QA	1647	1/1	0.96	0.14	37,37,37,37	0
57	MG	YA	3243	1/1	0.96	0.18	33,33,33,33	0
57	MG	RA	3051	1/1	0.96	0.10	27,27,27,27	0
57	MG	YA	3247	1/1	0.96	0.08	29,29,29,29	0
57	MG	RA	3278	1/1	0.96	0.17	47,47,47,47	0
57	MG	RE	301	1/1	0.96	0.16	21,21,21,21	0
57	MG	QA	1631	1/1	0.96	0.11	64,64,64,64	0
57	MG	YA	3069	1/1	0.96	0.11	19,19,19,19	0
57	MG	RA	3109	1/1	0.96	0.12	35,35,35,35	0
57	MG	XA	1625	1/1	0.96	0.20	24,24,24,24	0
57	MG	YA	3182	1/1	0.96	0.23	19,19,19,19	0
57	MG	XA	1697	1/1	0.96	0.17	22,22,22,22	0
57	MG	QA	1685	1/1	0.96	0.06	34,34,34,34	0
57	MG	XA	1663	1/1	0.96	0.07	16,16,16,16	0
57	MG	YA	3076	1/1	0.96	0.09	21,21,21,21	0
57	MG	RA	3206	1/1	0.96	0.18	25,25,25,25	0
57	MG	YA	3078	1/1	0.96	0.13	31,31,31,31	0
57	MG	YA	3027	1/1	0.96	0.09	12,12,12,12	0
57	MG	RA	3257	1/1	0.96	0.07	36,36,36,36	0
57	MG	RA	3125	1/1	0.96	0.09	21,21,21,21	0
57	MG	YA	3083	1/1	0.96	0.07	17,17,17,17	0
57	MG	XM	201	1/1	0.96	0.04	52,52,52,52	0
57	MG	YA	3268	1/1	0.96	0.05	37,37,37,37	0
57	MG	RA	3233	1/1	0.96	0.24	28,28,28,28	0
57	MG	QA	1601	1/1	0.96	0.11	28,28,28,28	0
57	MG	YB	203	1/1	0.96	0.17	28,28,28,28	0
57	MG	QA	1627	1/1	0.96	0.07	34,34,34,34	0
57	MG	RA	3292	1/1	0.96	0.10	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	Y0	101	1/1	0.96	0.07	9,9,9,9	0
57	MG	YA	3145	1/1	0.96	0.12	14,14,14,14	0
57	MG	YA	3146	1/1	0.96	0.10	21,21,21,21	0
57	MG	YA	3204	1/1	0.96	0.12	18,18,18,18	0
57	MG	RA	3159	1/1	0.96	0.09	32,32,32,32	0
57	MG	YA	3148	1/1	0.96	0.14	23,23,23,23	0
57	MG	YA	3040	1/1	0.96	0.05	16,16,16,16	0
57	MG	YA	3041	1/1	0.96	0.13	20,20,20,20	0
57	MG	RA	3068	1/1	0.96	0.18	12,12,12,12	0
57	MG	RA	3114	1/1	0.96	0.10	29,29,29,29	0
57	MG	YA	3213	1/1	0.96	0.07	16,16,16,16	0
57	MG	YA	3153	1/1	0.96	0.05	30,30,30,30	0
57	MG	YA	3285	1/1	0.96	0.09	36,36,36,36	0
57	MG	RA	3018	1/1	0.96	0.15	10,10,10,10	0
57	MG	RA	3267	1/1	0.96	0.05	32,32,32,32	0
57	MG	XA	1608	1/1	0.96	0.11	28,28,28,28	0
57	MG	QE	201	1/1	0.96	0.21	42,42,42,42	0
57	MG	RA	3269	1/1	0.96	0.12	34,34,34,34	0
57	MG	YA	3159	1/1	0.96	0.10	23,23,23,23	0
57	MG	YA	3050	1/1	0.96	0.16	22,22,22,22	0
57	MG	YA	3226	1/1	0.96	0.16	27,27,27,27	0
57	MG	YA	3245	1/1	0.97	0.20	24,24,24,24	0
57	MG	RA	3249	1/1	0.97	0.11	28,28,28,28	0
57	MG	YA	3144	1/1	0.97	0.07	25,25,25,25	0
57	MG	XA	1658	1/1	0.97	0.18	34,34,34,34	0
57	MG	YA	3250	1/1	0.97	0.12	35,35,35,35	0
57	MG	YA	3306	1/1	0.97	0.14	48,48,48,48	0
57	MG	YA	3307	1/1	0.97	0.05	24,24,24,24	0
57	MG	YA	3308	1/1	0.97	0.11	30,30,30,30	0
57	MG	RA	3199	1/1	0.97	0.17	17,17,17,17	0
57	MG	XA	1660	1/1	0.97	0.06	23,23,23,23	0
57	MG	QA	1609	1/1	0.97	0.08	31,31,31,31	0
57	MG	XA	1662	1/1	0.97	0.06	22,22,22,22	0
57	MG	XA	1627	1/1	0.97	0.08	37,37,37,37	0
57	MG	YA	3197	1/1	0.97	0.04	42,42,42,42	0
57	MG	YA	3106	1/1	0.97	0.12	25,25,25,25	0
57	MG	RA	3252	1/1	0.97	0.06	29,29,29,29	0
57	MG	YA	3200	1/1	0.97	0.22	23,23,23,23	0
57	MG	YA	3318	1/1	0.97	0.13	41,41,41,41	0
57	MG	RA	3284	1/1	0.97	0.05	16,16,16,16	0
57	MG	RA	3144	1/1	0.97	0.04	27,27,27,27	0
57	MG	RA	3145	1/1	0.97	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3070	1/1	0.97	0.09	25,25,25,25	0
57	MG	RA	3027	1/1	0.97	0.15	23,23,23,23	0
57	MG	QA	1629	1/1	0.97	0.05	33,33,33,33	0
57	MG	RA	3230	1/1	0.97	0.11	33,33,33,33	0
57	MG	RA	3040	1/1	0.97	0.12	10,10,10,10	0
57	MG	RA	3054	1/1	0.97	0.18	14,14,14,14	0
57	MG	RA	3187	1/1	0.97	0.14	5,5,5,5	0
57	MG	QA	1644	1/1	0.97	0.11	43,43,43,43	0
57	MG	RA	3001	1/1	0.97	0.13	8,8,8,8	0
57	MG	YA	3216	1/1	0.97	0.13	14,14,14,14	0
57	MG	YA	3217	1/1	0.97	0.05	37,37,37,37	0
57	MG	YA	3218	1/1	0.97	0.05	10,10,10,10	0
57	MG	RA	3019	1/1	0.97	0.11	13,13,13,13	0
57	MG	YA	3080	1/1	0.97	0.07	37,37,37,37	0
57	MG	QA	1663	1/1	0.97	0.16	36,36,36,36	0
57	MG	YA	3123	1/1	0.97	0.18	17,17,17,17	0
57	MG	RA	3011	1/1	0.97	0.05	30,30,30,30	0
57	MG	YA	3125	1/1	0.97	0.05	36,36,36,36	0
57	MG	YA	3126	1/1	0.97	0.11	15,15,15,15	0
57	MG	YA	3043	1/1	0.97	0.16	13,13,13,13	0
57	MG	YE	302	1/1	0.97	0.09	25,25,25,25	0
57	MG	YA	3227	1/1	0.97	0.20	36,36,36,36	0
57	MG	RA	3121	1/1	0.97	0.20	50,50,50,50	0
57	MG	RA	3214	1/1	0.97	0.17	35,35,35,35	0
57	MG	RA	3215	1/1	0.97	0.15	21,21,21,21	0
57	MG	XA	1615	1/1	0.97	0.11	28,28,28,28	0
57	MG	XA	1616	1/1	0.97	0.10	37,37,37,37	0
57	MG	YQ	201	1/1	0.97	0.12	58,58,58,58	0
57	MG	QA	1678	1/1	0.97	0.05	33,33,33,33	0
57	MG	RA	3004	1/1	0.97	0.10	26,26,26,26	0
57	MG	QA	1659	1/1	0.97	0.14	44,44,44,44	0
57	MG	RA	3275	1/1	0.97	0.23	40,40,40,40	0
57	MG	RA	3064	1/1	0.97	0.13	20,20,20,20	0
57	MG	YA	3238	1/1	0.97	0.16	27,27,27,27	0
57	MG	XA	1653	1/1	0.97	0.16	17,17,17,17	0
57	MG	RA	3220	1/1	0.97	0.13	34,34,34,34	0
57	MG	RA	3095	1/1	0.97	0.18	28,28,28,28	0
57	MG	YA	3242	1/1	0.97	0.14	10,10,10,10	0
59	ZN	XN	101	1/1	0.97	0.05	90,90,90,90	0
57	MG	YA	3188	1/1	0.97	0.17	8,8,8,8	0
57	MG	YA	3244	1/1	0.97	0.30	37,37,37,37	0
57	MG	RA	3070	1/1	0.98	0.12	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3035	1/1	0.98	0.17	2,2,2,2	0
57	MG	YA	3333	1/1	0.98	0.12	36,36,36,36	0
57	MG	RA	3259	1/1	0.98	0.15	26,26,26,26	0
57	MG	RA	3290	1/1	0.98	0.07	11,11,11,11	0
57	MG	YB	201	1/1	0.98	0.10	11,11,11,11	0
57	MG	YA	3206	1/1	0.98	0.12	14,14,14,14	0
57	MG	YA	3038	1/1	0.98	0.10	6,6,6,6	0
57	MG	YA	3208	1/1	0.98	0.18	17,17,17,17	0
57	MG	XA	1684	1/1	0.98	0.11	53,53,53,53	0
57	MG	YA	3065	1/1	0.98	0.07	38,38,38,38	0
57	MG	RA	3221	1/1	0.98	0.11	16,16,16,16	0
57	MG	XA	1665	1/1	0.98	0.05	34,34,34,34	0
57	MG	RA	3080	1/1	0.98	0.08	50,50,50,50	0
57	MG	YA	3214	1/1	0.98	0.15	22,22,22,22	0
57	MG	RA	3048	1/1	0.98	0.10	23,23,23,23	0
57	MG	RP	201	1/1	0.98	0.13	33,33,33,33	0
57	MG	YF	301	1/1	0.98	0.04	32,32,32,32	0
57	MG	RA	3063	1/1	0.98	0.22	12,12,12,12	0
57	MG	YA	3099	1/1	0.98	0.11	19,19,19,19	0
57	MG	QA	1674	1/1	0.98	0.15	36,36,36,36	0
57	MG	RA	3238	1/1	0.98	0.14	23,23,23,23	0
57	MG	YA	3129	1/1	0.98	0.09	25,25,25,25	0
57	MG	QA	1658	1/1	0.98	0.15	20,20,20,20	0
57	MG	RA	3281	1/1	0.98	0.18	44,44,44,44	0
57	MG	YA	3132	1/1	0.98	0.14	21,21,21,21	0
57	MG	XA	1654	1/1	0.98	0.15	28,28,28,28	0
57	MG	QA	1666	1/1	0.98	0.07	22,22,22,22	0
58	SF4	QD	302	8/8	0.98	0.07	59,76,106,109	0
58	SF4	XD	301	8/8	0.98	0.07	68,75,103,103	0
57	MG	YA	3028	1/1	0.98	0.05	14,14,14,14	0
57	MG	RA	3021	1/1	0.98	0.10	19,19,19,19	0
57	MG	QV	103	1/1	0.98	0.14	33,33,33,33	0
57	MG	RA	3256	1/1	0.98	0.19	37,37,37,37	0
57	MG	YA	3056	1/1	0.98	0.14	15,15,15,15	0
57	MG	QA	1670	1/1	0.98	0.12	37,37,37,37	0
57	MG	RA	3287	1/1	0.98	0.07	42,42,42,42	0
57	MG	RA	3253	1/1	0.99	0.06	10,10,10,10	0
57	MG	QA	1690	1/1	0.99	0.05	13,13,13,13	0
57	MG	RA	3153	1/1	0.99	0.04	23,23,23,23	0
57	MG	YA	3026	1/1	0.99	0.19	16,16,16,16	0
57	MG	YA	3170	1/1	0.99	0.03	56,56,56,56	0
57	MG	QA	1604	1/1	0.99	0.06	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	ZN	QN	101	1/1	0.99	0.05	112,112,112,112	0
57	MG	YA	3172	1/1	0.99	0.09	21,21,21,21	0
57	MG	QA	1655	1/1	0.99	0.11	33,33,33,33	0
57	MG	Y0	102	1/1	0.99	0.18	24,24,24,24	0
57	MG	QA	1668	1/1	0.99	0.06	44,44,44,44	0
57	MG	YA	3094	1/1	0.99	0.09	27,27,27,27	0
57	MG	YA	3249	1/1	0.99	0.05	18,18,18,18	0
57	MG	RA	3222	1/1	0.99	0.09	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.