wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2026 – 01:34 PM EDT

PDB ID	:	6NUO / pdb_00006nuo
Title	:	Modified tRNA(Pro) bound to Thermus thermophilus 70S (cognate)
Authors	:	Hoffer, E.D.; Subaramanian, S.; Hong, S.; Maehigashi, T.; Dunham, C.M.
Deposited on	:	2019-02-01
Resolution	:	3.20 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:

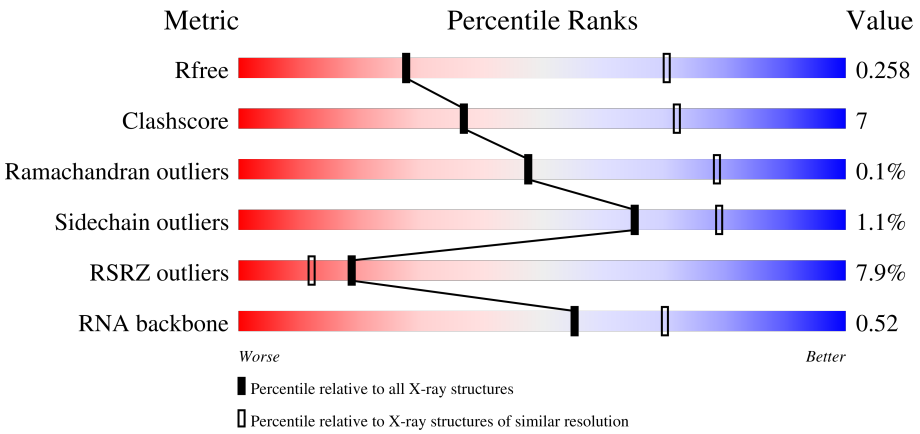
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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	5% 52% 39% 8% •
1	XA	1521	7% 53% 36% 9% •
2	QB	256	% 64% 26% • 8%
2	XB	256	7% 62% 28% • 8%

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Mol	Chain	Length	Quality of chain
3	QC	239	8% 61% 23% • 14%
3	XC	239	18% 66% 19% • 14%
4	QD	209	6% 76% 22% •
4	XD	209	25% 65% 30% •
5	QE	162	3% 66% 25% • 7%
5	XE	162	11% 75% 19% 7%
6	QF	101	8% 75% 24% •
6	XF	101	% 79% 20% •
7	QG	156	19% 78% 21% •
7	XG	156	22% 73% 24% • •
8	QH	138	4% 75% 24% •
8	XH	138	8% 75% 23% • •
9	QI	128	55% 69% 27% • •
9	XI	128	27% 59% 33% 6% •
10	QJ	105	20% 54% 36% • 6%
10	XJ	105	32% 66% 23% • 9%
11	QK	129	13% 64% 25% • 8%
11	XK	129	7% 71% 18% • 10%
12	QL	132	20% 77% 16% • 5%
12	XL	132	18% 67% 20% 5% 8%
13	QM	126	18% 63% 29% • 5%
13	XM	126	40% 52% 39% • 6%
14	QN	61	33% 51% 44% • •
14	XN	61	16% 75% 20% • •
15	QO	89	6% 84% 13% • •

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Mol	Chain	Length	Quality of chain
15	XO	89	3% 82% 16%
16	QP	88	2% 68% 26% 5%
16	XP	88	11% 69% 24% 5%
17	QQ	105	11% 62% 30% 5%
17	XQ	105	6% 78% 16% 5%
18	QR	88	7% 61% 18% 20%
18	XR	88	2% 59% 19% 20%
19	QS	93	20% 66% 20% 11%
19	XS	93	31% 58% 29% 10%
20	QT	106	9% 68% 24% 7%
20	XT	106	8% 58% 33% 7%
21	QU	27	33% 81% 11% 7%
21	XU	27	19% 56% 33% 7%
22	QV	77	8% 39% 51% 10%
22	XV	77	34% 48% 42% 10%
23	QX	19	21% 32% 63% 5%
23	XX	19	79% 32% 58% 11%
24	RA	2915	4% 58% 33% 8%
24	YA	2915	3% 63% 29% 7%
25	RB	122	% 69% 25%
25	YB	122	4% 61% 28% 10%
26	RD	276	5% 76% 22%
26	YD	276	2% 83% 15%
27	RE	206	4% 75% 25%
27	YE	206	% 75% 22%

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Mol	Chain	Length	Quality of chain
28	RF	210	4% 73% 23%
28	YF	210	3% 73% 22%
29	RG	182	15% 66% 30%
29	YG	182	12% 65% 32%
30	RH	180	12% 63% 31%
30	YH	180	3% 80% 16%
31	RI	148	14% 70% 26%
31	YI	148	14% 74% 23%
32	RN	140	13% 81% 15%
32	YN	140	% 80% 19%
33	RO	122	% 76% 22%
33	YO	122	4% 80% 20%
34	RP	150	8% 77% 19%
34	YP	150	3% 75% 23%
35	RQ	141	8% 61% 35%
35	YQ	141	% 85% 15%
36	RR	118	4% 75% 23%
36	YR	118	3% 82% 15%
37	RS	112	27% 71% 26%
37	YS	112	% 79% 20%
38	RT	146	5% 64% 25% 6%
38	YT	146	7% 66% 24% 6%
39	RU	118	14% 77% 19%
39	YU	118	6% 82% 14%
40	RV	101	5% 78% 20%

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Mol	Chain	Length	Quality of chain
40	YV	101	2% 82% 13% 5%
41	RW	113	4% 80% 20%
41	YW	113	4% 82% 17%
42	RX	96	5% 81% 14%
42	YX	96	85% 12%
43	RY	110	13% 77% 18%
43	YY	110	% 80% 16%
44	RZ	206	6% 54% 32% 11%
44	YZ	206	% 67% 20% 11%
45	R0	85	15% 71% 24% 5%
45	Y0	85	% 76% 12% 12%
46	R1	98	26% 79% 16%
46	Y1	98	14% 73% 18% 5%
47	R2	72	8% 72% 24%
47	Y2	72	8% 69% 22% 8%
48	R3	60	10% 73% 25%
48	Y3	60	3% 80% 17%
49	R4	71	11% 58% 37%
49	Y4	71	17% 56% 32% 8%
50	R5	60	2% 80% 18%
50	Y5	60	2% 85% 13%
51	R6	54	2% 81% 17%
51	Y6	54	80% 19%
52	R7	49	12% 78% 18%
52	Y7	49	4% 90% 8%

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Mol	Chain	Length	Quality of chain
53	R8	65	28% 60% 37%
53	Y8	65	15% 60% 37%
54	R9	37	3% 78% 22%
54	Y9	37	3% 68% 32%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	RA	3257	-	-	-	X
55	MG	YA	3144	-	-	-	X
55	MG	YA	3406	-	-	-	X

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 291964 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	1500	32247	14353	5981	10414	1499	0	0	0
1	XA	1500	32249	14354	5984	10412	1499	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	84	674	430	126	116	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-Pro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	QV	77	1648	734	295	542	77	0	0	0
22	XV	77	1648	734	295	542	77	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	19	418	186	86	127	19	0	0	0
23	XX	19	418	186	86	127	19	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	RD	274	2135	1347	426	359	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	YD	274	2135	1347	426	359	3	0	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	RN	138	1104	712	206	182	4	0	0	0
32	YN	140	1121	722	208	187	4	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	RP	149	1139	709	231	196	3	0	0	0
34	YP	147	1122	698	229	192	3	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
37	RS	111	882	556	176	150	0	0	0
37	YS	110	877	553	175	149	0	0	0

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	YX	94	742	482	134	125	1	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	R0	81	643	398	137	107	1	0	0	0
45	Y0	75	599	370	127	101	1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	R2	69	581	358	118	104	1	0	0	0
47	Y2	66	558	346	113	98	1	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
55	QA	64	64	64	0	0
55	QV	1	1	1	0	0
55	RA	444	444	444	0	0
55	RB	7	7	7	0	0
55	RE	5	5	5	0	0
55	RF	1	1	1	0	0
55	RN	1	1	1	0	0
55	RQ	1	1	1	0	0
55	RR	1	1	1	0	0
55	RT	1	1	1	0	0
55	RX	1	1	1	0	0
55	R0	2	2	2	0	0
55	R8	2	2	2	0	0
55	XA	78	78	78	0	0

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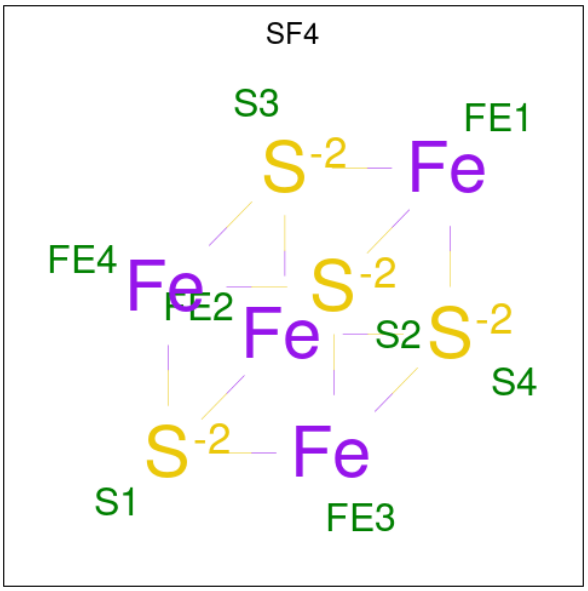
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
55	XE	1	1	1	0	0
55	XM	2	2	2	0	0
55	XV	1	1	1	0	0
55	YA	510	510	510	0	0
55	YB	7	7	7	0	0
55	YD	2	2	2	0	0
55	YE	5	5	5	0	0
55	YP	3	3	3	0	0
55	YQ	3	3	3	0	0
55	YR	1	1	1	0	0
55	Y0	2	2	2	0	0
55	Y1	2	2	2	0	0
55	Y3	1	1	1	0	0
55	Y5	1	1	1	0	0
55	Y7	1	1	1	0	0
55	Y8	1	1	1	0	0

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



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

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

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

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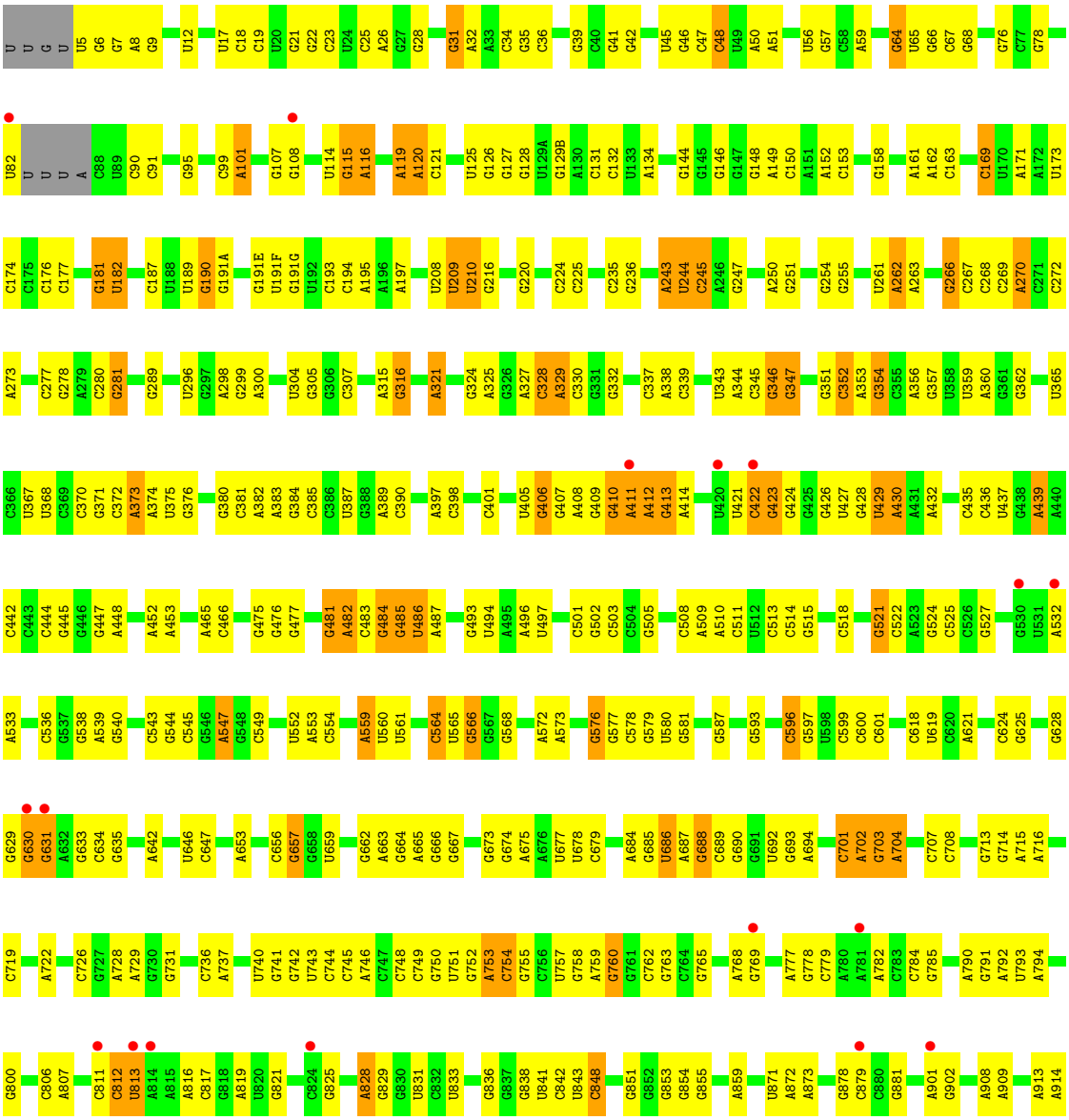
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
57	Y6	1	1	1	0	0
			Total	Zn		
57	Y9	1	1	1	0	0

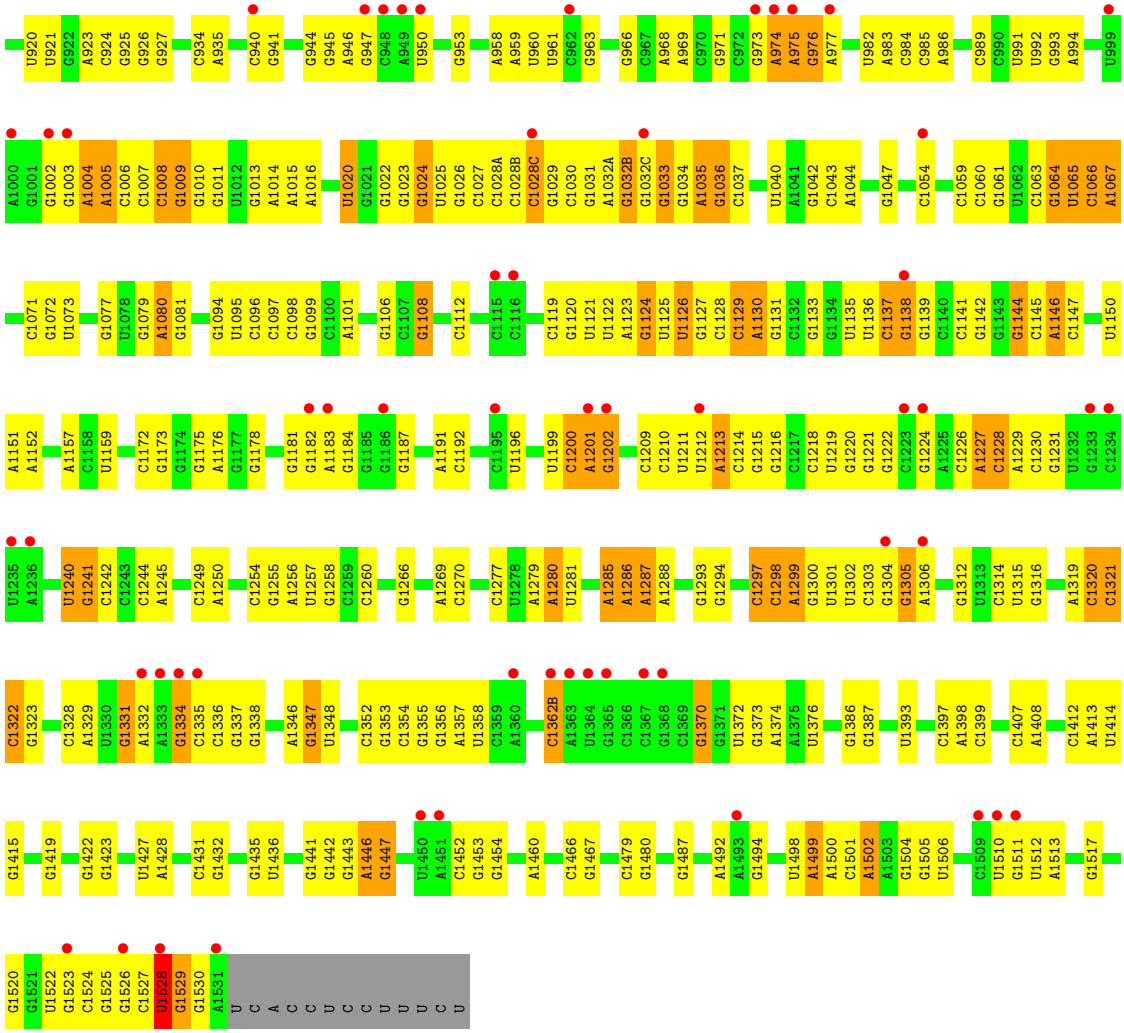
3 Residue-property plots (i)

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

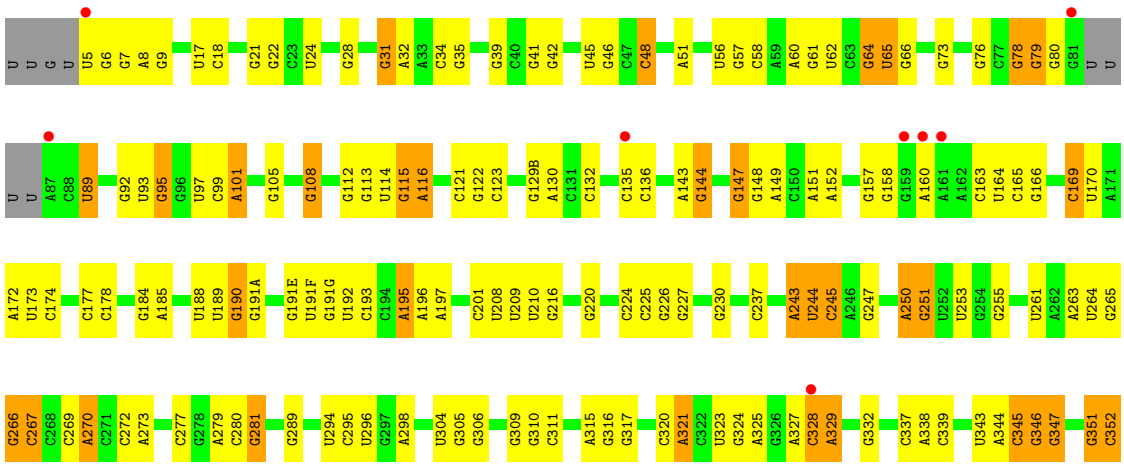
Chain QA:

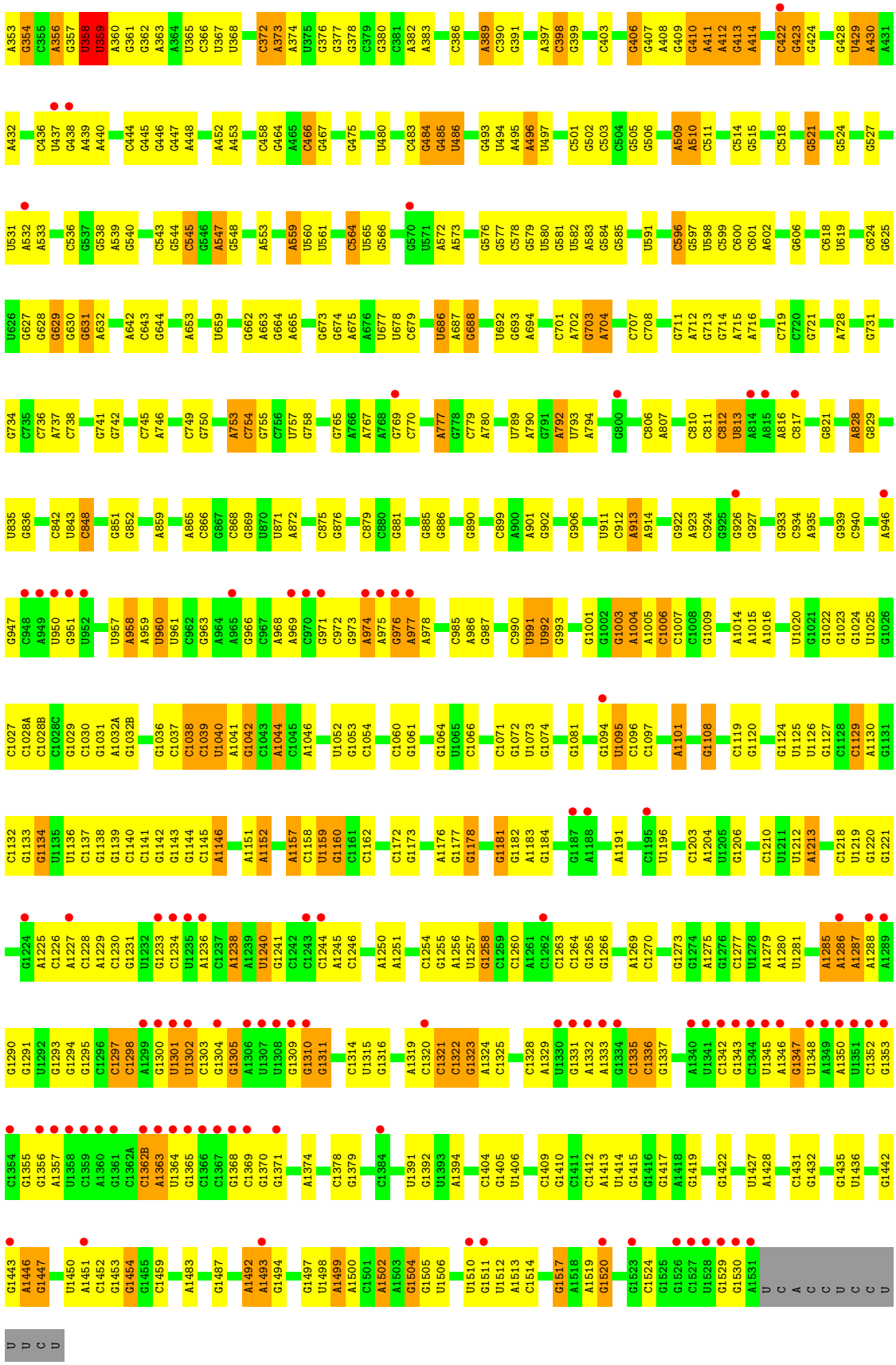




- Molecule 1: 16S rRNA

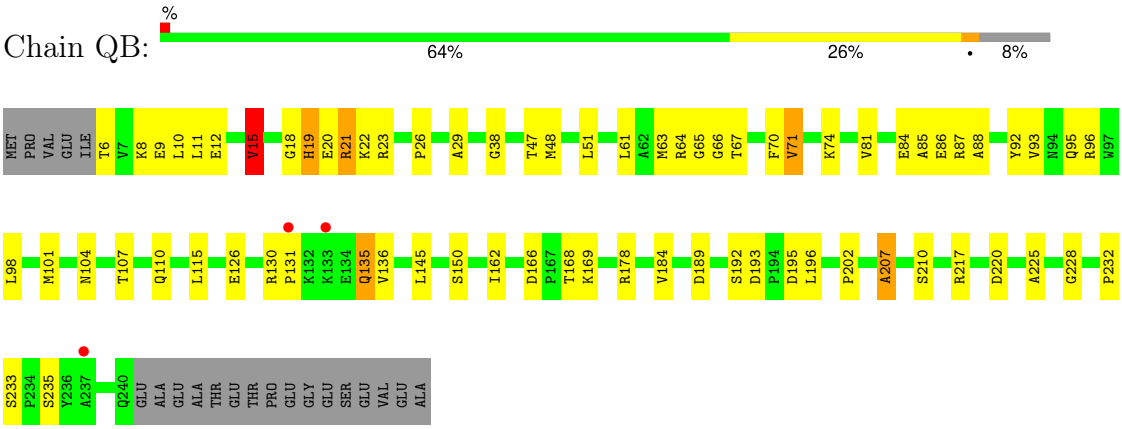
Chain XA:





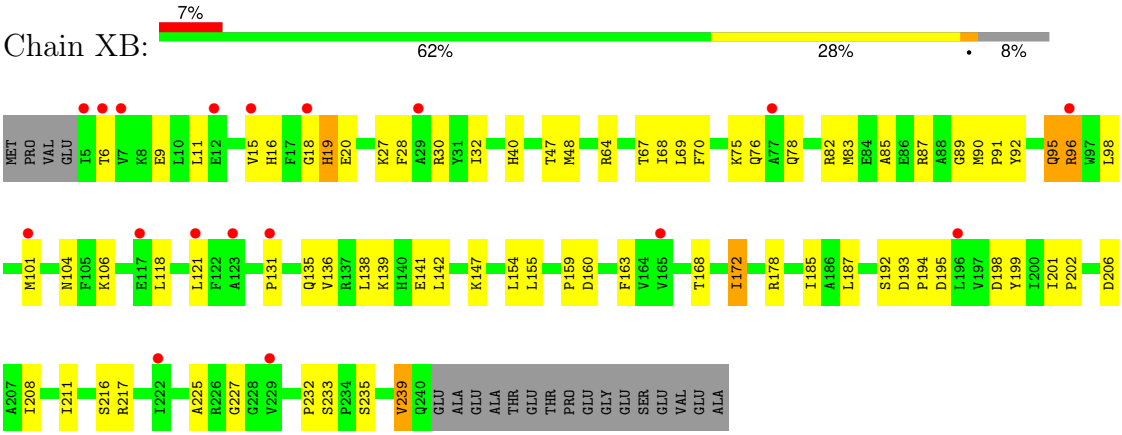
- Molecule 2: 30S ribosomal protein S2

Chain QB:



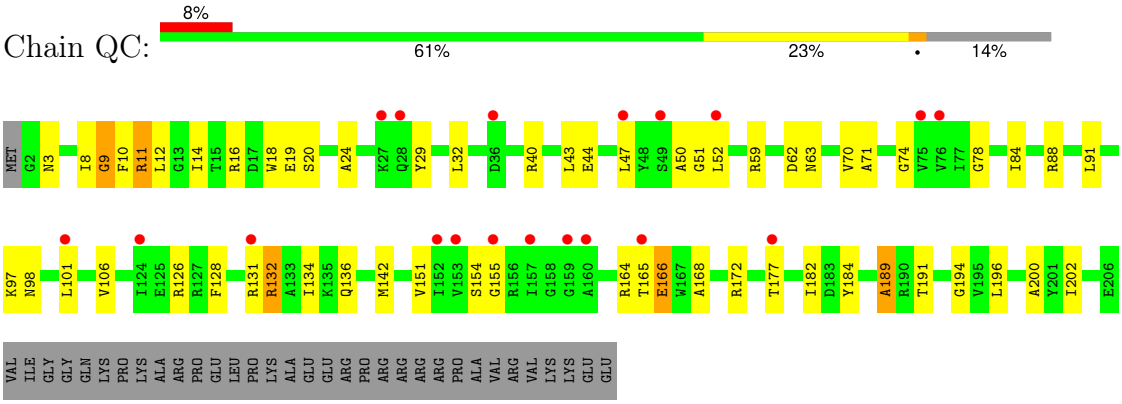
- Molecule 2: 30S ribosomal protein S2

Chain XB:



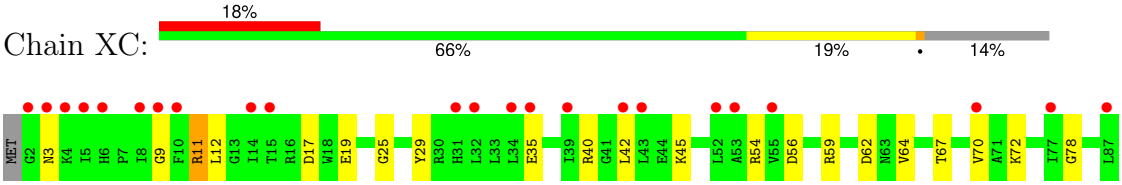
- Molecule 3: 30S ribosomal protein S3

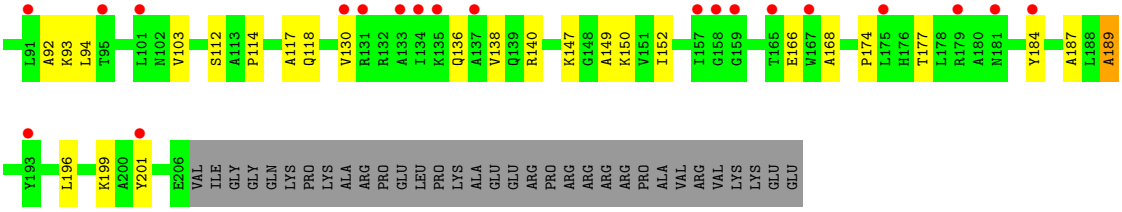
Chain QC:



- Molecule 3: 30S ribosomal protein S3

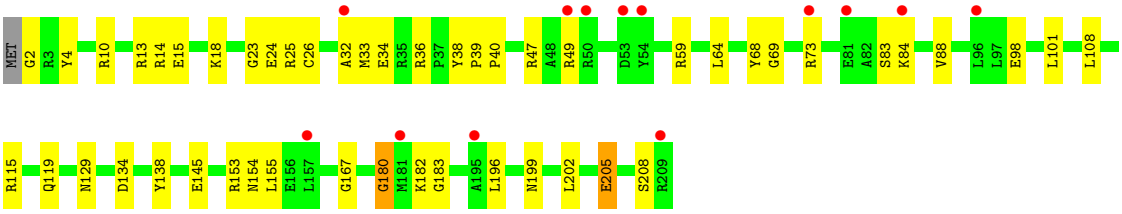
Chain XC:





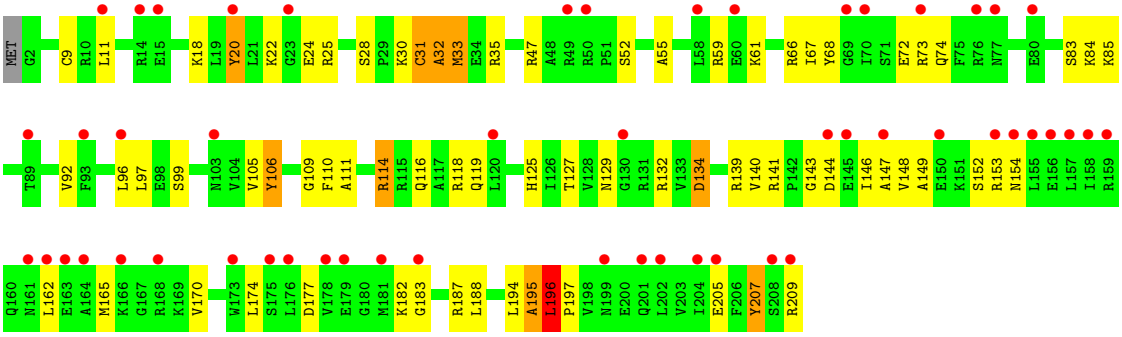
- Molecule 4: 30S ribosomal protein S4

Chain QD:



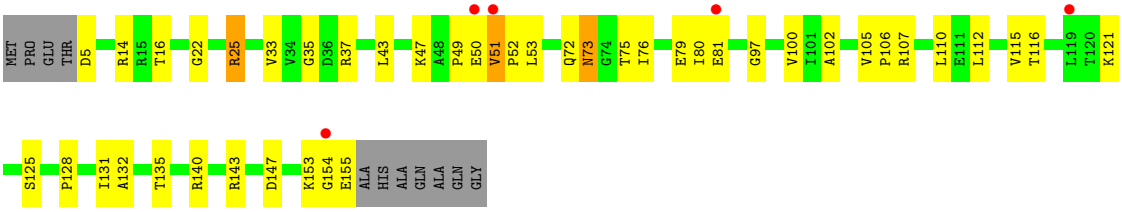
- Molecule 4: 30S ribosomal protein S4

Chain XD:



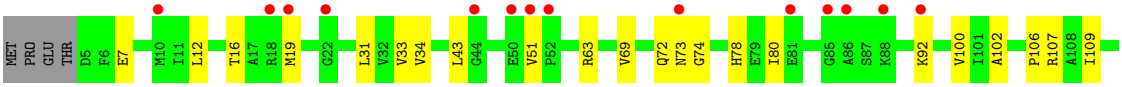
- Molecule 5: 30S ribosomal protein S5

Chain QE:



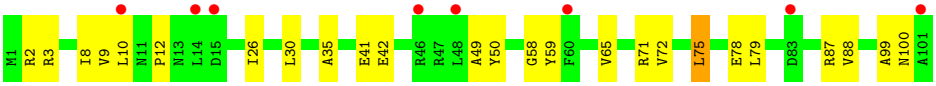
- Molecule 5: 30S ribosomal protein S5

Chain XE:



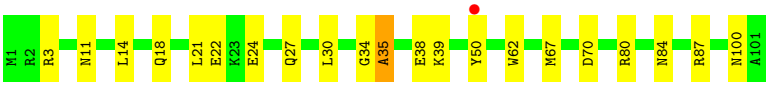
• Molecule 6: 30S ribosomal protein S6

Chain QF:



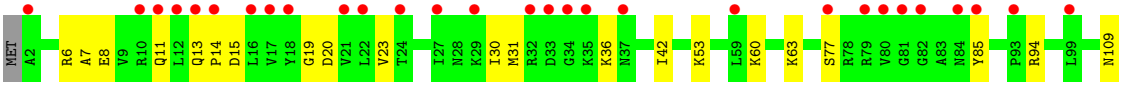
• Molecule 6: 30S ribosomal protein S6

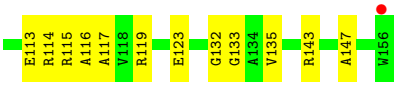
Chain XF:



• Molecule 7: 30S ribosomal protein S7

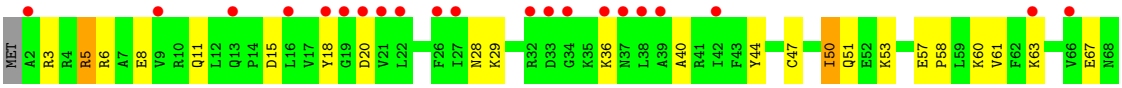
Chain QG:

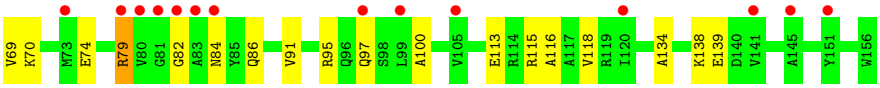




• Molecule 7: 30S ribosomal protein S7

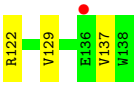
Chain XG:





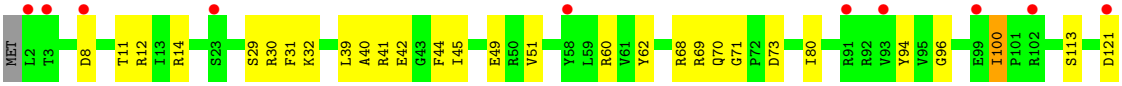
• Molecule 8: 30S ribosomal protein S8

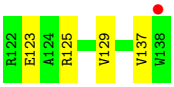
Chain QH:



• Molecule 8: 30S ribosomal protein S8

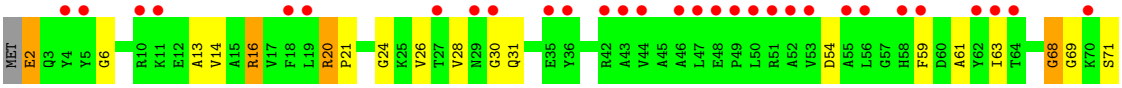
Chain XH:

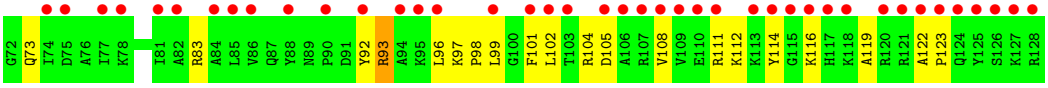




• Molecule 9: 30S ribosomal protein S9

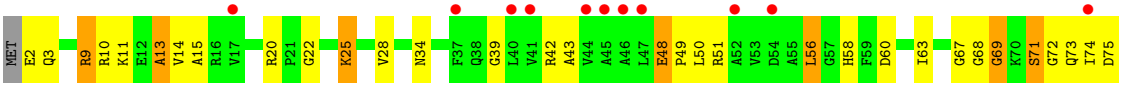
Chain QI:

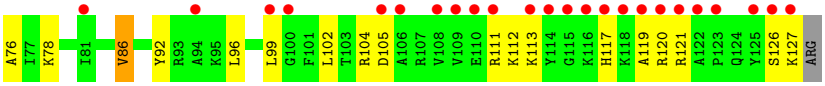




• Molecule 9: 30S ribosomal protein S9

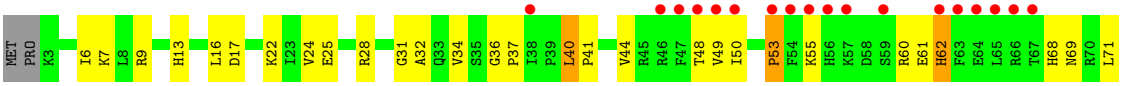
Chain XI:

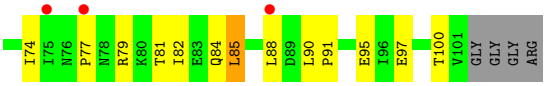




• Molecule 10: 30S ribosomal protein S10

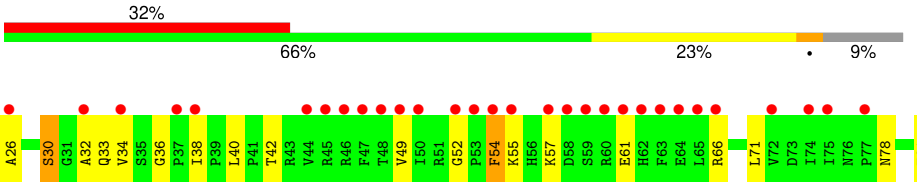
Chain QJ:

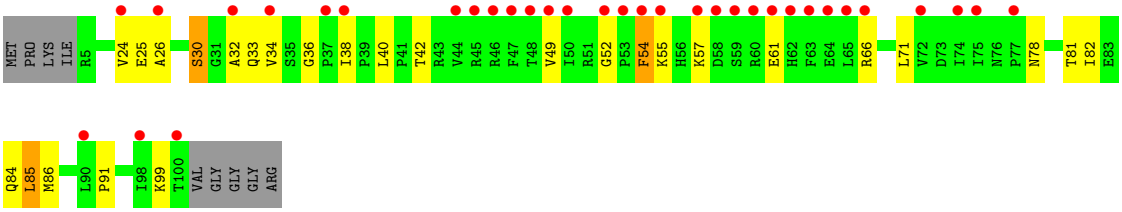




• Molecule 10: 30S ribosomal protein S10

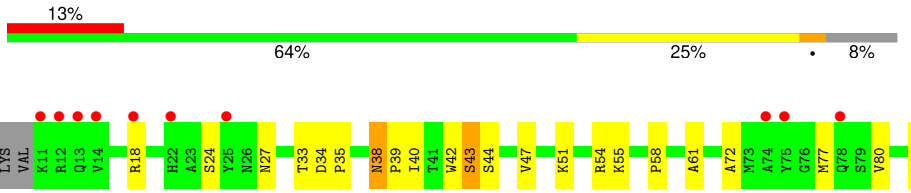
Chain XJ:

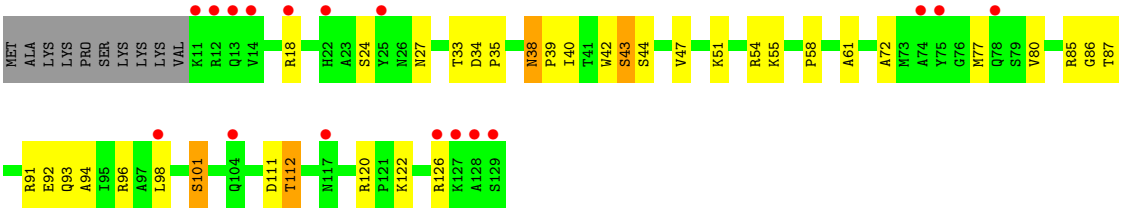




- Molecule 11: 30S ribosomal protein S11

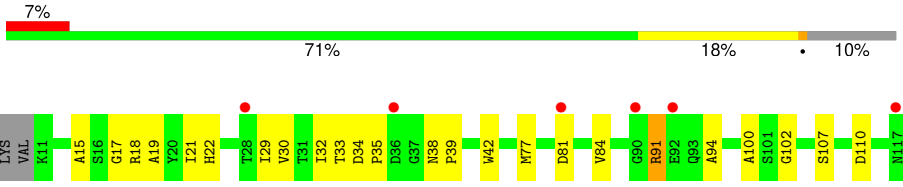
Chain QK:

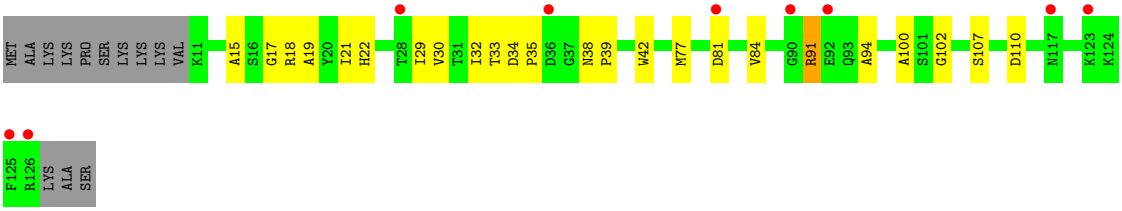




- Molecule 11: 30S ribosomal protein S11

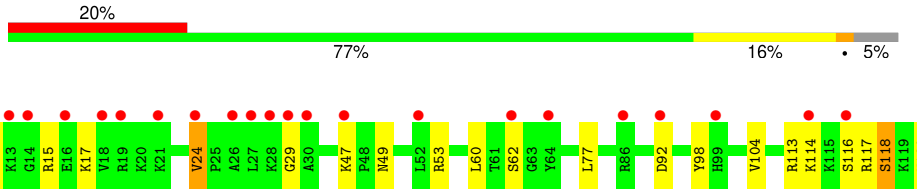
Chain XK:

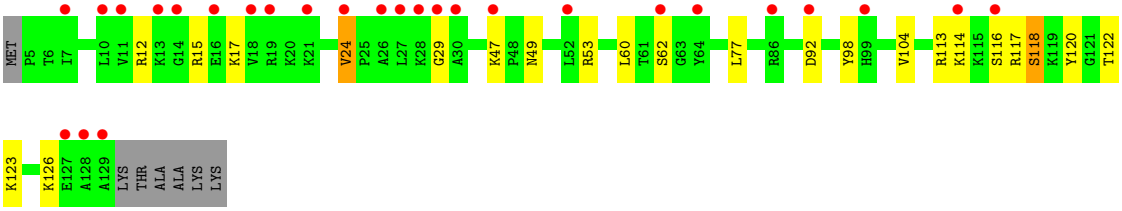




- Molecule 12: 30S ribosomal protein S12

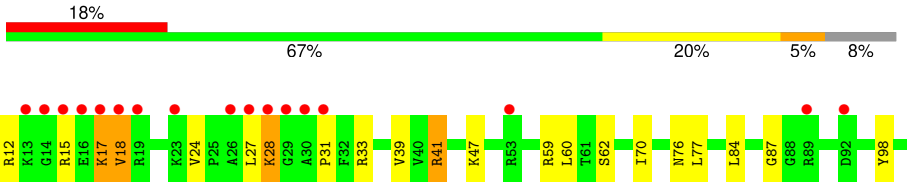
Chain QL:

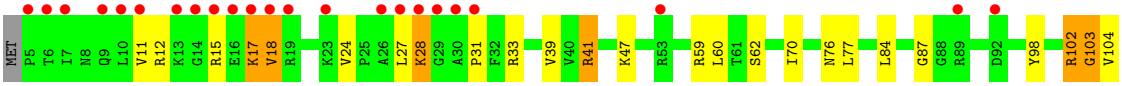


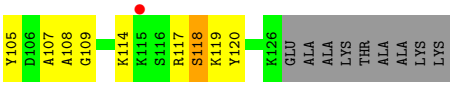


- Molecule 12: 30S ribosomal protein S12

Chain XL:





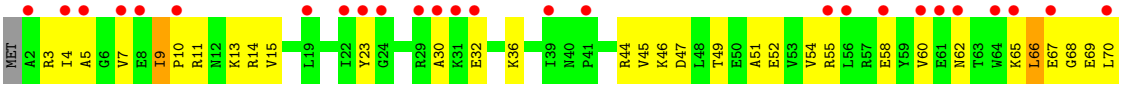


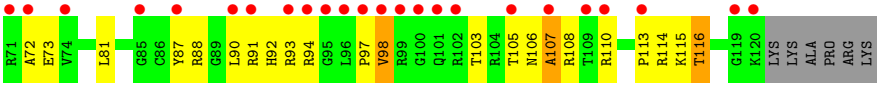
• Molecule 13: 30S ribosomal protein S13

Chain QM:

• Molecule 13: 30S ribosomal protein S13

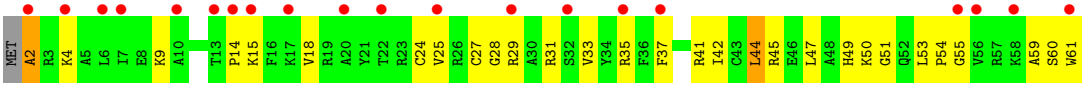
Chain XM:





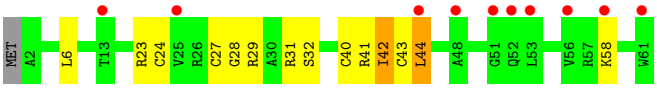
• Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:



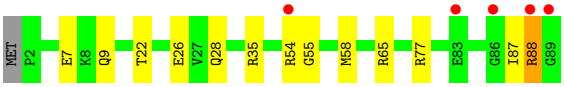
• Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:



• Molecule 15: 30S ribosomal protein S15

Chain QO:



• Molecule 15: 30S ribosomal protein S15

Chain XO: 3% 82% 16% •

MET P2 I3 T4 K5 E6 E7 K8 P19 G20 D21 R35 R38 Q62 R65 L66 L67 R68 R77 Y78 I82 I87 R88 GLY

• Molecule 16: 30S ribosomal protein S16

Chain QP: 2% 68% 26% • 5%

M1 V2 K3 T4 R5 R8 P15 I19 V20 V21 T22 D23 A24 R25 R28 D29 G30 E34 G37 K43 T44 T45 P46 D47 W48 L49 K50 R55 W59 T67 D68 E83 A84 ARG GLU GLY ALA

• Molecule 16: 30S ribosomal protein S16

Chain XP: 11% 69% 24% • 5%

M1 R5 F9 G10 S11 K12 P15 H16 Y17 R18 I19 V20 R25 R26 K27 R28 D29 G30 K31 Y32 I33 E34 K35 I36 R42 K43 T44 W48 V53 V62 G63 A64 T69 R72 R75 Q82 E83 A84 ARG GLU GLY ALA

• Molecule 17: 30S ribosomal protein S17

Chain QQ: 11% 62% 30% • 5%

MET P2 K3 L6 T7 V10 V11 S12 Q16 T20 V23 E24 P30 L31 Y32 I36 K37 R38 S39 K40 K41 Y42 L43 E49 V57 E58 I59 I60 E61 S66 K67 R68 K69 R70 V73 L76 V77 E78 S79 G80 R81 M82 D83 L84 Y88 L89 I90

R91 R92 Q93 N94 L98 S99 K100 R101 GLY GLY LYS ALA

• Molecule 17: 30S ribosomal protein S17

Chain XQ: 6% 78% 16% • 5%

MET P2 V5 E24 L31 Y32 V35 I36 K40 V57 I60 R63 P64 I65 S66 K67 R68 K69 R70 R81 M82 D83 Y88 R91 R92 K100 R101 GLY GLY LYS ALA

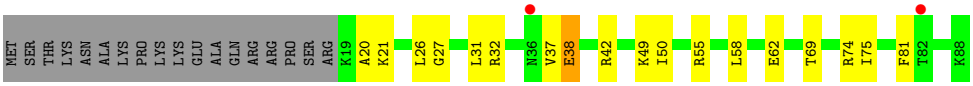
• Molecule 18: 30S ribosomal protein S18

Chain QR: 7% 61% 18% 20%

MET SER THR LYS ASN ALA LYS PRO LYS LYS GLU ALA GLN ARG ARG PRO SER ARG K19 V22 K23 A24 T25 L31 R32 D33 N36 V37 E38 E46 I50 R53 R54 R55 T56 S59 I70 R74 I75 L85 V86 R87 K88

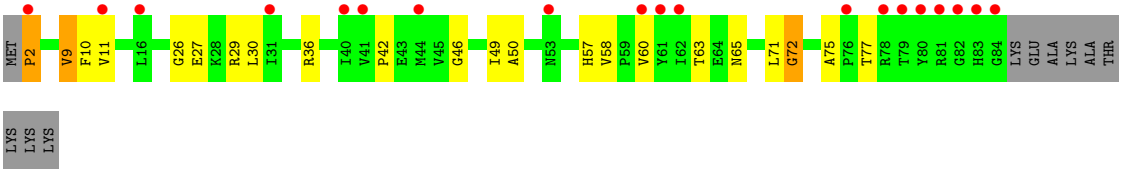
• Molecule 18: 30S ribosomal protein S18

Chain XR: 2% 59% 19% • 20%



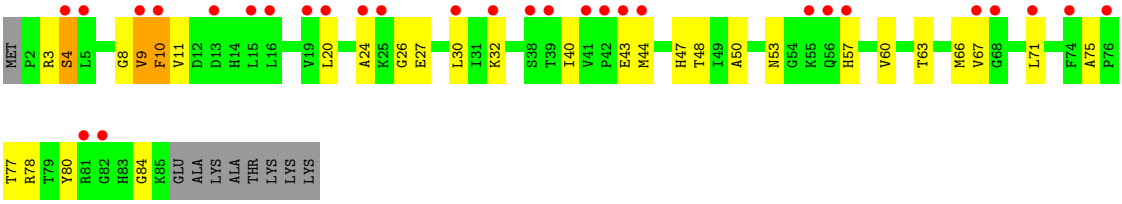
• Molecule 19: 30S ribosomal protein S19

Chain QS:



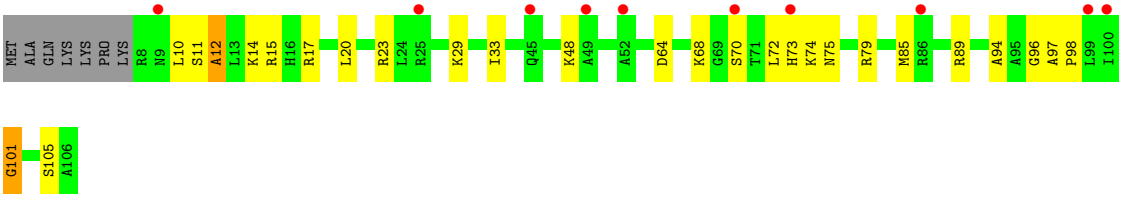
• Molecule 19: 30S ribosomal protein S19

Chain XS:



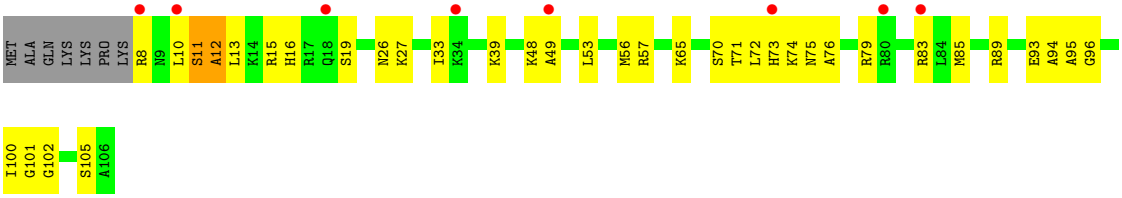
• Molecule 20: 30S ribosomal protein S20

Chain QT:



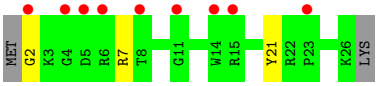
• Molecule 20: 30S ribosomal protein S20

Chain XT:



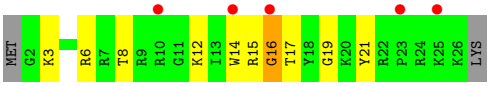
• Molecule 21: 30S ribosomal protein Thx

Chain QU:



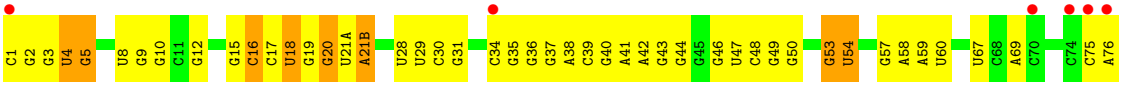
• Molecule 21: 30S ribosomal protein Thx

Chain XU:



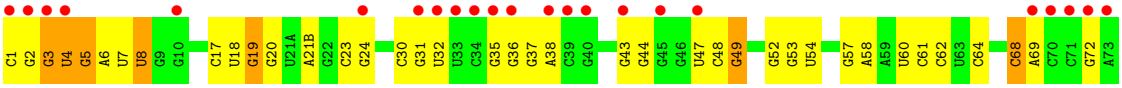
• Molecule 22: P-site tRNA-Pro

Chain QV:



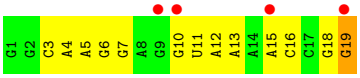
• Molecule 22: P-site tRNA-Pro

Chain XV:



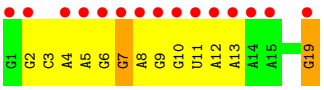
• Molecule 23: mRNA

Chain QX:



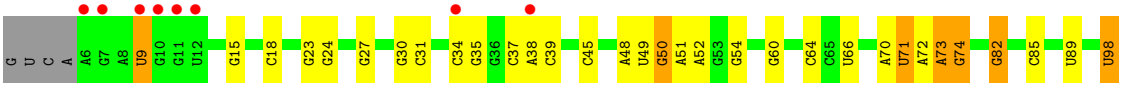
• Molecule 23: mRNA

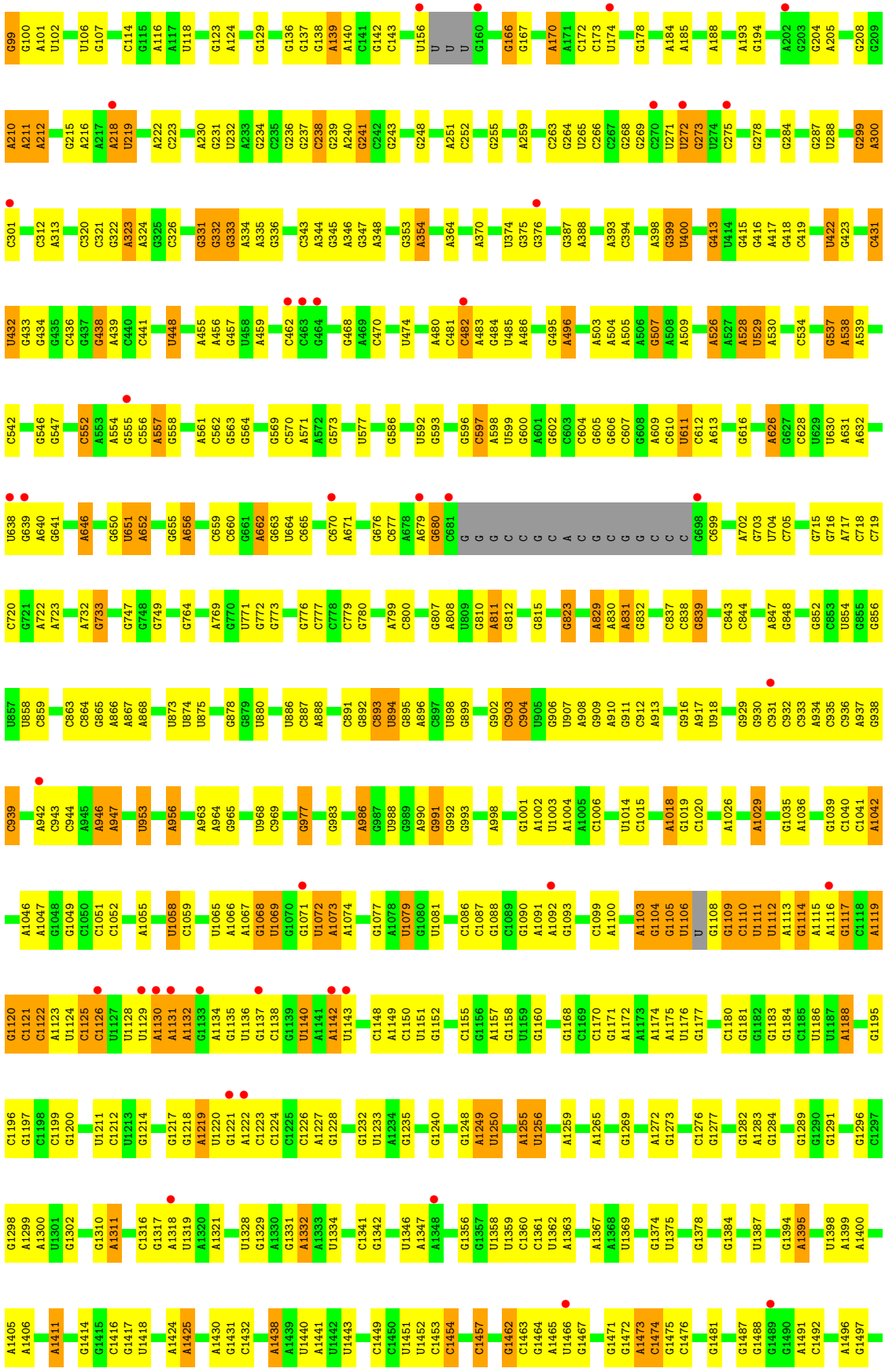
Chain XX:



• Molecule 24: 23S rRNA

Chain RA:

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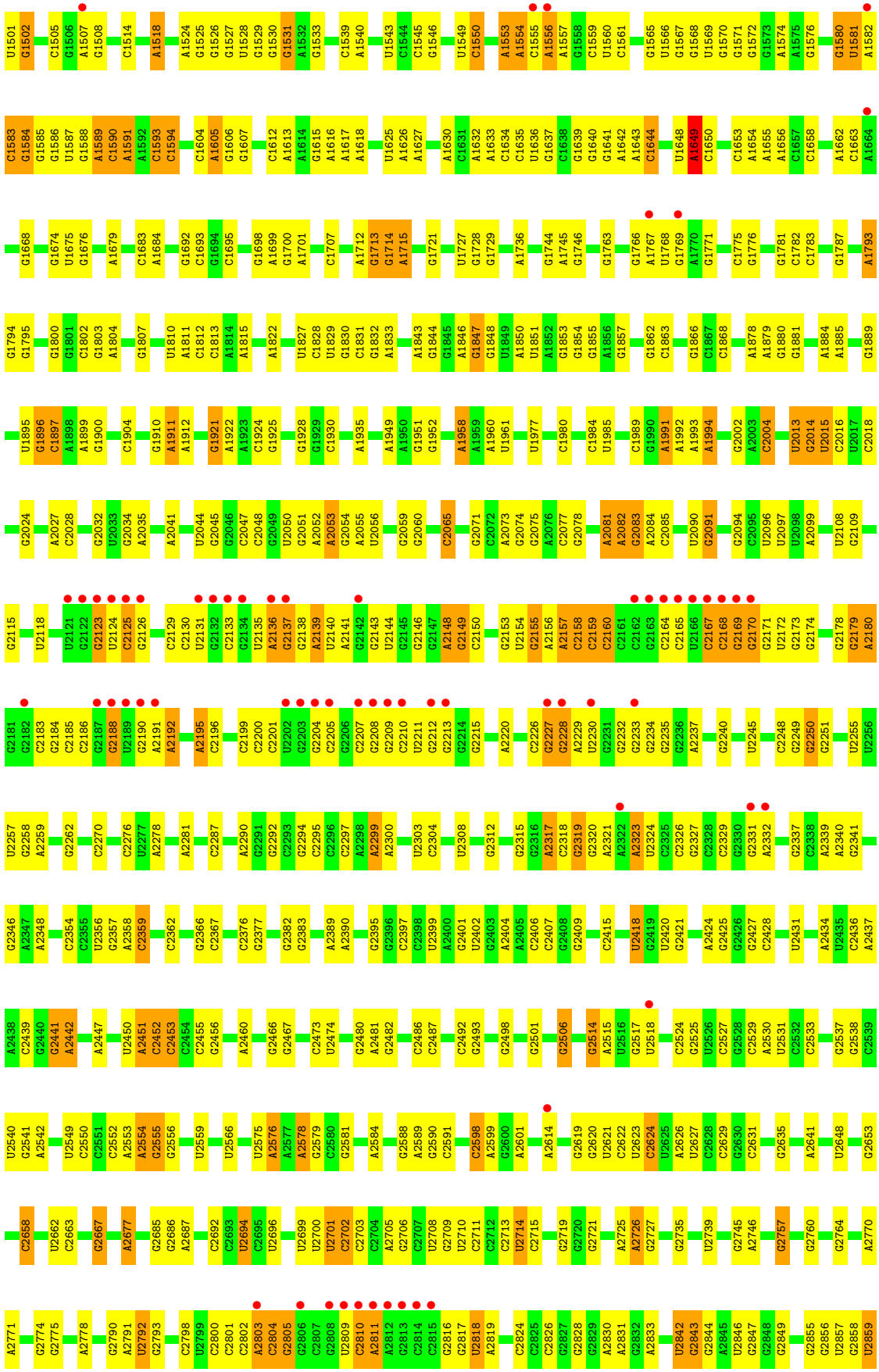
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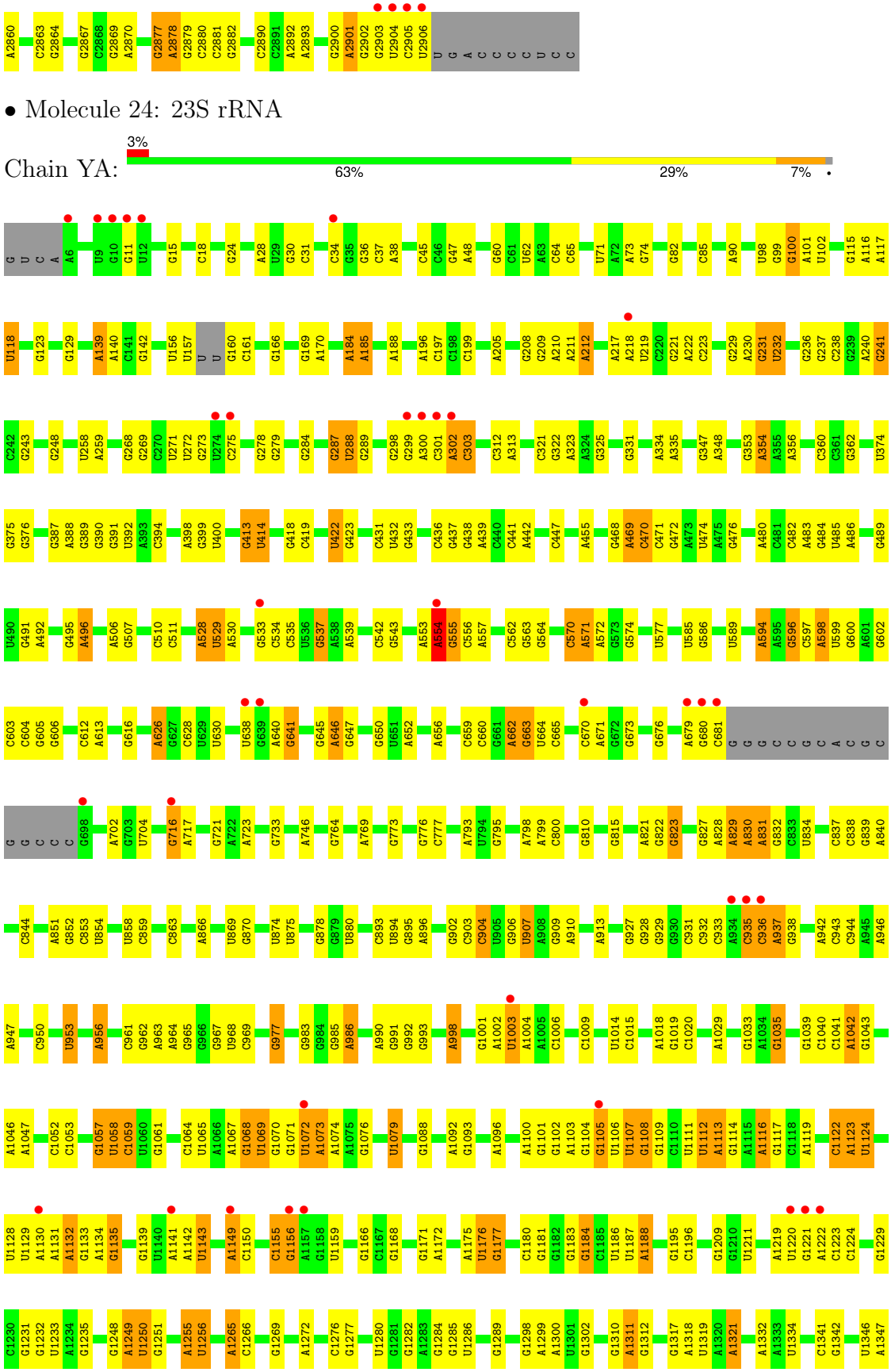
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• Molecule 24: 23S rRNA
Chain YA:
3%
63%
29%
7%
•
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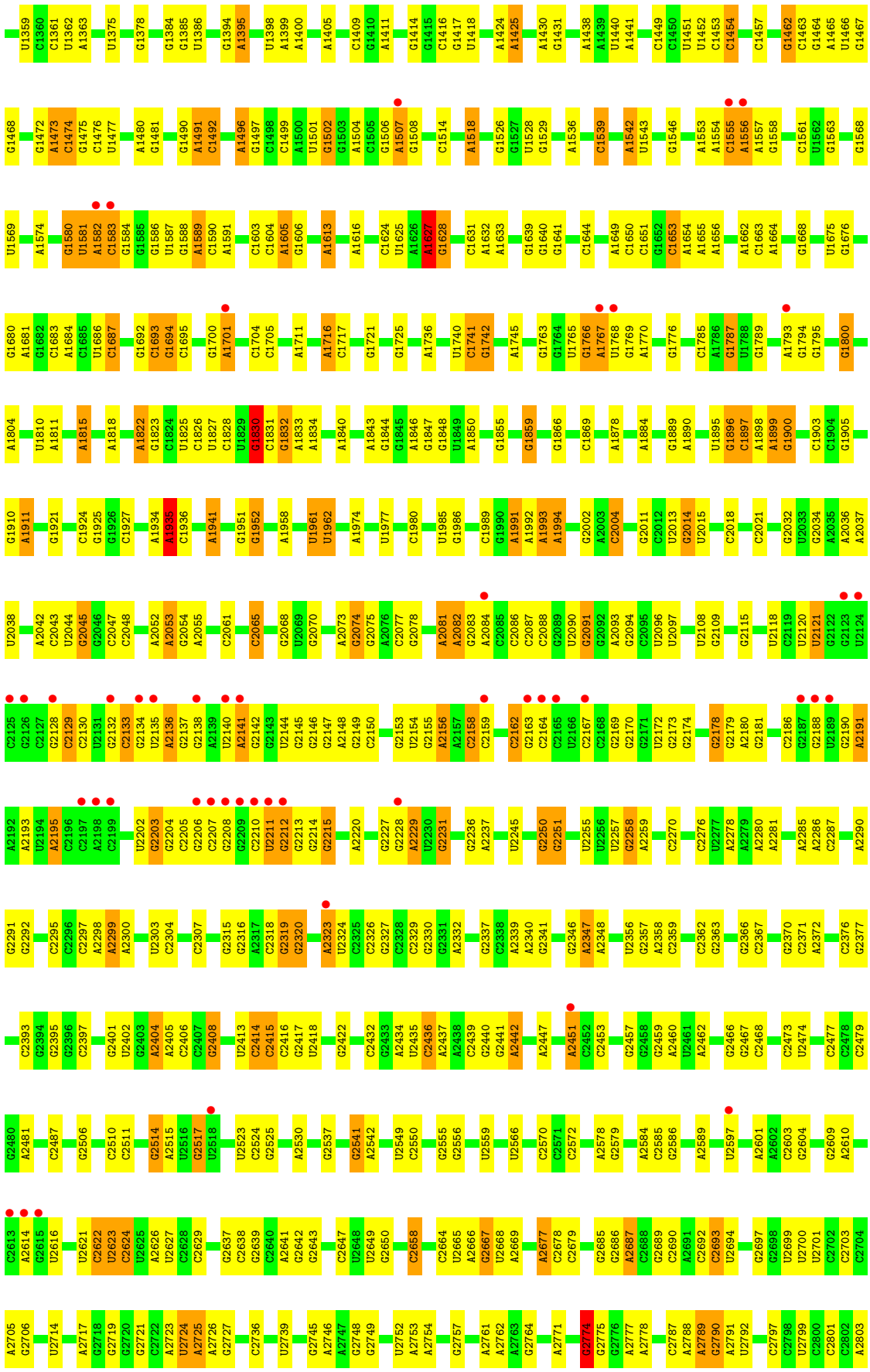
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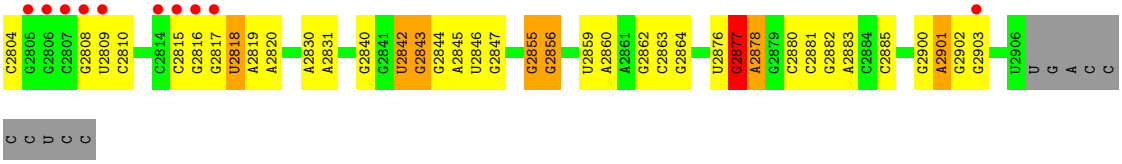
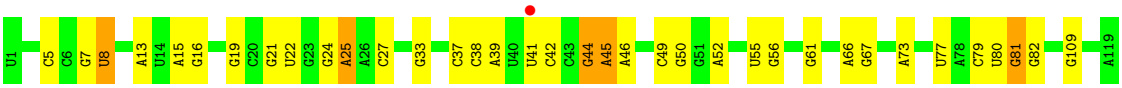


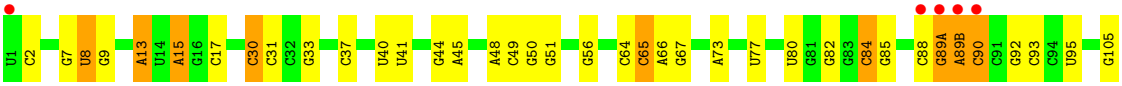
- Molecule 25: 5S rRNA

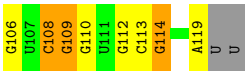
Chain RB:



- Molecule 25: 5S rRNA

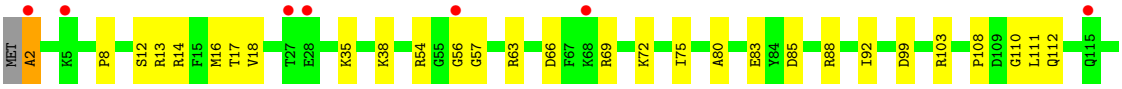
Chain YB:

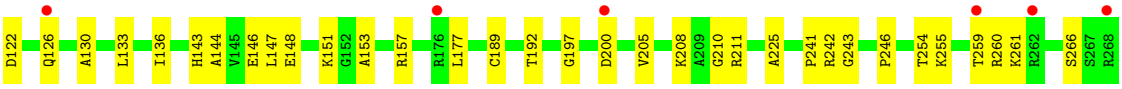


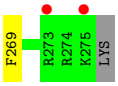


- Molecule 26: 50S ribosomal protein L2

Chain RD:

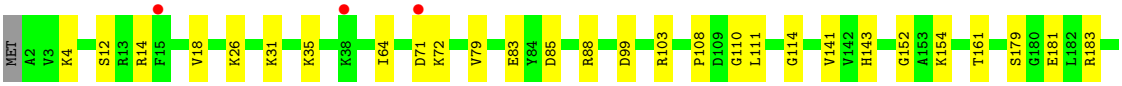


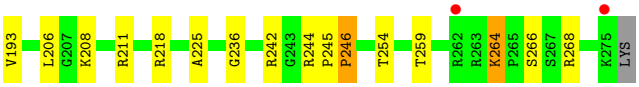




- Molecule 26: 50S ribosomal protein L2

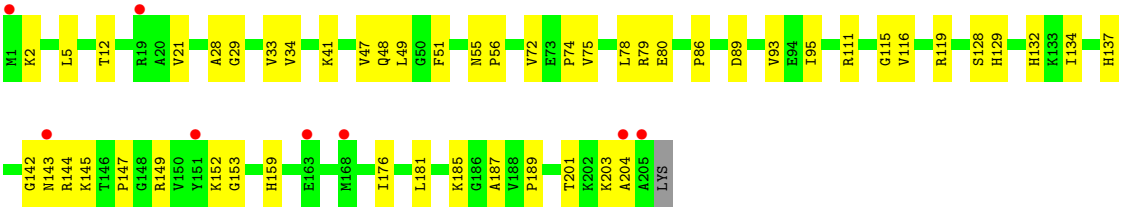
Chain YD:





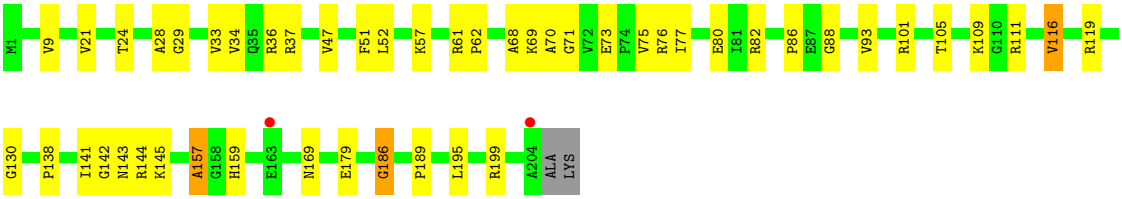
• Molecule 27: 50S ribosomal protein L3

Chain RE:



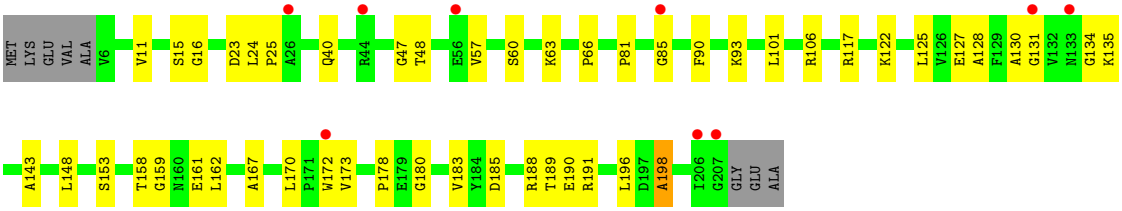
• Molecule 27: 50S ribosomal protein L3

Chain YE:



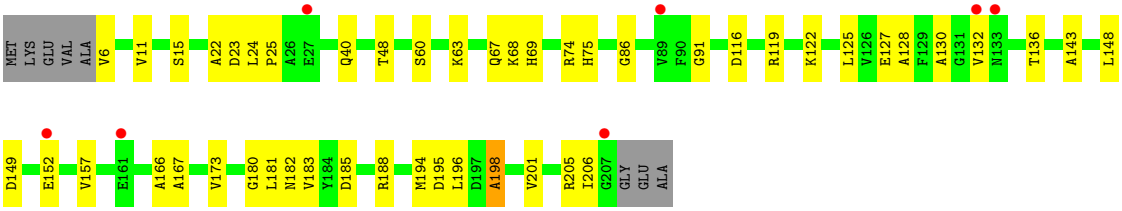
• Molecule 28: 50S ribosomal protein L4

Chain RF:



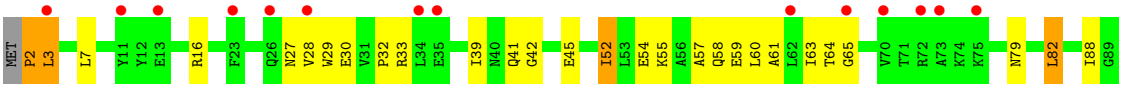
• Molecule 28: 50S ribosomal protein L4

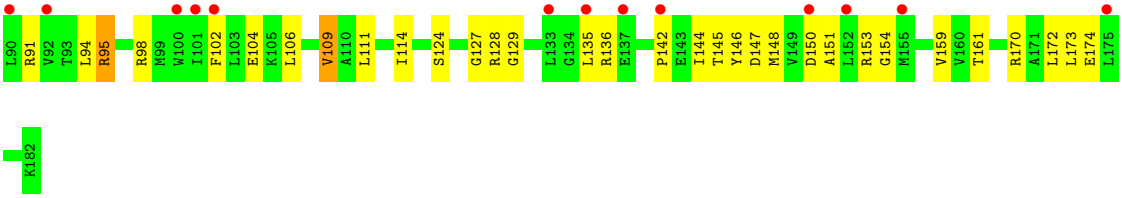
Chain YF:



• Molecule 29: 50S ribosomal protein L5

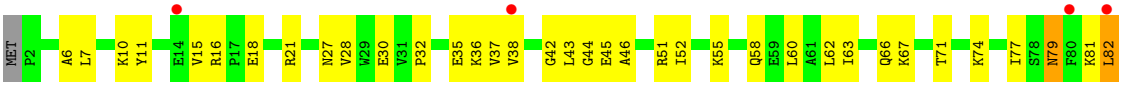
Chain RG:

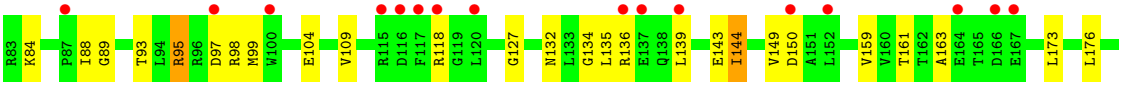




• Molecule 29: 50S ribosomal protein L5

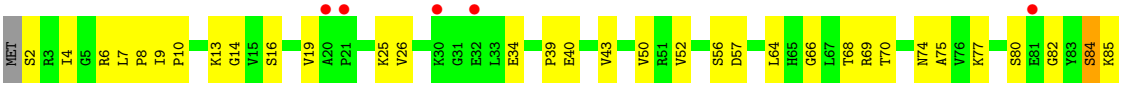
Chain YG:

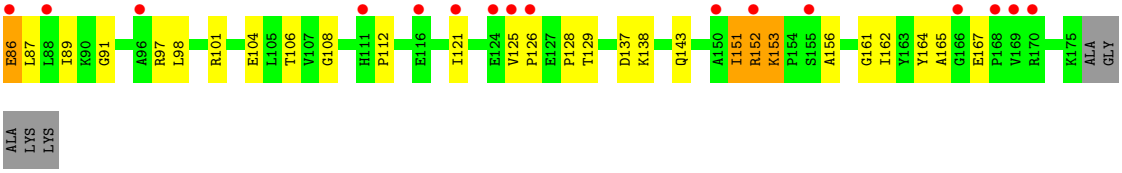




• Molecule 30: 50S ribosomal protein L6

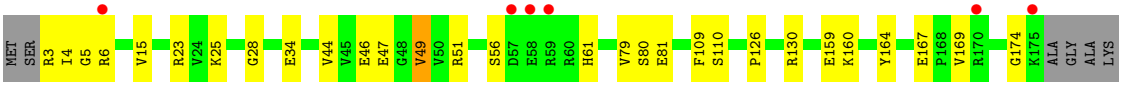
Chain RH:





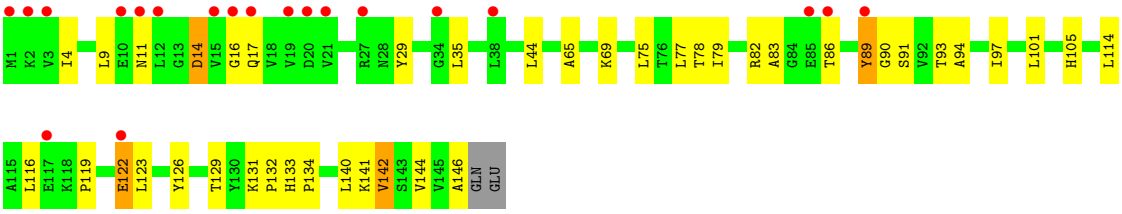
• Molecule 30: 50S ribosomal protein L6

Chain YH:



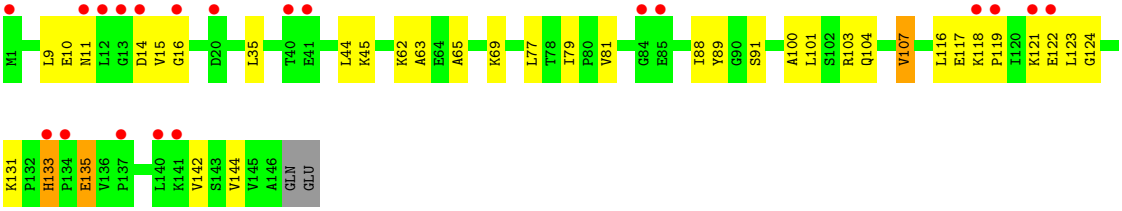
• Molecule 31: 50S ribosomal protein L9

Chain RI:



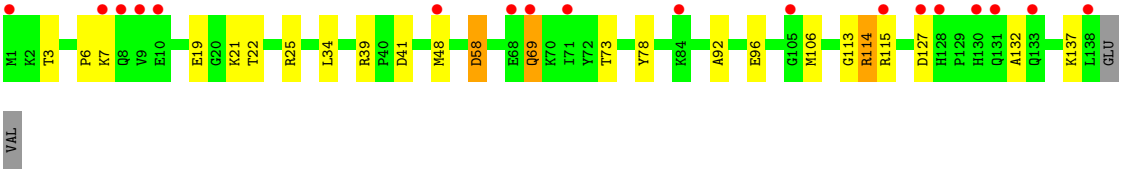
- Molecule 31: 50S ribosomal protein L9

Chain YI:



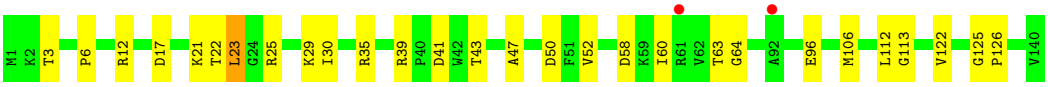
- Molecule 32: 50S ribosomal protein L13

Chain RN:



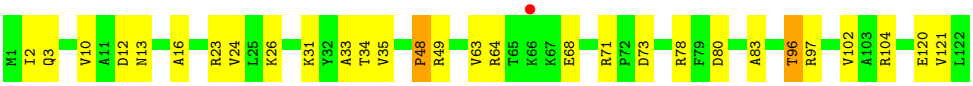
- Molecule 32: 50S ribosomal protein L13

Chain YN:



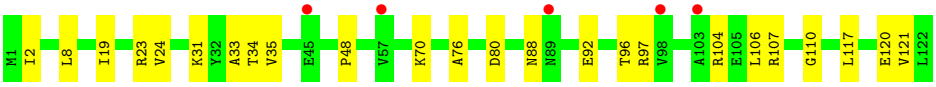
- Molecule 33: 50S ribosomal protein L14

Chain RO:



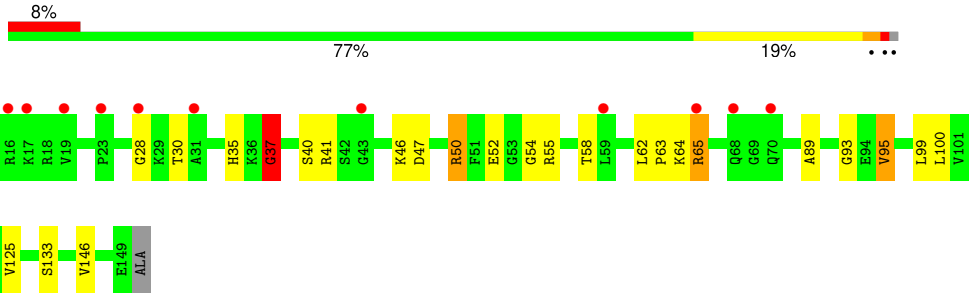
- Molecule 33: 50S ribosomal protein L14

Chain YO:



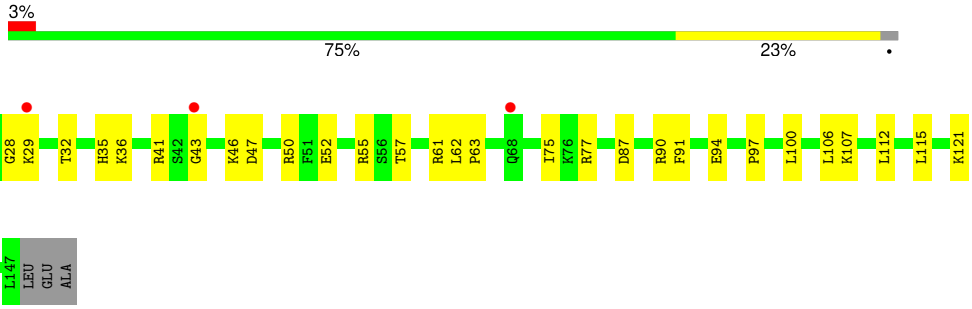
• Molecule 34: 50S ribosomal protein L15

Chain RP:



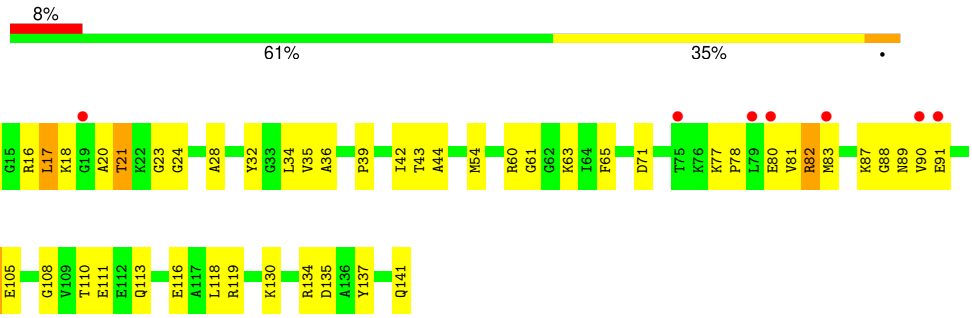
• Molecule 34: 50S ribosomal protein L15

Chain YP:



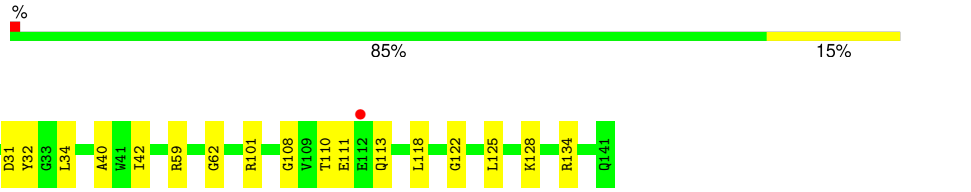
• Molecule 35: 50S ribosomal protein L16

Chain RQ:



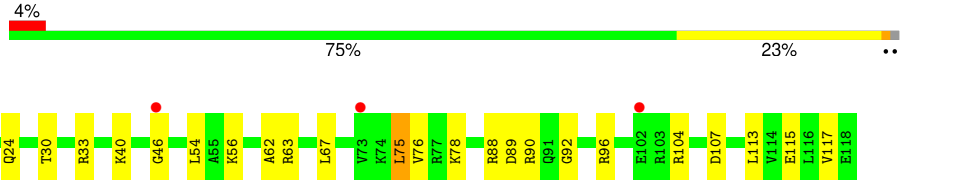
• Molecule 35: 50S ribosomal protein L16

Chain YQ:



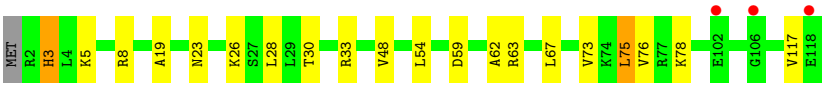
• Molecule 36: 50S ribosomal protein L17

Chain RR:



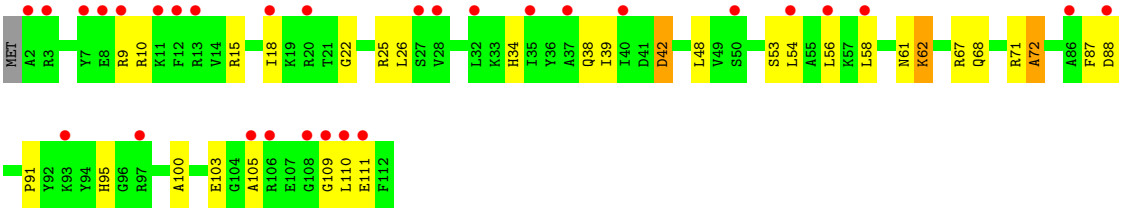
• Molecule 36: 50S ribosomal protein L17

Chain YR:



• Molecule 37: 50S ribosomal protein L18

Chain RS:



• Molecule 37: 50S ribosomal protein L18

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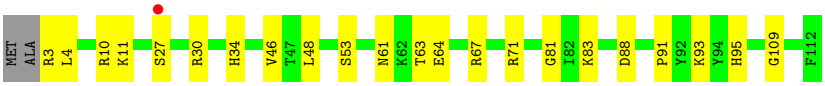
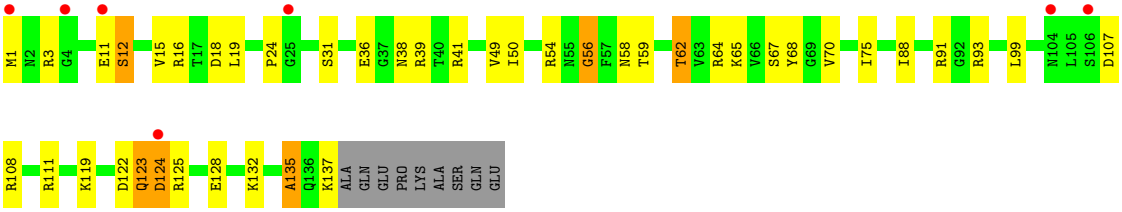


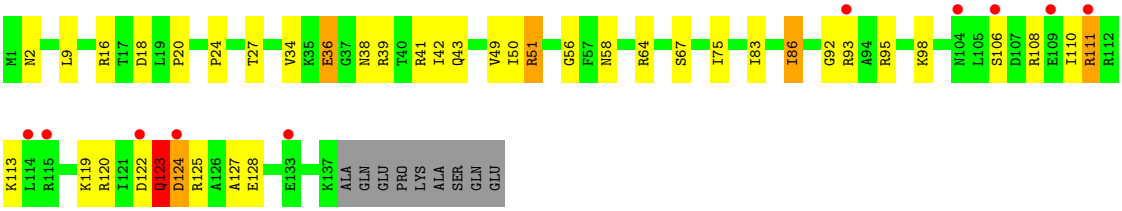
• Molecule 38: 50S ribosomal protein L19

Chain RT:



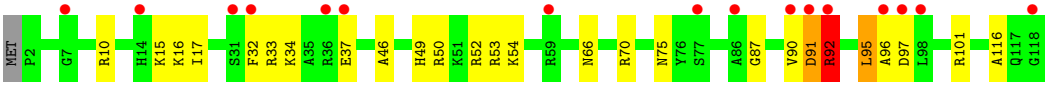
• Molecule 38: 50S ribosomal protein L19

Chain YT:



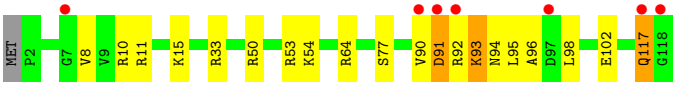
• Molecule 39: 50S ribosomal protein L20

Chain RU:



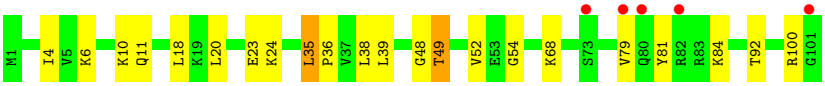
• Molecule 39: 50S ribosomal protein L20

Chain YU:



• Molecule 40: 50S ribosomal protein L21

Chain RV:

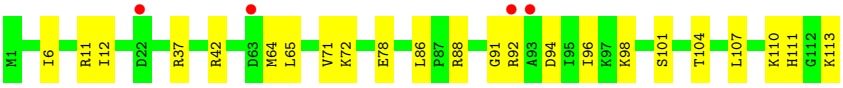


• Molecule 40: 50S ribosomal protein L21

Chain YV:

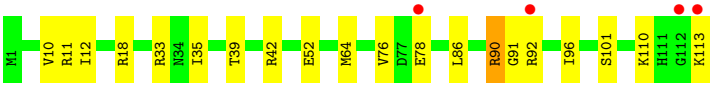
• Molecule 41: 50S ribosomal protein L22

Chain RW:



• Molecule 41: 50S ribosomal protein L22

Chain YW:



• Molecule 42: 50S ribosomal protein L23

Chain RX:

• Molecule 42: 50S ribosomal protein L23

Chain YX: 85% 12% •

M1 A10 K16 K25 Y26 T27 F28 W29 K33 A34 T35 K62 R76 I80 V81 Q82 E93 G94 LEU ILE

• Molecule 43: 50S ribosomal protein L24

Chain RY: 13% 77% 18% • •

M1 M5 K8 K9 G10 D11 L14 S17 G18 K21 G22 G25 K28 E29 V30 L31 P32 K33 K34 Y35 V39 E40 G41 V42 K47 A48 V49 S52 Y55 E62 K63 K71 V72 R73 R86 K95 V98 C102 G103 L106 D107 THR GLU GLU

• Molecule 43: 50S ribosomal protein L24

Chain YY: % 80% 16% • •

M1 K4 M5 S17 Y35 K46 K47 A48 V51 S52 P53 K54 K71 T83 R84 K87 N92 G93 K94 C102 G103 L106 D107 THR GLU GLU

• Molecule 44: 50S ribosomal protein L25

Chain RZ: 6% 54% 32% • 11%

M1 R4 L5 R10 E11 G12 R19 K23 G26 R31 H32 L33 V37 D40 D45 R49 Q50 A51 S52 I53 V58 L59 E60 L61 P62 D63 G64 Q65 T69 L70 L76 D77 K78 R79 R80 P83 E84 V90 L91 S92 D93 E94 P95 V96

Y99 F104 P108 A109 G110 A113 G114 R122 D123 I124 L125 V126 K127 V128 S129 P130 R131 N132 E138 V139 D140 V141 D148 H151 A152 S153 D154 L155 K156 L157 P158 P159 G160 V161 E162 L163 A164 V165 S166 P167 E168 V175 E178 D179 V180 E181 K182 L183 ALA GLU GLU

ALA ALA ALA GLU VAL ALA GLU PRO GLU VAL ILE LYS LYS GLY LYS GLU GLU GLU GLU GLU

• Molecule 44: 50S ribosomal protein L25

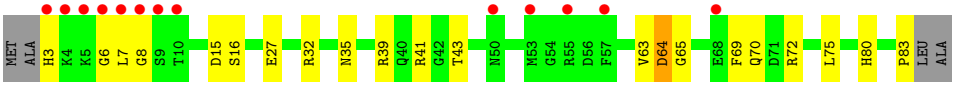
Chain YZ: % 67% 20% • 11%

M1 R10 E11 G12 S16 A17 L18 R19 K23 G26 Y29 R35 K36 V37 D40 D45 R49 Q50 A51 S52 I53 L61 P62 D63 G64 Q65 R72 R79 R80 E84 D93 A109 G110 V111 G114 E119 R122 D123 R131 F136

D140 V141 S142 G143 L144 L150 H151 A152 S153 D154 G160 E168 E169 T170 V174 L183 ALA GLU GLU ALA ALA ALA GLU VAL ALA GLU PRO GLU VAL ILE LYS LYS GLY LYS GLU GLU GLU GLU

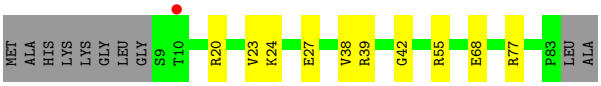
• Molecule 45: 50S ribosomal protein L27

Chain R0: 15% 71% 24% • 5%



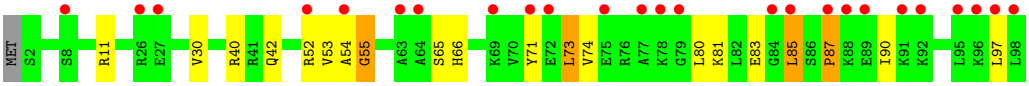
• Molecule 45: 50S ribosomal protein L27

Chain Y0:



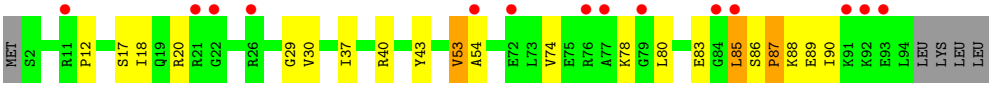
• Molecule 46: 50S ribosomal protein L28

Chain R1:



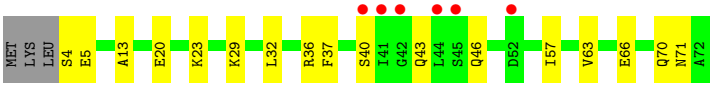
• Molecule 46: 50S ribosomal protein L28

Chain Y1:



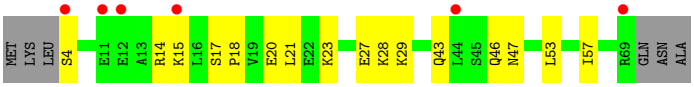
• Molecule 47: 50S ribosomal protein L29

Chain R2:



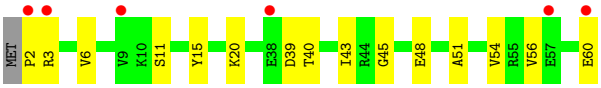
• Molecule 47: 50S ribosomal protein L29

Chain Y2:



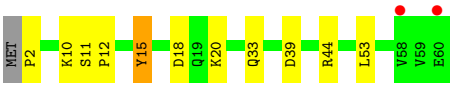
• Molecule 48: 50S ribosomal protein L30

Chain R3:



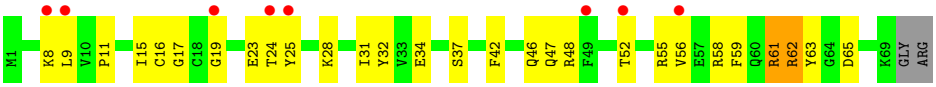
• Molecule 48: 50S ribosomal protein L30

Chain Y3:



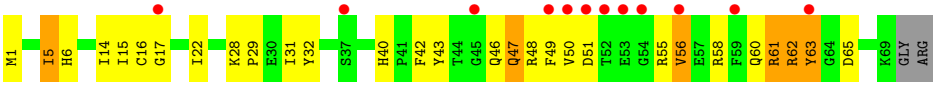
• Molecule 49: 50S ribosomal protein L31

Chain R4:



• Molecule 49: 50S ribosomal protein L31

Chain Y4:

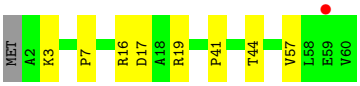


• Molecule 50: 50S ribosomal protein L32

Chain R5:

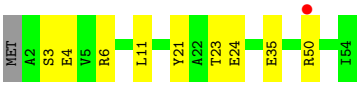
• Molecule 50: 50S ribosomal protein L32

Chain Y5:



• Molecule 51: 50S ribosomal protein L33

Chain R6:

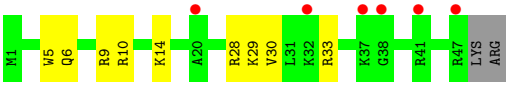


• Molecule 51: 50S ribosomal protein L33

Chain Y6:

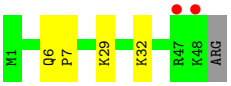
• Molecule 52: 50S ribosomal protein L34

Chain R7:



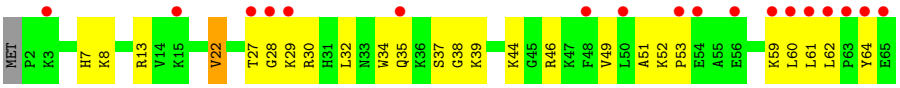
• Molecule 52: 50S ribosomal protein L34

Chain Y7:



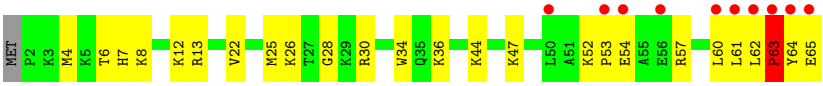
• Molecule 53: 50S ribosomal protein L35

Chain R8:



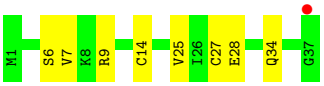
• Molecule 53: 50S ribosomal protein L35

Chain Y8:



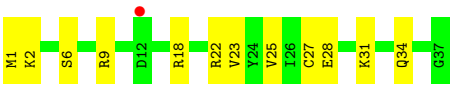
• Molecule 54: 50S ribosomal protein L36

Chain R9:



• Molecule 54: 50S ribosomal protein L36

Chain Y9:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.17Å 451.47Å 620.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.46 – 3.20 152.46 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (152.46-3.20) 99.2 (152.46-3.20)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.224 , 0.256 0.227 , 0.258	Depositor DCC
R_{free} test set	44319 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å^2)	71.2	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 87.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	291964	wwPDB-VP
Average B, all atoms (Å^2)	103.0	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: ZN, MG, SF4, 1MG

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	0.37	1/36098 (0.0%)	0.38	3/56341 (0.0%)
1	XA	0.37	1/36101 (0.0%)	0.38	8/56346 (0.0%)
2	QB	0.39	0/1942	0.74	5/2619 (0.2%)
2	XB	0.39	0/1950	0.63	0/2630
3	QC	0.34	0/1629	0.63	0/2195
3	XC	0.33	0/1629	0.58	0/2195
4	QD	0.46	0/1733	0.66	0/2318
4	XD	0.52	0/1733	0.81	5/2318 (0.2%)
5	QE	0.45	0/1171	0.67	1/1576 (0.1%)
5	XE	0.49	0/1171	0.59	0/1576
6	QF	0.40	0/856	0.57	0/1154
6	XF	0.48	0/856	0.54	0/1154
7	QG	0.31	0/1276	0.57	0/1709
7	XG	0.31	0/1276	0.58	0/1709
8	QH	0.48	0/1128	0.63	0/1517
8	XH	0.50	0/1128	0.59	0/1517
9	QI	0.31	0/1029	0.70	0/1379
9	XI	0.33	0/1017	0.67	0/1365
10	QJ	0.32	0/814	0.62	0/1095
10	XJ	0.31	0/790	0.58	0/1063
11	QK	0.47	0/900	0.62	0/1213
11	XK	0.49	0/879	0.54	0/1187
12	QL	0.58	0/991	0.62	0/1327
12	XL	0.55	0/972	0.70	1/1301 (0.1%)
13	QM	0.33	0/965	0.74	0/1292
13	XM	0.32	0/956	0.71	0/1281
14	QN	0.38	0/501	0.76	0/664
14	XN	0.37	0/501	0.69	0/664
15	QO	0.45	0/745	0.61	0/992
15	XO	0.53	0/740	0.50	0/987
16	QP	0.53	0/721	0.59	0/970
16	XP	0.43	0/721	0.58	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	QQ	0.50	0/847	0.57	0/1131
17	XQ	0.49	0/847	0.55	0/1131
18	QR	0.46	0/579	0.63	0/768
18	XR	0.52	0/579	0.60	0/768
19	QS	0.32	0/680	0.72	0/915
19	XS	0.32	0/689	0.67	0/926
20	QT	0.46	0/765	0.64	0/1007
20	XT	0.41	0/765	0.60	0/1007
21	QU	0.35	0/221	0.63	0/288
21	XU	0.31	0/221	0.61	0/288
22	QV	0.26	0/1814	0.38	0/2825
22	XV	0.25	0/1814	0.36	0/2825
23	QX	0.18	0/470	0.34	0/733
23	XX	0.20	0/470	0.35	0/733
24	RA	0.50	4/69498 (0.0%)	0.40	4/108491 (0.0%)
24	YA	0.60	0/69543	0.42	13/108563 (0.0%)
25	RB	0.35	0/2878	0.36	0/4490
25	YB	0.70	5/2878 (0.2%)	1.03	16/4490 (0.4%)
26	RD	0.75	1/2185 (0.0%)	0.62	0/2944
26	YD	0.91	1/2185 (0.0%)	0.78	2/2944 (0.1%)
27	RE	0.69	0/1601	0.66	2/2160 (0.1%)
27	YE	0.82	0/1596	0.71	0/2153
28	RF	0.63	0/1620	0.62	0/2194
28	YF	0.79	0/1620	0.66	0/2194
29	RG	0.40	0/1499	0.71	0/2016
29	YG	0.49	0/1499	0.68	0/2016
30	RH	0.43	0/1362	0.68	0/1841
30	YH	0.70	0/1356	0.60	0/1833
31	RI	0.44	0/1151	0.75	2/1558 (0.1%)
31	YI	0.50	0/1151	0.75	0/1558
32	RN	0.59	0/1131	0.65	2/1525 (0.1%)
32	YN	0.81	0/1148	0.68	0/1547
33	RO	0.69	0/943	0.60	0/1269
33	YO	0.81	1/943 (0.1%)	0.63	0/1269
34	RP	0.63	0/1156	0.68	1/1537 (0.1%)
34	YP	0.79	0/1139	0.72	0/1514
35	RQ	0.56	0/1143	0.68	0/1527
35	YQ	0.77	0/1143	0.59	0/1527
36	RR	0.71	0/974	0.65	0/1302
36	YR	0.82	0/974	0.73	0/1302
37	RS	0.45	0/892	0.71	0/1187
37	YS	0.65	0/887	0.60	0/1180
38	RT	0.59	0/1155	0.71	0/1542

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	YT	0.66	0/1155	0.72	0/1542
39	RU	0.66	0/982	0.67	2/1306 (0.2%)
39	YU	0.90	0/982	0.66	0/1306
40	RV	0.54	0/790	0.58	0/1057
40	YV	0.80	0/790	0.65	0/1057
41	RW	0.68	0/911	0.62	2/1220 (0.2%)
41	YW	0.86	0/911	0.63	0/1220
42	RX	0.62	0/739	0.63	0/993
42	YX	0.78	0/756	0.57	0/1014
43	RY	0.54	0/831	0.58	0/1108
43	YY	0.69	0/831	0.58	0/1108
44	RZ	0.43	0/1493	0.76	0/2026
44	YZ	0.59	0/1493	0.60	0/2026
45	R0	0.58	0/652	0.58	0/867
45	Y0	0.78	0/607	0.62	0/809
46	R1	0.67	0/770	0.66	0/1022
46	Y1	0.75	0/736	0.67	0/978
47	R2	0.50	0/583	0.55	0/771
47	Y2	0.70	0/560	0.61	0/741
48	R3	0.63	1/474 (0.2%)	0.60	0/635
48	Y3	0.76	0/474	0.71	1/635 (0.2%)
49	R4	0.32	0/578	0.75	0/776
49	Y4	0.36	0/578	0.82	5/776 (0.6%)
50	R5	0.72	0/473	0.64	0/639
50	Y5	0.87	0/473	0.68	0/639
51	R6	0.56	0/460	0.61	0/613
51	Y6	0.71	0/460	0.60	0/613
52	R7	0.77	0/417	0.62	0/550
52	Y7	0.94	0/426	0.66	0/561
53	R8	0.72	0/525	0.78	0/691
53	Y8	0.84	0/525	0.85	0/691
54	R9	0.55	0/310	0.53	0/407
54	Y9	0.78	0/310	0.54	0/407
All	All	0.53	15/315985 (0.0%)	0.49	75/472446 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	XA	0	1

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
27	RE	0	7
27	YE	0	10
28	RF	0	12
28	YF	0	15
29	RG	0	17
29	YG	0	20
30	RH	0	23
30	YH	0	1
31	RI	0	17
31	YI	0	21
32	RN	0	10
32	YN	0	7
33	RO	0	2
33	YO	0	1
34	RP	0	8
34	YP	0	5
35	RQ	0	18
35	YQ	0	6
36	RR	0	4
36	YR	0	5
37	RS	0	11
37	YS	0	1
38	RT	0	15
38	YT	0	11
39	RU	0	5
39	YU	0	5
40	RV	0	6
40	YV	0	7
41	RW	0	5
41	YW	0	5
42	RX	0	2
42	YX	0	1
43	RY	0	7
43	YY	0	5
44	RZ	0	38
44	YZ	0	10
45	R0	0	2
45	Y0	0	1
46	R1	0	10
46	Y1	0	7
47	R2	0	5
47	Y2	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
48	R3	0	1
48	Y3	0	2
49	R4	0	15
49	Y4	0	11
50	R5	0	1
52	R7	0	1
53	R8	0	11
53	Y8	0	6
All	All	0	781

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	YD	264	LYS	C-N	15.58	1.51	1.34
25	YB	112	G	N9-C4	12.28	1.62	1.38
25	YB	114	G	N9-C4	11.30	1.60	1.38
24	RA	1649	A	C5'-C4'	11.02	1.67	1.51
25	YB	112	G	N9-C8	-9.65	1.18	1.37

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	YB	114	G	N7-C8-N9	-24.75	38.86	113.10
25	YB	112	G	N7-C8-N9	-24.37	39.98	113.10
25	YB	114	G	C4-C5-N7	-23.53	40.20	110.80
25	YB	112	G	C4-C5-N7	-23.11	41.46	110.80
25	YB	112	G	C8-N9-C4	-17.30	54.49	106.40

There are no chirality outliers.

5 of 781 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	15	VAL	Peptide
2	QB	18	GLY	Peptide
2	QB	19	HIS	Peptide
2	QB	21	ARG	Peptide
2	QB	38	GLY	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	32247	0	16277	453	0
1	XA	32249	0	16278	463	3
2	QB	1907	0	1958	35	0
2	XB	1915	0	1969	38	0
3	QC	1605	0	1668	31	0
3	XC	1605	0	1668	21	0
4	QD	1703	0	1766	28	0
4	XD	1703	0	1764	37	0
5	QE	1155	0	1213	28	0
5	XE	1155	0	1213	14	0
6	QF	843	0	857	13	0
6	XF	843	0	857	12	0
7	QG	1257	0	1296	16	0
7	XG	1257	0	1296	22	0
8	QH	1108	0	1165	20	0
8	XH	1108	0	1165	22	0
9	QI	1010	0	1037	19	0
9	XI	998	0	1024	29	0
10	QJ	801	0	849	23	0
10	XJ	777	0	816	16	0
11	QK	885	0	904	27	0
11	XK	864	0	881	13	0
12	QL	975	0	1062	14	0
12	XL	956	0	1046	23	0
13	QM	955	0	1021	21	0
13	XM	946	0	1008	25	0
14	QN	492	0	529	19	0
14	XN	492	0	529	11	0
15	QO	734	0	771	11	0
15	XO	729	0	768	8	0
16	QP	705	0	725	15	0
16	XP	705	0	725	13	0
17	QQ	834	0	904	24	0
17	XQ	834	0	904	16	0
18	QR	574	0	644	7	0
18	XR	574	0	644	8	0
19	QS	665	0	686	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XS	674	0	699	11	0
20	QT	763	0	861	15	0
20	XT	763	0	861	23	0
21	QU	217	0	234	4	0
21	XU	217	0	234	4	0
22	QV	1648	0	834	27	0
22	XV	1648	0	834	23	0
23	QX	418	0	209	7	0
23	XX	418	0	209	7	0
24	RA	62051	0	31279	621	3
24	YA	62091	0	31292	533	0
25	RB	2573	0	1306	21	0
25	YB	2573	0	1304	41	0
26	RD	2135	0	2221	37	0
26	YD	2135	0	2221	32	0
27	RE	1568	0	1634	29	0
27	YE	1563	0	1628	29	0
28	RF	1585	0	1632	24	0
28	YF	1585	0	1632	23	0
29	RG	1474	0	1535	36	0
29	YG	1474	0	1535	30	0
30	RH	1336	0	1418	27	0
30	YH	1330	0	1413	19	0
31	RI	1136	0	1223	13	2
31	YI	1136	0	1223	12	0
32	RN	1104	0	1180	10	0
32	YN	1121	0	1195	15	0
33	RO	933	0	996	25	0
33	YO	933	0	996	18	0
34	RP	1139	0	1223	26	0
34	YP	1122	0	1206	26	0
35	RQ	1122	0	1179	29	0
35	YQ	1122	0	1179	10	0
36	RR	960	0	1021	18	0
36	YR	960	0	1021	11	0
37	RS	882	0	943	17	0
37	YS	877	0	938	15	0
38	RT	1141	0	1202	23	0
38	YT	1141	0	1202	27	0
39	RU	964	0	1022	26	0
39	YU	964	0	1021	19	0
40	RV	779	0	852	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	YV	779	0	852	12	0
41	RW	900	0	964	11	0
41	YW	900	0	964	11	0
42	RX	725	0	778	8	0
42	YX	742	0	803	8	0
43	RY	818	0	909	12	0
43	YY	818	0	909	14	0
44	RZ	1461	0	1493	26	0
44	YZ	1461	0	1493	22	0
45	R0	643	0	667	12	0
45	Y0	599	0	617	7	0
46	R1	763	0	848	9	0
46	Y1	729	0	801	10	0
47	R2	581	0	629	7	0
47	Y2	558	0	610	5	2
48	R3	469	0	518	7	0
48	Y3	469	0	518	8	0
49	R4	565	0	558	9	0
49	Y4	565	0	557	13	0
50	R5	459	0	476	9	0
50	Y5	459	0	476	9	0
51	R6	453	0	473	8	0
51	Y6	453	0	473	10	0
52	R7	409	0	454	7	0
52	Y7	418	0	467	3	0
53	R8	517	0	582	13	0
53	Y8	517	0	582	14	0
54	R9	307	0	335	6	0
54	Y9	307	0	335	8	0
55	QA	64	0	0	0	0
55	QV	1	0	0	0	0
55	R0	2	0	0	0	0
55	R8	2	0	0	0	0
55	RA	444	0	0	0	0
55	RB	7	0	0	0	0
55	RE	5	0	0	0	0
55	RF	1	0	0	0	0
55	RN	1	0	0	0	0
55	RQ	1	0	0	0	0
55	RR	1	0	0	0	0
55	RT	1	0	0	0	0
55	RX	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	XA	78	0	0	0	0
55	XE	1	0	0	0	0
55	XM	2	0	0	0	0
55	XV	1	0	0	0	0
55	Y0	2	0	0	0	0
55	Y1	2	0	0	0	0
55	Y3	1	0	0	0	0
55	Y5	1	0	0	0	0
55	Y7	1	0	0	0	0
55	Y8	1	0	0	0	0
55	YA	510	0	0	0	0
55	YB	7	0	0	0	0
55	YD	2	0	0	0	0
55	YE	5	0	0	0	0
55	YP	3	0	0	0	0
55	YQ	3	0	0	0	0
55	YR	1	0	0	0	0
56	QD	8	0	0	0	0
56	XD	8	0	0	0	0
57	QN	1	0	0	0	0
57	R4	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R9	1	0	0	0	0
57	RY	1	0	0	0	0
57	XN	1	0	0	0	0
57	Y4	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YY	1	0	0	0	0
All	All	291964	0	197875	3337	5

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

The worst 5 of 3337 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)
24:RA:1712:A:C2'	24:RA:1713:G:H5'	1.74	1.18
43:YY:92:ASN:ND2	43:YY:94:LYS:HG2	1.60	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:YA:1405:A:N6	24:YA:1418:U:H3	1.48	1.10
24:RA:2818:U:C2	24:RA:2901:A:N6	2.27	1.02
24:RA:2226:C:H1'	24:RA:2232:G:N2	1.74	1.01

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:RI:91:SER:OG	1:XA:368:U:OP1[4_555]	2.00	0.20
24:RA:331:G:OP2	47:Y2:17:SER:CA[3_555]	2.01	0.19
24:RA:331:G:OP2	47:Y2:17:SER:CB[3_555]	2.10	0.10
31:RI:89:TYR:O	1:XA:357:G:O2'[4_555]	2.10	0.10
24:RA:2158:C:O2'	1:XA:1042:G:O2'[4_555]	2.13	0.07

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%)	205 (88%)	28 (12%)	0	100 100
2	XB	234/256 (91%)	207 (88%)	27 (12%)	0	100 100
3	QC	203/239 (85%)	186 (92%)	17 (8%)	0	100 100
3	XC	203/239 (85%)	182 (90%)	21 (10%)	0	100 100
4	QD	206/209 (99%)	198 (96%)	8 (4%)	0	100 100
4	XD	206/209 (99%)	191 (93%)	12 (6%)	3 (2%)	8 37
5	QE	149/162 (92%)	140 (94%)	9 (6%)	0	100 100
5	XE	149/162 (92%)	140 (94%)	9 (6%)	0	100 100
6	QF	99/101 (98%)	97 (98%)	2 (2%)	0	100 100
6	XF	99/101 (98%)	97 (98%)	2 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	QG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
7	XG	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
8	QH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
8	XH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
9	QI	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
9	XI	124/128 (97%)	107 (86%)	17 (14%)	0	100	100
10	QJ	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
10	XJ	94/105 (90%)	88 (94%)	6 (6%)	0	100	100
11	QK	117/129 (91%)	101 (86%)	16 (14%)	0	100	100
11	XK	114/129 (88%)	102 (90%)	12 (10%)	0	100	100
12	QL	123/132 (93%)	110 (89%)	13 (11%)	0	100	100
12	XL	120/132 (91%)	100 (83%)	20 (17%)	0	100	100
13	QM	118/126 (94%)	102 (86%)	16 (14%)	0	100	100
13	XM	117/126 (93%)	99 (85%)	17 (14%)	1 (1%)	14	47
14	QN	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
14	XN	58/61 (95%)	50 (86%)	8 (14%)	0	100	100
15	QO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	XO	85/89 (96%)	84 (99%)	1 (1%)	0	100	100
16	QP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
16	XP	82/88 (93%)	74 (90%)	8 (10%)	0	100	100
17	QQ	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
17	XQ	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	QR	68/88 (77%)	63 (93%)	5 (7%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	81/93 (87%)	71 (88%)	10 (12%)	0	100	100
19	XS	82/93 (88%)	71 (87%)	11 (13%)	0	100	100
20	QT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
20	XT	97/106 (92%)	91 (94%)	6 (6%)	0	100	100
21	QU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	XU	23/27 (85%)	23 (100%)	0	0	100	100
26	RD	272/276 (99%)	259 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	YD	272/276 (99%)	253 (93%)	19 (7%)	0	100	100
27	RE	203/206 (98%)	187 (92%)	16 (8%)	0	100	100
27	YE	202/206 (98%)	189 (94%)	13 (6%)	0	100	100
28	RF	200/210 (95%)	186 (93%)	14 (7%)	0	100	100
28	YF	200/210 (95%)	185 (92%)	15 (8%)	0	100	100
29	RG	179/182 (98%)	155 (87%)	24 (13%)	0	100	100
29	YG	179/182 (98%)	151 (84%)	27 (15%)	1 (1%)	21	56
30	RH	172/180 (96%)	142 (83%)	29 (17%)	1 (1%)	21	56
30	YH	171/180 (95%)	163 (95%)	8 (5%)	0	100	100
31	RI	144/148 (97%)	124 (86%)	20 (14%)	0	100	100
31	YI	144/148 (97%)	120 (83%)	24 (17%)	0	100	100
32	RN	136/140 (97%)	119 (88%)	17 (12%)	0	100	100
32	YN	138/140 (99%)	126 (91%)	12 (9%)	0	100	100
33	RO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
33	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
34	RP	147/150 (98%)	142 (97%)	5 (3%)	0	100	100
34	YP	145/150 (97%)	138 (95%)	6 (4%)	1 (1%)	18	52
35	RQ	139/141 (99%)	116 (84%)	22 (16%)	1 (1%)	18	52
35	YQ	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
36	RR	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	14	47
36	YR	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
37	RS	109/112 (97%)	89 (82%)	20 (18%)	0	100	100
37	YS	108/112 (96%)	105 (97%)	3 (3%)	0	100	100
38	RT	135/146 (92%)	119 (88%)	14 (10%)	2 (2%)	8	37
38	YT	135/146 (92%)	120 (89%)	13 (10%)	2 (2%)	8	37
39	RU	115/118 (98%)	103 (90%)	12 (10%)	0	100	100
39	YU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	47
40	RV	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
40	YV	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
41	RW	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
41	YW	111/113 (98%)	104 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	RX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
42	YX	92/96 (96%)	90 (98%)	2 (2%)	0	100	100
43	RY	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
43	YY	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
44	RZ	181/206 (88%)	143 (79%)	38 (21%)	0	100	100
44	YZ	181/206 (88%)	176 (97%)	4 (2%)	1 (1%)	21	56
45	R0	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
45	Y0	73/85 (86%)	70 (96%)	3 (4%)	0	100	100
46	R1	95/98 (97%)	84 (88%)	11 (12%)	0	100	100
46	Y1	91/98 (93%)	84 (92%)	7 (8%)	0	100	100
47	R2	67/72 (93%)	65 (97%)	2 (3%)	0	100	100
47	Y2	64/72 (89%)	61 (95%)	3 (5%)	0	100	100
48	R3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
48	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
49	R4	67/71 (94%)	54 (81%)	13 (19%)	0	100	100
49	Y4	67/71 (94%)	55 (82%)	12 (18%)	0	100	100
50	R5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
50	Y5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
51	R6	51/54 (94%)	51 (100%)	0	0	100	100
51	Y6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
52	R7	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
52	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
53	R8	62/65 (95%)	49 (79%)	13 (21%)	0	100	100
53	Y8	62/65 (95%)	53 (86%)	8 (13%)	1 (2%)	7	36
54	R9	35/37 (95%)	35 (100%)	0	0	100	100
54	Y9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
All	All	11453/12128 (94%)	10502 (92%)	935 (8%)	16 (0%)	48	79

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
36	RR	4	LEU
4	XD	31	CYS

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Mol	Chain	Res	Type
44	YZ	52	SER
38	RT	123	GLN
38	RT	124	ASP

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%)	203 (100%)	0	100	100
2	XB	204/220 (93%)	201 (98%)	3 (2%)	57	76
3	QC	159/188 (85%)	158 (99%)	1 (1%)	78	84
3	XC	159/188 (85%)	156 (98%)	3 (2%)	50	73
4	QD	180/181 (99%)	178 (99%)	2 (1%)	65	79
4	XD	180/181 (99%)	170 (94%)	10 (6%)	19	52
5	QE	116/123 (94%)	114 (98%)	2 (2%)	53	75
5	XE	116/123 (94%)	115 (99%)	1 (1%)	70	81
6	QF	90/90 (100%)	89 (99%)	1 (1%)	65	79
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	125 (99%)	1 (1%)	73	82
7	XG	126/127 (99%)	124 (98%)	2 (2%)	55	75
8	QH	118/119 (99%)	116 (98%)	2 (2%)	53	75
8	XH	118/119 (99%)	117 (99%)	1 (1%)	73	82
9	QI	98/99 (99%)	98 (100%)	0	100	100
9	XI	97/99 (98%)	97 (100%)	0	100	100
10	QJ	89/92 (97%)	86 (97%)	3 (3%)	32	64
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	90/99 (91%)	89 (99%)	1 (1%)	65	79
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	XL	103/109 (94%)	103 (100%)	0	100	100
13	QM	96/101 (95%)	93 (97%)	3 (3%)	35	66
13	XM	95/101 (94%)	94 (99%)	1 (1%)	65	79
14	QN	49/50 (98%)	47 (96%)	2 (4%)	27	60
14	XN	49/50 (98%)	48 (98%)	1 (2%)	48	72
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%)	71 (99%)	1 (1%)	59	77
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	94 (99%)	1 (1%)	65	79
17	XQ	95/97 (98%)	94 (99%)	1 (1%)	65	79
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	60 (98%)	1 (2%)	55	75
19	QS	72/80 (90%)	71 (99%)	1 (1%)	59	77
19	XS	73/80 (91%)	72 (99%)	1 (1%)	59	77
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	22	55
26	RD	216/218 (99%)	216 (100%)	0	100	100
26	YD	216/218 (99%)	213 (99%)	3 (1%)	59	77
27	RE	165/166 (99%)	161 (98%)	4 (2%)	43	70
27	YE	165/166 (99%)	158 (96%)	7 (4%)	26	60
28	RF	161/166 (97%)	160 (99%)	1 (1%)	78	84
28	YF	161/166 (97%)	160 (99%)	1 (1%)	78	84
29	RG	155/156 (99%)	155 (100%)	0	100	100
29	YG	155/156 (99%)	154 (99%)	1 (1%)	78	84
30	RH	145/148 (98%)	144 (99%)	1 (1%)	76	83
30	YH	144/148 (97%)	140 (97%)	4 (3%)	38	68
31	RI	122/124 (98%)	120 (98%)	2 (2%)	55	75
31	YI	122/124 (98%)	121 (99%)	1 (1%)	73	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	RN	117/119 (98%)	113 (97%)	4 (3%)	32	64
32	YN	119/119 (100%)	119 (100%)	0	100	100
33	RO	100/100 (100%)	99 (99%)	1 (1%)	68	80
33	YO	100/100 (100%)	100 (100%)	0	100	100
34	RP	116/116 (100%)	115 (99%)	1 (1%)	70	81
34	YP	114/116 (98%)	114 (100%)	0	100	100
35	RQ	111/111 (100%)	110 (99%)	1 (1%)	70	81
35	YQ	111/111 (100%)	110 (99%)	1 (1%)	70	81
36	RR	100/101 (99%)	99 (99%)	1 (1%)	68	80
36	YR	100/101 (99%)	100 (100%)	0	100	100
37	RS	87/88 (99%)	87 (100%)	0	100	100
37	YS	87/88 (99%)	87 (100%)	0	100	100
38	RT	120/127 (94%)	118 (98%)	2 (2%)	53	75
38	YT	120/127 (94%)	116 (97%)	4 (3%)	33	65
39	RU	93/94 (99%)	92 (99%)	1 (1%)	65	79
39	YU	93/94 (99%)	91 (98%)	2 (2%)	45	71
40	RV	82/82 (100%)	80 (98%)	2 (2%)	43	70
40	YV	82/82 (100%)	79 (96%)	3 (4%)	30	63
41	RW	92/92 (100%)	92 (100%)	0	100	100
41	YW	92/92 (100%)	92 (100%)	0	100	100
42	RX	74/78 (95%)	73 (99%)	1 (1%)	59	77
42	YX	76/78 (97%)	75 (99%)	1 (1%)	61	78
43	RY	88/91 (97%)	87 (99%)	1 (1%)	65	79
43	YY	88/91 (97%)	88 (100%)	0	100	100
44	RZ	162/179 (90%)	160 (99%)	2 (1%)	63	79
44	YZ	162/179 (90%)	160 (99%)	2 (1%)	63	79
45	R0	65/67 (97%)	63 (97%)	2 (3%)	35	66
45	Y0	61/67 (91%)	61 (100%)	0	100	100
46	R1	82/83 (99%)	82 (100%)	0	100	100
46	Y1	78/83 (94%)	77 (99%)	1 (1%)	61	78
47	R2	64/67 (96%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	Y2	62/67 (92%)	62 (100%)	0	100	100
48	R3	51/52 (98%)	51 (100%)	0	100	100
48	Y3	51/52 (98%)	51 (100%)	0	100	100
49	R4	62/63 (98%)	62 (100%)	0	100	100
49	Y4	62/63 (98%)	61 (98%)	1 (2%)	55	75
50	R5	51/52 (98%)	51 (100%)	0	100	100
50	Y5	51/52 (98%)	51 (100%)	0	100	100
51	R6	51/52 (98%)	51 (100%)	0	100	100
51	Y6	51/52 (98%)	51 (100%)	0	100	100
52	R7	40/42 (95%)	40 (100%)	0	100	100
52	Y7	41/42 (98%)	41 (100%)	0	100	100
53	R8	54/55 (98%)	53 (98%)	1 (2%)	50	73
53	Y8	54/55 (98%)	54 (100%)	0	100	100
54	R9	34/34 (100%)	34 (100%)	0	100	100
54	Y9	34/34 (100%)	34 (100%)	0	100	100
All	All	9692/10066 (96%)	9585 (99%)	107 (1%)	65	79

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	XD	20	TYR
17	XQ	57	VAL
40	YV	72	VAL
4	XD	31	CYS
5	XE	51	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
27	YE	121	ASN
44	YZ	34	ASN
28	YF	40	GLN
35	YQ	113	GLN
31	RI	43	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1521 (98%)	289 (19%)	39 (2%)
1	XA	1499/1521 (98%)	271 (18%)	33 (2%)
22	QV	76/77 (98%)	22 (28%)	1 (1%)
22	XV	76/77 (98%)	18 (23%)	1 (1%)
23	QX	18/19 (94%)	7 (38%)	1 (5%)
23	XX	18/19 (94%)	6 (33%)	0
24	RA	2877/2915 (98%)	591 (20%)	37 (1%)
24	YA	2880/2915 (98%)	552 (19%)	43 (1%)
25	RB	119/122 (97%)	18 (15%)	1 (0%)
25	YB	119/122 (97%)	21 (17%)	1 (0%)
All	All	9181/9308 (98%)	1795 (19%)	157 (1%)

5 of 1795 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	32	A
1	QA	39	G
1	QA	47	C

5 of 157 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	YA	210	A
24	YA	1700	G
24	YA	302	A
24	YA	1068	G
24	YA	2622	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	1MG	QV	37	22	23,26,27	1.20	3 (13%)	33,39,42	1.73	5 (15%)
22	1MG	XV	37	22	23,26,27	1.19	3 (13%)	33,39,42	1.76	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	1MG	QV	37	22	-	0/7/25/26	0/3/3/3
22	1MG	XV	37	22	-	0/7/25/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	37	1MG	C5-C4	3.23	1.47	1.38
22	XV	37	1MG	C5-C4	3.19	1.47	1.38
22	XV	37	1MG	C2-N1	2.47	1.41	1.37
22	QV	37	1MG	C2-N1	2.40	1.41	1.37
22	QV	37	1MG	C5-N7	-2.17	1.34	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	XV	37	1MG	C5-C4-N3	-5.24	120.05	128.39
22	QV	37	1MG	C5-C4-N3	-5.17	120.16	128.39
22	XV	37	1MG	C2-N3-C4	4.35	121.76	111.98
22	QV	37	1MG	C2-N3-C4	4.28	121.61	111.98
22	QV	37	1MG	N9-C4-N3	3.90	133.76	125.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1166 ligands modelled in this entry, 1164 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	SF4	XD	301	4	0,12,12	-	-	-		
56	SF4	QD	301	4	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	SF4	XD	301	4	-	-	0/6/5/5
56	SF4	QD	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	1500/1521 (98%)	0.41	73 (4%)	35	22	58, 110, 240, 377	0
1	XA	1500/1521 (98%)	0.52	108 (7%)	21	14	54, 120, 257, 365	0
2	QB	235/256 (91%)	0.53	3 (1%)	75	55	109, 150, 192, 239	0
2	XB	236/256 (92%)	0.91	18 (7%)	20	13	104, 136, 180, 227	0
3	QC	205/239 (85%)	0.88	19 (9%)	14	9	123, 163, 203, 242	0
3	XC	205/239 (85%)	1.43	43 (20%)	2	2	119, 158, 198, 242	0
4	QD	208/209 (99%)	0.81	13 (6%)	26	17	84, 112, 140, 171	0
4	XD	208/209 (99%)	1.47	52 (25%)	2	2	92, 131, 170, 193	0
5	QE	151/162 (93%)	0.47	5 (3%)	49	30	86, 112, 152, 179	0
5	XE	151/162 (93%)	1.06	18 (11%)	9	6	78, 108, 140, 162	0
6	QF	101/101 (100%)	0.96	8 (7%)	18	12	96, 122, 156, 173	0
6	XF	101/101 (100%)	0.46	1 (0%)	79	63	76, 108, 135, 189	0
7	QG	155/156 (99%)	1.26	30 (19%)	3	2	130, 162, 199, 225	0
7	XG	155/156 (99%)	1.34	35 (22%)	2	2	122, 164, 201, 247	0
8	QH	137/138 (99%)	0.63	5 (3%)	46	28	87, 116, 138, 168	0
8	XH	137/138 (99%)	0.79	11 (8%)	18	12	83, 111, 148, 165	0
9	QI	127/128 (99%)	2.54	71 (55%)	0	0	129, 174, 219, 232	0
9	XI	126/128 (98%)	1.59	35 (27%)	1	1	132, 172, 203, 231	0
10	QJ	99/105 (94%)	1.12	21 (21%)	2	2	140, 178, 215, 240	0
10	XJ	96/105 (91%)	1.97	34 (35%)	1	1	144, 175, 211, 235	0
11	QK	119/129 (92%)	1.32	17 (14%)	6	5	91, 119, 158, 189	0
11	XK	116/129 (89%)	0.91	9 (7%)	19	12	64, 105, 149, 188	0
12	QL	125/132 (94%)	1.23	27 (21%)	2	2	64, 90, 133, 187	0
12	XL	122/132 (92%)	0.98	24 (19%)	3	2	60, 96, 126, 169	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	QM	120/126 (95%)	1.19	23 (19%)	3	2	129, 167, 203, 227	0
13	XM	119/126 (94%)	2.11	50 (42%)	0	1	137, 187, 227, 247	0
14	QN	60/61 (98%)	1.72	20 (33%)	1	1	139, 171, 209, 233	0
14	XN	60/61 (98%)	1.16	10 (16%)	4	3	132, 158, 190, 212	0
15	QO	88/89 (98%)	0.63	5 (5%)	29	19	67, 107, 144, 154	0
15	XO	87/89 (97%)	0.65	3 (3%)	48	30	62, 95, 139, 158	0
16	QP	84/88 (95%)	0.76	2 (2%)	59	40	80, 100, 140, 184	0
16	XP	84/88 (95%)	0.92	10 (11%)	9	6	93, 127, 165, 189	0
17	QQ	100/105 (95%)	0.98	12 (12%)	9	6	73, 99, 142, 155	0
17	XQ	100/105 (95%)	0.56	6 (6%)	27	17	68, 104, 134, 149	0
18	QR	70/88 (79%)	0.87	6 (8%)	16	11	95, 126, 152, 179	0
18	XR	70/88 (79%)	0.42	2 (2%)	53	35	73, 111, 152, 172	0
19	QS	83/93 (89%)	1.43	19 (22%)	2	2	153, 182, 217, 240	0
19	XS	84/93 (90%)	1.67	29 (34%)	1	1	160, 195, 230, 246	0
20	QT	99/106 (93%)	1.08	10 (10%)	12	8	67, 99, 143, 165	0
20	XT	99/106 (93%)	0.88	8 (8%)	18	11	76, 115, 152, 193	0
21	QU	25/27 (92%)	1.86	9 (36%)	1	1	124, 153, 183, 204	0
21	XU	25/27 (92%)	1.40	5 (20%)	3	2	108, 168, 192, 212	0
22	QV	76/77 (98%)	0.78	6 (7%)	18	12	151, 202, 240, 251	0
22	XV	76/77 (98%)	1.91	26 (34%)	1	1	225, 332, 347, 358	0
23	QX	19/19 (100%)	1.58	4 (21%)	2	2	116, 227, 311, 319	0
23	XX	19/19 (100%)	2.81	15 (78%)	0	0	131, 254, 297, 308	0
24	RA	2881/2915 (98%)	0.21	116 (4%)	42	26	40, 73, 215, 458	0
24	YA	2883/2915 (98%)	0.09	94 (3%)	49	30	28, 53, 212, 402	0
25	RB	120/122 (98%)	0.35	1 (0%)	82	67	82, 126, 171, 195	0
25	YB	120/122 (98%)	0.18	5 (4%)	40	25	49, 77, 109, 224	0
26	RD	274/276 (99%)	0.71	15 (5%)	30	19	42, 67, 101, 139	0
26	YD	274/276 (99%)	0.29	5 (1%)	67	48	35, 53, 81, 126	0
27	RE	205/206 (99%)	0.44	8 (3%)	43	27	37, 72, 114, 177	0
27	YE	204/206 (99%)	0.21	2 (0%)	79	63	25, 55, 91, 111	0
28	RF	202/210 (96%)	0.54	9 (4%)	38	24	46, 86, 135, 169	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	YF	202/210 (96%)	0.45	7 (3%) 47 29	29, 59, 134, 186	0
29	RG	181/182 (99%)	1.18	27 (14%) 5 4	112, 145, 188, 220	0
29	YG	181/182 (99%)	0.99	21 (11%) 9 7	73, 123, 172, 219	0
30	RH	174/180 (96%)	1.03	21 (12%) 8 6	90, 131, 176, 222	0
30	YH	173/180 (96%)	0.25	6 (3%) 47 29	48, 69, 97, 118	0
31	RI	146/148 (98%)	0.97	20 (13%) 6 5	72, 114, 150, 159	0
31	YI	146/148 (98%)	0.85	20 (13%) 6 5	65, 103, 139, 169	0
32	RN	138/140 (98%)	1.10	18 (13%) 7 6	50, 82, 129, 147	0
32	YN	140/140 (100%)	0.50	2 (1%) 73 54	33, 55, 91, 128	0
33	RO	122/122 (100%)	0.17	1 (0%) 82 67	47, 72, 99, 124	0
33	YO	122/122 (100%)	0.40	5 (4%) 41 25	38, 58, 90, 107	0
34	RP	149/150 (99%)	0.76	12 (8%) 18 11	50, 86, 131, 150	0
34	YP	147/150 (98%)	0.43	5 (3%) 48 30	30, 64, 105, 133	0
35	RQ	141/141 (100%)	0.85	11 (7%) 19 12	59, 91, 132, 189	0
35	YQ	141/141 (100%)	0.06	1 (0%) 84 69	39, 59, 88, 136	0
36	RR	117/118 (99%)	0.47	5 (4%) 40 24	53, 68, 100, 156	0
36	YR	117/118 (99%)	0.32	3 (2%) 57 37	39, 52, 83, 154	0
37	RS	111/112 (99%)	1.44	30 (27%) 1 1	98, 126, 166, 186	0
37	YS	110/112 (98%)	0.21	1 (0%) 81 64	52, 72, 103, 117	0
38	RT	137/146 (93%)	0.62	7 (5%) 33 21	50, 83, 143, 196	0
38	YT	137/146 (93%)	0.60	10 (7%) 21 13	47, 68, 125, 170	0
39	RU	117/118 (99%)	0.97	16 (13%) 6 5	47, 81, 131, 174	0
39	YU	117/118 (99%)	0.61	7 (5%) 27 17	29, 45, 88, 151	0
40	RV	101/101 (100%)	0.49	5 (4%) 34 22	57, 94, 123, 167	0
40	YV	101/101 (100%)	0.16	2 (1%) 65 45	28, 55, 89, 133	0
41	RW	113/113 (100%)	0.43	4 (3%) 47 29	46, 65, 114, 204	0
41	YW	113/113 (100%)	0.23	4 (3%) 47 29	29, 48, 82, 192	0
42	RX	92/96 (95%)	0.40	5 (5%) 31 20	52, 77, 114, 122	0
42	YX	94/96 (97%)	-0.03	0 100 100	34, 53, 83, 123	0
43	RY	107/110 (97%)	0.99	14 (13%) 7 6	64, 97, 130, 148	0
43	YY	107/110 (97%)	0.33	1 (0%) 81 64	45, 67, 97, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	RZ	183/206 (88%)	0.60	12 (6%) 24 15	98, 131, 173, 201	0
44	YZ	183/206 (88%)	0.20	2 (1%) 78 61	47, 84, 116, 174	0
45	R0	81/85 (95%)	1.00	13 (16%) 5 3	68, 90, 149, 208	0
45	Y0	75/85 (88%)	0.27	1 (1%) 75 55	42, 59, 85, 98	0
46	R1	97/98 (98%)	1.40	25 (25%) 1 2	49, 75, 139, 212	0
46	Y1	93/98 (94%)	0.87	14 (15%) 5 4	41, 65, 121, 135	0
47	R2	69/72 (95%)	0.65	6 (8%) 16 11	67, 93, 143, 158	0
47	Y2	66/72 (91%)	0.48	6 (9%) 15 9	41, 65, 105, 142	0
48	R3	59/60 (98%)	0.86	6 (10%) 12 8	56, 86, 144, 197	0
48	Y3	59/60 (98%)	0.20	2 (3%) 48 30	37, 53, 87, 140	0
49	R4	69/71 (97%)	1.01	8 (11%) 9 7	134, 176, 219, 247	0
49	Y4	69/71 (97%)	1.22	12 (17%) 4 3	102, 153, 229, 258	0
50	R5	59/60 (98%)	0.23	1 (1%) 69 49	43, 66, 105, 144	0
50	Y5	59/60 (98%)	0.26	1 (1%) 69 49	25, 53, 90, 114	0
51	R6	53/54 (98%)	0.36	1 (1%) 66 46	74, 83, 108, 119	0
51	Y6	53/54 (98%)	-0.05	0 100 100	49, 64, 85, 99	0
52	R7	47/49 (95%)	0.66	6 (12%) 7 6	48, 62, 85, 129	0
52	Y7	48/49 (97%)	0.33	2 (4%) 40 25	31, 45, 78, 108	0
53	R8	64/65 (98%)	1.48	18 (28%) 1 1	59, 77, 115, 163	0
53	Y8	64/65 (98%)	1.06	10 (15%) 5 4	37, 55, 92, 254	0
54	R9	37/37 (100%)	0.66	1 (2%) 56 36	76, 91, 120, 147	0
54	Y9	37/37 (100%)	0.18	1 (2%) 56 36	37, 57, 80, 99	0
All	All	20843/21436 (97%)	0.57	1654 (7%) 18 12	25, 91, 206, 458	0

The worst 5 of 1654 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	QK	128	ALA	14.3
11	QK	129	SER	13.6
9	QI	110	GLU	10.7
12	QL	28	LYS	10.2
13	XM	97	PRO	9.4

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
22	1MG	XV	37	24/25	0.53	0.25	287,291,295,297	0
22	1MG	QV	37	24/25	0.69	0.12	165,170,181,185	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	RA	3260	1/1	0.38	0.37	128,128,128,128	0
55	MG	YA	3449	1/1	0.43	0.20	85,85,85,85	0
55	MG	RA	3343	1/1	0.51	0.23	83,83,83,83	0
55	MG	RA	3257	1/1	0.52	0.45	93,93,93,93	0
55	MG	YA	3210	1/1	0.54	0.31	57,57,57,57	0
55	MG	XA	1620	1/1	0.55	0.11	85,85,85,85	0
55	MG	RA	3205	1/1	0.56	0.04	8,8,8,8	0
55	MG	YA	3028	1/1	0.56	0.11	10,10,10,10	0
55	MG	XA	1640	1/1	0.58	0.17	66,66,66,66	0
55	MG	RA	3297	1/1	0.58	0.25	79,79,79,79	0
55	MG	XM	202	1/1	0.59	0.14	75,75,75,75	0
55	MG	RA	3412	1/1	0.60	0.18	62,62,62,62	0
55	MG	RB	206	1/1	0.62	0.22	77,77,77,77	0
55	MG	RA	3265	1/1	0.64	0.27	83,83,83,83	0
55	MG	QA	1616	1/1	0.66	0.14	75,75,75,75	0
55	MG	YD	301	1/1	0.66	0.23	72,72,72,72	0
55	MG	YA	3326	1/1	0.67	0.33	62,62,62,62	0
55	MG	YA	3144	1/1	0.67	0.48	63,63,63,63	0
55	MG	YA	3270	1/1	0.67	0.17	66,66,66,66	0
55	MG	RA	3136	1/1	0.68	0.24	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	YA	3468	1/1	0.68	0.16	68,68,68,68	0
55	MG	RA	3143	1/1	0.68	0.15	76,76,76,76	0
55	MG	YA	3322	1/1	0.69	0.23	67,67,67,67	0
55	MG	RA	3346	1/1	0.69	0.33	71,71,71,71	0
55	MG	YA	3424	1/1	0.69	0.30	63,63,63,63	0
55	MG	XA	1645	1/1	0.69	0.11	70,70,70,70	0
55	MG	XM	201	1/1	0.69	0.24	77,77,77,77	0
55	MG	RA	3195	1/1	0.69	0.26	76,76,76,76	0
55	MG	XA	1610	1/1	0.70	0.11	67,67,67,67	0
55	MG	RA	3375	1/1	0.70	0.29	72,72,72,72	0
55	MG	RA	3147	1/1	0.70	0.11	64,64,64,64	0
55	MG	YA	3201	1/1	0.70	0.38	80,80,80,80	0
55	MG	RA	3437	1/1	0.70	0.18	32,32,32,32	0
55	MG	RA	3221	1/1	0.70	0.34	63,63,63,63	0
55	MG	RA	3330	1/1	0.71	0.13	70,70,70,70	0
55	MG	RA	3382	1/1	0.71	0.23	59,59,59,59	0
55	MG	RA	3258	1/1	0.71	0.40	69,69,69,69	0
55	MG	QA	1651	1/1	0.71	0.13	58,58,58,58	0
55	MG	YA	3118	1/1	0.71	0.11	42,42,42,42	0
55	MG	QA	1653	1/1	0.72	0.12	58,58,58,58	0
55	MG	YA	3290	1/1	0.72	0.23	65,65,65,65	0
55	MG	RA	3350	1/1	0.72	0.18	81,81,81,81	0
55	MG	YB	202	1/1	0.72	0.10	46,46,46,46	0
55	MG	RA	3318	1/1	0.72	0.20	84,84,84,84	0
55	MG	YA	3180	1/1	0.73	0.24	60,60,60,60	0
55	MG	YA	3379	1/1	0.73	0.16	57,57,57,57	0
55	MG	RA	3272	1/1	0.73	0.12	59,59,59,59	0
55	MG	RA	3171	1/1	0.73	0.15	60,60,60,60	0
55	MG	RA	3233	1/1	0.73	0.20	70,70,70,70	0
55	MG	RA	3175	1/1	0.73	0.20	67,67,67,67	0
55	MG	XA	1653	1/1	0.73	0.10	75,75,75,75	0
55	MG	YA	3353	1/1	0.74	0.21	50,50,50,50	0
55	MG	YA	3378	1/1	0.74	0.14	42,42,42,42	0
55	MG	RA	3170	1/1	0.74	0.16	73,73,73,73	0
55	MG	YA	3275	1/1	0.74	0.32	79,79,79,79	0
55	MG	YA	3429	1/1	0.74	0.14	62,62,62,62	0
55	MG	RA	3045	1/1	0.74	0.37	60,60,60,60	0
55	MG	YA	3301	1/1	0.74	0.16	54,54,54,54	0
55	MG	RA	3365	1/1	0.74	0.27	80,80,80,80	0
55	MG	YA	3234	1/1	0.74	0.15	66,66,66,66	0
55	MG	YA	3406	1/1	0.75	0.49	84,84,84,84	0
55	MG	RA	3396	1/1	0.75	0.18	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	YA	3021	1/1	0.75	0.08	9,9,9,9	0
55	MG	QA	1658	1/1	0.75	0.07	92,92,92,92	0
55	MG	RA	3268	1/1	0.75	0.13	52,52,52,52	0
55	MG	QA	1638	1/1	0.75	0.13	85,85,85,85	0
55	MG	QA	1657	1/1	0.75	0.10	44,44,44,44	0
55	MG	YA	3373	1/1	0.76	0.14	52,52,52,52	0
55	MG	RA	3223	1/1	0.76	0.13	44,44,44,44	0
55	MG	YA	3154	1/1	0.76	0.24	49,49,49,49	0
55	MG	RA	3414	1/1	0.76	0.13	71,71,71,71	0
55	MG	QA	1636	1/1	0.76	0.15	62,62,62,62	0
55	MG	XA	1666	1/1	0.76	0.10	74,74,74,74	0
55	MG	XA	1667	1/1	0.76	0.14	76,76,76,76	0
55	MG	YA	3457	1/1	0.76	0.26	87,87,87,87	0
55	MG	YA	3260	1/1	0.76	0.12	67,67,67,67	0
55	MG	YA	3368	1/1	0.76	0.15	57,57,57,57	0
55	MG	YA	3371	1/1	0.76	0.25	51,51,51,51	0
55	MG	RA	3090	1/1	0.77	0.16	40,40,40,40	0
55	MG	RA	3008	1/1	0.77	0.24	58,58,58,58	0
55	MG	RA	3161	1/1	0.77	0.11	43,43,43,43	0
55	MG	RA	3400	1/1	0.77	0.14	63,63,63,63	0
55	MG	RA	3410	1/1	0.77	0.16	80,80,80,80	0
55	MG	YA	3177	1/1	0.77	0.20	59,59,59,59	0
55	MG	YA	3510	1/1	0.77	0.13	29,29,29,29	0
55	MG	RA	3366	1/1	0.77	0.11	47,47,47,47	0
55	MG	YA	3194	1/1	0.77	0.13	46,46,46,46	0
55	MG	RA	3323	1/1	0.78	0.11	65,65,65,65	0
55	MG	RA	3237	1/1	0.78	0.13	52,52,52,52	0
55	MG	RA	3251	1/1	0.78	0.26	61,61,61,61	0
55	MG	YA	3413	1/1	0.78	0.14	42,42,42,42	0
55	MG	YA	3421	1/1	0.78	0.23	69,69,69,69	0
55	MG	QA	1623	1/1	0.78	0.11	50,50,50,50	0
55	MG	RA	3202	1/1	0.78	0.27	66,66,66,66	0
55	MG	YA	3015	1/1	0.78	0.14	48,48,48,48	0
55	MG	RA	3362	1/1	0.78	0.22	74,74,74,74	0
55	MG	YA	3462	1/1	0.78	0.10	46,46,46,46	0
55	MG	RA	3148	1/1	0.78	0.13	36,36,36,36	0
55	MG	YA	3227	1/1	0.78	0.13	57,57,57,57	0
55	MG	YA	3230	1/1	0.78	0.19	51,51,51,51	0
55	MG	YA	3057	1/1	0.78	0.15	19,19,19,19	0
55	MG	RQ	201	1/1	0.79	0.15	58,58,58,58	0
55	MG	RA	3103	1/1	0.79	0.10	52,52,52,52	0
55	MG	YA	3145	1/1	0.79	0.18	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	RA	3320	1/1	0.79	0.19	58,58,58,58	0
55	MG	YA	3175	1/1	0.79	0.16	49,49,49,49	0
55	MG	RA	3385	1/1	0.79	0.18	53,53,53,53	0
55	MG	RA	3091	1/1	0.79	0.16	43,43,43,43	0
55	MG	YA	3280	1/1	0.79	0.13	66,66,66,66	0
55	MG	RA	3441	1/1	0.79	0.32	72,72,72,72	0
55	MG	RA	3348	1/1	0.79	0.09	52,52,52,52	0
55	MG	RA	3192	1/1	0.80	0.17	39,39,39,39	0
55	MG	RA	3152	1/1	0.80	0.20	61,61,61,61	0
55	MG	YA	3285	1/1	0.80	0.12	45,45,45,45	0
55	MG	RA	3226	1/1	0.80	0.29	58,58,58,58	0
55	MG	RA	3093	1/1	0.80	0.15	39,39,39,39	0
55	MG	RA	3167	1/1	0.80	0.13	70,70,70,70	0
55	MG	YA	3446	1/1	0.80	0.12	64,64,64,64	0
55	MG	YA	3212	1/1	0.80	0.14	53,53,53,53	0
55	MG	YA	3341	1/1	0.80	0.08	64,64,64,64	0
55	MG	XA	1650	1/1	0.80	0.08	92,92,92,92	0
55	MG	RA	3424	1/1	0.80	0.24	72,72,72,72	0
55	MG	RA	3269	1/1	0.80	0.20	78,78,78,78	0
55	MG	RA	3219	1/1	0.80	0.19	51,51,51,51	0
55	MG	RA	3347	1/1	0.80	0.10	63,63,63,63	0
55	MG	YA	3337	1/1	0.81	0.12	35,35,35,35	0
55	MG	RA	3006	1/1	0.81	0.10	45,45,45,45	0
55	MG	YA	3203	1/1	0.81	0.16	42,42,42,42	0
55	MG	YA	3357	1/1	0.81	0.13	50,50,50,50	0
55	MG	RA	3357	1/1	0.81	0.20	43,43,43,43	0
55	MG	RA	3439	1/1	0.81	0.07	36,36,36,36	0
55	MG	RA	3271	1/1	0.81	0.15	49,49,49,49	0
55	MG	RA	3227	1/1	0.81	0.18	70,70,70,70	0
55	MG	YA	3233	1/1	0.81	0.19	48,48,48,48	0
55	MG	YA	3386	1/1	0.81	0.14	42,42,42,42	0
55	MG	RA	3231	1/1	0.81	0.22	36,36,36,36	0
55	MG	QA	1618	1/1	0.81	0.10	47,47,47,47	0
55	MG	RA	3194	1/1	0.81	0.14	66,66,66,66	0
55	MG	QA	1626	1/1	0.81	0.10	57,57,57,57	0
55	MG	RA	3107	1/1	0.81	0.21	63,63,63,63	0
55	MG	YA	3433	1/1	0.81	0.21	51,51,51,51	0
55	MG	YA	3434	1/1	0.81	0.14	68,68,68,68	0
55	MG	YA	3445	1/1	0.81	0.15	46,46,46,46	0
55	MG	YA	3281	1/1	0.81	0.10	35,35,35,35	0
55	MG	YA	3161	1/1	0.81	0.21	58,58,58,58	0
55	MG	RA	3164	1/1	0.81	0.14	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	RA	3061	1/1	0.81	0.23	45,45,45,45	0
55	MG	YA	3316	1/1	0.81	0.25	71,71,71,71	0
55	MG	RA	3141	1/1	0.81	0.10	58,58,58,58	0
55	MG	QA	1632	1/1	0.81	0.19	52,52,52,52	0
55	MG	YA	3327	1/1	0.81	0.12	53,53,53,53	0
55	MG	Y1	101	1/1	0.81	0.22	46,46,46,46	0
55	MG	YA	3289	1/1	0.82	0.12	36,36,36,36	0
55	MG	RA	3196	1/1	0.82	0.35	72,72,72,72	0
55	MG	YA	3058	1/1	0.82	0.20	34,34,34,34	0
55	MG	XA	1663	1/1	0.82	0.12	64,64,64,64	0
55	MG	YA	3220	1/1	0.82	0.11	27,27,27,27	0
55	MG	YA	3133	1/1	0.82	0.14	26,26,26,26	0
55	MG	RA	3298	1/1	0.82	0.18	45,45,45,45	0
55	MG	RA	3300	1/1	0.82	0.09	62,62,62,62	0
55	MG	RA	3301	1/1	0.82	0.15	57,57,57,57	0
55	MG	YA	3239	1/1	0.82	0.37	67,67,67,67	0
55	MG	QA	1615	1/1	0.82	0.11	69,69,69,69	0
55	MG	YA	3359	1/1	0.82	0.14	57,57,57,57	0
55	MG	YA	3363	1/1	0.82	0.09	55,55,55,55	0
55	MG	YA	3002	1/1	0.82	0.06	33,33,33,33	0
55	MG	YA	3492	1/1	0.82	0.23	49,49,49,49	0
55	MG	YA	3009	1/1	0.82	0.22	52,52,52,52	0
55	MG	RA	3430	1/1	0.82	0.17	69,69,69,69	0
55	MG	YB	207	1/1	0.82	0.06	48,48,48,48	0
55	MG	RA	3239	1/1	0.82	0.13	57,57,57,57	0
55	MG	RA	3174	1/1	0.82	0.12	36,36,36,36	0
55	MG	RA	3166	1/1	0.83	0.20	58,58,58,58	0
55	MG	YA	3004	1/1	0.83	0.11	35,35,35,35	0
55	MG	YA	3188	1/1	0.83	0.14	34,34,34,34	0
55	MG	YA	3384	1/1	0.83	0.14	36,36,36,36	0
55	MG	RA	3064	1/1	0.83	0.13	41,41,41,41	0
55	MG	RA	3228	1/1	0.83	0.13	49,49,49,49	0
55	MG	YA	3292	1/1	0.83	0.17	48,48,48,48	0
55	MG	YA	3417	1/1	0.83	0.10	43,43,43,43	0
55	MG	YA	3017	1/1	0.83	0.20	52,52,52,52	0
55	MG	YA	3310	1/1	0.83	0.35	84,84,84,84	0
55	MG	RA	3207	1/1	0.83	0.14	59,59,59,59	0
55	MG	XA	1643	1/1	0.83	0.11	59,59,59,59	0
55	MG	RA	3232	1/1	0.83	0.21	53,53,53,53	0
55	MG	YA	3224	1/1	0.83	0.11	32,32,32,32	0
55	MG	QA	1640	1/1	0.83	0.14	59,59,59,59	0
55	MG	QA	1659	1/1	0.83	0.11	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	YA	3345	1/1	0.83	0.27	59,59,59,59	0
55	MG	YA	3350	1/1	0.83	0.18	54,54,54,54	0
55	MG	YA	3352	1/1	0.83	0.08	45,45,45,45	0
55	MG	YA	3476	1/1	0.83	0.09	59,59,59,59	0
55	MG	XA	1654	1/1	0.83	0.19	63,63,63,63	0
55	MG	RA	3436	1/1	0.83	0.28	66,66,66,66	0
55	MG	RA	3372	1/1	0.83	0.20	63,63,63,63	0
55	MG	RA	3117	1/1	0.83	0.08	61,61,61,61	0
55	MG	RA	3245	1/1	0.83	0.24	57,57,57,57	0
55	MG	RA	3273	1/1	0.83	0.20	53,53,53,53	0
55	MG	RA	3247	1/1	0.84	0.17	45,45,45,45	0
55	MG	YA	3283	1/1	0.84	0.16	38,38,38,38	0
55	MG	YA	3181	1/1	0.84	0.14	45,45,45,45	0
55	MG	YA	3183	1/1	0.84	0.15	51,51,51,51	0
55	MG	YA	3398	1/1	0.84	0.21	66,66,66,66	0
55	MG	RA	3307	1/1	0.84	0.19	41,41,41,41	0
55	MG	RA	3316	1/1	0.84	0.18	58,58,58,58	0
55	MG	YA	3034	1/1	0.84	0.16	31,31,31,31	0
55	MG	YA	3306	1/1	0.84	0.29	61,61,61,61	0
55	MG	RA	3392	1/1	0.84	0.13	51,51,51,51	0
55	MG	RA	3156	1/1	0.84	0.18	60,60,60,60	0
55	MG	RA	3442	1/1	0.84	0.12	32,32,32,32	0
55	MG	YA	3120	1/1	0.84	0.16	36,36,36,36	0
55	MG	YA	3435	1/1	0.84	0.09	28,28,28,28	0
55	MG	YA	3440	1/1	0.84	0.18	63,63,63,63	0
55	MG	RA	3319	1/1	0.84	0.10	56,56,56,56	0
55	MG	RA	3287	1/1	0.84	0.10	55,55,55,55	0
55	MG	RA	3253	1/1	0.84	0.17	50,50,50,50	0
55	MG	XA	1613	1/1	0.84	0.12	61,61,61,61	0
55	MG	YA	3159	1/1	0.84	0.17	43,43,43,43	0
55	MG	YA	3238	1/1	0.84	0.26	57,57,57,57	0
55	MG	RA	3413	1/1	0.84	0.21	69,69,69,69	0
55	MG	YA	3246	1/1	0.84	0.20	39,39,39,39	0
55	MG	YA	3254	1/1	0.84	0.20	41,41,41,41	0
55	MG	YA	3166	1/1	0.84	0.12	40,40,40,40	0
55	MG	YA	3170	1/1	0.84	0.19	48,48,48,48	0
55	MG	RA	3177	1/1	0.84	0.10	41,41,41,41	0
55	MG	QA	1648	1/1	0.84	0.12	70,70,70,70	0
55	MG	RA	3280	1/1	0.85	0.20	52,52,52,52	0
55	MG	RA	3082	1/1	0.85	0.17	33,33,33,33	0
55	MG	RA	3250	1/1	0.85	0.18	59,59,59,59	0
55	MG	XA	1670	1/1	0.85	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	RA	3087	1/1	0.85	0.22	35,35,35,35	0
55	MG	YA	3392	1/1	0.85	0.10	27,27,27,27	0
55	MG	RA	3354	1/1	0.85	0.08	62,62,62,62	0
55	MG	RA	3112	1/1	0.85	0.12	36,36,36,36	0
55	MG	RA	3359	1/1	0.85	0.16	66,66,66,66	0
55	MG	RA	3113	1/1	0.85	0.32	42,42,42,42	0
55	MG	RA	3230	1/1	0.85	0.16	48,48,48,48	0
55	MG	RA	3309	1/1	0.85	0.15	57,57,57,57	0
55	MG	RA	3314	1/1	0.85	0.12	46,46,46,46	0
55	MG	RA	3203	1/1	0.85	0.15	62,62,62,62	0
55	MG	YA	3216	1/1	0.85	0.12	30,30,30,30	0
55	MG	RA	3378	1/1	0.85	0.13	49,49,49,49	0
55	MG	YA	3336	1/1	0.85	0.35	65,65,65,65	0
55	MG	YA	3442	1/1	0.85	0.08	59,59,59,59	0
55	MG	XA	1611	1/1	0.85	0.18	56,56,56,56	0
55	MG	RA	3049	1/1	0.85	0.11	46,46,46,46	0
55	MG	YA	3447	1/1	0.85	0.32	104,104,104,104	0
55	MG	YA	3343	1/1	0.85	0.10	45,45,45,45	0
55	MG	YA	3080	1/1	0.85	0.11	37,37,37,37	0
55	MG	YA	3459	1/1	0.85	0.17	49,49,49,49	0
55	MG	QA	1602	1/1	0.85	0.14	30,30,30,30	0
55	MG	YA	3463	1/1	0.85	0.25	70,70,70,70	0
55	MG	RA	3210	1/1	0.85	0.17	32,32,32,32	0
55	MG	RA	3394	1/1	0.85	0.12	45,45,45,45	0
55	MG	QA	1612	1/1	0.85	0.07	44,44,44,44	0
55	MG	XA	1646	1/1	0.85	0.12	57,57,57,57	0
55	MG	YA	3360	1/1	0.85	0.14	53,53,53,53	0
55	MG	RA	3242	1/1	0.85	0.11	30,30,30,30	0
55	MG	RA	3403	1/1	0.85	0.10	55,55,55,55	0
55	MG	YQ	203	1/1	0.85	0.12	55,55,55,55	0
55	MG	Y0	102	1/1	0.85	0.12	42,42,42,42	0
55	MG	RA	3165	1/1	0.85	0.20	55,55,55,55	0
55	MG	RA	3364	1/1	0.86	0.09	56,56,56,56	0
55	MG	YA	3396	1/1	0.86	0.10	42,42,42,42	0
55	MG	RA	3102	1/1	0.86	0.21	44,44,44,44	0
55	MG	YA	3018	1/1	0.86	0.24	49,49,49,49	0
55	MG	RA	3340	1/1	0.86	0.16	39,39,39,39	0
55	MG	RA	3302	1/1	0.86	0.19	53,53,53,53	0
55	MG	YA	3420	1/1	0.86	0.08	48,48,48,48	0
55	MG	RA	3159	1/1	0.86	0.20	69,69,69,69	0
55	MG	YA	3423	1/1	0.86	0.05	46,46,46,46	0
55	MG	RA	3160	1/1	0.86	0.09	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	RA	3281	1/1	0.86	0.09	58,58,58,58	0
55	MG	RA	3191	1/1	0.86	0.12	45,45,45,45	0
55	MG	YA	3081	1/1	0.86	0.13	41,41,41,41	0
55	MG	YA	3103	1/1	0.86	0.23	47,47,47,47	0
55	MG	XA	1655	1/1	0.86	0.07	46,46,46,46	0
55	MG	XA	1661	1/1	0.86	0.09	46,46,46,46	0
55	MG	YA	3228	1/1	0.86	0.18	56,56,56,56	0
55	MG	RA	3387	1/1	0.86	0.09	44,44,44,44	0
55	MG	YA	3137	1/1	0.86	0.11	33,33,33,33	0
55	MG	RA	3390	1/1	0.86	0.18	50,50,50,50	0
55	MG	YA	3450	1/1	0.86	0.07	52,52,52,52	0
55	MG	YA	3454	1/1	0.86	0.10	28,28,28,28	0
55	MG	RA	3295	1/1	0.86	0.15	39,39,39,39	0
55	MG	RA	3074	1/1	0.86	0.23	41,41,41,41	0
55	MG	YA	3156	1/1	0.86	0.13	30,30,30,30	0
55	MG	XA	1673	1/1	0.86	0.13	44,44,44,44	0
55	MG	YA	3464	1/1	0.86	0.08	49,49,49,49	0
55	MG	RA	3236	1/1	0.86	0.12	61,61,61,61	0
55	MG	YA	3267	1/1	0.86	0.15	47,47,47,47	0
55	MG	YA	3369	1/1	0.86	0.33	77,77,77,77	0
55	MG	RR	201	1/1	0.86	0.10	22,22,22,22	0
55	MG	RA	3397	1/1	0.86	0.11	56,56,56,56	0
55	MG	YA	3172	1/1	0.86	0.12	20,20,20,20	0
55	MG	RA	3360	1/1	0.86	0.07	40,40,40,40	0
55	MG	YE	304	1/1	0.86	0.13	60,60,60,60	0
55	MG	YA	3381	1/1	0.86	0.15	40,40,40,40	0
55	MG	Y0	101	1/1	0.86	0.12	34,34,34,34	0
55	MG	QA	1643	1/1	0.86	0.17	57,57,57,57	0
55	MG	YA	3178	1/1	0.86	0.17	36,36,36,36	0
55	MG	YA	3320	1/1	0.87	0.13	50,50,50,50	0
55	MG	RA	3438	1/1	0.87	0.13	46,46,46,46	0
55	MG	QA	1647	1/1	0.87	0.11	64,64,64,64	0
55	MG	RA	3218	1/1	0.87	0.36	55,55,55,55	0
55	MG	YA	3150	1/1	0.87	0.15	31,31,31,31	0
55	MG	YA	3151	1/1	0.87	0.15	45,45,45,45	0
55	MG	YA	3430	1/1	0.87	0.19	57,57,57,57	0
55	MG	YA	3152	1/1	0.87	0.07	21,21,21,21	0
55	MG	YA	3010	1/1	0.87	0.20	76,76,76,76	0
55	MG	YA	3011	1/1	0.87	0.15	47,47,47,47	0
55	MG	YA	3439	1/1	0.87	0.20	39,39,39,39	0
55	MG	YA	3347	1/1	0.87	0.08	31,31,31,31	0
55	MG	YA	3012	1/1	0.87	0.20	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	RA	3379	1/1	0.87	0.09	46,46,46,46	0
55	MG	RA	3305	1/1	0.87	0.15	54,54,54,54	0
55	MG	YA	3355	1/1	0.87	0.21	45,45,45,45	0
55	MG	RA	3198	1/1	0.87	0.15	42,42,42,42	0
55	MG	RA	3162	1/1	0.87	0.10	44,44,44,44	0
55	MG	RT	201	1/1	0.87	0.07	75,75,75,75	0
55	MG	YA	3456	1/1	0.87	0.14	52,52,52,52	0
55	MG	YA	3269	1/1	0.87	0.14	14,14,14,14	0
55	MG	YA	3458	1/1	0.87	0.12	66,66,66,66	0
55	MG	RA	3158	1/1	0.87	0.12	40,40,40,40	0
55	MG	XA	1665	1/1	0.87	0.12	57,57,57,57	0
55	MG	RA	3031	1/1	0.87	0.22	49,49,49,49	0
55	MG	RA	3393	1/1	0.87	0.16	60,60,60,60	0
55	MG	YA	3466	1/1	0.87	0.15	46,46,46,46	0
55	MG	RA	3133	1/1	0.87	0.13	27,27,27,27	0
55	MG	YA	3471	1/1	0.87	0.21	53,53,53,53	0
55	MG	XA	1622	1/1	0.87	0.08	55,55,55,55	0
55	MG	YA	3489	1/1	0.87	0.07	40,40,40,40	0
55	MG	XA	1631	1/1	0.87	0.10	62,62,62,62	0
55	MG	RA	3256	1/1	0.87	0.14	38,38,38,38	0
55	MG	YA	3128	1/1	0.87	0.20	28,28,28,28	0
55	MG	YA	3206	1/1	0.87	0.09	31,31,31,31	0
55	MG	YA	3132	1/1	0.87	0.18	31,31,31,31	0
55	MG	YA	3309	1/1	0.87	0.17	47,47,47,47	0
55	MG	YQ	201	1/1	0.87	0.16	48,48,48,48	0
55	MG	YA	3001	1/1	0.87	0.29	46,46,46,46	0
55	MG	YA	3408	1/1	0.87	0.16	53,53,53,53	0
55	MG	YA	3411	1/1	0.87	0.10	9,9,9,9	0
55	MG	YA	3213	1/1	0.87	0.12	29,29,29,29	0
55	MG	YA	3149	1/1	0.88	0.15	56,56,56,56	0
55	MG	YA	3333	1/1	0.88	0.17	45,45,45,45	0
55	MG	QA	1622	1/1	0.88	0.19	55,55,55,55	0
55	MG	RA	3313	1/1	0.88	0.15	50,50,50,50	0
55	MG	RA	3381	1/1	0.88	0.16	38,38,38,38	0
55	MG	YA	3432	1/1	0.88	0.18	46,46,46,46	0
55	MG	YA	3342	1/1	0.88	0.18	79,79,79,79	0
55	MG	RA	3423	1/1	0.88	0.22	52,52,52,52	0
55	MG	RA	3292	1/1	0.88	0.13	41,41,41,41	0
55	MG	RA	3243	1/1	0.88	0.12	22,22,22,22	0
55	MG	RA	3131	1/1	0.88	0.20	56,56,56,56	0
55	MG	RA	3075	1/1	0.88	0.11	39,39,39,39	0
55	MG	YA	3168	1/1	0.88	0.21	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	YA	3354	1/1	0.88	0.11	27,27,27,27	0
55	MG	QA	1624	1/1	0.88	0.10	80,80,80,80	0
55	MG	YA	3448	1/1	0.88	0.16	54,54,54,54	0
55	MG	YA	3257	1/1	0.88	0.29	54,54,54,54	0
55	MG	RA	3274	1/1	0.88	0.20	35,35,35,35	0
55	MG	YA	3451	1/1	0.88	0.16	59,59,59,59	0
55	MG	RA	3363	1/1	0.88	0.14	57,57,57,57	0
55	MG	YA	3361	1/1	0.88	0.26	63,63,63,63	0
55	MG	RA	3325	1/1	0.88	0.13	42,42,42,42	0
55	MG	RA	3444	1/1	0.88	0.14	45,45,45,45	0
55	MG	YA	3179	1/1	0.88	0.13	30,30,30,30	0
55	MG	YA	3070	1/1	0.88	0.17	27,27,27,27	0
55	MG	RB	202	1/1	0.88	0.08	41,41,41,41	0
55	MG	RA	3263	1/1	0.88	0.21	45,45,45,45	0
55	MG	YA	3184	1/1	0.88	0.14	35,35,35,35	0
55	MG	RE	301	1/1	0.88	0.10	56,56,56,56	0
55	MG	RA	3399	1/1	0.88	0.19	43,43,43,43	0
55	MG	RA	3140	1/1	0.88	0.16	48,48,48,48	0
55	MG	YA	3390	1/1	0.88	0.08	29,29,29,29	0
55	MG	XA	1671	1/1	0.88	0.16	35,35,35,35	0
55	MG	RA	3306	1/1	0.88	0.10	60,60,60,60	0
55	MG	R0	101	1/1	0.88	0.26	58,58,58,58	0
55	MG	YA	3405	1/1	0.88	0.16	31,31,31,31	0
55	MG	R8	101	1/1	0.88	0.16	40,40,40,40	0
55	MG	RA	3405	1/1	0.88	0.12	39,39,39,39	0
55	MG	YA	3319	1/1	0.88	0.19	59,59,59,59	0
55	MG	YA	3412	1/1	0.88	0.09	67,67,67,67	0
55	MG	YA	3214	1/1	0.88	0.07	45,45,45,45	0
55	MG	RA	3282	1/1	0.88	0.21	49,49,49,49	0
55	MG	YA	3218	1/1	0.88	0.10	31,31,31,31	0
55	MG	Y1	102	1/1	0.88	0.10	46,46,46,46	0
55	MG	XA	1658	1/1	0.89	0.17	37,37,37,37	0
55	MG	RA	3317	1/1	0.89	0.07	48,48,48,48	0
55	MG	YA	3418	1/1	0.89	0.17	61,61,61,61	0
55	MG	YA	3419	1/1	0.89	0.07	36,36,36,36	0
55	MG	YA	3312	1/1	0.89	0.14	44,44,44,44	0
55	MG	YA	3205	1/1	0.89	0.10	54,54,54,54	0
55	MG	RA	3361	1/1	0.89	0.17	60,60,60,60	0
55	MG	RA	3185	1/1	0.89	0.07	56,56,56,56	0
55	MG	YA	3125	1/1	0.89	0.11	27,27,27,27	0
55	MG	RA	3234	1/1	0.89	0.09	45,45,45,45	0
55	MG	YA	3431	1/1	0.89	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
55	MG	RA	3217	1/1	0.89	0.08	49,49,49,49	0
55	MG	XA	1669	1/1	0.89	0.19	49,49,49,49	0
55	MG	RA	3404	1/1	0.89	0.14	50,50,50,50	0
55	MG	RA	3149	1/1	0.89	0.07	48,48,48,48	0
55	MG	RA	3151	1/1	0.89	0.12	38,38,38,38	0
55	MG	XA	1603	1/1	0.89	0.14	58,58,58,58	0
55	MG	XA	1606	1/1	0.89	0.07	40,40,40,40	0
55	MG	YA	3443	1/1	0.89	0.17	44,44,44,44	0
55	MG	RA	3327	1/1	0.89	0.08	37,37,37,37	0
55	MG	YA	3231	1/1	0.89	0.12	38,38,38,38	0
55	MG	RA	3373	1/1	0.89	0.16	43,43,43,43	0
55	MG	RA	3138	1/1	0.89	0.14	40,40,40,40	0
55	MG	YA	3237	1/1	0.89	0.27	40,40,40,40	0
55	MG	XA	1615	1/1	0.89	0.07	66,66,66,66	0
55	MG	XA	1619	1/1	0.89	0.14	74,74,74,74	0
55	MG	RA	3417	1/1	0.89	0.16	50,50,50,50	0
55	MG	YA	3253	1/1	0.89	0.15	49,49,49,49	0
55	MG	YA	3164	1/1	0.89	0.07	27,27,27,27	0
55	MG	RA	3335	1/1	0.89	0.09	40,40,40,40	0
55	MG	QA	1656	1/1	0.89	0.10	48,48,48,48	0
55	MG	YA	3461	1/1	0.89	0.11	52,52,52,52	0
55	MG	YA	3261	1/1	0.89	0.12	21,21,21,21	0
55	MG	RA	3004	1/1	0.89	0.15	39,39,39,39	0
55	MG	RA	3246	1/1	0.89	0.20	36,36,36,36	0
55	MG	YA	3465	1/1	0.89	0.15	50,50,50,50	0
55	MG	XA	1644	1/1	0.89	0.10	54,54,54,54	0
55	MG	YA	3374	1/1	0.89	0.12	39,39,39,39	0
55	MG	YA	3469	1/1	0.89	0.08	39,39,39,39	0
55	MG	YA	3375	1/1	0.89	0.18	45,45,45,45	0
55	MG	QA	1637	1/1	0.89	0.08	77,77,77,77	0
55	MG	YA	3030	1/1	0.89	0.16	32,32,32,32	0
55	MG	YA	3490	1/1	0.89	0.18	30,30,30,30	0
55	MG	RA	3146	1/1	0.89	0.10	58,58,58,58	0
55	MG	YA	3504	1/1	0.89	0.17	39,39,39,39	0
55	MG	YA	3505	1/1	0.89	0.09	55,55,55,55	0
55	MG	YA	3509	1/1	0.89	0.14	56,56,56,56	0
55	MG	RA	3275	1/1	0.89	0.20	50,50,50,50	0
55	MG	RA	3111	1/1	0.89	0.17	32,32,32,32	0
55	MG	YA	3061	1/1	0.89	0.15	15,15,15,15	0
55	MG	YA	3066	1/1	0.89	0.14	41,41,41,41	0
55	MG	YA	3291	1/1	0.89	0.15	51,51,51,51	0
55	MG	QA	1628	1/1	0.89	0.17	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	YA	3295	1/1	0.89	0.27	64,64,64,64	0
55	MG	YA	3300	1/1	0.89	0.22	57,57,57,57	0
55	MG	RA	3182	1/1	0.89	0.11	22,22,22,22	0
55	MG	YA	3305	1/1	0.89	0.23	55,55,55,55	0
55	MG	YA	3199	1/1	0.89	0.14	34,34,34,34	0
55	MG	YA	3324	1/1	0.90	0.09	38,38,38,38	0
55	MG	RE	305	1/1	0.90	0.12	29,29,29,29	0
55	MG	RA	3303	1/1	0.90	0.11	32,32,32,32	0
55	MG	YA	3425	1/1	0.90	0.13	33,33,33,33	0
55	MG	YA	3331	1/1	0.90	0.06	35,35,35,35	0
55	MG	RA	3333	1/1	0.90	0.21	44,44,44,44	0
55	MG	YA	3334	1/1	0.90	0.20	56,56,56,56	0
55	MG	YA	3335	1/1	0.90	0.22	62,62,62,62	0
55	MG	YA	3050	1/1	0.90	0.13	16,16,16,16	0
55	MG	QA	1664	1/1	0.90	0.21	53,53,53,53	0
55	MG	RA	3276	1/1	0.90	0.26	60,60,60,60	0
55	MG	QV	101	1/1	0.90	0.14	69,69,69,69	0
55	MG	YA	3240	1/1	0.90	0.28	45,45,45,45	0
55	MG	RA	3201	1/1	0.90	0.11	40,40,40,40	0
55	MG	YA	3248	1/1	0.90	0.17	23,23,23,23	0
55	MG	RA	3415	1/1	0.90	0.12	52,52,52,52	0
55	MG	XA	1609	1/1	0.90	0.19	42,42,42,42	0
55	MG	YA	3256	1/1	0.90	0.08	20,20,20,20	0
55	MG	RA	3310	1/1	0.90	0.12	32,32,32,32	0
55	MG	YA	3086	1/1	0.90	0.20	25,25,25,25	0
55	MG	YA	3356	1/1	0.90	0.18	51,51,51,51	0
55	MG	YA	3095	1/1	0.90	0.10	28,28,28,28	0
55	MG	RA	3421	1/1	0.90	0.28	20,20,20,20	0
55	MG	QA	1606	1/1	0.90	0.07	51,51,51,51	0
55	MG	YA	3185	1/1	0.90	0.09	54,54,54,54	0
55	MG	RA	3284	1/1	0.90	0.05	42,42,42,42	0
55	MG	YA	3191	1/1	0.90	0.23	50,50,50,50	0
55	MG	YA	3193	1/1	0.90	0.14	48,48,48,48	0
55	MG	YA	3370	1/1	0.90	0.11	35,35,35,35	0
55	MG	YA	3122	1/1	0.90	0.08	22,22,22,22	0
55	MG	YA	3284	1/1	0.90	0.15	53,53,53,53	0
55	MG	YA	3195	1/1	0.90	0.20	47,47,47,47	0
55	MG	YA	3288	1/1	0.90	0.17	40,40,40,40	0
55	MG	QA	1642	1/1	0.90	0.12	73,73,73,73	0
55	MG	RA	3355	1/1	0.90	0.15	62,62,62,62	0
55	MG	RA	3124	1/1	0.90	0.19	24,24,24,24	0
55	MG	YA	3473	1/1	0.90	0.17	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	YA	3003	1/1	0.90	0.11	35,35,35,35	0
55	MG	YA	3485	1/1	0.90	0.13	9,9,9,9	0
55	MG	YA	3135	1/1	0.90	0.12	35,35,35,35	0
55	MG	YA	3299	1/1	0.90	0.15	46,46,46,46	0
55	MG	RA	3066	1/1	0.90	0.09	45,45,45,45	0
55	MG	YA	3394	1/1	0.90	0.07	39,39,39,39	0
55	MG	YA	3395	1/1	0.90	0.12	35,35,35,35	0
55	MG	XA	1635	1/1	0.90	0.06	54,54,54,54	0
55	MG	RA	3270	1/1	0.90	0.17	56,56,56,56	0
55	MG	RA	3072	1/1	0.90	0.19	51,51,51,51	0
55	MG	QA	1604	1/1	0.90	0.09	26,26,26,26	0
55	MG	RA	3137	1/1	0.90	0.11	47,47,47,47	0
55	MG	QA	1644	1/1	0.90	0.08	49,49,49,49	0
55	MG	YA	3313	1/1	0.90	0.15	58,58,58,58	0
55	MG	YA	3222	1/1	0.90	0.18	55,55,55,55	0
55	MG	RA	3401	1/1	0.90	0.11	55,55,55,55	0
55	MG	YA	3155	1/1	0.90	0.13	33,33,33,33	0
55	MG	YA	3321	1/1	0.90	0.10	44,44,44,44	0
55	MG	RA	3328	1/1	0.90	0.10	41,41,41,41	0
55	MG	YA	3153	1/1	0.91	0.11	31,31,31,31	0
55	MG	RA	3084	1/1	0.91	0.18	24,24,24,24	0
55	MG	YA	3215	1/1	0.91	0.08	26,26,26,26	0
55	MG	RA	3285	1/1	0.91	0.13	41,41,41,41	0
55	MG	YA	3367	1/1	0.91	0.10	57,57,57,57	0
55	MG	YA	3041	1/1	0.91	0.28	26,26,26,26	0
55	MG	YA	3219	1/1	0.91	0.06	11,11,11,11	0
55	MG	YA	3158	1/1	0.91	0.08	21,21,21,21	0
55	MG	RA	3062	1/1	0.91	0.13	30,30,30,30	0
55	MG	YA	3160	1/1	0.91	0.18	38,38,38,38	0
55	MG	RA	3180	1/1	0.91	0.23	42,42,42,42	0
55	MG	RA	3114	1/1	0.91	0.11	40,40,40,40	0
55	MG	YA	3376	1/1	0.91	0.12	37,37,37,37	0
55	MG	YA	3165	1/1	0.91	0.21	35,35,35,35	0
55	MG	RA	3409	1/1	0.91	0.17	47,47,47,47	0
55	MG	RA	3296	1/1	0.91	0.36	69,69,69,69	0
55	MG	RA	3184	1/1	0.91	0.13	54,54,54,54	0
55	MG	YA	3171	1/1	0.91	0.22	35,35,35,35	0
55	MG	XA	1604	1/1	0.91	0.08	50,50,50,50	0
55	MG	RA	3368	1/1	0.91	0.13	49,49,49,49	0
55	MG	RA	3267	1/1	0.91	0.22	43,43,43,43	0
55	MG	YA	3092	1/1	0.91	0.06	10,10,10,10	0
55	MG	RA	3010	1/1	0.91	0.13	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	RA	3121	1/1	0.91	0.08	38,38,38,38	0
55	MG	YA	3400	1/1	0.91	0.11	51,51,51,51	0
55	MG	YA	3401	1/1	0.91	0.08	39,39,39,39	0
55	MG	YA	3112	1/1	0.91	0.09	11,11,11,11	0
55	MG	YA	3255	1/1	0.91	0.18	45,45,45,45	0
55	MG	YA	3407	1/1	0.91	0.06	43,43,43,43	0
55	MG	QA	1629	1/1	0.91	0.06	59,59,59,59	0
55	MG	YA	3484	1/1	0.91	0.11	24,24,24,24	0
55	MG	YA	3409	1/1	0.91	0.13	18,18,18,18	0
55	MG	YA	3410	1/1	0.91	0.12	44,44,44,44	0
55	MG	RA	3336	1/1	0.91	0.08	36,36,36,36	0
55	MG	QA	1610	1/1	0.91	0.22	41,41,41,41	0
55	MG	YA	3493	1/1	0.91	0.07	31,31,31,31	0
55	MG	QA	1661	1/1	0.91	0.11	40,40,40,40	0
55	MG	RA	3224	1/1	0.91	0.10	26,26,26,26	0
55	MG	RA	3225	1/1	0.91	0.21	35,35,35,35	0
55	MG	RA	3051	1/1	0.91	0.07	25,25,25,25	0
55	MG	RA	3197	1/1	0.91	0.10	41,41,41,41	0
55	MG	YA	3349	1/1	0.91	0.12	25,25,25,25	0
55	MG	XA	1641	1/1	0.91	0.10	62,62,62,62	0
55	MG	YE	302	1/1	0.91	0.09	36,36,36,36	0
55	MG	RA	3353	1/1	0.91	0.14	55,55,55,55	0
55	MG	RA	3312	1/1	0.91	0.17	23,23,23,23	0
55	MG	YA	3428	1/1	0.91	0.07	19,19,19,19	0
55	MG	RA	3076	1/1	0.91	0.19	30,30,30,30	0
55	MG	RA	3255	1/1	0.91	0.17	43,43,43,43	0
55	MG	XA	1647	1/1	0.91	0.06	47,47,47,47	0
55	MG	QA	1652	1/1	0.91	0.10	45,45,45,45	0
55	MG	Y8	101	1/1	0.91	0.29	45,45,45,45	0
55	MG	RA	3293	1/1	0.92	0.09	51,51,51,51	0
55	MG	YA	3328	1/1	0.92	0.18	43,43,43,43	0
55	MG	RA	3018	1/1	0.92	0.14	22,22,22,22	0
55	MG	YA	3422	1/1	0.92	0.25	48,48,48,48	0
55	MG	RA	3426	1/1	0.92	0.06	32,32,32,32	0
55	MG	RA	3429	1/1	0.92	0.17	34,34,34,34	0
55	MG	YA	3236	1/1	0.92	0.11	40,40,40,40	0
55	MG	XA	1636	1/1	0.92	0.07	65,65,65,65	0
55	MG	RA	3209	1/1	0.92	0.16	23,23,23,23	0
55	MG	RA	3349	1/1	0.92	0.09	44,44,44,44	0
55	MG	RA	3054	1/1	0.92	0.10	72,72,72,72	0
55	MG	YA	3243	1/1	0.92	0.19	20,20,20,20	0
55	MG	RA	3254	1/1	0.92	0.25	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	YA	3169	1/1	0.92	0.09	39,39,39,39	0
55	MG	RA	3299	1/1	0.92	0.11	53,53,53,53	0
55	MG	RA	3092	1/1	0.92	0.12	40,40,40,40	0
55	MG	RA	3356	1/1	0.92	0.10	47,47,47,47	0
55	MG	YA	3173	1/1	0.92	0.09	26,26,26,26	0
55	MG	RA	3322	1/1	0.92	0.11	43,43,43,43	0
55	MG	YA	3258	1/1	0.92	0.13	10,10,10,10	0
55	MG	YA	3259	1/1	0.92	0.16	33,33,33,33	0
55	MG	RB	201	1/1	0.92	0.18	80,80,80,80	0
55	MG	RA	3060	1/1	0.92	0.14	47,47,47,47	0
55	MG	YA	3076	1/1	0.92	0.09	52,52,52,52	0
55	MG	QA	1627	1/1	0.92	0.10	84,84,84,84	0
55	MG	YA	3362	1/1	0.92	0.18	33,33,33,33	0
55	MG	YA	3452	1/1	0.92	0.13	37,37,37,37	0
55	MG	YA	3453	1/1	0.92	0.08	53,53,53,53	0
55	MG	RA	3037	1/1	0.92	0.15	25,25,25,25	0
55	MG	XA	1660	1/1	0.92	0.07	46,46,46,46	0
55	MG	YA	3276	1/1	0.92	0.19	36,36,36,36	0
55	MG	RE	302	1/1	0.92	0.17	28,28,28,28	0
55	MG	RA	3130	1/1	0.92	0.12	33,33,33,33	0
55	MG	RA	3179	1/1	0.92	0.09	71,71,71,71	0
55	MG	YA	3190	1/1	0.92	0.06	26,26,26,26	0
55	MG	QA	1646	1/1	0.92	0.08	50,50,50,50	0
55	MG	YA	3113	1/1	0.92	0.12	24,24,24,24	0
55	MG	RA	3334	1/1	0.92	0.14	38,38,38,38	0
55	MG	YA	3377	1/1	0.92	0.14	45,45,45,45	0
55	MG	RA	3406	1/1	0.92	0.13	52,52,52,52	0
55	MG	R0	102	1/1	0.92	0.07	33,33,33,33	0
55	MG	RA	3407	1/1	0.92	0.14	62,62,62,62	0
55	MG	RA	3181	1/1	0.92	0.24	31,31,31,31	0
55	MG	YA	3475	1/1	0.92	0.16	53,53,53,53	0
55	MG	YA	3298	1/1	0.92	0.09	24,24,24,24	0
55	MG	YA	3387	1/1	0.92	0.18	45,45,45,45	0
55	MG	YA	3389	1/1	0.92	0.13	33,33,33,33	0
55	MG	XA	1676	1/1	0.92	0.11	48,48,48,48	0
55	MG	XA	1677	1/1	0.92	0.09	54,54,54,54	0
55	MG	XA	1678	1/1	0.92	0.12	56,56,56,56	0
55	MG	YA	3302	1/1	0.92	0.13	48,48,48,48	0
55	MG	YA	3304	1/1	0.92	0.14	30,30,30,30	0
55	MG	QA	1633	1/1	0.92	0.16	53,53,53,53	0
55	MG	YA	3508	1/1	0.92	0.10	36,36,36,36	0
55	MG	RA	3411	1/1	0.92	0.09	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	XA	1607	1/1	0.92	0.22	40,40,40,40	0
55	MG	YA	3146	1/1	0.92	0.07	21,21,21,21	0
55	MG	YA	3147	1/1	0.92	0.09	19,19,19,19	0
55	MG	RA	3369	1/1	0.92	0.15	30,30,30,30	0
55	MG	RA	3339	1/1	0.92	0.09	21,21,21,21	0
55	MG	YA	3318	1/1	0.92	0.11	22,22,22,22	0
55	MG	RA	3311	1/1	0.92	0.09	33,33,33,33	0
55	MG	YA	3005	1/1	0.92	0.06	47,47,47,47	0
55	MG	RA	3134	1/1	0.92	0.16	44,44,44,44	0
55	MG	YA	3226	1/1	0.92	0.18	23,23,23,23	0
55	MG	YA	3416	1/1	0.92	0.07	29,29,29,29	0
55	MG	RA	3376	1/1	0.92	0.16	51,51,51,51	0
55	MG	RA	3345	1/1	0.92	0.18	48,48,48,48	0
57	ZN	Y4	101	1/1	0.92	0.07	270,270,270,270	0
55	MG	YA	3308	1/1	0.93	0.06	19,19,19,19	0
55	MG	XA	1642	1/1	0.93	0.10	46,46,46,46	0
55	MG	YA	3084	1/1	0.93	0.19	21,21,21,21	0
55	MG	RA	3321	1/1	0.93	0.06	42,42,42,42	0
55	MG	YA	3414	1/1	0.93	0.20	33,33,33,33	0
55	MG	YA	3090	1/1	0.93	0.06	20,20,20,20	0
55	MG	YA	3315	1/1	0.93	0.28	57,57,57,57	0
55	MG	YA	3091	1/1	0.93	0.19	24,24,24,24	0
55	MG	YA	3317	1/1	0.93	0.08	44,44,44,44	0
55	MG	RA	3241	1/1	0.93	0.05	67,67,67,67	0
55	MG	RA	3027	1/1	0.93	0.12	26,26,26,26	0
55	MG	RA	3428	1/1	0.93	0.06	27,27,27,27	0
55	MG	YA	3111	1/1	0.93	0.08	12,12,12,12	0
55	MG	RA	3168	1/1	0.93	0.16	35,35,35,35	0
55	MG	RA	3326	1/1	0.93	0.25	47,47,47,47	0
55	MG	YA	3426	1/1	0.93	0.14	47,47,47,47	0
55	MG	YA	3427	1/1	0.93	0.07	30,30,30,30	0
55	MG	XA	1652	1/1	0.93	0.07	39,39,39,39	0
55	MG	RA	3432	1/1	0.93	0.09	45,45,45,45	0
55	MG	RA	3433	1/1	0.93	0.21	59,59,59,59	0
55	MG	YA	3329	1/1	0.93	0.20	62,62,62,62	0
55	MG	RA	3104	1/1	0.93	0.08	30,30,30,30	0
55	MG	RA	3291	1/1	0.93	0.20	41,41,41,41	0
55	MG	YA	3130	1/1	0.93	0.12	18,18,18,18	0
55	MG	RA	3106	1/1	0.93	0.07	25,25,25,25	0
55	MG	YA	3438	1/1	0.93	0.11	46,46,46,46	0
55	MG	RA	3028	1/1	0.93	0.19	41,41,41,41	0
55	MG	RA	3294	1/1	0.93	0.18	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	YA	3339	1/1	0.93	0.10	36,36,36,36	0
55	MG	RA	3144	1/1	0.93	0.07	39,39,39,39	0
55	MG	RA	3443	1/1	0.93	0.17	52,52,52,52	0
55	MG	RA	3383	1/1	0.93	0.05	44,44,44,44	0
55	MG	RA	3384	1/1	0.93	0.23	50,50,50,50	0
55	MG	RA	3211	1/1	0.93	0.20	14,14,14,14	0
55	MG	YA	3348	1/1	0.93	0.07	29,29,29,29	0
55	MG	RA	3212	1/1	0.93	0.11	42,42,42,42	0
55	MG	RA	3213	1/1	0.93	0.21	45,45,45,45	0
55	MG	RA	3341	1/1	0.93	0.08	45,45,45,45	0
55	MG	RA	3030	1/1	0.93	0.18	24,24,24,24	0
55	MG	RA	3178	1/1	0.93	0.12	51,51,51,51	0
55	MG	YA	3250	1/1	0.93	0.20	18,18,18,18	0
55	MG	YA	3251	1/1	0.93	0.14	20,20,20,20	0
55	MG	RA	3395	1/1	0.93	0.05	71,71,71,71	0
55	MG	RA	3073	1/1	0.93	0.09	37,37,37,37	0
55	MG	QA	1631	1/1	0.93	0.15	51,51,51,51	0
55	MG	RA	3398	1/1	0.93	0.21	47,47,47,47	0
55	MG	QA	1641	1/1	0.93	0.07	68,68,68,68	0
55	MG	RA	3040	1/1	0.93	0.17	27,27,27,27	0
55	MG	RA	3183	1/1	0.93	0.14	82,82,82,82	0
55	MG	YA	3008	1/1	0.93	0.09	34,34,34,34	0
55	MG	YA	3467	1/1	0.93	0.13	29,29,29,29	0
55	MG	RA	3402	1/1	0.93	0.06	58,58,58,58	0
55	MG	YA	3263	1/1	0.93	0.11	42,42,42,42	0
55	MG	RA	3352	1/1	0.93	0.11	50,50,50,50	0
55	MG	YA	3268	1/1	0.93	0.10	23,23,23,23	0
55	MG	RA	3118	1/1	0.93	0.10	28,28,28,28	0
55	MG	RA	3120	1/1	0.93	0.25	45,45,45,45	0
55	MG	YA	3272	1/1	0.93	0.12	31,31,31,31	0
55	MG	YA	3014	1/1	0.93	0.18	24,24,24,24	0
55	MG	YA	3488	1/1	0.93	0.14	46,46,46,46	0
55	MG	RA	3187	1/1	0.93	0.11	38,38,38,38	0
55	MG	QA	1621	1/1	0.93	0.06	48,48,48,48	0
55	MG	XA	1614	1/1	0.93	0.09	21,21,21,21	0
55	MG	QA	1620	1/1	0.93	0.05	67,67,67,67	0
55	MG	YA	3495	1/1	0.93	0.14	24,24,24,24	0
55	MG	YA	3496	1/1	0.93	0.15	30,30,30,30	0
55	MG	YA	3499	1/1	0.93	0.16	23,23,23,23	0
55	MG	XA	1618	1/1	0.93	0.20	44,44,44,44	0
55	MG	RA	3358	1/1	0.93	0.09	34,34,34,34	0
55	MG	RA	3050	1/1	0.93	0.14	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	RA	3017	1/1	0.93	0.11	10,10,10,10	0
55	MG	XA	1623	1/1	0.93	0.12	44,44,44,44	0
55	MG	YA	3056	1/1	0.93	0.13	27,27,27,27	0
55	MG	YB	203	1/1	0.93	0.07	45,45,45,45	0
55	MG	YB	204	1/1	0.93	0.12	30,30,30,30	0
55	MG	XA	1626	1/1	0.93	0.08	32,32,32,32	0
55	MG	QA	1649	1/1	0.93	0.19	65,65,65,65	0
55	MG	YA	3397	1/1	0.93	0.15	48,48,48,48	0
55	MG	YA	3187	1/1	0.93	0.14	35,35,35,35	0
55	MG	RA	3019	1/1	0.93	0.13	15,15,15,15	0
55	MG	RA	3022	1/1	0.93	0.06	25,25,25,25	0
55	MG	YA	3404	1/1	0.93	0.14	40,40,40,40	0
55	MG	XA	1638	1/1	0.93	0.11	44,44,44,44	0
55	MG	YA	3074	1/1	0.93	0.14	19,19,19,19	0
55	MG	RA	3026	1/1	0.93	0.13	17,17,17,17	0
55	MG	YA	3078	1/1	0.93	0.15	23,23,23,23	0
55	MG	RA	3240	1/1	0.93	0.12	52,52,52,52	0
55	MG	RA	3029	1/1	0.94	0.26	24,24,24,24	0
55	MG	YA	3031	1/1	0.94	0.18	7,7,7,7	0
55	MG	XA	1630	1/1	0.94	0.09	13,13,13,13	0
55	MG	RA	3422	1/1	0.94	0.13	33,33,33,33	0
55	MG	YA	3044	1/1	0.94	0.15	13,13,13,13	0
55	MG	QA	1613	1/1	0.94	0.10	75,75,75,75	0
55	MG	RA	3100	1/1	0.94	0.20	31,31,31,31	0
55	MG	RA	3374	1/1	0.94	0.13	37,37,37,37	0
55	MG	YA	3297	1/1	0.94	0.18	31,31,31,31	0
55	MG	XA	1639	1/1	0.94	0.17	37,37,37,37	0
55	MG	YA	3059	1/1	0.94	0.08	10,10,10,10	0
55	MG	RA	3063	1/1	0.94	0.12	25,25,25,25	0
55	MG	RA	3331	1/1	0.94	0.14	46,46,46,46	0
55	MG	YA	3415	1/1	0.94	0.06	29,29,29,29	0
55	MG	RA	3377	1/1	0.94	0.17	40,40,40,40	0
55	MG	RA	3173	1/1	0.94	0.09	20,20,20,20	0
55	MG	RA	3011	1/1	0.94	0.12	26,26,26,26	0
55	MG	RA	3380	1/1	0.94	0.14	32,32,32,32	0
55	MG	YA	3307	1/1	0.94	0.18	50,50,50,50	0
55	MG	RA	3248	1/1	0.94	0.15	46,46,46,46	0
55	MG	RA	3015	1/1	0.94	0.18	41,41,41,41	0
55	MG	YA	3082	1/1	0.94	0.18	22,22,22,22	0
55	MG	YA	3311	1/1	0.94	0.07	39,39,39,39	0
55	MG	YA	3197	1/1	0.94	0.14	51,51,51,51	0
55	MG	RA	3337	1/1	0.94	0.07	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	YA	3314	1/1	0.94	0.09	39,39,39,39	0
55	MG	RA	3338	1/1	0.94	0.16	30,30,30,30	0
55	MG	RA	3070	1/1	0.94	0.16	31,31,31,31	0
55	MG	YA	3204	1/1	0.94	0.16	29,29,29,29	0
55	MG	RA	3386	1/1	0.94	0.07	46,46,46,46	0
55	MG	RA	3216	1/1	0.94	0.21	32,32,32,32	0
55	MG	YA	3207	1/1	0.94	0.05	23,23,23,23	0
55	MG	XA	1657	1/1	0.94	0.04	48,48,48,48	0
55	MG	YA	3211	1/1	0.94	0.08	33,33,33,33	0
55	MG	YA	3096	1/1	0.94	0.09	11,11,11,11	0
55	MG	YA	3325	1/1	0.94	0.15	62,62,62,62	0
55	MG	YA	3098	1/1	0.94	0.14	31,31,31,31	0
55	MG	RA	3071	1/1	0.94	0.12	13,13,13,13	0
55	MG	YA	3104	1/1	0.94	0.07	20,20,20,20	0
55	MG	YA	3444	1/1	0.94	0.12	37,37,37,37	0
55	MG	YA	3109	1/1	0.94	0.17	13,13,13,13	0
55	MG	XA	1659	1/1	0.94	0.05	42,42,42,42	0
55	MG	RA	3110	1/1	0.94	0.18	45,45,45,45	0
55	MG	RA	3039	1/1	0.94	0.13	16,16,16,16	0
55	MG	RA	3220	1/1	0.94	0.20	46,46,46,46	0
55	MG	XA	1664	1/1	0.94	0.09	41,41,41,41	0
55	MG	YA	3121	1/1	0.94	0.06	32,32,32,32	0
55	MG	QA	1662	1/1	0.94	0.09	29,29,29,29	0
55	MG	YA	3340	1/1	0.94	0.07	45,45,45,45	0
55	MG	YA	3124	1/1	0.94	0.17	27,27,27,27	0
55	MG	RA	3259	1/1	0.94	0.07	29,29,29,29	0
55	MG	QA	1663	1/1	0.94	0.13	76,76,76,76	0
55	MG	YA	3344	1/1	0.94	0.17	38,38,38,38	0
55	MG	YA	3129	1/1	0.94	0.07	5,5,5,5	0
55	MG	YA	3346	1/1	0.94	0.23	53,53,53,53	0
55	MG	XA	1668	1/1	0.94	0.05	41,41,41,41	0
55	MG	RA	3048	1/1	0.94	0.12	8,8,8,8	0
55	MG	RA	3351	1/1	0.94	0.16	42,42,42,42	0
55	MG	YA	3134	1/1	0.94	0.15	31,31,31,31	0
55	MG	YA	3351	1/1	0.94	0.11	36,36,36,36	0
55	MG	QA	1639	1/1	0.94	0.07	48,48,48,48	0
55	MG	RA	3154	1/1	0.94	0.08	16,16,16,16	0
55	MG	YA	3138	1/1	0.94	0.10	22,22,22,22	0
55	MG	YA	3142	1/1	0.94	0.06	29,29,29,29	0
55	MG	RA	3155	1/1	0.94	0.08	27,27,27,27	0
55	MG	YA	3474	1/1	0.94	0.07	37,37,37,37	0
55	MG	YA	3249	1/1	0.94	0.22	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	XA	1601	1/1	0.94	0.06	44,44,44,44	0
55	MG	YA	3478	1/1	0.94	0.12	25,25,25,25	0
55	MG	YA	3481	1/1	0.94	0.21	7,7,7,7	0
55	MG	QA	1614	1/1	0.94	0.07	47,47,47,47	0
55	MG	YA	3252	1/1	0.94	0.14	43,43,43,43	0
55	MG	QA	1645	1/1	0.94	0.07	60,60,60,60	0
55	MG	QA	1617	1/1	0.94	0.08	57,57,57,57	0
55	MG	RA	3088	1/1	0.94	0.14	13,13,13,13	0
55	MG	XA	1608	1/1	0.94	0.10	61,61,61,61	0
55	MG	RA	3125	1/1	0.94	0.09	22,22,22,22	0
55	MG	RA	3128	1/1	0.94	0.18	39,39,39,39	0
55	MG	RA	3235	1/1	0.94	0.20	38,38,38,38	0
55	MG	YA	3372	1/1	0.94	0.09	36,36,36,36	0
55	MG	YA	3502	1/1	0.94	0.32	42,42,42,42	0
55	MG	YA	3503	1/1	0.94	0.08	32,32,32,32	0
55	MG	XA	1612	1/1	0.94	0.17	54,54,54,54	0
55	MG	RA	3089	1/1	0.94	0.18	22,22,22,22	0
55	MG	YA	3262	1/1	0.94	0.10	7,7,7,7	0
55	MG	RA	3277	1/1	0.94	0.12	26,26,26,26	0
55	MG	YA	3264	1/1	0.94	0.15	28,28,28,28	0
55	MG	YA	3265	1/1	0.94	0.11	33,33,33,33	0
55	MG	RA	3199	1/1	0.94	0.15	69,69,69,69	0
55	MG	XA	1616	1/1	0.94	0.13	22,22,22,22	0
55	MG	YB	205	1/1	0.94	0.08	12,12,12,12	0
55	MG	RA	3057	1/1	0.94	0.15	31,31,31,31	0
55	MG	YA	3163	1/1	0.94	0.11	44,44,44,44	0
55	MG	QA	1660	1/1	0.94	0.08	59,59,59,59	0
55	MG	YA	3274	1/1	0.94	0.17	38,38,38,38	0
55	MG	RA	3416	1/1	0.94	0.06	35,35,35,35	0
55	MG	RA	3283	1/1	0.94	0.20	42,42,42,42	0
55	MG	YA	3393	1/1	0.94	0.08	48,48,48,48	0
55	MG	YA	3278	1/1	0.94	0.11	17,17,17,17	0
55	MG	RA	3418	1/1	0.94	0.16	17,17,17,17	0
55	MG	YA	3022	1/1	0.94	0.11	18,18,18,18	0
55	MG	Y3	101	1/1	0.94	0.17	25,25,25,25	0
55	MG	YA	3282	1/1	0.94	0.11	36,36,36,36	0
55	MG	XA	1624	1/1	0.94	0.07	23,23,23,23	0
55	MG	YA	3123	1/1	0.95	0.09	7,7,7,7	0
55	MG	RA	3003	1/1	0.95	0.11	24,24,24,24	0
55	MG	YA	3217	1/1	0.95	0.14	28,28,28,28	0
55	MG	YA	3007	1/1	0.95	0.09	45,45,45,45	0
55	MG	XA	1632	1/1	0.95	0.10	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	RA	3101	1/1	0.95	0.17	45,45,45,45	0
55	MG	RA	3013	1/1	0.95	0.05	7,7,7,7	0
55	MG	XA	1637	1/1	0.95	0.10	49,49,49,49	0
55	MG	YA	3225	1/1	0.95	0.11	33,33,33,33	0
55	MG	RA	3176	1/1	0.95	0.22	26,26,26,26	0
55	MG	RA	3079	1/1	0.95	0.11	27,27,27,27	0
55	MG	RA	3081	1/1	0.95	0.10	16,16,16,16	0
55	MG	YA	3229	1/1	0.95	0.10	49,49,49,49	0
55	MG	QA	1635	1/1	0.95	0.07	44,44,44,44	0
55	MG	RA	3367	1/1	0.95	0.07	37,37,37,37	0
55	MG	YA	3141	1/1	0.95	0.17	5,5,5,5	0
55	MG	YA	3330	1/1	0.95	0.14	23,23,23,23	0
55	MG	RE	304	1/1	0.95	0.14	28,28,28,28	0
55	MG	YA	3143	1/1	0.95	0.09	18,18,18,18	0
55	MG	RA	3132	1/1	0.95	0.07	40,40,40,40	0
55	MG	YA	3436	1/1	0.95	0.06	25,25,25,25	0
55	MG	YA	3437	1/1	0.95	0.06	37,37,37,37	0
55	MG	YA	3027	1/1	0.95	0.17	7,7,7,7	0
55	MG	RN	201	1/1	0.95	0.27	54,54,54,54	0
55	MG	YA	3029	1/1	0.95	0.08	13,13,13,13	0
55	MG	YA	3241	1/1	0.95	0.10	7,7,7,7	0
55	MG	YA	3242	1/1	0.95	0.09	13,13,13,13	0
55	MG	QA	1605	1/1	0.95	0.05	36,36,36,36	0
55	MG	RA	3408	1/1	0.95	0.18	48,48,48,48	0
55	MG	YA	3032	1/1	0.95	0.17	13,13,13,13	0
55	MG	XA	1649	1/1	0.95	0.04	37,37,37,37	0
55	MG	YA	3035	1/1	0.95	0.20	26,26,26,26	0
55	MG	RA	3370	1/1	0.95	0.08	42,42,42,42	0
55	MG	XA	1651	1/1	0.95	0.05	40,40,40,40	0
55	MG	YA	3047	1/1	0.95	0.16	21,21,21,21	0
55	MG	RX	101	1/1	0.95	0.07	31,31,31,31	0
55	MG	YA	3051	1/1	0.95	0.14	7,7,7,7	0
55	MG	QA	1625	1/1	0.95	0.06	46,46,46,46	0
55	MG	RA	3069	1/1	0.95	0.11	31,31,31,31	0
55	MG	YA	3162	1/1	0.95	0.16	34,34,34,34	0
55	MG	RA	3009	1/1	0.95	0.21	28,28,28,28	0
55	MG	XA	1656	1/1	0.95	0.05	35,35,35,35	0
55	MG	RA	3033	1/1	0.95	0.13	28,28,28,28	0
55	MG	YA	3065	1/1	0.95	0.15	7,7,7,7	0
55	MG	YA	3358	1/1	0.95	0.20	34,34,34,34	0
55	MG	RA	3304	1/1	0.95	0.05	6,6,6,6	0
55	MG	YA	3068	1/1	0.95	0.16	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	YA	3069	1/1	0.95	0.11	40,40,40,40	0
55	MG	RA	3186	1/1	0.95	0.14	40,40,40,40	0
55	MG	YA	3071	1/1	0.95	0.11	22,22,22,22	0
55	MG	YA	3364	1/1	0.95	0.05	40,40,40,40	0
55	MG	YA	3072	1/1	0.95	0.13	16,16,16,16	0
55	MG	YA	3472	1/1	0.95	0.22	60,60,60,60	0
55	MG	XA	1605	1/1	0.95	0.13	47,47,47,47	0
55	MG	YA	3271	1/1	0.95	0.16	29,29,29,29	0
55	MG	YA	3176	1/1	0.95	0.10	36,36,36,36	0
55	MG	YA	3273	1/1	0.95	0.07	26,26,26,26	0
55	MG	YA	3075	1/1	0.95	0.16	19,19,19,19	0
55	MG	RA	3244	1/1	0.95	0.31	57,57,57,57	0
55	MG	YA	3482	1/1	0.95	0.14	16,16,16,16	0
55	MG	YA	3483	1/1	0.95	0.13	10,10,10,10	0
55	MG	YA	3077	1/1	0.95	0.22	22,22,22,22	0
55	MG	XA	1662	1/1	0.95	0.05	45,45,45,45	0
55	MG	YA	3486	1/1	0.95	0.10	26,26,26,26	0
55	MG	YA	3487	1/1	0.95	0.14	9,9,9,9	0
55	MG	YA	3279	1/1	0.95	0.14	28,28,28,28	0
55	MG	RA	3139	1/1	0.95	0.06	30,30,30,30	0
55	MG	YA	3182	1/1	0.95	0.05	25,25,25,25	0
55	MG	RA	3308	1/1	0.95	0.10	39,39,39,39	0
55	MG	RA	3020	1/1	0.95	0.07	28,28,28,28	0
55	MG	RA	3116	1/1	0.95	0.06	31,31,31,31	0
55	MG	RA	3279	1/1	0.95	0.06	14,14,14,14	0
55	MG	YA	3498	1/1	0.95	0.12	28,28,28,28	0
55	MG	YA	3286	1/1	0.95	0.08	9,9,9,9	0
55	MG	YA	3501	1/1	0.95	0.05	7,7,7,7	0
55	MG	YA	3089	1/1	0.95	0.17	20,20,20,20	0
55	MG	RA	3222	1/1	0.95	0.15	60,60,60,60	0
55	MG	YA	3391	1/1	0.95	0.14	29,29,29,29	0
55	MG	RA	3059	1/1	0.95	0.07	28,28,28,28	0
55	MG	YA	3506	1/1	0.95	0.10	23,23,23,23	0
55	MG	YA	3507	1/1	0.95	0.23	48,48,48,48	0
55	MG	QA	1601	1/1	0.95	0.07	32,32,32,32	0
55	MG	RA	3315	1/1	0.95	0.11	28,28,28,28	0
55	MG	YA	3293	1/1	0.95	0.12	42,42,42,42	0
55	MG	RA	3388	1/1	0.95	0.05	40,40,40,40	0
55	MG	XA	1674	1/1	0.95	0.04	54,54,54,54	0
55	MG	YA	3198	1/1	0.95	0.18	55,55,55,55	0
55	MG	RA	3252	1/1	0.95	0.24	62,62,62,62	0
55	MG	RA	3169	1/1	0.95	0.06	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	RA	3434	1/1	0.95	0.08	25,25,25,25	0
55	MG	RA	3119	1/1	0.95	0.09	44,44,44,44	0
55	MG	YA	3303	1/1	0.95	0.07	30,30,30,30	0
55	MG	YP	202	1/1	0.95	0.10	23,23,23,23	0
55	MG	RA	3286	1/1	0.95	0.17	40,40,40,40	0
55	MG	XV	101	1/1	0.95	0.27	153,153,153,153	0
55	MG	YR	201	1/1	0.95	0.08	16,16,16,16	0
55	MG	YA	3114	1/1	0.95	0.12	17,17,17,17	0
55	MG	YA	3208	1/1	0.95	0.09	23,23,23,23	0
55	MG	YA	3116	1/1	0.95	0.18	29,29,29,29	0
55	MG	RA	3099	1/1	0.95	0.11	60,60,60,60	0
55	MG	XA	1625	1/1	0.95	0.07	30,30,30,30	0
55	MG	Y7	101	1/1	0.95	0.11	51,51,51,51	0
55	MG	RA	3288	1/1	0.95	0.11	34,34,34,34	0
57	ZN	R4	101	1/1	0.95	0.06	250,250,250,250	0
55	MG	RA	3289	1/1	0.95	0.10	32,32,32,32	0
55	MG	YA	3110	1/1	0.96	0.15	35,35,35,35	0
55	MG	YA	3174	1/1	0.96	0.13	38,38,38,38	0
55	MG	RA	3264	1/1	0.96	0.20	41,41,41,41	0
55	MG	YA	3244	1/1	0.96	0.15	7,7,7,7	0
55	MG	YA	3383	1/1	0.96	0.10	11,11,11,11	0
55	MG	RA	3078	1/1	0.96	0.13	29,29,29,29	0
55	MG	YA	3385	1/1	0.96	0.06	15,15,15,15	0
55	MG	YA	3247	1/1	0.96	0.20	20,20,20,20	0
55	MG	RA	3052	1/1	0.96	0.04	1,1,1,1	0
55	MG	YA	3388	1/1	0.96	0.08	24,24,24,24	0
55	MG	XA	1621	1/1	0.96	0.12	25,25,25,25	0
55	MG	YA	3039	1/1	0.96	0.10	7,7,7,7	0
55	MG	RA	3080	1/1	0.96	0.05	12,12,12,12	0
55	MG	YA	3042	1/1	0.96	0.12	15,15,15,15	0
55	MG	RA	3172	1/1	0.96	0.20	49,49,49,49	0
55	MG	YA	3045	1/1	0.96	0.08	17,17,17,17	0
55	MG	YA	3470	1/1	0.96	0.16	47,47,47,47	0
55	MG	RA	3123	1/1	0.96	0.20	21,21,21,21	0
55	MG	RB	204	1/1	0.96	0.11	33,33,33,33	0
55	MG	RA	3053	1/1	0.96	0.10	21,21,21,21	0
55	MG	YA	3126	1/1	0.96	0.10	21,21,21,21	0
55	MG	XA	1629	1/1	0.96	0.06	24,24,24,24	0
55	MG	RA	3206	1/1	0.96	0.05	16,16,16,16	0
55	MG	YA	3403	1/1	0.96	0.17	34,34,34,34	0
55	MG	QA	1608	1/1	0.96	0.09	27,27,27,27	0
55	MG	RA	3208	1/1	0.96	0.10	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	XA	1633	1/1	0.96	0.06	42,42,42,42	0
55	MG	YA	3064	1/1	0.96	0.10	15,15,15,15	0
55	MG	XA	1634	1/1	0.96	0.06	90,90,90,90	0
55	MG	YA	3266	1/1	0.96	0.10	22,22,22,22	0
55	MG	YA	3136	1/1	0.96	0.14	10,10,10,10	0
55	MG	RA	3150	1/1	0.96	0.09	40,40,40,40	0
55	MG	RA	3126	1/1	0.96	0.13	37,37,37,37	0
55	MG	YA	3139	1/1	0.96	0.06	23,23,23,23	0
55	MG	RA	3127	1/1	0.96	0.20	17,17,17,17	0
55	MG	RA	3153	1/1	0.96	0.14	43,43,43,43	0
55	MG	YA	3494	1/1	0.96	0.10	24,24,24,24	0
55	MG	RA	3083	1/1	0.96	0.18	21,21,21,21	0
55	MG	RA	3129	1/1	0.96	0.05	24,24,24,24	0
55	MG	YA	3497	1/1	0.96	0.08	21,21,21,21	0
55	MG	RA	3056	1/1	0.96	0.20	15,15,15,15	0
55	MG	RA	3085	1/1	0.96	0.10	14,14,14,14	0
55	MG	YA	3277	1/1	0.96	0.21	33,33,33,33	0
55	MG	RA	3419	1/1	0.96	0.13	23,23,23,23	0
55	MG	R8	102	1/1	0.96	0.06	26,26,26,26	0
55	MG	RA	3109	1/1	0.96	0.09	72,72,72,72	0
55	MG	RA	3001	1/1	0.96	0.10	22,22,22,22	0
55	MG	RA	3047	1/1	0.96	0.10	4,4,4,4	0
55	MG	RA	3023	1/1	0.96	0.13	5,5,5,5	0
55	MG	YA	3083	1/1	0.96	0.10	28,28,28,28	0
55	MG	RA	3188	1/1	0.96	0.12	38,38,38,38	0
55	MG	YA	3013	1/1	0.96	0.04	33,33,33,33	0
55	MG	YA	3157	1/1	0.96	0.05	7,7,7,7	0
55	MG	RA	3391	1/1	0.96	0.17	34,34,34,34	0
55	MG	RA	3163	1/1	0.96	0.06	36,36,36,36	0
55	MG	QA	1607	1/1	0.96	0.07	39,39,39,39	0
55	MG	YB	206	1/1	0.96	0.17	51,51,51,51	0
55	MG	QA	1655	1/1	0.96	0.19	29,29,29,29	0
55	MG	YA	3093	1/1	0.96	0.09	7,7,7,7	0
55	MG	YA	3094	1/1	0.96	0.14	7,7,7,7	0
55	MG	YA	3296	1/1	0.96	0.05	33,33,33,33	0
55	MG	RA	3324	1/1	0.96	0.11	26,26,26,26	0
55	MG	YP	203	1/1	0.96	0.05	4,4,4,4	0
55	MG	YA	3365	1/1	0.96	0.18	58,58,58,58	0
55	MG	YQ	202	1/1	0.96	0.11	36,36,36,36	0
55	MG	YA	3366	1/1	0.96	0.12	30,30,30,30	0
55	MG	RA	3005	1/1	0.96	0.14	24,24,24,24	0
55	MG	YA	3232	1/1	0.96	0.09	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	RA	3077	1/1	0.96	0.17	28,28,28,28	0
55	MG	YA	3167	1/1	0.96	0.25	32,32,32,32	0
55	MG	YA	3235	1/1	0.96	0.17	44,44,44,44	0
55	MG	YA	3102	1/1	0.96	0.19	12,12,12,12	0
55	MG	RA	3229	1/1	0.96	0.11	21,21,21,21	0
55	MG	RA	3262	1/1	0.96	0.15	34,34,34,34	0
55	MG	YA	3105	1/1	0.96	0.19	21,21,21,21	0
57	ZN	XN	101	1/1	0.96	0.10	155,155,155,155	0
55	MG	RA	3095	1/1	0.96	0.08	8,8,8,8	0
55	MG	XA	1648	1/1	0.97	0.17	27,27,27,27	0
55	MG	YA	3085	1/1	0.97	0.11	9,9,9,9	0
55	MG	RA	3425	1/1	0.97	0.06	23,23,23,23	0
55	MG	YA	3380	1/1	0.97	0.17	23,23,23,23	0
55	MG	YA	3087	1/1	0.97	0.12	11,11,11,11	0
55	MG	RA	3389	1/1	0.97	0.05	39,39,39,39	0
55	MG	RA	3427	1/1	0.97	0.09	17,17,17,17	0
55	MG	RA	3290	1/1	0.97	0.17	46,46,46,46	0
55	MG	YA	3019	1/1	0.97	0.12	29,29,29,29	0
55	MG	YA	3020	1/1	0.97	0.15	7,7,7,7	0
55	MG	RA	3098	1/1	0.97	0.06	30,30,30,30	0
55	MG	RA	3145	1/1	0.97	0.05	32,32,32,32	0
55	MG	YA	3023	1/1	0.97	0.07	20,20,20,20	0
55	MG	YA	3245	1/1	0.97	0.14	13,13,13,13	0
55	MG	RA	3058	1/1	0.97	0.08	15,15,15,15	0
55	MG	YA	3099	1/1	0.97	0.11	18,18,18,18	0
55	MG	YA	3101	1/1	0.97	0.13	13,13,13,13	0
55	MG	RA	3122	1/1	0.97	0.05	28,28,28,28	0
55	MG	QA	1650	1/1	0.97	0.04	31,31,31,31	0
55	MG	RA	3435	1/1	0.97	0.06	40,40,40,40	0
55	MG	RA	3042	1/1	0.97	0.13	22,22,22,22	0
55	MG	YA	3477	1/1	0.97	0.07	7,7,7,7	0
55	MG	YA	3399	1/1	0.97	0.07	26,26,26,26	0
55	MG	YA	3479	1/1	0.97	0.16	7,7,7,7	0
55	MG	YA	3108	1/1	0.97	0.09	11,11,11,11	0
55	MG	QA	1634	1/1	0.97	0.04	24,24,24,24	0
55	MG	YA	3402	1/1	0.97	0.08	30,30,30,30	0
55	MG	XA	1617	1/1	0.97	0.12	36,36,36,36	0
55	MG	RA	3046	1/1	0.97	0.10	26,26,26,26	0
55	MG	YA	3036	1/1	0.97	0.13	4,4,4,4	0
55	MG	RA	3329	1/1	0.97	0.07	40,40,40,40	0
55	MG	RA	3440	1/1	0.97	0.05	52,52,52,52	0
55	MG	YA	3332	1/1	0.97	0.15	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	QA	1611	1/1	0.97	0.06	32,32,32,32	0
55	MG	YA	3491	1/1	0.97	0.19	41,41,41,41	0
55	MG	YA	3043	1/1	0.97	0.14	8,8,8,8	0
55	MG	RA	3007	1/1	0.97	0.05	40,40,40,40	0
55	MG	RA	3332	1/1	0.97	0.17	59,59,59,59	0
55	MG	QA	1603	1/1	0.97	0.06	34,34,34,34	0
55	MG	YA	3338	1/1	0.97	0.20	43,43,43,43	0
55	MG	YA	3192	1/1	0.97	0.14	5,5,5,5	0
55	MG	YA	3048	1/1	0.97	0.10	22,22,22,22	0
55	MG	YA	3049	1/1	0.97	0.10	7,7,7,7	0
55	MG	YA	3500	1/1	0.97	0.04	22,22,22,22	0
55	MG	RA	3108	1/1	0.97	0.07	28,28,28,28	0
55	MG	YA	3196	1/1	0.97	0.08	41,41,41,41	0
55	MG	RA	3068	1/1	0.97	0.12	21,21,21,21	0
55	MG	YA	3127	1/1	0.97	0.11	37,37,37,37	0
55	MG	YA	3052	1/1	0.97	0.12	18,18,18,18	0
55	MG	YA	3053	1/1	0.97	0.09	7,7,7,7	0
55	MG	YA	3202	1/1	0.97	0.04	19,19,19,19	0
55	MG	YA	3054	1/1	0.97	0.04	18,18,18,18	0
55	MG	XA	1627	1/1	0.97	0.09	30,30,30,30	0
55	MG	RA	3157	1/1	0.97	0.05	19,19,19,19	0
55	MG	QA	1654	1/1	0.97	0.30	42,42,42,42	0
55	MG	RB	207	1/1	0.97	0.15	29,29,29,29	0
55	MG	RA	3214	1/1	0.97	0.26	40,40,40,40	0
55	MG	YA	3063	1/1	0.97	0.13	11,11,11,11	0
55	MG	RA	3032	1/1	0.97	0.06	19,19,19,19	0
55	MG	XE	201	1/1	0.97	0.09	71,71,71,71	0
55	MG	YA	3140	1/1	0.97	0.05	21,21,21,21	0
55	MG	YE	301	1/1	0.97	0.08	9,9,9,9	0
55	MG	RA	3002	1/1	0.97	0.04	20,20,20,20	0
55	MG	RA	3135	1/1	0.97	0.09	37,37,37,37	0
55	MG	YE	305	1/1	0.97	0.04	9,9,9,9	0
55	MG	YA	3287	1/1	0.97	0.15	7,7,7,7	0
55	MG	RA	3342	1/1	0.97	0.05	35,35,35,35	0
55	MG	RA	3034	1/1	0.97	0.08	26,26,26,26	0
55	MG	RA	3344	1/1	0.97	0.06	35,35,35,35	0
55	MG	RA	3249	1/1	0.97	0.07	19,19,19,19	0
55	MG	YA	3073	1/1	0.97	0.10	7,7,7,7	0
55	MG	RA	3035	1/1	0.97	0.12	24,24,24,24	0
55	MG	RA	3189	1/1	0.97	0.16	30,30,30,30	0
55	MG	YA	3006	1/1	0.97	0.10	24,24,24,24	0
55	MG	RA	3190	1/1	0.97	0.19	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	RA	3115	1/1	0.97	0.12	37,37,37,37	0
55	MG	Y5	102	1/1	0.97	0.09	32,32,32,32	0
55	MG	YA	3079	1/1	0.97	0.16	15,15,15,15	0
55	MG	RA	3055	1/1	0.97	0.20	16,16,16,16	0
56	SF4	XD	301	8/8	0.97	0.06	107,118,132,149	0
55	MG	QA	1630	1/1	0.97	0.07	49,49,49,49	0
55	MG	RA	3025	1/1	0.97	0.10	15,15,15,15	0
55	MG	RA	3096	1/1	0.97	0.05	20,20,20,20	0
55	MG	RA	3014	1/1	0.98	0.09	30,30,30,30	0
55	MG	YA	3223	1/1	0.98	0.03	25,25,25,25	0
55	MG	RA	3067	1/1	0.98	0.14	15,15,15,15	0
55	MG	RA	3215	1/1	0.98	0.12	9,9,9,9	0
55	MG	YA	3067	1/1	0.98	0.07	0,0,0,0	0
55	MG	XA	1602	1/1	0.98	0.05	43,43,43,43	0
55	MG	YA	3106	1/1	0.98	0.11	7,7,7,7	0
55	MG	YA	3107	1/1	0.98	0.24	20,20,20,20	0
55	MG	YA	3186	1/1	0.98	0.03	25,25,25,25	0
55	MG	YA	3148	1/1	0.98	0.07	19,19,19,19	0
55	MG	XA	1628	1/1	0.98	0.05	41,41,41,41	0
55	MG	YA	3455	1/1	0.98	0.25	55,55,55,55	0
55	MG	YA	3189	1/1	0.98	0.10	12,12,12,12	0
55	MG	QA	1609	1/1	0.98	0.07	36,36,36,36	0
55	MG	YA	3033	1/1	0.98	0.05	11,11,11,11	0
55	MG	RA	3420	1/1	0.98	0.12	7,7,7,7	0
55	MG	YA	3460	1/1	0.98	0.04	35,35,35,35	0
55	MG	RA	3142	1/1	0.98	0.07	22,22,22,22	0
55	MG	RA	3043	1/1	0.98	0.08	13,13,13,13	0
55	MG	YB	201	1/1	0.98	0.09	17,17,17,17	0
55	MG	YA	3037	1/1	0.98	0.16	7,7,7,7	0
55	MG	RA	3044	1/1	0.98	0.06	13,13,13,13	0
55	MG	RB	203	1/1	0.98	0.04	63,63,63,63	0
55	MG	YA	3119	1/1	0.98	0.10	6,6,6,6	0
55	MG	RA	3105	1/1	0.98	0.06	11,11,11,11	0
55	MG	RB	205	1/1	0.98	0.21	38,38,38,38	0
55	MG	RA	3238	1/1	0.98	0.05	42,42,42,42	0
55	MG	YD	302	1/1	0.98	0.04	22,22,22,22	0
55	MG	RA	3204	1/1	0.98	0.10	26,26,26,26	0
55	MG	YA	3046	1/1	0.98	0.08	1,1,1,1	0
55	MG	YE	303	1/1	0.98	0.09	7,7,7,7	0
55	MG	RA	3278	1/1	0.98	0.07	27,27,27,27	0
55	MG	RA	3036	1/1	0.98	0.06	17,17,17,17	0
55	MG	YP	201	1/1	0.98	0.05	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	RA	3024	1/1	0.98	0.07	29,29,29,29	0
55	MG	YA	3294	1/1	0.98	0.19	38,38,38,38	0
55	MG	RA	3094	1/1	0.98	0.13	31,31,31,31	0
55	MG	YA	3209	1/1	0.98	0.04	30,30,30,30	0
55	MG	RA	3261	1/1	0.98	0.06	43,43,43,43	0
55	MG	YA	3016	1/1	0.98	0.14	23,23,23,23	0
55	MG	YA	3480	1/1	0.98	0.12	7,7,7,7	0
55	MG	RA	3038	1/1	0.98	0.04	13,13,13,13	0
55	MG	RA	3021	1/1	0.98	0.07	8,8,8,8	0
55	MG	RA	3193	1/1	0.98	0.07	30,30,30,30	0
55	MG	RA	3065	1/1	0.98	0.08	19,19,19,19	0
55	MG	XA	1675	1/1	0.98	0.06	20,20,20,20	0
55	MG	RA	3266	1/1	0.98	0.05	54,54,54,54	0
55	MG	YA	3060	1/1	0.98	0.12	7,7,7,7	0
56	SF4	QD	301	8/8	0.98	0.05	67,98,117,173	0
55	MG	RA	3086	1/1	0.98	0.15	20,20,20,20	0
57	ZN	QN	101	1/1	0.98	0.08	175,175,175,175	0
57	ZN	RY	201	1/1	0.98	0.06	112,112,112,112	0
55	MG	YA	3441	1/1	0.98	0.09	53,53,53,53	0
57	ZN	R5	101	1/1	0.98	0.04	124,124,124,124	0
55	MG	YA	3026	1/1	0.98	0.10	12,12,12,12	0
57	ZN	YY	201	1/1	0.98	0.04	72,72,72,72	0
55	MG	YA	3221	1/1	0.98	0.13	36,36,36,36	0
57	ZN	Y5	101	1/1	0.98	0.05	88,88,88,88	0
57	ZN	Y9	101	1/1	0.98	0.06	66,66,66,66	0
55	MG	YA	3117	1/1	0.99	0.03	9,9,9,9	0
55	MG	YA	3323	1/1	0.99	0.09	4,4,4,4	0
55	MG	YA	3062	1/1	0.99	0.05	0,0,0,0	0
55	MG	QA	1619	1/1	0.99	0.10	40,40,40,40	0
55	MG	YA	3088	1/1	0.99	0.12	9,9,9,9	0
55	MG	RA	3097	1/1	0.99	0.05	23,23,23,23	0
55	MG	RA	3016	1/1	0.99	0.11	7,7,7,7	0
55	MG	RE	303	1/1	0.99	0.03	7,7,7,7	0
55	MG	YA	3055	1/1	0.99	0.07	17,17,17,17	0
55	MG	RA	3041	1/1	0.99	0.04	19,19,19,19	0
55	MG	RA	3431	1/1	0.99	0.07	10,10,10,10	0
55	MG	RF	301	1/1	0.99	0.04	34,34,34,34	0
55	MG	YA	3200	1/1	0.99	0.14	27,27,27,27	0
55	MG	XA	1672	1/1	0.99	0.03	32,32,32,32	0
55	MG	YA	3097	1/1	0.99	0.03	7,7,7,7	0
55	MG	RA	3200	1/1	0.99	0.05	25,25,25,25	0
57	ZN	R6	101	1/1	0.99	0.03	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	ZN	R9	101	1/1	0.99	0.06	65,65,65,65	0
55	MG	YA	3131	1/1	0.99	0.06	9,9,9,9	0
55	MG	YA	3040	1/1	0.99	0.14	7,7,7,7	0
55	MG	YA	3115	1/1	0.99	0.03	8,8,8,8	0
55	MG	YA	3100	1/1	0.99	0.05	3,3,3,3	0
57	ZN	Y6	101	1/1	0.99	0.03	55,55,55,55	0
55	MG	YA	3382	1/1	0.99	0.07	4,4,4,4	0
55	MG	RA	3012	1/1	1.00	0.06	1,1,1,1	0
55	MG	RA	3371	1/1	1.00	0.03	3,3,3,3	0
55	MG	YA	3024	1/1	1.00	0.05	8,8,8,8	0
55	MG	YA	3025	1/1	1.00	0.11	7,7,7,7	0
55	MG	YA	3038	1/1	1.00	0.03	7,7,7,7	0

6.5 Other polymers (i)

There are no such residues in this entry.