wwPDB X-ray Structure Validation Summary Report (i)

Mar 27, 2026 – 01:06 AM UTC

PDB ID	:	6NWY / pdb_00006nwy
Title	:	Modified tRNA(Pro) bound to Thermus thermophilus 70S (near-cognate)
Authors	:	Hoffer, E.D.; Subaramanian, S.; Hong, S.; Maehigashi, T.; Dunham, C.M.
Deposited on	:	2019-02-07
Resolution	:	3.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

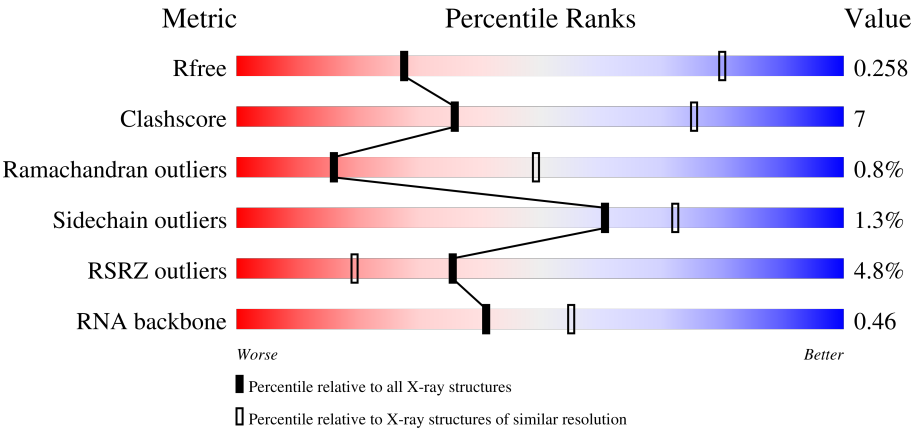
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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

Mol	Chain	Length	Quality of chain
1	QA	1521	7% 55% 38% 7%
1	XA	1521	3% 55% 38% 7%
2	QB	256	3% 63% 28% 8%
2	XB	256	% 67% 24% 8%

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Mol	Chain	Length	Quality of chain
3	QC	239	2% 64% 19% 14%
3	XC	239	3% 70% 15% 14%
4	QD	209	6% 73% 24%
4	XD	209	7% 67% 30%
5	QE	162	2% 69% 24% 7%
5	XE	162	70% 23% 7%
6	QF	101	2% 77% 22%
6	XF	101	79% 21%
7	QG	156	8% 78% 21%
7	XG	156	4% 76% 22%
8	QH	138	7% 77% 22%
8	XH	138	6% 75% 23%
9	QI	128	23% 67% 30%
9	XI	128	14% 76% 22%
10	QJ	105	21% 62% 30% 6%
10	XJ	105	10% 73% 18% 9%
11	QK	129	5% 83% 9% 8%
11	XK	129	2% 74% 16% 10%
12	QL	132	10% 70% 23% 5%
12	XL	132	8% 72% 20% 8%
13	QM	126	6% 63% 32% 5%
13	XM	126	6% 67% 21% 10%
14	QN	61	18% 62% 33%
14	XN	61	11% 62% 31%
15	QO	89	88% 11%

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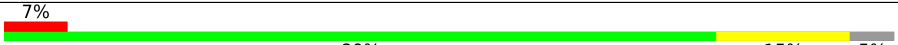
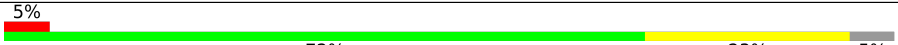
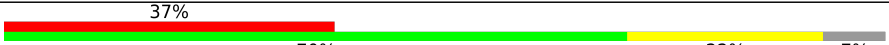
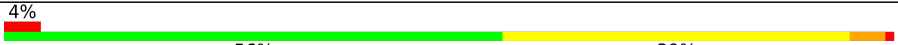
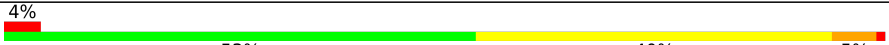
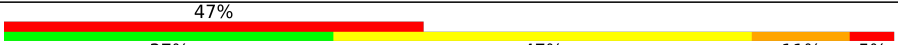
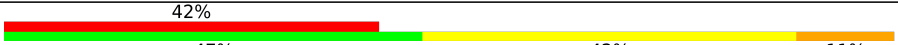
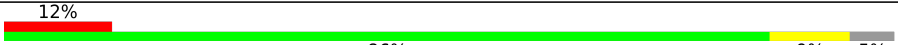
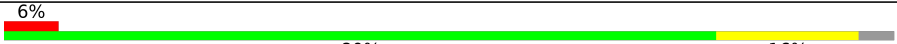
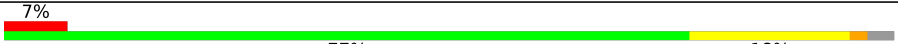
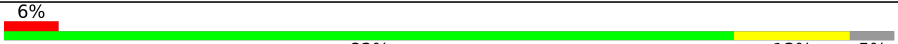
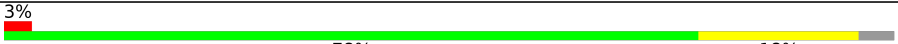
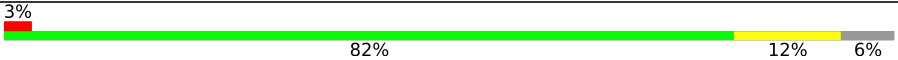
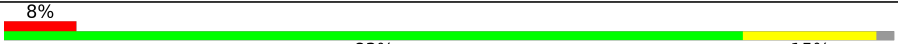
Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	19	
23	XX	19	
24	R0	85	
24	Y0	85	
25	R1	98	
25	Y1	98	
26	R2	72	
26	Y2	72	
27	R3	60	
27	Y3	60	

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Mol	Chain	Length	Quality of chain
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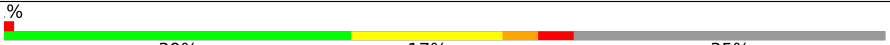
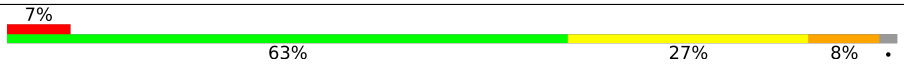
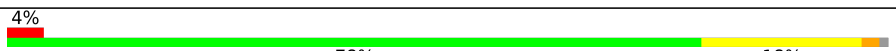
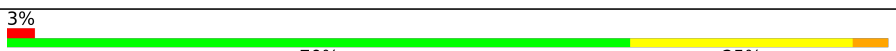
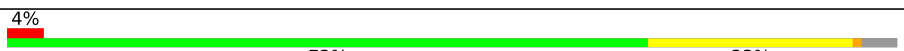
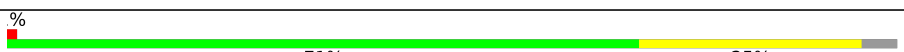
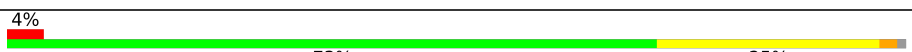
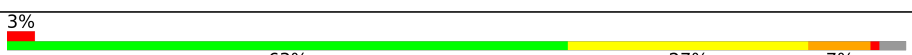
28	Y4	71	
29	R5	60	
29	Y5	60	
30	R6	54	
30	Y6	54	
31	R7	49	
31	Y7	49	
32	R8	65	
32	Y8	65	
33	R9	37	
33	Y9	37	
34	RA	2915	
34	YA	2915	
35	RB	122	
35	YB	122	
36	RD	276	
36	YD	276	
37	RE	206	
37	YE	206	
38	RF	210	
38	YF	210	
39	RG	182	
39	YG	182	
40	RH	180	

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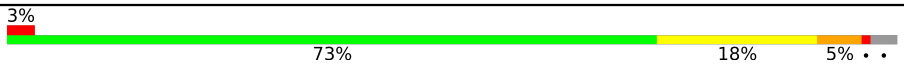
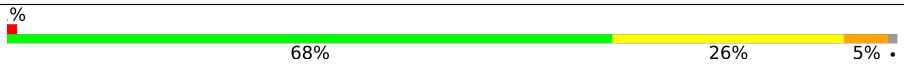
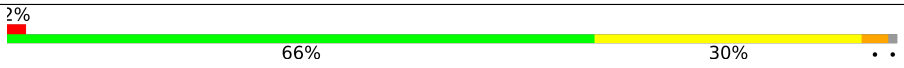
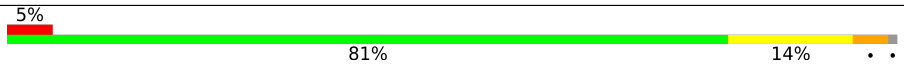
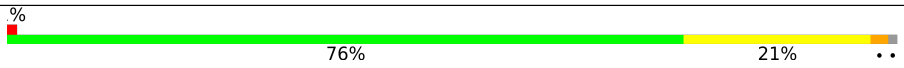
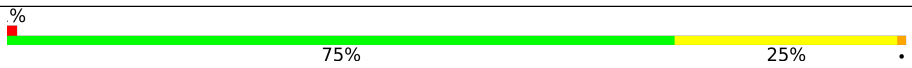
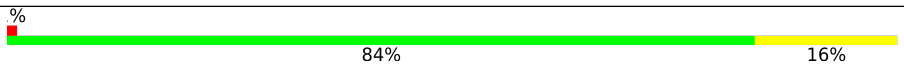
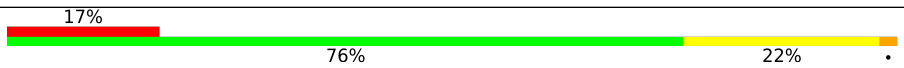
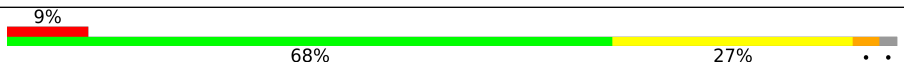
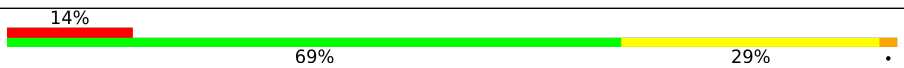
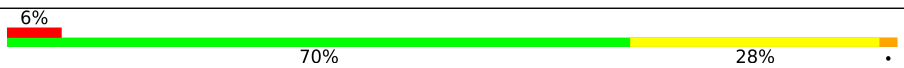
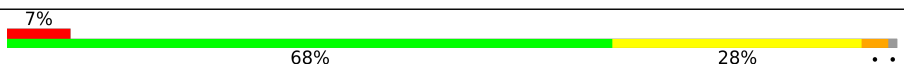
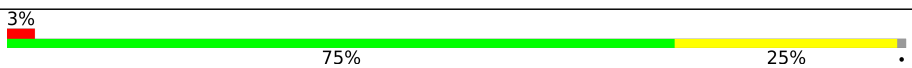
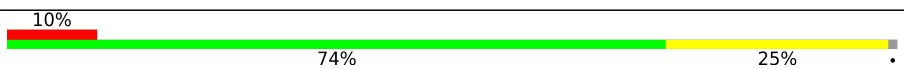
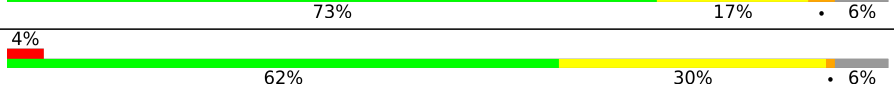
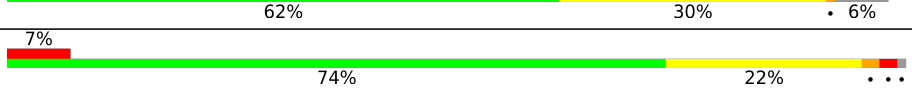
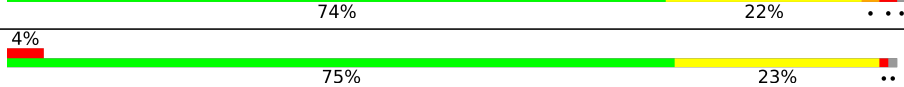
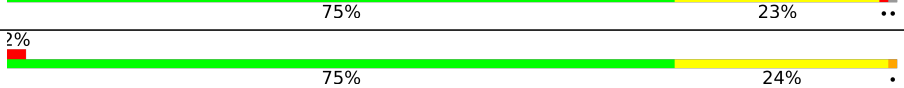
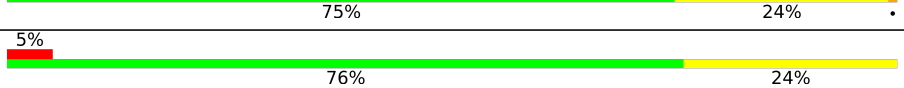
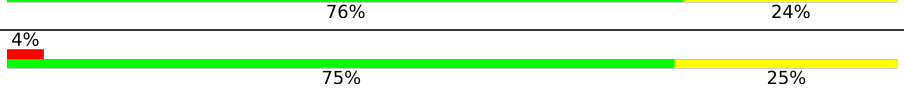
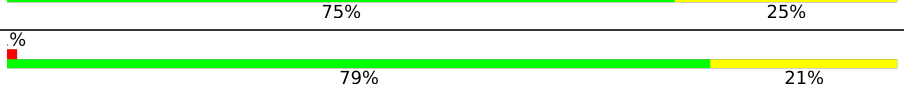
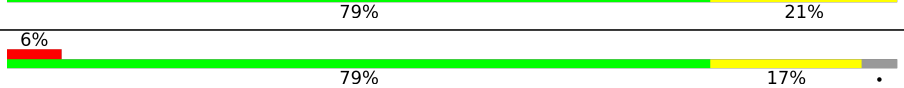
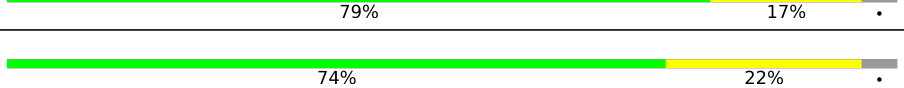
Mol	Chain	Length	Quality of chain
40	YH	180	
41	RI	148	
41	YI	148	
42	RN	140	
42	YN	140	
43	RO	122	
43	YO	122	
44	RP	150	
44	YP	150	
45	RQ	141	
45	YQ	141	
46	RR	118	
46	YR	118	
47	RS	112	
47	YS	112	
48	RT	146	
48	YT	146	
49	RU	118	
49	YU	118	
50	RV	101	
50	YV	101	
51	RW	113	
51	YW	113	
52	RX	96	
52	YX	96	

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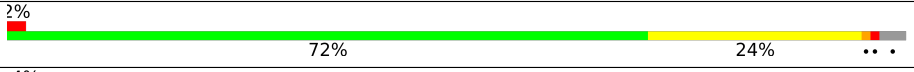
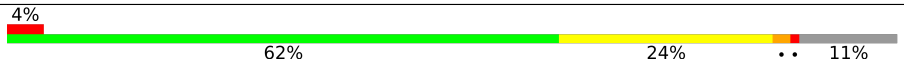
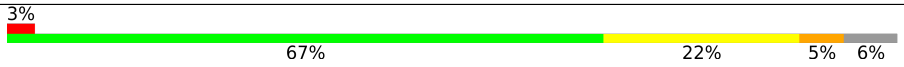
Mol	Chain	Length	Quality of chain
53	RY	110	
53	YY	110	
54	RZ	206	
54	YZ	206	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	YA	3245	-	-	-	X
56	SF4	QD	301	-	-	X	-

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 292039 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1511	Total	C	N	O	P	0	0	0
			32469	14453	6011	10495	1510			
1	XA	1515	Total	C	N	O	P	0	0	0
			32551	14490	6022	10525	1514			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	120	Total	C	N	O	S	0	0	0
			955	591	197	165	2			
13	XM	114	Total	C	N	O	S	0	0	0
			914	565	189	158	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called E-site tRNA-Pro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total 1647	C 734	N 295	O 541	P 77	0	0	0
22	XV	77	Total 1647	C 734	N 295	O 541	P 77	0	0	0

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	19	Total 409	C 184	N 81	O 126	P 18	0	0	0
23	XX	19	Total 409	C 184	N 81	O 126	P 18	0	0	0

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

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

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R1	95	Total 746	C 469	N 148	O 128	S 1	0	0	0
25	Y1	93	Total 729	C 457	N 145	O 126	S 1	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L29.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y2	68	Total	C	N	O	S	0	0	0
			575	355	117	102	1			

- Molecule 27 is a protein called 50S ribosomal protein L30.

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

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R4	45	Total	C	N	O	S	0	0	0
			348	224	57	62	5			
28	Y4	46	Total	C	N	O	S	0	0	0
			357	229	59	64	5			

- Molecule 29 is a protein called 50S ribosomal protein L32.

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

- Molecule 30 is a protein called 50S ribosomal protein L33.

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

- Molecule 31 is a protein called 50S ribosomal protein L34.

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

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	RA	2882	Total	C	N	O	P	0	0	0
			62070	27627	11611	19951	2881			
34	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- Molecule 35 is a RNA chain called 5S rRNA.

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

- Molecule 36 is a protein called 50S ribosomal protein L2.

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

- Molecule 37 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
37	YE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 38 is a protein called 50S ribosomal protein L4.

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

- Molecule 39 is a protein called 50S ribosomal protein L5.

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

- Molecule 40 is a protein called 50S ribosomal protein L6.

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

- Molecule 41 is a protein called 50S ribosomal protein L9.

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

- Molecule 42 is a protein called 50S ribosomal protein L13.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L14.

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

- Molecule 44 is a protein called 50S ribosomal protein L15.

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

- Molecule 45 is a protein called 50S ribosomal protein L16.

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

- Molecule 46 is a protein called 50S ribosomal protein L17.

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

- Molecule 47 is a protein called 50S ribosomal protein L18.

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

- Molecule 48 is a protein called 50S ribosomal protein L19.

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

- Molecule 49 is a protein called 50S ribosomal protein L20.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L22.

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

- Molecule 52 is a protein called 50S ribosomal protein L23.

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

- Molecule 53 is a protein called 50S ribosomal protein L24.

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

- Molecule 54 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RZ	183	Total 1461	C 933	N 260	O 265	S 3	0	0	0
54	YZ	193	Total 1529	C 973	N 270	O 283	S 3	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	87	Total 87	Mg 87	0	0
55	QF	1	Total 1	Mg 1	0	0
55	QH	2	Total 2	Mg 2	0	0
55	QL	1	Total 1	Mg 1	0	0
55	R0	2	Total 2	Mg 2	0	0
55	R1	1	Total 1	Mg 1	0	0
55	R3	1	Total 1	Mg 1	0	0
55	R8	1	Total 1	Mg 1	0	0
55	RA	429	Total 429	Mg 429	0	0
55	RB	11	Total 11	Mg 11	0	0
55	RD	1	Total 1	Mg 1	0	0
55	RE	4	Total 4	Mg 4	0	0
55	RF	2	Total 2	Mg 2	0	0
55	RN	1	Total 1	Mg 1	0	0

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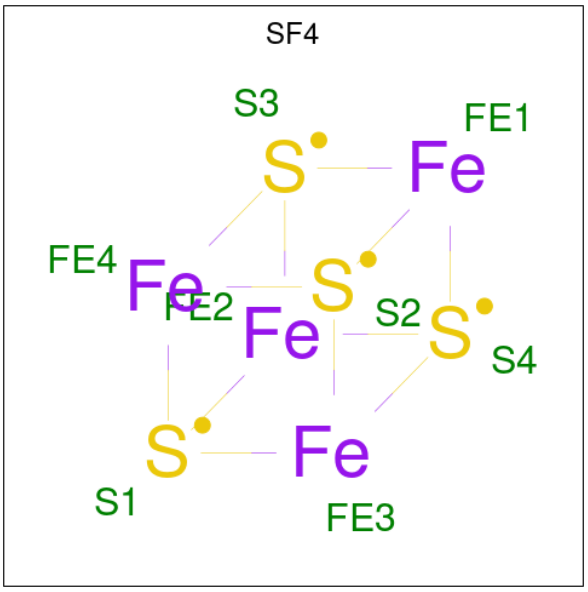
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	RO	1	Total Mg 1 1	0	0
55	RP	1	Total Mg 1 1	0	0
55	RQ	1	Total Mg 1 1	0	0
55	XA	89	Total Mg 89 89	0	0
55	XE	1	Total Mg 1 1	0	0
55	Y1	1	Total Mg 1 1	0	0
55	Y2	1	Total Mg 1 1	0	0
55	Y5	1	Total Mg 1 1	0	0
55	Y7	1	Total Mg 1 1	0	0
55	Y8	1	Total Mg 1 1	0	0
55	YA	439	Total Mg 439 439	0	0
55	YB	8	Total Mg 8 8	0	0
55	YD	1	Total Mg 1 1	0	0
55	YE	2	Total Mg 2 2	0	0
55	YF	1	Total Mg 1 1	0	0
55	YQ	1	Total Mg 1 1	0	0
55	YR	2	Total Mg 2 2	0	0
55	YU	1	Total Mg 1 1	0	0
55	YX	1	Total Mg 1 1	0	0

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



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

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

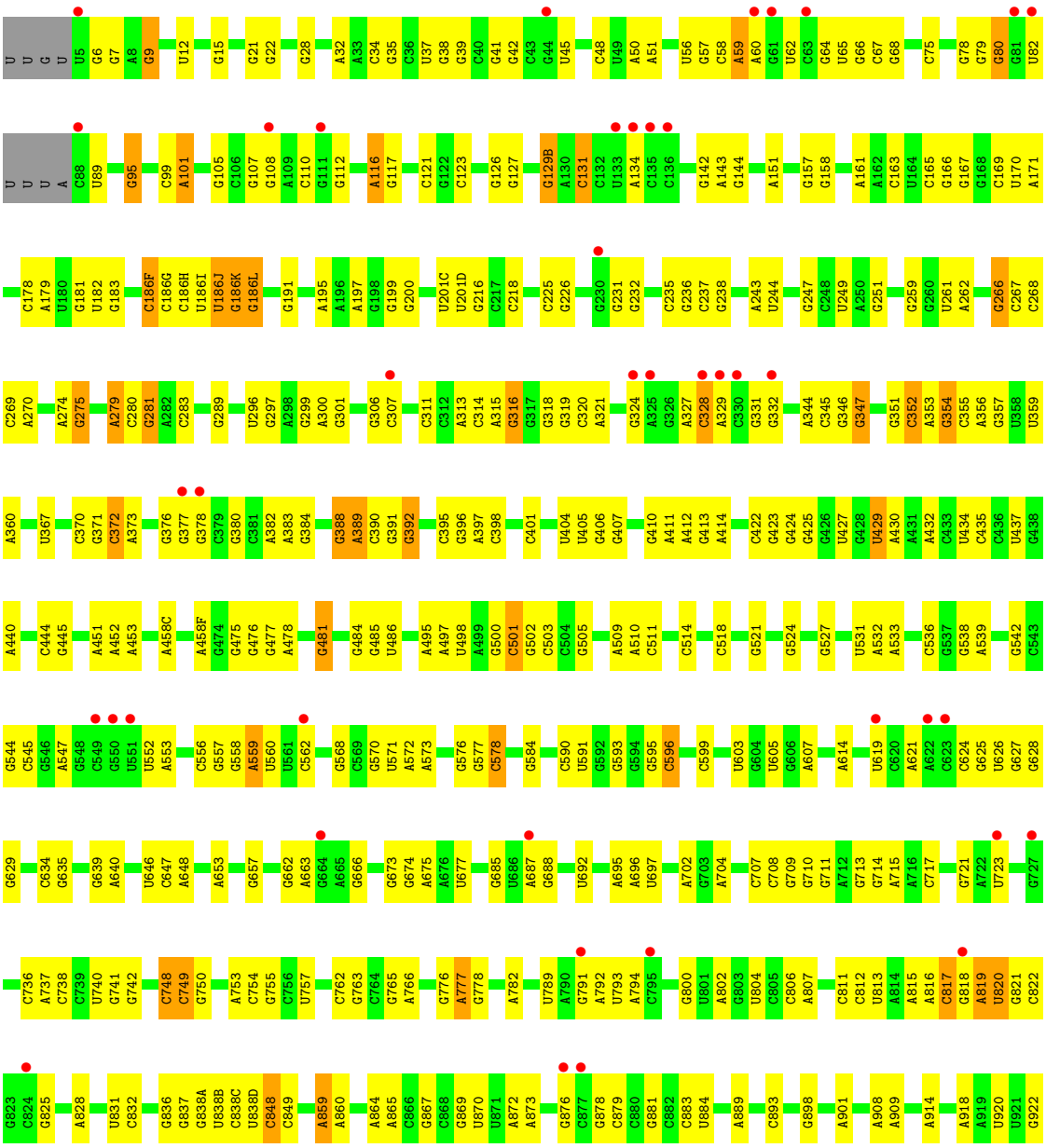
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	QN	1	Total Zn 1 1	0	0
57	R5	1	Total Zn 1 1	0	0
57	R6	1	Total Zn 1 1	0	0
57	R9	1	Total Zn 1 1	0	0
57	RY	1	Total Zn 1 1	0	0
57	XN	1	Total Zn 1 1	0	0
57	Y5	1	Total Zn 1 1	0	0
57	Y6	1	Total Zn 1 1	0	0
57	Y9	1	Total Zn 1 1	0	0
57	YY	1	Total Zn 1 1	0	0

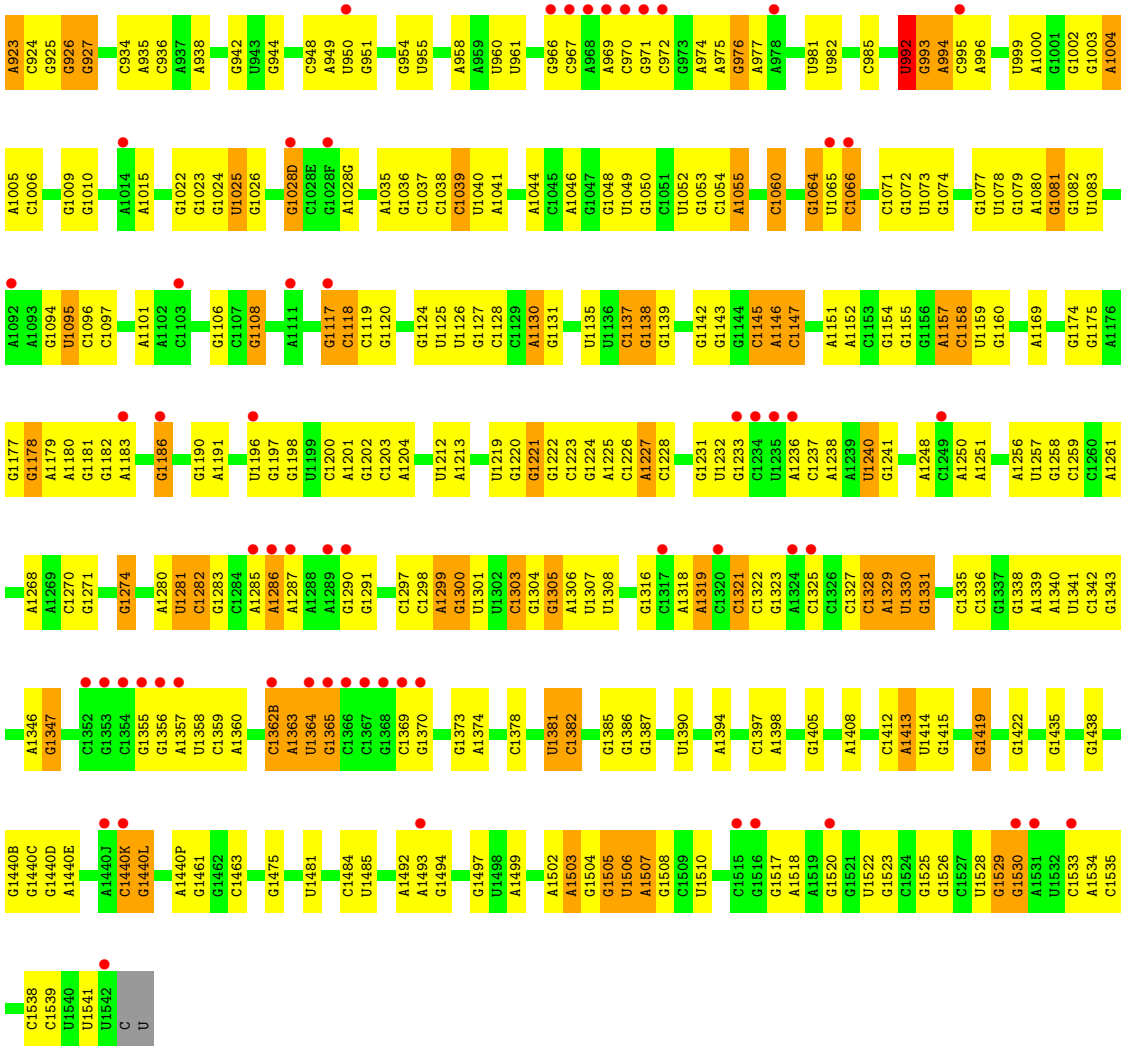
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

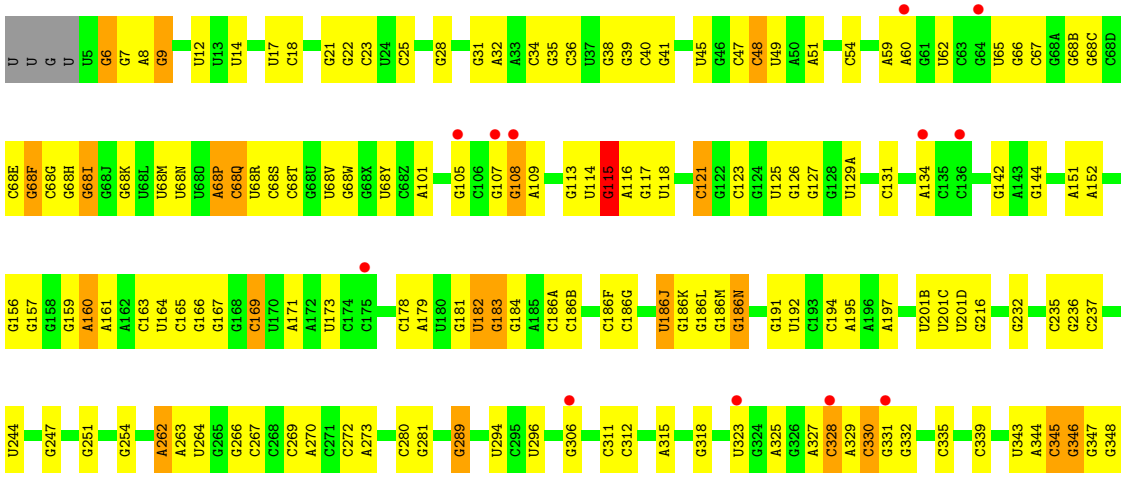
Chain QA:

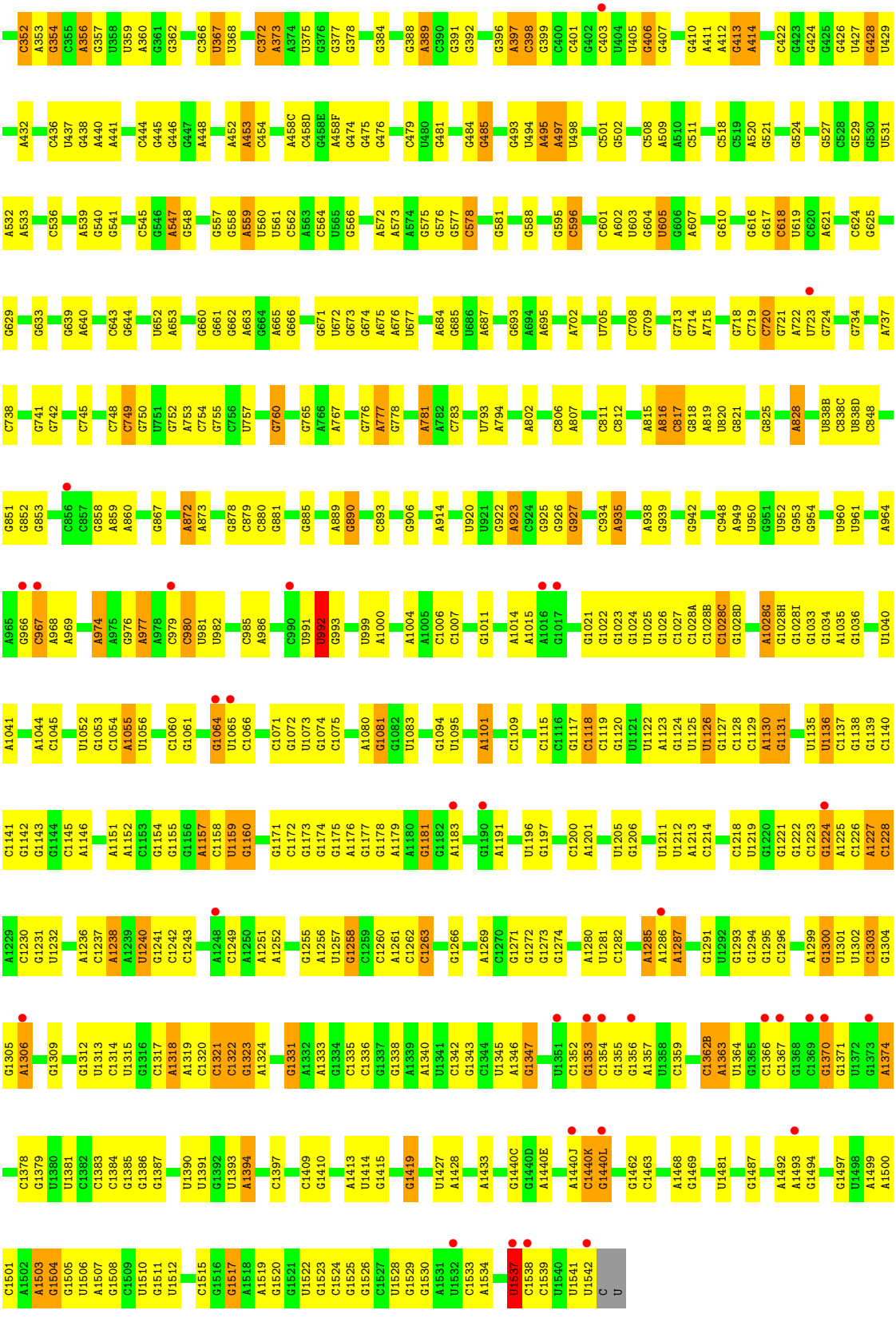




• Molecule 1: 16S rRNA

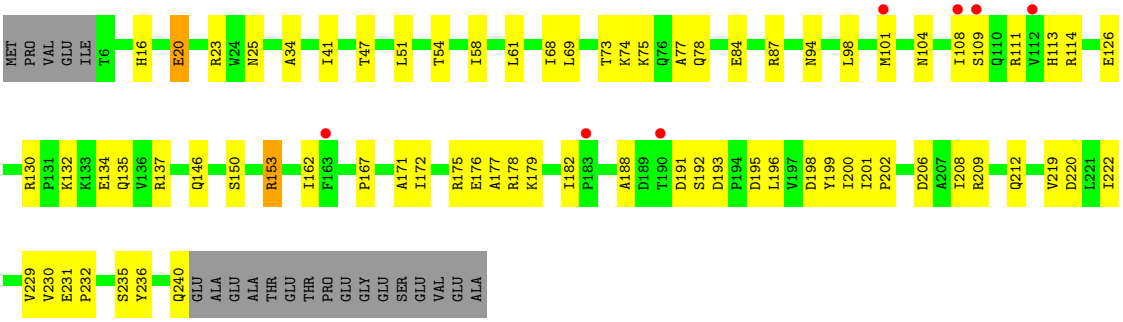
Chain XA:





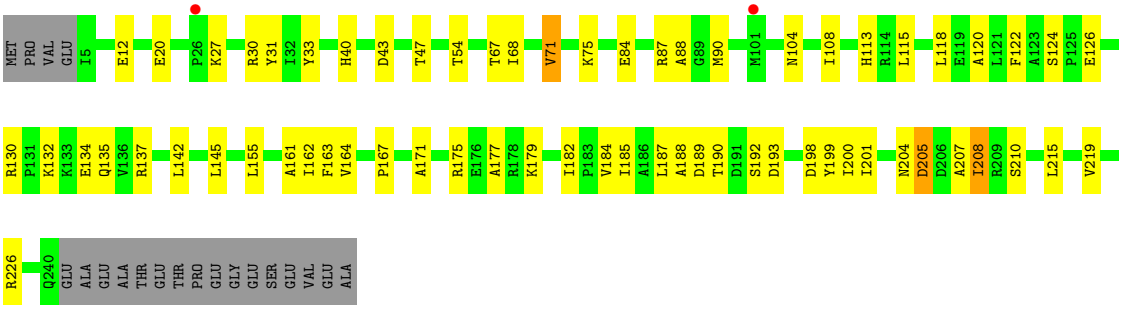
• Molecule 2: 30S ribosomal protein S2

Chain QB:



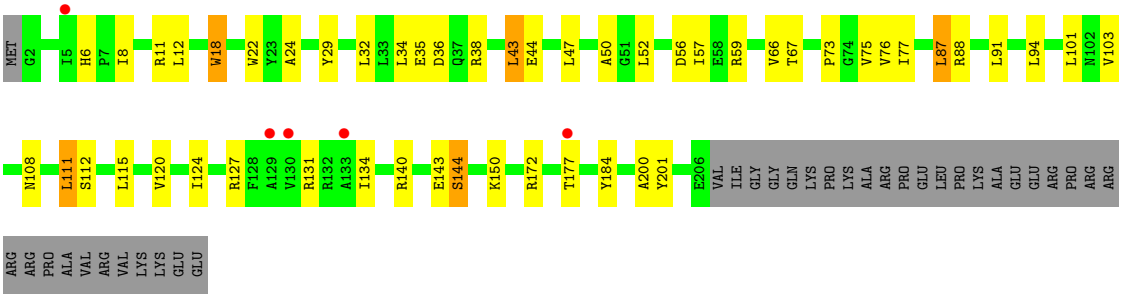
• Molecule 2: 30S ribosomal protein S2

Chain XB:



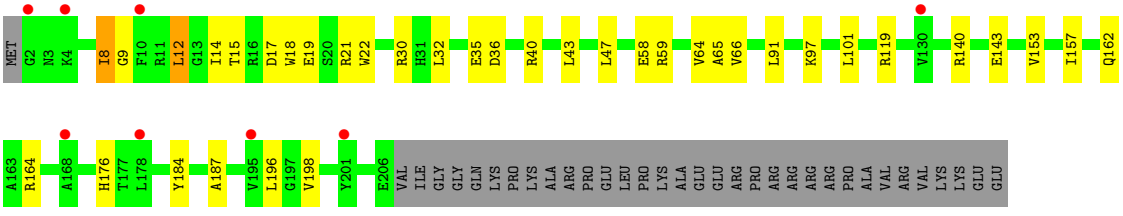
• Molecule 3: 30S ribosomal protein S3

Chain QC:



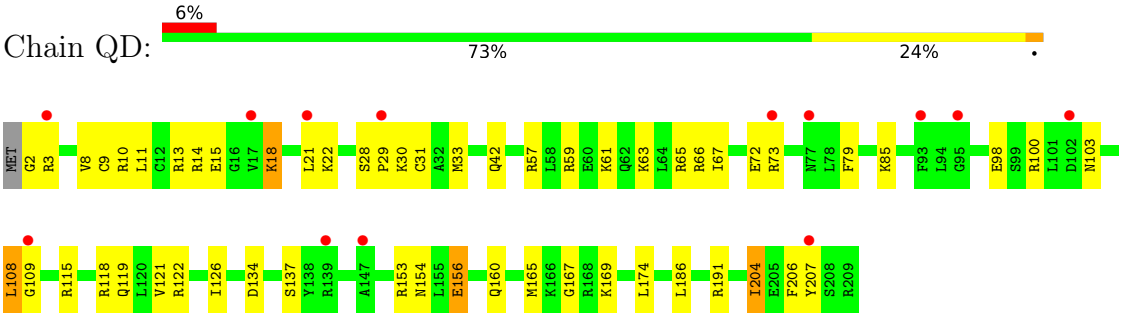
• Molecule 3: 30S ribosomal protein S3

Chain XC:



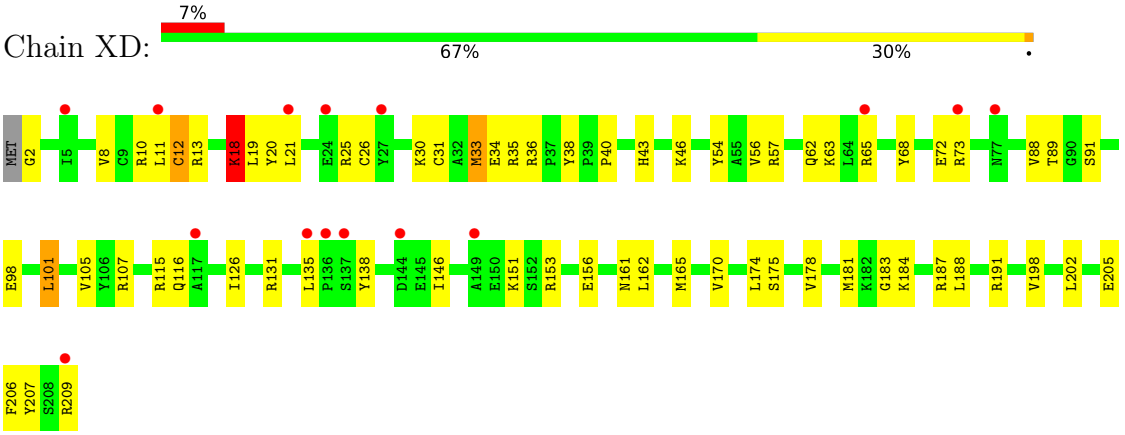
• Molecule 4: 30S ribosomal protein S4

Chain QD:



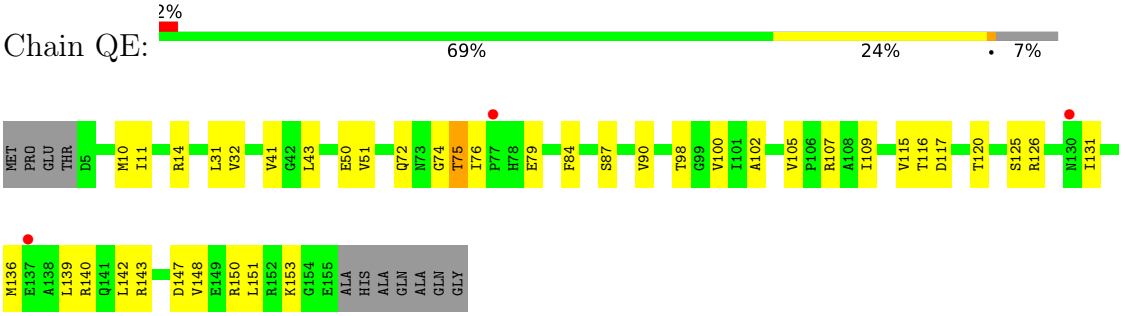
• Molecule 4: 30S ribosomal protein S4

Chain XD:



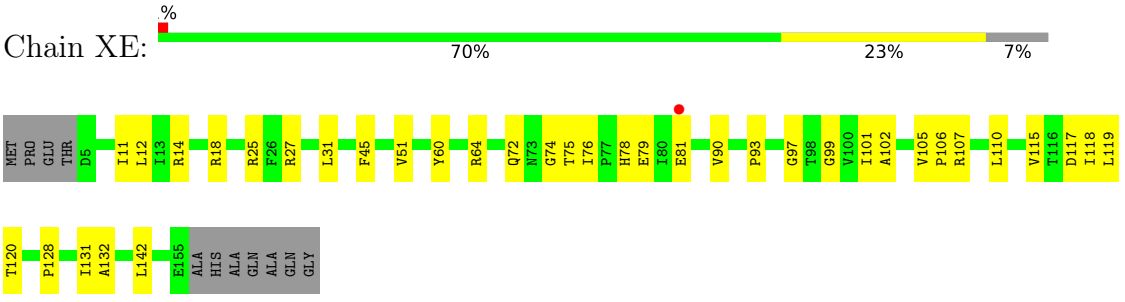
• Molecule 5: 30S ribosomal protein S5

Chain QE:



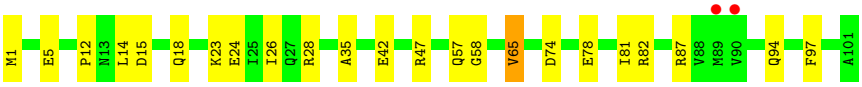
• Molecule 5: 30S ribosomal protein S5

Chain XE:

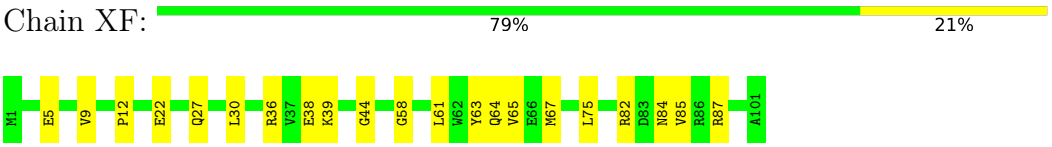


• Molecule 6: 30S ribosomal protein S6

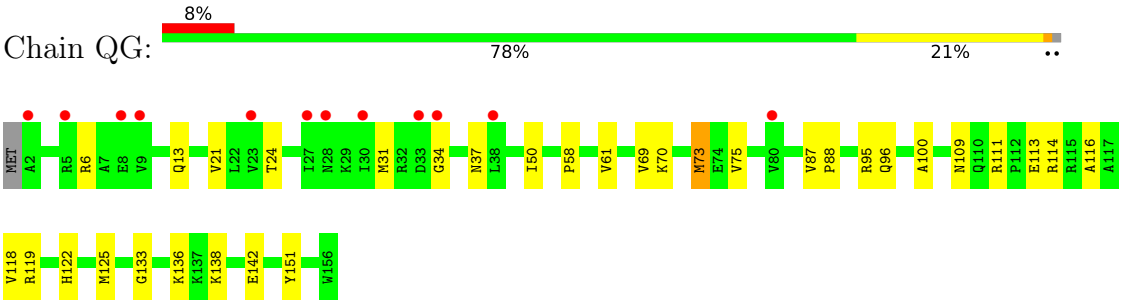
Chain QF:



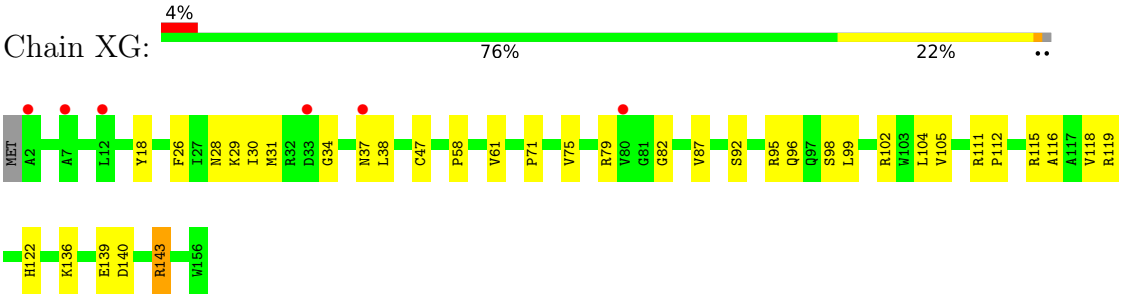
• Molecule 6: 30S ribosomal protein S6



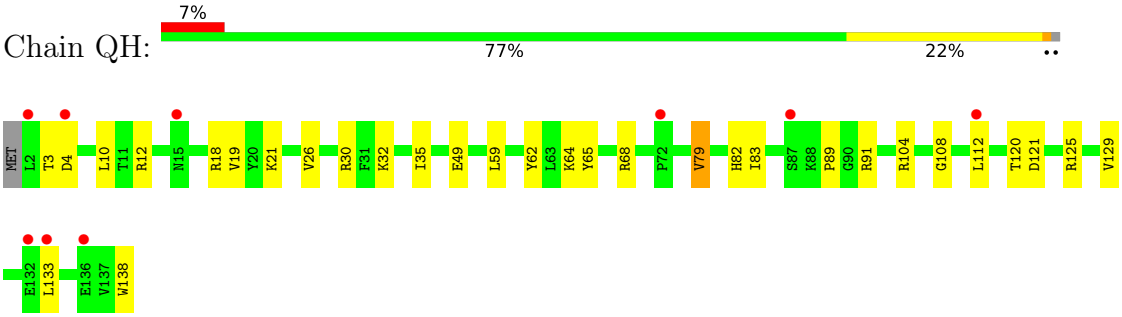
• Molecule 7: 30S ribosomal protein S7



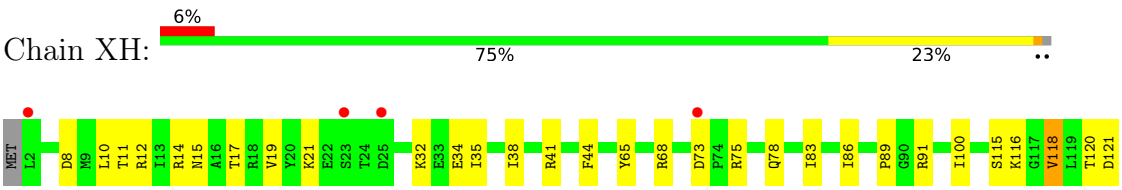
• Molecule 7: 30S ribosomal protein S7

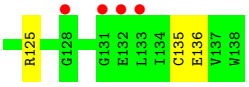


• Molecule 8: 30S ribosomal protein S8



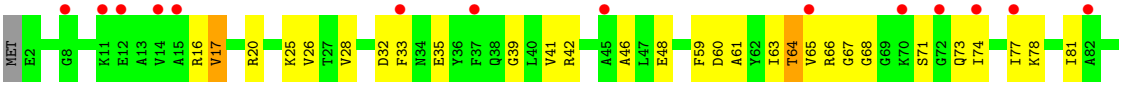
• Molecule 8: 30S ribosomal protein S8

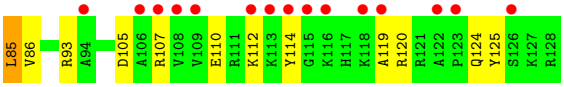




• Molecule 9: 30S ribosomal protein S9

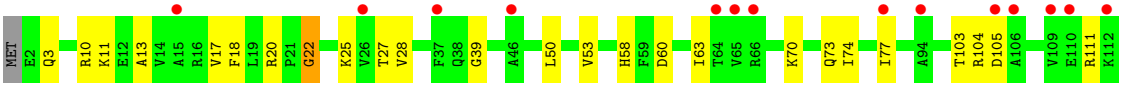
Chain QI:

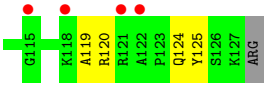




• Molecule 9: 30S ribosomal protein S9

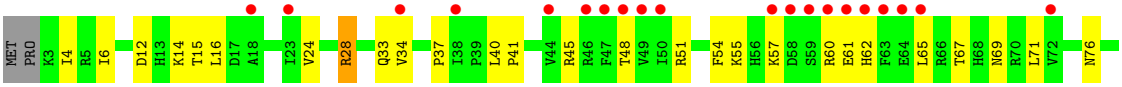
Chain XI:

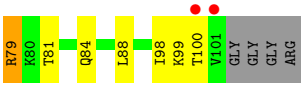




• Molecule 10: 30S ribosomal protein S10

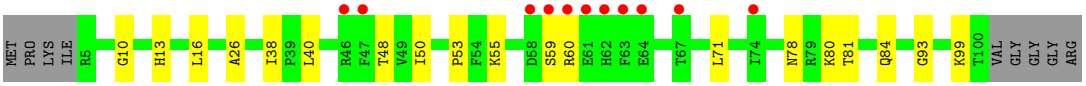
Chain QJ:





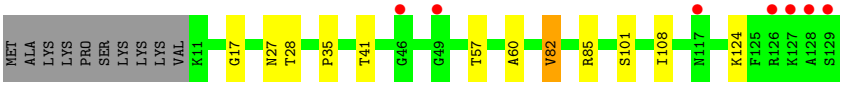
• Molecule 10: 30S ribosomal protein S10

Chain XJ:



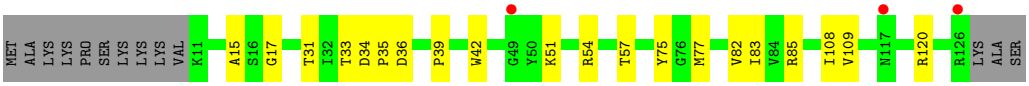
• Molecule 11: 30S ribosomal protein S11

Chain QK:



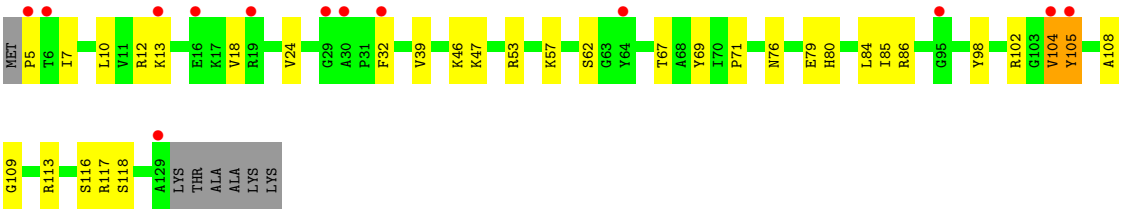
• Molecule 11: 30S ribosomal protein S11

Chain XK:



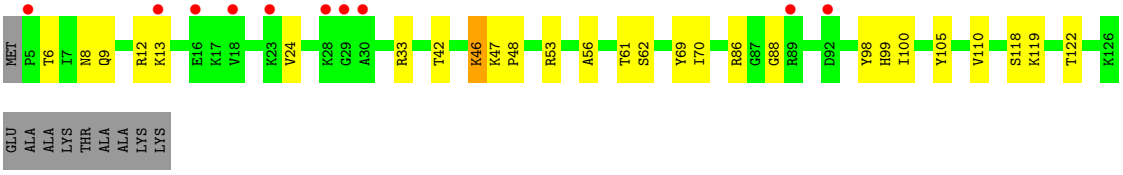
• Molecule 12: 30S ribosomal protein S12

Chain QL:



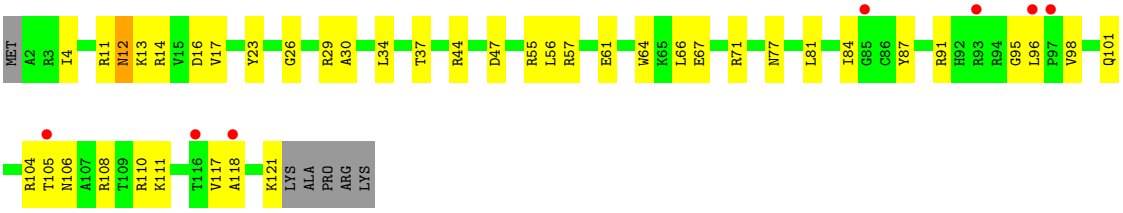
• Molecule 12: 30S ribosomal protein S12

Chain XL:



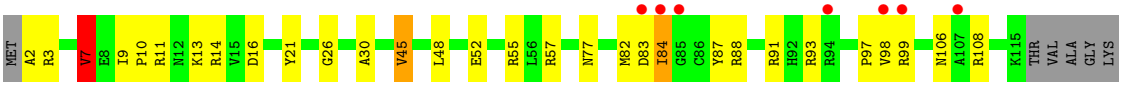
• Molecule 13: 30S ribosomal protein S13

Chain QM:



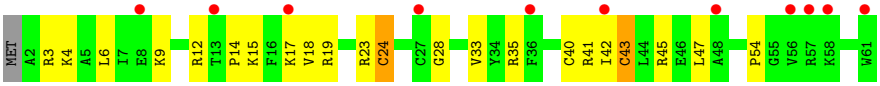
• Molecule 13: 30S ribosomal protein S13

Chain XM:



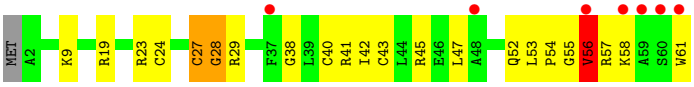
• Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:



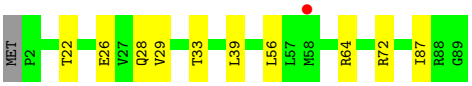
• Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:



• Molecule 15: 30S ribosomal protein S15

Chain QO:

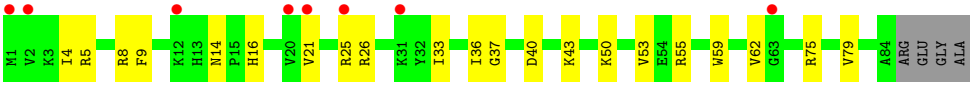


• Molecule 15: 30S ribosomal protein S15

Chain XO:

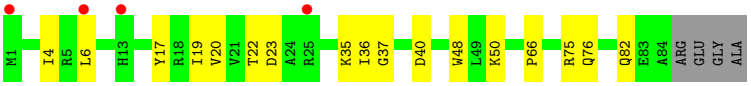
• Molecule 16: 30S ribosomal protein S16

Chain QP:



• Molecule 16: 30S ribosomal protein S16

Chain XP:

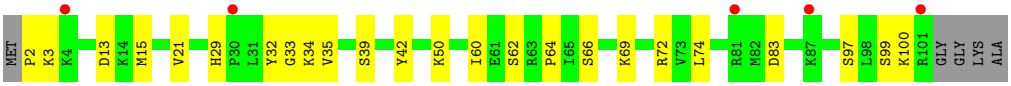


• Molecule 17: 30S ribosomal protein S17

Chain QQ:

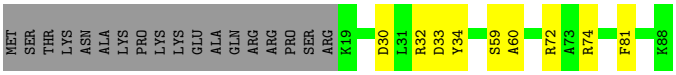
• Molecule 17: 30S ribosomal protein S17

Chain XQ:



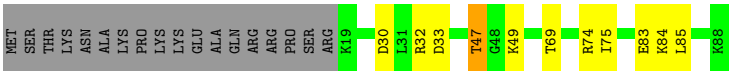
• Molecule 18: 30S ribosomal protein S18

Chain QR:



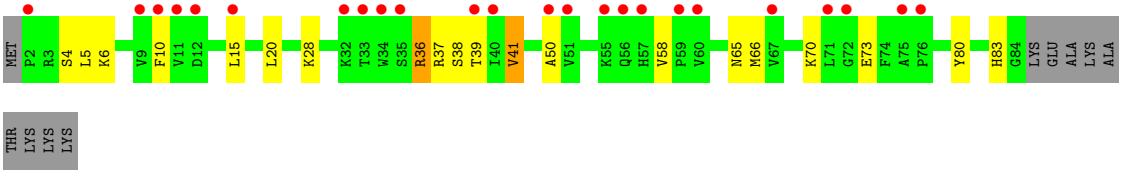
• Molecule 18: 30S ribosomal protein S18

Chain XR:



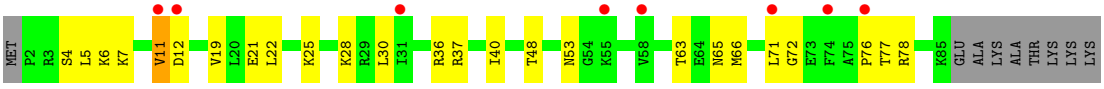
• Molecule 19: 30S ribosomal protein S19

Chain QS:



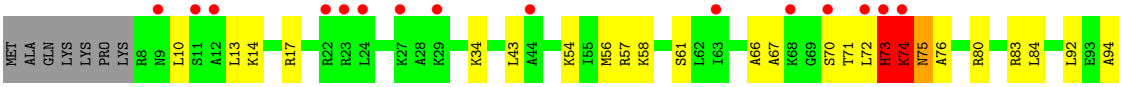
• Molecule 19: 30S ribosomal protein S19

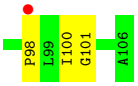
Chain XS:



• Molecule 20: 30S ribosomal protein S20

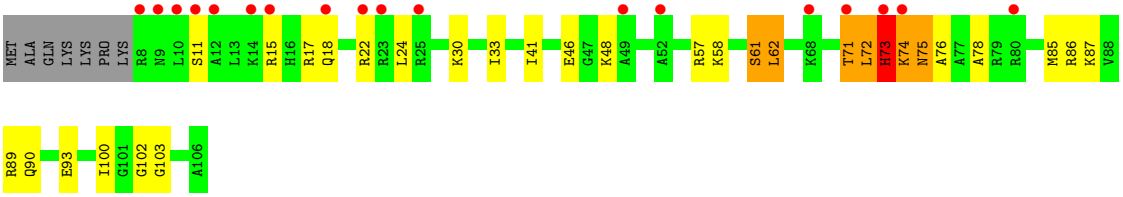
Chain QT:





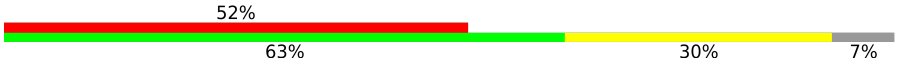
• Molecule 20: 30S ribosomal protein S20

Chain XT:



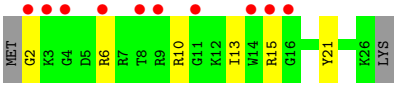
• Molecule 21: 30S ribosomal protein Thx

Chain QU:



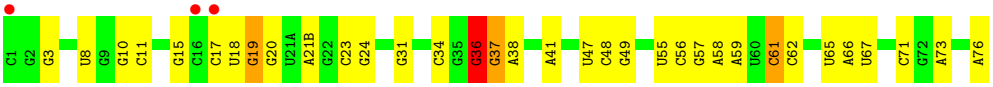
• Molecule 21: 30S ribosomal protein Thx

Chain XU:



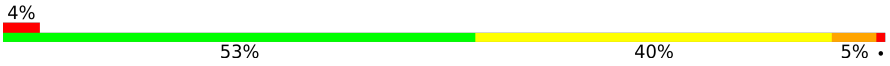
• Molecule 22: E-site tRNA-Pro

Chain QV:



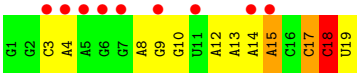
• Molecule 22: E-site tRNA-Pro

Chain XV:



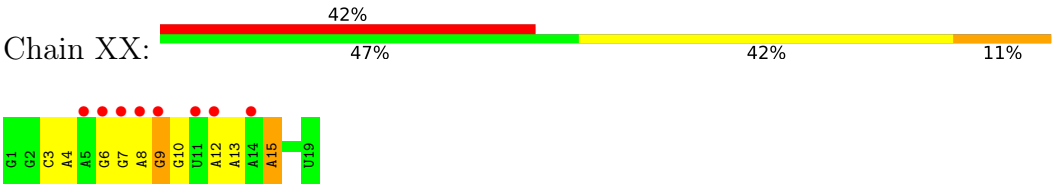
• Molecule 23: mRNA

Chain QX:



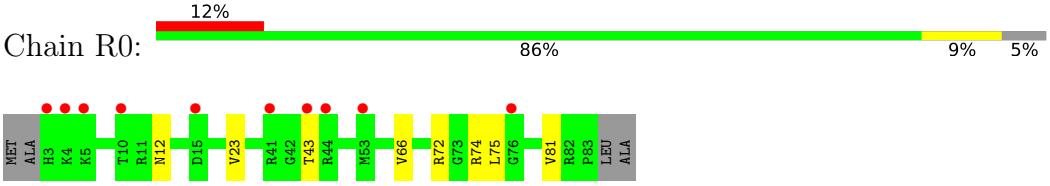
• Molecule 23: mRNA

Chain XX:



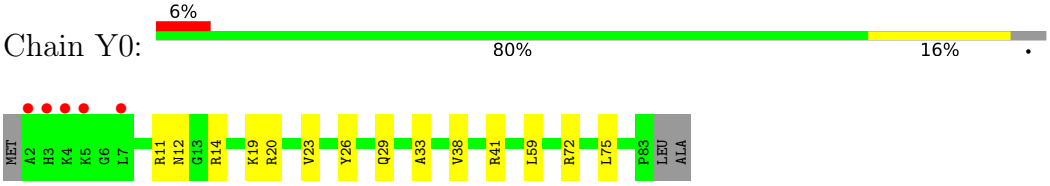
• Molecule 24: 50S ribosomal protein L27

Chain R0:



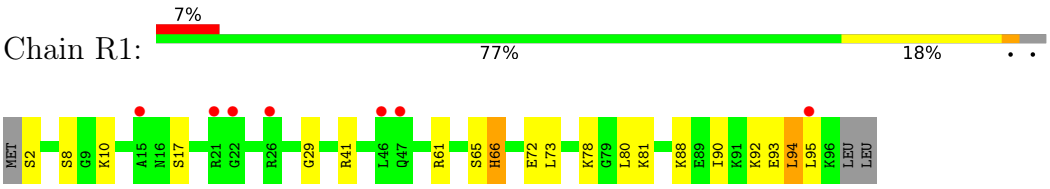
• Molecule 24: 50S ribosomal protein L27

Chain Y0:



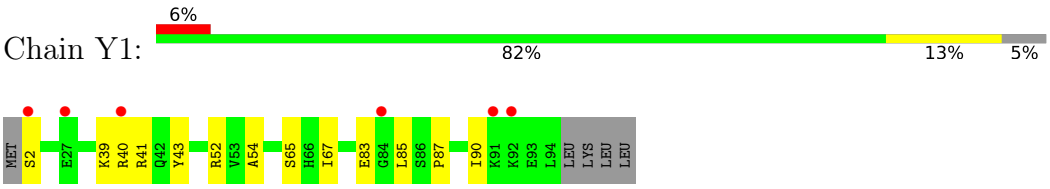
• Molecule 25: 50S ribosomal protein L28

Chain R1:



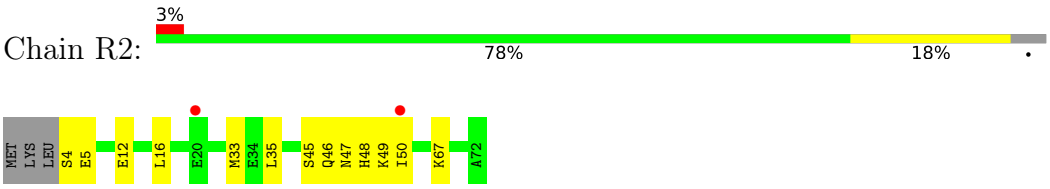
• Molecule 25: 50S ribosomal protein L28

Chain Y1:



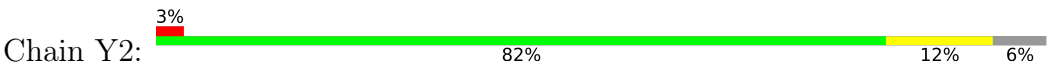
• Molecule 26: 50S ribosomal protein L29

Chain R2:



• Molecule 26: 50S ribosomal protein L29

Chain Y2:

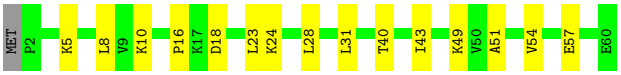


• Molecule 27: 50S ribosomal protein L30

Chain R3:

• Molecule 27: 50S ribosomal protein L30

Chain Y3:

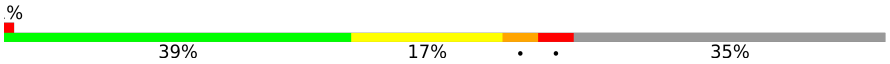


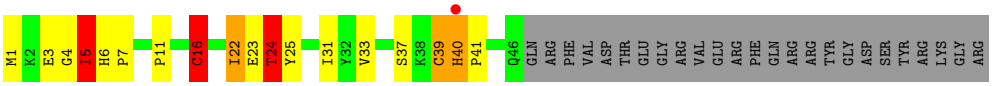
• Molecule 28: 50S ribosomal protein L31

Chain R4:

• Molecule 28: 50S ribosomal protein L31

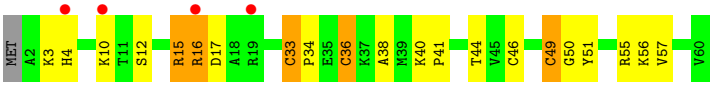
Chain Y4:





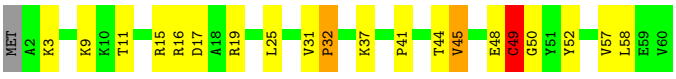
• Molecule 29: 50S ribosomal protein L32

Chain R5:



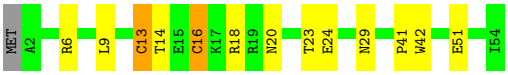
• Molecule 29: 50S ribosomal protein L32

Chain Y5:



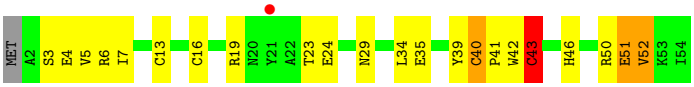
• Molecule 30: 50S ribosomal protein L33

Chain R6:



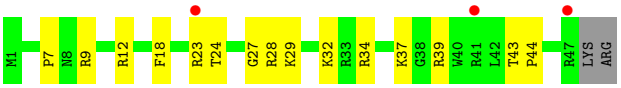
• Molecule 30: 50S ribosomal protein L33

Chain Y6:



• Molecule 31: 50S ribosomal protein L34

Chain R7:

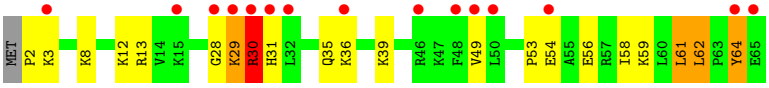


• Molecule 31: 50S ribosomal protein L34

Chain Y7:

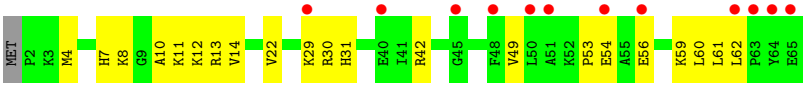
• Molecule 32: 50S ribosomal protein L35

Chain R8:



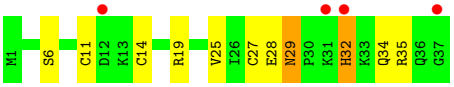
• Molecule 32: 50S ribosomal protein L35

Chain Y8:



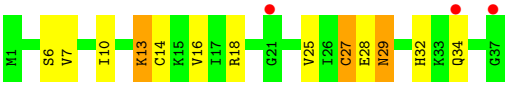
• Molecule 33: 50S ribosomal protein L36

Chain R9:



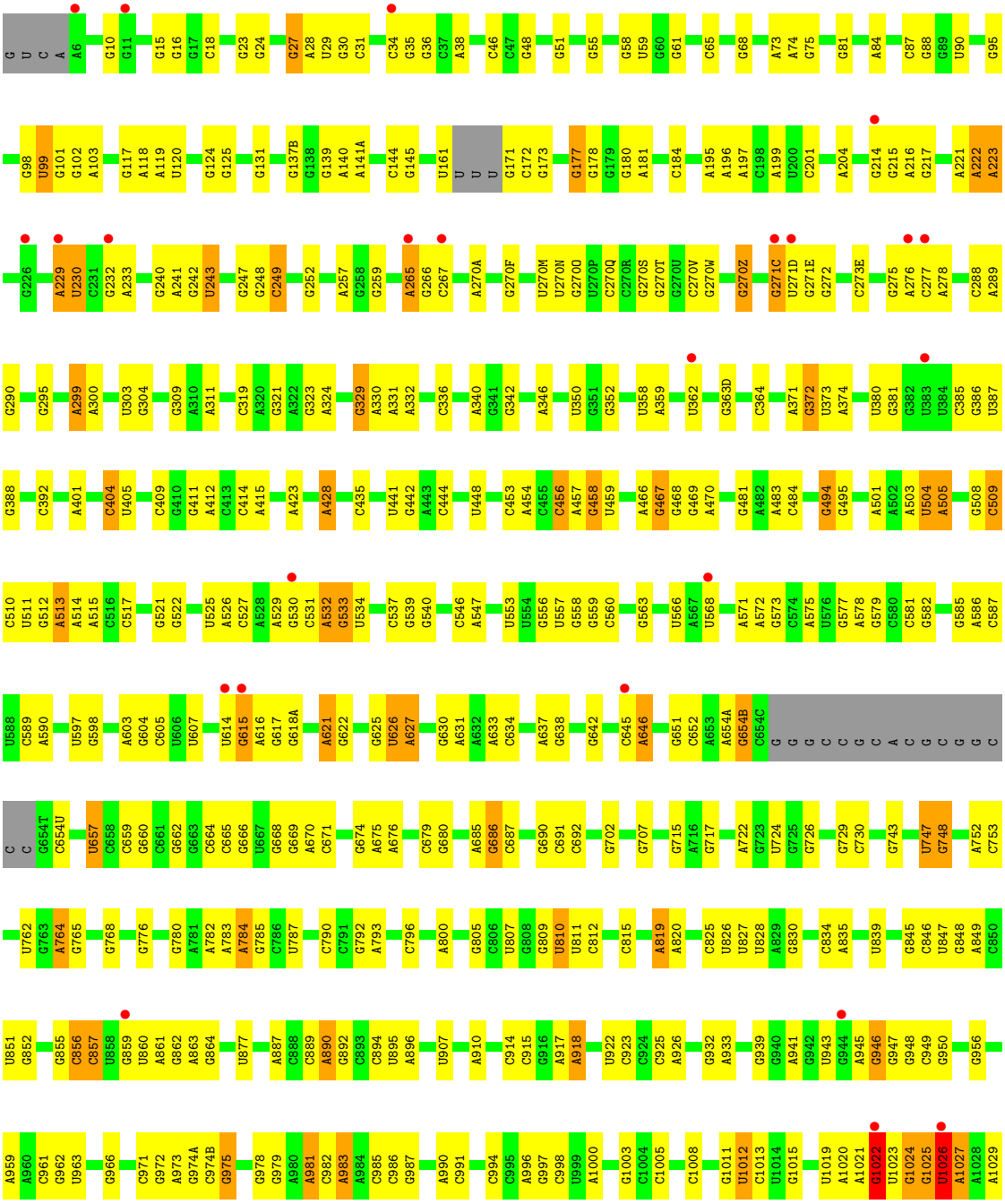
• Molecule 33: 50S ribosomal protein L36

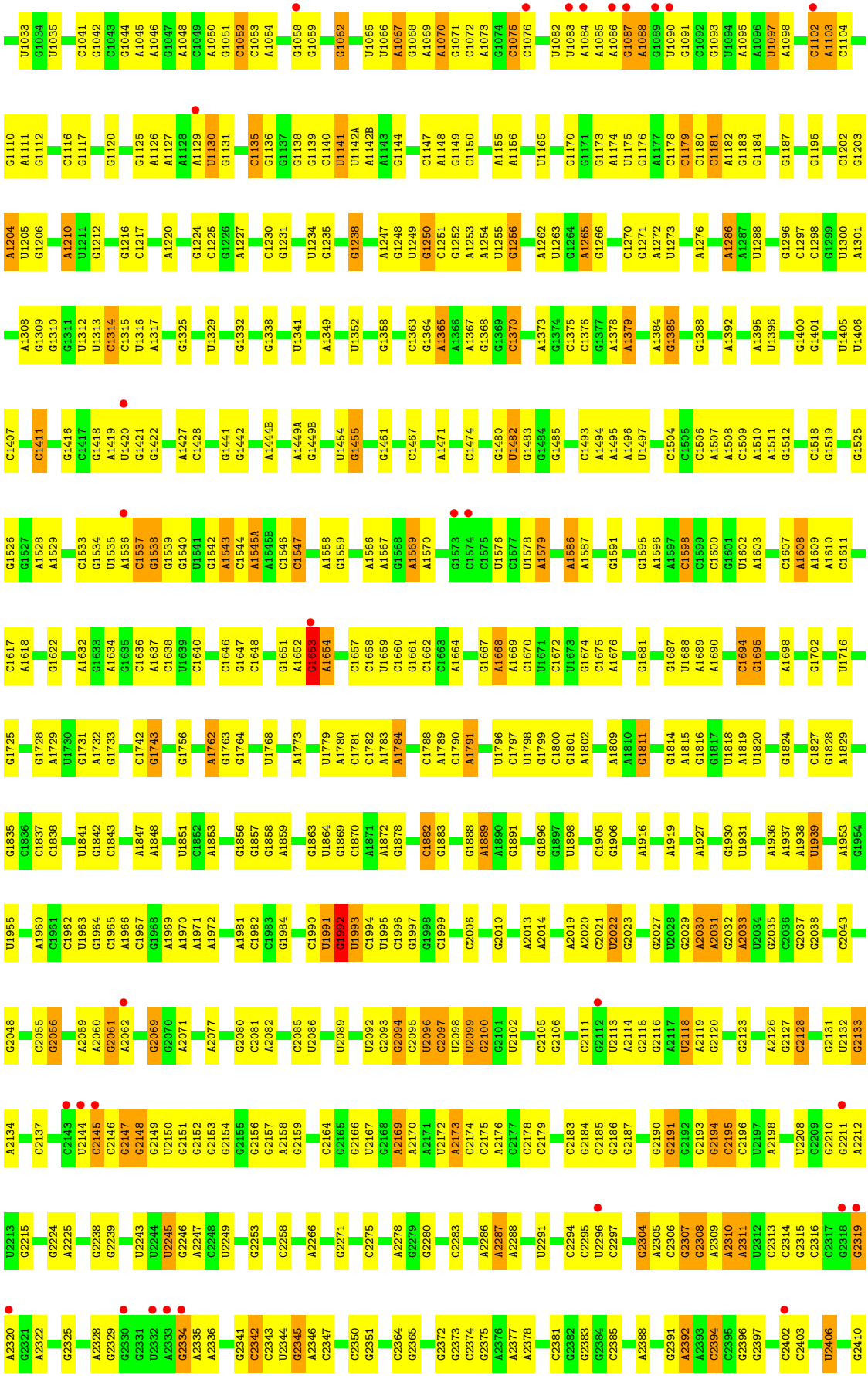
Chain Y9:

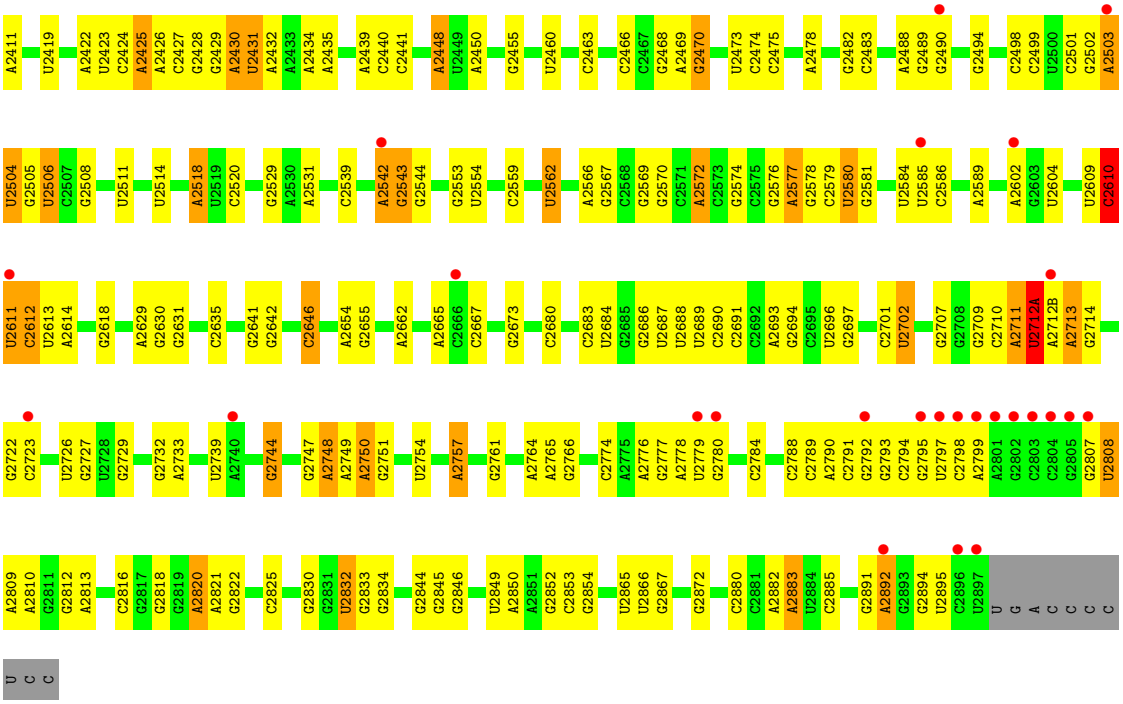


• Molecule 34: 23S rRNA

Chain RA:

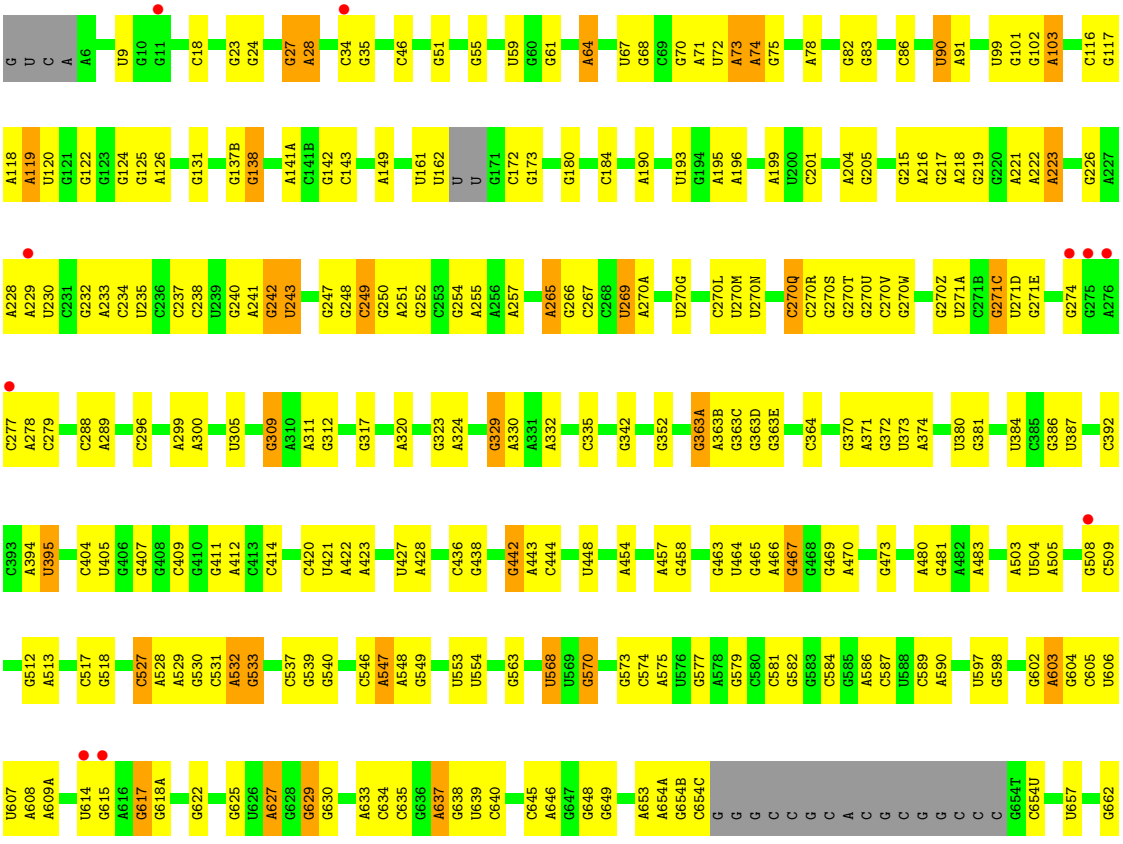


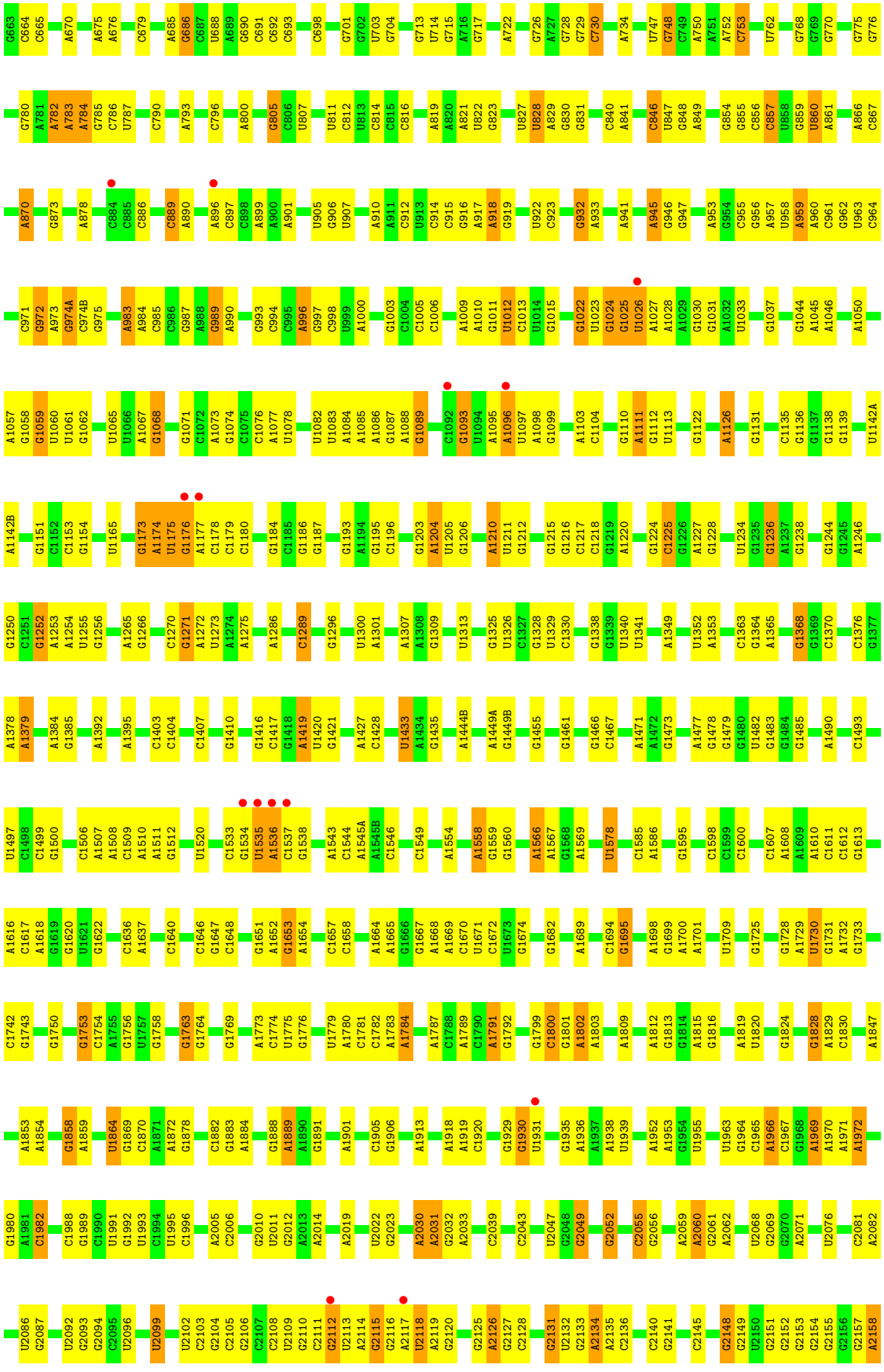


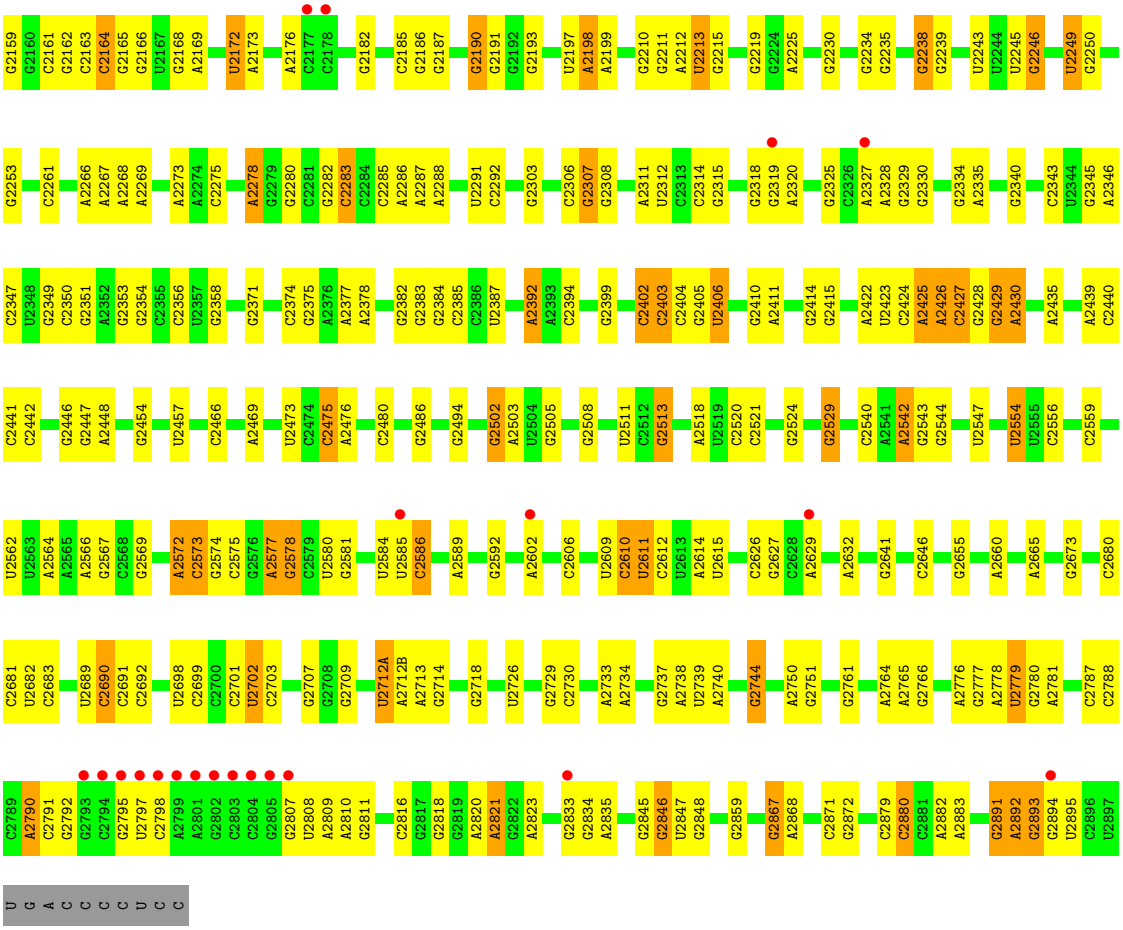


• Molecule 34: 23S rRNA

Chain YA:

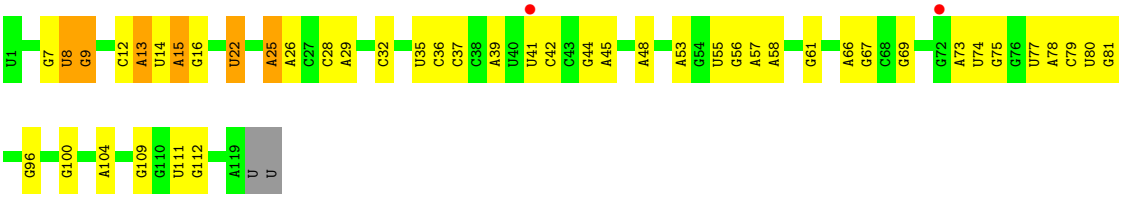






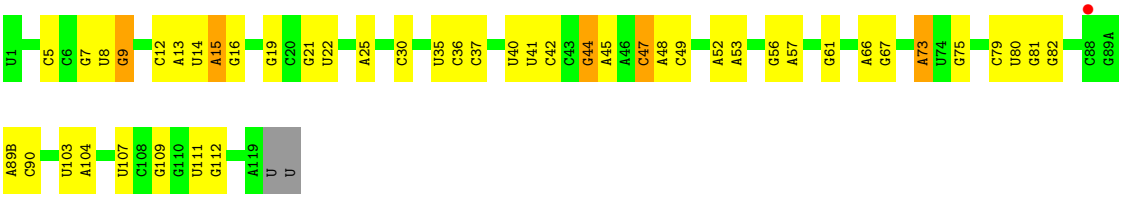
• Molecule 35: 5S rRNA

Chain RB:



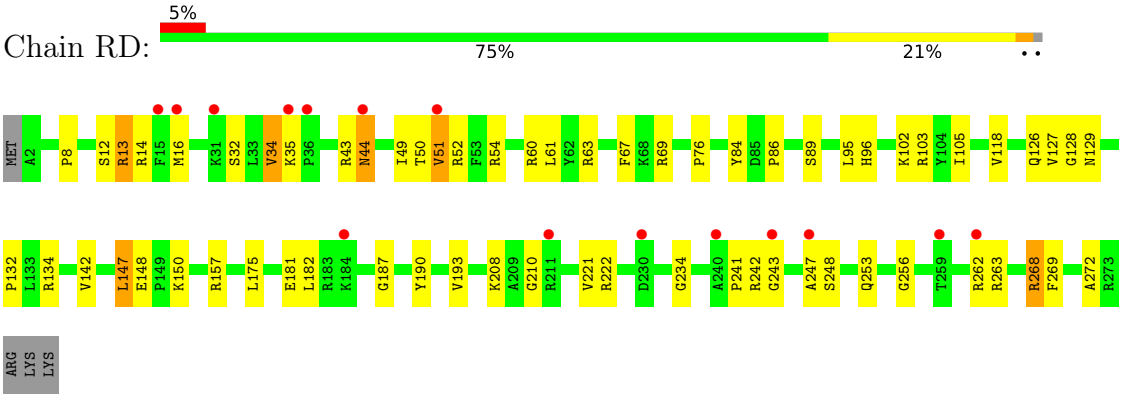
• Molecule 35: 5S rRNA

Chain YB:



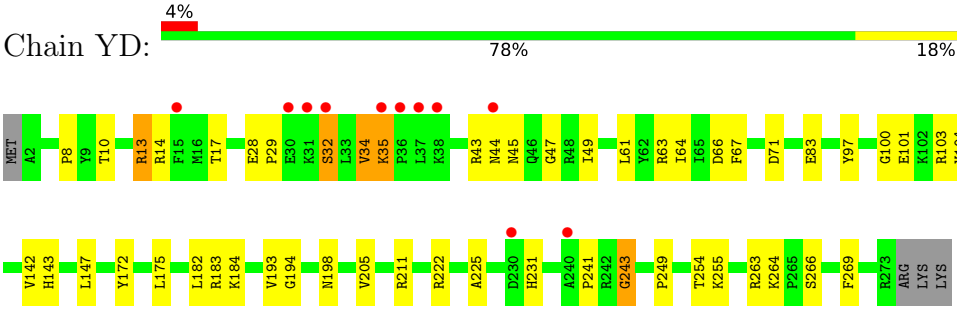
• Molecule 36: 50S ribosomal protein L2

Chain RD:



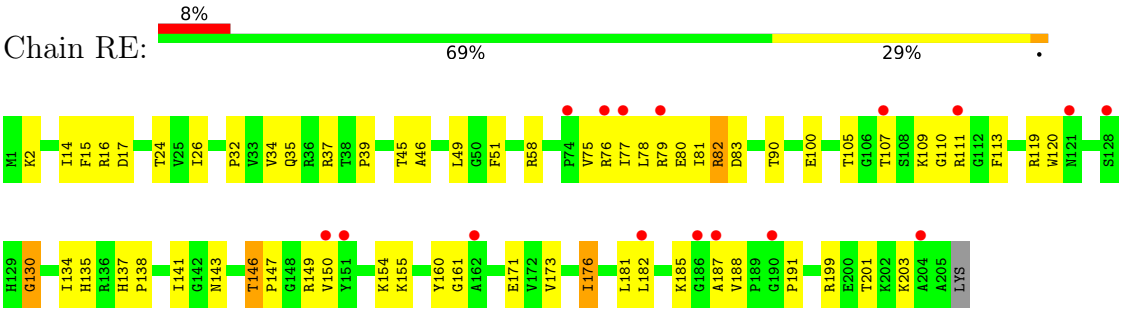
• Molecule 36: 50S ribosomal protein L2

Chain YD:



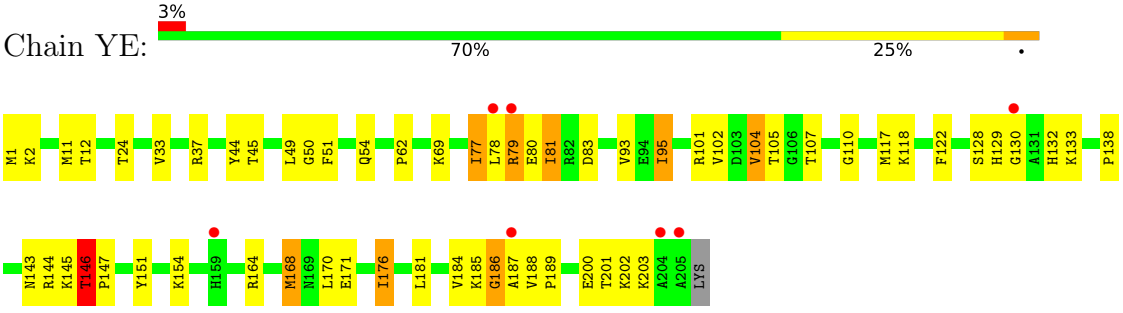
• Molecule 37: 50S ribosomal protein L3

Chain RE:



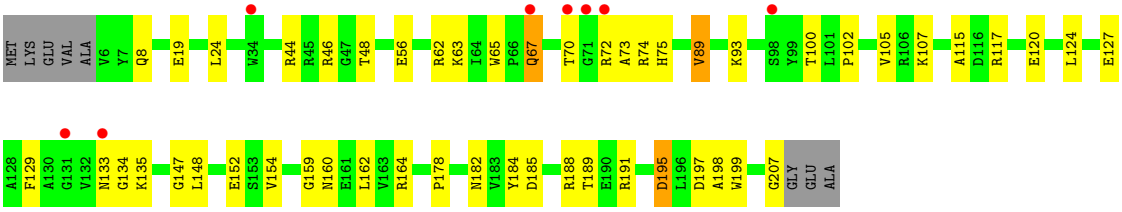
• Molecule 37: 50S ribosomal protein L3

Chain YE:

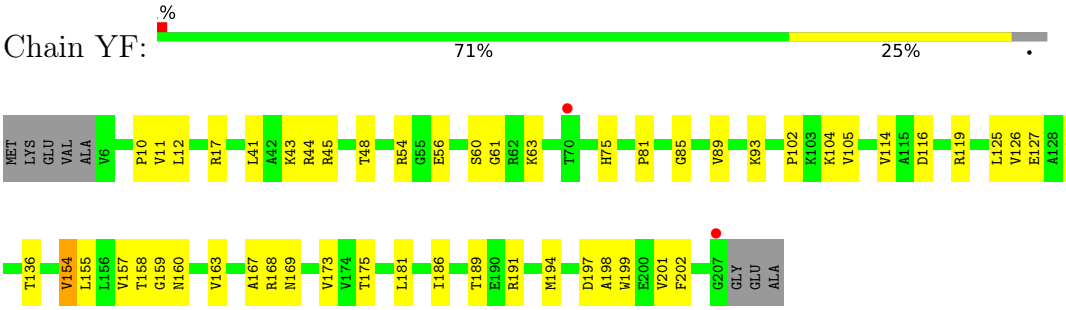


• Molecule 38: 50S ribosomal protein L4

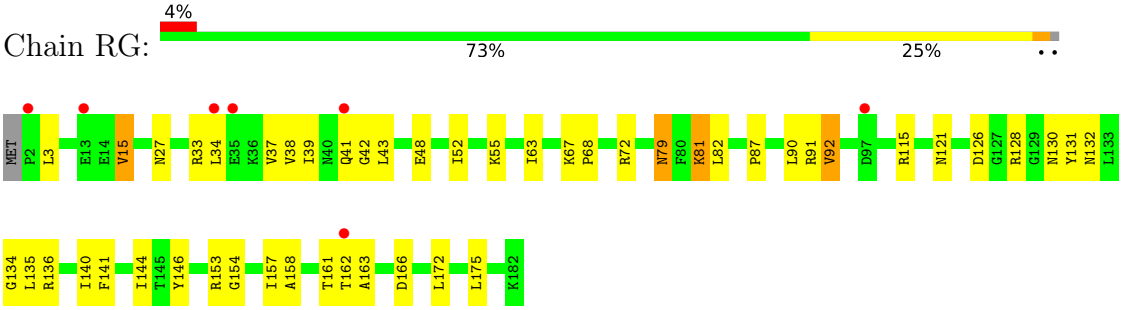
Chain RF:



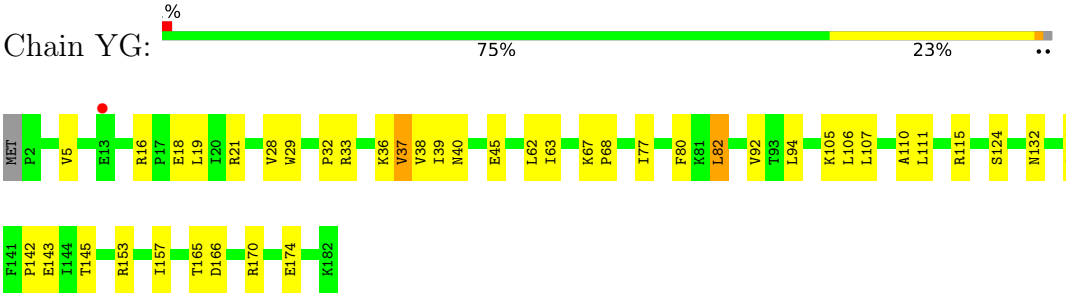
• Molecule 38: 50S ribosomal protein L4



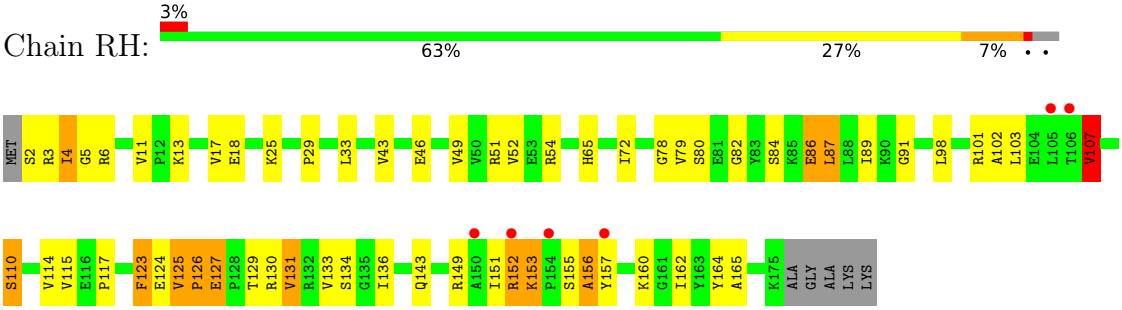
• Molecule 39: 50S ribosomal protein L5



• Molecule 39: 50S ribosomal protein L5

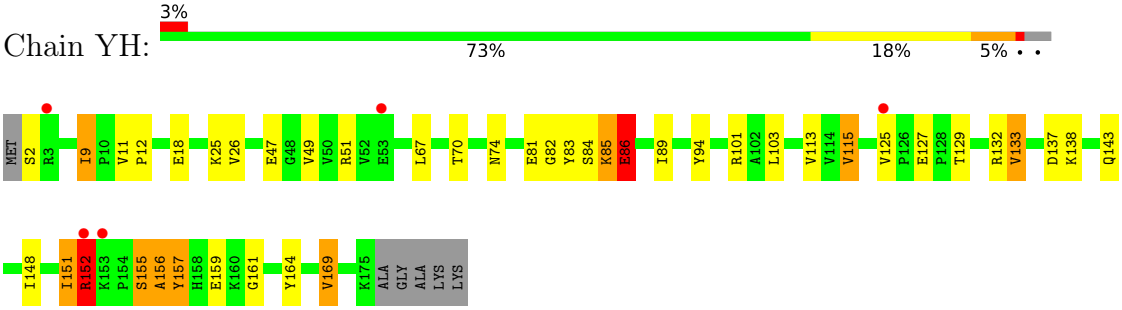


• Molecule 40: 50S ribosomal protein L6



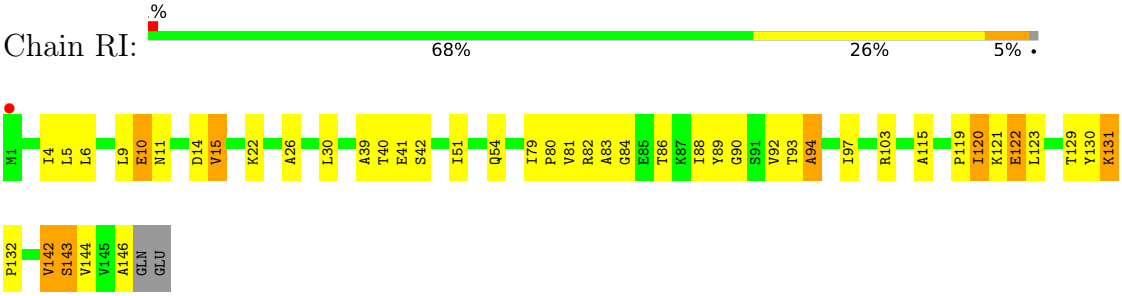
• Molecule 40: 50S ribosomal protein L6

Chain YH:



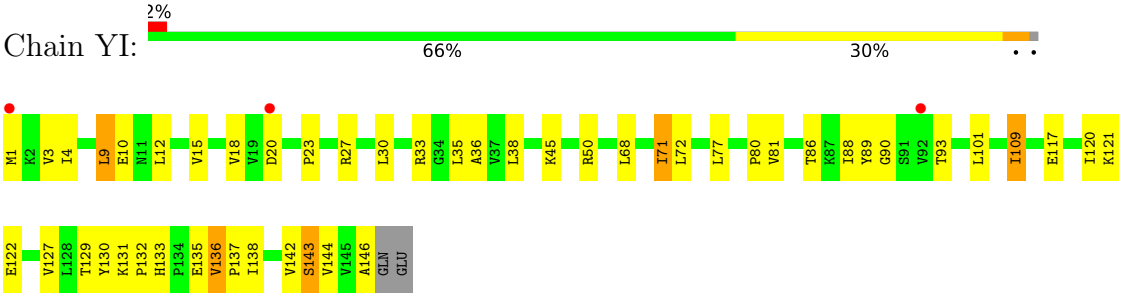
• Molecule 41: 50S ribosomal protein L9

Chain RI:



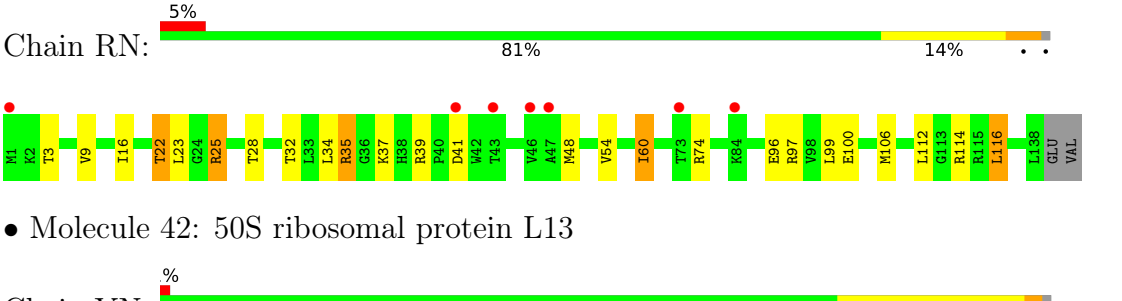
• Molecule 41: 50S ribosomal protein L9

Chain YI:



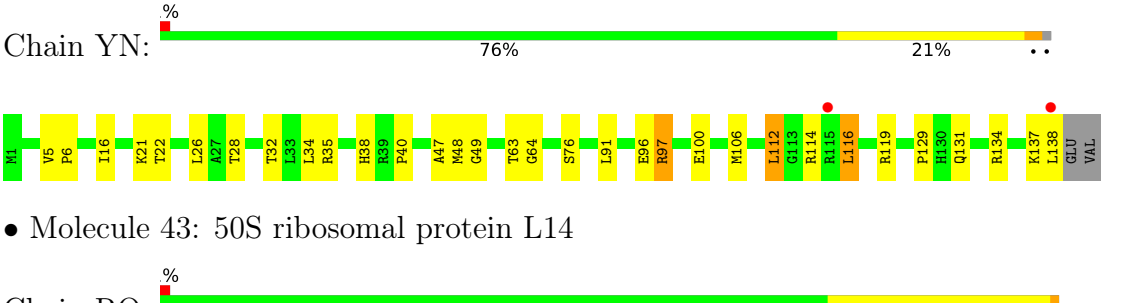
• Molecule 42: 50S ribosomal protein L13

Chain RN:



• Molecule 42: 50S ribosomal protein L13

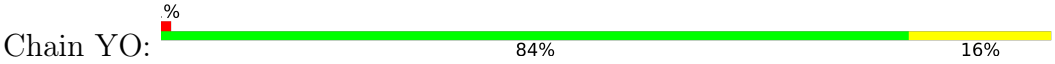
Chain YN:

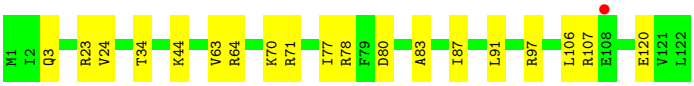


• Molecule 43: 50S ribosomal protein L14

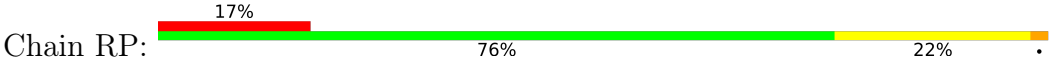
Chain RO:

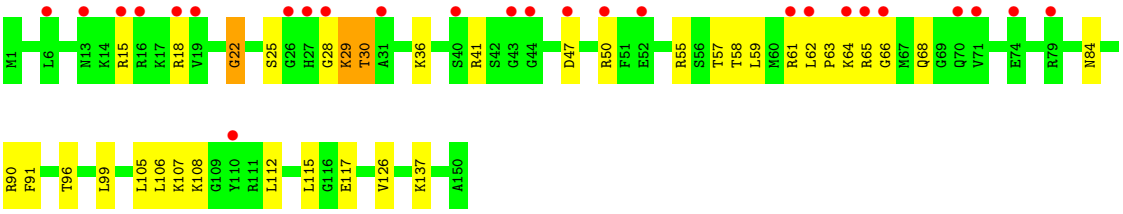
• Molecule 43: 50S ribosomal protein L14



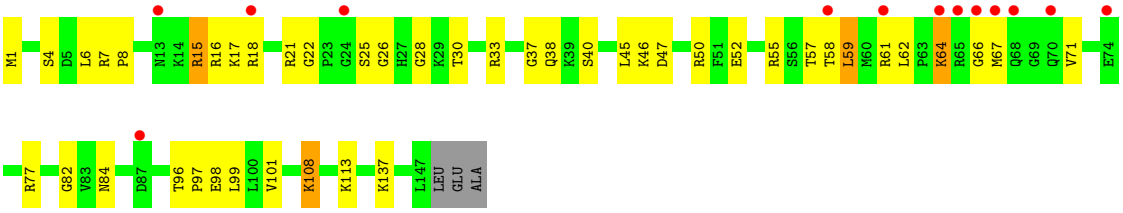


• Molecule 44: 50S ribosomal protein L15

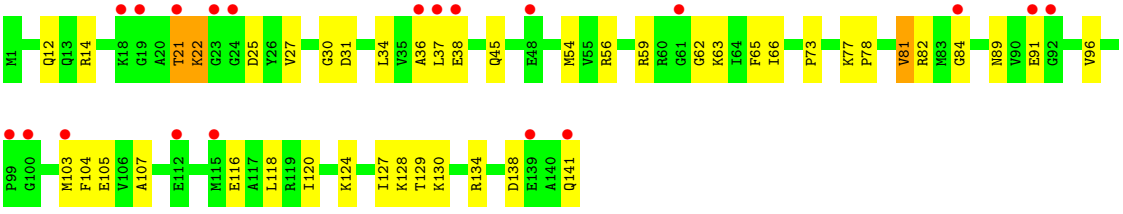




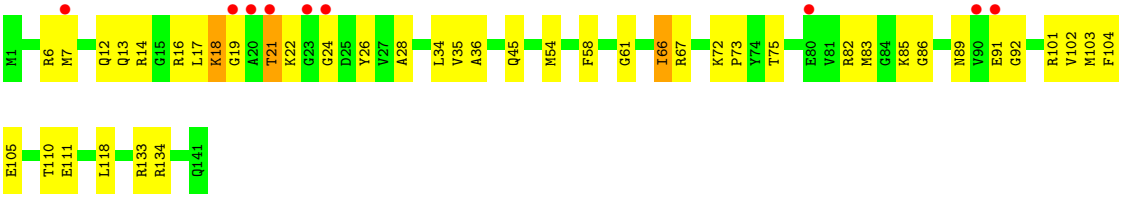
• Molecule 44: 50S ribosomal protein L15



• Molecule 45: 50S ribosomal protein L16

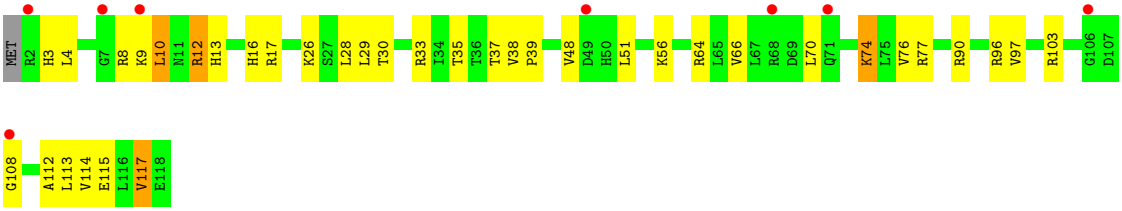


• Molecule 45: 50S ribosomal protein L16



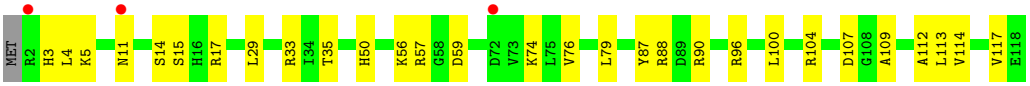
• Molecule 46: 50S ribosomal protein L17

Chain RR:



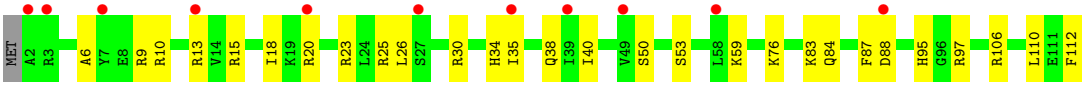
• Molecule 46: 50S ribosomal protein L17

Chain YR:



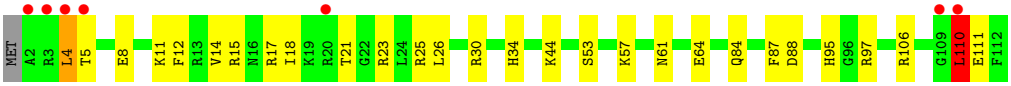
• Molecule 47: 50S ribosomal protein L18

Chain RS:



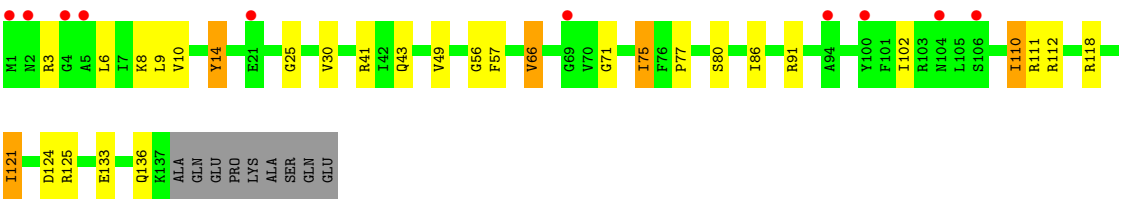
• Molecule 47: 50S ribosomal protein L18

Chain YS:



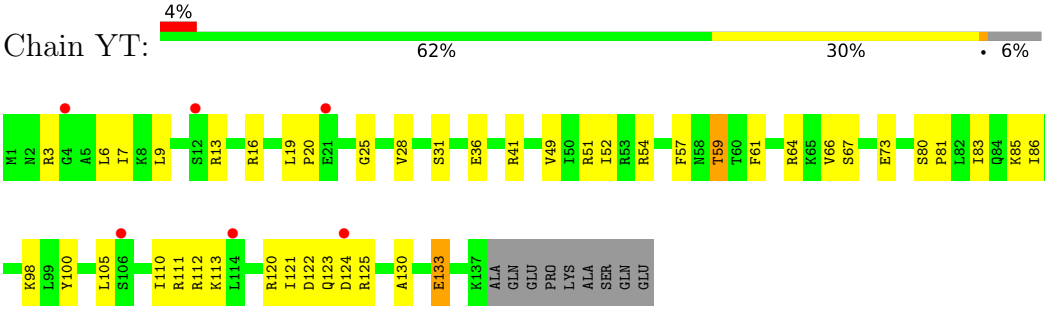
• Molecule 48: 50S ribosomal protein L19

Chain RT:



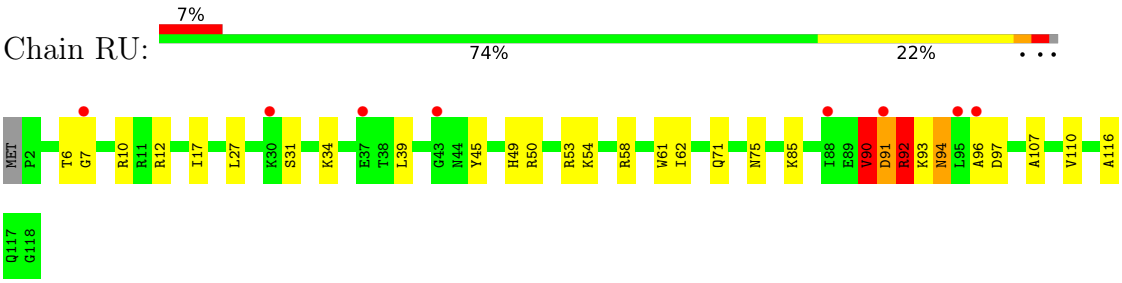
• Molecule 48: 50S ribosomal protein L19

Chain YT:



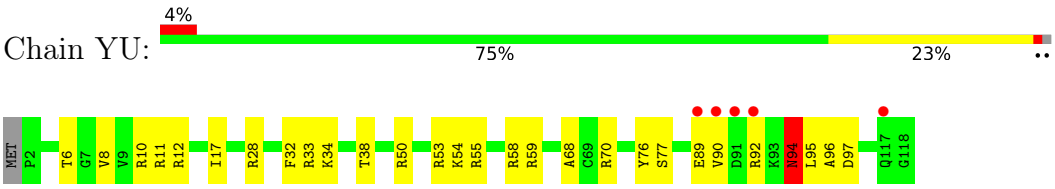
• Molecule 49: 50S ribosomal protein L20

Chain RU:



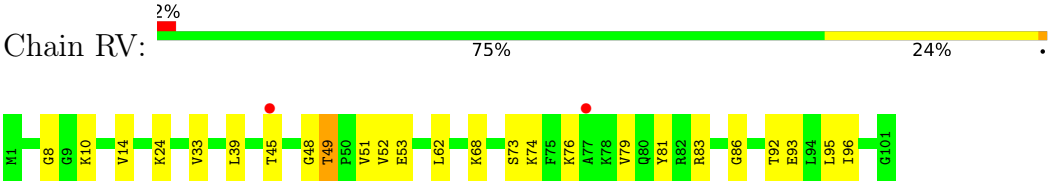
• Molecule 49: 50S ribosomal protein L20

Chain YU:



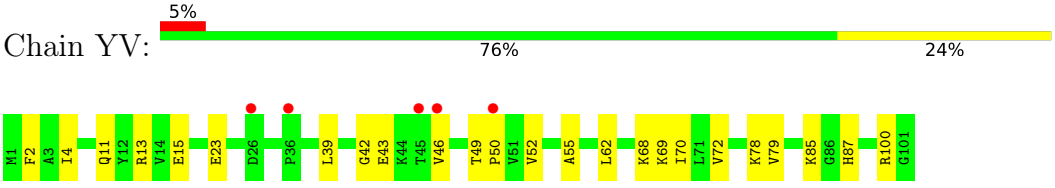
• Molecule 50: 50S ribosomal protein L21

Chain RV:



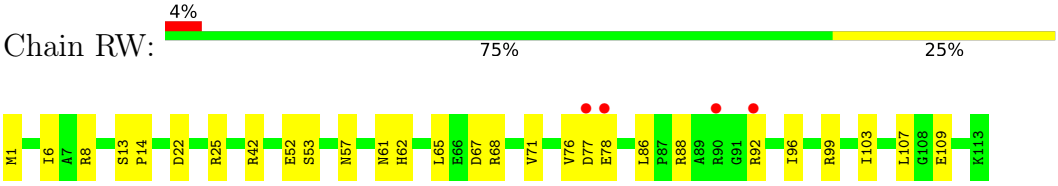
• Molecule 50: 50S ribosomal protein L21

Chain YV:



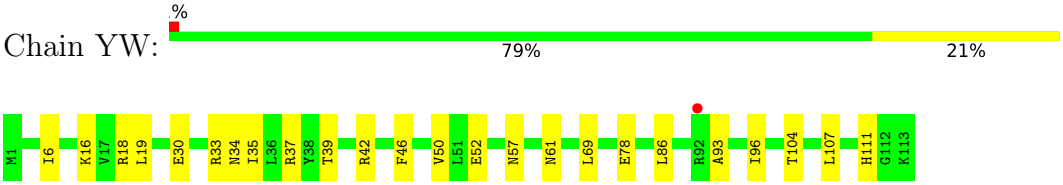
• Molecule 51: 50S ribosomal protein L22

Chain RW:



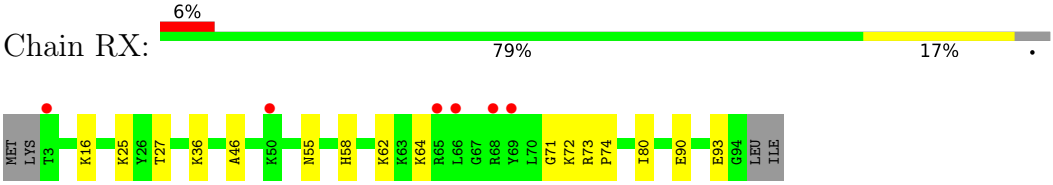
• Molecule 51: 50S ribosomal protein L22

Chain YW:



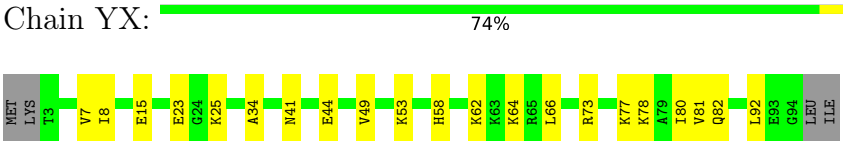
• Molecule 52: 50S ribosomal protein L23

Chain RX:



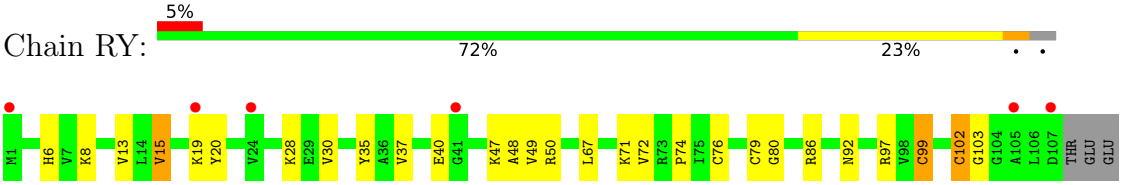
• Molecule 52: 50S ribosomal protein L23

Chain YX:



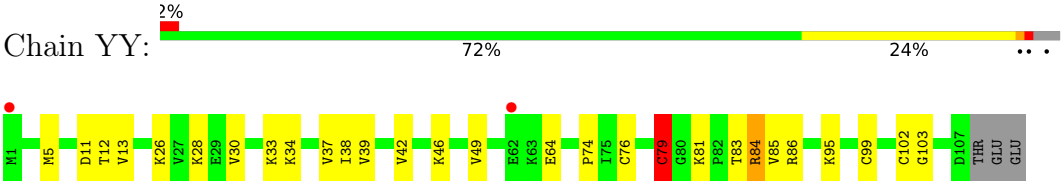
• Molecule 53: 50S ribosomal protein L24

Chain RY:



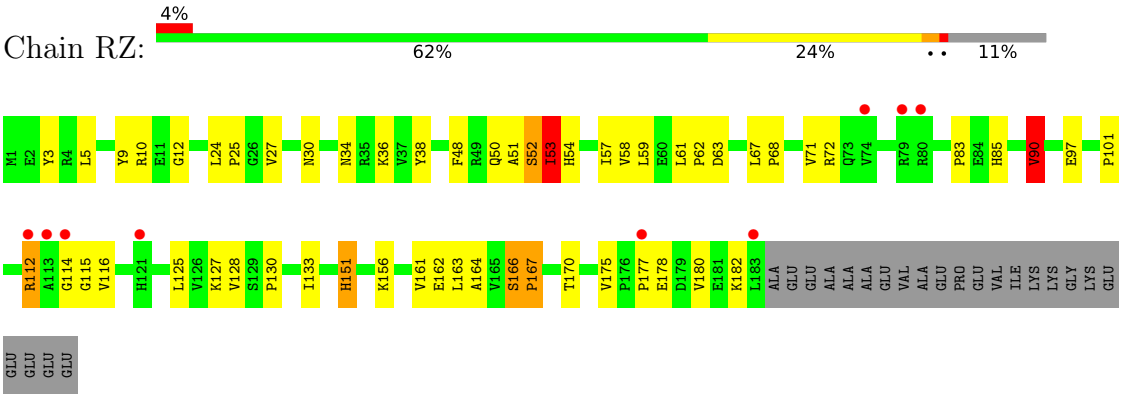
• Molecule 53: 50S ribosomal protein L24

Chain YY:



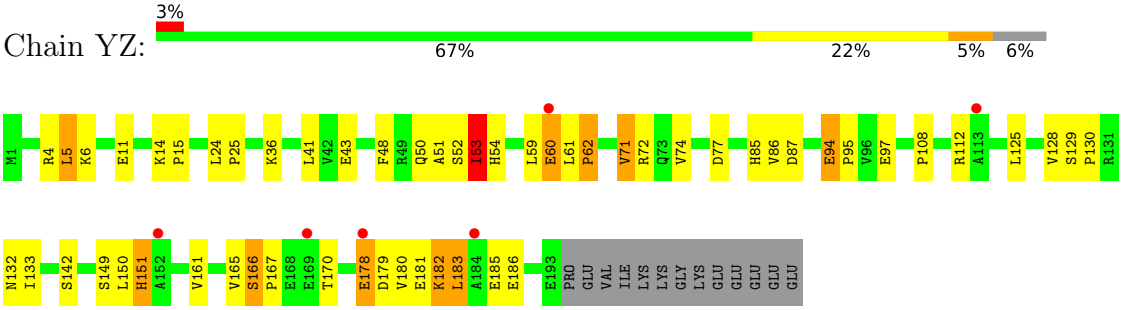
• Molecule 54: 50S ribosomal protein L25

Chain RZ:



• Molecule 54: 50S ribosomal protein L25

Chain YZ:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.74Å 450.26Å 626.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.94 – 3.50 49.94 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.94-3.50) 97.5 (49.94-3.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.240 , 0.258 0.240 , 0.258	Depositor DCC
R_{free} test set	40067 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å^2)	75.0	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 74.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	292039	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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: SF4, MG, 1MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	QA	0.36	0/36343	0.44	2/56720 (0.0%)
1	XA	0.39	0/36435	0.45	5/56865 (0.0%)
2	QB	0.33	0/1942	0.98	12/2619 (0.5%)
2	XB	0.33	0/1950	0.93	7/2630 (0.3%)
3	QC	0.32	0/1629	0.94	7/2195 (0.3%)
3	XC	0.31	0/1629	0.86	3/2195 (0.1%)
4	QD	0.39	0/1733	0.98	6/2318 (0.3%)
4	XD	0.43	1/1733 (0.1%)	0.96	6/2318 (0.3%)
5	QE	0.35	0/1171	0.96	11/1576 (0.7%)
5	XE	0.43	1/1171 (0.1%)	0.84	4/1576 (0.3%)
6	QF	0.34	0/856	0.94	6/1154 (0.5%)
6	XF	0.35	0/856	0.81	2/1154 (0.2%)
7	QG	0.32	0/1276	0.93	2/1709 (0.1%)
7	XG	0.31	0/1276	0.83	3/1709 (0.2%)
8	QH	0.37	0/1128	0.90	2/1517 (0.1%)
8	XH	0.40	0/1128	0.93	2/1517 (0.1%)
9	QI	0.43	1/1029 (0.1%)	1.10	10/1379 (0.7%)
9	XI	0.33	0/1017	0.99	5/1365 (0.4%)
10	QJ	0.34	0/814	1.01	4/1095 (0.4%)
10	XJ	0.32	0/790	0.86	1/1063 (0.1%)
11	QK	0.33	0/900	0.81	0/1213
11	XK	0.36	0/879	0.84	4/1187 (0.3%)
12	QL	0.38	0/991	1.00	5/1327 (0.4%)
12	XL	0.43	0/972	1.08	6/1301 (0.5%)
13	QM	0.33	0/965	1.12	10/1292 (0.8%)
13	XM	0.32	0/924	0.98	3/1238 (0.2%)
14	QN	0.55	1/501 (0.2%)	1.14	7/664 (1.1%)
14	XN	0.57	1/501 (0.2%)	1.20	5/664 (0.8%)
15	QO	0.35	0/745	0.77	0/992
15	XO	0.36	0/740	0.75	0/987
16	QP	0.38	0/721	0.92	4/970 (0.4%)
16	XP	0.34	0/721	0.92	1/970 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	QQ	0.33	0/847	0.87	3/1131 (0.3%)
17	XQ	0.46	0/847	0.93	3/1131 (0.3%)
18	QR	0.35	0/579	0.81	0/768
18	XR	0.36	0/579	0.77	1/768 (0.1%)
19	QS	0.32	0/680	1.05	6/915 (0.7%)
19	XS	0.33	0/689	1.00	3/926 (0.3%)
20	QT	1.05	3/765 (0.4%)	1.53	12/1007 (1.2%)
20	XT	0.37	0/765	1.14	10/1007 (1.0%)
21	QU	0.29	0/221	0.75	0/288
21	XU	0.30	0/221	0.77	1/288 (0.3%)
22	QV	0.39	0/1813	0.54	2/2825 (0.1%)
22	XV	0.35	0/1813	0.46	0/2825
23	QX	0.52	0/459	0.93	2/715 (0.3%)
23	XX	0.30	0/459	0.48	0/715
24	R0	0.38	0/652	0.83	0/867
24	Y0	0.58	0/657	0.86	0/874
25	R1	0.58	0/753	0.99	6/1000 (0.6%)
25	Y1	0.60	1/736 (0.1%)	1.03	1/978 (0.1%)
26	R2	0.35	0/583	0.94	2/771 (0.3%)
26	Y2	0.47	0/577	0.89	1/764 (0.1%)
27	R3	0.38	0/474	0.93	0/635
27	Y3	0.65	1/474 (0.2%)	0.85	1/635 (0.2%)
28	R4	0.25	0/357	0.85	0/483
28	Y4	2.19	2/366 (0.5%)	2.02	17/495 (3.4%)
29	R5	0.88	2/473 (0.4%)	1.26	7/639 (1.1%)
29	Y5	1.10	1/473 (0.2%)	1.33	4/639 (0.6%)
30	R6	0.69	2/460 (0.4%)	0.94	2/613 (0.3%)
30	Y6	1.20	7/460 (1.5%)	1.55	9/613 (1.5%)
31	R7	0.55	0/417	0.89	1/550 (0.2%)
31	Y7	0.64	0/426	0.83	0/561
32	R8	0.47	0/525	1.19	8/691 (1.2%)
32	Y8	0.61	0/525	1.19	5/691 (0.7%)
33	R9	0.86	1/310 (0.3%)	1.33	3/407 (0.7%)
33	Y9	0.63	0/310	1.01	2/407 (0.5%)
34	RA	0.47	0/69520	0.51	16/108527 (0.0%)
34	YA	0.65	0/69543	0.55	7/108563 (0.0%)
35	RB	0.36	0/2878	0.43	0/4490
35	YB	0.55	0/2878	0.52	0/4490
36	RD	0.52	0/2165	0.99	9/2919 (0.3%)
36	YD	0.63	0/2165	1.03	12/2919 (0.4%)
37	RE	0.50	0/1601	1.44	13/2160 (0.6%)
37	YE	0.63	0/1601	1.50	16/2160 (0.7%)
38	RF	0.45	0/1620	1.00	10/2194 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	YF	0.61	0/1620	0.96	8/2194 (0.4%)
39	RG	0.36	0/1499	1.01	9/2016 (0.4%)
39	YG	0.42	0/1499	0.97	7/2016 (0.3%)
40	RH	0.41	0/1362	1.19	15/1841 (0.8%)
40	YH	0.59	0/1362	1.22	19/1841 (1.0%)
41	RI	0.60	2/1151 (0.2%)	1.25	19/1558 (1.2%)
41	YI	0.48	1/1151 (0.1%)	1.10	10/1558 (0.6%)
42	RN	0.44	0/1131	0.99	5/1525 (0.3%)
42	YN	0.62	0/1131	1.05	7/1525 (0.5%)
43	RO	0.46	0/943	0.87	1/1269 (0.1%)
43	YO	0.59	0/943	0.86	0/1269
44	RP	0.47	0/1162	1.05	6/1544 (0.4%)
44	YP	0.58	0/1139	1.19	10/1514 (0.7%)
45	RQ	0.42	0/1143	1.00	9/1527 (0.6%)
45	YQ	0.56	0/1143	1.09	8/1527 (0.5%)
46	RR	0.50	0/974	1.00	6/1302 (0.5%)
46	YR	0.58	0/974	1.01	2/1302 (0.2%)
47	RS	0.37	0/892	0.94	1/1187 (0.1%)
47	YS	0.50	0/892	0.98	4/1187 (0.3%)
48	RT	0.41	0/1155	1.09	8/1542 (0.5%)
48	YT	0.51	0/1155	1.06	9/1542 (0.6%)
49	RU	0.45	0/982	0.99	6/1306 (0.5%)
49	YU	0.65	0/982	0.95	6/1306 (0.5%)
50	RV	0.44	0/790	1.08	8/1057 (0.8%)
50	YV	0.61	0/790	1.01	4/1057 (0.4%)
51	RW	0.50	0/911	0.88	1/1220 (0.1%)
51	YW	0.64	0/911	0.87	2/1220 (0.2%)
52	RX	0.48	0/739	0.84	1/993 (0.1%)
52	YX	0.61	0/739	0.95	2/993 (0.2%)
53	RY	0.51	1/831 (0.1%)	0.93	1/1108 (0.1%)
53	YY	0.61	1/831 (0.1%)	0.99	6/1108 (0.5%)
54	RZ	0.42	0/1493	1.55	18/2026 (0.9%)
54	YZ	0.50	0/1561	1.46	14/2119 (0.7%)
All	All	0.50	30/316163 (0.0%)	0.69	572/472822 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
28	Y4	1	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
37	RE	0	1
37	YE	0	1
50	RV	0	2
54	RZ	0	1
54	YZ	0	1
All	All	1	7

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y4	5	ILE	CA-CB	-36.42	1.04	1.54
20	QT	73	HIS	N-CA	-19.14	1.21	1.46
28	Y4	4	GLY	N-CA	-18.88	1.18	1.45
20	QT	74	LYS	CA-CB	-17.57	1.23	1.53
29	Y5	32	PRO	N-CA	17.50	1.69	1.47

The worst 5 of 572 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	YE	146	THR	CA-C-N	33.70	161.97	119.84
37	YE	146	THR	C-N-CA	33.70	161.97	119.84
54	RZ	166	SER	CA-C-N	32.44	160.39	119.84
54	RZ	166	SER	C-N-CA	32.44	160.39	119.84
54	YZ	166	SER	CA-C-N	30.31	157.72	119.84

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	Y4	5	ILE	CA

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
37	RE	146	THR	Peptide
50	RV	49	THR	Peptide,Mainchain
54	RZ	166	SER	Peptide
28	Y4	5	ILE	Mainchain
37	YE	146	THR	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	32469	0	16393	392	0
1	XA	32551	0	16433	387	1
2	QB	1907	0	1958	39	0
2	XB	1915	0	1969	39	0
3	QC	1605	0	1668	31	0
3	XC	1605	0	1668	21	0
4	QD	1703	0	1763	56	0
4	XD	1703	0	1763	48	0
5	QE	1155	0	1213	22	0
5	XE	1155	0	1213	22	0
6	QF	843	0	857	11	0
6	XF	843	0	857	12	0
7	QG	1257	0	1296	26	0
7	XG	1257	0	1296	24	0
8	QH	1108	0	1165	23	0
8	XH	1108	0	1165	24	0
9	QI	1010	0	1037	22	0
9	XI	998	0	1024	21	0
10	QJ	801	0	849	22	0
10	XJ	777	0	816	14	0
11	QK	885	0	904	7	0
11	XK	864	0	881	12	0
12	QL	975	0	1062	23	0
12	XL	956	0	1046	14	0
13	QM	955	0	1021	27	0
13	XM	914	0	971	23	0
14	QN	492	0	532	18	0
14	XN	492	0	531	16	0
15	QO	734	0	771	6	0
15	XO	729	0	768	10	0
16	QP	705	0	725	12	0
16	XP	705	0	725	11	0
17	QQ	834	0	904	12	0
17	XQ	834	0	904	13	0
18	QR	574	0	644	6	0
18	XR	574	0	644	11	0
19	QS	665	0	686	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XS	674	0	699	17	0
20	QT	763	0	861	16	0
20	XT	763	0	861	19	0
21	QU	217	0	234	8	0
21	XU	217	0	234	4	0
22	QV	1647	0	834	21	0
22	XV	1647	0	834	18	0
23	QX	409	0	209	11	0
23	XX	409	0	209	6	0
24	R0	643	0	667	6	0
24	Y0	648	0	672	14	0
25	R1	746	0	826	21	0
25	Y1	729	0	802	7	0
26	R2	581	0	629	7	0
26	Y2	575	0	624	5	0
27	R3	469	0	518	6	0
27	Y3	469	0	518	10	0
28	R4	348	0	354	6	0
28	Y4	357	0	362	13	0
29	R5	459	0	477	24	0
29	Y5	459	0	476	17	0
30	R6	453	0	474	7	0
30	Y6	453	0	473	13	0
31	R7	409	0	454	9	0
31	Y7	418	0	467	8	0
32	R8	517	0	582	19	0
32	Y8	517	0	582	16	0
33	R9	307	0	335	9	0
33	Y9	307	0	336	17	0
34	RA	62070	0	31284	625	0
34	YA	62091	0	31294	499	0
35	RB	2573	0	1306	27	0
35	YB	2573	0	1306	24	0
36	RD	2115	0	2195	51	0
36	YD	2115	0	2195	41	0
37	RE	1568	0	1634	36	0
37	YE	1568	0	1633	37	0
38	RF	1585	0	1632	32	0
38	YF	1585	0	1632	31	0
39	RG	1474	0	1535	32	0
39	YG	1474	0	1535	24	0
40	RH	1336	0	1418	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	YH	1336	0	1418	21	0
41	RI	1136	0	1223	32	1
41	YI	1136	0	1223	25	0
42	RN	1104	0	1180	14	0
42	YN	1104	0	1180	18	0
43	RO	933	0	996	21	0
43	YO	933	0	996	15	0
44	RP	1145	0	1228	27	0
44	YP	1122	0	1206	31	0
45	RQ	1122	0	1179	25	0
45	YQ	1122	0	1179	27	0
46	RR	960	0	1021	32	0
46	YR	960	0	1021	19	0
47	RS	882	0	943	21	0
47	YS	882	0	943	20	0
48	RT	1141	0	1202	17	0
48	YT	1141	0	1202	27	0
49	RU	964	0	1022	27	0
49	YU	964	0	1022	22	0
50	RV	779	0	852	14	0
50	YV	779	0	852	12	0
51	RW	900	0	964	20	0
51	YW	900	0	964	16	0
52	RX	725	0	778	11	0
52	YX	725	0	778	14	0
53	RY	818	0	911	25	0
53	YY	818	0	910	21	0
54	RZ	1461	0	1493	32	0
54	YZ	1529	0	1551	29	0
55	QA	87	0	0	0	0
55	QF	1	0	0	0	0
55	QH	2	0	0	0	0
55	QL	1	0	0	0	0
55	R0	2	0	0	0	0
55	R1	1	0	0	0	0
55	R3	1	0	0	0	0
55	R8	1	0	0	0	0
55	RA	429	0	0	0	0
55	RB	11	0	0	0	0
55	RD	1	0	0	0	0
55	RE	4	0	0	0	0
55	RF	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	RN	1	0	0	0	0
55	RO	1	0	0	0	0
55	RP	1	0	0	0	0
55	RQ	1	0	0	0	0
55	XA	89	0	0	0	0
55	XE	1	0	0	0	0
55	Y1	1	0	0	0	0
55	Y2	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	439	0	0	0	0
55	YB	8	0	0	0	0
55	YD	1	0	0	0	0
55	YE	2	0	0	0	0
55	YF	1	0	0	0	0
55	YQ	1	0	0	0	0
55	YR	2	0	0	0	0
55	YU	1	0	0	0	0
55	YX	1	0	0	0	0
56	QD	8	0	0	2	0
56	XD	8	0	0	0	0
57	QN	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	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	1	0
All	All	292039	0	197761	3384	1

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

The worst 5 of 3384 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)
14:QN:24:CYS:SG	14:QN:40:CYS:HB2	1.24	1.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:RH:98:LEU:CD2	40:RH:125:VAL:HG11	1.44	1.45
29:Y5:32:PRO:N	29:Y5:32:PRO:CA	1.69	1.44
30:R6:16:CYS:SG	30:R6:16:CYS:CB	2.06	1.44
14:QN:24:CYS:SG	14:QN:40:CYS:CB	2.14	1.35

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:RI:89:TYR:O	1:XA:357:G:O2'[4_555]	1.70	0.50

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%)	206 (88%)	27 (12%)	0	100	100
2	XB	234/256 (91%)	202 (86%)	31 (13%)	1 (0%)	30	62
3	QC	203/239 (85%)	180 (89%)	23 (11%)	0	100	100
3	XC	203/239 (85%)	182 (90%)	21 (10%)	0	100	100
4	QD	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	24	57
4	XD	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	24	57
5	QE	149/162 (92%)	134 (90%)	14 (9%)	1 (1%)	18	51
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	18	51
6	QF	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
8	QH	135/138 (98%)	127 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	XH	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
9	QI	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
9	XI	124/128 (97%)	110 (89%)	13 (10%)	1 (1%)	16	49
10	QJ	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	12	44
10	XJ	94/105 (90%)	86 (92%)	8 (8%)	0	100	100
11	QK	117/129 (91%)	108 (92%)	9 (8%)	0	100	100
11	XK	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
12	QL	123/132 (93%)	98 (80%)	24 (20%)	1 (1%)	16	49
12	XL	120/132 (91%)	99 (82%)	21 (18%)	0	100	100
13	QM	118/126 (94%)	99 (84%)	17 (14%)	2 (2%)	7	35
13	XM	112/126 (89%)	101 (90%)	10 (9%)	1 (1%)	14	47
14	QN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	7	35
14	XN	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	23
15	QO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	XO	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
16	QP	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
17	XQ	98/105 (93%)	94 (96%)	4 (4%)	0	100	100
18	QR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
18	XR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
19	QS	81/93 (87%)	66 (82%)	15 (18%)	0	100	100
19	XS	82/93 (88%)	65 (79%)	17 (21%)	0	100	100
20	QT	97/106 (92%)	86 (89%)	8 (8%)	3 (3%)	3	25
20	XT	97/106 (92%)	84 (87%)	10 (10%)	3 (3%)	3	25
21	QU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	XU	23/27 (85%)	19 (83%)	4 (17%)	0	100	100
24	R0	79/85 (93%)	71 (90%)	8 (10%)	0	100	100
24	Y0	80/85 (94%)	75 (94%)	5 (6%)	0	100	100
25	R1	93/98 (95%)	76 (82%)	17 (18%)	0	100	100
25	Y1	91/98 (93%)	78 (86%)	12 (13%)	1 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	R2	67/72 (93%)	63 (94%)	4 (6%)	0	100	100
26	Y2	66/72 (92%)	64 (97%)	2 (3%)	0	100	100
27	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	R4	43/71 (61%)	41 (95%)	2 (5%)	0	100	100
28	Y4	44/71 (62%)	28 (64%)	13 (30%)	3 (7%)	1	10
29	R5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	6	34
29	Y5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	6	34
30	R6	51/54 (94%)	46 (90%)	5 (10%)	0	100	100
30	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
31	R7	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
31	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
32	R8	62/65 (95%)	51 (82%)	9 (14%)	2 (3%)	3	24
32	Y8	62/65 (95%)	48 (77%)	14 (23%)	0	100	100
33	R9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	Y9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
36	RD	270/276 (98%)	244 (90%)	24 (9%)	2 (1%)	18	51
36	YD	270/276 (98%)	241 (89%)	28 (10%)	1 (0%)	30	62
37	RE	203/206 (98%)	159 (78%)	39 (19%)	5 (2%)	4	28
37	YE	203/206 (98%)	163 (80%)	38 (19%)	2 (1%)	12	44
38	RF	200/210 (95%)	183 (92%)	15 (8%)	2 (1%)	12	44
38	YF	200/210 (95%)	183 (92%)	16 (8%)	1 (0%)	24	57
39	RG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	21	54
39	YG	179/182 (98%)	152 (85%)	27 (15%)	0	100	100
40	RH	172/180 (96%)	145 (84%)	24 (14%)	3 (2%)	7	35
40	YH	172/180 (96%)	147 (86%)	20 (12%)	5 (3%)	3	26
41	RI	144/148 (97%)	115 (80%)	23 (16%)	6 (4%)	2	19
41	YI	144/148 (97%)	118 (82%)	22 (15%)	4 (3%)	4	26
42	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	18	51
42	YN	136/140 (97%)	123 (90%)	12 (9%)	1 (1%)	18	51
43	RO	120/122 (98%)	109 (91%)	11 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
43	YO	120/122 (98%)	111 (92%)	9 (8%)	0	100 100
44	RP	148/150 (99%)	114 (77%)	31 (21%)	3 (2%)	6 32
44	YP	145/150 (97%)	116 (80%)	28 (19%)	1 (1%)	18 51
45	RQ	139/141 (99%)	120 (86%)	18 (13%)	1 (1%)	18 51
45	YQ	139/141 (99%)	111 (80%)	27 (19%)	1 (1%)	18 51
46	RR	115/118 (98%)	103 (90%)	12 (10%)	0	100 100
46	YR	115/118 (98%)	104 (90%)	10 (9%)	1 (1%)	14 47
47	RS	109/112 (97%)	94 (86%)	15 (14%)	0	100 100
47	YS	109/112 (97%)	95 (87%)	13 (12%)	1 (1%)	14 47
48	RT	135/146 (92%)	116 (86%)	19 (14%)	0	100 100
48	YT	135/146 (92%)	121 (90%)	14 (10%)	0	100 100
49	RU	115/118 (98%)	106 (92%)	6 (5%)	3 (3%)	4 27
49	YU	115/118 (98%)	109 (95%)	6 (5%)	0	100 100
50	RV	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	12 44
50	YV	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	12 44
51	RW	111/113 (98%)	104 (94%)	7 (6%)	0	100 100
51	YW	111/113 (98%)	107 (96%)	4 (4%)	0	100 100
52	RX	90/96 (94%)	85 (94%)	5 (6%)	0	100 100
52	YX	90/96 (94%)	84 (93%)	6 (7%)	0	100 100
53	RY	105/110 (96%)	102 (97%)	3 (3%)	0	100 100
53	YY	105/110 (96%)	99 (94%)	6 (6%)	0	100 100
54	RZ	181/206 (88%)	139 (77%)	38 (21%)	4 (2%)	5 30
54	YZ	191/206 (93%)	145 (76%)	39 (20%)	7 (4%)	2 21
All	All	11414/12128 (94%)	10111 (89%)	1217 (11%)	86 (1%)	16 49

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	QL	105	TYR
20	QT	75	ASN
32	R8	30	ARG
37	RE	147	PRO
40	RH	157	TYR

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%)	202 (100%)	1 (0%)	81	80
2	XB	204/220 (93%)	203 (100%)	1 (0%)	81	80
3	QC	159/188 (85%)	158 (99%)	1 (1%)	78	79
3	XC	159/188 (85%)	157 (99%)	2 (1%)	61	72
4	QD	180/181 (99%)	179 (99%)	1 (1%)	78	79
4	XD	180/181 (99%)	177 (98%)	3 (2%)	53	70
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	115 (99%)	1 (1%)	70	76
6	QF	90/90 (100%)	89 (99%)	1 (1%)	65	74
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	125 (99%)	1 (1%)	73	77
8	QH	118/119 (99%)	117 (99%)	1 (1%)	73	77
8	XH	118/119 (99%)	117 (99%)	1 (1%)	73	77
9	QI	98/99 (99%)	95 (97%)	3 (3%)	35	59
9	XI	97/99 (98%)	96 (99%)	1 (1%)	68	75
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	90/99 (91%)	88 (98%)	2 (2%)	45	65
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	103 (99%)	1 (1%)	68	75
12	XL	103/109 (94%)	101 (98%)	2 (2%)	50	68
13	QM	96/101 (95%)	96 (100%)	0	100	100
13	XM	92/101 (91%)	92 (100%)	0	100	100
14	QN	49/50 (98%)	47 (96%)	2 (4%)	27	53
14	XN	49/50 (98%)	47 (96%)	2 (4%)	27	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	QO	79/80 (99%)	77 (98%)	2 (2%)	42 63
15	XO	79/80 (99%)	79 (100%)	0	100 100
16	QP	72/74 (97%)	72 (100%)	0	100 100
16	XP	72/74 (97%)	72 (100%)	0	100 100
17	QQ	95/97 (98%)	95 (100%)	0	100 100
17	XQ	95/97 (98%)	93 (98%)	2 (2%)	47 66
18	QR	61/77 (79%)	61 (100%)	0	100 100
18	XR	61/77 (79%)	61 (100%)	0	100 100
19	QS	72/80 (90%)	72 (100%)	0	100 100
19	XS	73/80 (91%)	72 (99%)	1 (1%)	59 71
20	QT	76/82 (93%)	75 (99%)	1 (1%)	61 72
20	XT	76/82 (93%)	75 (99%)	1 (1%)	61 72
21	QU	20/22 (91%)	20 (100%)	0	100 100
21	XU	20/22 (91%)	20 (100%)	0	100 100
24	R0	65/67 (97%)	65 (100%)	0	100 100
24	Y0	65/67 (97%)	65 (100%)	0	100 100
25	R1	80/83 (96%)	78 (98%)	2 (2%)	42 63
25	Y1	78/83 (94%)	78 (100%)	0	100 100
26	R2	64/67 (96%)	64 (100%)	0	100 100
26	Y2	64/67 (96%)	64 (100%)	0	100 100
27	R3	51/52 (98%)	50 (98%)	1 (2%)	48 67
27	Y3	51/52 (98%)	51 (100%)	0	100 100
28	R4	40/63 (64%)	40 (100%)	0	100 100
28	Y4	41/63 (65%)	39 (95%)	2 (5%)	22 48
29	R5	51/52 (98%)	50 (98%)	1 (2%)	48 67
29	Y5	51/52 (98%)	48 (94%)	3 (6%)	18 44
30	R6	51/52 (98%)	50 (98%)	1 (2%)	48 67
30	Y6	51/52 (98%)	50 (98%)	1 (2%)	48 67
31	R7	40/42 (95%)	40 (100%)	0	100 100
31	Y7	41/42 (98%)	41 (100%)	0	100 100
32	R8	54/55 (98%)	54 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Y8	54/55 (98%)	54 (100%)	0	100	100
33	R9	34/34 (100%)	34 (100%)	0	100	100
33	Y9	34/34 (100%)	32 (94%)	2 (6%)	18	44
36	RD	214/218 (98%)	211 (99%)	3 (1%)	59	71
36	YD	214/218 (98%)	214 (100%)	0	100	100
37	RE	165/166 (99%)	162 (98%)	3 (2%)	51	69
37	YE	165/166 (99%)	159 (96%)	6 (4%)	31	57
38	RF	161/166 (97%)	158 (98%)	3 (2%)	50	68
38	YF	161/166 (97%)	161 (100%)	0	100	100
39	RG	155/156 (99%)	154 (99%)	1 (1%)	78	79
39	YG	155/156 (99%)	152 (98%)	3 (2%)	50	68
40	RH	145/148 (98%)	137 (94%)	8 (6%)	19	46
40	YH	145/148 (98%)	138 (95%)	7 (5%)	23	49
41	RI	122/124 (98%)	121 (99%)	1 (1%)	73	77
41	YI	122/124 (98%)	118 (97%)	4 (3%)	33	58
42	RN	117/119 (98%)	114 (97%)	3 (3%)	40	62
42	YN	117/119 (98%)	116 (99%)	1 (1%)	70	76
43	RO	100/100 (100%)	100 (100%)	0	100	100
43	YO	100/100 (100%)	98 (98%)	2 (2%)	48	67
44	RP	116/116 (100%)	116 (100%)	0	100	100
44	YP	114/116 (98%)	113 (99%)	1 (1%)	70	76
45	RQ	111/111 (100%)	109 (98%)	2 (2%)	51	69
45	YQ	111/111 (100%)	111 (100%)	0	100	100
46	RR	100/101 (99%)	98 (98%)	2 (2%)	48	67
46	YR	100/101 (99%)	100 (100%)	0	100	100
47	RS	87/88 (99%)	87 (100%)	0	100	100
47	YS	87/88 (99%)	84 (97%)	3 (3%)	32	57
48	RT	120/127 (94%)	118 (98%)	2 (2%)	53	70
48	YT	120/127 (94%)	118 (98%)	2 (2%)	53	70
49	RU	93/94 (99%)	92 (99%)	1 (1%)	65	74
49	YU	93/94 (99%)	92 (99%)	1 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
50	RV	82/82 (100%)	80 (98%)	2 (2%)	43 64
50	YV	82/82 (100%)	78 (95%)	4 (5%)	22 48
51	RW	92/92 (100%)	91 (99%)	1 (1%)	65 74
51	YW	92/92 (100%)	92 (100%)	0	100 100
52	RX	74/78 (95%)	73 (99%)	1 (1%)	59 71
52	YX	74/78 (95%)	72 (97%)	2 (3%)	39 62
53	RY	88/91 (97%)	87 (99%)	1 (1%)	65 74
53	YY	88/91 (97%)	87 (99%)	1 (1%)	65 74
54	RZ	162/179 (90%)	161 (99%)	1 (1%)	78 79
54	YZ	167/179 (93%)	164 (98%)	3 (2%)	51 69
All	All	9648/10066 (96%)	9526 (99%)	122 (1%)	61 72

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	XC	12	LEU
48	YT	105	LEU
17	XQ	74	LEU
48	YT	66	VAL
53	YY	79	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
39	YG	79	ASN
40	YH	74	ASN
39	RG	79	ASN
39	RG	66	GLN
41	YI	105	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1509/1521 (99%)	309 (20%)	9 (0%)
1	XA	1514/1521 (99%)	322 (21%)	10 (0%)
22	QV	76/77 (98%)	17 (22%)	2 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	XV	76/77 (98%)	21 (27%)	1 (1%)
23	QX	18/19 (94%)	4 (22%)	1 (5%)
23	XX	18/19 (94%)	5 (27%)	0
34	RA	2877/2915 (98%)	619 (21%)	40 (1%)
34	YA	2880/2915 (98%)	638 (22%)	44 (1%)
35	RB	119/122 (97%)	21 (17%)	1 (0%)
35	YB	119/122 (97%)	25 (21%)	1 (0%)
All	All	9206/9308 (98%)	1981 (21%)	109 (1%)

5 of 1981 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	32	A
1	QA	38	G
1	QA	39	G

5 of 109 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	748	C
34	YA	278	A
34	YA	2402	C
1	XA	1064	G
34	YA	102	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	1MG	XV	37	22	23,26,27	1.18	3 (13%)	33,39,42	1.95	8 (24%)

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	1.83	5 (21%)	33,39,42	2.38	8 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	1MG	XV	37	22	-	2/7/25/26	0/3/3/3
22	1MG	QV	37	22	-	2/7/25/26	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	37	1MG	C5-C4	4.60	1.51	1.38
22	QV	37	1MG	C2-N1	3.89	1.44	1.37
22	QV	37	1MG	C2-N3	3.16	1.38	1.33
22	XV	37	1MG	C5-C4	3.10	1.47	1.38
22	QV	37	1MG	C5-C6	2.65	1.52	1.45

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	QV	37	1MG	C5-C4-N3	-8.11	115.49	128.39
22	QV	37	1MG	C2-N3-C4	5.68	124.75	111.98
22	XV	37	1MG	C5-C4-N3	-5.44	119.73	128.39
22	QV	37	1MG	N9-C4-N3	5.43	136.81	125.95
22	XV	37	1MG	C2-N3-C4	4.78	122.73	111.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	XV	37	1MG	O4'-C4'-C5'-O5'
22	XV	37	1MG	C3'-C4'-C5'-O5'
22	QV	37	1MG	C3'-C4'-C5'-O5'
22	QV	37	1MG	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	XV	37	1MG	2	0
22	QV	37	1MG	4	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1110 ligands modelled in this entry, 1108 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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	QD	301	SF4	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
41	RI	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	RI	82:ARG	C	83:ALA	N	1.18

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	QA	1511/1521 (99%)	0.65	101 (6%) 24 15	96, 139, 274, 366	0
1	XA	1515/1521 (99%)	0.46	45 (2%) 52 30	72, 129, 225, 307	0
2	QB	235/256 (91%)	0.46	7 (2%) 52 30	128, 165, 188, 207	0
2	XB	236/256 (92%)	0.20	2 (0%) 82 60	106, 138, 172, 188	0
3	QC	205/239 (85%)	0.43	5 (2%) 59 35	140, 169, 191, 211	0
3	XC	205/239 (85%)	0.42	8 (3%) 43 23	127, 152, 176, 192	0
4	QD	208/209 (99%)	0.72	13 (6%) 26 15	95, 130, 151, 168	0
4	XD	208/209 (99%)	0.61	15 (7%) 21 14	91, 134, 156, 172	0
5	QE	151/162 (93%)	0.38	3 (1%) 65 39	111, 132, 161, 167	0
5	XE	151/162 (93%)	0.11	1 (0%) 84 63	89, 109, 139, 182	0
6	QF	101/101 (100%)	0.10	2 (1%) 65 39	80, 124, 146, 170	0
6	XF	101/101 (100%)	0.16	0 100 100	87, 117, 142, 159	0
7	QG	155/156 (99%)	0.34	12 (7%) 19 13	158, 186, 212, 249	0
7	XG	155/156 (99%)	0.22	6 (3%) 43 23	141, 168, 194, 274	0
8	QH	137/138 (99%)	0.72	9 (6%) 24 15	100, 125, 147, 182	0
8	XH	137/138 (99%)	0.57	8 (5%) 29 17	89, 119, 146, 157	0
9	QI	127/128 (99%)	1.17	29 (22%) 2 2	148, 190, 219, 230	0
9	XI	126/128 (98%)	0.90	18 (14%) 6 5	126, 173, 193, 218	0
10	QJ	99/105 (94%)	1.46	22 (22%) 2 2	152, 196, 212, 227	0
10	XJ	96/105 (91%)	0.95	11 (11%) 9 6	134, 169, 192, 207	0
11	QK	119/129 (92%)	0.59	7 (5%) 28 16	100, 125, 158, 177	0
11	XK	116/129 (89%)	0.32	3 (2%) 57 33	72, 115, 142, 153	0
12	QL	125/132 (94%)	0.90	13 (10%) 11 8	99, 118, 143, 181	0
12	XL	122/132 (92%)	0.76	10 (8%) 17 11	84, 102, 125, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	QM	120/126 (95%)	0.65	7 (5%) 29 17	150, 184, 210, 224	0
13	XM	114/126 (90%)	0.68	7 (6%) 27 16	121, 175, 195, 213	0
14	QN	60/61 (98%)	1.34	11 (18%) 3 4	124, 163, 182, 191	0
14	XN	60/61 (98%)	1.13	7 (11%) 9 6	123, 150, 185, 200	0
15	QO	88/89 (98%)	0.39	1 (1%) 78 54	92, 112, 135, 150	0
15	XO	87/89 (97%)	0.30	0 100 100	83, 101, 132, 146	0
16	QP	84/88 (95%)	0.91	8 (9%) 14 9	89, 124, 149, 169	0
16	XP	84/88 (95%)	0.55	4 (4%) 35 19	102, 132, 153, 197	0
17	QQ	100/105 (95%)	0.77	7 (7%) 22 14	103, 119, 132, 135	0
17	XQ	100/105 (95%)	0.61	5 (5%) 34 19	84, 104, 127, 141	0
18	QR	70/88 (79%)	0.12	0 100 100	83, 121, 148, 165	0
18	XR	70/88 (79%)	0.16	0 100 100	96, 116, 144, 160	0
19	QS	83/93 (89%)	1.44	24 (28%) 1 1	171, 204, 229, 245	0
19	XS	84/93 (90%)	0.93	8 (9%) 14 9	126, 167, 200, 228	0
20	QT	99/106 (93%)	1.03	16 (16%) 4 4	86, 118, 165, 176	0
20	XT	99/106 (93%)	1.07	18 (18%) 3 4	88, 116, 160, 173	0
21	QU	25/27 (92%)	2.50	14 (56%) 0 0	153, 183, 204, 213	0
21	XU	25/27 (92%)	2.28	10 (40%) 1 1	145, 158, 182, 187	0
22	QV	76/77 (98%)	0.55	3 (3%) 43 23	119, 205, 269, 284	0
22	XV	76/77 (98%)	0.44	3 (3%) 43 23	74, 177, 222, 267	0
23	QX	19/19 (100%)	2.07	9 (47%) 0 1	143, 241, 287, 290	0
23	XX	19/19 (100%)	2.08	8 (42%) 0 1	126, 234, 286, 304	0
24	R0	81/85 (95%)	0.91	10 (12%) 8 6	84, 104, 169, 198	0
24	Y0	82/85 (96%)	0.56	5 (6%) 27 16	44, 65, 146, 190	0
25	R1	95/98 (96%)	0.79	7 (7%) 20 13	70, 91, 121, 136	0
25	Y1	93/98 (94%)	0.71	6 (6%) 25 15	46, 70, 96, 115	0
26	R2	69/72 (95%)	0.51	2 (2%) 53 31	81, 98, 134, 156	0
26	Y2	68/72 (94%)	0.59	2 (2%) 53 31	44, 73, 104, 125	0
27	R3	59/60 (98%)	0.62	5 (8%) 16 11	80, 106, 135, 187	0
27	Y3	59/60 (98%)	0.12	0 100 100	27, 53, 96, 147	0
28	R4	45/71 (63%)	0.18	0 100 100	121, 174, 203, 225	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	Y4	46/71 (64%)	0.25	1 (2%) 62 37	105, 153, 169, 188	0
29	R5	59/60 (98%)	0.42	4 (6%) 23 14	66, 91, 113, 148	0
29	Y5	59/60 (98%)	0.10	0 100 100	29, 47, 77, 134	0
30	R6	53/54 (98%)	0.23	0 100 100	90, 101, 119, 126	0
30	Y6	53/54 (98%)	0.17	1 (1%) 66 41	49, 69, 97, 104	0
31	R7	47/49 (95%)	0.70	3 (6%) 25 15	58, 72, 93, 96	0
31	Y7	48/49 (97%)	0.55	3 (6%) 26 15	32, 45, 85, 106	0
32	R8	64/65 (98%)	1.47	15 (23%) 2 2	80, 98, 125, 183	0
32	Y8	64/65 (98%)	1.04	12 (18%) 3 3	48, 58, 82, 143	0
33	R9	37/37 (100%)	1.00	4 (10%) 11 8	86, 110, 136, 145	0
33	Y9	37/37 (100%)	0.84	3 (8%) 18 12	53, 66, 84, 98	0
34	RA	2882/2915 (98%)	0.41	80 (2%) 55 32	55, 100, 221, 404	0
34	YA	2883/2915 (98%)	0.18	45 (1%) 70 45	28, 58, 166, 367	0
35	RB	120/122 (98%)	0.33	2 (1%) 69 43	111, 144, 166, 214	0
35	YB	120/122 (98%)	-0.01	1 (0%) 82 60	55, 83, 103, 128	0
36	RD	272/276 (98%)	0.65	15 (5%) 30 18	62, 86, 105, 141	0
36	YD	272/276 (98%)	0.39	11 (4%) 42 23	41, 60, 83, 116	0
37	RE	205/206 (99%)	0.62	16 (7%) 19 12	72, 101, 130, 153	0
37	YE	205/206 (99%)	0.39	7 (3%) 48 27	37, 59, 101, 127	0
38	RF	202/210 (96%)	0.49	8 (3%) 42 23	69, 101, 135, 161	0
38	YF	202/210 (96%)	0.17	2 (0%) 79 56	28, 64, 102, 125	0
39	RG	181/182 (99%)	0.66	7 (3%) 43 23	121, 153, 191, 218	0
39	YG	181/182 (99%)	0.27	1 (0%) 85 65	71, 117, 157, 187	0
40	RH	174/180 (96%)	0.64	6 (3%) 48 27	112, 154, 176, 195	0
40	YH	174/180 (96%)	0.38	5 (2%) 53 31	42, 77, 103, 147	0
41	RI	146/148 (98%)	0.30	1 (0%) 84 63	94, 126, 156, 193	0
41	YI	146/148 (98%)	0.27	3 (2%) 63 38	69, 117, 137, 144	0
42	RN	138/140 (98%)	0.54	7 (5%) 33 19	62, 103, 138, 161	0
42	YN	138/140 (98%)	0.35	2 (1%) 73 48	32, 54, 96, 115	0
43	RO	122/122 (100%)	0.42	1 (0%) 82 60	65, 100, 123, 133	0
43	YO	122/122 (100%)	0.09	1 (0%) 82 60	36, 63, 90, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	RP	150/150 (100%)	1.01	26 (17%) 4 4	74, 114, 142, 182	0
44	YP	147/150 (98%)	0.79	13 (8%) 15 10	41, 76, 105, 120	0
45	RQ	141/141 (100%)	0.93	20 (14%) 6 5	87, 116, 143, 165	0
45	YQ	141/141 (100%)	0.61	9 (6%) 25 15	34, 68, 104, 144	0
46	RR	117/118 (99%)	0.67	8 (6%) 23 14	64, 87, 111, 134	0
46	YR	117/118 (99%)	0.50	3 (2%) 57 33	41, 57, 83, 141	0
47	RS	111/112 (99%)	0.80	11 (9%) 13 8	83, 132, 187, 218	0
47	YS	111/112 (99%)	0.45	7 (6%) 26 15	58, 83, 123, 190	0
48	RT	137/146 (93%)	0.57	10 (7%) 21 13	76, 114, 153, 183	0
48	YT	137/146 (93%)	0.44	6 (4%) 39 21	53, 76, 141, 171	0
49	RU	117/118 (99%)	0.75	8 (6%) 23 14	75, 109, 146, 173	0
49	YU	117/118 (99%)	0.45	5 (4%) 40 21	33, 44, 88, 121	0
50	RV	101/101 (100%)	0.32	2 (1%) 65 39	71, 114, 151, 194	0
50	YV	101/101 (100%)	0.24	5 (4%) 34 19	30, 60, 111, 172	0
51	RW	113/113 (100%)	0.51	4 (3%) 47 26	59, 74, 106, 167	0
51	YW	113/113 (100%)	0.11	1 (0%) 81 58	31, 43, 80, 148	0
52	RX	92/96 (95%)	0.53	6 (6%) 25 15	59, 80, 109, 136	0
52	YX	92/96 (95%)	0.28	0 100 100	38, 55, 81, 100	0
53	RY	107/110 (97%)	0.57	6 (5%) 30 17	68, 104, 134, 175	0
53	YY	107/110 (97%)	0.24	2 (1%) 66 41	39, 66, 91, 130	0
54	RZ	183/206 (88%)	0.45	9 (4%) 35 19	108, 142, 172, 208	0
54	YZ	193/206 (93%)	0.39	6 (3%) 51 29	57, 93, 129, 169	0
All	All	20831/21436 (97%)	0.48	991 (4%) 35 19	27, 108, 200, 404	0

The worst 5 of 991 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	QK	129	SER	11.8
21	QU	16	GLY	10.4
9	QI	123	PRO	7.6
1	XA	966	G	7.2
34	YA	2602	A	7.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	1MG	QV	37	24/25	0.72	0.13	187,197,202,203	0
22	1MG	XV	37	24/25	0.73	0.13	183,186,189,189	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	YA	3323	1/1	0.15	0.22	208,208,208,208	0
55	MG	RA	3288	1/1	0.35	0.25	110,110,110,110	0
55	MG	YA	3216	1/1	0.43	0.17	53,53,53,53	0
55	MG	RA	3221	1/1	0.44	0.14	74,74,74,74	0
55	MG	QA	1615	1/1	0.48	0.09	79,79,79,79	0
55	MG	RA	3214	1/1	0.49	0.20	43,43,43,43	0
55	MG	YA	3016	1/1	0.49	0.38	39,39,39,39	0
55	MG	RA	3185	1/1	0.50	0.11	56,56,56,56	0
55	MG	RA	3166	1/1	0.52	0.13	70,70,70,70	0
55	MG	YA	3075	1/1	0.52	0.26	56,56,56,56	0
55	MG	YA	3289	1/1	0.53	0.07	11,11,11,11	0
55	MG	XA	1660	1/1	0.54	0.14	62,62,62,62	0
55	MG	YA	3062	1/1	0.54	0.25	63,63,63,63	0
55	MG	Y2	101	1/1	0.55	0.13	79,79,79,79	0
55	MG	YA	3044	1/1	0.57	0.11	90,90,90,90	0
55	MG	YA	3175	1/1	0.58	0.17	54,54,54,54	0
55	MG	YA	3055	1/1	0.58	0.19	35,35,35,35	0
55	MG	YA	3291	1/1	0.59	0.39	64,64,64,64	0
55	MG	YA	3045	1/1	0.61	0.15	53,53,53,53	0
55	MG	XA	1674	1/1	0.61	0.14	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	RA	3294	1/1	0.61	0.10	52,52,52,52	0
55	MG	YA	3220	1/1	0.62	0.23	47,47,47,47	0
55	MG	XA	1623	1/1	0.63	0.08	102,102,102,102	0
55	MG	RA	3371	1/1	0.66	0.12	74,74,74,74	0
55	MG	XA	1688	1/1	0.67	0.16	67,67,67,67	0
55	MG	YA	3383	1/1	0.67	0.14	47,47,47,47	0
55	MG	YA	3025	1/1	0.68	0.29	50,50,50,50	0
55	MG	YA	3422	1/1	0.68	0.10	52,52,52,52	0
55	MG	XA	1627	1/1	0.69	0.16	55,55,55,55	0
55	MG	YA	3384	1/1	0.69	0.13	66,66,66,66	0
55	MG	RA	3001	1/1	0.69	0.16	50,50,50,50	0
55	MG	YA	3195	1/1	0.70	0.19	46,46,46,46	0
55	MG	XA	1679	1/1	0.70	0.14	62,62,62,62	0
55	MG	YA	3015	1/1	0.70	0.39	76,76,76,76	0
55	MG	RA	3186	1/1	0.71	0.19	63,63,63,63	0
55	MG	YA	3419	1/1	0.71	0.10	35,35,35,35	0
55	MG	YA	3317	1/1	0.71	0.17	31,31,31,31	0
55	MG	YA	3438	1/1	0.71	0.05	13,13,13,13	0
55	MG	RA	3089	1/1	0.72	0.29	65,65,65,65	0
55	MG	RB	209	1/1	0.72	0.11	51,51,51,51	0
55	MG	RA	3042	1/1	0.73	0.09	52,52,52,52	0
55	MG	XA	1643	1/1	0.73	0.15	52,52,52,52	0
55	MG	RA	3202	1/1	0.73	0.20	38,38,38,38	0
55	MG	YA	3425	1/1	0.73	0.23	11,11,11,11	0
55	MG	RA	3299	1/1	0.73	0.20	46,46,46,46	0
55	MG	YA	3126	1/1	0.74	0.13	51,51,51,51	0
55	MG	YA	3397	1/1	0.74	0.15	42,42,42,42	0
55	MG	RA	3055	1/1	0.74	0.10	53,53,53,53	0
55	MG	YA	3279	1/1	0.74	0.07	7,7,7,7	0
55	MG	YA	3368	1/1	0.74	0.21	24,24,24,24	0
55	MG	RB	210	1/1	0.74	0.08	44,44,44,44	0
55	MG	YA	3268	1/1	0.75	0.18	45,45,45,45	0
55	MG	RA	3048	1/1	0.75	0.10	52,52,52,52	0
55	MG	YA	3040	1/1	0.75	0.16	23,23,23,23	0
55	MG	RA	3330	1/1	0.75	0.29	47,47,47,47	0
55	MG	YA	3316	1/1	0.75	0.10	44,44,44,44	0
55	MG	RA	3133	1/1	0.75	0.10	76,76,76,76	0
55	MG	YA	3227	1/1	0.75	0.09	51,51,51,51	0
55	MG	YA	3330	1/1	0.75	0.14	50,50,50,50	0
55	MG	QA	1601	1/1	0.76	0.10	50,50,50,50	0
55	MG	RA	3084	1/1	0.76	0.09	61,61,61,61	0
55	MG	RA	3015	1/1	0.76	0.15	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	RA	3365	1/1	0.76	0.13	65,65,65,65	0
55	MG	RA	3370	1/1	0.76	0.12	52,52,52,52	0
55	MG	RA	3119	1/1	0.76	0.11	48,48,48,48	0
55	MG	RA	3379	1/1	0.76	0.16	66,66,66,66	0
55	MG	QA	1645	1/1	0.76	0.15	49,49,49,49	0
55	MG	RA	3254	1/1	0.76	0.20	68,68,68,68	0
55	MG	RA	3255	1/1	0.76	0.09	57,57,57,57	0
55	MG	RA	3274	1/1	0.76	0.09	55,55,55,55	0
55	MG	R0	102	1/1	0.76	0.06	40,40,40,40	0
55	MG	QA	1679	1/1	0.77	0.07	48,48,48,48	0
55	MG	YA	3245	1/1	0.77	0.44	62,62,62,62	0
55	MG	RO	201	1/1	0.77	0.11	69,69,69,69	0
55	MG	RA	3265	1/1	0.77	0.09	66,66,66,66	0
55	MG	RA	3387	1/1	0.77	0.10	67,67,67,67	0
55	MG	RA	3424	1/1	0.77	0.20	40,40,40,40	0
55	MG	RB	202	1/1	0.77	0.10	53,53,53,53	0
55	MG	RB	207	1/1	0.77	0.27	56,56,56,56	0
55	MG	QA	1677	1/1	0.77	0.20	50,50,50,50	0
55	MG	RA	3167	1/1	0.78	0.10	48,48,48,48	0
55	MG	RA	3400	1/1	0.78	0.24	43,43,43,43	0
55	MG	RA	3423	1/1	0.78	0.34	52,52,52,52	0
55	MG	YA	3068	1/1	0.78	0.16	45,45,45,45	0
55	MG	QA	1607	1/1	0.78	0.07	58,58,58,58	0
55	MG	YA	3120	1/1	0.78	0.25	27,27,27,27	0
55	MG	RA	3068	1/1	0.78	0.11	41,41,41,41	0
55	MG	XA	1689	1/1	0.78	0.17	51,51,51,51	0
55	MG	RA	3002	1/1	0.78	0.12	50,50,50,50	0
55	MG	QA	1685	1/1	0.78	0.10	56,56,56,56	0
55	MG	RA	3024	1/1	0.78	0.08	77,77,77,77	0
55	MG	YA	3224	1/1	0.78	0.20	59,59,59,59	0
55	MG	RA	3127	1/1	0.78	0.13	49,49,49,49	0
55	MG	QH	201	1/1	0.78	0.10	57,57,57,57	0
55	MG	QA	1621	1/1	0.78	0.17	65,65,65,65	0
55	MG	RA	3160	1/1	0.79	0.12	65,65,65,65	0
55	MG	QA	1614	1/1	0.79	0.07	45,45,45,45	0
55	MG	YA	3031	1/1	0.79	0.07	48,48,48,48	0
55	MG	RA	3122	1/1	0.79	0.13	37,37,37,37	0
55	MG	YA	3276	1/1	0.79	0.13	41,41,41,41	0
55	MG	RA	3049	1/1	0.79	0.10	57,57,57,57	0
55	MG	RA	3103	1/1	0.79	0.20	64,64,64,64	0
55	MG	RA	3368	1/1	0.79	0.12	45,45,45,45	0
55	MG	YA	3217	1/1	0.79	0.16	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	3135	1/1	0.79	0.10	108,108,108,108	0
55	MG	YB	206	1/1	0.79	0.10	51,51,51,51	0
55	MG	QA	1660	1/1	0.80	0.08	59,59,59,59	0
55	MG	YA	3043	1/1	0.80	0.10	33,33,33,33	0
55	MG	RA	3417	1/1	0.80	0.18	55,55,55,55	0
55	MG	RA	3304	1/1	0.80	0.09	37,37,37,37	0
55	MG	RA	3097	1/1	0.80	0.09	54,54,54,54	0
55	MG	RA	3345	1/1	0.80	0.18	64,64,64,64	0
55	MG	RA	3168	1/1	0.80	0.13	49,49,49,49	0
55	MG	RA	3098	1/1	0.80	0.15	50,50,50,50	0
55	MG	RA	3070	1/1	0.80	0.24	51,51,51,51	0
55	MG	RA	3187	1/1	0.80	0.06	81,81,81,81	0
55	MG	RA	3025	1/1	0.80	0.07	49,49,49,49	0
55	MG	RA	3211	1/1	0.80	0.15	37,37,37,37	0
55	MG	RA	3252	1/1	0.81	0.13	60,60,60,60	0
55	MG	RA	3316	1/1	0.81	0.09	41,41,41,41	0
55	MG	XA	1651	1/1	0.81	0.08	25,25,25,25	0
55	MG	RA	3121	1/1	0.81	0.24	40,40,40,40	0
55	MG	RA	3118	1/1	0.81	0.22	35,35,35,35	0
55	MG	XA	1612	1/1	0.81	0.18	61,61,61,61	0
55	MG	RA	3250	1/1	0.81	0.10	51,51,51,51	0
55	MG	RA	3010	1/1	0.82	0.17	76,76,76,76	0
55	MG	RA	3178	1/1	0.82	0.24	48,48,48,48	0
55	MG	RA	3131	1/1	0.82	0.10	57,57,57,57	0
55	MG	YA	3088	1/1	0.82	0.09	34,34,34,34	0
55	MG	RA	3354	1/1	0.82	0.10	54,54,54,54	0
55	MG	RA	3032	1/1	0.82	0.25	76,76,76,76	0
55	MG	RA	3096	1/1	0.82	0.11	66,66,66,66	0
55	MG	RB	211	1/1	0.82	0.07	62,62,62,62	0
55	MG	YA	3333	1/1	0.82	0.18	44,44,44,44	0
55	MG	YA	3214	1/1	0.82	0.09	49,49,49,49	0
55	MG	RA	3158	1/1	0.82	0.20	42,42,42,42	0
55	MG	RA	3285	1/1	0.82	0.07	48,48,48,48	0
55	MG	YA	3394	1/1	0.82	0.13	34,34,34,34	0
55	MG	RA	3120	1/1	0.82	0.15	40,40,40,40	0
55	MG	QA	1669	1/1	0.82	0.27	47,47,47,47	0
55	MG	QA	1647	1/1	0.82	0.13	64,64,64,64	0
55	MG	YA	3233	1/1	0.82	0.14	62,62,62,62	0
55	MG	RA	3248	1/1	0.82	0.09	45,45,45,45	0
55	MG	RA	3421	1/1	0.82	0.21	14,14,14,14	0
55	MG	RA	3021	1/1	0.83	0.12	62,62,62,62	0
55	MG	YA	3242	1/1	0.83	0.23	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	QA	1634	1/1	0.83	0.12	30,30,30,30	0
55	MG	QA	1676	1/1	0.83	0.07	50,50,50,50	0
55	MG	QA	1648	1/1	0.83	0.17	44,44,44,44	0
55	MG	YA	3048	1/1	0.83	0.17	36,36,36,36	0
55	MG	YA	3051	1/1	0.83	0.19	36,36,36,36	0
55	MG	RA	3184	1/1	0.83	0.11	44,44,44,44	0
55	MG	XA	1626	1/1	0.83	0.10	54,54,54,54	0
55	MG	RA	3094	1/1	0.83	0.12	54,54,54,54	0
55	MG	QA	1659	1/1	0.83	0.13	49,49,49,49	0
55	MG	YA	3087	1/1	0.83	0.16	35,35,35,35	0
55	MG	RA	3276	1/1	0.83	0.09	48,48,48,48	0
55	MG	QA	1646	1/1	0.83	0.08	63,63,63,63	0
55	MG	RA	3401	1/1	0.83	0.09	83,83,83,83	0
55	MG	RA	3416	1/1	0.83	0.12	49,49,49,49	0
55	MG	YA	3390	1/1	0.83	0.21	39,39,39,39	0
55	MG	RA	3014	1/1	0.83	0.10	55,55,55,55	0
55	MG	RA	3203	1/1	0.83	0.20	44,44,44,44	0
55	MG	RA	3143	1/1	0.83	0.16	52,52,52,52	0
55	MG	QA	1687	1/1	0.83	0.08	70,70,70,70	0
55	MG	RA	3312	1/1	0.83	0.12	64,64,64,64	0
55	MG	RA	3220	1/1	0.83	0.15	72,72,72,72	0
55	MG	RA	3060	1/1	0.83	0.07	62,62,62,62	0
55	MG	RA	3043	1/1	0.84	0.07	57,57,57,57	0
55	MG	RA	3384	1/1	0.84	0.14	27,27,27,27	0
55	MG	RA	3305	1/1	0.84	0.16	48,48,48,48	0
55	MG	QA	1686	1/1	0.84	0.11	49,49,49,49	0
55	MG	QA	1637	1/1	0.84	0.08	46,46,46,46	0
55	MG	RA	3231	1/1	0.84	0.15	50,50,50,50	0
55	MG	RA	3279	1/1	0.84	0.12	28,28,28,28	0
55	MG	YA	3391	1/1	0.84	0.20	44,44,44,44	0
55	MG	YA	3107	1/1	0.84	0.09	27,27,27,27	0
55	MG	QA	1612	1/1	0.84	0.12	71,71,71,71	0
55	MG	YA	3417	1/1	0.84	0.12	39,39,39,39	0
55	MG	XA	1642	1/1	0.84	0.10	43,43,43,43	0
55	MG	RA	3035	1/1	0.84	0.16	40,40,40,40	0
55	MG	RA	3289	1/1	0.84	0.17	38,38,38,38	0
55	MG	RA	3169	1/1	0.84	0.07	44,44,44,44	0
55	MG	RA	3009	1/1	0.84	0.14	59,59,59,59	0
57	ZN	R9	101	1/1	0.84	0.13	110,110,110,110	0
55	MG	QA	1627	1/1	0.85	0.14	41,41,41,41	0
55	MG	RA	3303	1/1	0.85	0.19	47,47,47,47	0
55	MG	RA	3005	1/1	0.85	0.09	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	RA	3207	1/1	0.85	0.10	52,52,52,52	0
55	MG	RA	3110	1/1	0.85	0.08	45,45,45,45	0
55	MG	RA	3175	1/1	0.85	0.11	51,51,51,51	0
55	MG	YA	3387	1/1	0.85	0.23	47,47,47,47	0
55	MG	Y5	102	1/1	0.85	0.12	18,18,18,18	0
55	MG	RA	3219	1/1	0.85	0.15	55,55,55,55	0
55	MG	RA	3023	1/1	0.85	0.07	28,28,28,28	0
55	MG	R0	101	1/1	0.85	0.12	69,69,69,69	0
55	MG	YA	3271	1/1	0.85	0.10	15,15,15,15	0
55	MG	XA	1632	1/1	0.85	0.12	40,40,40,40	0
55	MG	QA	1663	1/1	0.85	0.13	51,51,51,51	0
55	MG	RA	3030	1/1	0.85	0.23	57,57,57,57	0
55	MG	YA	3180	1/1	0.85	0.16	14,14,14,14	0
55	MG	YA	3183	1/1	0.85	0.09	47,47,47,47	0
55	MG	QA	1613	1/1	0.85	0.13	69,69,69,69	0
55	MG	RA	3190	1/1	0.86	0.18	61,61,61,61	0
55	MG	RA	3222	1/1	0.86	0.15	68,68,68,68	0
55	MG	RA	3427	1/1	0.86	0.10	47,47,47,47	0
55	MG	RA	3226	1/1	0.86	0.11	37,37,37,37	0
55	MG	XA	1687	1/1	0.86	0.15	47,47,47,47	0
55	MG	QH	202	1/1	0.86	0.19	45,45,45,45	0
55	MG	QA	1674	1/1	0.86	0.09	41,41,41,41	0
55	MG	RA	3181	1/1	0.86	0.15	55,55,55,55	0
55	MG	YA	3143	1/1	0.86	0.08	9,9,9,9	0
55	MG	YA	3145	1/1	0.86	0.12	38,38,38,38	0
55	MG	RA	3378	1/1	0.86	0.12	53,53,53,53	0
55	MG	YA	3349	1/1	0.86	0.07	48,48,48,48	0
55	MG	RA	3296	1/1	0.86	0.16	65,65,65,65	0
55	MG	RP	201	1/1	0.86	0.27	48,48,48,48	0
55	MG	YA	3188	1/1	0.86	0.10	52,52,52,52	0
55	MG	XA	1601	1/1	0.86	0.10	69,69,69,69	0
55	MG	YA	3199	1/1	0.86	0.11	58,58,58,58	0
55	MG	YA	3201	1/1	0.86	0.21	40,40,40,40	0
55	MG	YA	3028	1/1	0.86	0.20	1,1,1,1	0
55	MG	QA	1655	1/1	0.86	0.07	44,44,44,44	0
55	MG	QA	1658	1/1	0.86	0.18	49,49,49,49	0
55	MG	RA	3218	1/1	0.86	0.18	34,34,34,34	0
55	MG	RA	3262	1/1	0.86	0.13	56,56,56,56	0
55	MG	XA	1629	1/1	0.86	0.16	41,41,41,41	0
55	MG	QA	1642	1/1	0.86	0.08	62,62,62,62	0
55	MG	RA	3269	1/1	0.86	0.16	52,52,52,52	0
55	MG	RA	3080	1/1	0.86	0.11	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	QA	1628	1/1	0.87	0.10	40,40,40,40	0
55	MG	YA	3177	1/1	0.87	0.19	41,41,41,41	0
55	MG	YA	3034	1/1	0.87	0.21	15,15,15,15	0
55	MG	RA	3216	1/1	0.87	0.13	59,59,59,59	0
55	MG	RA	3253	1/1	0.87	0.09	28,28,28,28	0
55	MG	QA	1605	1/1	0.87	0.16	45,45,45,45	0
55	MG	RB	206	1/1	0.87	0.11	24,24,24,24	0
55	MG	YA	3336	1/1	0.87	0.14	56,56,56,56	0
55	MG	YA	3348	1/1	0.87	0.09	27,27,27,27	0
55	MG	RA	3040	1/1	0.87	0.27	53,53,53,53	0
55	MG	YA	3352	1/1	0.87	0.13	15,15,15,15	0
55	MG	RA	3258	1/1	0.87	0.06	49,49,49,49	0
55	MG	YA	3215	1/1	0.87	0.09	60,60,60,60	0
55	MG	RA	3134	1/1	0.87	0.07	83,83,83,83	0
55	MG	YA	3060	1/1	0.87	0.13	38,38,38,38	0
55	MG	RA	3195	1/1	0.87	0.22	32,32,32,32	0
55	MG	RA	3266	1/1	0.87	0.08	59,59,59,59	0
55	MG	RA	3395	1/1	0.87	0.08	54,54,54,54	0
55	MG	XE	201	1/1	0.87	0.08	53,53,53,53	0
55	MG	QA	1618	1/1	0.87	0.14	60,60,60,60	0
55	MG	XA	1604	1/1	0.87	0.08	61,61,61,61	0
55	MG	QA	1662	1/1	0.87	0.15	45,45,45,45	0
55	MG	RA	3018	1/1	0.87	0.23	48,48,48,48	0
55	MG	RA	3099	1/1	0.87	0.09	32,32,32,32	0
55	MG	YA	3278	1/1	0.87	0.14	34,34,34,34	0
55	MG	RA	3346	1/1	0.87	0.12	61,61,61,61	0
55	MG	RA	3420	1/1	0.88	0.12	40,40,40,40	0
55	MG	QA	1668	1/1	0.88	0.11	53,53,53,53	0
55	MG	RA	3033	1/1	0.88	0.11	59,59,59,59	0
55	MG	YA	3004	1/1	0.88	0.18	33,33,33,33	0
55	MG	RA	3126	1/1	0.88	0.06	46,46,46,46	0
55	MG	RA	3237	1/1	0.88	0.06	39,39,39,39	0
55	MG	RA	3429	1/1	0.88	0.12	40,40,40,40	0
55	MG	QA	1617	1/1	0.88	0.18	54,54,54,54	0
55	MG	YA	3234	1/1	0.88	0.20	27,27,27,27	0
55	MG	RA	3091	1/1	0.88	0.09	36,36,36,36	0
55	MG	RA	3311	1/1	0.88	0.16	58,58,58,58	0
55	MG	QA	1670	1/1	0.88	0.07	40,40,40,40	0
55	MG	QA	1623	1/1	0.88	0.11	49,49,49,49	0
55	MG	RA	3020	1/1	0.88	0.18	38,38,38,38	0
55	MG	RF	302	1/1	0.88	0.12	46,46,46,46	0
55	MG	RA	3137	1/1	0.88	0.20	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	YA	3281	1/1	0.88	0.09	51,51,51,51	0
55	MG	RA	3138	1/1	0.88	0.10	45,45,45,45	0
55	MG	YA	3053	1/1	0.88	0.11	25,25,25,25	0
55	MG	YA	3054	1/1	0.88	0.16	36,36,36,36	0
55	MG	RA	3351	1/1	0.88	0.10	22,22,22,22	0
55	MG	RA	3261	1/1	0.88	0.09	32,32,32,32	0
55	MG	XA	1609	1/1	0.88	0.11	53,53,53,53	0
55	MG	YA	3067	1/1	0.88	0.17	43,43,43,43	0
55	MG	QA	1638	1/1	0.88	0.09	58,58,58,58	0
55	MG	RA	3150	1/1	0.88	0.10	47,47,47,47	0
55	MG	YA	3080	1/1	0.88	0.17	52,52,52,52	0
55	MG	RA	3209	1/1	0.88	0.06	53,53,53,53	0
55	MG	YA	3357	1/1	0.88	0.15	37,37,37,37	0
55	MG	YA	3360	1/1	0.88	0.24	6,6,6,6	0
55	MG	RA	3268	1/1	0.88	0.09	62,62,62,62	0
55	MG	YA	3369	1/1	0.88	0.12	39,39,39,39	0
55	MG	YA	3377	1/1	0.88	0.12	47,47,47,47	0
55	MG	YA	3095	1/1	0.88	0.08	21,21,21,21	0
55	MG	QA	1609	1/1	0.88	0.06	46,46,46,46	0
55	MG	XA	1630	1/1	0.88	0.09	53,53,53,53	0
55	MG	YA	3388	1/1	0.88	0.11	20,20,20,20	0
55	MG	QA	1620	1/1	0.88	0.14	50,50,50,50	0
55	MG	RA	3383	1/1	0.88	0.10	31,31,31,31	0
55	MG	RA	3162	1/1	0.88	0.16	47,47,47,47	0
55	MG	RA	3278	1/1	0.88	0.07	47,47,47,47	0
55	MG	YA	3412	1/1	0.88	0.11	31,31,31,31	0
55	MG	XA	1658	1/1	0.88	0.17	31,31,31,31	0
55	MG	RA	3388	1/1	0.88	0.12	41,41,41,41	0
55	MG	QA	1630	1/1	0.88	0.11	43,43,43,43	0
55	MG	RA	3284	1/1	0.88	0.12	30,30,30,30	0
55	MG	YA	3430	1/1	0.88	0.10	27,27,27,27	0
55	MG	YA	3431	1/1	0.88	0.11	31,31,31,31	0
55	MG	QA	1633	1/1	0.88	0.23	43,43,43,43	0
55	MG	RA	3069	1/1	0.88	0.16	22,22,22,22	0
55	MG	RA	3031	1/1	0.88	0.10	17,17,17,17	0
55	MG	RA	3249	1/1	0.89	0.08	58,58,58,58	0
55	MG	QA	1654	1/1	0.89	0.17	36,36,36,36	0
55	MG	XA	1638	1/1	0.89	0.12	49,49,49,49	0
55	MG	YA	3325	1/1	0.89	0.12	61,61,61,61	0
55	MG	QA	1622	1/1	0.89	0.09	43,43,43,43	0
55	MG	YA	3036	1/1	0.89	0.24	18,18,18,18	0
55	MG	RA	3059	1/1	0.89	0.06	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	YA	3338	1/1	0.89	0.22	49,49,49,49	0
55	MG	YA	3341	1/1	0.89	0.13	32,32,32,32	0
55	MG	XA	1648	1/1	0.89	0.08	46,46,46,46	0
55	MG	XA	1649	1/1	0.89	0.13	46,46,46,46	0
55	MG	YA	3196	1/1	0.89	0.15	33,33,33,33	0
55	MG	RA	3356	1/1	0.89	0.07	47,47,47,47	0
55	MG	YA	3047	1/1	0.89	0.16	48,48,48,48	0
55	MG	YA	3361	1/1	0.89	0.13	16,16,16,16	0
55	MG	RA	3407	1/1	0.89	0.12	44,44,44,44	0
55	MG	RA	3362	1/1	0.89	0.15	67,67,67,67	0
55	MG	XA	1667	1/1	0.89	0.10	48,48,48,48	0
55	MG	XA	1670	1/1	0.89	0.06	56,56,56,56	0
55	MG	RA	3152	1/1	0.89	0.12	44,44,44,44	0
55	MG	YA	3385	1/1	0.89	0.08	32,32,32,32	0
55	MG	XA	1677	1/1	0.89	0.10	42,42,42,42	0
55	MG	XA	1678	1/1	0.89	0.17	40,40,40,40	0
55	MG	RA	3418	1/1	0.89	0.20	43,43,43,43	0
55	MG	RA	3013	1/1	0.89	0.14	66,66,66,66	0
55	MG	RA	3093	1/1	0.89	0.07	20,20,20,20	0
55	MG	QA	1606	1/1	0.89	0.26	40,40,40,40	0
55	MG	YA	3261	1/1	0.89	0.08	19,19,19,19	0
55	MG	YA	3413	1/1	0.89	0.24	62,62,62,62	0
55	MG	YA	3416	1/1	0.89	0.15	41,41,41,41	0
55	MG	XA	1619	1/1	0.89	0.09	39,39,39,39	0
55	MG	XA	1620	1/1	0.89	0.19	54,54,54,54	0
55	MG	YA	3421	1/1	0.89	0.09	44,44,44,44	0
55	MG	YA	3092	1/1	0.89	0.17	38,38,38,38	0
55	MG	RA	3045	1/1	0.89	0.07	41,41,41,41	0
55	MG	RA	3286	1/1	0.89	0.16	35,35,35,35	0
55	MG	QA	1653	1/1	0.89	0.08	49,49,49,49	0
55	MG	RA	3341	1/1	0.89	0.10	52,52,52,52	0
55	MG	YB	201	1/1	0.89	0.08	17,17,17,17	0
55	MG	YA	3136	1/1	0.89	0.08	29,29,29,29	0
55	MG	YD	301	1/1	0.89	0.11	28,28,28,28	0
55	MG	YA	3304	1/1	0.89	0.17	37,37,37,37	0
55	MG	RA	3306	1/1	0.90	0.06	55,55,55,55	0
55	MG	RA	3046	1/1	0.90	0.08	56,56,56,56	0
55	MG	RA	3027	1/1	0.90	0.12	44,44,44,44	0
55	MG	RA	3376	1/1	0.90	0.12	59,59,59,59	0
55	MG	XA	1605	1/1	0.90	0.08	46,46,46,46	0
55	MG	QA	1629	1/1	0.90	0.07	41,41,41,41	0
55	MG	YA	3244	1/1	0.90	0.14	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	YA	3370	1/1	0.90	0.07	19,19,19,19	0
55	MG	XA	1668	1/1	0.90	0.15	73,73,73,73	0
55	MG	YA	3380	1/1	0.90	0.15	34,34,34,34	0
55	MG	QA	1639	1/1	0.90	0.06	41,41,41,41	0
55	MG	YA	3139	1/1	0.90	0.15	41,41,41,41	0
55	MG	RA	3291	1/1	0.90	0.13	46,46,46,46	0
55	MG	YA	3274	1/1	0.90	0.20	38,38,38,38	0
55	MG	YA	3275	1/1	0.90	0.14	45,45,45,45	0
55	MG	RA	3293	1/1	0.90	0.09	27,27,27,27	0
55	MG	YA	3147	1/1	0.90	0.15	39,39,39,39	0
55	MG	YA	3170	1/1	0.90	0.17	17,17,17,17	0
55	MG	RA	3224	1/1	0.90	0.15	44,44,44,44	0
55	MG	YA	3176	1/1	0.90	0.16	26,26,26,26	0
55	MG	RA	3213	1/1	0.90	0.09	56,56,56,56	0
55	MG	YA	3298	1/1	0.90	0.12	28,28,28,28	0
55	MG	YA	3299	1/1	0.90	0.09	11,11,11,11	0
55	MG	RA	3394	1/1	0.90	0.08	44,44,44,44	0
55	MG	YA	3420	1/1	0.90	0.07	35,35,35,35	0
55	MG	RA	3192	1/1	0.90	0.14	48,48,48,48	0
55	MG	RA	3399	1/1	0.90	0.06	45,45,45,45	0
55	MG	YA	3423	1/1	0.90	0.18	52,52,52,52	0
55	MG	RA	3012	1/1	0.90	0.08	31,31,31,31	0
55	MG	XA	1633	1/1	0.90	0.09	47,47,47,47	0
55	MG	RA	3283	1/1	0.90	0.06	49,49,49,49	0
55	MG	YA	3436	1/1	0.90	0.08	23,23,23,23	0
55	MG	RA	3008	1/1	0.90	0.13	45,45,45,45	0
55	MG	YA	3071	1/1	0.90	0.07	38,38,38,38	0
55	MG	YB	202	1/1	0.90	0.09	26,26,26,26	0
55	MG	RN	201	1/1	0.90	0.06	48,48,48,48	0
55	MG	YA	3079	1/1	0.90	0.19	18,18,18,18	0
55	MG	YF	301	1/1	0.90	0.09	26,26,26,26	0
57	ZN	QN	101	1/1	0.90	0.08	158,158,158,158	0
55	MG	XA	1646	1/1	0.90	0.06	69,69,69,69	0
55	MG	YA	3003	1/1	0.91	0.09	21,21,21,21	0
55	MG	RA	3161	1/1	0.91	0.07	39,39,39,39	0
55	MG	QA	1673	1/1	0.91	0.09	51,51,51,51	0
55	MG	RA	3163	1/1	0.91	0.04	28,28,28,28	0
55	MG	RA	3165	1/1	0.91	0.16	50,50,50,50	0
55	MG	YA	3342	1/1	0.91	0.06	59,59,59,59	0
55	MG	YA	3345	1/1	0.91	0.12	43,43,43,43	0
55	MG	RA	3406	1/1	0.91	0.06	28,28,28,28	0
55	MG	RA	3085	1/1	0.91	0.04	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	YA	3032	1/1	0.91	0.04	60,60,60,60	0
55	MG	RA	3410	1/1	0.91	0.14	36,36,36,36	0
55	MG	RA	3415	1/1	0.91	0.10	35,35,35,35	0
55	MG	RA	3086	1/1	0.91	0.06	30,30,30,30	0
55	MG	YA	3364	1/1	0.91	0.12	16,16,16,16	0
55	MG	YA	3367	1/1	0.91	0.16	31,31,31,31	0
55	MG	RA	3217	1/1	0.91	0.08	52,52,52,52	0
55	MG	RA	3270	1/1	0.91	0.07	53,53,53,53	0
55	MG	RA	3058	1/1	0.91	0.04	63,63,63,63	0
55	MG	RA	3016	1/1	0.91	0.17	51,51,51,51	0
55	MG	QA	1682	1/1	0.91	0.08	38,38,38,38	0
55	MG	RA	3177	1/1	0.91	0.09	42,42,42,42	0
55	MG	RA	3061	1/1	0.91	0.13	25,25,25,25	0
55	MG	XA	1647	1/1	0.91	0.05	49,49,49,49	0
55	MG	RA	3364	1/1	0.91	0.08	36,36,36,36	0
55	MG	RB	201	1/1	0.91	0.11	61,61,61,61	0
55	MG	YA	3238	1/1	0.91	0.13	37,37,37,37	0
55	MG	RA	3066	1/1	0.91	0.20	43,43,43,43	0
55	MG	YA	3066	1/1	0.91	0.23	35,35,35,35	0
55	MG	RB	204	1/1	0.91	0.10	48,48,48,48	0
55	MG	YA	3404	1/1	0.91	0.09	26,26,26,26	0
55	MG	YA	3405	1/1	0.91	0.09	22,22,22,22	0
55	MG	YA	3409	1/1	0.91	0.28	43,43,43,43	0
55	MG	YA	3410	1/1	0.91	0.17	45,45,45,45	0
55	MG	YA	3258	1/1	0.91	0.13	56,56,56,56	0
55	MG	RA	3067	1/1	0.91	0.10	28,28,28,28	0
55	MG	QA	1683	1/1	0.91	0.07	51,51,51,51	0
55	MG	QA	1635	1/1	0.91	0.18	50,50,50,50	0
55	MG	RA	3101	1/1	0.91	0.08	43,43,43,43	0
55	MG	XA	1672	1/1	0.91	0.07	47,47,47,47	0
55	MG	RA	3147	1/1	0.91	0.06	34,34,34,34	0
55	MG	RD	301	1/1	0.91	0.23	38,38,38,38	0
55	MG	RE	301	1/1	0.91	0.10	36,36,36,36	0
55	MG	YA	3094	1/1	0.91	0.28	40,40,40,40	0
55	MG	QL	201	1/1	0.91	0.06	55,55,55,55	0
55	MG	YA	3101	1/1	0.91	0.07	22,22,22,22	0
55	MG	XA	1685	1/1	0.91	0.18	41,41,41,41	0
55	MG	RA	3072	1/1	0.91	0.06	24,24,24,24	0
55	MG	RA	3079	1/1	0.91	0.06	40,40,40,40	0
55	MG	YA	3312	1/1	0.91	0.16	12,12,12,12	0
55	MG	RA	3006	1/1	0.91	0.11	30,30,30,30	0
55	MG	RA	3204	1/1	0.91	0.17	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	3318	1/1	0.91	0.17	40,40,40,40	0
55	MG	XA	1603	1/1	0.91	0.07	44,44,44,44	0
55	MG	RA	3257	1/1	0.91	0.11	47,47,47,47	0
55	MG	YA	3302	1/1	0.92	0.12	20,20,20,20	0
55	MG	YA	3081	1/1	0.92	0.21	51,51,51,51	0
55	MG	RA	3179	1/1	0.92	0.06	44,44,44,44	0
55	MG	YA	3315	1/1	0.92	0.04	47,47,47,47	0
55	MG	RA	3275	1/1	0.92	0.13	62,62,62,62	0
55	MG	YA	3089	1/1	0.92	0.07	19,19,19,19	0
55	MG	RA	3140	1/1	0.92	0.13	50,50,50,50	0
55	MG	RA	3363	1/1	0.92	0.17	37,37,37,37	0
55	MG	QA	1624	1/1	0.92	0.16	55,55,55,55	0
55	MG	YA	3327	1/1	0.92	0.10	26,26,26,26	0
55	MG	YA	3100	1/1	0.92	0.12	28,28,28,28	0
55	MG	RB	208	1/1	0.92	0.17	57,57,57,57	0
55	MG	YA	3103	1/1	0.92	0.05	22,22,22,22	0
55	MG	XA	1675	1/1	0.92	0.20	46,46,46,46	0
55	MG	YA	3109	1/1	0.92	0.06	36,36,36,36	0
55	MG	QA	1651	1/1	0.92	0.16	36,36,36,36	0
55	MG	RA	3280	1/1	0.92	0.13	56,56,56,56	0
55	MG	RA	3075	1/1	0.92	0.13	13,13,13,13	0
55	MG	XA	1682	1/1	0.92	0.06	33,33,33,33	0
55	MG	RA	3230	1/1	0.92	0.07	43,43,43,43	0
55	MG	YA	3354	1/1	0.92	0.20	15,15,15,15	0
55	MG	RA	3374	1/1	0.92	0.10	37,37,37,37	0
55	MG	RA	3375	1/1	0.92	0.06	46,46,46,46	0
55	MG	YA	3148	1/1	0.92	0.12	32,32,32,32	0
55	MG	QA	1640	1/1	0.92	0.09	49,49,49,49	0
55	MG	RA	3236	1/1	0.92	0.18	57,57,57,57	0
55	MG	RA	3189	1/1	0.92	0.10	35,35,35,35	0
55	MG	RA	3238	1/1	0.92	0.16	23,23,23,23	0
55	MG	YA	3002	1/1	0.92	0.09	29,29,29,29	0
55	MG	YA	3375	1/1	0.92	0.09	22,22,22,22	0
55	MG	YA	3182	1/1	0.92	0.07	49,49,49,49	0
55	MG	QA	1641	1/1	0.92	0.15	41,41,41,41	0
55	MG	QA	1608	1/1	0.92	0.07	44,44,44,44	0
55	MG	RA	3029	1/1	0.92	0.16	42,42,42,42	0
55	MG	XA	1606	1/1	0.92	0.16	51,51,51,51	0
55	MG	RA	3389	1/1	0.92	0.09	46,46,46,46	0
55	MG	QA	1643	1/1	0.92	0.16	38,38,38,38	0
55	MG	YA	3206	1/1	0.92	0.22	9,9,9,9	0
55	MG	XA	1613	1/1	0.92	0.08	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	XA	1617	1/1	0.92	0.15	36,36,36,36	0
55	MG	XA	1618	1/1	0.92	0.09	42,42,42,42	0
55	MG	YA	3401	1/1	0.92	0.11	17,17,17,17	0
55	MG	QA	1616	1/1	0.92	0.06	64,64,64,64	0
55	MG	RA	3300	1/1	0.92	0.20	13,13,13,13	0
55	MG	QA	1602	1/1	0.92	0.12	49,49,49,49	0
55	MG	QA	1678	1/1	0.92	0.09	41,41,41,41	0
55	MG	RA	3402	1/1	0.92	0.07	67,67,67,67	0
55	MG	RA	3208	1/1	0.92	0.12	27,27,27,27	0
55	MG	RA	3062	1/1	0.92	0.27	44,44,44,44	0
55	MG	YA	3050	1/1	0.92	0.04	19,19,19,19	0
55	MG	R8	101	1/1	0.92	0.14	35,35,35,35	0
55	MG	RA	3038	1/1	0.92	0.12	25,25,25,25	0
55	MG	RA	3314	1/1	0.92	0.10	37,37,37,37	0
55	MG	RA	3171	1/1	0.92	0.19	38,38,38,38	0
55	MG	YA	3057	1/1	0.92	0.10	12,12,12,12	0
55	MG	YA	3059	1/1	0.92	0.16	26,26,26,26	0
55	MG	RA	3327	1/1	0.92	0.08	47,47,47,47	0
55	MG	QA	1661	1/1	0.92	0.10	50,50,50,50	0
55	MG	RA	3337	1/1	0.92	0.18	25,25,25,25	0
55	MG	RA	3176	1/1	0.92	0.06	33,33,33,33	0
55	MG	QA	1610	1/1	0.92	0.14	54,54,54,54	0
55	MG	YA	3070	1/1	0.92	0.13	57,57,57,57	0
55	MG	RA	3139	1/1	0.92	0.05	58,58,58,58	0
55	MG	YB	207	1/1	0.92	0.08	42,42,42,42	0
55	MG	XA	1657	1/1	0.92	0.12	44,44,44,44	0
55	MG	YA	3293	1/1	0.92	0.17	31,31,31,31	0
55	MG	YR	201	1/1	0.92	0.14	25,25,25,25	0
55	MG	RA	3272	1/1	0.92	0.06	53,53,53,53	0
55	MG	XA	1659	1/1	0.92	0.08	29,29,29,29	0
55	MG	YA	3114	1/1	0.93	0.22	1,1,1,1	0
55	MG	RA	3295	1/1	0.93	0.08	38,38,38,38	0
55	MG	YA	3013	1/1	0.93	0.15	15,15,15,15	0
55	MG	YA	3127	1/1	0.93	0.22	12,12,12,12	0
55	MG	QA	1681	1/1	0.93	0.06	52,52,52,52	0
55	MG	YA	3137	1/1	0.93	0.08	26,26,26,26	0
55	MG	XA	1625	1/1	0.93	0.06	56,56,56,56	0
55	MG	YA	3141	1/1	0.93	0.12	20,20,20,20	0
55	MG	YA	3024	1/1	0.93	0.09	35,35,35,35	0
55	MG	QA	1649	1/1	0.93	0.09	40,40,40,40	0
55	MG	RA	3422	1/1	0.93	0.18	37,37,37,37	0
55	MG	RA	3164	1/1	0.93	0.06	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	YA	3149	1/1	0.93	0.15	1,1,1,1	0
55	MG	YA	3152	1/1	0.93	0.10	17,17,17,17	0
55	MG	RA	3369	1/1	0.93	0.07	41,41,41,41	0
55	MG	RA	3301	1/1	0.93	0.11	46,46,46,46	0
55	MG	QA	1650	1/1	0.93	0.14	36,36,36,36	0
55	MG	YA	3353	1/1	0.93	0.09	34,34,34,34	0
55	MG	YA	3037	1/1	0.93	0.26	8,8,8,8	0
55	MG	XA	1635	1/1	0.93	0.07	69,69,69,69	0
55	MG	RA	3372	1/1	0.93	0.06	59,59,59,59	0
55	MG	RA	3057	1/1	0.93	0.09	63,63,63,63	0
55	MG	RB	203	1/1	0.93	0.11	45,45,45,45	0
55	MG	YA	3190	1/1	0.93	0.12	32,32,32,32	0
55	MG	XA	1645	1/1	0.93	0.06	49,49,49,49	0
55	MG	RA	3198	1/1	0.93	0.09	41,41,41,41	0
55	MG	QA	1672	1/1	0.93	0.10	40,40,40,40	0
55	MG	RA	3308	1/1	0.93	0.05	26,26,26,26	0
55	MG	RA	3310	1/1	0.93	0.05	57,57,57,57	0
55	MG	YA	3378	1/1	0.93	0.13	36,36,36,36	0
55	MG	YA	3207	1/1	0.93	0.13	13,13,13,13	0
55	MG	QA	1656	1/1	0.93	0.11	46,46,46,46	0
55	MG	RA	3116	1/1	0.93	0.19	29,29,29,29	0
55	MG	RA	3242	1/1	0.93	0.16	25,25,25,25	0
55	MG	RA	3170	1/1	0.93	0.07	45,45,45,45	0
55	MG	RA	3319	1/1	0.93	0.14	16,16,16,16	0
55	MG	YA	3061	1/1	0.93	0.07	14,14,14,14	0
55	MG	YA	3225	1/1	0.93	0.10	30,30,30,30	0
55	MG	RA	3392	1/1	0.93	0.09	51,51,51,51	0
55	MG	YA	3063	1/1	0.93	0.22	36,36,36,36	0
55	MG	RA	3325	1/1	0.93	0.08	23,23,23,23	0
55	MG	YA	3403	1/1	0.93	0.08	26,26,26,26	0
55	MG	YA	3235	1/1	0.93	0.15	38,38,38,38	0
55	MG	XA	1669	1/1	0.93	0.05	45,45,45,45	0
55	MG	YA	3407	1/1	0.93	0.05	29,29,29,29	0
55	MG	YA	3240	1/1	0.93	0.11	39,39,39,39	0
55	MG	RA	3019	1/1	0.93	0.14	57,57,57,57	0
55	MG	QA	1626	1/1	0.93	0.09	50,50,50,50	0
55	MG	RA	3333	1/1	0.93	0.17	22,22,22,22	0
55	MG	YA	3414	1/1	0.93	0.06	41,41,41,41	0
55	MG	YA	3073	1/1	0.93	0.26	42,42,42,42	0
55	MG	XA	1602	1/1	0.93	0.08	41,41,41,41	0
55	MG	RA	3144	1/1	0.93	0.19	25,25,25,25	0
55	MG	QA	1664	1/1	0.93	0.14	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	QA	1665	1/1	0.93	0.07	39,39,39,39	0
55	MG	QA	1666	1/1	0.93	0.23	51,51,51,51	0
55	MG	RA	3153	1/1	0.93	0.10	33,33,33,33	0
55	MG	XA	1611	1/1	0.93	0.10	24,24,24,24	0
55	MG	RA	3411	1/1	0.93	0.17	36,36,36,36	0
55	MG	RA	3412	1/1	0.93	0.06	39,39,39,39	0
55	MG	YA	3284	1/1	0.93	0.15	9,9,9,9	0
55	MG	YA	3286	1/1	0.93	0.17	9,9,9,9	0
55	MG	XA	1614	1/1	0.93	0.07	39,39,39,39	0
55	MG	XA	1616	1/1	0.93	0.15	36,36,36,36	0
55	MG	YB	204	1/1	0.93	0.17	16,16,16,16	0
55	MG	RA	3011	1/1	0.93	0.05	66,66,66,66	0
55	MG	Y8	101	1/1	0.93	0.12	5,5,5,5	0
55	MG	QA	1632	1/1	0.93	0.07	33,33,33,33	0
55	MG	YE	302	1/1	0.93	0.17	51,51,51,51	0
55	MG	RA	3130	1/1	0.93	0.14	57,57,57,57	0
55	MG	YA	3110	1/1	0.93	0.20	29,29,29,29	0
55	MG	YA	3310	1/1	0.93	0.10	30,30,30,30	0
55	MG	YA	3111	1/1	0.93	0.17	30,30,30,30	0
55	MG	RA	3240	1/1	0.94	0.06	38,38,38,38	0
55	MG	YA	3308	1/1	0.94	0.19	15,15,15,15	0
55	MG	YA	3035	1/1	0.94	0.20	10,10,10,10	0
55	MG	YA	3138	1/1	0.94	0.14	20,20,20,20	0
55	MG	YA	3313	1/1	0.94	0.14	50,50,50,50	0
55	MG	RA	3196	1/1	0.94	0.19	16,16,16,16	0
55	MG	RA	3307	1/1	0.94	0.14	33,33,33,33	0
55	MG	RA	3183	1/1	0.94	0.12	36,36,36,36	0
55	MG	XA	1655	1/1	0.94	0.14	20,20,20,20	0
55	MG	XA	1656	1/1	0.94	0.07	43,43,43,43	0
55	MG	RA	3125	1/1	0.94	0.14	50,50,50,50	0
55	MG	YA	3046	1/1	0.94	0.09	18,18,18,18	0
55	MG	YA	3329	1/1	0.94	0.07	25,25,25,25	0
55	MG	RA	3419	1/1	0.94	0.13	47,47,47,47	0
55	MG	YA	3155	1/1	0.94	0.10	42,42,42,42	0
55	MG	XA	1608	1/1	0.94	0.17	22,22,22,22	0
55	MG	YA	3171	1/1	0.94	0.15	43,43,43,43	0
55	MG	RA	3148	1/1	0.94	0.15	40,40,40,40	0
55	MG	XA	1661	1/1	0.94	0.06	48,48,48,48	0
55	MG	YA	3052	1/1	0.94	0.09	14,14,14,14	0
55	MG	YA	3178	1/1	0.94	0.08	26,26,26,26	0
55	MG	XA	1610	1/1	0.94	0.15	67,67,67,67	0
55	MG	YA	3350	1/1	0.94	0.10	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	RA	3251	1/1	0.94	0.08	41,41,41,41	0
55	MG	RA	3281	1/1	0.94	0.17	56,56,56,56	0
55	MG	YA	3184	1/1	0.94	0.08	42,42,42,42	0
55	MG	YA	3186	1/1	0.94	0.15	28,28,28,28	0
55	MG	RA	3081	1/1	0.94	0.18	41,41,41,41	0
55	MG	YA	3058	1/1	0.94	0.15	25,25,25,25	0
55	MG	YA	3193	1/1	0.94	0.15	11,11,11,11	0
55	MG	XA	1671	1/1	0.94	0.11	47,47,47,47	0
55	MG	QA	1611	1/1	0.94	0.11	58,58,58,58	0
55	MG	XA	1615	1/1	0.94	0.05	53,53,53,53	0
55	MG	RA	3324	1/1	0.94	0.08	40,40,40,40	0
55	MG	YA	3205	1/1	0.94	0.10	18,18,18,18	0
55	MG	RA	3188	1/1	0.94	0.16	54,54,54,54	0
55	MG	YA	3065	1/1	0.94	0.16	29,29,29,29	0
55	MG	RA	3225	1/1	0.94	0.14	34,34,34,34	0
55	MG	RA	3386	1/1	0.94	0.10	41,41,41,41	0
55	MG	RA	3107	1/1	0.94	0.07	50,50,50,50	0
55	MG	XA	1683	1/1	0.94	0.07	31,31,31,31	0
55	MG	YA	3218	1/1	0.94	0.09	22,22,22,22	0
55	MG	XA	1684	1/1	0.94	0.08	37,37,37,37	0
55	MG	RA	3228	1/1	0.94	0.20	39,39,39,39	0
55	MG	XA	1686	1/1	0.94	0.15	41,41,41,41	0
55	MG	YA	3078	1/1	0.94	0.27	32,32,32,32	0
55	MG	YA	3229	1/1	0.94	0.15	31,31,31,31	0
55	MG	YA	3398	1/1	0.94	0.08	42,42,42,42	0
55	MG	YA	3400	1/1	0.94	0.17	31,31,31,31	0
55	MG	YA	3230	1/1	0.94	0.16	39,39,39,39	0
55	MG	XA	1624	1/1	0.94	0.05	58,58,58,58	0
55	MG	RA	3259	1/1	0.94	0.04	30,30,30,30	0
55	MG	RA	3339	1/1	0.94	0.17	12,12,12,12	0
55	MG	YA	3086	1/1	0.94	0.21	9,9,9,9	0
55	MG	RA	3229	1/1	0.94	0.07	52,52,52,52	0
55	MG	RA	3210	1/1	0.94	0.09	35,35,35,35	0
55	MG	YA	3411	1/1	0.94	0.13	36,36,36,36	0
55	MG	RA	3263	1/1	0.94	0.17	27,27,27,27	0
55	MG	YA	3091	1/1	0.94	0.04	24,24,24,24	0
55	MG	YA	3249	1/1	0.94	0.22	13,13,13,13	0
55	MG	RA	3051	1/1	0.94	0.12	27,27,27,27	0
55	MG	RA	3234	1/1	0.94	0.08	51,51,51,51	0
55	MG	XA	1634	1/1	0.94	0.07	46,46,46,46	0
55	MG	RA	3007	1/1	0.94	0.07	34,34,34,34	0
55	MG	YA	3272	1/1	0.94	0.18	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	YA	3273	1/1	0.94	0.19	9,9,9,9	0
55	MG	XA	1637	1/1	0.94	0.05	43,43,43,43	0
55	MG	RA	3359	1/1	0.94	0.17	36,36,36,36	0
55	MG	YA	3427	1/1	0.94	0.12	18,18,18,18	0
55	MG	YA	3428	1/1	0.94	0.17	58,58,58,58	0
55	MG	YA	3105	1/1	0.94	0.10	9,9,9,9	0
55	MG	XA	1640	1/1	0.94	0.12	54,54,54,54	0
55	MG	YA	3020	1/1	0.94	0.17	7,7,7,7	0
55	MG	RA	3193	1/1	0.94	0.09	52,52,52,52	0
55	MG	YA	3439	1/1	0.94	0.12	42,42,42,42	0
55	MG	YA	3283	1/1	0.94	0.09	3,3,3,3	0
55	MG	RA	3123	1/1	0.94	0.05	30,30,30,30	0
55	MG	XA	1644	1/1	0.94	0.10	32,32,32,32	0
55	MG	YA	3116	1/1	0.94	0.16	32,32,32,32	0
55	MG	YA	3029	1/1	0.94	0.14	17,17,17,17	0
55	MG	YA	3125	1/1	0.94	0.24	36,36,36,36	0
55	MG	YA	3295	1/1	0.94	0.19	8,8,8,8	0
55	MG	RA	3239	1/1	0.94	0.08	44,44,44,44	0
55	MG	RQ	201	1/1	0.94	0.06	34,34,34,34	0
55	MG	YX	101	1/1	0.94	0.07	37,37,37,37	0
55	MG	YA	3131	1/1	0.94	0.20	2,2,2,2	0
55	MG	YA	3303	1/1	0.94	0.11	33,33,33,33	0
55	MG	RA	3052	1/1	0.95	0.12	28,28,28,28	0
55	MG	YA	3297	1/1	0.95	0.20	26,26,26,26	0
55	MG	YA	3033	1/1	0.95	0.15	12,12,12,12	0
55	MG	R3	3101	1/1	0.95	0.06	42,42,42,42	0
55	MG	RA	3071	1/1	0.95	0.07	74,74,74,74	0
55	MG	RA	3282	1/1	0.95	0.04	37,37,37,37	0
55	MG	XA	1641	1/1	0.95	0.12	37,37,37,37	0
55	MG	YA	3306	1/1	0.95	0.20	43,43,43,43	0
55	MG	YA	3307	1/1	0.95	0.15	55,55,55,55	0
55	MG	YA	3146	1/1	0.95	0.18	33,33,33,33	0
55	MG	YA	3309	1/1	0.95	0.21	33,33,33,33	0
55	MG	RA	3428	1/1	0.95	0.06	45,45,45,45	0
55	MG	YA	3042	1/1	0.95	0.12	9,9,9,9	0
55	MG	RA	3355	1/1	0.95	0.04	29,29,29,29	0
55	MG	YA	3314	1/1	0.95	0.10	30,30,30,30	0
55	MG	YA	3151	1/1	0.95	0.09	21,21,21,21	0
55	MG	RA	3095	1/1	0.95	0.08	64,64,64,64	0
55	MG	RA	3357	1/1	0.95	0.09	25,25,25,25	0
55	MG	YA	3157	1/1	0.95	0.10	25,25,25,25	0
55	MG	YA	3321	1/1	0.95	0.07	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	YA	3159	1/1	0.95	0.14	6,6,6,6	0
55	MG	YA	3163	1/1	0.95	0.12	15,15,15,15	0
55	MG	YA	3164	1/1	0.95	0.16	5,5,5,5	0
55	MG	YA	3167	1/1	0.95	0.08	15,15,15,15	0
55	MG	RA	3197	1/1	0.95	0.07	66,66,66,66	0
55	MG	RA	3128	1/1	0.95	0.06	54,54,54,54	0
55	MG	RA	3199	1/1	0.95	0.11	30,30,30,30	0
55	MG	YA	3337	1/1	0.95	0.04	24,24,24,24	0
55	MG	RA	3287	1/1	0.95	0.09	38,38,38,38	0
55	MG	YA	3340	1/1	0.95	0.12	48,48,48,48	0
55	MG	XA	1650	1/1	0.95	0.06	43,43,43,43	0
55	MG	RA	3200	1/1	0.95	0.06	30,30,30,30	0
55	MG	YA	3179	1/1	0.95	0.11	18,18,18,18	0
55	MG	YA	3346	1/1	0.95	0.06	41,41,41,41	0
55	MG	YA	3347	1/1	0.95	0.06	26,26,26,26	0
55	MG	RA	3367	1/1	0.95	0.06	53,53,53,53	0
55	MG	RA	3129	1/1	0.95	0.05	58,58,58,58	0
55	MG	RA	3290	1/1	0.95	0.12	47,47,47,47	0
55	MG	RA	3244	1/1	0.95	0.20	45,45,45,45	0
55	MG	RA	3247	1/1	0.95	0.10	39,39,39,39	0
55	MG	QA	1657	1/1	0.95	0.10	37,37,37,37	0
55	MG	RA	3074	1/1	0.95	0.06	24,24,24,24	0
55	MG	YA	3359	1/1	0.95	0.18	22,22,22,22	0
55	MG	XA	1663	1/1	0.95	0.12	41,41,41,41	0
55	MG	YA	3194	1/1	0.95	0.13	8,8,8,8	0
55	MG	QA	1625	1/1	0.95	0.19	39,39,39,39	0
55	MG	RA	3077	1/1	0.95	0.05	28,28,28,28	0
55	MG	YA	3064	1/1	0.95	0.06	42,42,42,42	0
55	MG	YA	3200	1/1	0.95	0.09	18,18,18,18	0
55	MG	RA	3078	1/1	0.95	0.15	16,16,16,16	0
55	MG	YA	3372	1/1	0.95	0.25	19,19,19,19	0
55	MG	RA	3044	1/1	0.95	0.11	35,35,35,35	0
55	MG	RA	3380	1/1	0.95	0.04	37,37,37,37	0
55	MG	RA	3382	1/1	0.95	0.07	33,33,33,33	0
55	MG	YA	3213	1/1	0.95	0.09	24,24,24,24	0
55	MG	YA	3381	1/1	0.95	0.06	11,11,11,11	0
55	MG	RA	3174	1/1	0.95	0.06	8,8,8,8	0
55	MG	RA	3212	1/1	0.95	0.09	23,23,23,23	0
55	MG	RA	3256	1/1	0.95	0.13	56,56,56,56	0
55	MG	YA	3386	1/1	0.95	0.07	35,35,35,35	0
55	MG	YA	3074	1/1	0.95	0.14	1,1,1,1	0
55	MG	RA	3104	1/1	0.95	0.09	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	YA	3219	1/1	0.95	0.09	36,36,36,36	0
55	MG	YA	3076	1/1	0.95	0.10	28,28,28,28	0
55	MG	YA	3393	1/1	0.95	0.12	29,29,29,29	0
55	MG	RA	3106	1/1	0.95	0.07	31,31,31,31	0
55	MG	XA	1680	1/1	0.95	0.08	38,38,38,38	0
55	MG	RA	3215	1/1	0.95	0.07	17,17,17,17	0
55	MG	YA	3399	1/1	0.95	0.14	36,36,36,36	0
55	MG	YA	3228	1/1	0.95	0.13	20,20,20,20	0
55	MG	RA	3309	1/1	0.95	0.06	96,96,96,96	0
55	MG	YA	3084	1/1	0.95	0.23	16,16,16,16	0
55	MG	YA	3231	1/1	0.95	0.14	39,39,39,39	0
55	MG	RA	3260	1/1	0.95	0.09	45,45,45,45	0
55	MG	YA	3406	1/1	0.95	0.20	33,33,33,33	0
55	MG	QA	1619	1/1	0.95	0.09	56,56,56,56	0
55	MG	YA	3408	1/1	0.95	0.18	45,45,45,45	0
55	MG	RA	3003	1/1	0.95	0.04	42,42,42,42	0
55	MG	YA	3236	1/1	0.95	0.07	26,26,26,26	0
55	MG	YA	3237	1/1	0.95	0.20	39,39,39,39	0
55	MG	RA	3313	1/1	0.95	0.12	54,54,54,54	0
55	MG	YA	3239	1/1	0.95	0.08	30,30,30,30	0
55	MG	RA	3115	1/1	0.95	0.09	22,22,22,22	0
55	MG	RA	3082	1/1	0.95	0.09	57,57,57,57	0
55	MG	RA	3318	1/1	0.95	0.11	32,32,32,32	0
55	MG	RA	3083	1/1	0.95	0.04	44,44,44,44	0
55	MG	RA	3149	1/1	0.95	0.12	27,27,27,27	0
55	MG	YA	3256	1/1	0.95	0.08	39,39,39,39	0
55	MG	XA	1621	1/1	0.95	0.06	45,45,45,45	0
55	MG	YA	3260	1/1	0.95	0.09	35,35,35,35	0
55	MG	XA	1622	1/1	0.95	0.13	41,41,41,41	0
55	MG	QA	1684	1/1	0.95	0.05	42,42,42,42	0
55	MG	YA	3269	1/1	0.95	0.10	32,32,32,32	0
55	MG	YA	3429	1/1	0.95	0.21	26,26,26,26	0
55	MG	YA	3270	1/1	0.95	0.16	17,17,17,17	0
55	MG	RA	3223	1/1	0.95	0.17	35,35,35,35	0
55	MG	YA	3011	1/1	0.95	0.21	13,13,13,13	0
55	MG	RA	3413	1/1	0.95	0.19	30,30,30,30	0
55	MG	RA	3329	1/1	0.95	0.15	46,46,46,46	0
55	MG	YA	3112	1/1	0.95	0.06	49,49,49,49	0
55	MG	QA	1631	1/1	0.95	0.10	35,35,35,35	0
55	MG	XA	1628	1/1	0.95	0.10	44,44,44,44	0
55	MG	YA	3023	1/1	0.95	0.10	17,17,17,17	0
55	MG	YA	3121	1/1	0.95	0.07	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	YA	3124	1/1	0.95	0.11	10,10,10,10	0
55	MG	RA	3050	1/1	0.95	0.14	24,24,24,24	0
55	MG	RA	3334	1/1	0.95	0.20	19,19,19,19	0
55	MG	RA	3155	1/1	0.95	0.09	26,26,26,26	0
55	MG	YR	202	1/1	0.95	0.12	33,33,33,33	0
55	MG	YU	201	1/1	0.95	0.09	37,37,37,37	0
55	MG	RA	3156	1/1	0.95	0.09	18,18,18,18	0
55	MG	QA	1652	1/1	0.95	0.17	33,33,33,33	0
55	MG	YA	3294	1/1	0.95	0.20	0,0,0,0	0
57	ZN	RY	201	1/1	0.95	0.05	137,137,137,137	0
55	MG	XA	1662	1/1	0.96	0.08	26,26,26,26	0
55	MG	RA	3366	1/1	0.96	0.10	29,29,29,29	0
55	MG	YA	3117	1/1	0.96	0.09	26,26,26,26	0
55	MG	YA	3118	1/1	0.96	0.10	21,21,21,21	0
55	MG	YA	3119	1/1	0.96	0.11	36,36,36,36	0
55	MG	YA	3041	1/1	0.96	0.19	12,12,12,12	0
55	MG	XA	1666	1/1	0.96	0.04	48,48,48,48	0
55	MG	YA	3122	1/1	0.96	0.10	12,12,12,12	0
55	MG	RA	3037	1/1	0.96	0.14	26,26,26,26	0
55	MG	RA	3145	1/1	0.96	0.07	24,24,24,24	0
55	MG	RA	3026	1/1	0.96	0.06	20,20,20,20	0
55	MG	RA	3191	1/1	0.96	0.13	28,28,28,28	0
55	MG	RA	3039	1/1	0.96	0.13	29,29,29,29	0
55	MG	YA	3365	1/1	0.96	0.06	6,6,6,6	0
55	MG	YA	3241	1/1	0.96	0.06	14,14,14,14	0
55	MG	RA	3315	1/1	0.96	0.10	31,31,31,31	0
55	MG	YA	3049	1/1	0.96	0.13	18,18,18,18	0
55	MG	XA	1673	1/1	0.96	0.04	33,33,33,33	0
55	MG	RA	3373	1/1	0.96	0.08	25,25,25,25	0
55	MG	YA	3373	1/1	0.96	0.16	19,19,19,19	0
55	MG	YA	3254	1/1	0.96	0.16	49,49,49,49	0
55	MG	QA	1671	1/1	0.96	0.04	34,34,34,34	0
55	MG	YA	3257	1/1	0.96	0.04	14,14,14,14	0
55	MG	YA	3379	1/1	0.96	0.13	29,29,29,29	0
55	MG	XA	1676	1/1	0.96	0.10	29,29,29,29	0
55	MG	RA	3317	1/1	0.96	0.09	20,20,20,20	0
55	MG	RA	3194	1/1	0.96	0.17	42,42,42,42	0
55	MG	YA	3264	1/1	0.96	0.15	41,41,41,41	0
55	MG	YA	3266	1/1	0.96	0.06	23,23,23,23	0
55	MG	YA	3267	1/1	0.96	0.10	9,9,9,9	0
55	MG	YA	3056	1/1	0.96	0.16	31,31,31,31	0
55	MG	RA	3087	1/1	0.96	0.07	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	RA	3320	1/1	0.96	0.14	30,30,30,30	0
55	MG	RA	3173	1/1	0.96	0.18	34,34,34,34	0
55	MG	YA	3392	1/1	0.96	0.13	14,14,14,14	0
55	MG	RA	3073	1/1	0.96	0.06	23,23,23,23	0
55	MG	RA	3113	1/1	0.96	0.11	14,14,14,14	0
55	MG	RA	3154	1/1	0.96	0.14	17,17,17,17	0
55	MG	RA	3132	1/1	0.96	0.08	40,40,40,40	0
55	MG	YA	3160	1/1	0.96	0.14	11,11,11,11	0
55	MG	YA	3161	1/1	0.96	0.07	18,18,18,18	0
55	MG	RA	3201	1/1	0.96	0.07	38,38,38,38	0
55	MG	RA	3292	1/1	0.96	0.05	40,40,40,40	0
55	MG	QA	1667	1/1	0.96	0.15	44,44,44,44	0
55	MG	QA	1604	1/1	0.96	0.11	46,46,46,46	0
55	MG	RA	3180	1/1	0.96	0.14	31,31,31,31	0
55	MG	YA	3173	1/1	0.96	0.15	12,12,12,12	0
55	MG	RE	302	1/1	0.96	0.08	25,25,25,25	0
55	MG	Y7	101	1/1	0.96	0.11	24,24,24,24	0
55	MG	YA	3072	1/1	0.96	0.14	6,6,6,6	0
55	MG	RE	303	1/1	0.96	0.16	16,16,16,16	0
55	MG	RA	3344	1/1	0.96	0.06	39,39,39,39	0
55	MG	RA	3397	1/1	0.96	0.11	29,29,29,29	0
55	MG	YA	3181	1/1	0.96	0.07	22,22,22,22	0
55	MG	YA	3301	1/1	0.96	0.15	12,12,12,12	0
55	MG	RA	3398	1/1	0.96	0.09	36,36,36,36	0
55	MG	YA	3005	1/1	0.96	0.22	26,26,26,26	0
55	MG	YA	3006	1/1	0.96	0.12	3,3,3,3	0
55	MG	YA	3185	1/1	0.96	0.05	41,41,41,41	0
55	MG	RA	3264	1/1	0.96	0.10	25,25,25,25	0
55	MG	YA	3012	1/1	0.96	0.12	7,7,7,7	0
55	MG	YA	3424	1/1	0.96	0.16	39,39,39,39	0
55	MG	RA	3298	1/1	0.96	0.11	49,49,49,49	0
55	MG	YA	3085	1/1	0.96	0.07	24,24,24,24	0
55	MG	YA	3311	1/1	0.96	0.13	18,18,18,18	0
55	MG	YA	3014	1/1	0.96	0.14	4,4,4,4	0
55	MG	RA	3206	1/1	0.96	0.10	47,47,47,47	0
55	MG	R1	101	1/1	0.96	0.22	40,40,40,40	0
55	MG	YA	3434	1/1	0.96	0.07	23,23,23,23	0
55	MG	YA	3019	1/1	0.96	0.11	1,1,1,1	0
55	MG	YA	3437	1/1	0.96	0.07	23,23,23,23	0
55	MG	RA	3404	1/1	0.96	0.17	37,37,37,37	0
55	MG	YA	3021	1/1	0.96	0.07	13,13,13,13	0
55	MG	RA	3182	1/1	0.96	0.11	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	QA	1644	1/1	0.96	0.09	40,40,40,40	0
55	MG	YA	3096	1/1	0.96	0.18	0,0,0,0	0
55	MG	YB	205	1/1	0.96	0.14	41,41,41,41	0
55	MG	YA	3098	1/1	0.96	0.16	2,2,2,2	0
55	MG	XA	1653	1/1	0.96	0.10	41,41,41,41	0
55	MG	XA	1654	1/1	0.96	0.16	27,27,27,27	0
55	MG	YE	301	1/1	0.96	0.16	24,24,24,24	0
55	MG	QA	1675	1/1	0.96	0.07	46,46,46,46	0
55	MG	RA	3034	1/1	0.96	0.08	27,27,27,27	0
55	MG	RA	3273	1/1	0.96	0.04	63,63,63,63	0
55	MG	QA	1603	1/1	0.96	0.05	41,41,41,41	0
55	MG	RA	3414	1/1	0.96	0.08	41,41,41,41	0
55	MG	YA	3223	1/1	0.96	0.12	12,12,12,12	0
55	MG	RA	3036	1/1	0.96	0.11	32,32,32,32	0
55	MG	RA	3246	1/1	0.96	0.14	44,44,44,44	0
55	MG	YA	3226	1/1	0.96	0.22	45,45,45,45	0
55	MG	RF	301	1/1	0.97	0.10	37,37,37,37	0
55	MG	YA	3334	1/1	0.97	0.07	31,31,31,31	0
55	MG	YA	3335	1/1	0.97	0.14	2,2,2,2	0
55	MG	RA	3358	1/1	0.97	0.16	19,19,19,19	0
55	MG	YA	3222	1/1	0.97	0.14	8,8,8,8	0
55	MG	RA	3022	1/1	0.97	0.06	48,48,48,48	0
55	MG	YA	3128	1/1	0.97	0.14	10,10,10,10	0
55	MG	YA	3129	1/1	0.97	0.13	10,10,10,10	0
55	MG	YA	3130	1/1	0.97	0.10	22,22,22,22	0
55	MG	YA	3343	1/1	0.97	0.06	39,39,39,39	0
55	MG	RA	3403	1/1	0.97	0.04	25,25,25,25	0
55	MG	YA	3132	1/1	0.97	0.17	1,1,1,1	0
55	MG	YA	3133	1/1	0.97	0.07	6,6,6,6	0
55	MG	YA	3134	1/1	0.97	0.10	28,28,28,28	0
55	MG	YA	3001	1/1	0.97	0.04	16,16,16,16	0
55	MG	YA	3232	1/1	0.97	0.16	24,24,24,24	0
55	MG	YA	3351	1/1	0.97	0.16	22,22,22,22	0
55	MG	RA	3361	1/1	0.97	0.14	37,37,37,37	0
55	MG	RA	3405	1/1	0.97	0.14	24,24,24,24	0
55	MG	RA	3243	1/1	0.97	0.10	17,17,17,17	0
55	MG	YA	3140	1/1	0.97	0.15	10,10,10,10	0
55	MG	RA	3076	1/1	0.97	0.04	19,19,19,19	0
55	MG	YA	3142	1/1	0.97	0.25	1,1,1,1	0
55	MG	RA	3408	1/1	0.97	0.14	21,21,21,21	0
55	MG	YA	3363	1/1	0.97	0.07	9,9,9,9	0
55	MG	YA	3008	1/1	0.97	0.09	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	RA	3245	1/1	0.97	0.13	32,32,32,32	0
55	MG	YA	3366	1/1	0.97	0.13	25,25,25,25	0
55	MG	YA	3069	1/1	0.97	0.07	15,15,15,15	0
55	MG	QF	301	1/1	0.97	0.06	46,46,46,46	0
55	MG	RA	3017	1/1	0.97	0.12	16,16,16,16	0
55	MG	YA	3247	1/1	0.97	0.09	2,2,2,2	0
55	MG	YA	3371	1/1	0.97	0.10	21,21,21,21	0
55	MG	RA	3271	1/1	0.97	0.17	47,47,47,47	0
55	MG	YA	3250	1/1	0.97	0.22	30,30,30,30	0
55	MG	YA	3374	1/1	0.97	0.10	27,27,27,27	0
55	MG	RA	3205	1/1	0.97	0.07	40,40,40,40	0
55	MG	YA	3376	1/1	0.97	0.16	9,9,9,9	0
55	MG	YA	3255	1/1	0.97	0.08	18,18,18,18	0
55	MG	YA	3153	1/1	0.97	0.11	16,16,16,16	0
55	MG	YA	3154	1/1	0.97	0.06	21,21,21,21	0
55	MG	RA	3326	1/1	0.97	0.03	21,21,21,21	0
55	MG	YA	3259	1/1	0.97	0.08	31,31,31,31	0
55	MG	RA	3088	1/1	0.97	0.06	36,36,36,36	0
55	MG	YA	3158	1/1	0.97	0.11	8,8,8,8	0
55	MG	YA	3263	1/1	0.97	0.11	4,4,4,4	0
55	MG	RA	3328	1/1	0.97	0.15	22,22,22,22	0
55	MG	RA	3172	1/1	0.97	0.17	36,36,36,36	0
55	MG	RA	3102	1/1	0.97	0.09	46,46,46,46	0
55	MG	YA	3162	1/1	0.97	0.12	20,20,20,20	0
55	MG	RA	3331	1/1	0.97	0.14	36,36,36,36	0
55	MG	RA	3136	1/1	0.97	0.09	52,52,52,52	0
55	MG	YA	3026	1/1	0.97	0.07	5,5,5,5	0
55	MG	XA	1665	1/1	0.97	0.18	34,34,34,34	0
55	MG	YA	3395	1/1	0.97	0.06	31,31,31,31	0
55	MG	YA	3396	1/1	0.97	0.11	38,38,38,38	0
55	MG	RA	3277	1/1	0.97	0.04	28,28,28,28	0
55	MG	YA	3172	1/1	0.97	0.12	3,3,3,3	0
55	MG	YA	3030	1/1	0.97	0.14	0,0,0,0	0
55	MG	YA	3174	1/1	0.97	0.04	20,20,20,20	0
55	MG	YA	3277	1/1	0.97	0.18	40,40,40,40	0
55	MG	YA	3402	1/1	0.97	0.21	44,44,44,44	0
55	MG	RA	3377	1/1	0.97	0.10	30,30,30,30	0
55	MG	RA	3335	1/1	0.97	0.07	51,51,51,51	0
55	MG	YA	3280	1/1	0.97	0.12	4,4,4,4	0
55	MG	YA	3090	1/1	0.97	0.04	27,27,27,27	0
55	MG	RA	3336	1/1	0.97	0.12	31,31,31,31	0
55	MG	RA	3028	1/1	0.97	0.05	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	3093	1/1	0.97	0.16	3,3,3,3	0
55	MG	YA	3287	1/1	0.97	0.12	31,31,31,31	0
55	MG	YA	3288	1/1	0.97	0.05	37,37,37,37	0
55	MG	RA	3338	1/1	0.97	0.12	28,28,28,28	0
55	MG	RA	3090	1/1	0.97	0.27	27,27,27,27	0
55	MG	YA	3292	1/1	0.97	0.20	29,29,29,29	0
55	MG	RA	3124	1/1	0.97	0.11	18,18,18,18	0
55	MG	YA	3097	1/1	0.97	0.17	1,1,1,1	0
55	MG	YA	3038	1/1	0.97	0.09	7,7,7,7	0
55	MG	YA	3099	1/1	0.97	0.15	0,0,0,0	0
55	MG	YA	3039	1/1	0.97	0.12	1,1,1,1	0
55	MG	YA	3189	1/1	0.97	0.13	40,40,40,40	0
55	MG	RA	3385	1/1	0.97	0.08	41,41,41,41	0
55	MG	YA	3192	1/1	0.97	0.23	50,50,50,50	0
55	MG	RA	3232	1/1	0.97	0.11	20,20,20,20	0
55	MG	RB	205	1/1	0.97	0.08	24,24,24,24	0
55	MG	YA	3305	1/1	0.97	0.14	28,28,28,28	0
55	MG	RA	3105	1/1	0.97	0.03	15,15,15,15	0
55	MG	RA	3235	1/1	0.97	0.09	35,35,35,35	0
55	MG	YA	3197	1/1	0.97	0.06	27,27,27,27	0
55	MG	YA	3432	1/1	0.97	0.08	12,12,12,12	0
55	MG	RA	3347	1/1	0.97	0.04	57,57,57,57	0
55	MG	RA	3348	1/1	0.97	0.10	54,54,54,54	0
55	MG	RA	3142	1/1	0.97	0.06	11,11,11,11	0
55	MG	YA	3203	1/1	0.97	0.14	10,10,10,10	0
55	MG	YA	3204	1/1	0.97	0.11	10,10,10,10	0
55	MG	RA	3353	1/1	0.97	0.17	36,36,36,36	0
55	MG	RA	3041	1/1	0.97	0.06	46,46,46,46	0
55	MG	YB	203	1/1	0.97	0.10	13,13,13,13	0
55	MG	XA	1636	1/1	0.97	0.07	26,26,26,26	0
55	MG	YA	3208	1/1	0.97	0.07	20,20,20,20	0
55	MG	YA	3209	1/1	0.97	0.22	21,21,21,21	0
55	MG	RA	3047	1/1	0.97	0.10	37,37,37,37	0
55	MG	YA	3322	1/1	0.97	0.14	18,18,18,18	0
55	MG	RA	3064	1/1	0.97	0.08	22,22,22,22	0
55	MG	YA	3324	1/1	0.97	0.04	33,33,33,33	0
55	MG	XA	1639	1/1	0.97	0.07	38,38,38,38	0
55	MG	YA	3326	1/1	0.97	0.05	18,18,18,18	0
55	MG	RA	3056	1/1	0.97	0.08	46,46,46,46	0
55	MG	YA	3328	1/1	0.97	0.09	9,9,9,9	0
55	MG	RE	304	1/1	0.97	0.12	14,14,14,14	0
56	SF4	QD	301	8/8	0.97	0.05	96,109,113,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	Y1	101	1/1	0.97	0.05	31,31,31,31	0
55	MG	YA	3331	1/1	0.97	0.08	40,40,40,40	0
55	MG	YA	3332	1/1	0.97	0.07	39,39,39,39	0
57	ZN	Y9	101	1/1	0.97	0.05	54,54,54,54	0
55	MG	RA	3381	1/1	0.98	0.04	22,22,22,22	0
55	MG	YA	3191	1/1	0.98	0.03	56,56,56,56	0
55	MG	YA	3252	1/1	0.98	0.15	1,1,1,1	0
55	MG	YA	3389	1/1	0.98	0.07	15,15,15,15	0
55	MG	RA	3100	1/1	0.98	0.06	29,29,29,29	0
55	MG	YA	3319	1/1	0.98	0.03	1,1,1,1	0
55	MG	RA	3267	1/1	0.98	0.08	10,10,10,10	0
55	MG	XA	1664	1/1	0.98	0.09	28,28,28,28	0
55	MG	RA	3111	1/1	0.98	0.05	29,29,29,29	0
55	MG	XA	1631	1/1	0.98	0.03	36,36,36,36	0
55	MG	YA	3007	1/1	0.98	0.11	1,1,1,1	0
55	MG	RA	3233	1/1	0.98	0.09	16,16,16,16	0
55	MG	YA	3144	1/1	0.98	0.06	14,14,14,14	0
55	MG	YA	3010	1/1	0.98	0.10	9,9,9,9	0
55	MG	YA	3202	1/1	0.98	0.03	17,17,17,17	0
55	MG	YA	3265	1/1	0.98	0.10	21,21,21,21	0
55	MG	RA	3151	1/1	0.98	0.20	39,39,39,39	0
55	MG	RA	3360	1/1	0.98	0.13	39,39,39,39	0
55	MG	QA	1636	1/1	0.98	0.03	38,38,38,38	0
55	MG	RA	3114	1/1	0.98	0.12	6,6,6,6	0
55	MG	YA	3150	1/1	0.98	0.13	2,2,2,2	0
55	MG	RA	3390	1/1	0.98	0.07	41,41,41,41	0
55	MG	RA	3004	1/1	0.98	0.06	21,21,21,21	0
55	MG	YA	3210	1/1	0.98	0.23	25,25,25,25	0
55	MG	YA	3339	1/1	0.98	0.04	20,20,20,20	0
55	MG	YA	3211	1/1	0.98	0.16	19,19,19,19	0
55	MG	YA	3017	1/1	0.98	0.12	7,7,7,7	0
55	MG	YA	3102	1/1	0.98	0.06	1,1,1,1	0
55	MG	YA	3018	1/1	0.98	0.14	1,1,1,1	0
55	MG	YA	3415	1/1	0.98	0.15	38,38,38,38	0
55	MG	YA	3344	1/1	0.98	0.09	11,11,11,11	0
55	MG	YA	3104	1/1	0.98	0.03	26,26,26,26	0
55	MG	YA	3418	1/1	0.98	0.25	42,42,42,42	0
55	MG	RA	3393	1/1	0.98	0.04	38,38,38,38	0
55	MG	XA	1607	1/1	0.98	0.06	28,28,28,28	0
55	MG	RA	3053	1/1	0.98	0.13	23,23,23,23	0
55	MG	YA	3282	1/1	0.98	0.10	3,3,3,3	0
55	MG	RA	3141	1/1	0.98	0.06	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	YA	3221	1/1	0.98	0.10	26,26,26,26	0
55	MG	RA	3396	1/1	0.98	0.03	29,29,29,29	0
55	MG	RA	3157	1/1	0.98	0.13	24,24,24,24	0
55	MG	RA	3117	1/1	0.98	0.07	35,35,35,35	0
55	MG	YA	3115	1/1	0.98	0.16	3,3,3,3	0
55	MG	YA	3358	1/1	0.98	0.07	13,13,13,13	0
55	MG	YA	3290	1/1	0.98	0.10	1,1,1,1	0
55	MG	YA	3168	1/1	0.98	0.05	22,22,22,22	0
55	MG	YA	3027	1/1	0.98	0.12	5,5,5,5	0
55	MG	YA	3435	1/1	0.98	0.04	17,17,17,17	0
55	MG	YA	3362	1/1	0.98	0.10	18,18,18,18	0
55	MG	XA	1681	1/1	0.98	0.14	20,20,20,20	0
55	MG	RA	3065	1/1	0.98	0.06	18,18,18,18	0
55	MG	RA	3342	1/1	0.98	0.04	31,31,31,31	0
55	MG	YA	3296	1/1	0.98	0.12	17,17,17,17	0
55	MG	RA	3343	1/1	0.98	0.12	14,14,14,14	0
55	MG	RA	3297	1/1	0.98	0.07	26,26,26,26	0
55	MG	RA	3054	1/1	0.98	0.04	21,21,21,21	0
55	MG	YA	3300	1/1	0.98	0.08	5,5,5,5	0
55	MG	YA	3123	1/1	0.98	0.23	22,22,22,22	0
55	MG	QA	1680	1/1	0.98	0.03	32,32,32,32	0
55	MG	YB	208	1/1	0.98	0.03	25,25,25,25	0
55	MG	RA	3146	1/1	0.98	0.19	18,18,18,18	0
55	MG	RA	3323	1/1	0.98	0.07	11,11,11,11	0
55	MG	YA	3077	1/1	0.98	0.15	12,12,12,12	0
55	MG	RA	3349	1/1	0.98	0.05	25,25,25,25	0
55	MG	YQ	201	1/1	0.98	0.04	30,30,30,30	0
55	MG	RA	3092	1/1	0.98	0.03	50,50,50,50	0
55	MG	RA	3409	1/1	0.98	0.07	24,24,24,24	0
55	MG	RA	3352	1/1	0.98	0.05	35,35,35,35	0
55	MG	YA	3243	1/1	0.98	0.16	0,0,0,0	0
55	MG	YA	3083	1/1	0.98	0.04	11,11,11,11	0
55	MG	YA	3382	1/1	0.98	0.12	24,24,24,24	0
55	MG	RA	3302	1/1	0.98	0.03	37,37,37,37	0
55	MG	YA	3246	1/1	0.98	0.07	3,3,3,3	0
57	ZN	XN	101	1/1	0.98	0.05	144,144,144,144	0
55	MG	RA	3108	1/1	0.98	0.09	10,10,10,10	0
55	MG	RA	3227	1/1	0.99	0.06	20,20,20,20	0
55	MG	YA	3156	1/1	0.99	0.04	6,6,6,6	0
55	MG	YA	3433	1/1	0.99	0.04	18,18,18,18	0
55	MG	YA	3251	1/1	0.99	0.18	5,5,5,5	0
55	MG	RA	3159	1/1	0.99	0.04	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	YA	3253	1/1	0.99	0.03	1,1,1,1	0
55	MG	RA	3340	1/1	0.99	0.06	11,11,11,11	0
55	MG	XA	1652	1/1	0.99	0.05	26,26,26,26	0
55	MG	RA	3426	1/1	0.99	0.04	34,34,34,34	0
55	MG	YA	3285	1/1	0.99	0.10	1,1,1,1	0
55	MG	YA	3106	1/1	0.99	0.03	18,18,18,18	0
55	MG	RA	3109	1/1	0.99	0.07	21,21,21,21	0
55	MG	YA	3108	1/1	0.99	0.10	2,2,2,2	0
55	MG	RA	3350	1/1	0.99	0.03	29,29,29,29	0
55	MG	YA	3187	1/1	0.99	0.04	22,22,22,22	0
55	MG	YA	3320	1/1	0.99	0.06	42,42,42,42	0
55	MG	YA	3262	1/1	0.99	0.20	5,5,5,5	0
55	MG	YA	3165	1/1	0.99	0.17	13,13,13,13	0
55	MG	YA	3212	1/1	0.99	0.06	22,22,22,22	0
55	MG	YA	3022	1/1	0.99	0.07	8,8,8,8	0
55	MG	YA	3356	1/1	0.99	0.03	0,0,0,0	0
55	MG	YA	3009	1/1	0.99	0.15	1,1,1,1	0
55	MG	YA	3169	1/1	0.99	0.05	15,15,15,15	0
55	MG	RA	3112	1/1	0.99	0.06	26,26,26,26	0
55	MG	RA	3241	1/1	0.99	0.18	5,5,5,5	0
55	MG	YA	3082	1/1	0.99	0.04	10,10,10,10	0
55	MG	RA	3063	1/1	0.99	0.09	17,17,17,17	0
56	SF4	XD	301	8/8	0.99	0.03	95,101,103,103	0
55	MG	RA	3321	1/1	0.99	0.05	23,23,23,23	0
57	ZN	R5	101	1/1	0.99	0.04	84,84,84,84	0
57	ZN	R6	101	1/1	0.99	0.05	70,70,70,70	0
55	MG	YA	3135	1/1	0.99	0.02	32,32,32,32	0
55	MG	YA	3198	1/1	0.99	0.21	5,5,5,5	0
55	MG	RA	3391	1/1	0.99	0.07	25,25,25,25	0
57	ZN	Y5	101	1/1	0.99	0.03	66,66,66,66	0
55	MG	YA	3248	1/1	0.99	0.04	1,1,1,1	0
57	ZN	YY	201	1/1	0.99	0.02	69,69,69,69	0
55	MG	YA	3426	1/1	1.00	0.17	4,4,4,4	0
55	MG	RA	3332	1/1	1.00	0.04	4,4,4,4	0
55	MG	YA	3355	1/1	1.00	0.06	5,5,5,5	0
55	MG	YA	3113	1/1	1.00	0.07	10,10,10,10	0
55	MG	YA	3166	1/1	1.00	0.13	9,9,9,9	0
57	ZN	Y6	101	1/1	1.00	0.02	44,44,44,44	0
55	MG	RA	3425	1/1	1.00	0.02	25,25,25,25	0
55	MG	RA	3322	1/1	1.00	0.03	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.