



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:21 PM GMT

PDB ID : 1VVJ
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 bound to Codon CCC-G on the Ribosome
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-05-24
Resolution : 3.44 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

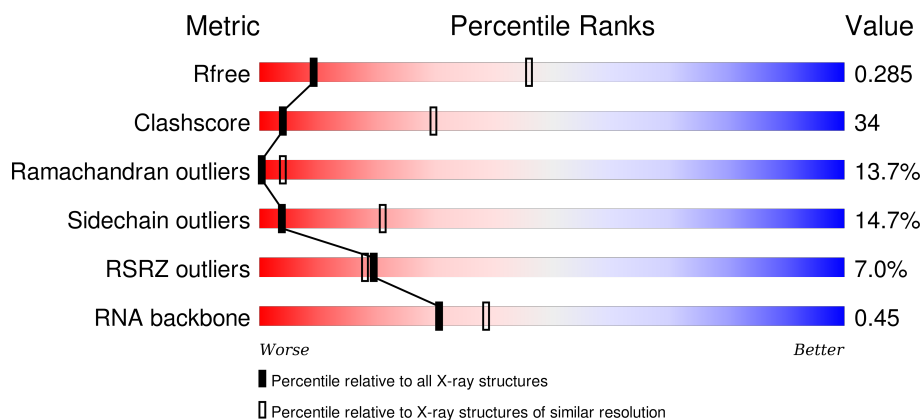
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.44 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}	91344	1007 (3.54-3.34)
Clashscore	102246	1044 (3.52-3.36)
Ramachandran outliers	100387	1013 (3.52-3.36)
Sidechain outliers	100360	1014 (3.52-3.36)
RSRZ outliers	91569	1012 (3.54-3.34)
RNA backbone	2183	1042 (4.02-2.80)

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

Mol	Chain	Length	Quality of chain
1	QA	1522	<div> <div>4%</div> <div>36%</div> <div>46%</div> <div>15%</div> <div>..</div> </div>
1	XA	1522	<div> <div>3%</div> <div>38%</div> <div>45%</div> <div>14%</div> <div>..</div> </div>
2	QB	256	<div> <div>13%</div> <div>16%</div> <div>59%</div> <div>16%</div> <div>7%</div> </div>
2	XB	256	<div> <div>11%</div> <div>16%</div> <div>60%</div> <div>16%</div> <div>7%</div> </div>

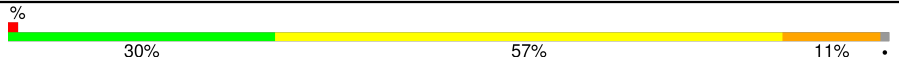
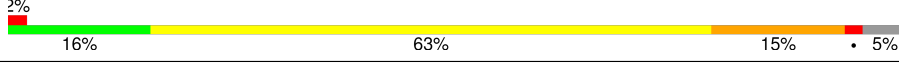
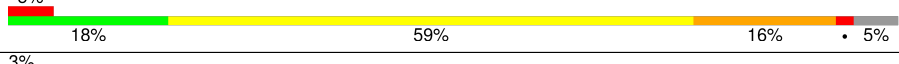
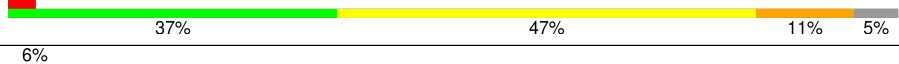
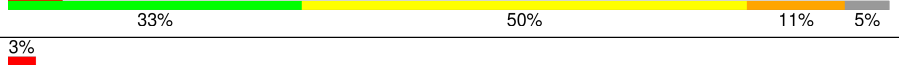
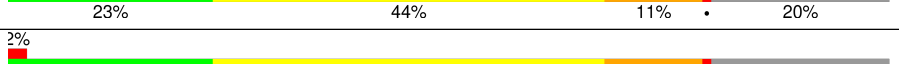
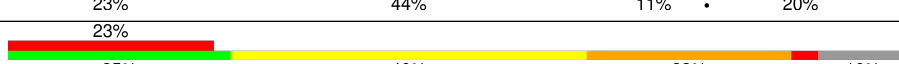
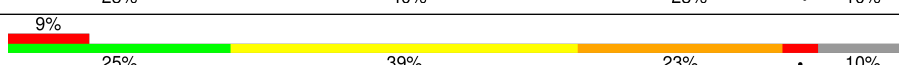
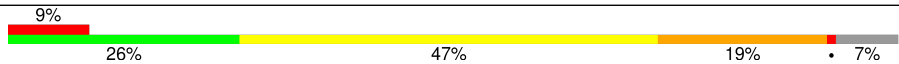
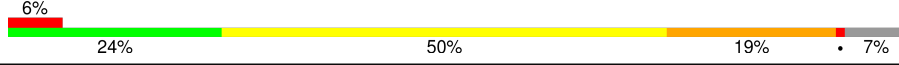
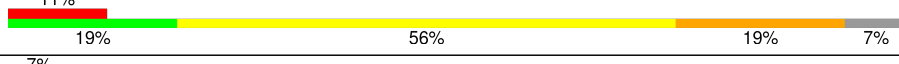
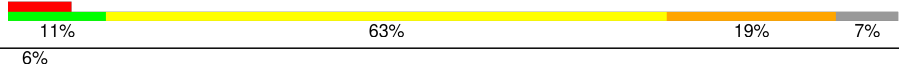
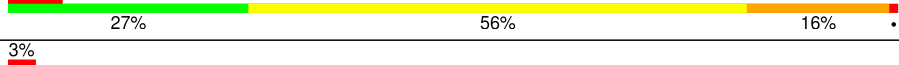


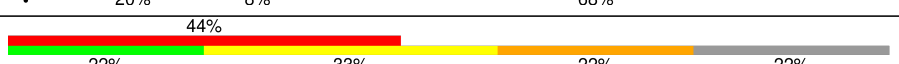
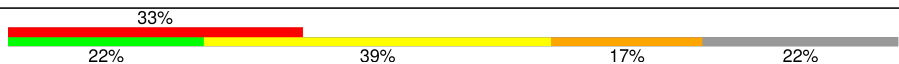
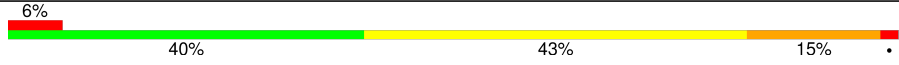
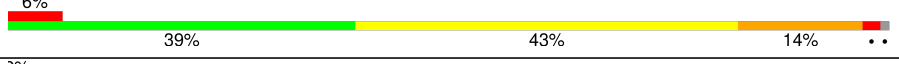


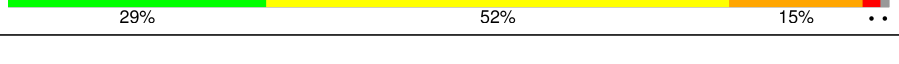



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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126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

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Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	25	
23	XX	25	
24	QY	18	
24	XY	18	
25	RA	2916	
25	YA	2916	
26	RB	122	
26	YB	122	
27	RD	276	
27	YD	276	

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Mol	Chain	Length	Quality of chain
28	RE	206	
28	YE	206	
29	RF	210	
29	YF	210	
30	RG	182	
30	YG	182	
31	RH	180	
31	YH	180	
32	RI	148	
32	YI	148	
33	RN	140	
33	YN	140	
34	RO	122	
34	YO	122	
35	RP	150	
35	YP	150	
36	RQ	141	
36	YQ	141	
37	RR	118	
37	YR	118	
38	RS	112	
38	YS	112	
39	RT	146	
39	YT	146	
40	RU	118	

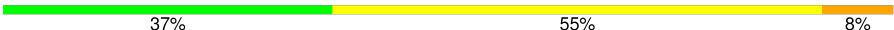




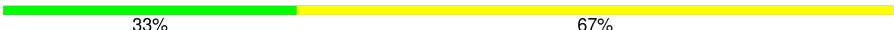
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Mol	Chain	Length	Quality of chain
40	YU	118	
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	71	
51	R5	60	
51	Y5	60	
52	R6	54	
52	Y6	54	

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Mol	Chain	Length	Quality of chain
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	Z6	3	
55	Z8	3	

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
56	MG	QA	1601	-	-	-	X
56	MG	QA	1609	-	-	-	X
56	MG	QA	1620	-	-	-	X
56	MG	QA	1626	-	-	-	X
56	MG	QA	1627	-	-	-	X
56	MG	QA	1638	-	-	-	X
56	MG	QA	1649	-	-	-	X
56	MG	RA	3005	-	-	-	X
56	MG	RA	3012	-	-	-	X
56	MG	RA	3014	-	-	-	X
56	MG	RA	3016	-	-	-	X
56	MG	RA	3018	-	-	-	X
56	MG	RA	3021	-	-	-	X
56	MG	RA	3023	-	-	-	X
56	MG	RA	3024	-	-	-	X
56	MG	RA	3030	-	-	-	X
56	MG	RA	3039	-	-	-	X
56	MG	RA	3044	-	-	-	X
56	MG	RA	3045	-	-	-	X
56	MG	RA	3046	-	-	-	X
56	MG	RA	3048	-	-	-	X
56	MG	RA	3051	-	-	-	X
56	MG	RA	3052	-	-	-	X
56	MG	RA	3054	-	-	-	X
56	MG	RA	3058	-	-	-	X
56	MG	RA	3060	-	-	-	X
56	MG	RA	3062	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3064	-	-	-	X
56	MG	RA	3069	-	-	-	X
56	MG	RA	3070	-	-	-	X
56	MG	RA	3074	-	-	-	X
56	MG	RA	3076	-	-	-	X
56	MG	RA	3077	-	-	-	X
56	MG	RA	3078	-	-	-	X
56	MG	RA	3080	-	-	-	X
56	MG	RA	3081	-	-	-	X
56	MG	RA	3089	-	-	-	X
56	MG	RA	3103	-	-	-	X
56	MG	RA	3104	-	-	-	X
56	MG	RA	3106	-	-	-	X
56	MG	RA	3112	-	-	-	X
56	MG	RA	3117	-	-	-	X
56	MG	RA	3124	-	-	-	X
56	MG	RA	3130	-	-	-	X
56	MG	RA	3136	-	-	-	X
56	MG	RA	3141	-	-	-	X
56	MG	RA	3152	-	-	-	X
56	MG	RA	3166	-	-	-	X
56	MG	RA	3179	-	-	-	X
56	MG	RA	3185	-	-	-	X
56	MG	RA	3189	-	-	-	X
56	MG	RA	3200	-	-	-	X
56	MG	RA	3201	-	-	-	X
56	MG	RA	3202	-	-	-	X
56	MG	RA	3210	-	-	-	X
56	MG	RA	3211	-	-	-	X
56	MG	RE	302	-	-	-	X
56	MG	RP	201	-	-	-	X
56	MG	XA	1605	-	-	-	X
56	MG	XA	1606	-	-	-	X
56	MG	XA	1627	-	-	-	X
56	MG	XA	1642	-	-	-	X
56	MG	XA	1647	-	-	-	X
56	MG	YA	3002	-	-	-	X
56	MG	YA	3004	-	-	-	X
56	MG	YA	3008	-	-	-	X
56	MG	YA	3009	-	-	-	X
56	MG	YA	3011	-	-	-	X
56	MG	YA	3014	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3015	-	-	-	X
56	MG	YA	3023	-	-	-	X
56	MG	YA	3024	-	-	-	X
56	MG	YA	3026	-	-	-	X
56	MG	YA	3031	-	-	-	X
56	MG	YA	3032	-	-	-	X
56	MG	YA	3035	-	-	-	X
56	MG	YA	3036	-	-	-	X
56	MG	YA	3037	-	-	-	X
56	MG	YA	3042	-	-	-	X
56	MG	YA	3044	-	-	-	X
56	MG	YA	3047	-	-	-	X
56	MG	YA	3049	-	-	-	X
56	MG	YA	3050	-	-	-	X
56	MG	YA	3057	-	-	-	X
56	MG	YA	3058	-	-	-	X
56	MG	YA	3068	-	-	-	X
56	MG	YA	3079	-	-	-	X
56	MG	YA	3080	-	-	-	X
56	MG	YA	3081	-	-	-	X
56	MG	YA	3087	-	-	-	X
56	MG	YA	3090	-	-	-	X
56	MG	YA	3100	-	-	-	X
56	MG	YA	3101	-	-	-	X
56	MG	YA	3105	-	-	-	X
56	MG	YA	3107	-	-	-	X
56	MG	YA	3109	-	-	-	X
56	MG	YA	3113	-	-	-	X
56	MG	YA	3117	-	-	-	X
56	MG	YA	3119	-	-	-	X
56	MG	YA	3140	-	-	-	X
56	MG	YA	3152	-	-	-	X
56	MG	YA	3159	-	-	-	X
56	MG	YA	3162	-	-	-	X
56	MG	YA	3164	-	-	-	X
56	MG	YA	3165	-	-	-	X
56	MG	YA	3166	-	-	-	X
56	MG	YA	3170	-	-	-	X
56	MG	YA	3179	-	-	-	X
56	MG	YA	3192	-	-	-	X
56	MG	YA	3194	-	-	-	X
56	MG	YA	3208	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3233	-	-	-	X
56	MG	YA	3234	-	-	-	X
56	MG	YA	3238	-	-	-	X
56	MG	YA	3241	-	-	-	X
56	MG	YA	3242	-	-	-	X
57	PAR	QA	1661	-	-	-	X
57	PAR	XA	1664	-	-	-	X

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 291123 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1500	Total	C	N	O	P	0	0	0
			32247	14353	5981	10414	1499			
1	XA	1501	Total	C	N	O	P	0	0	0
			32269	14363	5986	10420	1500			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
2	XB	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	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	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	XH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- 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	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- 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	99	Total	C	N	O	S	0	0	0
			801	504	157	139	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	119	Total	C	N	O	S	0	0	0
			885	549	168	165	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	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	121	Total	C	N	O	S	0	0	0
			964	597	199	166	2			
13	XM	121	Total	C	N	O	S	0	0	0
			964	597	199	166	2			

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

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	88	Total	C	N	O	S	0	0	0
			734	459	147	126	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	84	Total	C	N	O	S	0	0	0
			674	430	126	116	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 S21.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	XV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 23 is a RNA chain called A-site ASL SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total	C	N	O	P	0	0	0
			170	76	31	55	8			
23	XX	8	Total	C	N	O	P	0	0	0
			170	76	31	55	8			

- Molecule 24 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	14	Total	C	N	O	P	0	0	0
			303	135	55	99	14			
24	XY	14	Total	C	N	O	P	0	0	0
			303	135	55	99	14			

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	RA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			
25	YA	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			

- Molecule 26 is a RNA chain called 5S rRNA.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	RH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
31	YH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
37	YR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
44	YY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RZ	172	Total	C	N	O	S	0	0	0
			1378	879	248	248	3			
45	YZ	172	Total	C	N	O	S	0	0	0
			1378	879	248	248	3			

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			
46	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
47	Y1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	R4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			
50	Y4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	R6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			
52	Y6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	R7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
53	Y7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 54 is a protein called tRNA acceptor end mimic.

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

- Molecule 55 is a RNA chain called RNA (5'-R(*CP*CP*(PPU))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	Z6	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
55	Z8	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

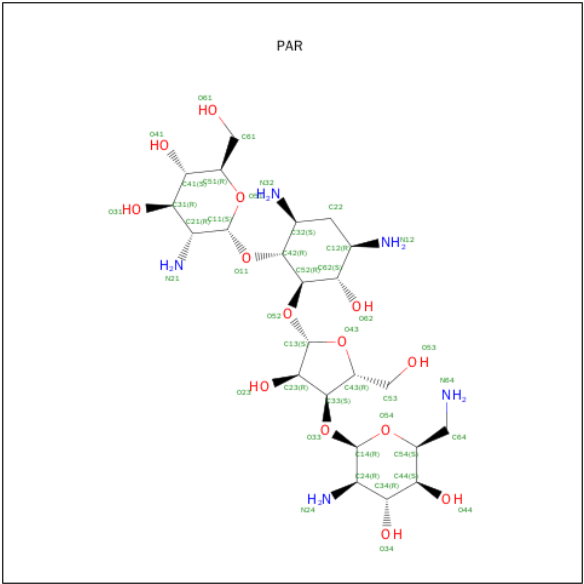
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	RE	2	Total	Mg	0	0
			2	2		
56	YX	1	Total	Mg	0	0
			1	1		
56	XA	63	Total	Mg	0	0
			63	63		
56	QA	60	Total	Mg	0	0
			60	60		
56	Y5	1	Total	Mg	0	0
			1	1		
56	RP	1	Total	Mg	0	0
			1	1		
56	QX	2	Total	Mg	0	0
			2	2		
56	YA	242	Total	Mg	0	0
			242	242		
56	YB	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QF	1	Total	Mg	0	0
			1	1		
56	QM	1	Total	Mg	0	0
			1	1		
56	R5	1	Total	Mg	0	0
			1	1		
56	RB	2	Total	Mg	0	0
			2	2		
56	RA	212	Total	Mg	0	0
			212	212		
56	XM	2	Total	Mg	0	0
			2	2		
56	QH	1	Total	Mg	0	0
			1	1		
56	XV	2	Total	Mg	0	0
			2	2		
56	RF	1	Total	Mg	0	0
			1	1		
56	QV	2	Total	Mg	0	0
			2	2		
56	YE	2	Total	Mg	0	0
			2	2		

- Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	QA	1	Total	C	N	O	0	0
			42	23	5	14		
57	XA	1	Total	C	N	O	0	0
			42	23	5	14		

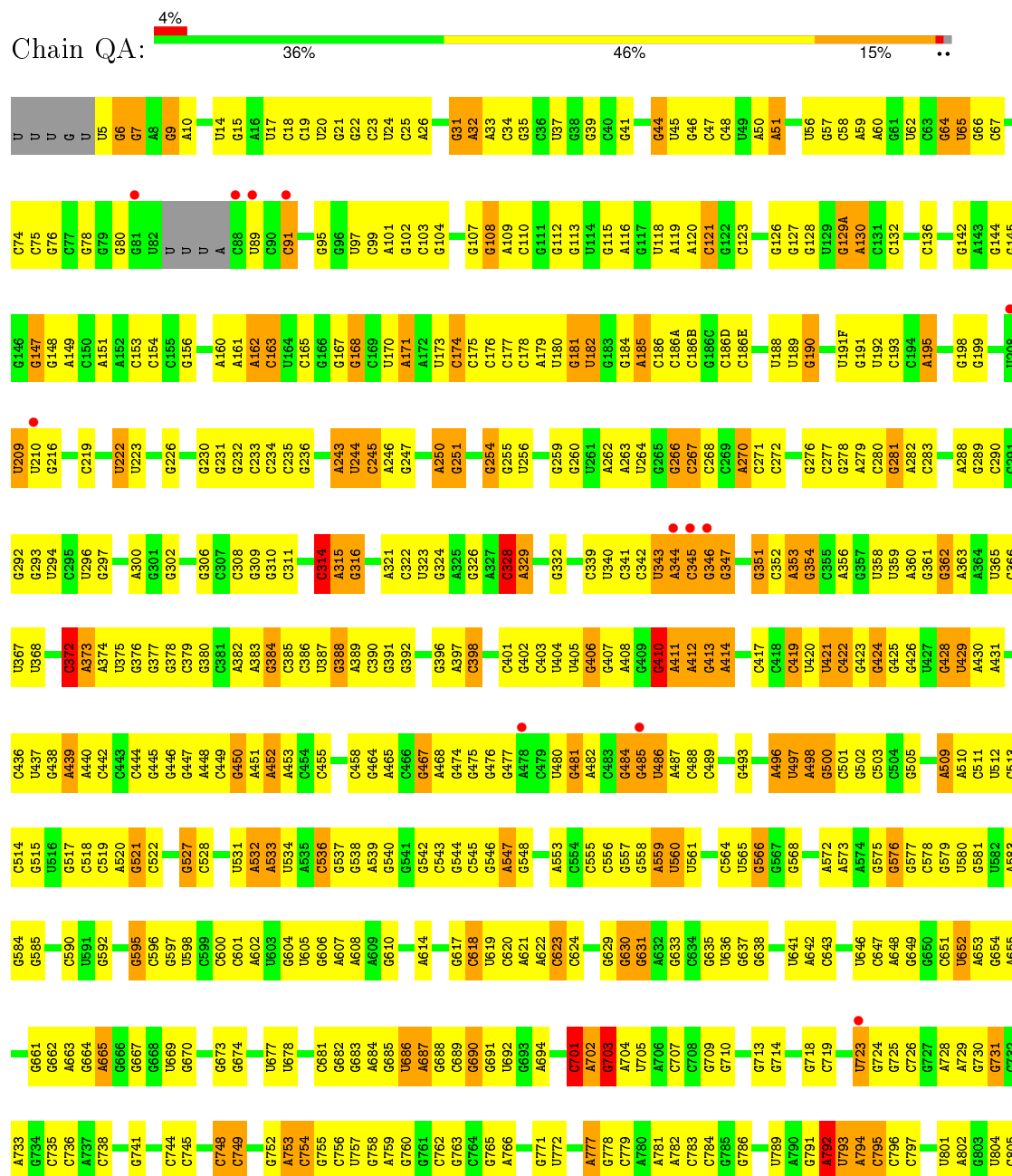
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

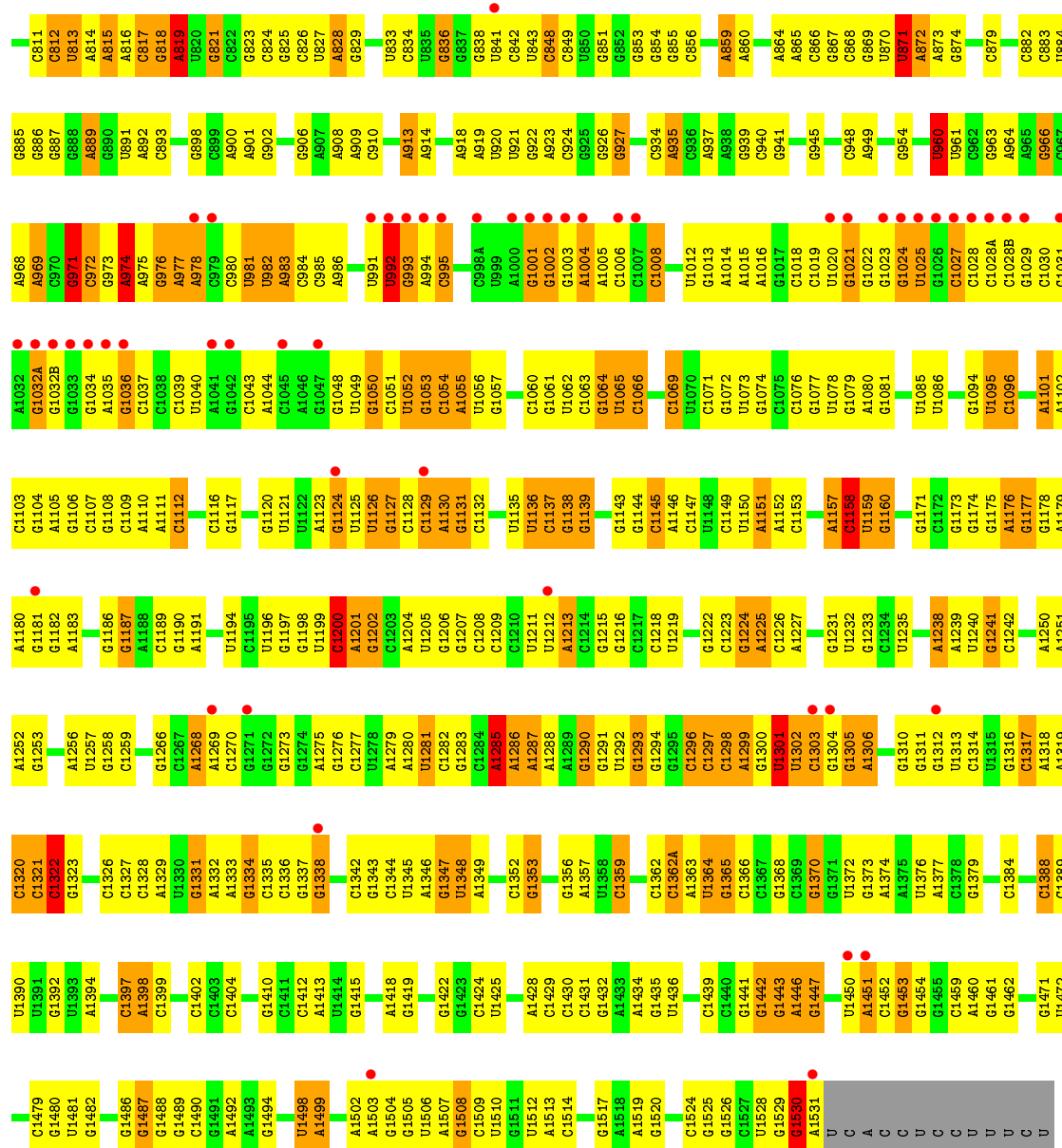
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	XD	1	Total	Zn	0	0
			1	1		
58	QD	1	Total	Zn	0	0
			1	1		
58	QN	1	Total	Zn	0	0
			1	1		
58	XN	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

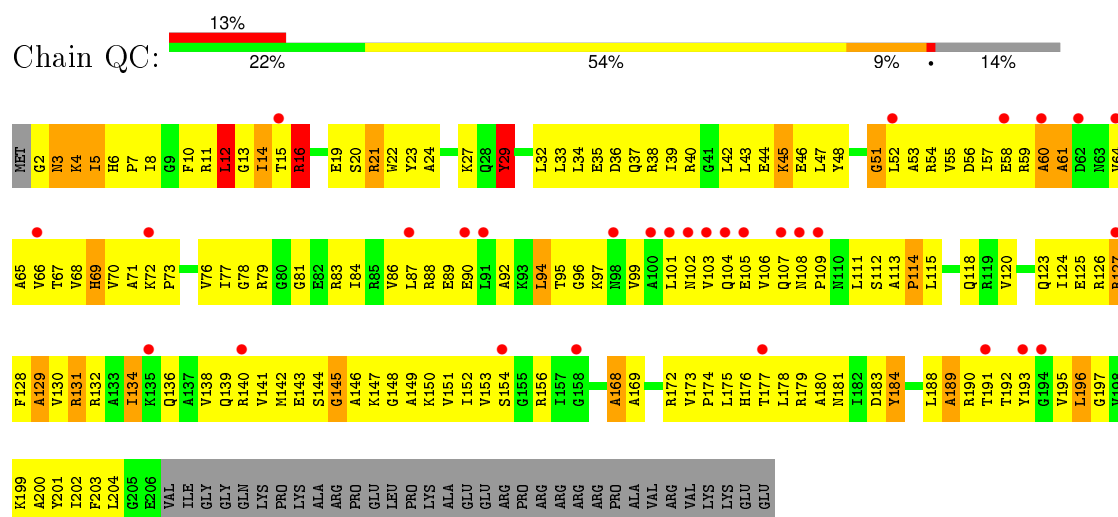
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

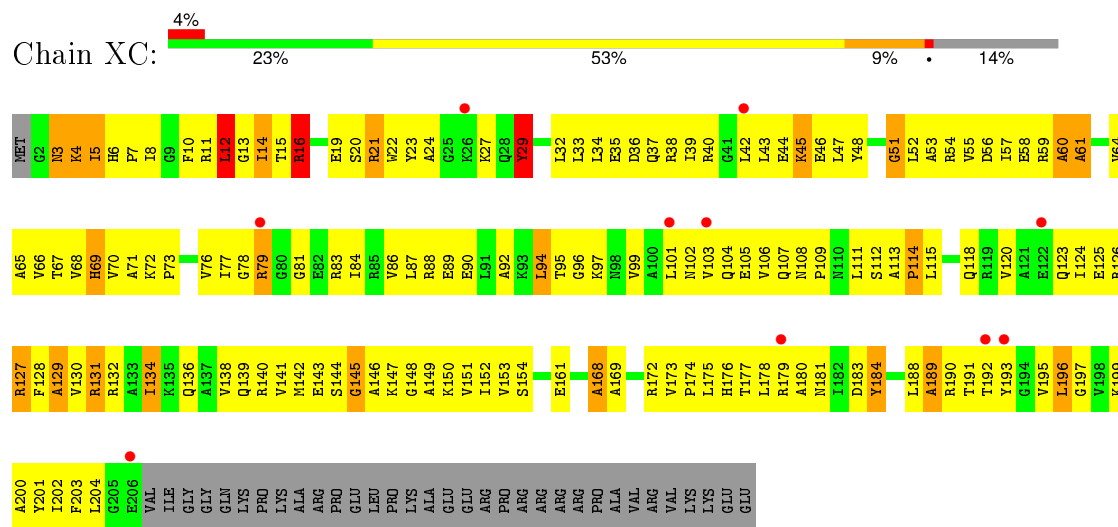




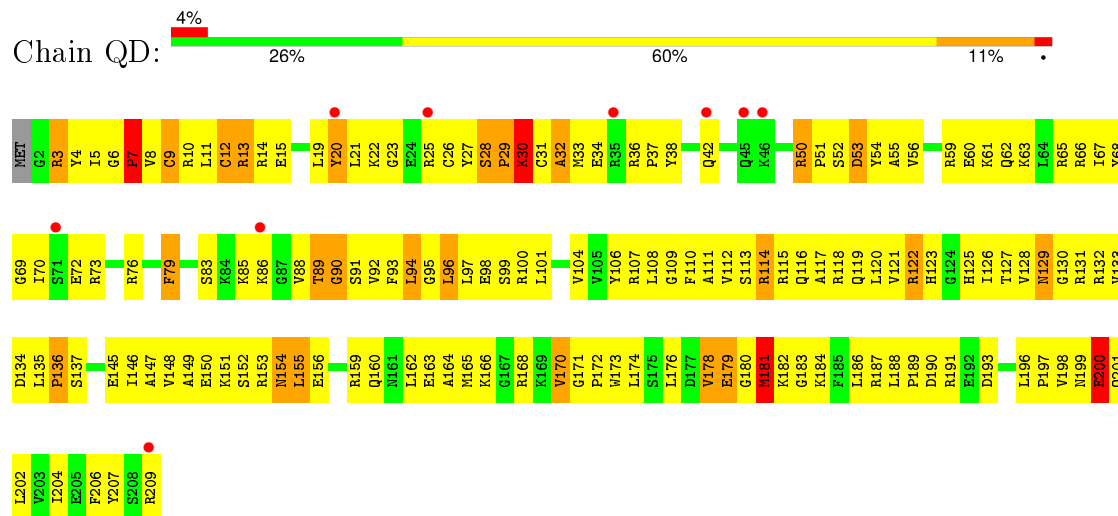
A1285	C1218	C1153	U1078	A1014	A937	A864	G769	C701	A607	A535	A453	G371	A300	C235
A1286	U1219	G1154	G1079	A1015	A938	A865	G773	A702	A608	C536	C454	C372	G301	G236
A1287	G1220	G1155	A1080	A1016	G939	A866	G774	A703	G630	G537	C455	A374	A303	G237
A1288	G1221	G1156	U1085	U1017	G940	G867	A777	A704	G631	G538	C456	U375	A303	G238
G1291	C1223	A1157	U1086	U1020	G941	G867	A777	C707	A632	A539	C457	G376	G309	C240
U1292	G1224	G1158	U1086	U1021	G942	U871	G778	C708	G633	G540	C458	G377	G310	C241
G1293	A1225	U1159	U1091	G1022	A946	A872	G779	A711	C634	G542	A465	G384	G311	C242
G1294	C1226	C1161	G1094	G1023	G947	A873	A780	A712	G637	C545	C466	G384	A313	U243
G1295	A1227	G1162	G1094	G1024	G948	A874	G784	G713	G638	G546	A468	G388	A313	U244
C1296	C1228	U1095	U1095	U1025	A949	C875	G785	G713	G639	A547	A468	A389	A313	C245
C1297	G1229	G1164	C1096	G1026	U950	G876	G785	A715	A640	U547	G474	C390	G316	A246
C1298	C1230	C1165	U1097	G1027	G951	G877	A777	G716	A641	G548	G475	G377	G317	G247
A1299	G1231	G1166	G1099	C1028	U952	C879	U789	C719	U642	G550	U480	G392	G319	A250
G1300	U1232	A1167	C1100	C1028A	G953	C880	A789	C720	A643	C554	G481	G392	G320	G251
G1301	G1233	U1101	A1101	C1028B	G954	G881	A791	G721	C644	C555	C482	A397	A321	U252
U1302	C1234	G1171	A1102	G1029	U955	C882	A792	G722	G644	C556	C483	C398	A321	U253
C1303	U1235	C1172	C1103	C1030	U956	C883	U793	A723	C645	C557	C484	G401	A325	G254
G1304	A1236	U1173	G1104	G1031	U960	U884	A794	U723	U646	G557	G485	G402	A328	U256
G1305	C1237	G1175	A1105	A1032	U961	G885	C795	G724	U648	G558	G486	G402	A329	G257
A1306	A1238	U1176	G1106	G1032A	G962	G886	C796	G725	A648	A559	A487	G403	A329	G258
U1307	C1239	G1177	C1107	G1032B	G963	G887	C797	G726	G649	U560	C488	G406	C330	G259
U1308	U1240	G1178	G1108	G1033	A964	G888	G798	G727	G650	U561	C489	G407	G331	G260
G1309	G1241	A1179	C1109	A964	A965	C889	G798	A728	C651	C562	G490	G410	A411	A261
G1310	C1242	U1180	A1110	G1034	A966	G890	C811	A729	U652	C563	G491	G410	A411	A262
G1311	C1243	G1181	C1111	G1036	U967	U891	C812	G730	A653	C564	G492	G411	A412	A263
C1312	G1244	G1182	C1112	C1037	A968	A892	U813	G731	G654	U565	G493	C335	A412	G264
A1245	C1245	A1183	C1113	C1038	A969	C893	U813	G731		G566	U494	G413	C336	U264
C1246	C1246	G1184	C1114	G1039	C970	G894	A816	G732	U859	C567	U495	G414	C336	U264
U1315	U1040	G1185	C1115	U1040	G971	C895	C817	G735	G660	G570	A496	A414	C337	G265
G1316	G1252	G1186	C1116	C1043	C972	C896	G818	C736	G661	U571	U497	C417	A338	G266
G1317	G1253	G1187	G1117	G1043	G973	C896	A819	A737	G662	A572	A500	C418	C339	G267
A1318	U1254	A1188	U1122	G1047	A974	A900	U820	C738	A663	A573	G500	C419	U340	C268
A1319	A1256	C1189	A1123	G1047	A975	A901	G821	G741	G664	A574	C501	U420	U343	C269
U1257	G1257	G1190	A1123	U1049	A976	G902	G825	G742	G665	A574	G502	U421	U344	A270
G1258	C1258	A1191	G1124	U1049	A977	G903	G825	U743	G666	G575	G502	C422	C345	C271
C1321	U1125	C1192	U1125	G1050	A978	C904	C826	C744	G667	G576	C507	G424	G347	A273
G1322	C1260	G1193	G1126	G1051	C979	U905	U827	C744	G668	C578	C508	G424	G347	G276
A1323	A1261	U1194	G1127	G1052	C980	G906	A828	C745	G668	U580	A510	U427	G350	G277
C1325	C1262	C1195	C1128	C1054	U981	A907	G829	U746	G673	G579	A510	G428	G351	C278
C1263	C1263	U1196	C1129	A1055	U982	A908	G830	C747	G674	U580	C511	C428	G352	A279
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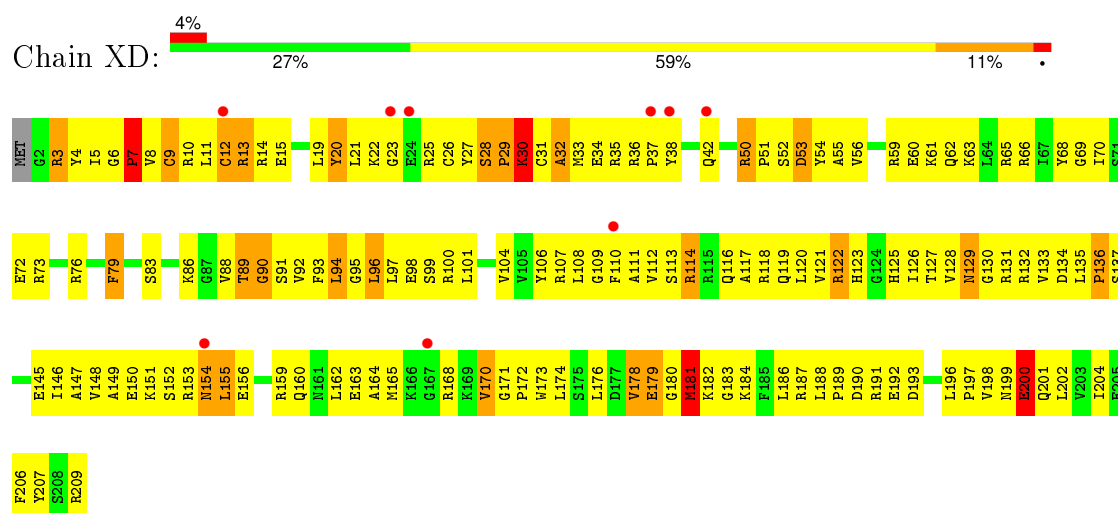
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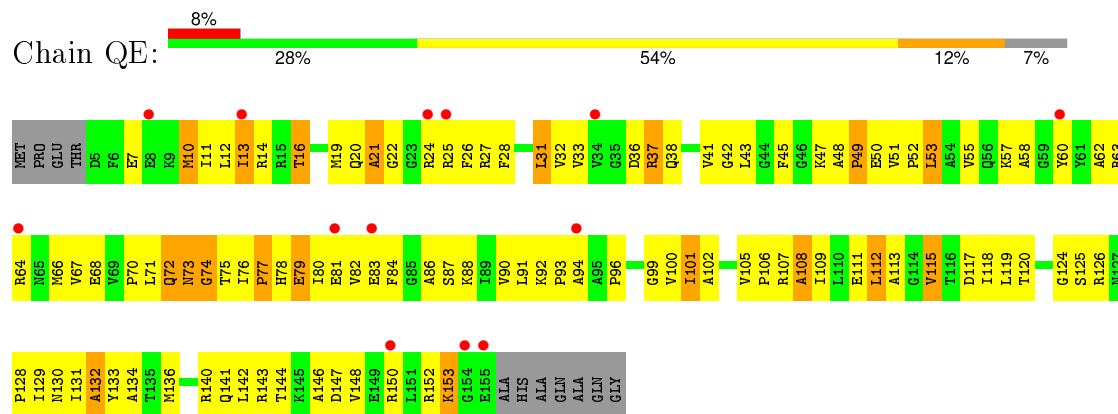
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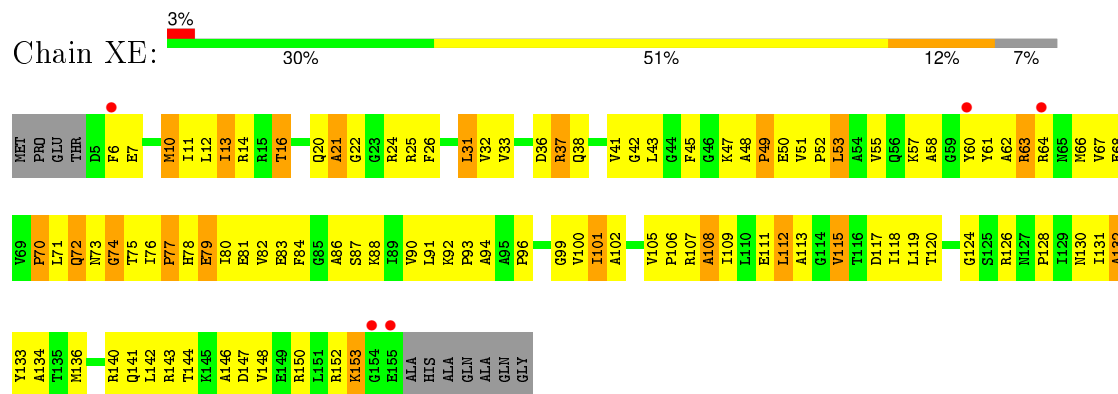
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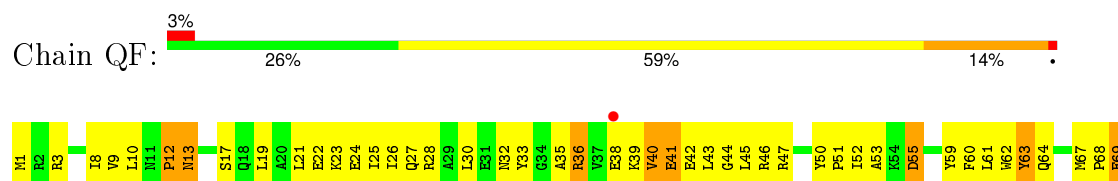
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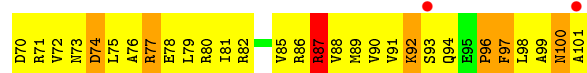


• Molecule 5: 30S ribosomal protein S5

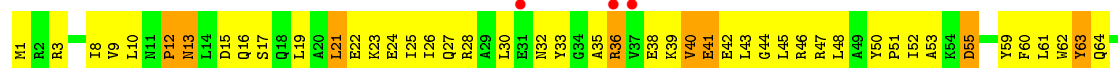


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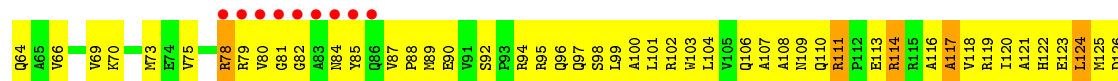




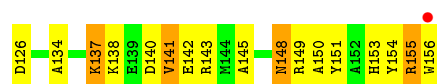
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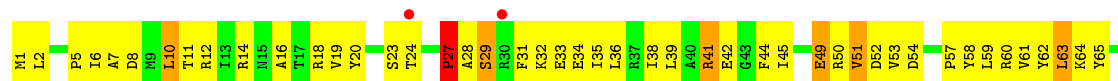
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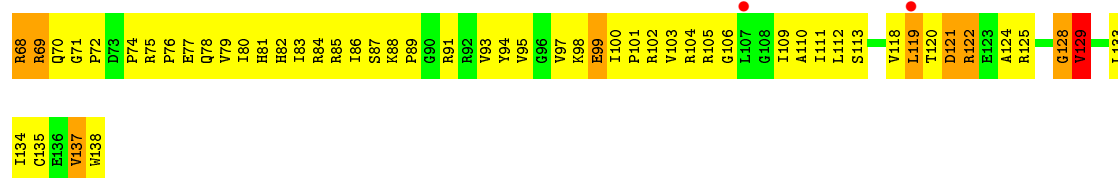


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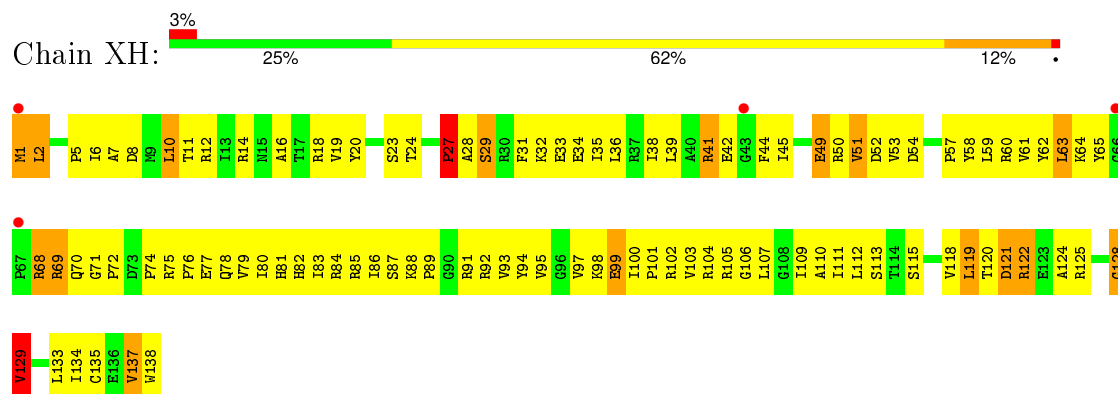


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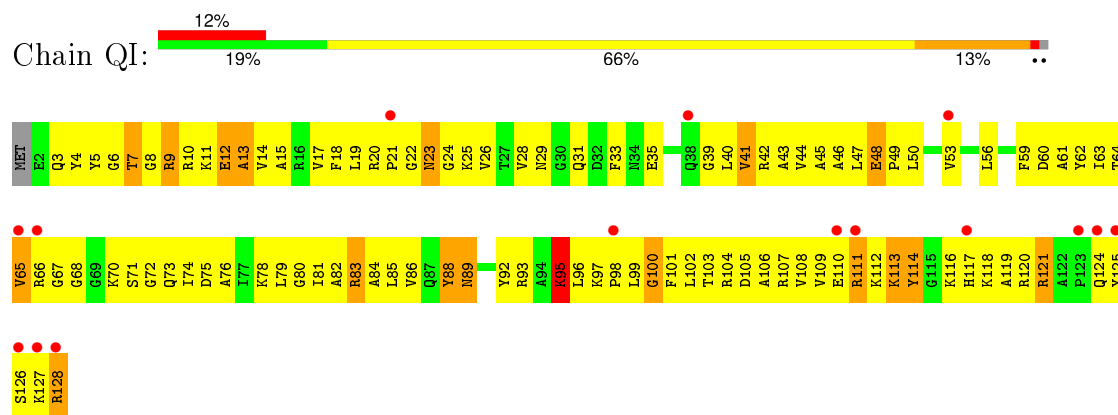




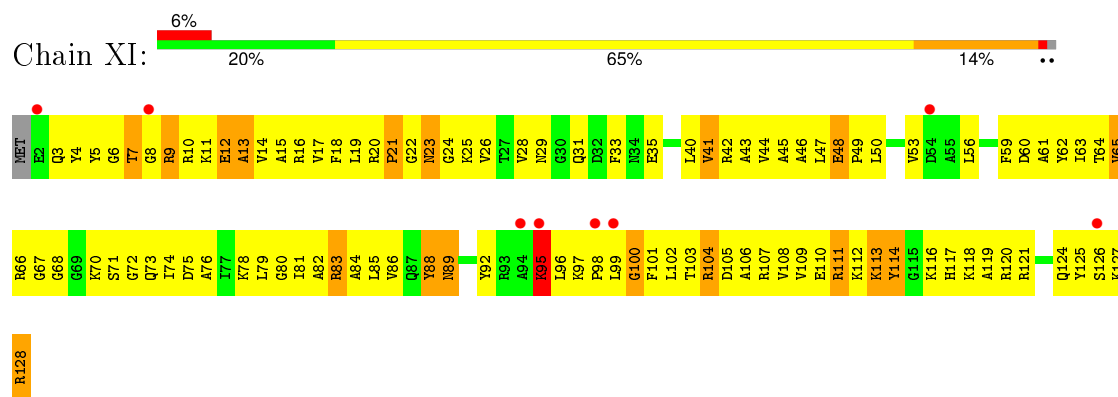
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• Molecule 9: 30S ribosomal protein S9

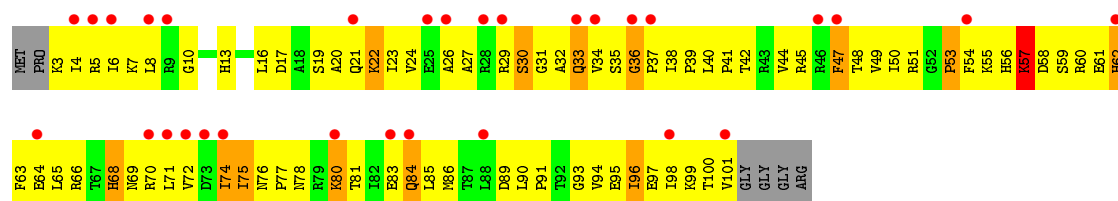


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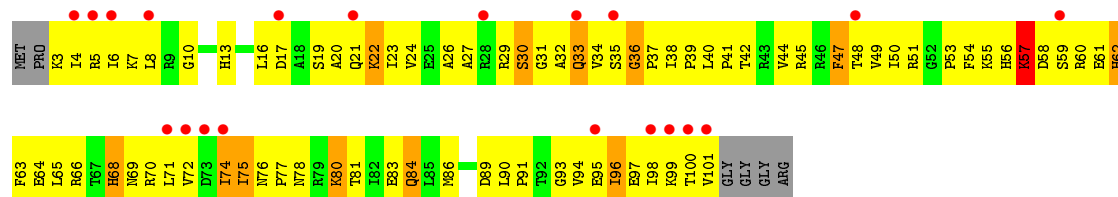


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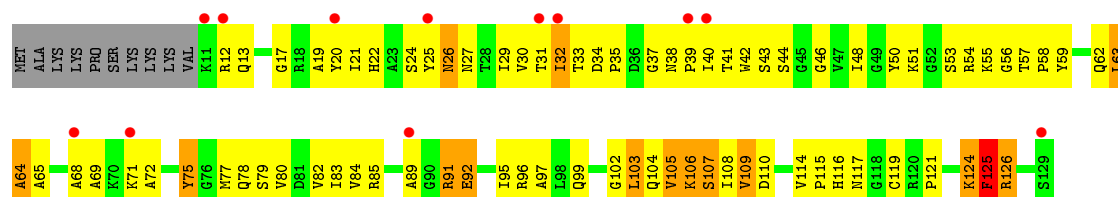




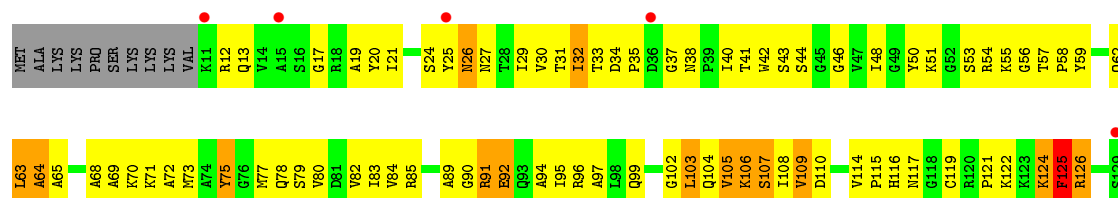
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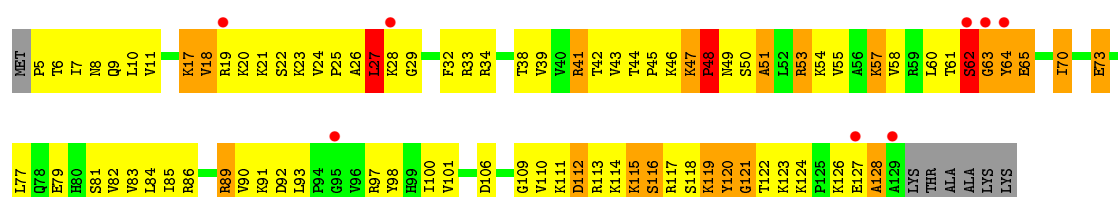
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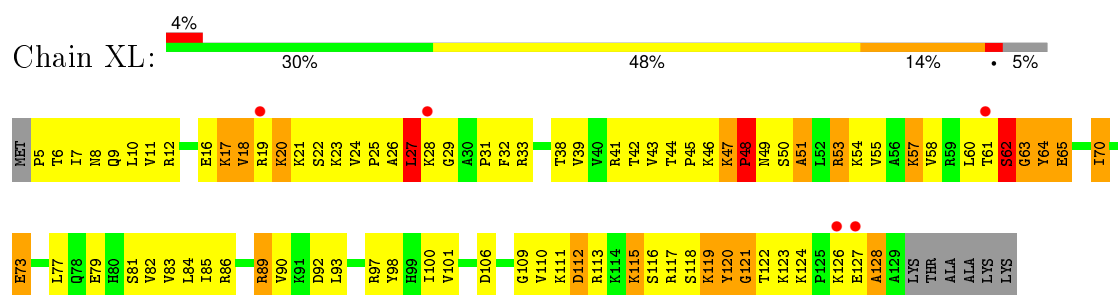
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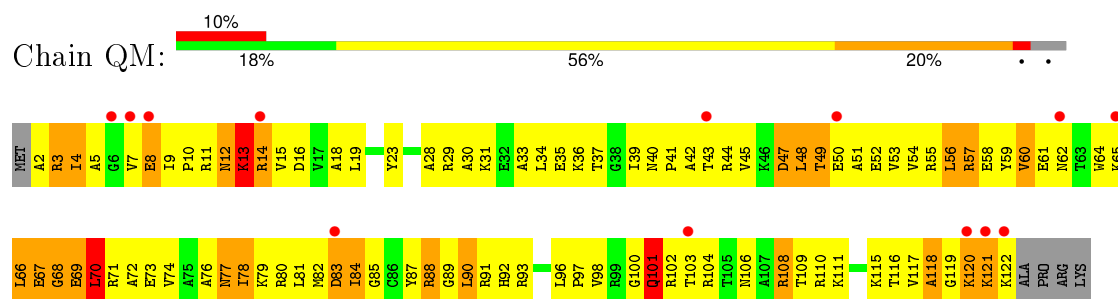
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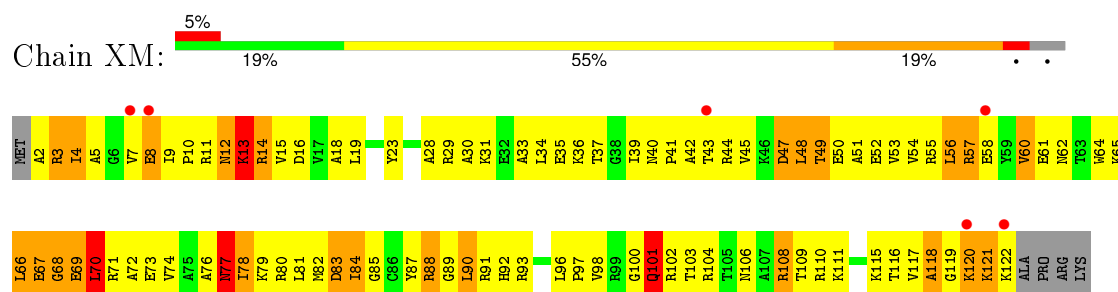
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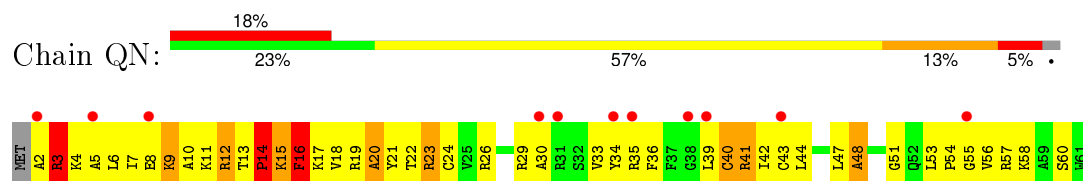
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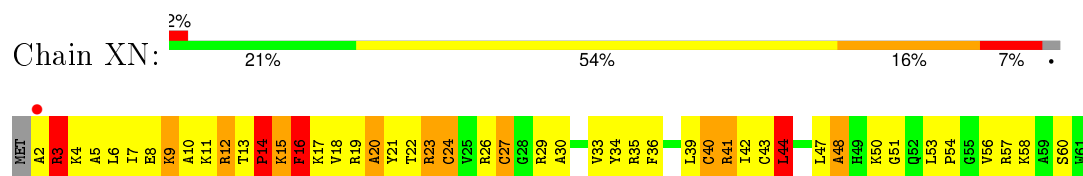
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- Molecule 14: 30S ribosomal protein S14

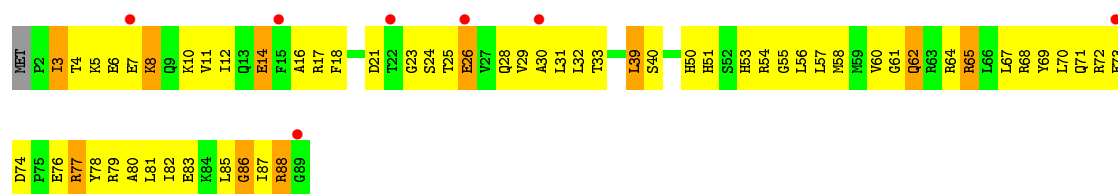


- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15

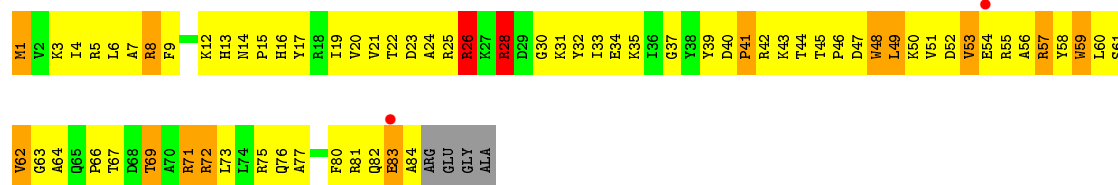




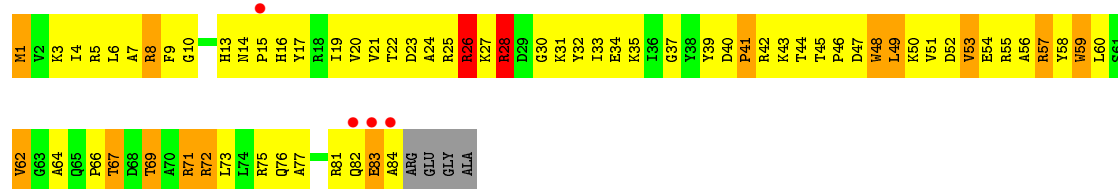
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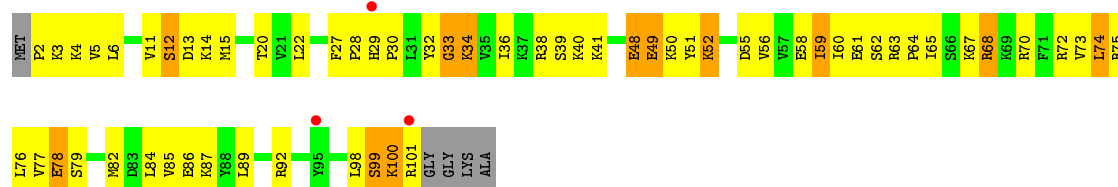
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16

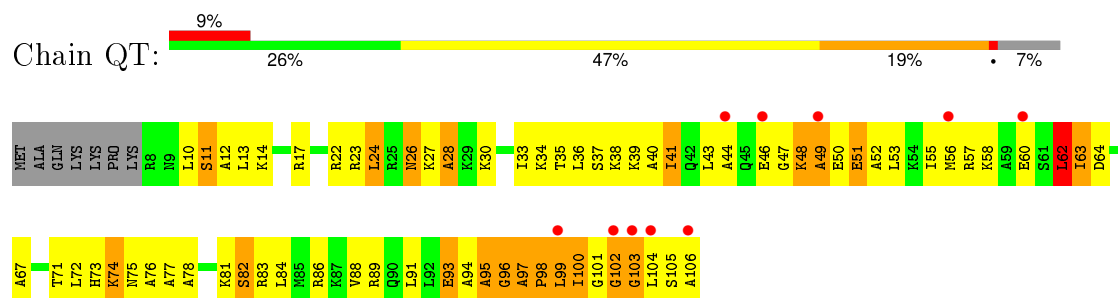


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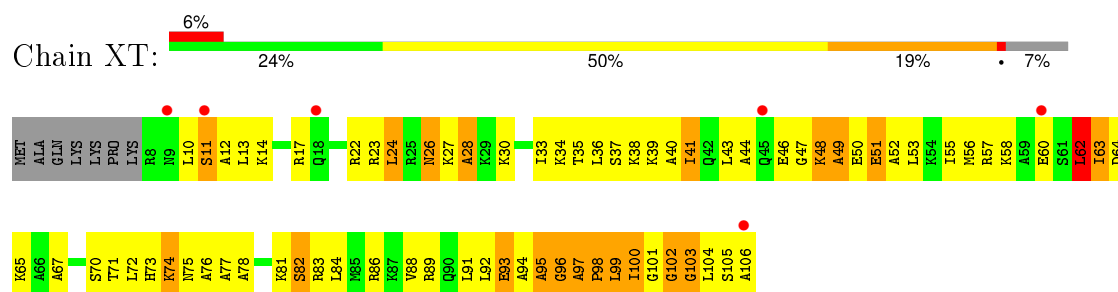


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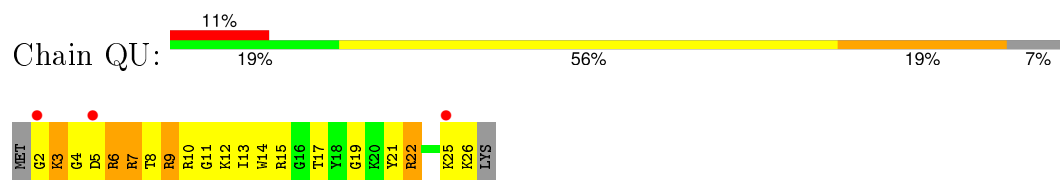
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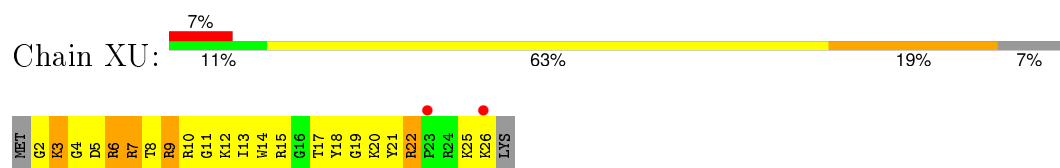
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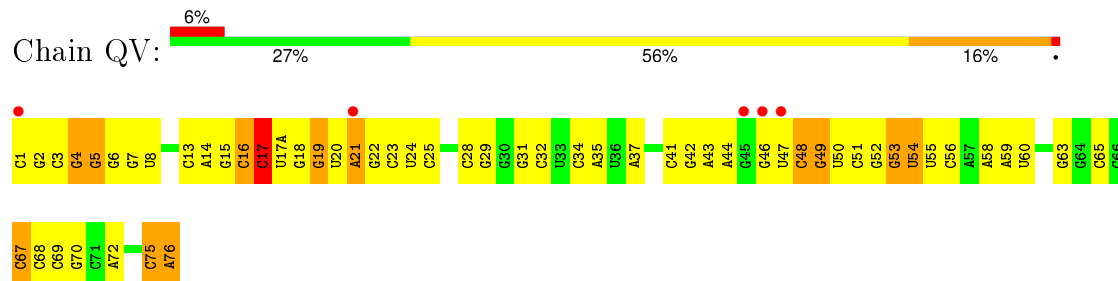
- Molecule 21: 30S ribosomal protein S21



- Molecule 21: 30S ribosomal protein S21



- Molecule 22: P-site tRNA fMet

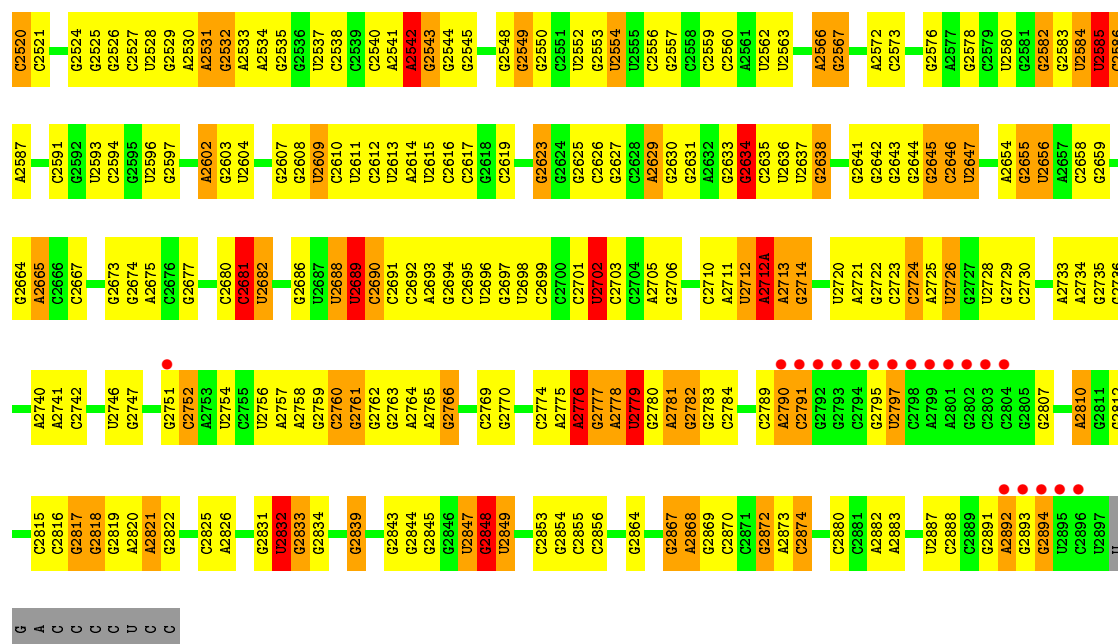


- Molecule 22: P-site tRNA fMet

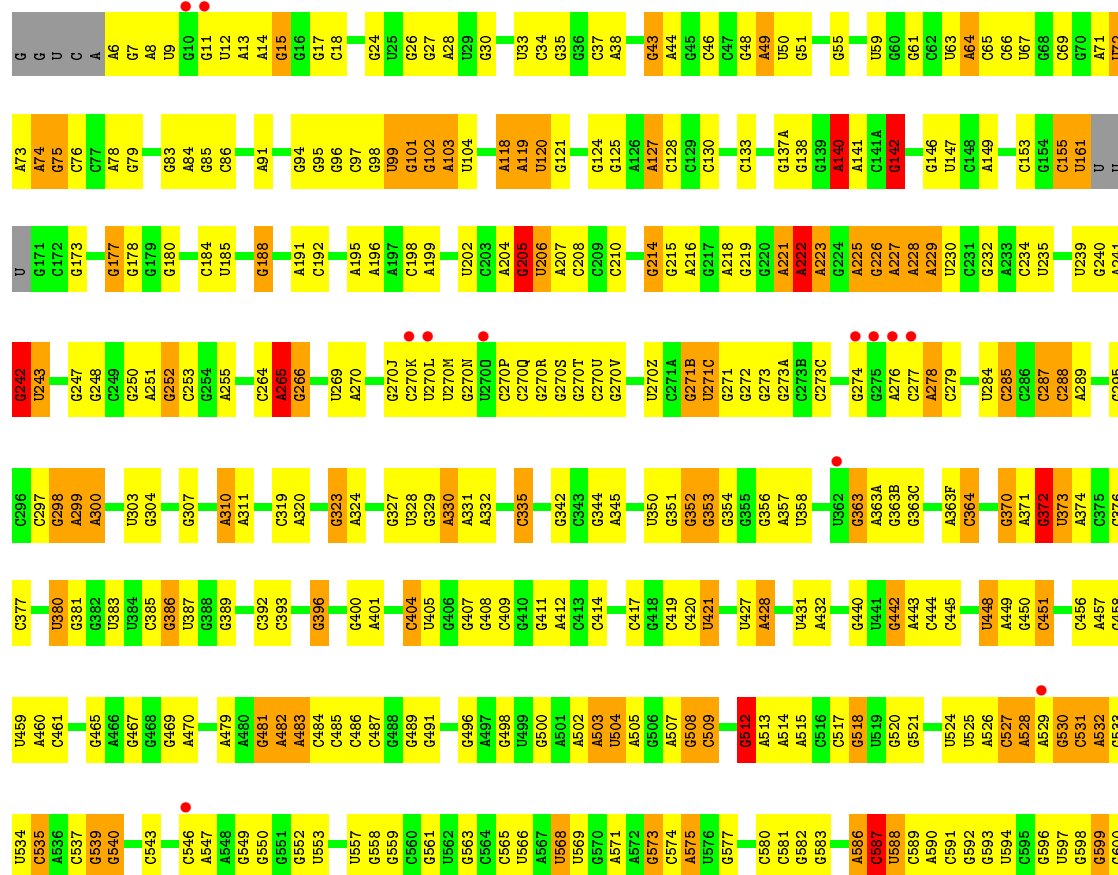


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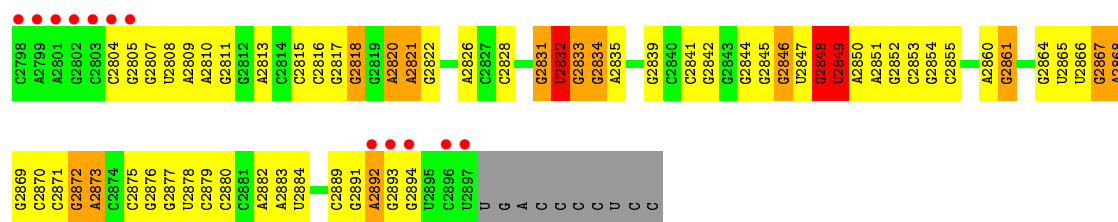


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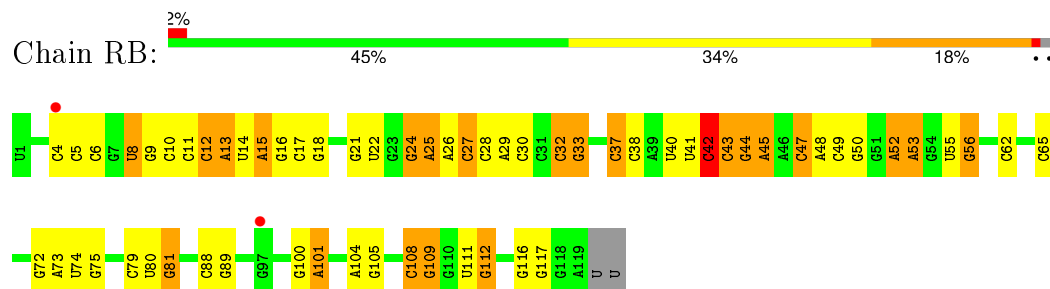


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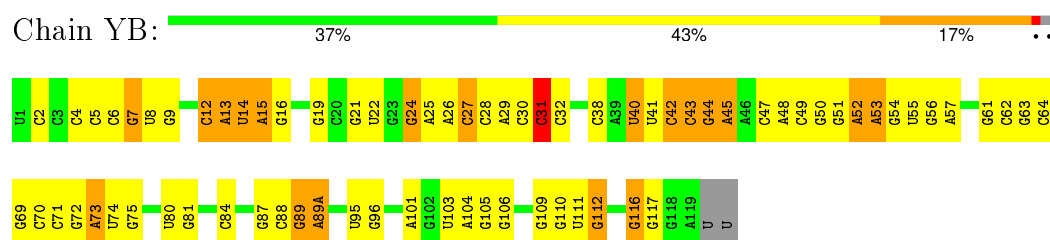
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G2778	U2701	C2626	U2555	G2477	U2401	G2334	C2263	G2186	G2125		G1967	G1896	A1819	G1757
U2702	U2702		C2556	A2478	C2402	A2335	C2268	G2187	A2126	G2048	A1968	G1897	U1820	U1757
G2703		A2629	G2557		C2403	A2336		C2188	G2127	G2049	A1969	G1898	A1821	G1758
G2710	G2710	G2630	C2558	G2481	C2404		U2269	U2189	C2128	C2050	A1970	G1899	G1822	A1759
A2711		G2632	C2559	G2482	G2405	G2342	A2273	G2190	C2129	A2051	A1971	A1900	G1823	
U2712	U2712	G2633	G2560	G2483	U2406	C2343	A2274	G2191	U2130	G2052	A1972	A1901	G1824	A1762
A2713			A2561	G2484	G2407	C2344	A2275	G2192	G2131			C1902	A1825	G1763
G2714	G2714	U2636	U2562	G2485	U2408	U2345	C2276	G2193	G2132	C2055	C1979	G1903	G1764	
G2715	G2715	G2637	U2563	A2411		G2346	A2277	G2194	G2133	G2056	G1980	G1906	C1765	C1765
G2716	A2638	U2638	A2564	G2489		A2347	A2278	A2134	A2134	A2059	A1981	G1907	U1766	U1766
U2717	U2717	G2639	A2565		A2411	A2348	G2279	G2135	C2136	A2060	C1982	C1908	U1768	U1768
G2718	G2718	G2640	U2566	G2494	G2415	U2349	G2280	U2197	C2137	G2061	G1985	C1909	G1769	G1769
G2719			G2567	G2495		G2349	G2281	A2198	C2138	A2062		C1909	U1833	U1833
G2720	G2720	G2641	U2568	U2419	U2419	G2349	G2282	A2199	C2139	G2063	C1988	G1910	G1770	G1770
G2721			G2569	A2497		G2351	G2283	C2205	C2138				G1835	G1835
	A2721			G2498	A2422			C2207	C2140		G1989		A1913	G1772



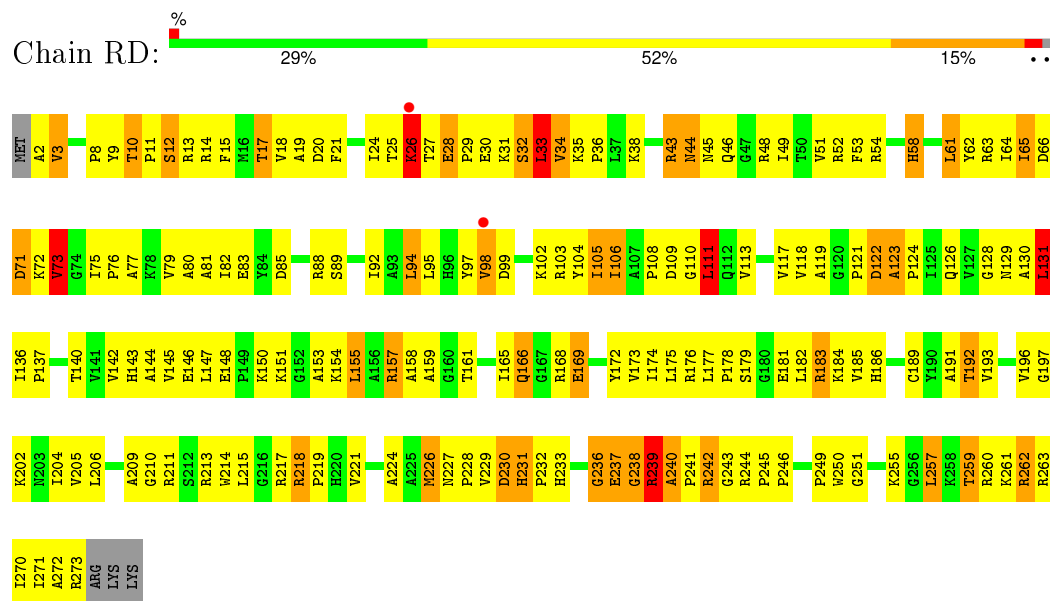
• Molecule 26: 5S rRNA



• Molecule 26: 5S rRNA

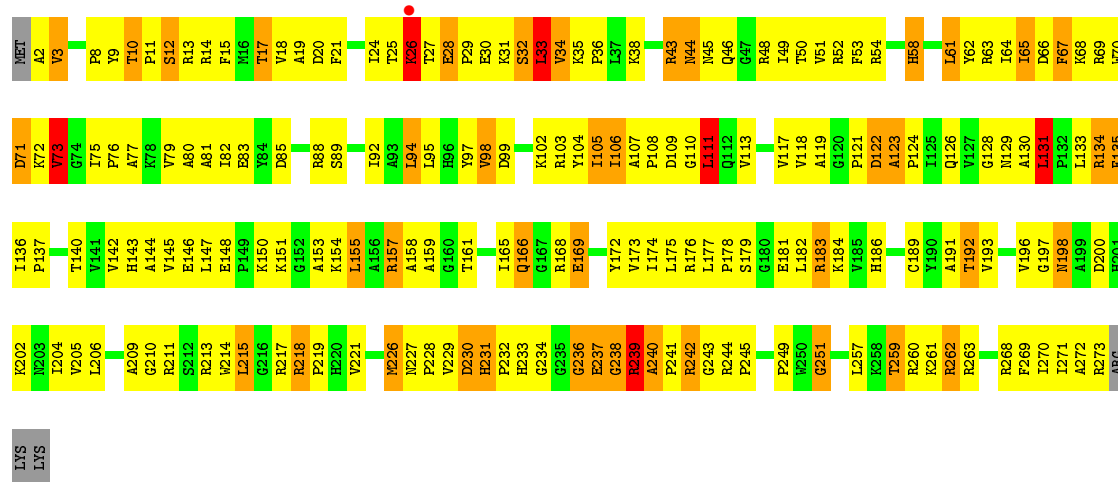


• Molecule 27: 50S ribosomal protein L2

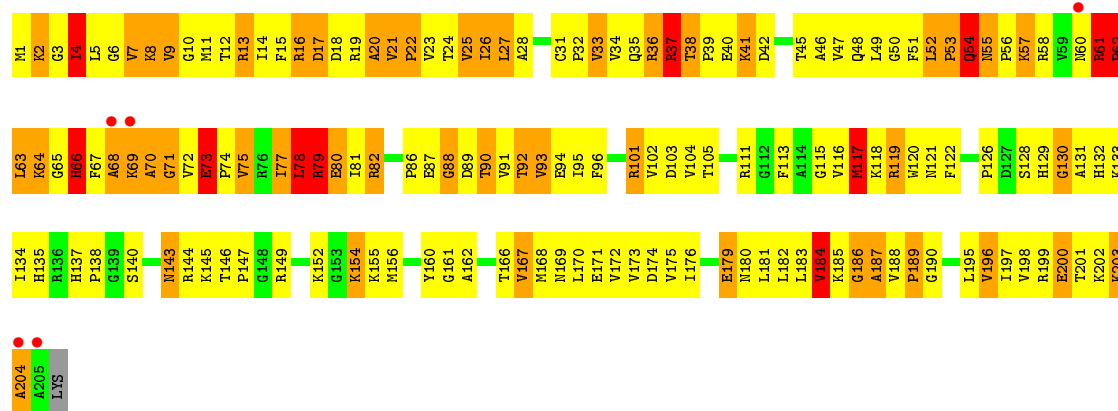


• Molecule 27: 50S ribosomal protein L2

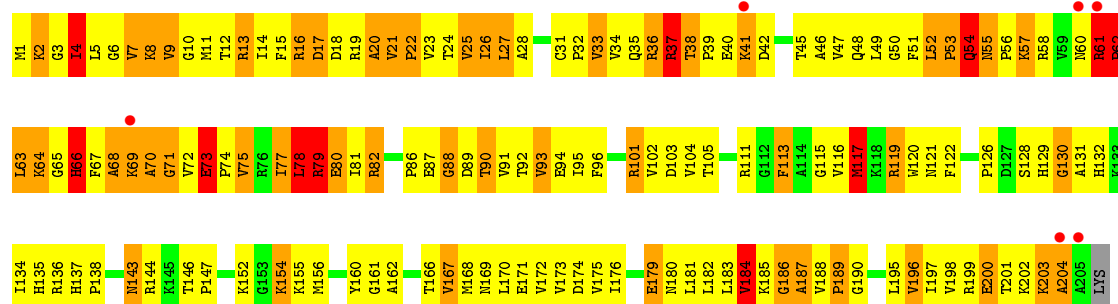




• Molecule 28: 50S ribosomal protein L3

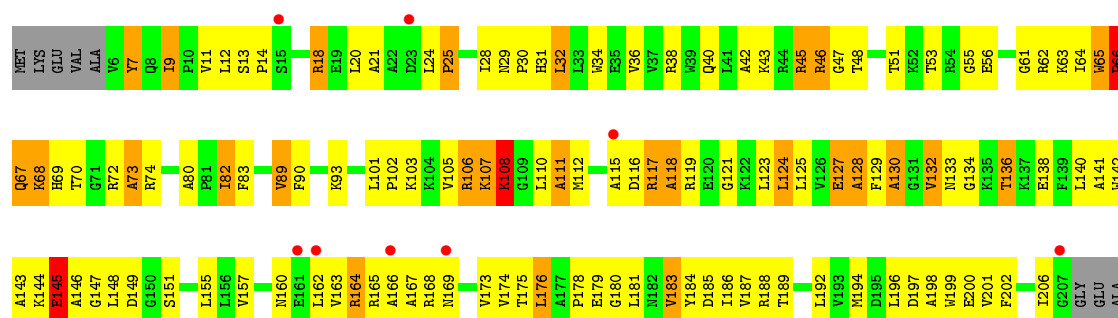


• Molecule 28: 50S ribosomal protein L3

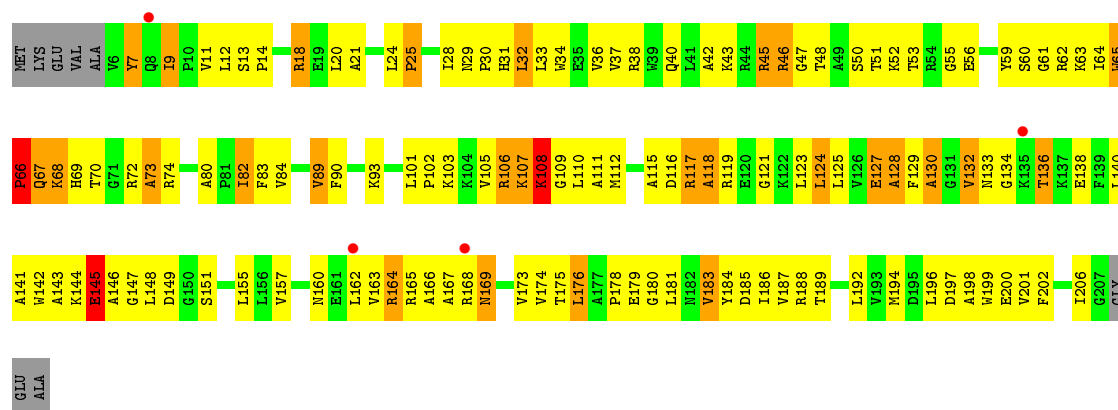


• Molecule 29: 50S ribosomal protein L4

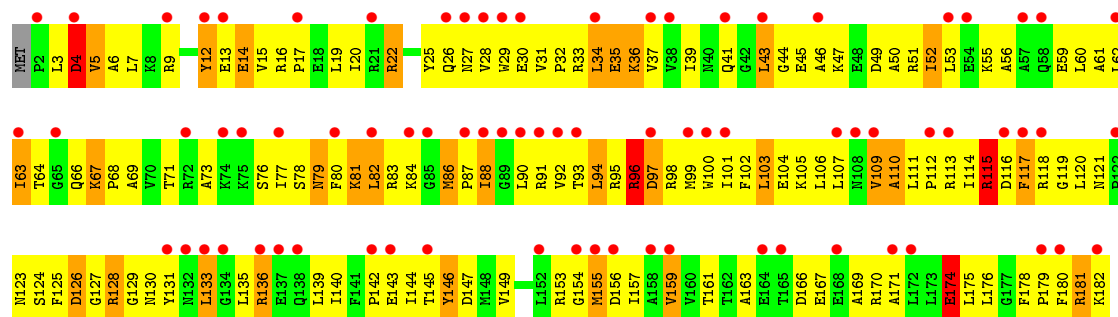




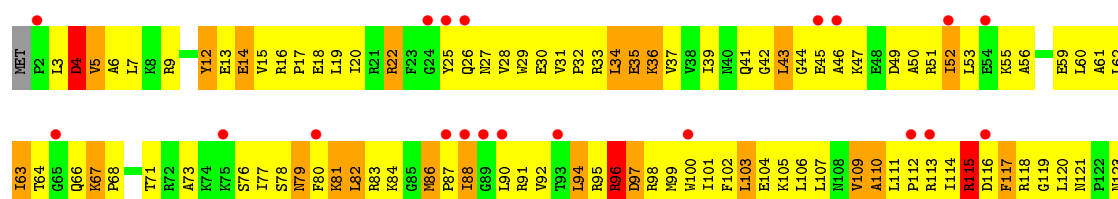
• Molecule 29: 50S ribosomal protein L4

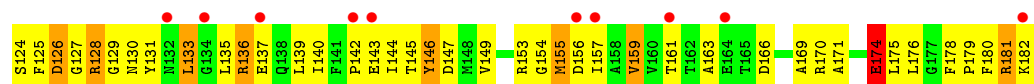


• Molecule 30: 50S ribosomal protein L5

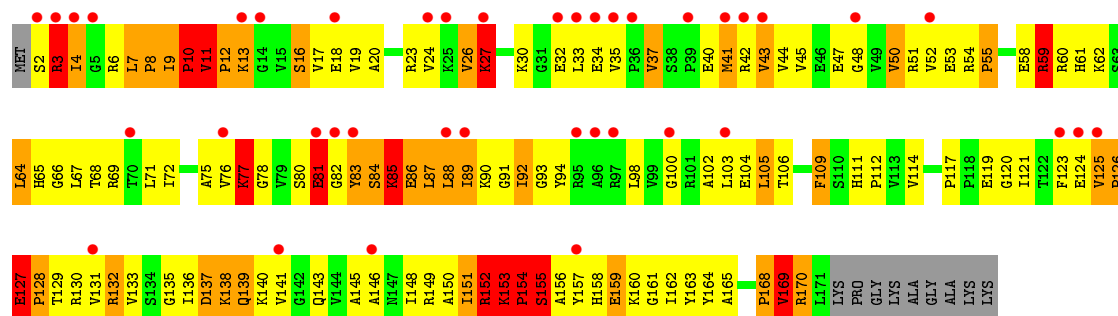
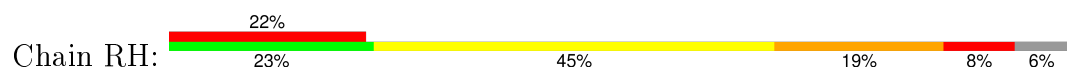


• Molecule 30: 50S ribosomal protein L5

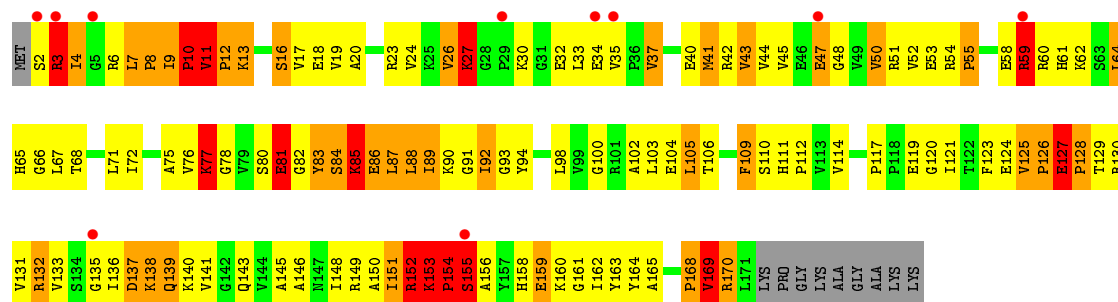
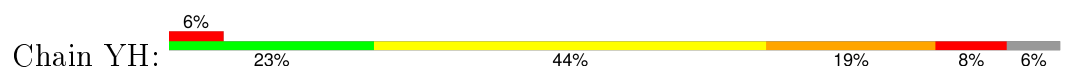




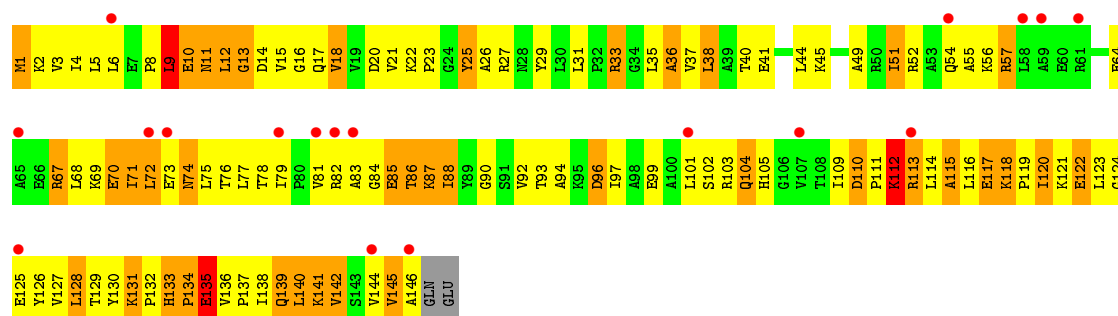
• Molecule 31: 50S ribosomal protein L6



• Molecule 31: 50S ribosomal protein L6

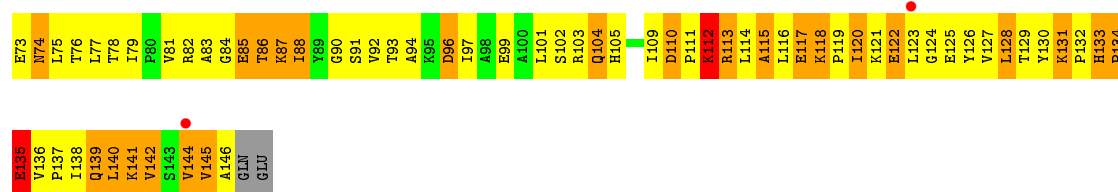


• Molecule 32: 50S ribosomal protein L9

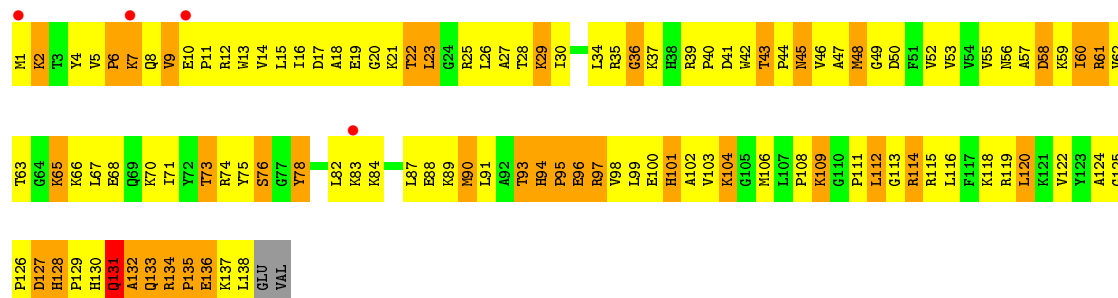
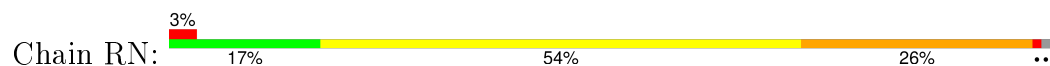


• Molecule 32: 50S ribosomal protein L9

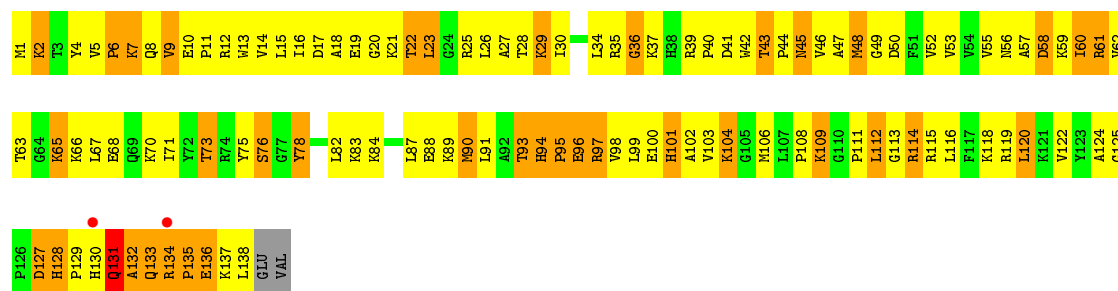




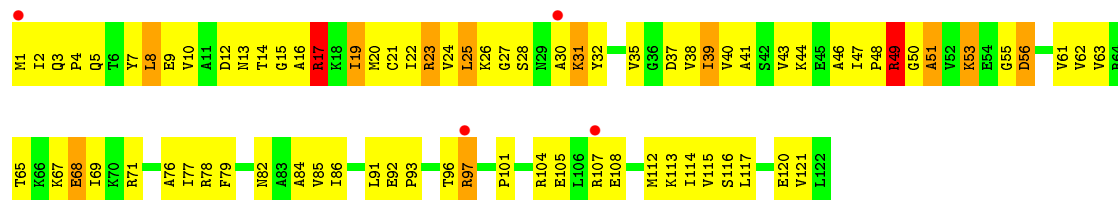
• Molecule 33: 50S ribosomal protein L13



• Molecule 33: 50S ribosomal protein L13

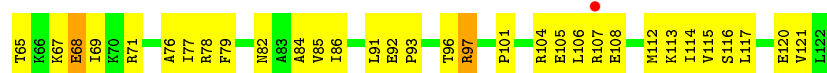


• Molecule 34: 50S ribosomal protein L14

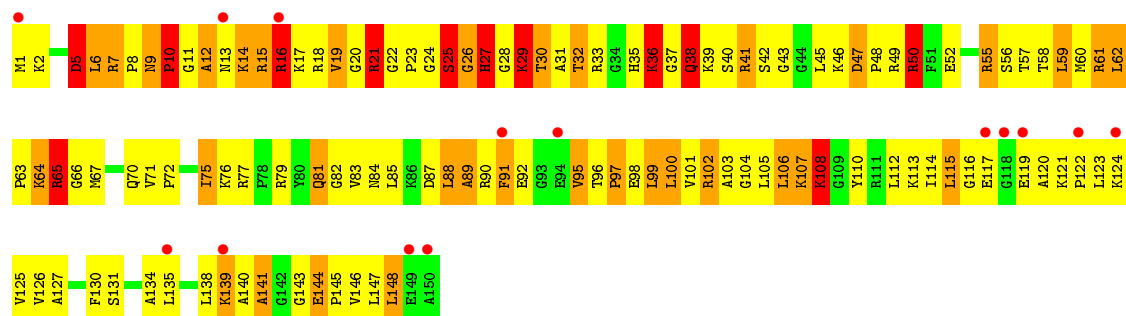
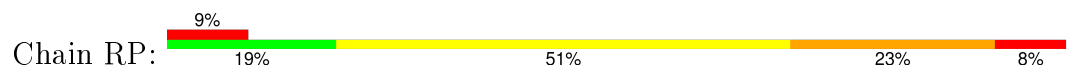


• Molecule 34: 50S ribosomal protein L14

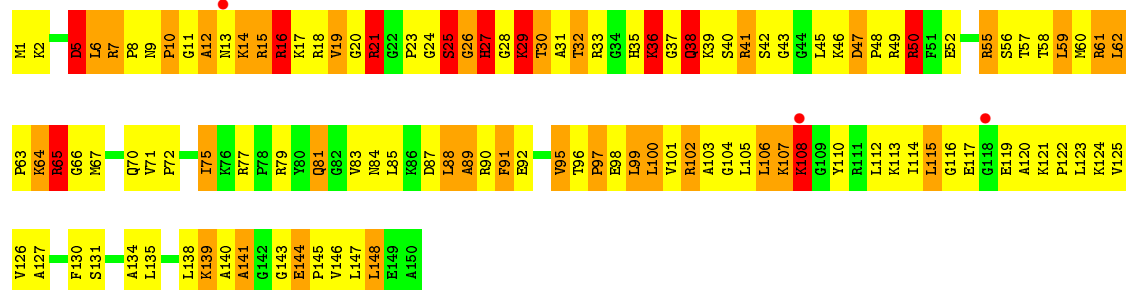
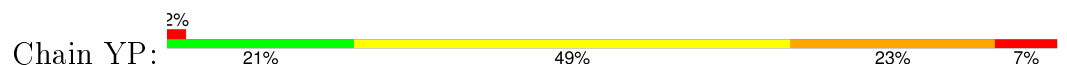




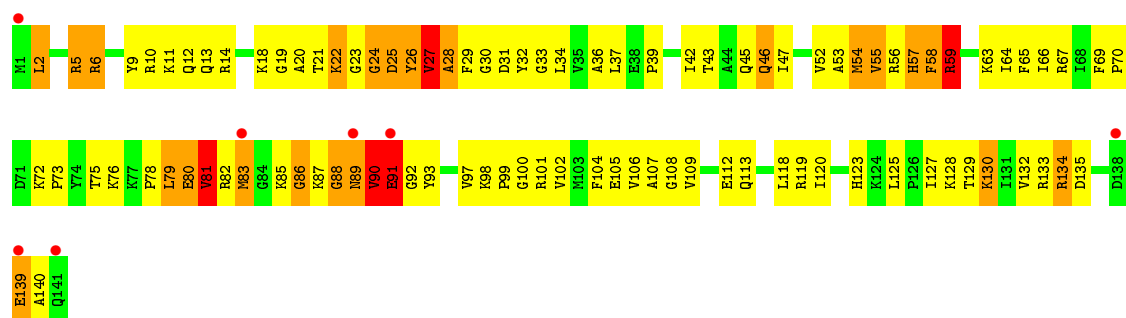
• Molecule 35: 50S ribosomal protein L15



• Molecule 35: 50S ribosomal protein L15

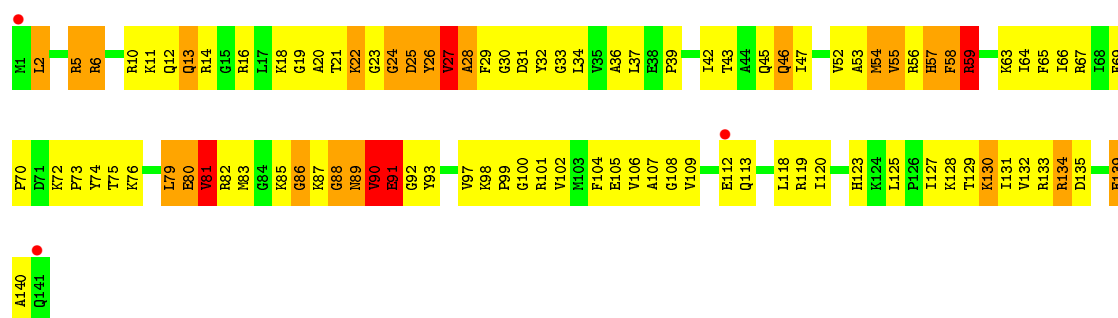


• Molecule 36: 50S ribosomal protein L16



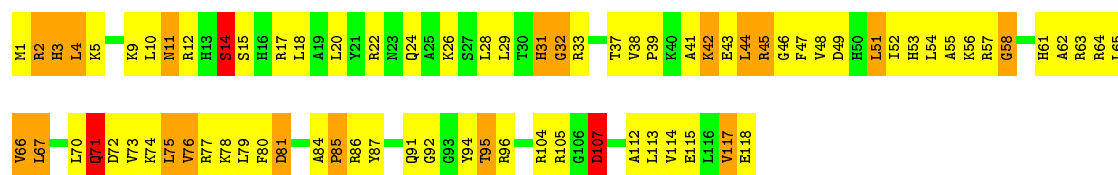
• Molecule 36: 50S ribosomal protein L16





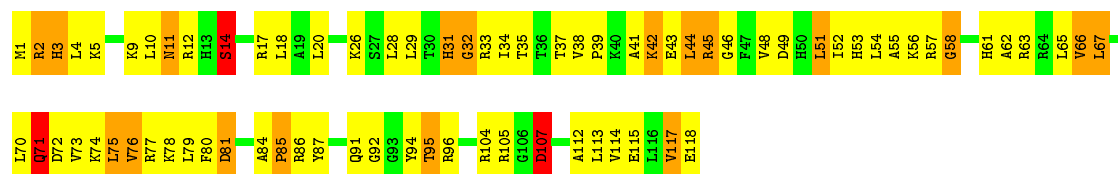
- Molecule 37: 50S ribosomal protein L17

Chain RR: 33% 48% 16% •



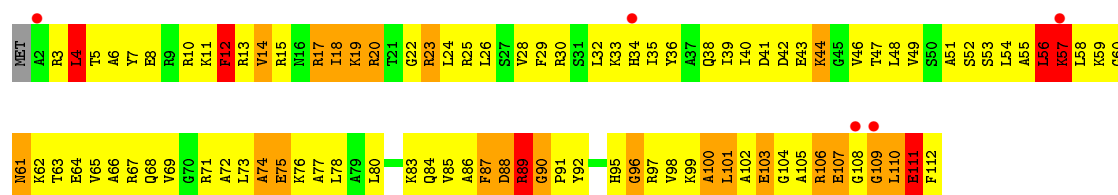
- Molecule 37: 50S ribosomal protein L17

Chain YR: 36% 47% 15% •



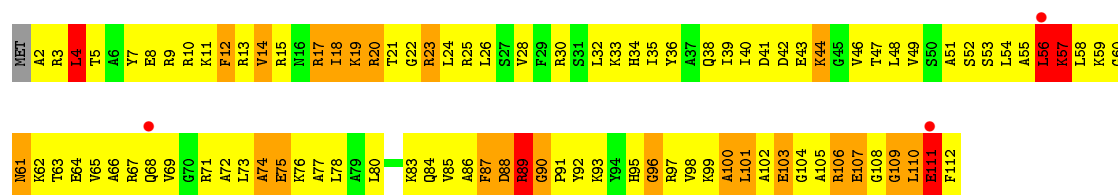
- Molecule 38: 50S ribosomal protein L18

Chain RS: 4% 13% 62% 19% 5% •

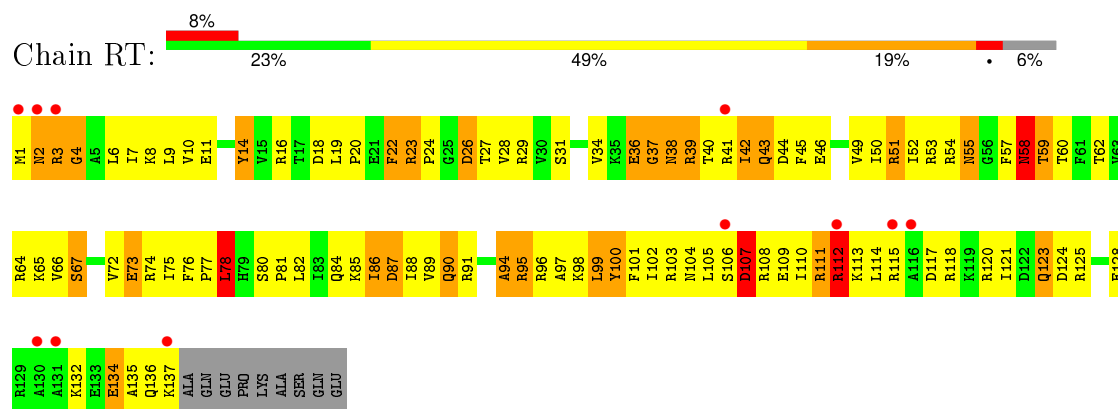


- Molecule 38: 50S ribosomal protein L18

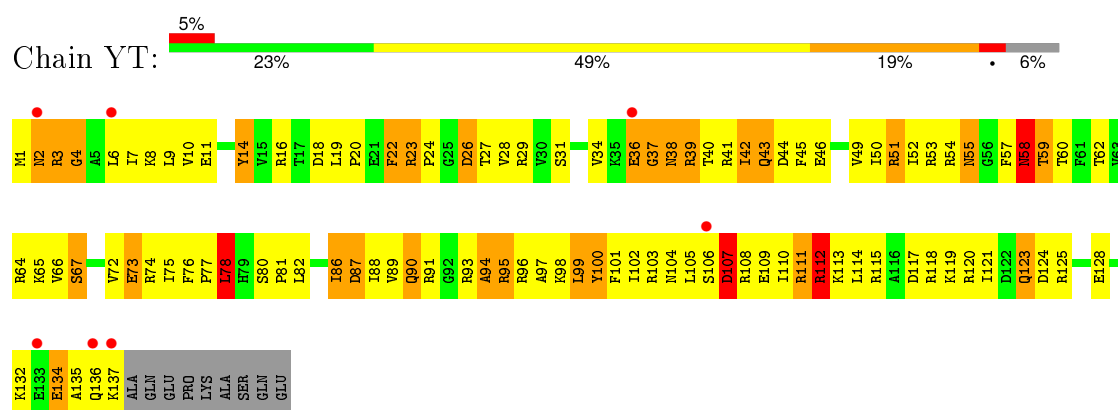
Chain YS: 3% 12% 63% 20% •



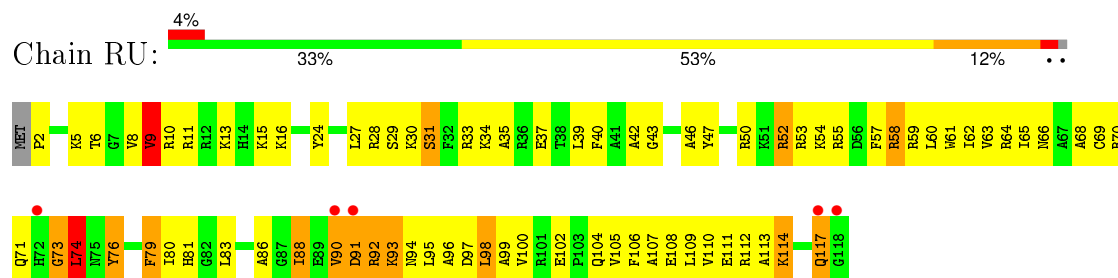
- Molecule 39: 50S ribosomal protein L19



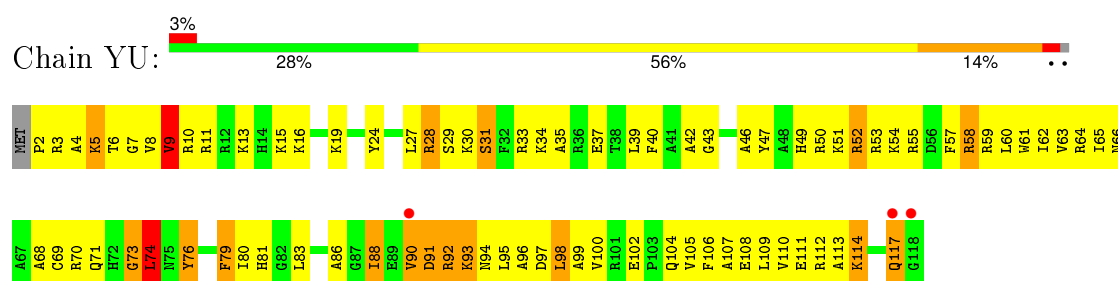
- Molecule 39: 50S ribosomal protein L19



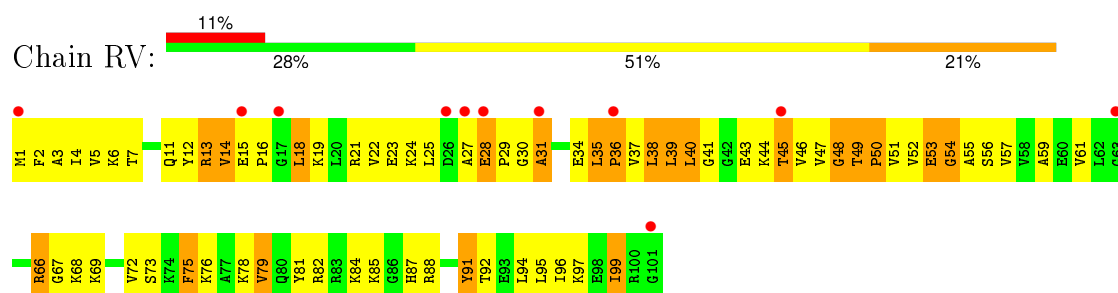
- Molecule 40: 50S ribosomal protein L20



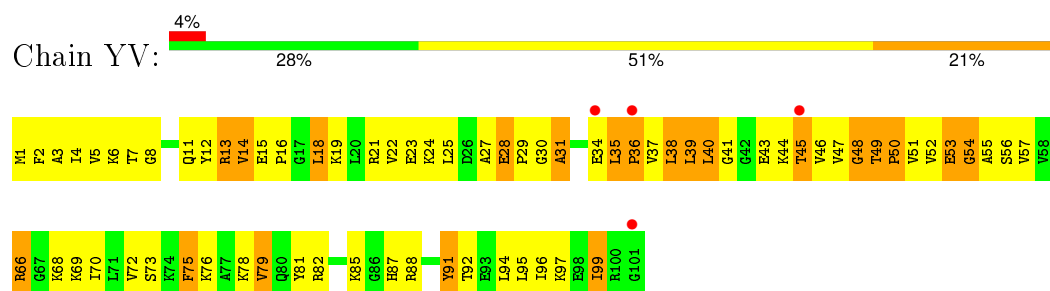
- Molecule 40: 50S ribosomal protein L20



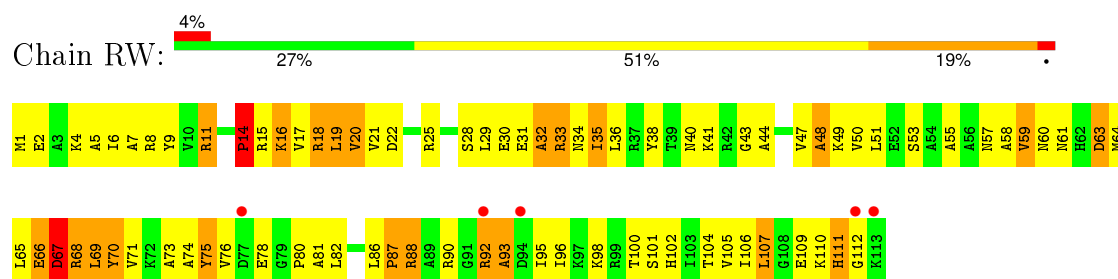
- Molecule 41: 50S ribosomal protein L21



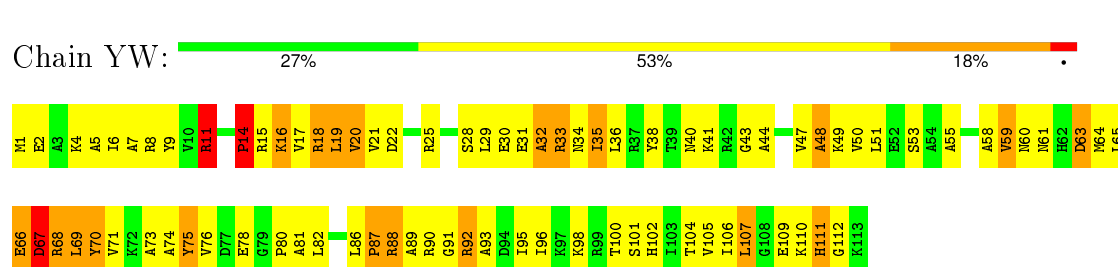
• Molecule 41: 50S ribosomal protein L21



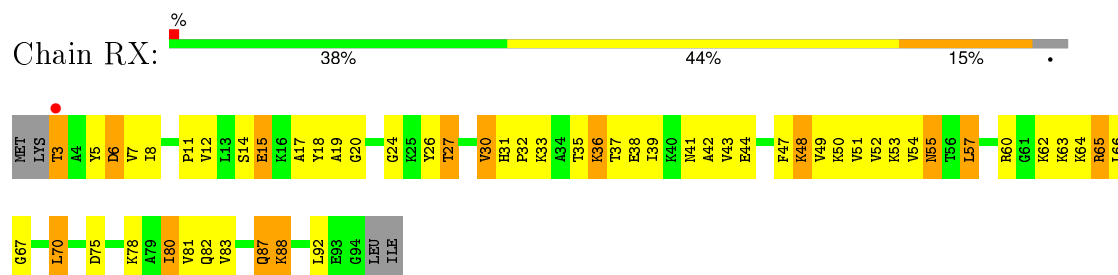
• Molecule 42: 50S ribosomal protein L22



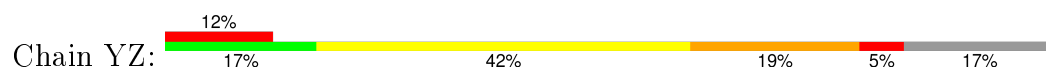
• Molecule 42: 50S ribosomal protein L22



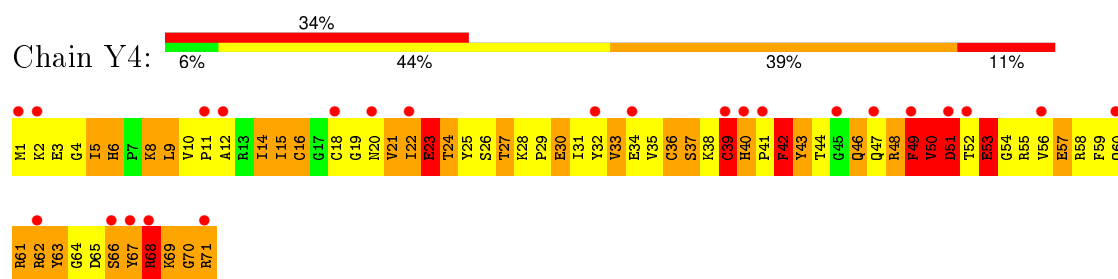
• Molecule 43: 50S ribosomal protein L23



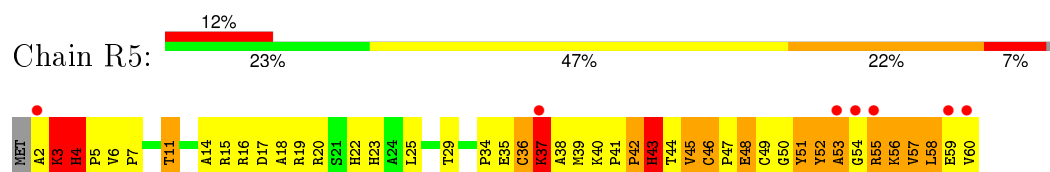
• Molecule 43: 50S ribosomal protein L23



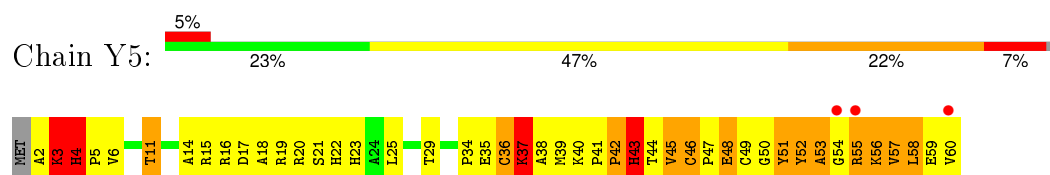




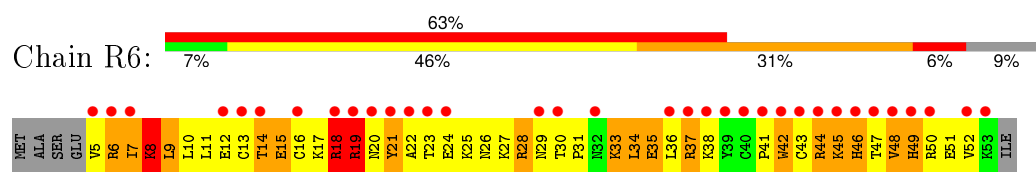
- Molecule 51: 50S ribosomal protein L33



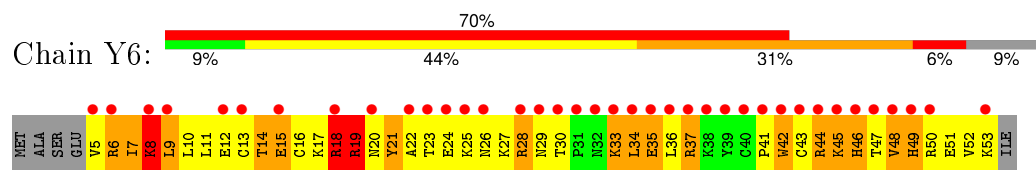
- Molecule 51: 50S ribosomal protein L33



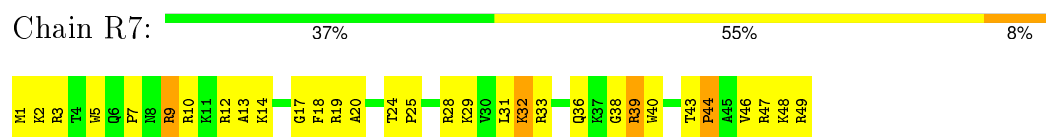
- Molecule 52: 50S ribosomal protein L34



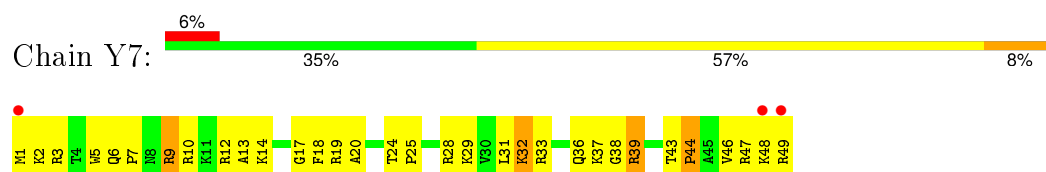
- Molecule 52: 50S ribosomal protein L34



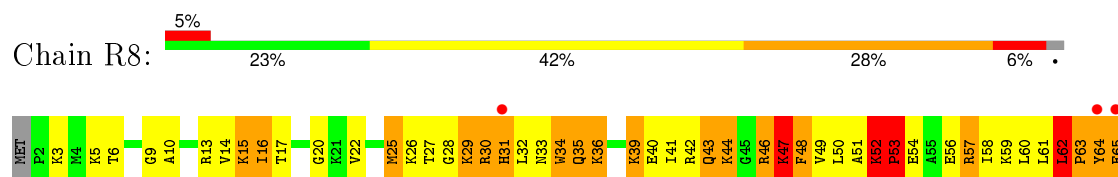
- Molecule 53: 50S ribosomal protein L35



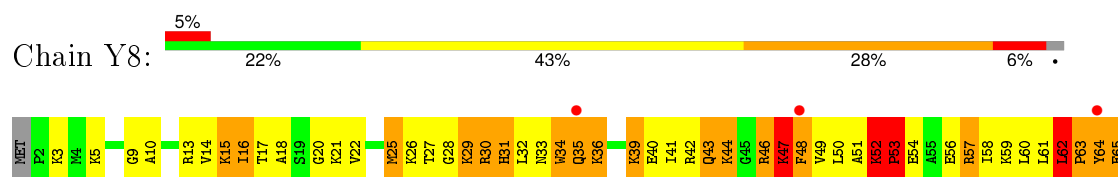
- Molecule 53: 50S ribosomal protein L35



- Molecule 54: tRNA acceptor end mimic



- Molecule 54: tRNA acceptor end mimic



- Molecule 55: RNA (5'-R(*CP*CP*(PPU))-3')



- Molecule 55: RNA (5'-R(*CP*CP*(PPU))-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.55Å 449.21Å 619.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.81 – 3.44 34.81 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.7 (34.81-3.44) 98.2 (34.81-3.26)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.243 , 0.285 0.246 , 0.285	Depositor DCC
R_{free} test set	34687 reflections (4.81%)	DCC
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 63.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 881904 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	291123	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PAR, 1MG, PPU

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	0.42	0/36098	0.97	58/56341 (0.1%)
1	XA	0.45	0/36123	1.00	71/56380 (0.1%)
2	QB	0.35	0/1959	0.65	0/2642
2	XB	0.35	0/1959	0.65	0/2642
3	QC	0.36	0/1629	0.60	0/2195
3	XC	0.36	0/1629	0.60	0/2195
4	QD	0.42	0/1733	0.69	1/2318 (0.0%)
4	XD	0.42	0/1733	0.70	1/2318 (0.0%)
5	QE	0.38	0/1171	0.66	0/1576
5	XE	0.38	0/1171	0.66	0/1576
6	QF	0.43	0/856	0.68	0/1154
6	XF	0.43	0/856	0.68	0/1154
7	QG	0.37	0/1276	0.60	0/1709
7	XG	0.37	0/1276	0.61	0/1709
8	QH	0.40	0/1136	0.69	0/1527
8	XH	0.40	0/1136	0.69	0/1527
9	QI	0.36	0/1029	0.67	0/1379
9	XI	0.36	0/1029	0.67	0/1379
10	QJ	0.35	0/814	0.61	0/1095
10	XJ	0.36	0/814	0.61	0/1095
11	QK	0.40	0/900	0.67	0/1213
11	XK	0.40	0/900	0.67	0/1213
12	QL	0.45	0/991	1.00	4/1327 (0.3%)
12	XL	0.45	0/991	1.00	4/1327 (0.3%)
13	QM	0.34	0/974	0.66	0/1303
13	XM	0.35	0/974	0.66	0/1303
14	QN	0.43	0/501	0.70	1/664 (0.2%)
14	XN	0.43	0/501	0.70	1/664 (0.2%)
15	QO	0.39	0/745	0.66	0/992
15	XO	0.39	0/745	0.66	0/992
16	QP	0.37	0/721	0.67	0/970
16	XP	0.37	0/721	0.67	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.38	0/847	0.68	0/1131
17	XQ	0.38	0/847	0.68	0/1131
18	QR	0.39	0/579	0.72	0/768
18	XR	0.39	0/579	0.73	0/768
19	QS	0.36	0/689	0.84	2/926 (0.2%)
19	XS	0.36	0/689	0.84	2/926 (0.2%)
20	QT	0.34	0/765	0.69	0/1007
20	XT	0.33	0/765	0.69	0/1007
21	QU	0.37	0/221	0.63	0/288
21	XU	0.37	0/221	0.62	0/288
22	QV	0.52	0/1836	0.99	6/2859 (0.2%)
22	XV	0.52	0/1836	0.99	6/2859 (0.2%)
23	QX	0.40	0/189	0.75	0/292
23	XX	0.66	0/189	1.09	2/292 (0.7%)
24	QY	0.51	0/311	0.88	0/483
24	XY	0.52	0/311	0.89	0/483
25	RA	0.52	2/69543 (0.0%)	1.06	149/108563 (0.1%)
25	YA	0.59	2/69521 (0.0%)	1.10	200/108529 (0.2%)
26	RB	0.44	0/2878	1.04	7/4490 (0.2%)
26	YB	0.46	0/2878	1.03	2/4490 (0.0%)
27	RD	0.62	2/2165 (0.1%)	0.90	3/2919 (0.1%)
27	YD	0.62	2/2165 (0.1%)	0.90	3/2919 (0.1%)
28	RE	0.52	0/1601	0.91	2/2160 (0.1%)
28	YE	0.52	0/1601	0.91	2/2160 (0.1%)
29	RF	0.50	0/1620	0.76	0/2194
29	YF	0.50	0/1620	0.76	0/2194
30	RG	0.40	0/1499	0.66	0/2016
30	YG	0.40	0/1499	0.66	0/2016
31	RH	0.45	0/1332	0.85	4/1802 (0.2%)
31	YH	0.45	0/1332	0.85	4/1802 (0.2%)
32	RI	0.40	0/1151	0.80	1/1558 (0.1%)
32	YI	0.40	0/1151	0.79	1/1558 (0.1%)
33	RN	0.46	0/1131	0.78	1/1525 (0.1%)
33	YN	0.46	0/1131	0.78	1/1525 (0.1%)
34	RO	0.53	0/943	0.71	0/1269
34	YO	0.53	0/943	0.71	0/1269
35	RP	0.50	0/1162	0.94	3/1544 (0.2%)
35	YP	0.49	0/1162	0.95	3/1544 (0.2%)
36	RQ	0.53	0/1143	0.89	3/1527 (0.2%)
36	YQ	0.53	0/1143	0.89	3/1527 (0.2%)
37	RR	0.45	0/982	0.80	1/1312 (0.1%)
37	YR	0.45	0/982	0.80	1/1312 (0.1%)
38	RS	0.46	0/892	0.82	1/1187 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YS	0.45	0/892	0.82	1/1187 (0.1%)
39	RT	0.47	0/1155	0.73	2/1542 (0.1%)
39	YT	0.47	0/1155	0.73	2/1542 (0.1%)
40	RU	0.48	0/982	0.78	0/1306
40	YU	0.48	0/982	0.78	0/1306
41	RV	0.47	0/790	0.82	0/1057
41	YV	0.47	0/790	0.82	0/1057
42	RW	0.45	0/911	0.75	0/1220
42	YW	0.45	0/911	0.75	0/1220
43	RX	0.56	0/739	0.78	0/993
43	YX	0.56	0/739	0.77	0/993
44	RY	0.52	0/798	0.80	0/1064
44	YY	0.52	0/798	0.80	0/1064
45	RZ	0.47	0/1408	0.77	1/1908 (0.1%)
45	YZ	0.47	0/1408	0.77	1/1908 (0.1%)
46	R0	0.57	0/657	0.80	0/874
46	Y0	0.60	0/657	0.85	0/874
47	R1	0.49	0/770	0.85	1/1022 (0.1%)
47	Y1	0.49	0/770	0.85	1/1022 (0.1%)
48	R2	0.50	0/583	0.83	1/771 (0.1%)
48	Y2	0.50	0/583	0.84	1/771 (0.1%)
49	R3	0.43	0/474	0.71	0/635
49	Y3	0.43	0/474	0.71	0/635
50	R4	0.38	0/594	0.78	1/795 (0.1%)
50	Y4	0.38	0/594	0.78	1/795 (0.1%)
51	R5	0.51	0/473	0.74	0/639
51	Y5	0.51	0/473	0.74	0/639
52	R6	0.42	0/431	0.76	0/575
52	Y6	0.42	0/431	0.76	0/575
53	R7	0.56	0/438	0.76	0/575
53	Y7	0.56	0/438	0.76	0/575
54	R8	0.62	0/525	0.93	1/691 (0.1%)
54	Y8	0.62	0/525	0.93	1/691 (0.1%)
55	Z6	0.82	0/40	1.81	1/60 (1.7%)
55	Z8	0.80	0/40	1.80	1/60 (1.7%)
All	All	0.50	8/315563 (0.0%)	0.98	571/471909 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	YD	236	GLY	C-N	8.59	1.53	1.34
27	RD	236	GLY	C-N	8.55	1.53	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	YD	239	ARG	CA-C	-6.77	1.35	1.52
27	RD	239	ARG	CA-C	-6.76	1.35	1.52
25	YA	783	A	N7-C5	-5.95	1.35	1.39

The worst 5 of 571 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	QL	47	LYS	C-N-CD	-20.50	75.51	120.60
12	XL	47	LYS	C-N-CD	-20.46	75.58	120.60
25	YA	761	A	N1-C6-N6	12.76	126.25	118.60
25	YA	945	A	N9-C1'-C2'	12.75	130.58	114.00
22	QV	17	C	C2-N1-C1'	11.85	131.84	118.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16275	828	0
1	XA	32269	0	16289	816	0
2	QB	1924	0	1975	291	0
2	XB	1924	0	1975	301	0
3	QC	1605	0	1668	208	0
3	XC	1605	0	1668	209	1
4	QD	1703	0	1762	240	0
4	XD	1703	0	1763	215	0
5	QE	1155	0	1213	147	0
5	XE	1155	0	1213	142	0
6	QF	843	0	857	93	0
6	XF	843	0	857	99	0
7	QG	1257	0	1296	149	0
7	XG	1257	0	1296	147	0
8	QH	1116	0	1176	155	0
8	XH	1116	0	1177	164	0
9	QI	1010	0	1037	151	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	XI	1010	0	1037	160	0
10	QJ	801	0	849	138	0
10	XJ	801	0	849	136	0
11	QK	885	0	904	108	1
11	XK	885	0	904	118	0
12	QL	975	0	1062	109	0
12	XL	975	0	1062	113	0
13	QM	964	0	1034	171	0
13	XM	964	0	1034	180	0
14	QN	492	0	531	89	0
14	XN	492	0	529	87	0
15	QO	734	0	771	75	0
15	XO	734	0	771	74	0
16	QP	705	0	725	114	0
16	XP	705	0	725	113	0
17	QQ	834	0	904	84	0
17	XQ	834	0	904	82	0
18	QR	574	0	644	68	0
18	XR	574	0	644	67	0
19	QS	674	0	699	104	0
19	XS	674	0	699	143	0
20	QT	763	0	860	108	0
20	XT	763	0	861	102	0
21	QU	217	0	234	30	0
21	XU	217	0	234	29	0
22	QV	1644	0	836	41	0
22	XV	1644	0	836	40	0
23	QX	170	0	87	16	0
23	XX	170	0	88	10	0
24	QY	303	0	154	13	0
24	XY	303	0	154	17	0
25	RA	62091	0	31301	1401	0
25	YA	62071	0	31286	1351	0
26	RB	2573	0	1306	70	0
26	YB	2573	0	1306	61	0
27	RD	2115	0	2195	324	0
27	YD	2115	0	2195	350	0
28	RE	1568	0	1634	277	0
28	YE	1568	0	1634	266	0
29	RF	1585	0	1632	174	0
29	YF	1585	0	1632	182	0
30	RG	1474	0	1535	212	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	YG	1474	0	1535	206	0
31	RH	1307	0	1382	217	0
31	YH	1307	0	1382	219	1
32	RI	1136	0	1223	179	0
32	YI	1136	0	1223	176	0
33	RN	1104	0	1180	194	0
33	YN	1104	0	1180	186	0
34	RO	933	0	996	123	0
34	YO	933	0	996	124	0
35	RP	1145	0	1228	248	0
35	YP	1145	0	1228	247	0
36	RQ	1122	0	1179	168	0
36	YQ	1122	0	1179	168	0
37	RR	968	0	1033	115	0
37	YR	968	0	1033	112	0
38	RS	882	0	943	158	0
38	YS	882	0	943	163	0
39	RT	1141	0	1202	152	0
39	YT	1141	0	1202	156	0
40	RU	964	0	1022	130	0
40	YU	964	0	1022	138	0
41	RV	779	0	852	132	0
41	YV	779	0	852	130	1
42	RW	900	0	964	101	0
42	YW	900	0	964	108	0
43	RX	725	0	778	68	0
43	YX	725	0	778	82	0
44	RY	785	0	878	163	0
44	YY	785	0	878	154	1
45	RZ	1378	0	1407	227	0
45	YZ	1378	0	1407	227	0
46	R0	648	0	672	88	0
46	Y0	648	0	672	85	0
47	R1	763	0	848	141	0
47	Y1	763	0	848	145	0
48	R2	581	0	629	80	0
48	Y2	581	0	629	75	0
49	R3	469	0	518	40	0
49	Y3	469	0	518	41	0
50	R4	581	0	574	159	0
50	Y4	581	0	574	180	0
51	R5	459	0	480	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	Y5	459	0	480	75	1
52	R6	424	0	450	93	0
52	Y6	424	0	450	90	0
53	R7	430	0	480	47	0
53	Y7	430	0	480	42	0
54	R8	517	0	582	106	0
54	Y8	517	0	582	100	0
55	Z6	74	0	51	10	0
55	Z8	74	0	51	4	0
56	QA	60	0	0	0	0
56	QF	1	0	0	0	0
56	QH	1	0	0	0	0
56	QM	1	0	0	0	0
56	QV	2	0	0	0	0
56	QX	2	0	0	0	0
56	R5	1	0	0	0	0
56	RA	212	0	0	0	0
56	RB	2	0	0	0	0
56	RE	2	0	0	0	0
56	RF	1	0	0	0	0
56	RP	1	0	0	0	0
56	XA	63	0	0	0	0
56	XM	2	0	0	0	0
56	XV	2	0	0	0	0
56	Y5	1	0	0	0	0
56	YA	242	0	0	0	0
56	YB	2	0	0	0	0
56	YE	2	0	0	0	0
56	YX	1	0	0	0	0
57	QA	42	0	45	4	0
57	XA	42	0	45	1	0
58	QD	1	0	0	0	0
58	QN	1	0	0	0	0
58	XD	1	0	0	0	0
58	XN	1	0	0	0	0
All	All	291123	0	197505	16608	3

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 34.

The worst 5 of 16608 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:39:LEU:HD22	14:QN:43:CYS:SG	1.33	1.63
36:YQ:81:VAL:HG23	46:Y0:7:LEU:CD2	1.21	1.60
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.35	1.54
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.35	1.52
19:QS:5:LEU:HD22	50:R4:67:TYR:CE2	1.45	1.51

All (3) 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:YV:51:VAL:N	51:Y5:60:VAL:O[4_445]	1.98	0.22
31:YH:47:GLU:OE2	44:YY:79:CYS:CB[4_445]	2.04	0.16
11:QK:99:GLN:NE2	3:XC:79:ARG:NH2[4_555]	2.06	0.14

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	5
2	XB	235/256 (92%)	152 (65%)	53 (23%)	30 (13%)	0	5
3	QC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	1	10
3	XC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	1	10
4	QD	206/209 (99%)	133 (65%)	51 (25%)	22 (11%)	0	8
4	XD	206/209 (99%)	133 (65%)	50 (24%)	23 (11%)	0	7
5	QE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	0	8
5	XE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	1	9
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	10
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	10
7	QG	153/156 (98%)	102 (67%)	37 (24%)	14 (9%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	XG	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	1	9
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	8
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	8
9	QI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	5
9	XI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	5
10	QJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	1	8
10	XJ	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	1	10
11	QK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	14
11	XK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	14
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	7
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	7
13	QM	119/126 (94%)	71 (60%)	27 (23%)	21 (18%)	0	2
13	XM	119/126 (94%)	71 (60%)	27 (23%)	21 (18%)	0	2
14	QN	58/61 (95%)	33 (57%)	15 (26%)	10 (17%)	0	2
14	XN	58/61 (95%)	33 (57%)	15 (26%)	10 (17%)	0	2
15	QO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	16
15	XO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	16
16	QP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	4
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	4
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	12
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	12
18	QR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	6
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	6
19	QS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	1
19	XS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	1
20	QT	97/106 (92%)	63 (65%)	16 (16%)	18 (19%)	0	2
20	XT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	0	2
21	QU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	2
21	XU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	2
27	RD	270/276 (98%)	204 (76%)	46 (17%)	20 (7%)	1	15
27	YD	270/276 (98%)	204 (76%)	46 (17%)	20 (7%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
29	RF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	9
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	9
30	RG	179/182 (98%)	120 (67%)	38 (21%)	21 (12%)	0	6
30	YG	179/182 (98%)	120 (67%)	38 (21%)	21 (12%)	0	6
31	RH	168/180 (93%)	94 (56%)	35 (21%)	39 (23%)	0	1
31	YH	168/180 (93%)	95 (56%)	35 (21%)	38 (23%)	0	1
32	RI	144/148 (97%)	83 (58%)	33 (23%)	28 (19%)	0	2
32	YI	144/148 (97%)	85 (59%)	32 (22%)	27 (19%)	0	2
33	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	2
33	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	2
34	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	14
34	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	14
35	RP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	1
35	YP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	1
36	RQ	139/141 (99%)	94 (68%)	30 (22%)	15 (11%)	0	8
36	YQ	139/141 (99%)	94 (68%)	30 (22%)	15 (11%)	0	8
37	RR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	6
37	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	6
38	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	2
38	YS	109/112 (97%)	63 (58%)	27 (25%)	19 (17%)	0	2
39	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	3
39	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	3
40	RU	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	13
40	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	13
41	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	9
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	9
42	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	5
42	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	5
43	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	22
44	RY	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	1
44	YY	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	1
45	RZ	170/206 (82%)	91 (54%)	40 (24%)	39 (23%)	0	1
45	YZ	170/206 (82%)	91 (54%)	40 (24%)	39 (23%)	0	1
46	R0	80/85 (94%)	61 (76%)	14 (18%)	5 (6%)	2	19
46	Y0	80/85 (94%)	62 (78%)	12 (15%)	6 (8%)	1	14
47	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	7
47	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	7
48	R2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	4
48	Y2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	4
49	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	23
49	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	23
50	R4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
50	Y4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
51	R5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	1
51	Y5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	1
52	R6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
52	Y6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
53	R7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	19
53	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	19
54	R8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	2
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	2
All	All	11378/12054 (94%)	7461 (66%)	2359 (21%)	1558 (14%)	0	4

5 of 1558 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	6	THR
2	QB	15	VAL
2	QB	26	PRO
2	QB	84	GLU
2	QB	88	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	181 (88%)	24 (12%)	7	30
2	XB	205/220 (93%)	181 (88%)	24 (12%)	7	30
3	QC	159/188 (85%)	143 (90%)	16 (10%)	9	39
3	XC	159/188 (85%)	143 (90%)	16 (10%)	9	39
4	QD	180/181 (99%)	164 (91%)	16 (9%)	12	46
4	XD	180/181 (99%)	164 (91%)	16 (9%)	12	46
5	QE	116/123 (94%)	107 (92%)	9 (8%)	16	52
5	XE	116/123 (94%)	108 (93%)	8 (7%)	19	59
6	QF	90/90 (100%)	77 (86%)	13 (14%)	4	22
6	XF	90/90 (100%)	77 (86%)	13 (14%)	4	22
7	QG	126/127 (99%)	115 (91%)	11 (9%)	13	47
7	XG	126/127 (99%)	115 (91%)	11 (9%)	13	47
8	QH	119/119 (100%)	106 (89%)	13 (11%)	8	35
8	XH	119/119 (100%)	106 (89%)	13 (11%)	8	35
9	QI	98/99 (99%)	87 (89%)	11 (11%)	7	33
9	XI	98/99 (99%)	87 (89%)	11 (11%)	7	33
10	QJ	89/92 (97%)	81 (91%)	8 (9%)	12	46
10	XJ	89/92 (97%)	81 (91%)	8 (9%)	12	46
11	QK	90/99 (91%)	81 (90%)	9 (10%)	9	40
11	XK	90/99 (91%)	81 (90%)	9 (10%)	9	40
12	QL	104/109 (95%)	90 (86%)	14 (14%)	5	25
12	XL	104/109 (95%)	90 (86%)	14 (14%)	5	25
13	QM	97/101 (96%)	81 (84%)	16 (16%)	3	15
13	XM	97/101 (96%)	80 (82%)	17 (18%)	2	13
14	QN	49/50 (98%)	45 (92%)	4 (8%)	14	50
14	XN	49/50 (98%)	42 (86%)	7 (14%)	4	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	QO	79/80 (99%)	73 (92%)	6 (8%)	16	54
15	XO	79/80 (99%)	73 (92%)	6 (8%)	16	54
16	QP	72/74 (97%)	63 (88%)	9 (12%)	6	28
16	XP	72/74 (97%)	63 (88%)	9 (12%)	6	28
17	QQ	95/97 (98%)	89 (94%)	6 (6%)	22	63
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	22	63
18	QR	61/77 (79%)	54 (88%)	7 (12%)	7	31
18	XR	61/77 (79%)	54 (88%)	7 (12%)	7	31
19	QS	73/80 (91%)	62 (85%)	11 (15%)	3	20
19	XS	73/80 (91%)	62 (85%)	11 (15%)	3	20
20	QT	76/82 (93%)	68 (90%)	8 (10%)	8	37
20	XT	76/82 (93%)	68 (90%)	8 (10%)	8	37
21	QU	20/22 (91%)	19 (95%)	1 (5%)	30	69
21	XU	20/22 (91%)	19 (95%)	1 (5%)	30	69
27	RD	214/218 (98%)	177 (83%)	37 (17%)	2	13
27	YD	214/218 (98%)	177 (83%)	37 (17%)	2	13
28	RE	165/166 (99%)	127 (77%)	38 (23%)	1	4
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	4
29	RF	161/166 (97%)	140 (87%)	21 (13%)	5	26
29	YF	161/166 (97%)	139 (86%)	22 (14%)	4	24
30	RG	155/156 (99%)	130 (84%)	25 (16%)	3	17
30	YG	155/156 (99%)	131 (84%)	24 (16%)	3	18
31	RH	142/148 (96%)	115 (81%)	27 (19%)	2	9
31	YH	142/148 (96%)	115 (81%)	27 (19%)	2	9
32	RI	122/124 (98%)	98 (80%)	24 (20%)	1	8
32	YI	122/124 (98%)	97 (80%)	25 (20%)	1	7
33	RN	117/119 (98%)	98 (84%)	19 (16%)	3	16
33	YN	117/119 (98%)	98 (84%)	19 (16%)	3	16
34	RO	100/100 (100%)	90 (90%)	10 (10%)	9	40
34	YO	100/100 (100%)	90 (90%)	10 (10%)	9	40
35	RP	116/116 (100%)	89 (77%)	27 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	YP	116/116 (100%)	89 (77%)	27 (23%)	1	4
36	RQ	111/111 (100%)	92 (83%)	19 (17%)	2	14
36	YQ	111/111 (100%)	92 (83%)	19 (17%)	2	14
37	RR	101/101 (100%)	84 (83%)	17 (17%)	2	14
37	YR	101/101 (100%)	84 (83%)	17 (17%)	2	14
38	RS	87/88 (99%)	74 (85%)	13 (15%)	4	20
38	YS	87/88 (99%)	74 (85%)	13 (15%)	4	20
39	RT	120/127 (94%)	97 (81%)	23 (19%)	2	8
39	YT	120/127 (94%)	97 (81%)	23 (19%)	2	8
40	RU	93/94 (99%)	80 (86%)	13 (14%)	4	23
40	YU	93/94 (99%)	80 (86%)	13 (14%)	4	23
41	RV	82/82 (100%)	71 (87%)	11 (13%)	5	25
41	YV	82/82 (100%)	71 (87%)	11 (13%)	5	25
42	RW	92/92 (100%)	77 (84%)	15 (16%)	3	16
42	YW	92/92 (100%)	77 (84%)	15 (16%)	3	16
43	RX	74/78 (95%)	63 (85%)	11 (15%)	4	20
43	YX	74/78 (95%)	63 (85%)	11 (15%)	4	20
44	RY	85/91 (93%)	70 (82%)	15 (18%)	2	12
44	YY	85/91 (93%)	70 (82%)	15 (18%)	2	12
45	RZ	152/179 (85%)	124 (82%)	28 (18%)	2	10
45	YZ	152/179 (85%)	124 (82%)	28 (18%)	2	10
46	R0	65/67 (97%)	55 (85%)	10 (15%)	3	19
46	Y0	65/67 (97%)	56 (86%)	9 (14%)	4	24
47	R1	82/83 (99%)	67 (82%)	15 (18%)	2	10
47	Y1	82/83 (99%)	67 (82%)	15 (18%)	2	10
48	R2	64/67 (96%)	57 (89%)	7 (11%)	8	35
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	8	35
49	R3	51/52 (98%)	40 (78%)	11 (22%)	1	6
49	Y3	51/52 (98%)	40 (78%)	11 (22%)	1	6
50	R4	63/63 (100%)	44 (70%)	19 (30%)	0	3
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	4
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	4
52	R6	48/52 (92%)	38 (79%)	10 (21%)	1	7
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	7
53	R7	42/42 (100%)	39 (93%)	3 (7%)	18	58
53	Y7	42/42 (100%)	39 (93%)	3 (7%)	18	58
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	3
54	Y8	54/55 (98%)	39 (72%)	15 (28%)	0	3
All	All	9614/9998 (96%)	8197 (85%)	1417 (15%)	4	21

5 of 1417 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	R3	17	LYS
7	XG	148	ASN
45	YZ	132	ASN
50	R4	53	GLU
2	XB	94	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
47	R1	56	GLN
5	XE	78	HIS
43	YX	87	GLN
48	R2	9	GLN
2	XB	135	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	343 (22%)	51 (3%)
1	XA	1499/1522 (98%)	333 (22%)	55 (3%)
22	QV	76/77 (98%)	30 (39%)	1 (1%)
22	XV	76/77 (98%)	30 (39%)	1 (1%)
23	QX	7/25 (28%)	6 (85%)	1 (14%)
23	XX	7/25 (28%)	2 (28%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	QY	13/18 (72%)	6 (46%)	1 (7%)
24	XY	13/18 (72%)	5 (38%)	1 (7%)
25	RA	2880/2916 (98%)	734 (25%)	76 (2%)
25	YA	2879/2916 (98%)	747 (25%)	75 (2%)
26	RB	119/122 (97%)	30 (25%)	2 (1%)
26	YB	119/122 (97%)	38 (31%)	1 (0%)
55	Z6	1/3 (33%)	0	0
55	Z8	1/3 (33%)	0	0
All	All	9189/9366 (98%)	2304 (25%)	265 (2%)

5 of 2304 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	7	G
1	QA	9	G
1	QA	32	A
1	QA	39	G

5 of 265 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2566	A
1	XA	481	G
25	YA	2198	A
25	RA	2689	U
1	XA	64	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	1MG	QY	37	24	16,26,27	2.92	3 (18%)	19,39,42	1.57	4 (21%)
24	1MG	XY	37	24	16,26,27	2.89	3 (18%)	19,39,42	1.58	4 (21%)
55	PPU	Z6	76	55,25	30,40,41	2.57	6 (20%)	37,57,60	3.25	11 (29%)
55	PPU	Z8	76	55,25	30,40,41	2.57	6 (20%)	37,57,60	3.25	11 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	1MG	QY	37	24	-	0/3/25/26	0/3/3/3
24	1MG	XY	37	24	-	0/3/25/26	0/3/3/3
55	PPU	Z6	76	55,25	-	0/21/43/44	0/4/4/4
55	PPU	Z8	76	55,25	-	0/21/43/44	0/4/4/4

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	Z6	76	PPU	C9-N6	-5.62	1.32	1.45
55	Z8	76	PPU	C9-N6	-5.58	1.32	1.45
55	Z8	76	PPU	C10-N6	-5.31	1.32	1.45
55	Z6	76	PPU	C10-N6	-5.31	1.32	1.45
55	Z6	76	PPU	C5-N7	-2.03	1.32	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	Z6	76	PPU	C2'-C1'-N9	-10.35	98.48	114.29
55	Z8	76	PPU	C2'-C1'-N9	-10.35	98.48	114.29
55	Z6	76	PPU	N3-C2-N1	-9.86	121.35	128.89
55	Z8	76	PPU	N3-C2-N1	-9.82	121.38	128.89
55	Z8	76	PPU	C3'-N3'-C	-8.20	110.27	123.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	XY	37	IMG	1	0
55	Z6	76	PPU	10	0
55	Z8	76	PPU	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 607 ligands modelled in this entry, 605 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	$\# Z > 2$
57	PAR	QA	1661	-	45,45,45	1.27	6 (13%)	59,67,67	1.38	6 (10%)
57	PAR	XA	1664	-	45,45,45	1.31	7 (15%)	59,67,67	1.35	7 (11%)

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
57	PAR	QA	1661	-	-	0/18/94/94	0/4/4/4
57	PAR	XA	1664	-	-	0/18/94/94	0/4/4/4

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	XA	1664	PAR	C31-C21	2.00	1.56	1.53
57	XA	1664	PAR	C14-C24	2.14	1.56	1.52
57	QA	1661	PAR	C31-C21	2.16	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	QA	1661	PAR	C11-C21	2.20	1.56	1.52
57	QA	1661	PAR	O51-C11	2.28	1.47	1.41

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	XA	1664	PAR	O11-C42-C32	-2.83	102.06	108.92
57	QA	1661	PAR	O11-C42-C32	-2.74	102.29	108.92
57	QA	1661	PAR	C22-C12-C62	-2.43	106.38	110.11
57	XA	1664	PAR	C31-C41-C51	-2.07	106.59	110.20
57	XA	1664	PAR	C11-O51-C51	2.19	118.00	113.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	QA	1661	PAR	4	0
57	XA	1664	PAR	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1522 (98%)	0.21	65 (4%) 39 33	30, 83, 175, 356	0
1	XA	1501/1522 (98%)	0.08	53 (3%) 48 41	30, 76, 171, 324	0
2	QB	237/256 (92%)	0.89	34 (14%) 4 4	56, 138, 222, 266	0
2	XB	237/256 (92%)	0.55	27 (11%) 7 7	55, 126, 194, 238	0
3	QC	205/239 (85%)	0.74	30 (14%) 3 4	54, 122, 199, 216	0
3	XC	205/239 (85%)	0.29	10 (4%) 33 28	39, 95, 158, 217	0
4	QD	208/209 (99%)	0.20	9 (4%) 39 33	44, 92, 154, 184	0
4	XD	208/209 (99%)	0.34	9 (4%) 39 33	39, 95, 161, 234	0
5	QE	151/162 (93%)	0.61	13 (8%) 13 13	29, 104, 175, 237	0
5	XE	151/162 (93%)	0.16	5 (3%) 50 44	34, 79, 149, 229	0
6	QF	101/101 (100%)	0.15	3 (2%) 54 47	44, 86, 125, 222	0
6	XF	101/101 (100%)	0.13	4 (3%) 42 36	36, 86, 144, 209	0
7	QG	155/156 (99%)	0.55	16 (10%) 9 9	51, 106, 181, 215	0
7	XG	155/156 (99%)	0.30	10 (6%) 22 20	46, 103, 177, 230	0
8	QH	138/138 (100%)	0.28	4 (2%) 55 49	48, 108, 167, 204	0
8	XH	138/138 (100%)	0.21	4 (2%) 55 49	48, 96, 158, 208	0
9	QI	127/128 (99%)	0.74	15 (11%) 6 7	53, 124, 188, 214	0
9	XI	127/128 (99%)	0.60	8 (6%) 23 21	43, 116, 194, 219	0
10	QJ	99/105 (94%)	1.39	30 (30%) 1 1	67, 145, 212, 246	0
10	XJ	99/105 (94%)	0.96	20 (20%) 1 2	37, 119, 193, 210	0
11	QK	119/129 (92%)	0.57	12 (10%) 9 10	42, 92, 152, 199	0
11	XK	119/129 (92%)	0.35	5 (4%) 40 34	39, 89, 165, 204	0
12	QL	125/132 (94%)	0.43	8 (6%) 23 21	42, 84, 176, 269	0
12	XL	125/132 (94%)	0.12	5 (4%) 42 36	30, 66, 131, 242	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	0.58	13 (10%) 8 8	43, 124, 197, 254	0
13	XM	121/126 (96%)	0.28	6 (4%) 32 28	44, 98, 183, 264	0
14	QN	60/61 (98%)	1.13	11 (18%) 2 2	61, 128, 195, 227	0
14	XN	60/61 (98%)	0.12	1 (1%) 73 67	47, 87, 134, 161	0
15	QO	88/89 (98%)	0.48	7 (7%) 15 14	42, 97, 165, 235	0
15	XO	88/89 (98%)	-0.04	1 (1%) 82 76	39, 79, 130, 178	0
16	QP	84/88 (95%)	0.31	2 (2%) 62 56	41, 79, 136, 206	0
16	XP	84/88 (95%)	0.42	4 (4%) 34 30	54, 92, 151, 203	0
17	QQ	100/105 (95%)	0.31	3 (3%) 54 47	53, 102, 165, 210	0
17	XQ	100/105 (95%)	0.47	6 (6%) 25 22	38, 101, 159, 213	0
18	QR	70/88 (79%)	0.15	3 (4%) 39 33	34, 90, 156, 213	0
18	XR	70/88 (79%)	0.13	2 (2%) 55 49	30, 88, 138, 206	0
19	QS	84/93 (90%)	1.30	21 (25%) 1 1	87, 149, 204, 237	0
19	XS	84/93 (90%)	0.60	8 (9%) 10 11	55, 105, 176, 244	0
20	QT	99/106 (93%)	0.57	10 (10%) 9 10	48, 101, 192, 233	0
20	XT	99/106 (93%)	0.29	6 (6%) 25 22	50, 107, 163, 197	0
21	QU	25/27 (92%)	1.14	3 (12%) 6 7	41, 100, 139, 189	0
21	XU	25/27 (92%)	0.78	2 (8%) 15 14	52, 96, 135, 165	0
22	QV	77/77 (100%)	0.48	5 (6%) 22 20	40, 91, 151, 170	0
22	XV	77/77 (100%)	0.21	2 (2%) 59 53	34, 77, 126, 180	0
23	QX	8/25 (32%)	0.67	1 (12%) 5 6	61, 82, 137, 169	0
23	XX	8/25 (32%)	0.69	1 (12%) 5 6	39, 67, 104, 175	0
24	QY	13/18 (72%)	4.19	8 (61%) 0 0	93, 213, 294, 312	0
24	XY	13/18 (72%)	2.92	6 (46%) 0 0	69, 188, 276, 278	0
25	RA	2883/2916 (98%)	0.15	180 (6%) 24 22	24, 57, 221, 389	0
25	YA	2882/2916 (98%)	0.02	162 (5%) 28 25	17, 48, 215, 377	0
26	RB	120/122 (98%)	0.13	3 (2%) 61 54	52, 91, 141, 150	0
26	YB	120/122 (98%)	-0.10	0 100 100	44, 74, 109, 158	0
27	RD	272/276 (98%)	0.09	2 (0%) 89 84	19, 60, 98, 243	0
27	YD	272/276 (98%)	-0.09	1 (0%) 93 90	13, 50, 85, 221	0
28	RE	205/206 (99%)	0.19	5 (2%) 62 56	24, 78, 165, 260	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YE	205/206 (99%)	0.23	6 (2%) 55 49	22, 76, 161, 238	0
29	RF	202/210 (96%)	0.25	8 (3%) 42 36	21, 82, 158, 250	0
29	YF	202/210 (96%)	0.07	4 (1%) 68 63	13, 64, 130, 197	0
30	RG	181/182 (99%)	1.96	77 (42%) 0 0	58, 164, 258, 303	0
30	YG	181/182 (99%)	0.95	30 (16%) 2 2	59, 108, 186, 248	0
31	RH	170/180 (94%)	1.37	40 (23%) 1 1	78, 171, 239, 267	0
31	YH	170/180 (94%)	0.50	10 (5%) 26 23	39, 100, 156, 260	0
32	RI	146/148 (98%)	0.72	18 (12%) 5 6	56, 118, 204, 240	0
32	YI	146/148 (98%)	0.27	4 (2%) 58 51	40, 104, 169, 214	0
33	RN	138/140 (98%)	0.11	4 (2%) 55 49	32, 84, 153, 194	0
33	YN	138/140 (98%)	-0.03	2 (1%) 78 72	31, 78, 128, 166	0
34	RO	122/122 (100%)	0.07	4 (3%) 50 44	24, 71, 133, 170	0
34	YO	122/122 (100%)	0.10	1 (0%) 87 81	23, 66, 114, 153	0
35	RP	150/150 (100%)	0.39	14 (9%) 11 11	15, 79, 185, 232	0
35	YP	150/150 (100%)	0.16	3 (2%) 68 63	5, 68, 135, 230	0
36	RQ	141/141 (100%)	0.35	7 (4%) 32 28	38, 85, 149, 219	0
36	YQ	141/141 (100%)	0.05	3 (2%) 67 62	27, 66, 118, 196	0
37	RR	118/118 (100%)	-0.07	0 100 100	28, 68, 107, 171	0
37	YR	118/118 (100%)	-0.05	0 100 100	20, 64, 114, 153	0
38	RS	111/112 (99%)	0.30	5 (4%) 37 32	40, 90, 146, 203	0
38	YS	111/112 (99%)	0.10	3 (2%) 58 51	36, 77, 134, 207	0
39	RT	137/146 (93%)	0.35	11 (8%) 15 14	39, 90, 189, 221	0
39	YT	137/146 (93%)	0.30	7 (5%) 32 27	41, 78, 176, 220	0
40	RU	117/118 (99%)	0.18	5 (4%) 39 33	27, 73, 155, 249	0
40	YU	117/118 (99%)	-0.02	3 (2%) 59 53	20, 59, 129, 212	0
41	RV	101/101 (100%)	0.50	11 (10%) 7 8	28, 88, 167, 278	0
41	YV	101/101 (100%)	0.20	4 (3%) 42 36	25, 82, 143, 255	0
42	RW	113/113 (100%)	0.13	5 (4%) 38 33	28, 63, 127, 241	0
42	YW	113/113 (100%)	-0.08	0 100 100	22, 60, 109, 204	0
43	RX	92/96 (95%)	0.03	1 (1%) 82 76	31, 65, 108, 137	0
43	YX	92/96 (95%)	0.15	2 (2%) 65 59	21, 50, 92, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RY	102/110 (92%)	1.01	22 (21%) 1 1	46, 106, 214, 270	0
44	YY	102/110 (92%)	0.38	7 (6%) 20 18	25, 85, 144, 243	0
45	RZ	172/206 (83%)	1.58	46 (26%) 1 1	62, 130, 264, 332	0
45	YZ	172/206 (83%)	0.94	25 (14%) 3 4	33, 111, 243, 361	0
46	R0	82/85 (96%)	0.28	1 (1%) 81 75	35, 72, 105, 143	0
46	Y0	82/85 (96%)	0.07	1 (1%) 81 75	28, 63, 99, 116	0
47	R1	97/98 (98%)	0.44	4 (4%) 41 36	24, 67, 167, 259	0
47	Y1	97/98 (98%)	0.31	7 (7%) 18 17	20, 65, 161, 211	0
48	R2	69/72 (95%)	0.09	3 (4%) 39 33	34, 82, 149, 217	0
48	Y2	69/72 (95%)	0.13	2 (2%) 55 49	22, 72, 138, 203	0
49	R3	59/60 (98%)	0.27	1 (1%) 73 67	35, 81, 147, 173	0
49	Y3	59/60 (98%)	0.09	2 (3%) 49 43	33, 67, 108, 178	0
50	R4	71/71 (100%)	3.22	42 (59%) 0 0	102, 207, 283, 352	0
50	Y4	71/71 (100%)	1.87	24 (33%) 0 0	88, 160, 251, 277	0
51	R5	59/60 (98%)	0.54	7 (11%) 6 7	12, 64, 224, 264	0
51	Y5	59/60 (98%)	-0.04	3 (5%) 32 27	20, 71, 220, 229	0
52	R6	49/54 (90%)	4.38	34 (69%) 0 0	119, 196, 290, 297	0
52	Y6	49/54 (90%)	3.85	38 (77%) 0 0	120, 182, 235, 265	0
53	R7	49/49 (100%)	-0.22	0 100 100	19, 44, 100, 216	0
53	Y7	49/49 (100%)	-0.03	3 (6%) 25 22	15, 37, 100, 216	0
54	R8	64/65 (98%)	0.26	3 (4%) 35 31	18, 62, 156, 228	0
54	Y8	64/65 (98%)	0.27	3 (4%) 35 31	20, 61, 116, 173	0
55	Z6	2/3 (66%)	0.43	0 100 100	49, 49, 49, 51	0
55	Z8	2/3 (66%)	0.26	0 100 100	36, 36, 36, 37	0
All	All	20776/21420 (96%)	0.31	1454 (6%) 19 18	5, 78, 195, 389	0

The worst 5 of 1454 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	YA	2173	A	17.6
25	RA	2116	G	16.2
24	QY	32	U	15.6
52	R6	43	CYS	15.6
25	YA	2175	C	15.4

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	PPU	Z6	76	37/38	0.94	0.28	-	53,53,53,53	0
24	1MG	QY	37	24/25	0.83	0.24	-	124,124,124,124	0
24	1MG	XY	37	24/25	0.93	0.15	-	89,89,89,89	0
55	PPU	Z8	76	37/38	0.95	0.25	-	40,40,40,40	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	MG	RA	3081	1/1	0.97	0.47	30.94	28,28,28,28	0
56	MG	YA	3152	1/1	0.92	0.40	29.69	38,38,38,38	0
56	MG	XA	1647	1/1	0.84	0.53	26.33	58,58,58,58	0
56	MG	YA	3009	1/1	0.96	0.46	23.75	27,27,27,27	0
56	MG	YA	3090	1/1	0.97	0.39	19.64	11,11,11,11	0
56	MG	YA	3179	1/1	0.96	0.41	18.98	31,31,31,31	0
56	MG	YA	3015	1/1	0.98	0.43	17.76	10,10,10,10	0
56	MG	YA	3170	1/1	0.94	0.35	16.70	10,10,10,10	0
56	MG	YA	3057	1/1	0.97	0.49	15.69	22,22,22,22	0
56	MG	RA	3024	1/1	0.99	0.45	15.61	4,4,4,4	0
56	MG	YA	3119	1/1	0.96	0.37	14.64	35,35,35,35	0
56	MG	YA	3002	1/1	1.00	0.38	14.62	15,15,15,15	0
56	MG	RA	3012	1/1	0.93	0.36	14.19	26,26,26,26	0
56	MG	YA	3026	1/1	0.97	0.40	13.86	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3100	1/1	0.96	0.32	13.62	1,1,1,1	0
56	MG	RA	3130	1/1	0.90	0.31	13.45	44,44,44,44	0
56	MG	YA	3159	1/1	0.94	0.30	13.08	43,43,43,43	0
56	MG	RA	3074	1/1	0.97	0.32	12.68	8,8,8,8	0
56	MG	RA	3141	1/1	0.73	0.37	12.61	43,43,43,43	0
56	MG	RA	3103	1/1	0.91	0.62	12.51	48,48,48,48	0
56	MG	RA	3023	1/1	0.96	0.29	12.42	24,24,24,24	0
56	MG	RA	3051	1/1	0.96	0.40	12.30	1,1,1,1	0
56	MG	RA	3106	1/1	0.90	0.50	12.12	24,24,24,24	0
56	MG	YA	3080	1/1	0.97	0.30	11.98	3,3,3,3	0
56	MG	YA	3031	1/1	0.99	0.35	11.89	6,6,6,6	0
56	MG	RA	3045	1/1	0.98	0.30	11.06	12,12,12,12	0
56	MG	YA	3058	1/1	0.99	0.30	10.97	16,16,16,16	0
56	MG	RA	3052	1/1	0.96	0.42	10.75	24,24,24,24	0
56	MG	RA	3062	1/1	0.98	0.38	10.50	21,21,21,21	0
56	MG	RA	3089	1/1	0.98	0.28	10.04	26,26,26,26	0
56	MG	RA	3112	1/1	0.98	0.28	9.98	50,50,50,50	0
56	MG	YA	3008	1/1	0.96	0.27	9.52	17,17,17,17	0
56	MG	RA	3030	1/1	0.98	0.28	9.52	15,15,15,15	0
56	MG	YA	3164	1/1	0.86	0.30	9.37	25,25,25,25	0
56	MG	YA	3081	1/1	0.97	0.30	9.36	18,18,18,18	0
56	MG	YA	3068	1/1	0.98	0.31	9.18	12,12,12,12	0
56	MG	RA	3021	1/1	0.97	0.42	9.12	27,27,27,27	0
56	MG	RA	3070	1/1	0.98	0.31	8.91	37,37,37,37	0
56	MG	YA	3165	1/1	0.84	0.24	8.86	42,42,42,42	0
56	MG	RA	3124	1/1	0.96	0.32	8.81	21,21,21,21	0
56	MG	RA	3201	1/1	0.72	0.34	8.65	22,22,22,22	0
56	MG	RA	3202	1/1	0.78	0.40	8.49	84,84,84,84	0
56	MG	RA	3117	1/1	0.87	0.24	8.28	42,42,42,42	0
56	MG	YA	3087	1/1	0.98	0.25	8.21	7,7,7,7	0
56	MG	YA	3192	1/1	0.90	0.28	8.05	40,40,40,40	0
56	MG	YA	3014	1/1	0.97	0.39	7.87	12,12,12,12	0
56	MG	QA	1627	1/1	0.84	0.35	7.85	57,57,57,57	0
56	MG	YA	3242	1/1	0.93	0.32	7.78	34,34,34,34	0
56	MG	RA	3005	1/1	0.95	0.26	7.69	8,8,8,8	0
56	MG	YA	3140	1/1	0.97	0.29	7.33	2,2,2,2	0
56	MG	QA	1620	1/1	0.85	0.50	7.33	40,40,40,40	0
56	MG	YA	3233	1/1	0.97	0.37	7.14	44,44,44,44	0
56	MG	RA	3076	1/1	0.97	0.40	7.12	22,22,22,22	0
56	MG	QA	1626	1/1	0.96	0.32	7.06	77,77,77,77	0
56	MG	YA	3234	1/1	0.89	0.22	6.84	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3044	1/1	0.96	0.29	6.83	21,21,21,21	0
56	MG	RA	3014	1/1	0.99	0.24	6.66	10,10,10,10	0
56	MG	RA	3064	1/1	0.98	0.40	6.60	25,25,25,25	0
56	MG	RA	3185	1/1	0.91	0.36	6.56	44,44,44,44	0
56	MG	RA	3104	1/1	0.94	0.24	6.52	44,44,44,44	0
56	MG	RA	3136	1/1	0.95	0.24	6.52	49,49,49,49	0
56	MG	YA	3004	1/1	0.95	0.23	6.38	13,13,13,13	0
56	MG	XA	1605	1/1	0.65	0.41	6.25	126,126,126,126	0
56	MG	YA	3117	1/1	0.90	0.34	5.92	60,60,60,60	0
56	MG	XA	1642	1/1	0.87	0.26	5.77	49,49,49,49	0
56	MG	YA	3035	1/1	0.97	0.20	5.64	10,10,10,10	0
56	MG	YA	3241	1/1	0.94	0.29	5.48	33,33,33,33	0
56	MG	RA	3211	1/1	0.97	0.28	5.41	13,13,13,13	0
56	MG	RA	3080	1/1	0.89	0.27	5.13	44,44,44,44	0
56	MG	YA	3194	1/1	0.91	0.31	4.98	42,42,42,42	0
56	MG	YA	3042	1/1	0.99	0.31	4.92	28,28,28,28	0
56	MG	YA	3011	1/1	0.99	0.26	4.61	13,13,13,13	0
56	MG	YA	3079	1/1	0.98	0.26	4.57	18,18,18,18	0
56	MG	RA	3058	1/1	0.98	0.21	4.52	13,13,13,13	0
56	MG	YA	3023	1/1	0.99	0.26	4.50	4,4,4,4	0
56	MG	RA	3039	1/1	0.98	0.26	4.42	18,18,18,18	0
56	MG	RE	302	1/1	0.96	0.38	4.36	22,22,22,22	0
56	MG	YA	3101	1/1	0.97	0.27	4.34	5,5,5,5	0
56	MG	RA	3060	1/1	0.97	0.22	4.31	25,25,25,25	0
56	MG	YA	3109	1/1	0.98	0.25	4.31	25,25,25,25	0
56	MG	YA	3238	1/1	0.98	0.25	4.29	34,34,34,34	0
56	MG	YA	3113	1/1	0.96	0.26	4.26	21,21,21,21	0
56	MG	RA	3166	1/1	0.95	0.23	4.25	56,56,56,56	0
56	MG	RA	3078	1/1	0.94	0.19	4.10	15,15,15,15	0
56	MG	YA	3044	1/1	0.98	0.22	4.09	9,9,9,9	0
56	MG	QA	1649	1/1	0.95	0.34	3.97	45,45,45,45	0
56	MG	YA	3049	1/1	0.98	0.27	3.90	15,15,15,15	0
56	MG	RA	3046	1/1	0.98	0.35	3.87	31,31,31,31	0
56	MG	QA	1609	1/1	0.97	0.28	3.74	34,34,34,34	0
56	MG	YA	3208	1/1	0.93	0.22	3.69	53,53,53,53	0
56	MG	YA	3107	1/1	0.89	0.23	3.57	25,25,25,25	0
56	MG	XA	1606	1/1	0.98	0.25	3.52	17,17,17,17	0
56	MG	RA	3077	1/1	0.97	0.32	3.50	14,14,14,14	0
56	MG	RA	3200	1/1	0.84	0.24	3.45	58,58,58,58	0
56	MG	RA	3189	1/1	0.94	0.23	3.31	34,34,34,34	0
56	MG	YA	3047	1/1	0.97	0.26	3.24	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3037	1/1	0.99	0.20	3.08	3,3,3,3	0
56	MG	RA	3179	1/1	0.94	0.21	3.01	22,22,22,22	0
56	MG	RA	3069	1/1	0.93	0.30	2.98	43,43,43,43	0
56	MG	YA	3105	1/1	0.83	0.22	2.94	16,16,16,16	0
56	MG	RA	3048	1/1	0.95	0.22	2.93	13,13,13,13	0
56	MG	YA	3024	1/1	0.98	0.19	2.69	10,10,10,10	0
56	MG	YA	3162	1/1	0.88	0.27	2.67	34,34,34,34	0
56	MG	YA	3166	1/1	0.98	0.19	2.64	51,51,51,51	0
57	PAR	XA	1664	42/42	0.91	0.25	2.57	57,57,57,57	0
56	MG	RP	201	1/1	0.95	0.35	2.50	37,37,37,37	0
56	MG	YA	3036	1/1	0.98	0.23	2.49	3,3,3,3	0
56	MG	RA	3210	1/1	0.87	0.34	2.47	38,38,38,38	0
56	MG	RA	3018	1/1	0.95	0.22	2.41	6,6,6,6	0
56	MG	QA	1601	1/1	0.91	0.23	2.28	27,27,27,27	0
56	MG	RA	3152	1/1	0.90	0.18	2.23	26,26,26,26	0
56	MG	XA	1627	1/1	0.95	0.29	2.17	31,31,31,31	0
57	PAR	QA	1661	42/42	0.89	0.23	2.15	75,75,75,75	0
56	MG	YA	3050	1/1	0.98	0.18	2.13	2,2,2,2	0
56	MG	RA	3054	1/1	0.99	0.23	2.11	5,5,5,5	0
56	MG	RA	3016	1/1	0.96	0.26	2.08	2,2,2,2	0
56	MG	QA	1638	1/1	0.91	0.30	2.03	53,53,53,53	0
56	MG	YA	3032	1/1	0.98	0.21	2.01	9,9,9,9	0
56	MG	XA	1609	1/1	0.95	0.25	1.97	15,15,15,15	0
56	MG	RA	3053	1/1	0.99	0.17	1.95	5,5,5,5	0
56	MG	YA	3095	1/1	0.99	0.29	1.93	5,5,5,5	0
56	MG	XA	1650	1/1	0.94	0.26	1.91	39,39,39,39	0
56	MG	RA	3113	1/1	0.98	0.27	1.90	24,24,24,24	0
56	MG	RA	3138	1/1	0.97	0.17	1.86	21,21,21,21	0
56	MG	YA	3204	1/1	0.99	0.17	1.85	43,43,43,43	0
56	MG	RA	3150	1/1	0.93	0.25	1.84	26,26,26,26	0
56	MG	RA	3102	1/1	0.93	0.25	1.80	32,32,32,32	0
56	MG	YA	3074	1/1	0.96	0.17	1.79	28,28,28,28	0
56	MG	XA	1644	1/1	0.83	0.28	1.78	59,59,59,59	0
56	MG	YE	302	1/1	0.79	0.19	1.76	13,13,13,13	0
56	MG	XA	1656	1/1	0.90	0.18	1.72	37,37,37,37	0
56	MG	RA	3042	1/1	0.97	0.20	1.66	11,11,11,11	0
56	MG	RA	3049	1/1	0.99	0.15	1.66	10,10,10,10	0
56	MG	RA	3155	1/1	0.97	0.21	1.65	12,12,12,12	0
56	MG	RA	3047	1/1	0.95	0.23	1.63	7,7,7,7	0
56	MG	RA	3083	1/1	0.87	0.20	1.63	26,26,26,26	0
56	MG	RA	3002	1/1	0.97	0.24	1.61	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3160	1/1	0.94	0.17	1.60	25,25,25,25	0
56	MG	YA	3111	1/1	0.98	0.23	1.46	30,30,30,30	0
56	MG	RA	3026	1/1	0.97	0.22	1.45	6,6,6,6	0
56	MG	YA	3028	1/1	0.99	0.19	1.36	23,23,23,23	0
56	MG	YA	3174	1/1	0.94	0.19	1.35	29,29,29,29	0
56	MG	RA	3158	1/1	0.93	0.16	1.34	14,14,14,14	0
56	MG	XA	1626	1/1	0.89	0.32	1.28	27,27,27,27	0
56	MG	YA	3144	1/1	0.96	0.16	1.27	13,13,13,13	0
56	MG	RA	3157	1/1	0.93	0.37	1.22	20,20,20,20	0
56	MG	YA	3033	1/1	0.94	0.24	1.20	6,6,6,6	0
56	MG	RA	3009	1/1	0.94	0.17	1.18	21,21,21,21	0
56	MG	RA	3122	1/1	0.87	0.24	1.17	70,70,70,70	0
56	MG	YA	3006	1/1	0.98	0.24	1.13	0,0,0,0	0
56	MG	YA	3199	1/1	0.94	0.21	1.12	42,42,42,42	0
56	MG	XA	1661	1/1	0.95	0.19	1.09	38,38,38,38	0
56	MG	QA	1646	1/1	0.98	0.26	1.07	14,14,14,14	0
56	MG	RA	3140	1/1	0.96	0.19	1.07	45,45,45,45	0
56	MG	RA	3028	1/1	0.98	0.19	1.07	12,12,12,12	0
56	MG	YA	3022	1/1	0.98	0.21	0.98	6,6,6,6	0
56	MG	YA	3197	1/1	0.94	0.15	0.94	33,33,33,33	0
56	MG	YA	3114	1/1	0.99	0.24	0.90	6,6,6,6	0
56	MG	RA	3144	1/1	0.88	0.18	0.90	36,36,36,36	0
56	MG	YA	3184	1/1	0.94	0.17	0.90	33,33,33,33	0
56	MG	RA	3071	1/1	0.97	0.19	0.88	32,32,32,32	0
56	MG	QA	1656	1/1	0.94	0.22	0.87	53,53,53,53	0
56	MG	XM	202	1/1	0.72	0.31	0.86	43,43,43,43	0
56	MG	XA	1652	1/1	0.90	0.16	0.82	64,64,64,64	0
56	MG	YA	3176	1/1	0.81	0.17	0.75	54,54,54,54	0
56	MG	YA	3136	1/1	0.97	0.15	0.75	4,4,4,4	0
56	MG	YA	3056	1/1	0.90	0.19	0.72	9,9,9,9	0
56	MG	RA	3167	1/1	0.86	0.19	0.72	35,35,35,35	0
56	MG	RA	3063	1/1	0.96	0.20	0.63	27,27,27,27	0
56	MG	RA	3131	1/1	0.94	0.20	0.60	77,77,77,77	0
56	MG	YA	3205	1/1	0.94	0.15	0.57	28,28,28,28	0
56	MG	XV	101	1/1	0.98	0.22	0.55	14,14,14,14	0
56	MG	YA	3138	1/1	0.97	0.16	0.52	15,15,15,15	0
56	MG	RA	3011	1/1	0.99	0.16	0.46	30,30,30,30	0
56	MG	QA	1605	1/1	0.97	0.17	0.41	51,51,51,51	0
56	MG	YA	3034	1/1	0.96	0.19	0.40	3,3,3,3	0
56	MG	YA	3154	1/1	0.95	0.16	0.35	15,15,15,15	0
56	MG	RA	3088	1/1	0.96	0.17	0.32	24,24,24,24	0
56	MG	RA	3193	1/1	0.93	0.14	0.29	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3142	1/1	0.93	0.15	0.28	30,30,30,30	0
56	MG	YA	3169	1/1	0.77	0.21	0.15	84,84,84,84	0
56	MG	RA	3156	1/1	0.99	0.16	0.07	22,22,22,22	0
56	MG	QV	101	1/1	0.96	0.20	0.06	17,17,17,17	0
56	MG	YA	3025	1/1	0.98	0.18	0.05	6,6,6,6	0
56	MG	QA	1644	1/1	0.90	0.19	0.03	23,23,23,23	0
56	MG	YA	3228	1/1	0.87	0.17	0.02	45,45,45,45	0
56	MG	RA	3173	1/1	0.76	0.18	-0.00	71,71,71,71	0
56	MG	RA	3029	1/1	0.98	0.15	-0.02	2,2,2,2	0
56	MG	YA	3126	1/1	0.94	0.17	-0.04	27,27,27,27	0
56	MG	XA	1640	1/1	0.97	0.19	-0.05	47,47,47,47	0
56	MG	YA	3227	1/1	0.88	0.14	-0.06	22,22,22,22	0
56	MG	QA	1617	1/1	0.95	0.22	-0.09	41,41,41,41	0
56	MG	QA	1608	1/1	0.97	0.18	-0.11	27,27,27,27	0
56	MG	RA	3190	1/1	0.88	0.18	-0.12	50,50,50,50	0
56	MG	QA	1640	1/1	0.89	0.18	-0.13	54,54,54,54	0
56	MG	QA	1651	1/1	0.98	0.21	-0.15	70,70,70,70	0
56	MG	YA	3092	1/1	0.97	0.16	-0.21	11,11,11,11	0
56	MG	RA	3032	1/1	0.99	0.17	-0.26	17,17,17,17	0
56	MG	XA	1602	1/1	0.97	0.15	-0.28	15,15,15,15	0
56	MG	RA	3015	1/1	0.92	0.15	-0.31	15,15,15,15	0
56	MG	XA	1619	1/1	0.76	0.14	-0.40	46,46,46,46	0
56	MG	XA	1646	1/1	0.93	0.18	-0.41	23,23,23,23	0
56	MG	YA	3048	1/1	0.98	0.16	-0.42	4,4,4,4	0
56	MG	XA	1611	1/1	0.98	0.17	-0.44	29,29,29,29	0
56	MG	YA	3070	1/1	0.95	0.13	-0.49	22,22,22,22	0
56	MG	RF	301	1/1	0.90	0.24	-0.58	45,45,45,45	0
56	MG	YA	3071	1/1	0.92	0.13	-0.60	18,18,18,18	0
56	MG	XA	1624	1/1	0.99	0.14	-0.65	35,35,35,35	0
56	MG	YA	3203	1/1	0.96	0.13	-0.66	24,24,24,24	0
56	MG	YA	3038	1/1	0.98	0.13	-0.66	12,12,12,12	0
56	MG	QA	1652	1/1	0.90	0.17	-0.67	36,36,36,36	0
56	MG	YB	202	1/1	0.92	0.16	-0.68	42,42,42,42	0
56	MG	RA	3110	1/1	0.98	0.12	-0.69	51,51,51,51	0
56	MG	YA	3210	1/1	0.96	0.11	-0.70	35,35,35,35	0
56	MG	YA	3183	1/1	0.86	0.12	-0.81	36,36,36,36	0
56	MG	RA	3098	1/1	0.91	0.13	-0.82	11,11,11,11	0
56	MG	QA	1641	1/1	0.98	0.17	-0.86	25,25,25,25	0
56	MG	RA	3139	1/1	0.93	0.13	-0.87	31,31,31,31	0
56	MG	XA	1629	1/1	0.97	0.13	-0.87	49,49,49,49	0
56	MG	RA	3169	1/1	0.89	0.13	-0.90	23,23,23,23	0
56	MG	QM	201	1/1	0.98	0.15	-0.91	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3177	1/1	0.96	0.15	-0.91	59,59,59,59	0
56	MG	RA	3025	1/1	0.99	0.14	-0.91	9,9,9,9	0
56	MG	RA	3040	1/1	0.94	0.14	-0.98	9,9,9,9	0
56	MG	XA	1628	1/1	0.98	0.17	-1.02	24,24,24,24	0
56	MG	YA	3091	1/1	0.98	0.13	-1.05	23,23,23,23	0
56	MG	YA	3214	1/1	0.94	0.15	-1.06	42,42,42,42	0
56	MG	RA	3082	1/1	0.94	0.14	-1.12	13,13,13,13	0
56	MG	QA	1654	1/1	0.98	0.15	-1.13	14,14,14,14	0
56	MG	YA	3005	1/1	0.94	0.12	-1.15	19,19,19,19	0
56	MG	RA	3207	1/1	0.88	0.12	-1.21	51,51,51,51	0
58	ZN	QD	301	1/1	0.96	0.19	-1.24	59,59,59,59	0
56	MG	YA	3065	1/1	0.91	0.13	-1.32	12,12,12,12	0
56	MG	RA	3109	1/1	0.99	0.07	-1.38	26,26,26,26	0
56	MG	YA	3027	1/1	0.98	0.11	-1.40	5,5,5,5	0
56	MG	YA	3016	1/1	0.89	0.14	-1.45	19,19,19,19	0
58	ZN	XD	301	1/1	0.98	0.23	-1.45	49,49,49,49	0
56	MG	QA	1625	1/1	0.89	0.14	-1.49	66,66,66,66	0
56	MG	QA	1616	1/1	0.96	0.09	-1.51	42,42,42,42	0
56	MG	RA	3094	1/1	0.95	0.12	-1.57	19,19,19,19	0
56	MG	RA	3007	1/1	0.93	0.13	-1.57	8,8,8,8	0
58	ZN	QN	101	1/1	0.76	0.13	-1.59	155,155,155,155	0
56	MG	QX	102	1/1	0.94	0.09	-1.59	42,42,42,42	0
58	ZN	XN	101	1/1	0.98	0.12	-1.60	107,107,107,107	0
56	MG	YA	3218	1/1	0.97	0.11	-1.76	19,19,19,19	0
56	MG	RA	3099	1/1	0.95	0.13	-1.77	21,21,21,21	0
56	MG	XA	1637	1/1	0.95	0.11	-1.78	39,39,39,39	0
56	MG	RA	3004	1/1	0.96	0.11	-1.79	5,5,5,5	0
56	MG	YA	3216	1/1	0.97	0.09	-1.83	42,42,42,42	0
56	MG	QA	1630	1/1	0.97	0.12	-1.85	66,66,66,66	0
56	MG	XA	1635	1/1	0.99	0.07	-1.91	36,36,36,36	0
56	MG	XA	1651	1/1	0.92	0.13	-1.92	18,18,18,18	0
56	MG	YA	3132	1/1	0.97	0.10	-1.96	13,13,13,13	0
56	MG	RA	3105	1/1	0.97	0.12	-1.99	50,50,50,50	0
56	MG	YA	3017	1/1	0.98	0.11	-2.01	16,16,16,16	0
56	MG	XA	1613	1/1	0.99	0.13	-2.02	45,45,45,45	0
56	MG	XA	1601	1/1	0.98	0.12	-2.06	15,15,15,15	0
56	MG	YA	3112	1/1	0.97	0.11	-2.10	41,41,41,41	0
56	MG	YA	3237	1/1	0.98	0.08	-2.12	15,15,15,15	0
56	MG	RA	3068	1/1	0.97	0.13	-2.13	16,16,16,16	0
56	MG	QA	1606	1/1	0.97	0.15	-2.13	7,7,7,7	0
56	MG	RA	3114	1/1	0.93	0.11	-2.14	30,30,30,30	0
56	MG	YA	3185	1/1	0.94	0.09	-2.27	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3135	1/1	0.99	0.10	-2.42	33,33,33,33	0
56	MG	YA	3059	1/1	0.97	0.15	-2.42	74,74,74,74	0
56	MG	QA	1634	1/1	0.92	0.10	-2.44	48,48,48,48	0
56	MG	RA	3090	1/1	0.96	0.11	-2.48	14,14,14,14	0
56	MG	XA	1616	1/1	0.99	0.11	-2.51	20,20,20,20	0
56	MG	YA	3108	1/1	0.99	0.11	-2.52	5,5,5,5	0
56	MG	YA	3072	1/1	0.97	0.13	-2.61	10,10,10,10	0
56	MG	YA	3129	1/1	0.97	0.07	-2.76	22,22,22,22	0
56	MG	YA	3189	1/1	0.97	0.11	-2.96	31,31,31,31	0
56	MG	RA	3204	1/1	0.97	0.12	-2.98	30,30,30,30	0
56	MG	YA	3137	1/1	0.98	0.08	-3.12	15,15,15,15	0
56	MG	YA	3223	1/1	0.94	0.09	-3.40	30,30,30,30	0
56	MG	RA	3067	1/1	0.98	0.06	-3.45	7,7,7,7	0
56	MG	RA	3085	1/1	0.97	0.11	-3.48	15,15,15,15	0
56	MG	RA	3118	1/1	0.97	0.14	-3.56	14,14,14,14	0
56	MG	YA	3167	1/1	0.97	0.06	-3.74	12,12,12,12	0
56	MG	RA	3165	1/1	0.98	0.09	-3.78	5,5,5,5	0
56	MG	RB	201	1/1	0.98	0.05	-4.05	13,13,13,13	0
56	MG	XA	1603	1/1	0.98	0.07	-4.13	23,23,23,23	0
56	MG	YA	3161	1/1	0.98	0.09	-4.27	30,30,30,30	0
56	MG	YA	3217	1/1	0.98	0.09	-4.29	35,35,35,35	0
56	MG	YA	3206	1/1	0.98	0.10	-4.29	24,24,24,24	0
56	MG	QA	1603	1/1	0.99	0.05	-4.30	28,28,28,28	0
56	MG	QA	1611	1/1	0.92	0.08	-4.57	32,32,32,32	0
56	MG	RA	3057	1/1	0.94	0.06	-4.83	22,22,22,22	0
56	MG	YA	3052	1/1	0.98	0.23	-	17,17,17,17	0
56	MG	YA	3182	1/1	0.91	0.24	-	30,30,30,30	0
56	MG	XA	1620	1/1	0.96	0.10	-	55,55,55,55	0
56	MG	XA	1648	1/1	0.68	0.33	-	25,25,25,25	0
56	MG	YA	3219	1/1	0.96	0.26	-	29,29,29,29	0
56	MG	XA	1641	1/1	0.89	0.13	-	24,24,24,24	0
56	MG	YA	3235	1/1	0.99	0.13	-	26,26,26,26	0
56	MG	YA	3084	1/1	0.83	0.19	-	23,23,23,23	0
56	MG	RA	3192	1/1	0.84	0.29	-	56,56,56,56	0
56	MG	YA	3102	1/1	0.96	0.25	-	5,5,5,5	0
56	MG	YA	3093	1/1	0.99	0.14	-	18,18,18,18	0
56	MG	RA	3075	1/1	0.92	0.35	-	4,4,4,4	0
56	MG	YA	3013	1/1	0.99	0.31	-	3,3,3,3	0
56	MG	XA	1643	1/1	0.97	0.17	-	47,47,47,47	0
56	MG	YA	3173	1/1	0.67	0.21	-	43,43,43,43	0
56	MG	YA	3040	1/1	0.97	0.12	-	1,1,1,1	0
56	MG	YA	3064	1/1	0.98	0.18	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3012	1/1	0.70	1.51	-	80,80,80,80	0
56	MG	YA	3200	1/1	0.92	0.11	-	15,15,15,15	0
56	MG	YA	3212	1/1	0.94	0.10	-	21,21,21,21	0
56	MG	RA	3209	1/1	0.88	0.25	-	49,49,49,49	0
56	MG	XA	1645	1/1	0.89	0.19	-	31,31,31,31	0
56	MG	RA	3178	1/1	0.92	0.25	-	62,62,62,62	0
56	MG	QA	1650	1/1	0.95	0.14	-	36,36,36,36	0
56	MG	RA	3146	1/1	0.92	0.30	-	44,44,44,44	0
56	MG	RA	3183	1/1	0.90	0.33	-	49,49,49,49	0
56	MG	RA	3127	1/1	0.94	0.18	-	47,47,47,47	0
56	MG	RA	3184	1/1	0.96	0.30	-	33,33,33,33	0
56	MG	YA	3177	1/1	0.77	0.16	-	35,35,35,35	0
56	MG	YA	3030	1/1	0.97	0.27	-	24,24,24,24	0
56	MG	QA	1629	1/1	0.95	0.17	-	68,68,68,68	0
56	MG	RA	3186	1/1	0.86	0.21	-	90,90,90,90	0
56	MG	YA	3240	1/1	0.84	0.14	-	45,45,45,45	0
56	MG	YA	3163	1/1	0.96	0.20	-	40,40,40,40	0
56	MG	QA	1637	1/1	0.91	0.17	-	49,49,49,49	0
56	MG	RA	3174	1/1	0.90	0.39	-	68,68,68,68	0
56	MG	QA	1612	1/1	0.96	0.07	-	37,37,37,37	0
56	MG	YA	3156	1/1	0.80	0.15	-	33,33,33,33	0
56	MG	XA	1657	1/1	0.96	0.13	-	28,28,28,28	0
56	MG	QA	1657	1/1	0.88	0.10	-	76,76,76,76	0
56	MG	YA	3088	1/1	0.94	0.26	-	20,20,20,20	0
56	MG	YA	3098	1/1	0.92	0.17	-	49,49,49,49	0
56	MG	YA	3178	1/1	0.93	0.22	-	68,68,68,68	0
56	MG	YA	3193	1/1	0.97	0.14	-	39,39,39,39	0
56	MG	YA	3131	1/1	0.94	0.14	-	20,20,20,20	0
56	MG	RA	3084	1/1	0.98	0.30	-	17,17,17,17	0
56	MG	RA	3163	1/1	0.87	0.19	-	38,38,38,38	0
56	MG	XA	1625	1/1	0.94	0.14	-	20,20,20,20	0
56	MG	RA	3050	1/1	0.99	0.14	-	0,0,0,0	0
56	MG	XA	1654	1/1	0.89	0.12	-	50,50,50,50	0
56	MG	YA	3010	1/1	0.98	0.15	-	3,3,3,3	0
56	MG	RA	3086	1/1	0.98	0.22	-	33,33,33,33	0
56	MG	YA	3236	1/1	0.73	0.24	-	57,57,57,57	0
56	MG	RA	3038	1/1	0.96	0.15	-	14,14,14,14	0
56	MG	RA	3033	1/1	0.92	0.20	-	62,62,62,62	0
56	MG	YA	3155	1/1	0.95	0.23	-	22,22,22,22	0
56	MG	RA	3120	1/1	0.93	0.11	-	10,10,10,10	0
56	MG	YA	3073	1/1	0.98	0.25	-	24,24,24,24	0
56	MG	XA	1663	1/1	0.91	0.30	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3147	1/1	0.99	0.11	-	11,11,11,11	0
56	MG	YA	3157	1/1	0.96	0.17	-	29,29,29,29	0
56	MG	QA	1653	1/1	0.96	0.27	-	39,39,39,39	0
56	MG	YA	3209	1/1	0.98	0.18	-	41,41,41,41	0
56	MG	XA	1630	1/1	0.98	0.14	-	39,39,39,39	0
56	MG	QA	1643	1/1	0.84	0.20	-	24,24,24,24	0
56	MG	YA	3188	1/1	0.89	0.20	-	38,38,38,38	0
56	MG	YA	3139	1/1	0.90	0.22	-	32,32,32,32	0
56	MG	RA	3187	1/1	0.82	0.49	-	68,68,68,68	0
56	MG	YA	3069	1/1	0.97	0.16	-	16,16,16,16	0
56	MG	YA	3181	1/1	0.84	0.28	-	51,51,51,51	0
56	MG	XM	201	1/1	0.94	0.12	-	28,28,28,28	0
56	MG	YA	3096	1/1	0.99	0.22	-	15,15,15,15	0
56	MG	QA	1619	1/1	0.93	0.30	-	48,48,48,48	0
56	MG	RA	3121	1/1	0.94	0.65	-	35,35,35,35	0
56	MG	QV	102	1/1	0.92	0.19	-	8,8,8,8	0
56	MG	QA	1602	1/1	0.96	0.34	-	19,19,19,19	0
56	MG	XV	102	1/1	0.93	0.12	-	22,22,22,22	0
56	MG	RA	3205	1/1	0.88	0.23	-	54,54,54,54	0
56	MG	XA	1636	1/1	0.94	0.15	-	58,58,58,58	0
56	MG	YA	3007	1/1	0.99	0.17	-	6,6,6,6	0
56	MG	YA	3231	1/1	0.94	0.29	-	32,32,32,32	0
56	MG	RA	3196	1/1	0.88	0.23	-	53,53,53,53	0
56	MG	RA	3115	1/1	0.92	0.26	-	59,59,59,59	0
56	MG	RA	3072	1/1	0.90	0.27	-	24,24,24,24	0
56	MG	QA	1648	1/1	0.99	0.03	-	100,100,100,100	0
56	MG	YA	3145	1/1	0.95	0.15	-	42,42,42,42	0
56	MG	YA	3196	1/1	0.94	0.13	-	33,33,33,33	0
56	MG	RA	3176	1/1	0.71	0.53	-	71,71,71,71	0
56	MG	YA	3127	1/1	0.94	0.53	-	44,44,44,44	0
56	MG	XA	1634	1/1	0.97	0.29	-	28,28,28,28	0
56	MG	YA	3061	1/1	0.92	0.12	-	35,35,35,35	0
56	MG	RA	3194	1/1	0.98	0.14	-	14,14,14,14	0
56	MG	YA	3054	1/1	0.97	0.15	-	14,14,14,14	0
56	MG	YA	3130	1/1	0.90	0.18	-	16,16,16,16	0
56	MG	XA	1631	1/1	0.91	0.32	-	45,45,45,45	0
56	MG	XA	1614	1/1	0.92	0.11	-	14,14,14,14	0
56	MG	RA	3147	1/1	0.89	0.42	-	49,49,49,49	0
56	MG	YA	3153	1/1	0.98	0.21	-	26,26,26,26	0
56	MG	YA	3118	1/1	0.97	0.17	-	12,12,12,12	0
56	MG	YA	3003	1/1	0.91	0.13	-	13,13,13,13	0
56	MG	YA	3150	1/1	0.92	0.19	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3119	1/1	0.95	0.38	-	34,34,34,34	0
56	MG	XA	1639	1/1	0.95	0.17	-	32,32,32,32	0
56	MG	YA	3213	1/1	0.97	0.13	-	41,41,41,41	0
56	MG	YA	3043	1/1	0.98	0.40	-	9,9,9,9	0
56	MG	YA	3045	1/1	0.95	0.37	-	22,22,22,22	0
56	MG	YA	3222	1/1	0.98	0.05	-	9,9,9,9	0
56	MG	RA	3096	1/1	0.84	0.16	-	8,8,8,8	0
56	MG	RA	3168	1/1	0.93	0.10	-	31,31,31,31	0
56	MG	YA	3019	1/1	0.97	0.39	-	21,21,21,21	0
56	MG	XA	1658	1/1	0.90	0.27	-	50,50,50,50	0
56	MG	YA	3171	1/1	0.72	0.30	-	72,72,72,72	0
56	MG	RA	3056	1/1	0.89	0.15	-	26,26,26,26	0
56	MG	RA	3073	1/1	0.92	0.38	-	5,5,5,5	0
56	MG	YA	3120	1/1	0.80	0.23	-	36,36,36,36	0
56	MG	QA	1604	1/1	0.96	0.10	-	33,33,33,33	0
56	MG	YA	3175	1/1	0.94	0.12	-	12,12,12,12	0
56	MG	YA	3075	1/1	0.98	0.10	-	14,14,14,14	0
56	MG	YA	3160	1/1	0.93	0.19	-	37,37,37,37	0
56	MG	RA	3135	1/1	0.94	0.27	-	32,32,32,32	0
56	MG	YA	3128	1/1	0.95	0.22	-	23,23,23,23	0
56	MG	RA	3107	1/1	0.99	0.28	-	21,21,21,21	0
56	MG	YB	201	1/1	0.98	0.15	-	21,21,21,21	0
56	MG	YA	3046	1/1	0.99	0.13	-	4,4,4,4	0
56	MG	YA	3172	1/1	0.75	0.17	-	55,55,55,55	0
56	MG	YA	3051	1/1	0.97	0.23	-	4,4,4,4	0
56	MG	RA	3128	1/1	0.94	0.20	-	27,27,27,27	0
56	MG	XA	1607	1/1	0.99	0.07	-	5,5,5,5	0
56	MG	RA	3191	1/1	0.90	0.17	-	62,62,62,62	0
56	MG	YX	101	1/1	0.91	0.09	-	28,28,28,28	0
56	MG	QA	1655	1/1	0.95	0.35	-	50,50,50,50	0
56	MG	XA	1610	1/1	0.97	0.18	-	37,37,37,37	0
56	MG	RA	3159	1/1	0.91	0.42	-	26,26,26,26	0
56	MG	YA	3221	1/1	0.95	0.21	-	26,26,26,26	0
56	MG	XA	1617	1/1	0.96	0.14	-	26,26,26,26	0
56	MG	XA	1649	1/1	0.97	0.36	-	28,28,28,28	0
56	MG	YA	3226	1/1	0.93	0.15	-	14,14,14,14	0
56	MG	RA	3079	1/1	0.98	0.20	-	32,32,32,32	0
56	MG	YA	3104	1/1	0.99	0.24	-	6,6,6,6	0
56	MG	YA	3225	1/1	0.96	0.15	-	32,32,32,32	0
56	MG	RA	3195	1/1	0.88	0.25	-	28,28,28,28	0
56	MG	XA	1615	1/1	0.96	0.24	-	19,19,19,19	0
56	MG	XA	1621	1/1	0.88	0.15	-	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3134	1/1	0.95	0.10	-	29,29,29,29	0
56	MG	YA	3180	1/1	0.97	0.11	-	53,53,53,53	0
56	MG	RA	3142	1/1	0.98	0.11	-	15,15,15,15	0
56	MG	QA	1628	1/1	0.98	0.28	-	14,14,14,14	0
56	MG	YA	3187	1/1	0.96	0.36	-	58,58,58,58	0
56	MG	RA	3175	1/1	0.84	0.25	-	99,99,99,99	0
56	MG	YA	3149	1/1	0.94	0.30	-	26,26,26,26	0
56	MG	RA	3093	1/1	0.97	0.07	-	24,24,24,24	0
56	MG	QA	1618	1/1	0.91	0.16	-	41,41,41,41	0
56	MG	YA	3039	1/1	0.88	0.20	-	30,30,30,30	0
56	MG	YA	3123	1/1	0.96	0.12	-	15,15,15,15	0
56	MG	RA	3162	1/1	0.86	0.28	-	56,56,56,56	0
56	MG	XA	1653	1/1	0.91	0.23	-	44,44,44,44	0
56	MG	YA	3215	1/1	0.94	0.15	-	51,51,51,51	0
56	MG	QA	1607	1/1	0.97	0.14	-	22,22,22,22	0
56	MG	YA	3133	1/1	0.86	0.72	-	43,43,43,43	0
56	MG	YA	3220	1/1	0.95	0.14	-	18,18,18,18	0
56	MG	RA	3123	1/1	0.92	0.14	-	32,32,32,32	0
56	MG	YA	3082	1/1	0.93	0.15	-	13,13,13,13	0
56	MG	RA	3125	1/1	0.95	0.32	-	24,24,24,24	0
56	MG	QA	1645	1/1	0.93	0.17	-	22,22,22,22	0
56	MG	YA	3097	1/1	0.96	0.24	-	19,19,19,19	0
56	MG	Y5	101	1/1	0.98	0.15	-	25,25,25,25	0
56	MG	YA	3067	1/1	0.93	0.14	-	15,15,15,15	0
56	MG	QA	1636	1/1	0.97	0.07	-	15,15,15,15	0
56	MG	QX	101	1/1	0.97	0.10	-	24,24,24,24	0
56	MG	RA	3161	1/1	0.94	0.15	-	32,32,32,32	0
56	MG	YA	3041	1/1	0.97	0.28	-	6,6,6,6	0
56	MG	RA	3132	1/1	0.97	0.21	-	12,12,12,12	0
56	MG	RA	3097	1/1	0.90	0.21	-	24,24,24,24	0
56	MG	RA	3171	1/1	0.91	0.32	-	49,49,49,49	0
56	MG	RA	3145	1/1	0.97	0.22	-	37,37,37,37	0
56	MG	YA	3106	1/1	0.97	0.30	-	32,32,32,32	0
56	MG	YA	3202	1/1	0.96	0.07	-	21,21,21,21	0
56	MG	YA	3124	1/1	0.93	0.22	-	22,22,22,22	0
56	MG	RA	3133	1/1	0.88	0.13	-	32,32,32,32	0
56	MG	YA	3077	1/1	0.97	0.15	-	8,8,8,8	0
56	MG	YA	3060	1/1	0.96	0.23	-	13,13,13,13	0
56	MG	YA	3116	1/1	0.85	0.20	-	28,28,28,28	0
56	MG	RA	3172	1/1	0.97	0.21	-	29,29,29,29	0
56	MG	RB	202	1/1	0.95	0.08	-	31,31,31,31	0
56	MG	RA	3164	1/1	0.93	0.15	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3230	1/1	0.92	0.39	-	43,43,43,43	0
56	MG	QA	1632	1/1	0.90	0.24	-	41,41,41,41	0
56	MG	YA	3168	1/1	0.93	0.30	-	65,65,65,65	0
56	MG	QA	1660	1/1	0.91	0.19	-	45,45,45,45	0
56	MG	RA	3170	1/1	0.97	0.09	-	41,41,41,41	0
56	MG	QA	1622	1/1	0.90	0.27	-	60,60,60,60	0
56	MG	RA	3017	1/1	0.99	0.12	-	13,13,13,13	0
56	MG	YA	3086	1/1	0.98	0.14	-	3,3,3,3	0
56	MG	YA	3083	1/1	0.95	0.42	-	21,21,21,21	0
56	MG	YA	3099	1/1	0.98	0.34	-	11,11,11,11	0
56	MG	RA	3043	1/1	0.98	0.11	-	30,30,30,30	0
56	MG	YA	3158	1/1	0.83	0.12	-	20,20,20,20	0
56	MG	YA	3103	1/1	0.98	0.08	-	12,12,12,12	0
56	MG	YA	3224	1/1	0.95	0.18	-	18,18,18,18	0
56	MG	RA	3003	1/1	0.96	0.23	-	17,17,17,17	0
56	MG	RA	3129	1/1	0.97	0.19	-	26,26,26,26	0
56	MG	YA	3121	1/1	0.93	0.15	-	23,23,23,23	0
56	MG	YA	3110	1/1	0.97	0.08	-	10,10,10,10	0
56	MG	YA	3190	1/1	0.89	0.24	-	51,51,51,51	0
56	MG	RA	3180	1/1	0.89	0.21	-	28,28,28,28	0
56	MG	QA	1623	1/1	0.94	0.15	-	28,28,28,28	0
56	MG	RA	3116	1/1	0.95	0.22	-	69,69,69,69	0
56	MG	RA	3065	1/1	0.95	0.28	-	21,21,21,21	0
56	MG	QA	1610	1/1	0.91	0.21	-	33,33,33,33	0
56	MG	RA	3111	1/1	0.91	0.28	-	52,52,52,52	0
56	MG	YA	3115	1/1	0.96	0.15	-	21,21,21,21	0
56	MG	RA	3100	1/1	0.97	0.16	-	44,44,44,44	0
56	MG	RA	3151	1/1	0.97	0.23	-	23,23,23,23	0
56	MG	YA	3207	1/1	0.87	0.30	-	66,66,66,66	0
56	MG	QA	1659	1/1	0.92	0.26	-	79,79,79,79	0
56	MG	YA	3191	1/1	0.94	0.13	-	24,24,24,24	0
56	MG	RA	3022	1/1	0.98	0.33	-	3,3,3,3	0
56	MG	RA	3153	1/1	0.91	0.16	-	36,36,36,36	0
56	MG	YA	3141	1/1	0.93	0.49	-	43,43,43,43	0
56	MG	YA	3198	1/1	0.93	0.27	-	32,32,32,32	0
56	MG	YA	3143	1/1	0.97	0.13	-	33,33,33,33	0
56	MG	RA	3035	1/1	0.98	0.12	-	21,21,21,21	0
56	MG	YA	3063	1/1	0.92	0.12	-	6,6,6,6	0
56	MG	YA	3195	1/1	0.98	0.09	-	55,55,55,55	0
56	MG	RA	3199	1/1	0.95	0.19	-	47,47,47,47	0
56	MG	QH	201	1/1	0.62	0.31	-	124,124,124,124	0
56	MG	XA	1662	1/1	0.94	0.23	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	XA	1638	1/1	0.86	0.21	-	55,55,55,55	0
56	MG	YA	3062	1/1	0.99	0.11	-	6,6,6,6	0
56	MG	YA	3201	1/1	0.91	0.10	-	122,122,122,122	0
56	MG	RA	3108	1/1	0.90	0.17	-	26,26,26,26	0
56	MG	RA	3027	1/1	0.91	0.74	-	80,80,80,80	0
56	MG	RA	3061	1/1	0.98	0.21	-	28,28,28,28	0
56	MG	YE	301	1/1	0.93	0.11	-	1,1,1,1	0
56	MG	RA	3055	1/1	0.99	0.15	-	12,12,12,12	0
56	MG	RA	3206	1/1	0.90	0.28	-	38,38,38,38	0
56	MG	RA	3197	1/1	0.88	0.15	-	50,50,50,50	0
56	MG	RA	3036	1/1	0.99	0.33	-	10,10,10,10	0
56	MG	RE	301	1/1	0.97	0.12	-	22,22,22,22	0
56	MG	YA	3066	1/1	0.94	0.48	-	18,18,18,18	0
56	MG	QA	1639	1/1	0.64	0.13	-	44,44,44,44	0
56	MG	YA	3029	1/1	0.97	0.35	-	17,17,17,17	0
56	MG	YA	3125	1/1	0.96	0.13	-	18,18,18,18	0
56	MG	YA	3094	1/1	0.98	0.30	-	10,10,10,10	0
56	MG	R5	101	1/1	0.97	0.14	-	27,27,27,27	0
56	MG	YA	3239	1/1	0.81	0.45	-	48,48,48,48	0
56	MG	RA	3143	1/1	0.93	0.47	-	16,16,16,16	0
56	MG	RA	3041	1/1	0.96	0.17	-	5,5,5,5	0
56	MG	QA	1658	1/1	0.98	0.08	-	68,68,68,68	0
56	MG	YA	3211	1/1	0.94	0.18	-	42,42,42,42	0
56	MG	RA	3149	1/1	0.94	0.19	-	48,48,48,48	0
56	MG	RA	3087	1/1	0.96	0.12	-	9,9,9,9	0
56	MG	YA	3021	1/1	0.98	0.32	-	12,12,12,12	0
56	MG	RA	3010	1/1	0.98	0.36	-	4,4,4,4	0
56	MG	XA	1660	1/1	0.95	0.09	-	61,61,61,61	0
56	MG	RA	3020	1/1	0.96	0.27	-	29,29,29,29	0
56	MG	YA	3151	1/1	0.91	0.50	-	26,26,26,26	0
56	MG	YA	3146	1/1	0.97	0.11	-	50,50,50,50	0
56	MG	QA	1631	1/1	0.93	0.15	-	55,55,55,55	0
56	MG	YA	3148	1/1	0.95	0.11	-	25,25,25,25	0
56	MG	RA	3091	1/1	0.92	0.16	-	21,21,21,21	0
56	MG	XA	1618	1/1	0.86	0.14	-	24,24,24,24	0
56	MG	XA	1612	1/1	0.96	0.31	-	21,21,21,21	0
56	MG	XA	1623	1/1	0.97	0.39	-	31,31,31,31	0
56	MG	RA	3101	1/1	0.91	0.11	-	50,50,50,50	0
56	MG	RA	3059	1/1	0.99	0.28	-	21,21,21,21	0
56	MG	YA	3085	1/1	0.95	0.10	-	41,41,41,41	0
56	MG	XA	1622	1/1	0.98	0.07	-	40,40,40,40	0
56	MG	YA	3076	1/1	0.98	0.37	-	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	XA	1632	1/1	0.93	0.19	-	11,11,11,11	0
56	MG	RA	3034	1/1	0.96	0.28	-	16,16,16,16	0
56	MG	QA	1635	1/1	0.93	0.18	-	31,31,31,31	0
56	MG	RA	3198	1/1	0.97	0.09	-	53,53,53,53	0
56	MG	QA	1633	1/1	0.93	0.37	-	50,50,50,50	0
56	MG	XA	1655	1/1	0.94	0.21	-	33,33,33,33	0
56	MG	RA	3208	1/1	0.86	0.14	-	47,47,47,47	0
56	MG	QA	1642	1/1	0.97	0.09	-	49,49,49,49	0
56	MG	RA	3008	1/1	0.96	0.20	-	13,13,13,13	0
56	MG	RA	3037	1/1	0.97	0.25	-	10,10,10,10	0
56	MG	RA	3066	1/1	0.92	0.24	-	12,12,12,12	0
56	MG	RA	3126	1/1	0.98	0.24	-	27,27,27,27	0
56	MG	XA	1633	1/1	0.98	0.23	-	32,32,32,32	0
56	MG	RA	3019	1/1	0.98	0.16	-	10,10,10,10	0
56	MG	QA	1615	1/1	0.67	0.76	-	46,46,46,46	0
56	MG	RA	3013	1/1	0.99	0.22	-	10,10,10,10	0
56	MG	YA	3001	1/1	0.98	0.43	-	13,13,13,13	0
56	MG	YA	3232	1/1	0.95	0.29	-	43,43,43,43	0
56	MG	YA	3078	1/1	0.98	0.38	-	25,25,25,25	0
56	MG	QA	1613	1/1	0.84	0.33	-	56,56,56,56	0
56	MG	RA	3148	1/1	0.95	0.20	-	21,21,21,21	0
56	MG	YA	3089	1/1	0.99	0.23	-	2,2,2,2	0
56	MG	QF	201	1/1	0.86	0.17	-	56,56,56,56	0
56	MG	XA	1604	1/1	0.99	0.07	-	31,31,31,31	0
56	MG	QA	1647	1/1	0.97	0.11	-	41,41,41,41	0
56	MG	RA	3031	1/1	0.98	0.29	-	26,26,26,26	0
56	MG	YA	3186	1/1	0.88	0.28	-	50,50,50,50	0
56	MG	RA	3095	1/1	0.92	0.14	-	31,31,31,31	0
56	MG	RA	3001	1/1	0.96	0.18	-	36,36,36,36	0
56	MG	XA	1659	1/1	0.96	0.09	-	60,60,60,60	0
56	MG	YA	3229	1/1	0.98	0.10	-	52,52,52,52	0
56	MG	RA	3006	1/1	0.99	0.17	-	3,3,3,3	0
56	MG	QA	1614	1/1	0.86	0.25	-	38,38,38,38	0
56	MG	YA	3122	1/1	0.87	0.17	-	35,35,35,35	0
56	MG	YA	3018	1/1	0.94	0.32	-	24,24,24,24	0
56	MG	XA	1608	1/1	0.98	0.16	-	7,7,7,7	0
56	MG	RA	3182	1/1	0.98	0.35	-	25,25,25,25	0
56	MG	RA	3154	1/1	0.98	0.13	-	12,12,12,12	0
56	MG	RA	3137	1/1	0.94	0.17	-	36,36,36,36	0
56	MG	RA	3092	1/1	0.92	0.10	-	18,18,18,18	0
56	MG	RA	3212	1/1	0.96	0.28	-	18,18,18,18	0
56	MG	RA	3188	1/1	0.92	0.28	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3053	1/1	0.99	0.15	-	4,4,4,4	0
56	MG	YA	3055	1/1	0.97	0.23	-	16,16,16,16	0
56	MG	QA	1624	1/1	0.96	0.35	-	24,24,24,24	0
56	MG	YA	3020	1/1	0.97	0.34	-	8,8,8,8	0
56	MG	RA	3134	1/1	0.93	0.21	-	18,18,18,18	0
56	MG	RA	3181	1/1	0.91	0.28	-	34,34,34,34	0
56	MG	RA	3203	1/1	0.57	0.27	-	73,73,73,73	0
56	MG	QA	1621	1/1	0.97	0.18	-	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.