



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 16, 2024 – 09:31 AM EST

PDB ID : 6OSI  
Title : Unmodified tRNA(Pro) bound to Thermus thermophilus 70S (near cognate)  
Authors : Hoffer, E.D.; Subaramanian, S.; Hong, S.; Maehigashi, T.; Dunham, C.M.  
Deposited on : 2019-05-01  
Resolution : 4.14 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

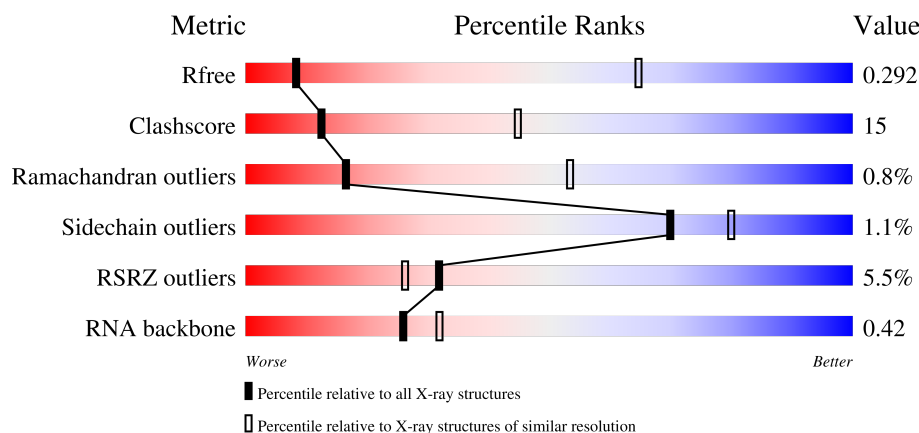
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.14 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))
$R_{free}$	164625	1166 (4.48-3.80)
Clashscore	180529	1233 (4.48-3.80)
Ramachandran outliers	177936	1158 (4.48-3.80)
Sidechain outliers	177891	1145 (4.48-3.80)
RSRZ outliers	164620	1164 (4.48-3.80)
RNA backbone	3690	1145 (5.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	1521	<div> <div>24%</div> <div>48%</div> <div>23%</div> <div>• •</div> </div>
1	XA	1521	<div> <div>28%</div> <div>44%</div> <div>21%</div> <div>7%</div> </div>
2	QB	256	<div> <div>4%</div> <div>64%</div> <div>28%</div> <div>8%</div> </div>
2	XB	256	<div> <div>7%</div> <div>69%</div> <div>23%</div> <div>8%</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	19	
23	XX	19	
24	R0	85	
24	Y0	85	
25	R1	98	
25	Y1	98	
26	R2	72	
26	Y2	72	
27	R3	60	
27	Y3	60	

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Mol	Chain	Length	Quality of chain
28	R4	71	
28	Y4	71	
29	R5	60	
29	Y5	60	
30	R6	54	
30	Y6	54	
31	R7	49	
31	Y7	49	
32	R8	65	
32	Y8	65	
33	R9	37	
33	Y9	37	
34	RA	2905	
34	YA	2905	
35	RB	122	
35	YB	122	
36	RD	276	
36	YD	276	
37	RE	206	
37	YE	206	
38	RF	210	
38	YF	210	
39	RG	182	
39	YG	182	
40	RH	180	

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	QA	1622	-	-	-	X
55	MG	QE	201	-	-	-	X
55	MG	RA	2912	-	-	-	X
55	MG	RA	2921	-	-	-	X
55	MG	RA	2954	-	-	-	X
55	MG	RA	2970	-	-	-	X
55	MG	RA	2975	-	-	-	X
55	MG	RA	2976	-	-	-	X
55	MG	RA	3013	-	-	-	X
55	MG	RA	3051	-	-	-	X
55	MG	RA	3057	-	-	-	X
55	MG	RA	3064	-	-	-	X
55	MG	RA	3071	-	-	-	X
55	MG	RA	3075	-	-	-	X
55	MG	RA	3078	-	-	-	X
55	MG	RA	3083	-	-	-	X
55	MG	RA	3101	-	-	-	X
55	MG	RA	3103	-	-	-	X
55	MG	RA	3133	-	-	-	X
55	MG	RA	3139	-	-	-	X
55	MG	RA	3144	-	-	-	X
55	MG	RA	3147	-	-	-	X
55	MG	RA	3152	-	-	-	X
55	MG	RA	3162	-	-	-	X
55	MG	RA	3195	-	-	-	X
55	MG	RA	3220	-	-	-	X
55	MG	RA	3221	-	-	-	X
55	MG	RA	3223	-	-	-	X
55	MG	RA	3260	-	-	-	X
55	MG	RA	3286	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	RA	3307	-	-	-	X
55	MG	RA	3310	-	-	-	X
55	MG	RA	3318	-	-	-	X
55	MG	RE	304	-	-	-	X
55	MG	XA	1605	-	-	-	X
55	MG	XA	1610	-	-	-	X
55	MG	XA	1612	-	-	-	X
55	MG	XA	1613	-	-	-	X
55	MG	XA	1621	-	-	-	X
55	MG	XA	1657	-	-	-	X
55	MG	XA	1665	-	-	-	X
55	MG	XA	1688	-	-	X	-
55	MG	Y8	101	-	-	-	X
55	MG	YA	2904	-	-	-	X
55	MG	YA	2905	-	-	-	X
55	MG	YA	2907	-	-	-	X
55	MG	YA	2921	-	-	-	X
55	MG	YA	2930	-	-	-	X
55	MG	YA	2931	-	-	-	X
55	MG	YA	2932	-	-	-	X
55	MG	YA	2933	-	-	-	X
55	MG	YA	2934	-	-	-	X
55	MG	YA	2936	-	-	-	X
55	MG	YA	2952	-	-	-	X
55	MG	YA	2953	-	-	-	X
55	MG	YA	2954	-	-	-	X
55	MG	YA	2955	-	-	-	X
55	MG	YA	2958	-	-	-	X
55	MG	YA	2962	-	-	-	X
55	MG	YA	2974	-	-	-	X
55	MG	YA	2983	-	-	-	X
55	MG	YA	2984	-	-	-	X
55	MG	YA	3004	-	-	-	X
55	MG	YA	3010	-	-	-	X
55	MG	YA	3017	-	-	-	X
55	MG	YA	3018	-	-	-	X
55	MG	YA	3087	-	-	-	X
55	MG	YA	3097	-	-	-	X
55	MG	YA	3101	-	-	-	X
55	MG	YA	3117	-	-	-	X
55	MG	YA	3120	-	-	-	X
55	MG	YA	3122	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	YA	3126	-	-	-	X
55	MG	YA	3153	-	-	-	X
55	MG	YA	3168	-	-	-	X
55	MG	YA	3175	-	-	-	X
55	MG	YA	3192	-	-	X	-
55	MG	YA	3194	-	-	-	X
55	MG	YA	3205	-	-	-	X
55	MG	YA	3210	-	-	-	X
55	MG	YA	3211	-	-	-	X
55	MG	YA	3237	-	-	-	X
55	MG	YA	3239	-	-	-	X
55	MG	YA	3245	-	-	-	X
55	MG	YA	3262	-	-	-	X
55	MG	YA	3276	-	-	-	X
55	MG	YA	3281	-	-	-	X
55	MG	YA	3288	-	-	-	X
55	MG	YA	3290	-	-	-	X
56	SF4	QD	301	-	-	X	-

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 291185 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	QI	105	Total	C	N	O		0	0	0
			816	519	152	145				
9	XI	107	Total	C	N	O		0	0	0
			834	530	157	147				

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	115	Total	C	N	O	S	0	0	0
			921	569	190	160	2			
13	XM	114	Total	C	N	O	S	0	0	0
			914	565	189	158	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	QU	25	Total	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 tRNA(Pro).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	68	Total	C	N	O	P	0	0	0
			1452	647	260	477	68			
22	XV	68	Total	C	N	O	P	0	0	0
			1452	647	260	477	68			

- Molecule 23 is a RNA chain called mRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

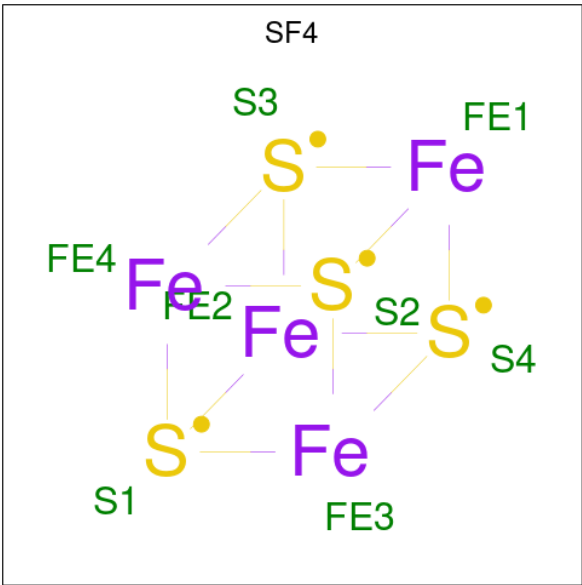
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	70	Total	Mg	0	0
			70	70		
55	QE	1	Total	Mg	0	0
			1	1		
55	QF	1	Total	Mg	0	0
			1	1		
55	QH	2	Total	Mg	0	0
			2	2		
55	QL	2	Total	Mg	0	0
			2	2		
55	R0	2	Total	Mg	0	0
			2	2		
55	R3	1	Total	Mg	0	0
			1	1		
55	R8	2	Total	Mg	0	0
			2	2		
55	RA	432	Total	Mg	0	0
			432	432		
55	RD	1	Total	Mg	0	0
			1	1		
55	RE	4	Total	Mg	0	0
			4	4		
55	RF	2	Total	Mg	0	0
			2	2		
55	RN	1	Total	Mg	0	0
			1	1		
55	RO	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	XA	88	Total 88	Mg 88	0	0
55	XE	1	Total 1	Mg 1	0	0
55	XO	1	Total 1	Mg 1	0	0
55	Y1	1	Total 1	Mg 1	0	0
55	Y2	1	Total 1	Mg 1	0	0
55	Y5	1	Total 1	Mg 1	0	0
55	Y7	1	Total 1	Mg 1	0	0
55	Y8	2	Total 2	Mg 2	0	0
55	YA	394	Total 394	Mg 394	0	0
55	YB	1	Total 1	Mg 1	0	0
55	YD	2	Total 2	Mg 2	0	0
55	YE	4	Total 4	Mg 4	0	0
55	YF	1	Total 1	Mg 1	0	0
55	YP	1	Total 1	Mg 1	0	0
55	YQ	1	Total 1	Mg 1	0	0
55	YR	2	Total 2	Mg 2	0	0
55	YU	1	Total 1	Mg 1	0	0
55	YX	1	Total 1	Mg 1	0	0

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

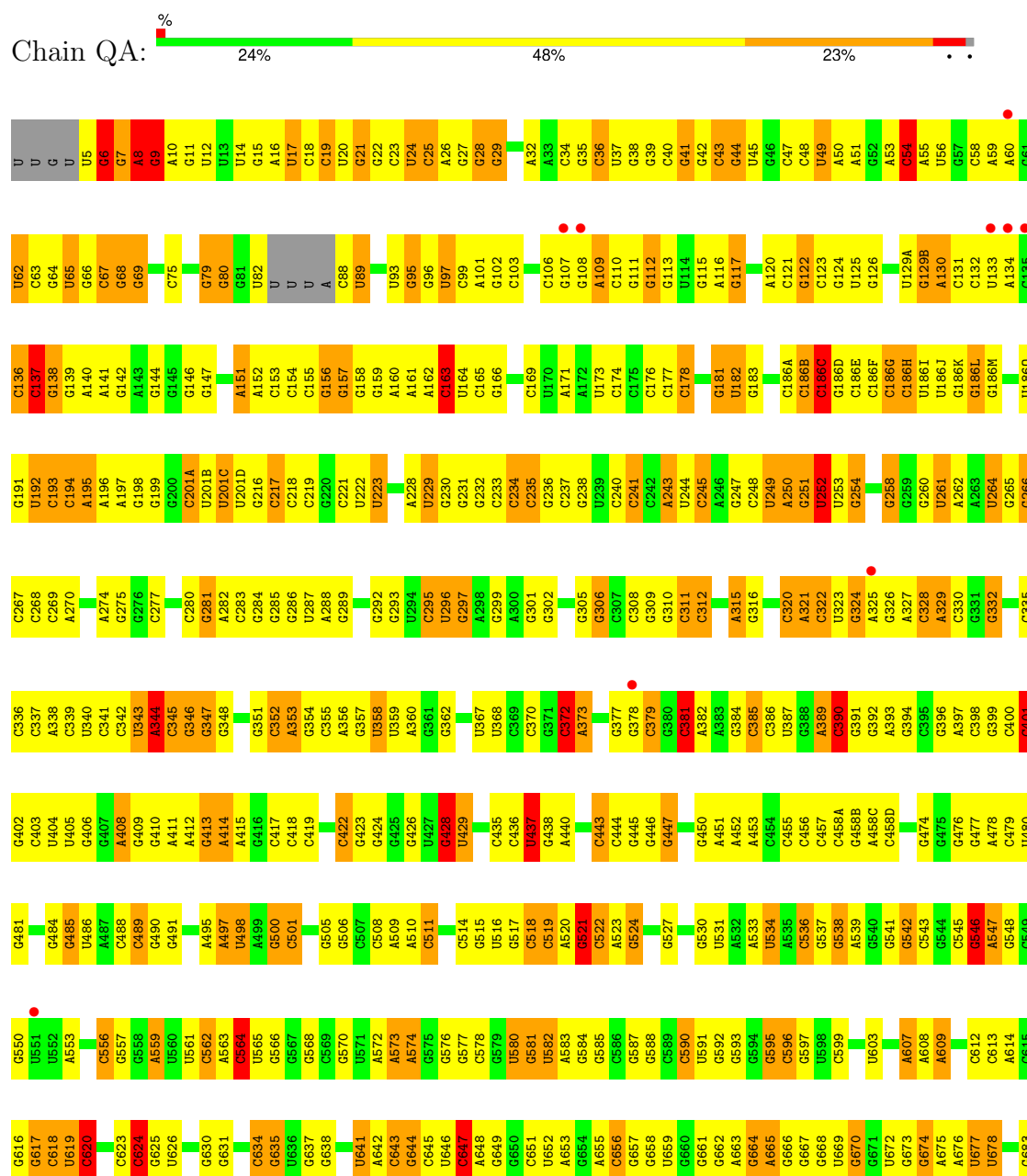
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

### 3 Residue-property plots

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

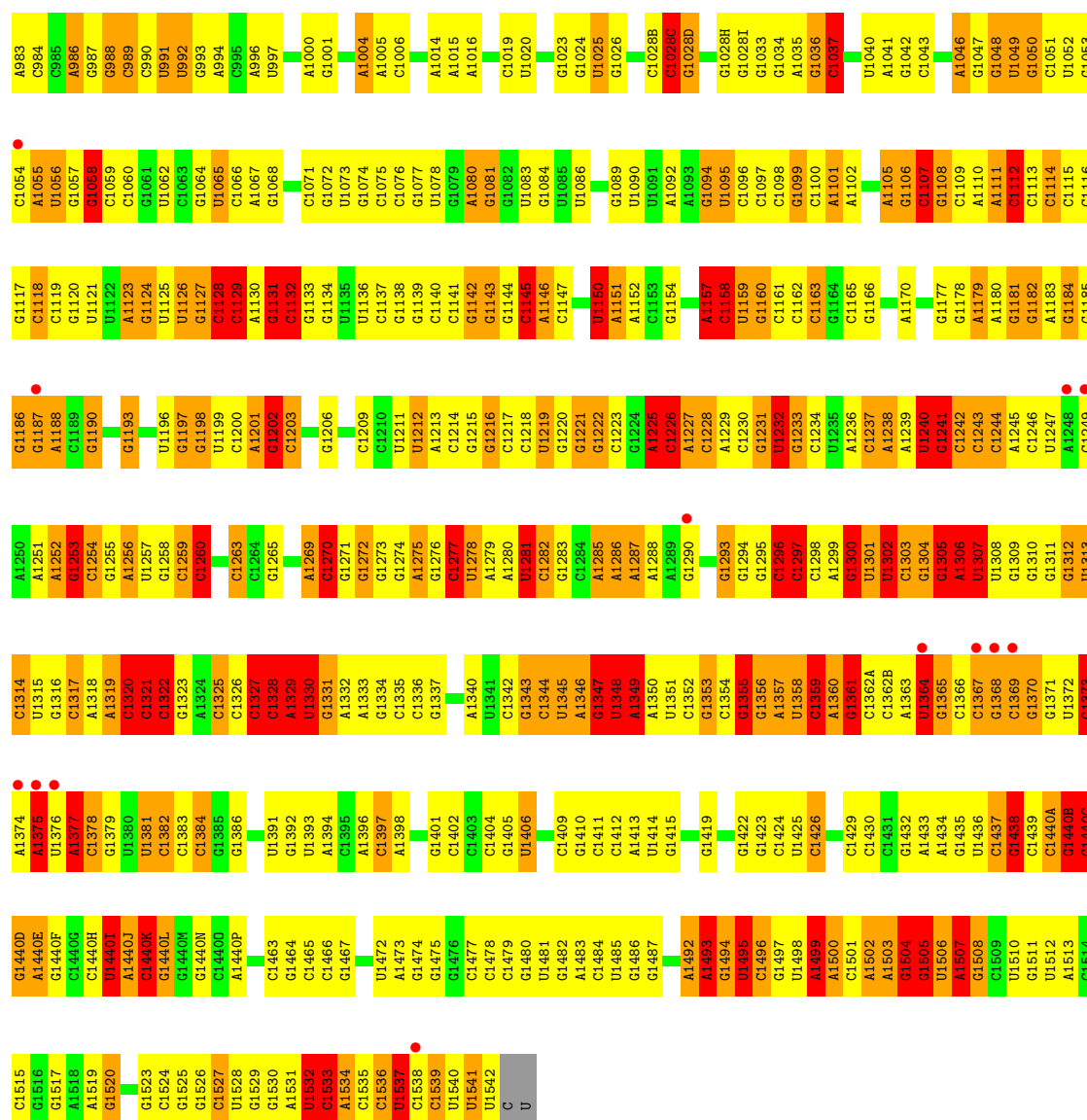
#### • Molecule 1: 16S rRNA



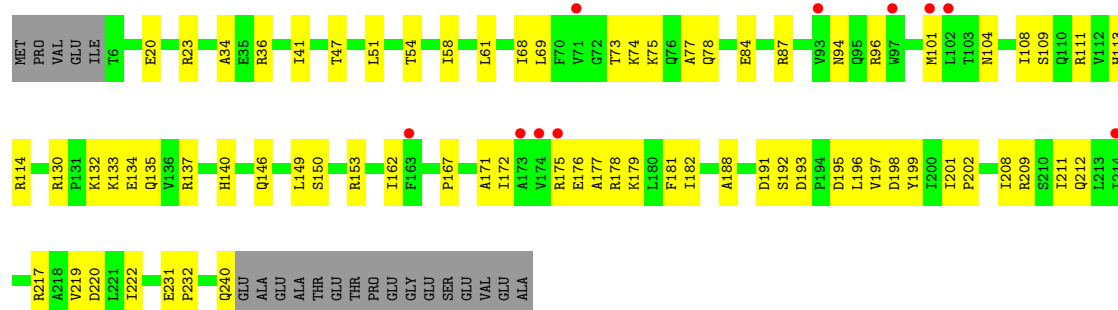
- Molecule 1: 16S rRNA





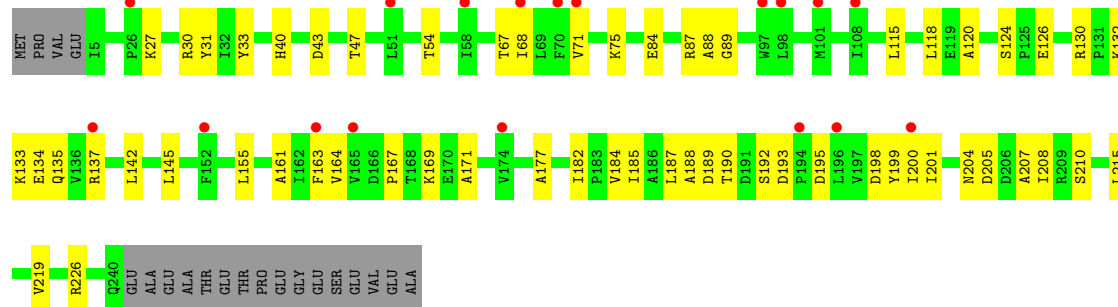


### • Molecule 2: 30S ribosomal protein S2



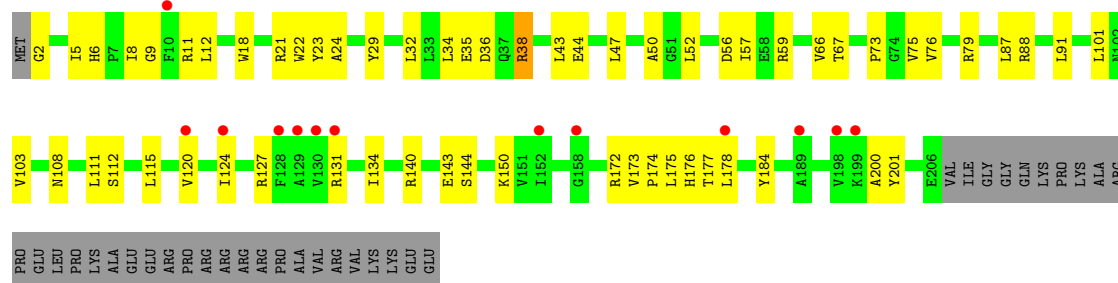
### • Molecule 2: 30S ribosomal protein S2

Chain XB:



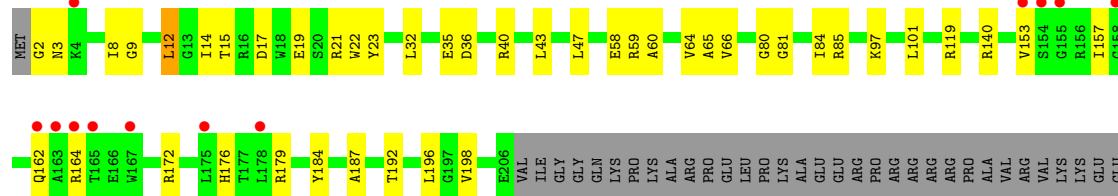
- Molecule 3: 30S ribosomal protein S3

Chain QC:



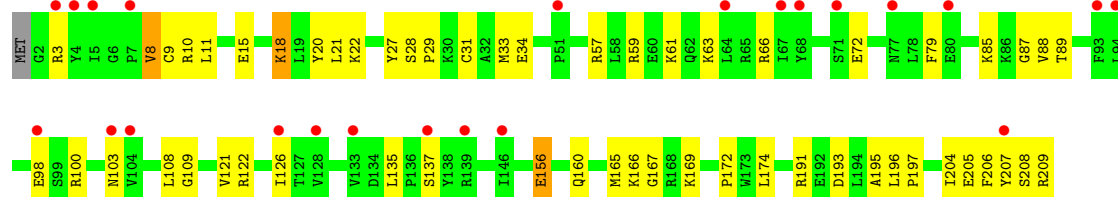
- Molecule 3: 30S ribosomal protein S3

Chain XC:

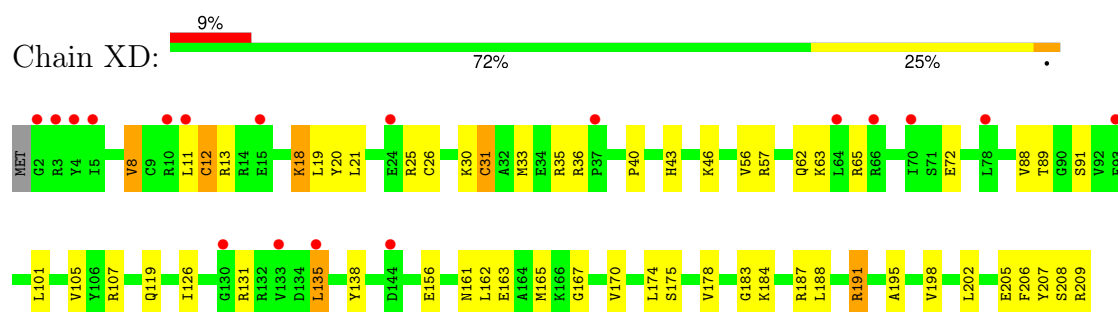


- Molecule 4: 30S ribosomal protein S4

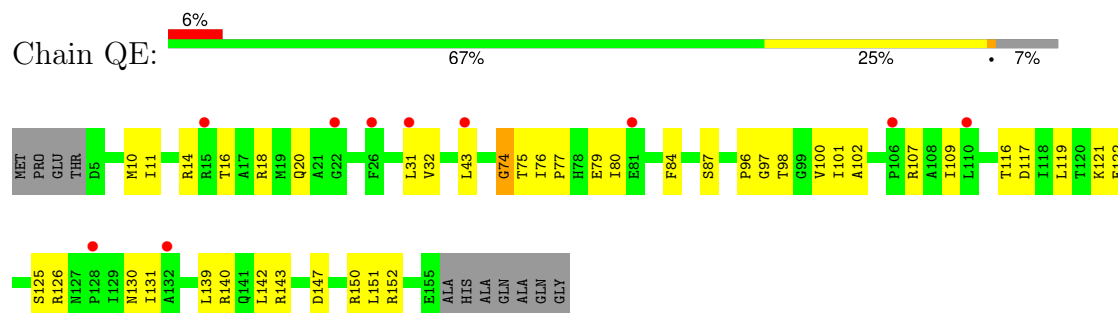
Chain QD:



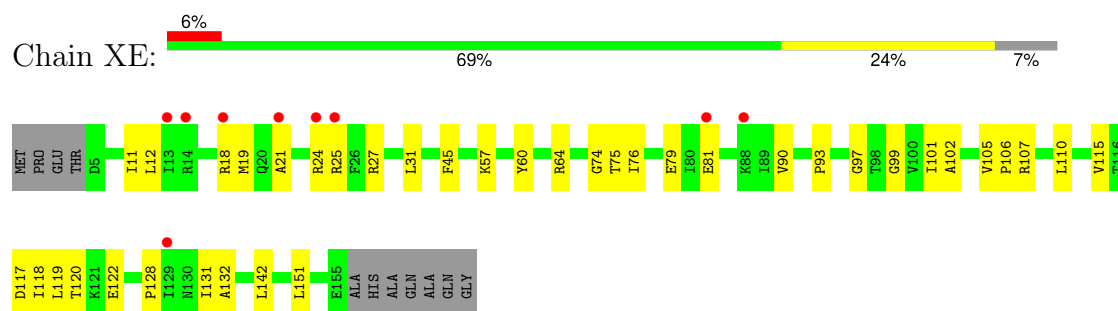
- Molecule 4: 30S ribosomal protein S4



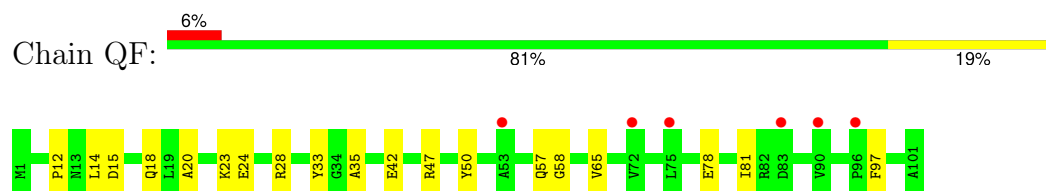
- Molecule 5: 30S ribosomal protein S5



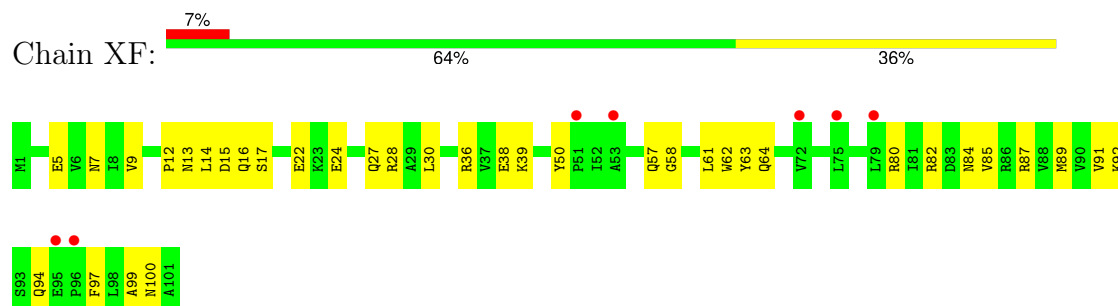
- Molecule 5: 30S ribosomal protein S5



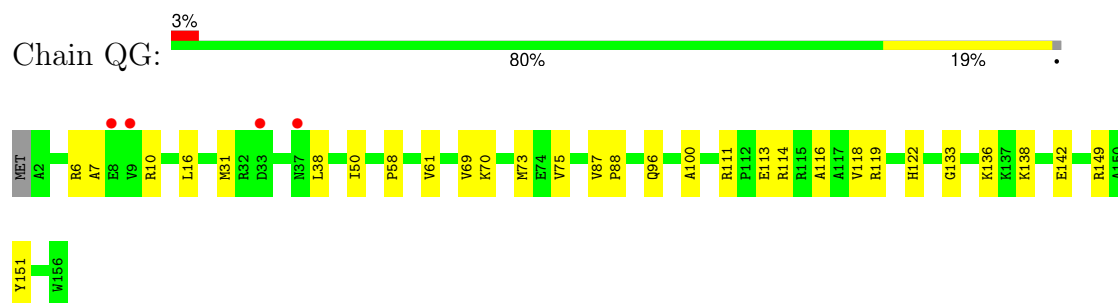
- Molecule 6: 30S ribosomal protein S6



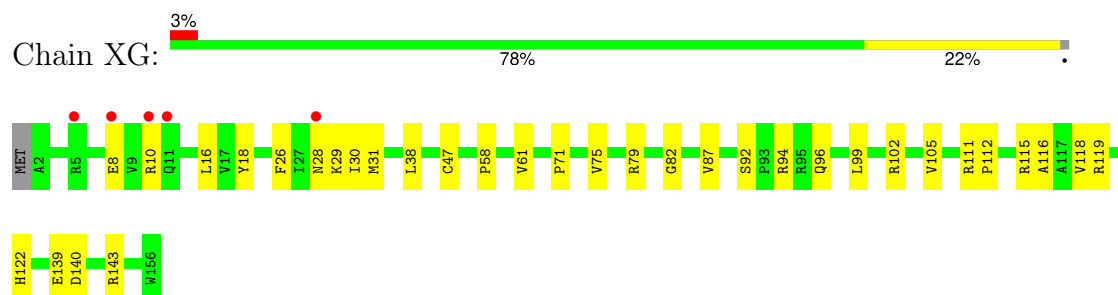
- Molecule 6: 30S ribosomal protein S6



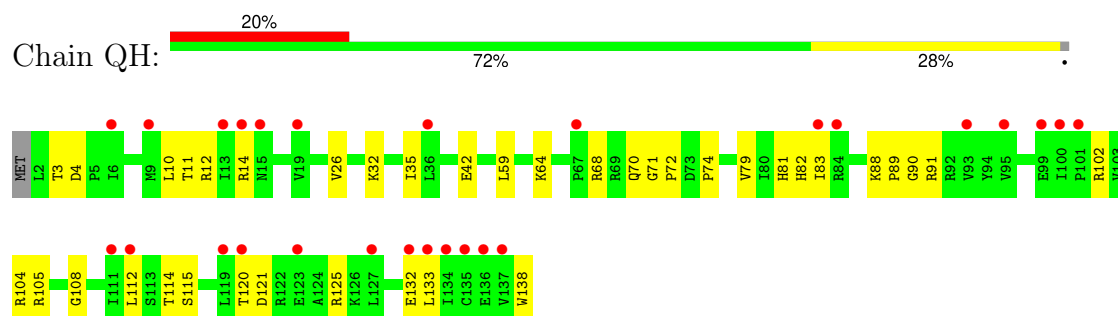
- Molecule 7: 30S ribosomal protein S7



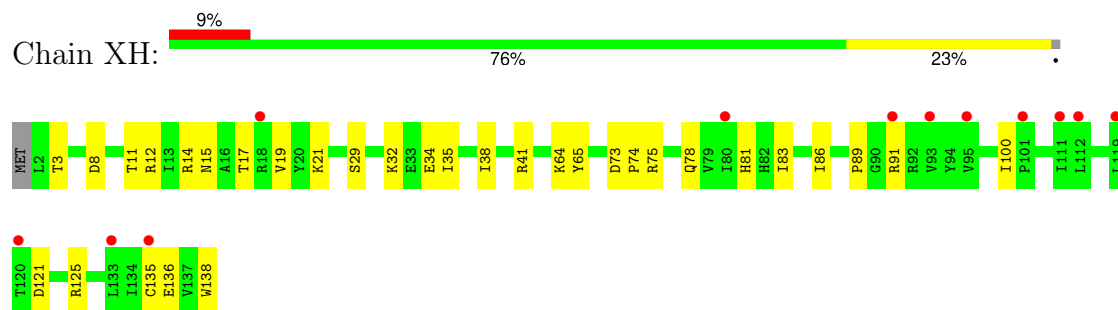
- Molecule 7: 30S ribosomal protein S7



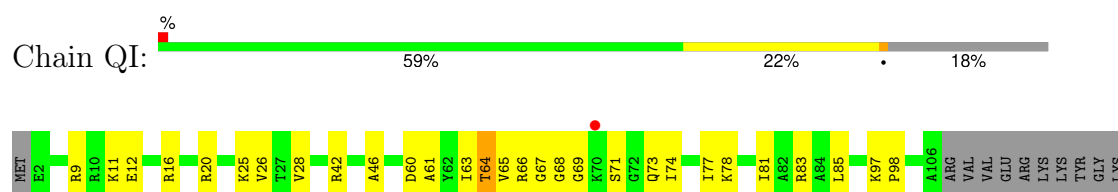
- Molecule 8: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S8



- Molecule 9: 30S ribosomal protein S9



HIS  
LYS  
ALA  
ARG  
ARG  
ALA  
PRO  
GLN  
TYR  
SER  
LYS  
ARG

• Molecule 9: 30S ribosomal protein S9



MET E2 T7 R10 K11 E12 A13 V17 F18 L19 R20 P21 G22 T27 V28 V44 A45 H58 I63 G68 G69 K70 S71 G72 Q73 I74 I77 D105 A106 R107 V108 VAL GLU ARG LYS LYS TYR GLY LYS HIS LYS ALA ARG ARG ALA PRO GLN TYR SER LYS

ARG

• Molecule 10: 30S ribosomal protein S10



MET PRO K3 I4 R5 I6 R9 G10 F11 D12 H13 K14 T15 L16 D17 V24 R28 Q33 V34 S35 G36 P37 I38 P39 L40 P41 T42 R43 R44 R45 R46 F47 T48 V49 I50 R51 G52 P53 P54 F55 H56 K57 D58 S59 H62 L65 R66 T67 H68 N69 R70 V72 D73

N76 R79 G83 V94 E95 I98 K99 T100 V101 GLY GLY GLY ARG

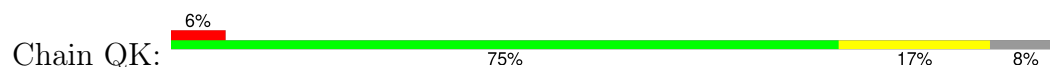
• Molecule 10: 30S ribosomal protein S10



MET PRO LYS ILE R5 I6 K7 L8 R9 G10 H13 K14 T15 L16 V24 E25 A26 G36 P37 I38 P39 L40 P41 T42 R43 V44 R45 R46 F47 T48 V49 I50 P53 F54 K55 D58 S59 R60 E61 H62 E63 E64 L65 R66 T67 H68 N69 R70 L71 V72 N78 R79 R80 T81

Q84 L90 P91 T92 G93 V94 E95 I96 E97 I98 K99 T100 VAL GLY GLY ARG

• Molecule 11: 30S ribosomal protein S11



MET ALA LYS LYS PRO SER LYS LYS VAL K11 R12 Q13 G17 N27 T28 T32 P35 P39 T40 T41 G52 S53 R54 K55 G56 T57 A60 K70 K71 V82 I83 V84 S101 I108 V109 D110 P115 H116 N117 G118 C119 G119 F125 R126 K127 A128 S129

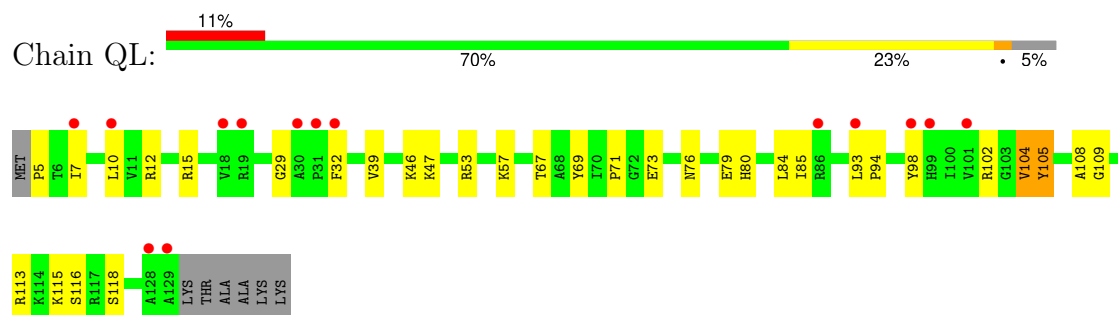
• Molecule 11: 30S ribosomal protein S11



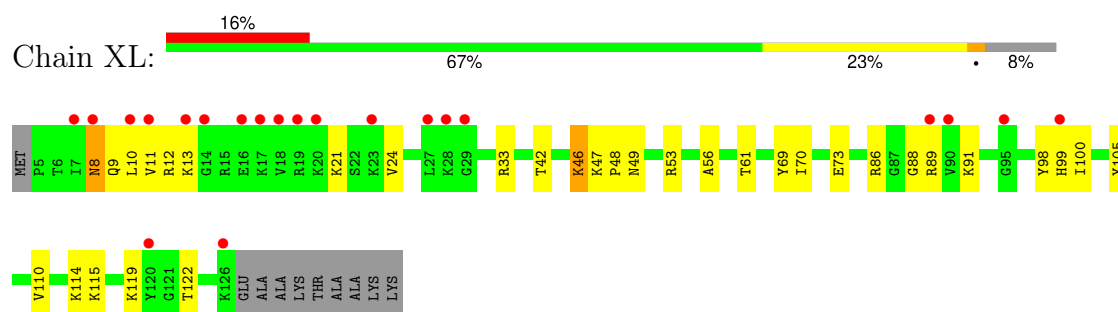
MET ALA LYS LYS PRO SER LYS LYS VAL K11 A15 S16 G17 T31 T35 W42 K51 R54 T57 M77 V82 I83 V84 R85 R91 Q104 V105 K106 I107 I108 V109 D110 P113 V114 P115 H116 N117 G118 C119 R120 P121 K122 K123 K124 F125 R126 LYS

ALA  
SER

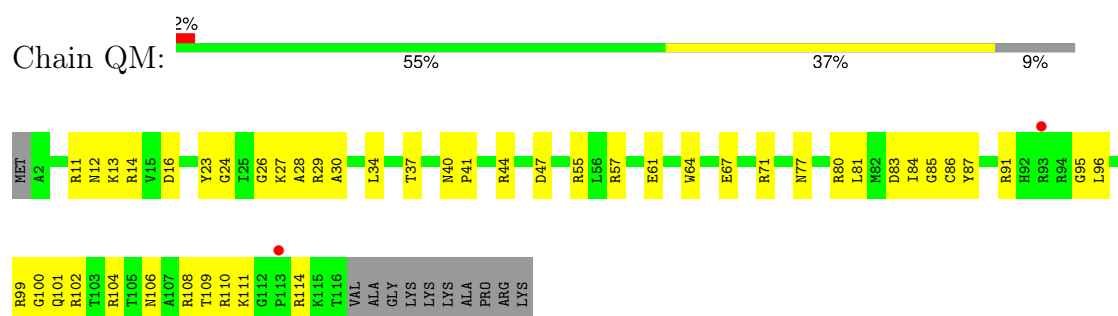
- Molecule 12: 30S ribosomal protein S12



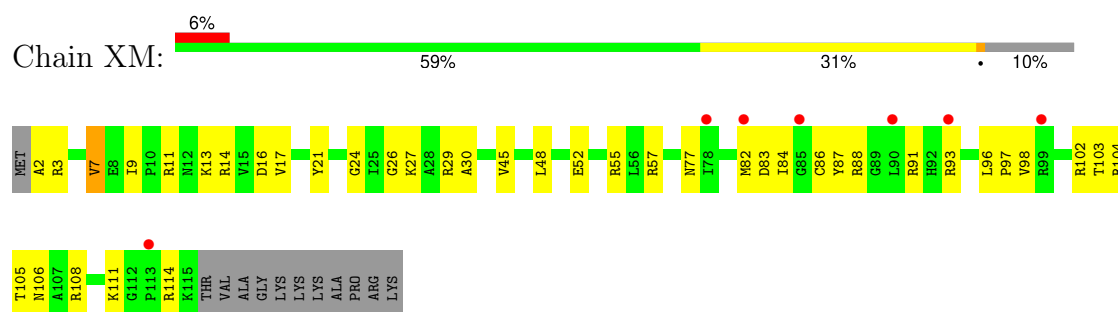
- Molecule 12: 30S ribosomal protein S12



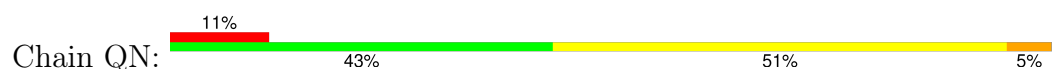
- Molecule 13: 30S ribosomal protein S13

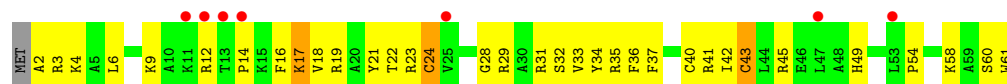


- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z

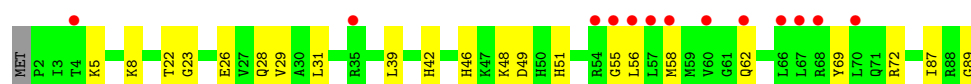
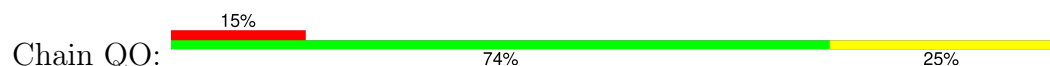




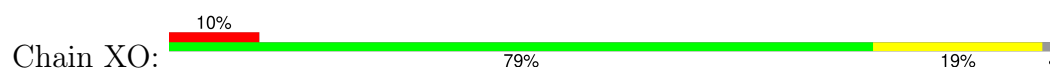
- Molecule 14: 30S ribosomal protein S14 type Z



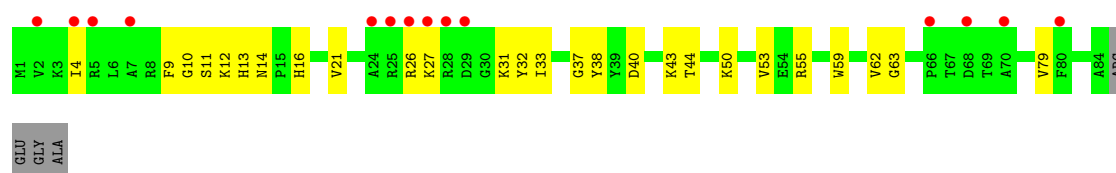
- Molecule 15: 30S ribosomal protein S15



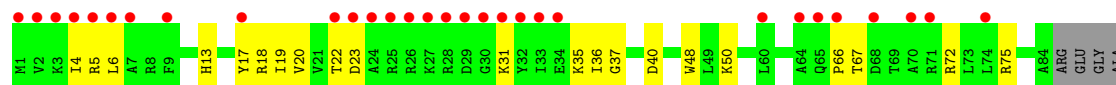
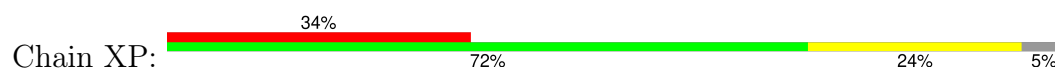
- Molecule 15: 30S ribosomal protein S15



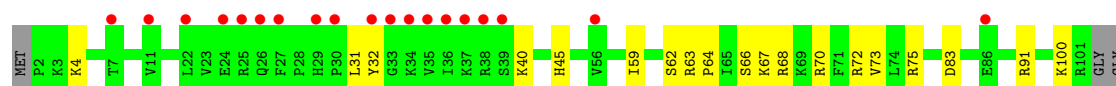
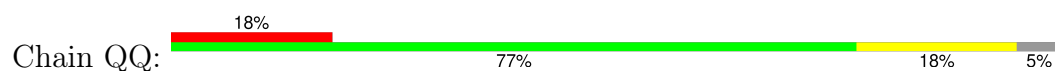
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16




- Molecule 17: 30S ribosomal protein S17

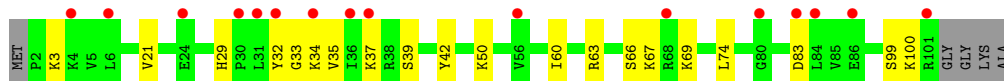




LYS  
ALA

- Molecule 17: 30S ribosomal protein S17

Chain XQ: 



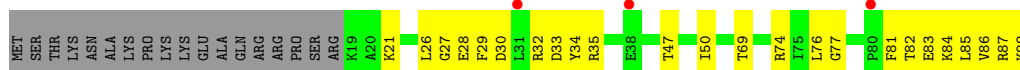
- Molecule 18: 30S ribosomal protein S18

Chain QR: 



- Molecule 18: 30S ribosomal protein S18

Chain XR: 



- Molecule 19: 30S ribosomal protein S19

Chain QS: 



LYS  
LYS  
LYS

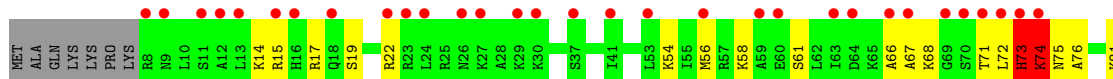
- Molecule 19: 30S ribosomal protein S19

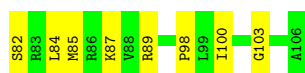
Chain XS: 



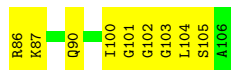
- Molecule 20: 30S ribosomal protein S20

Chain QT: 

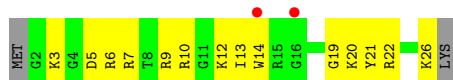
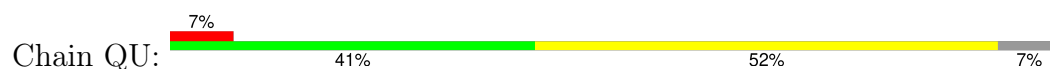




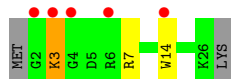
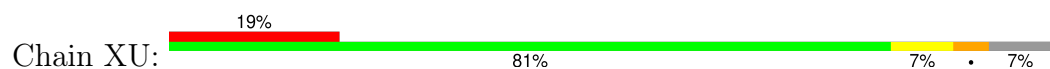
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: tRNA(Pro)



- Molecule 22: tRNA(Pro)

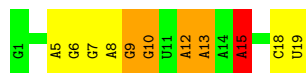


- Molecule 23: mRNA




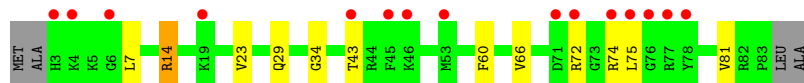
- Molecule 23: mRNA

Chain XX: 




- Molecule 24: 50S ribosomal protein L27

Chain R0: 




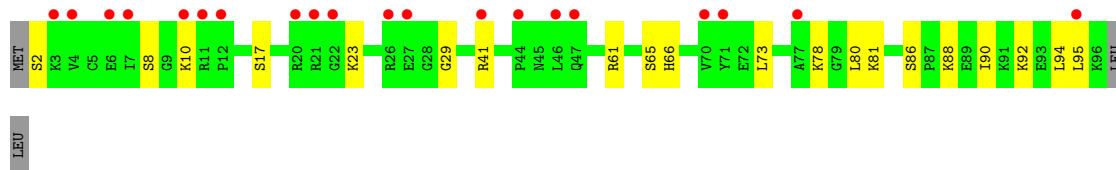
- Molecule 24: 50S ribosomal protein L27

Chain Y0: 




- Molecule 25: 50S ribosomal protein L28

Chain R1: 




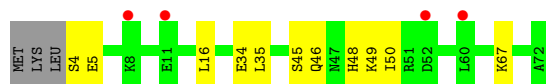
- Molecule 25: 50S ribosomal protein L28

Chain Y1: 




- Molecule 26: 50S ribosomal protein L29

Chain R2: 

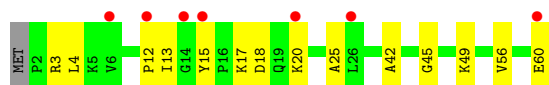
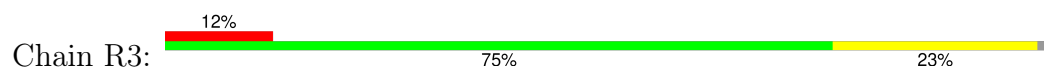


- Molecule 26: 50S ribosomal protein L29

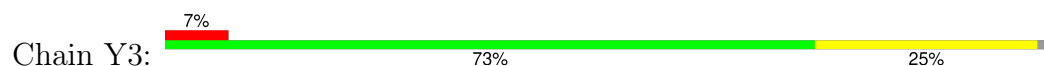
Chain Y2: 



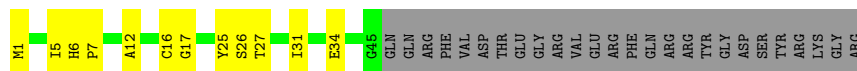
- Molecule 27: 50S ribosomal protein L30



- Molecule 27: 50S ribosomal protein L30



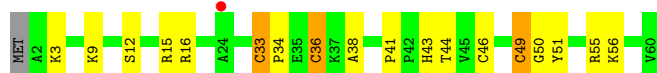
- Molecule 28: 50S ribosomal protein L31



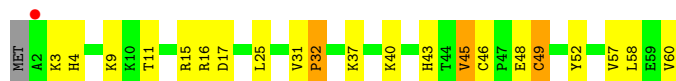
- Molecule 28: 50S ribosomal protein L31



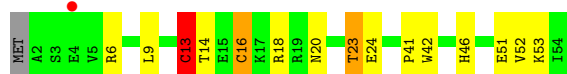
- Molecule 29: 50S ribosomal protein L32



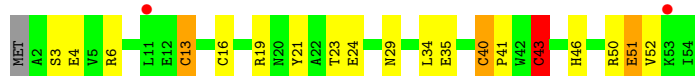
- Molecule 29: 50S ribosomal protein L32



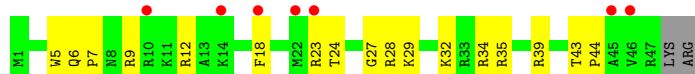
- Molecule 30: 50S ribosomal protein L33



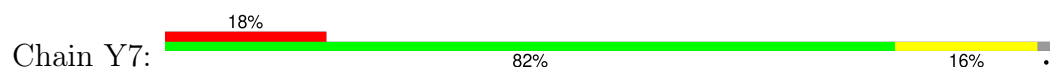
- Molecule 30: 50S ribosomal protein L33



- Molecule 31: 50S ribosomal protein L34



- Molecule 31: 50S ribosomal protein L34



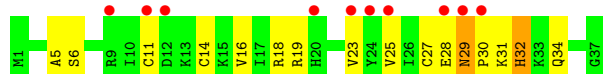
- Molecule 32: 50S ribosomal protein L35

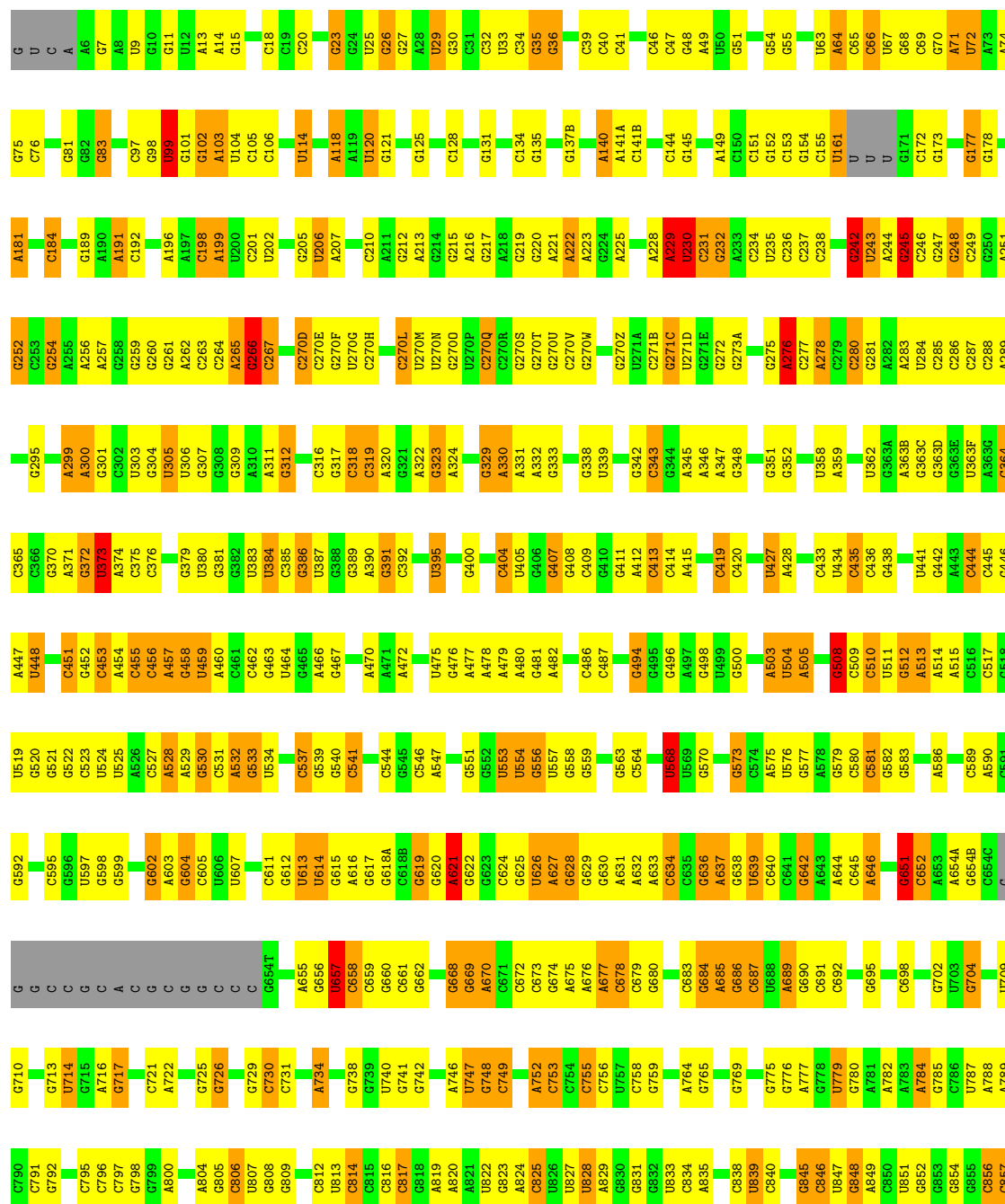


- Molecule 32: 50S ribosomal protein L35



- Molecule 33: 50S ribosomal protein L36





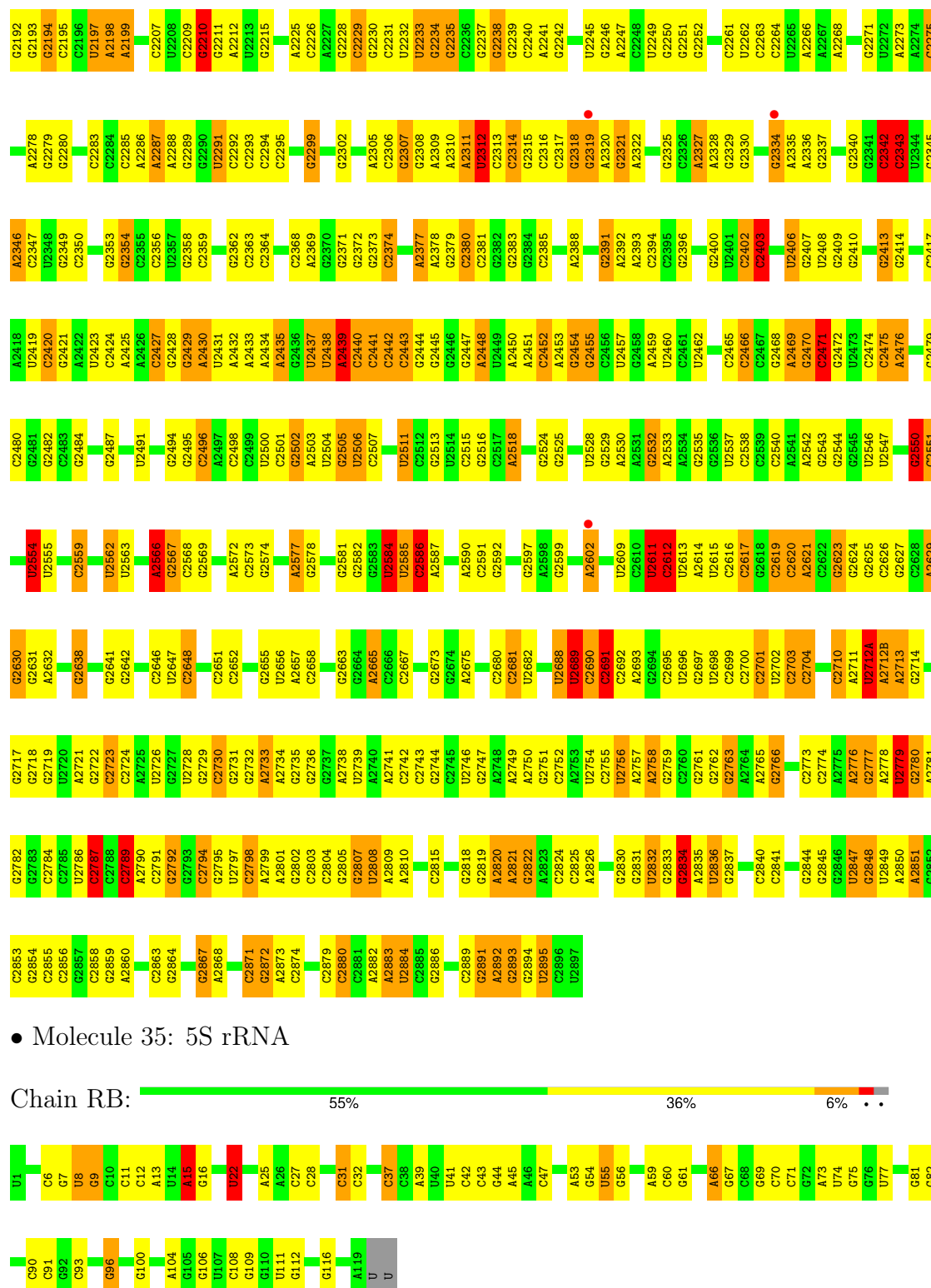
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U1956	C1883	A1872	C1694	C1545A	G1474	C1475	G1401	C1161	G1087	U1019	G944	U860
G1959	C1884	A1873	A1545B	A1545B	C1475	A1476	C1402	G1162	A1088	G1020	A945	A863
A1960	C1885	A1874	C1546	C1546	C1476	A1477	C1403	U1165	G1089	A1021	G946	G864
C1961	C1886	A1875	C1547	C1547	C1404	C1547	U1405	U1166	G1090	G1022	C949	C865
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A1971	C1896	A1885	G1414	G1414	G1414	A1494	C1333	U1176	U1105	A1032	A960	C884
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A1981	C1899	A1888	U1417	U1417	U1417	U1497	C1336	C1179	C1108	C1041	G966	C889
C1982	C1900	A1889	U1418	U1418	U1418	C1498	C1337	C1180	C1109	G1042	C967	A890
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C1992	C1903	A1892	C1421	C1421	C1421	U1503	C1340	C1183	G1112	A1045	C970	A896
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C1994	C1905	A1894	C1423	C1423	C1423	C1505	C1342	C1185	G1114	G1047	G972	C904
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C1996	C1907	A1896	C1425	C1425	C1425	C1507	C1344	C1187	G1116	C1049	G974A	C974B
C1999	C1908	A1897	U1426	U1426	U1426	U1508	C1345	C1188	G1117	A1050	U905	U905
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C2006	C1910	A1899	U1428	U1428	U1428	C1510	C1347	C1190	G1122	C1052	A980	U907
C2007	C1911	A1900	C1429	C1429	C1429	A1511	C1348	C1191	C1123	G1053	A983	A910
C2008	C1912	A1901	U1430	U1430	U1430	G1512	C1349	C1192	G1054	A1054	A984	A911
G2009	C1913	A1902	C1431	C1431	C1431	C1513	C1350	C1193	G1055	G1056	C985	C914
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C2012	C1915	A1904	C1433	C1433	C1433	C1515	C1352	C1195	A1129	G1058	G987	G916
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G2024	C1923	A1912	C1441	C1441	C1441	C1523	C1360	C1203	U1142B	A1069	A996	C926
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C2026	C1925	A1914	C1443	C1443	C1443	C1525	C1362	C1205	G1144	G1071	G998	G929
G2027	C1926	A1915	U1444	U1444	U1444	C1526	C1363	C1206	C1145	A1072	U999	U930
C2028	C1927	A1916	C1445	C1445	C1445	C1527	C1364	C1207	C1146	G1073	C1000	G932
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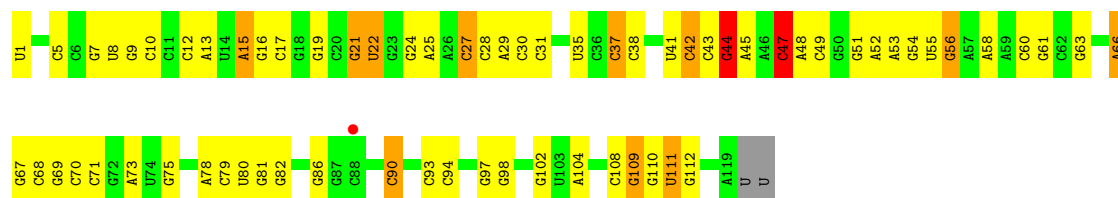




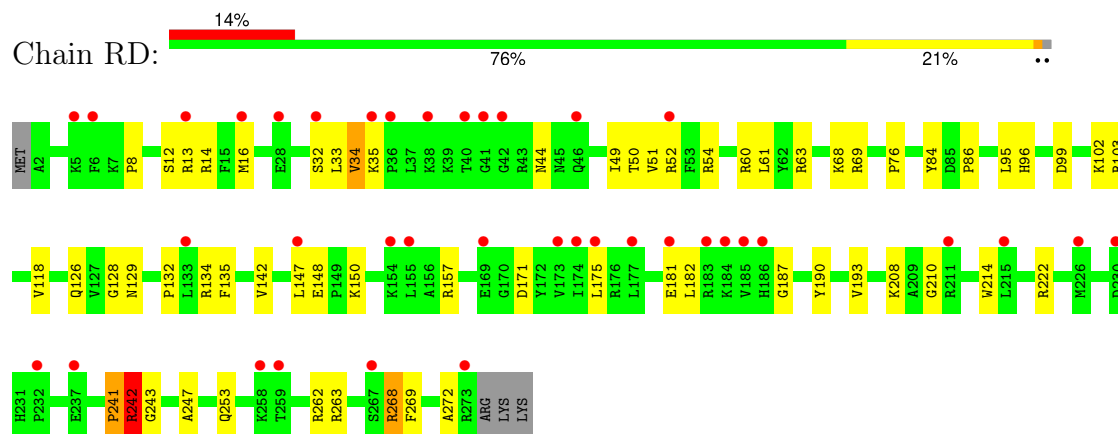




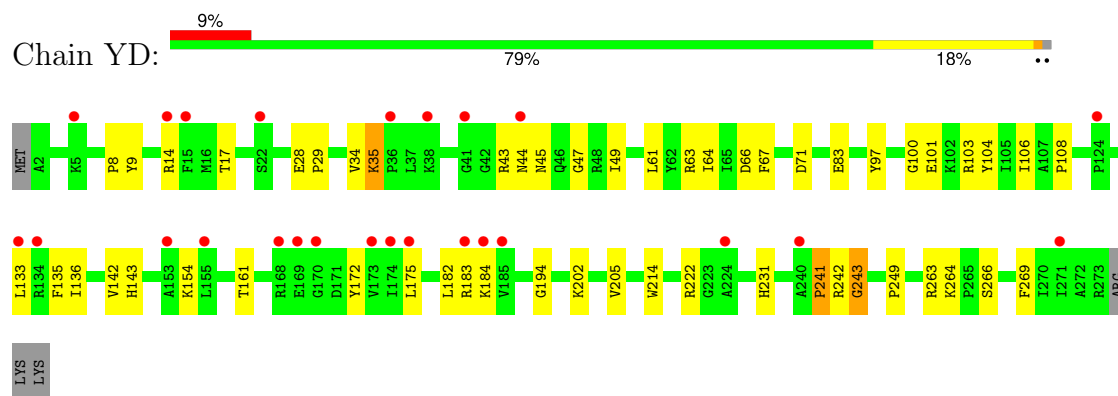




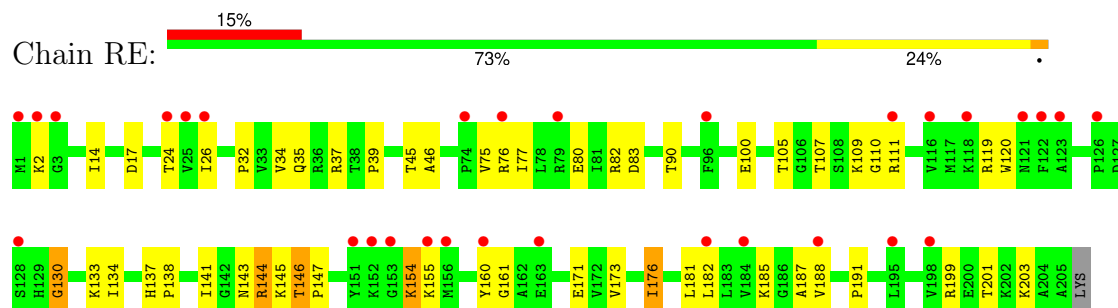
• Molecule 36: 50S ribosomal protein L2



• Molecule 36: 50S ribosomal protein L2

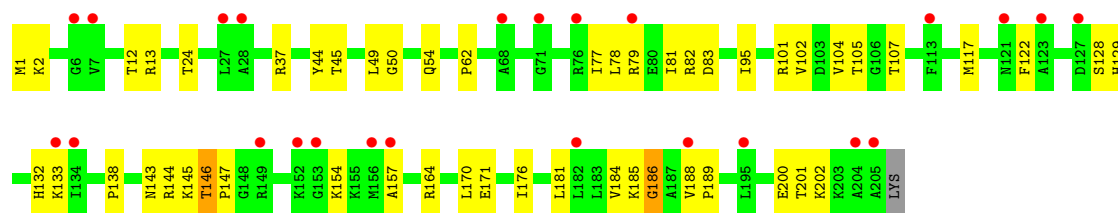


• Molecule 37: 50S ribosomal protein L3

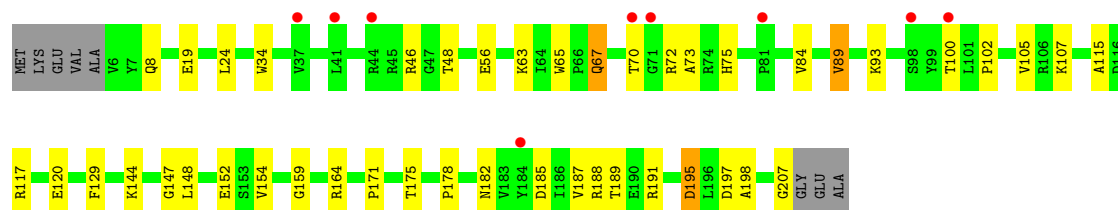
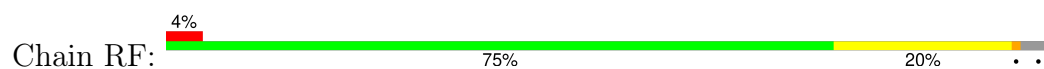


• Molecule 37: 50S ribosomal protein L3

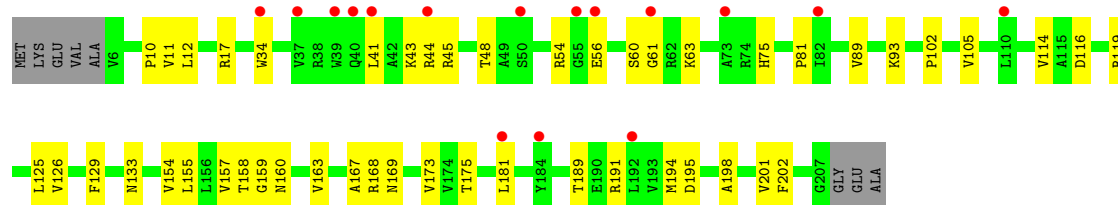
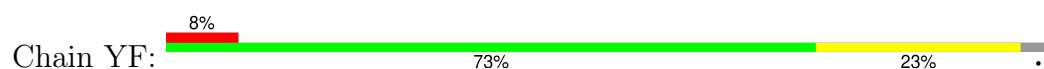




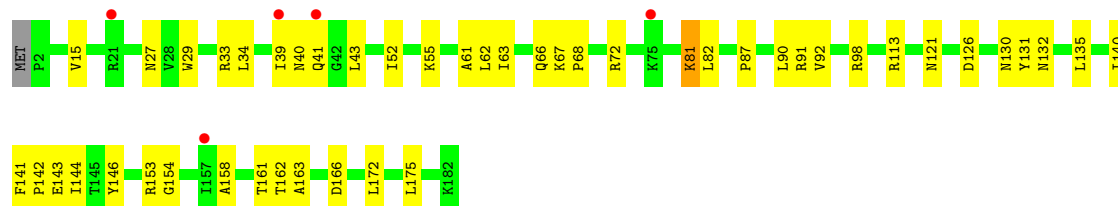
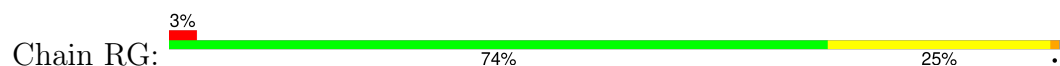
• Molecule 38: 50S ribosomal protein L4



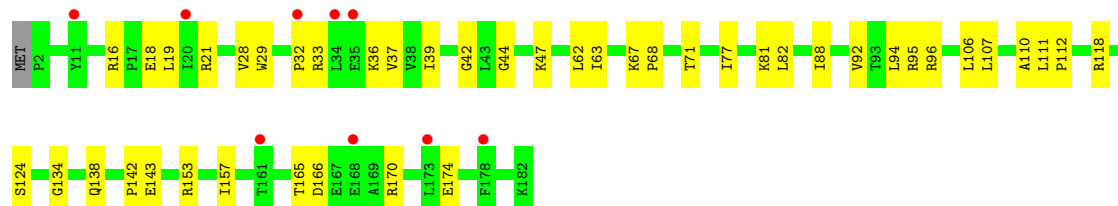
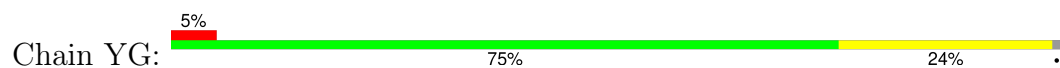
• Molecule 38: 50S ribosomal protein L4



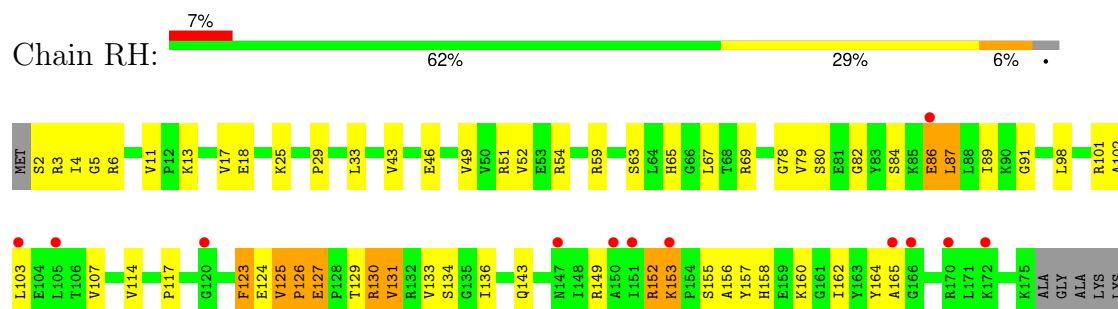
• Molecule 39: 50S ribosomal protein L5



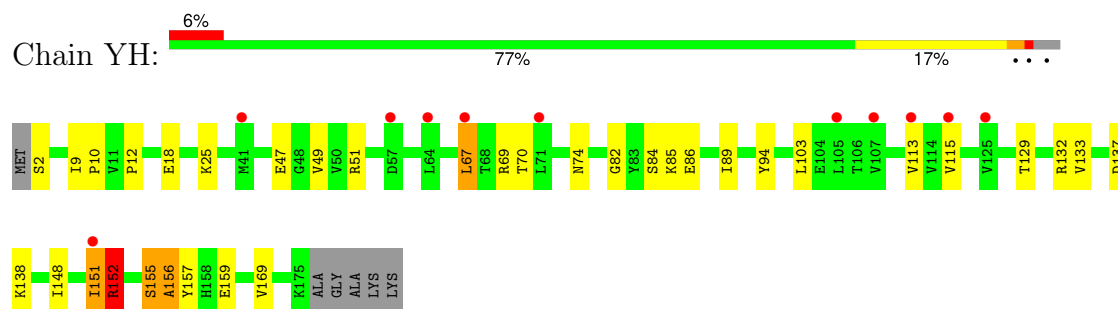
• Molecule 39: 50S ribosomal protein L5



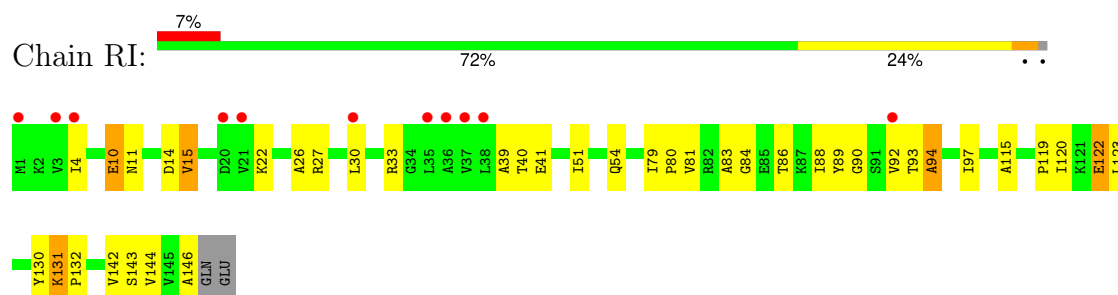
- Molecule 40: 50S ribosomal protein L6



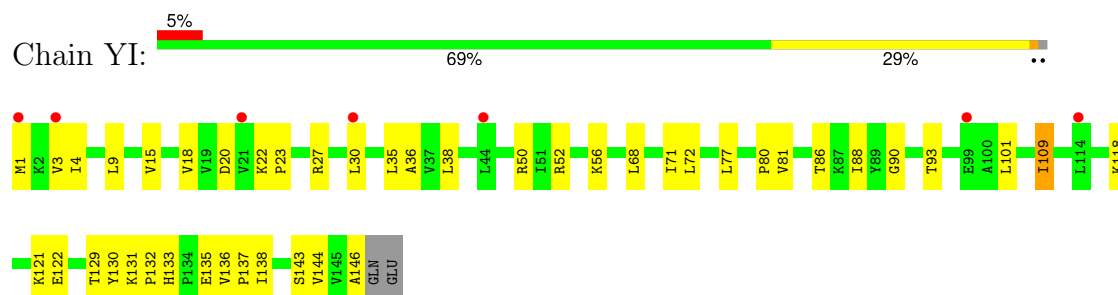
- Molecule 40: 50S ribosomal protein L6



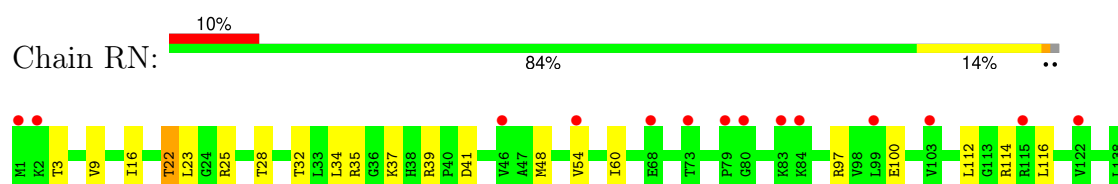
- Molecule 41: 50S ribosomal protein L9



- Molecule 41: 50S ribosomal protein L9

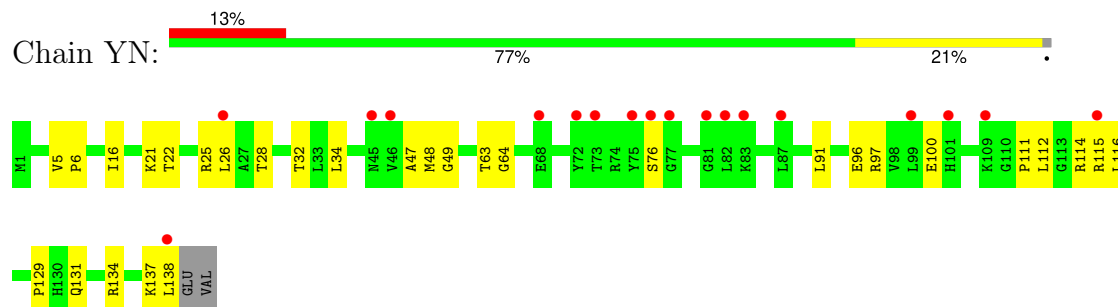


- Molecule 42: 50S ribosomal protein L13

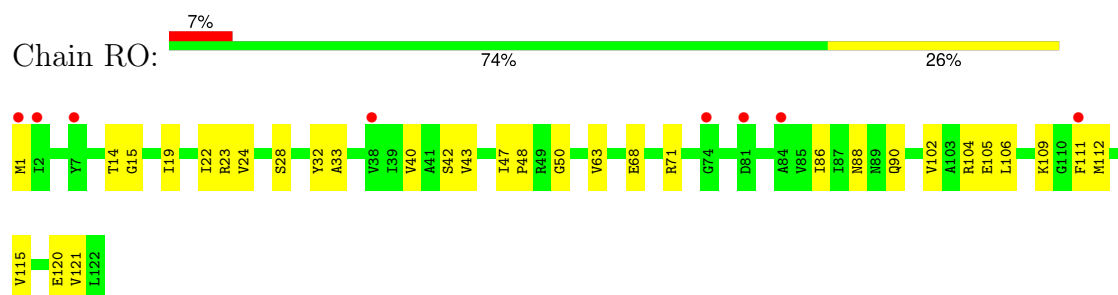


GLU  
VAL

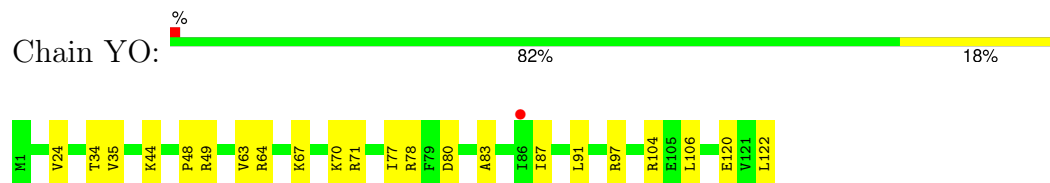
- Molecule 42: 50S ribosomal protein L13



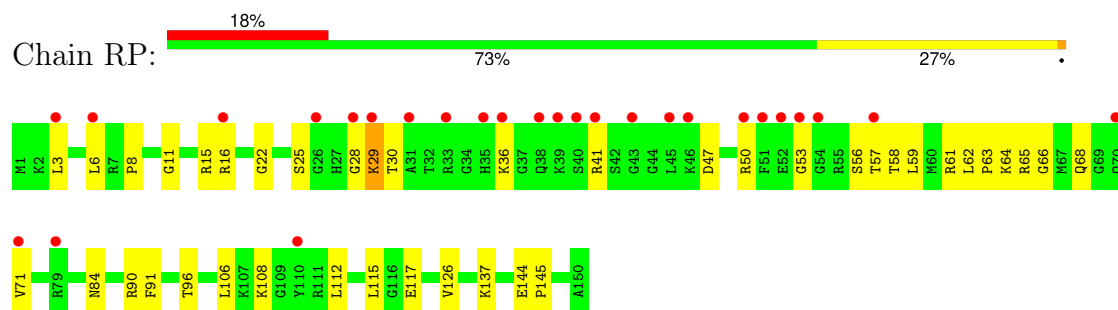
- Molecule 43: 50S ribosomal protein L14



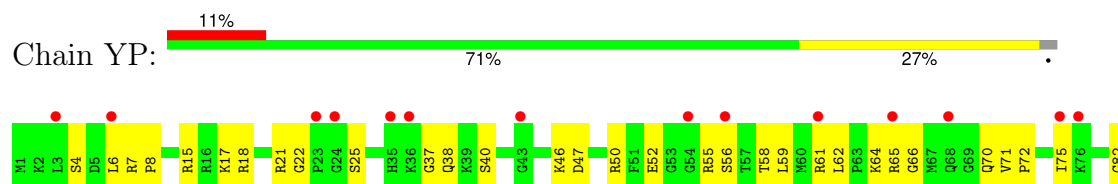
- Molecule 43: 50S ribosomal protein L14

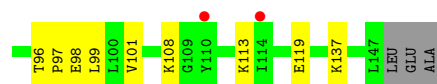


- Molecule 44: 50S ribosomal protein L15

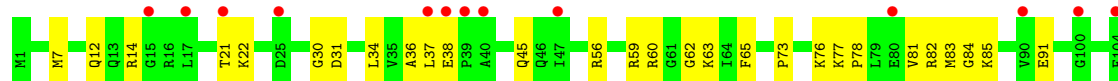
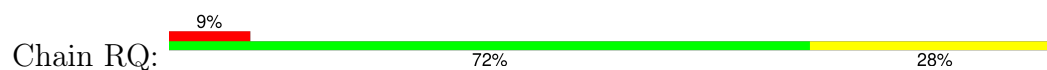


- Molecule 44: 50S ribosomal protein L15

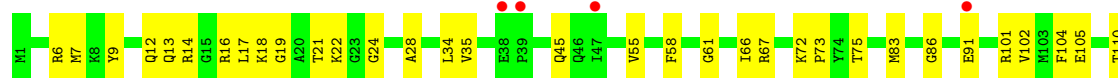
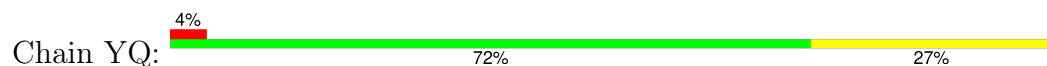




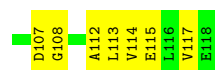
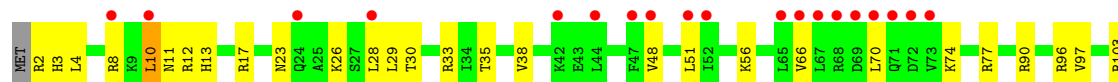
- Molecule 45: 50S ribosomal protein L16



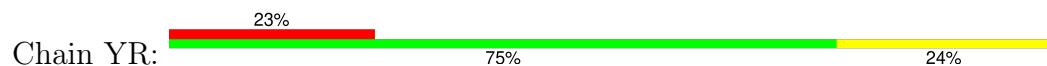
- Molecule 45: 50S ribosomal protein L16



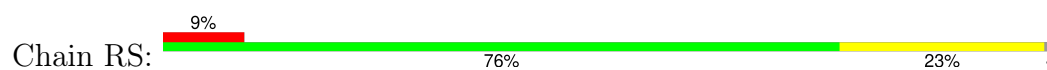
- Molecule 46: 50S ribosomal protein L17



- Molecule 46: 50S ribosomal protein L17



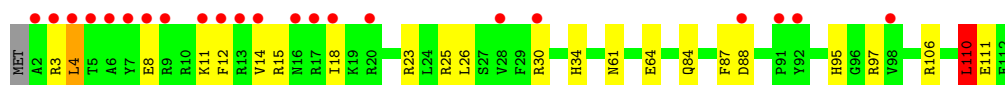
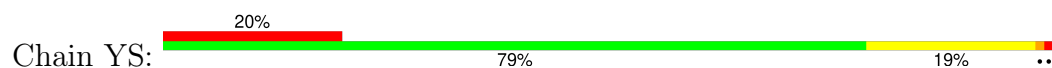
- Molecule 47: 50S ribosomal protein L18



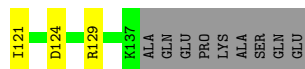
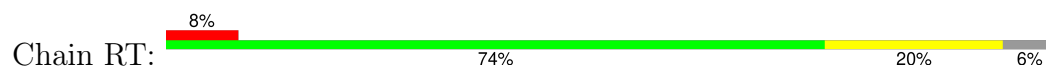




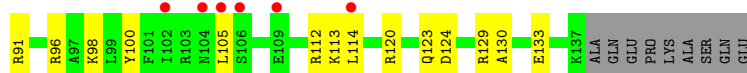
- Molecule 47: 50S ribosomal protein L18



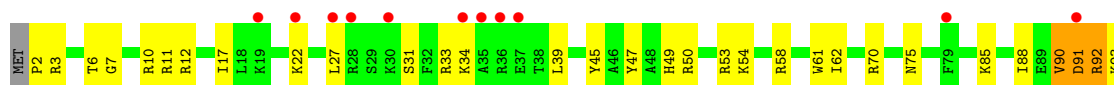
- Molecule 48: 50S ribosomal protein L19



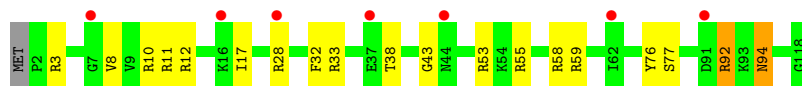
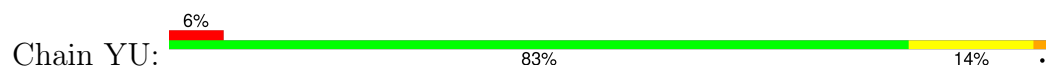
- Molecule 48: 50S ribosomal protein L19



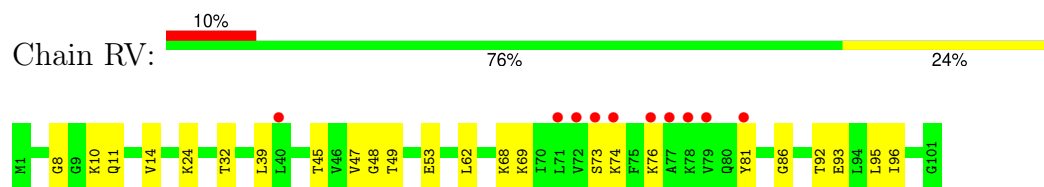
- Molecule 49: 50S ribosomal protein L20



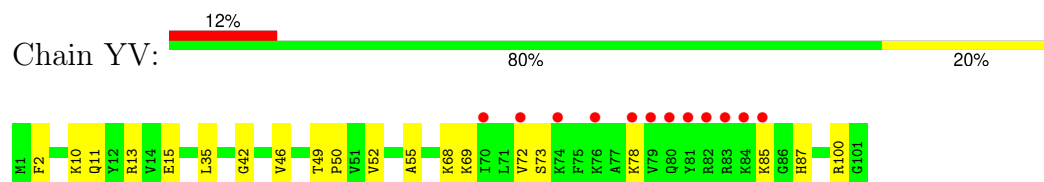
- Molecule 49: 50S ribosomal protein L20



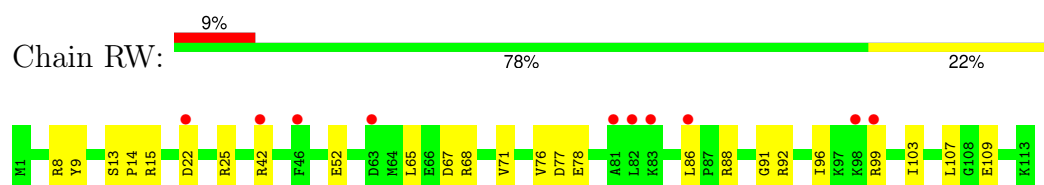
- Molecule 50: 50S ribosomal protein L21



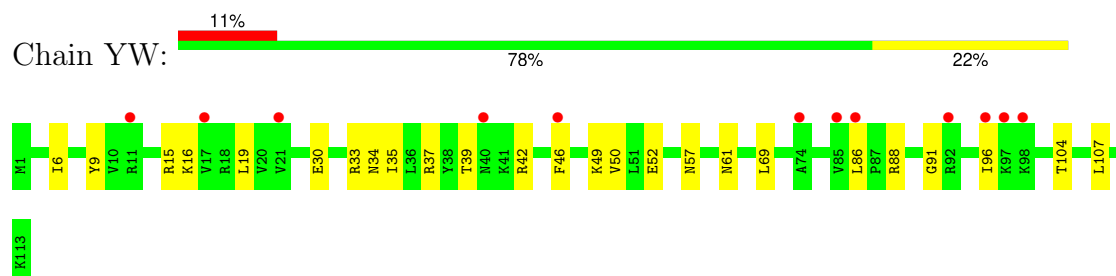
- Molecule 50: 50S ribosomal protein L21

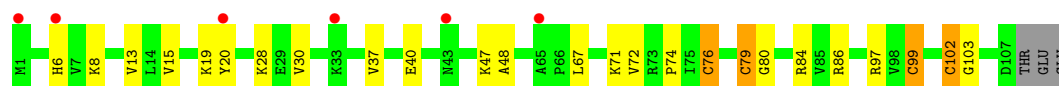


- Molecule 51: 50S ribosomal protein L22

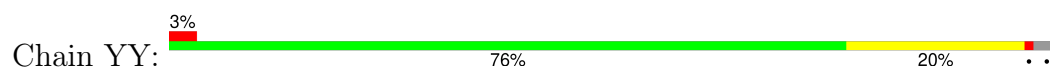


- Molecule 51: 50S ribosomal protein L22

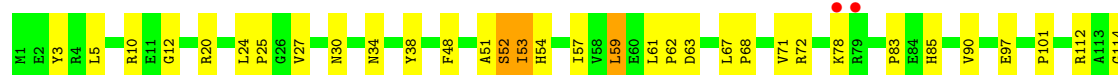




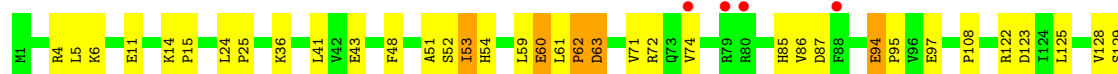
- Molecule 53: 50S ribosomal protein L24



- Molecule 54: 50S ribosomal protein L25



- Molecule 54: 50S ribosomal protein L25



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.09Å 450.32Å 622.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 4.14 49.85 – 4.14	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.85-4.14) 98.4 (49.85-4.14)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.248 , 0.294 0.246 , 0.292	Depositor DCC
$R_{free}$ test set	427005 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	171.1	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.19 , 97.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	291185	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	247.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	QA	0.31	0/36343	1.10	485/56720 (0.9%)
1	XA	0.44	28/36435 (0.1%)	1.31	648/56865 (1.1%)
2	QB	0.36	0/1942	0.67	0/2619
2	XB	0.37	0/1950	0.64	1/2630 (0.0%)
3	QC	0.36	0/1629	0.66	0/2195
3	XC	0.37	0/1629	0.61	0/2195
4	QD	0.45	1/1733 (0.1%)	0.65	0/2318
4	XD	0.52	2/1733 (0.1%)	0.70	2/2318 (0.1%)
5	QE	0.37	0/1171	0.67	0/1576
5	XE	0.43	0/1171	0.62	0/1576
6	QF	0.39	0/856	0.68	0/1154
6	XF	0.41	0/856	0.62	0/1154
7	QG	0.35	0/1276	0.63	1/1709 (0.1%)
7	XG	0.36	0/1276	0.61	0/1709
8	QH	0.40	0/1128	0.62	0/1517
8	XH	0.42	0/1128	0.66	0/1517
9	QI	0.42	0/831	0.74	0/1120
9	XI	0.36	0/849	0.72	0/1144
10	QJ	0.35	0/814	0.67	0/1095
10	XJ	0.68	1/790 (0.1%)	0.80	1/1063 (0.1%)
11	QK	0.36	0/900	0.57	0/1213
11	XK	0.39	0/879	0.59	0/1187
12	QL	0.41	0/991	0.70	1/1327 (0.1%)
12	XL	0.45	0/972	0.76	2/1301 (0.2%)
13	QM	0.35	0/931	0.75	0/1248
13	XM	0.37	0/924	0.66	0/1238
14	QN	0.67	1/501 (0.2%)	0.84	3/664 (0.5%)
14	XN	0.69	1/501 (0.2%)	0.89	2/664 (0.3%)
15	QO	0.38	0/745	0.57	0/992
15	XO	0.40	0/740	0.56	0/987
16	QP	0.40	0/721	0.64	0/970
16	XP	0.38	0/721	0.66	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	QQ	0.38	0/847	0.62	0/1131
17	XQ	0.47	0/847	0.64	0/1131
18	QR	0.38	0/579	0.56	0/768
18	XR	0.39	0/579	0.58	0/768
19	QS	0.35	0/680	0.72	1/915 (0.1%)
19	XS	0.36	0/689	0.70	0/926
20	QT	0.77	2/765 (0.3%)	1.14	8/1007 (0.8%)
20	XT	0.37	0/765	0.75	2/1007 (0.2%)
21	QU	0.34	0/221	0.58	0/288
21	XU	0.52	0/221	0.61	0/288
22	QV	0.28	0/1621	0.84	5/2523 (0.2%)
22	XV	0.44	0/1621	1.24	15/2523 (0.6%)
23	QX	0.41	0/459	1.04	0/715
23	XX	0.60	0/459	1.31	2/715 (0.3%)
24	R0	0.40	0/652	0.63	0/867
24	Y0	0.59	0/657	0.60	0/874
25	R1	0.54	0/753	0.68	0/1000
25	Y1	0.59	0/736	0.74	0/978
26	R2	0.37	0/583	0.62	0/771
26	Y2	0.47	0/577	0.62	0/764
27	R3	0.39	0/474	0.59	0/635
27	Y3	0.62	0/474	0.59	0/635
28	R4	0.33	0/357	0.60	0/483
28	Y4	1.56	2/366 (0.5%)	1.47	9/495 (1.8%)
29	R5	0.87	3/473 (0.6%)	0.79	2/639 (0.3%)
29	Y5	0.94	2/473 (0.4%)	0.77	1/639 (0.2%)
30	R6	0.95	3/460 (0.7%)	0.81	2/613 (0.3%)
30	Y6	1.33	6/460 (1.3%)	1.01	3/613 (0.5%)
31	R7	0.53	0/417	0.62	0/550
31	Y7	0.63	0/426	0.66	0/561
32	R8	0.43	0/525	0.88	4/691 (0.6%)
32	Y8	0.59	0/525	0.84	0/691
33	R9	0.62	1/310 (0.3%)	0.72	1/407 (0.2%)
33	Y9	0.64	0/310	0.73	0/407
34	RA	0.26	0/69520	1.00	605/108527 (0.6%)
34	YA	0.29	2/69543 (0.0%)	1.02	662/108563 (0.6%)
35	RB	0.57	0/2878	1.40	38/4490 (0.8%)
35	YB	0.72	0/2878	1.67	85/4490 (1.9%)
36	RD	0.52	0/2165	0.71	3/2919 (0.1%)
36	YD	0.64	0/2165	0.74	4/2919 (0.1%)
37	RE	0.50	0/1601	0.83	3/2160 (0.1%)
37	YE	0.66	0/1601	0.85	3/2160 (0.1%)
38	RF	0.49	0/1620	0.70	1/2194 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	YF	0.67	0/1620	0.65	1/2194 (0.0%)
39	RG	0.41	0/1499	0.69	0/2016
39	YG	0.43	0/1499	0.68	0/2016
40	RH	0.39	0/1362	0.83	5/1841 (0.3%)
40	YH	0.68	1/1362 (0.1%)	0.86	6/1841 (0.3%)
41	RI	0.45	1/1151 (0.1%)	0.81	3/1558 (0.2%)
41	YI	0.45	1/1151 (0.1%)	0.79	0/1558
42	RN	0.45	0/1131	0.68	1/1525 (0.1%)
42	YN	0.63	0/1131	0.71	2/1525 (0.1%)
43	RO	0.51	0/943	0.65	0/1269
43	YO	0.60	0/943	0.63	0/1269
44	RP	0.44	0/1162	0.76	1/1544 (0.1%)
44	YP	0.54	0/1139	0.83	1/1514 (0.1%)
45	RQ	0.45	0/1143	0.73	0/1527
45	YQ	0.61	0/1143	0.77	2/1527 (0.1%)
46	RR	0.48	0/974	0.68	0/1302
46	YR	0.57	0/974	0.70	0/1302
47	RS	0.40	0/892	0.66	0/1187
47	YS	0.52	0/892	0.67	0/1187
48	RT	0.43	0/1155	0.69	0/1542
48	YT	0.54	0/1155	0.72	1/1542 (0.1%)
49	RU	0.49	0/982	0.62	0/1306
49	YU	0.70	0/982	0.62	0/1306
50	RV	0.48	0/790	0.74	1/1057 (0.1%)
50	YV	0.63	0/790	0.76	1/1057 (0.1%)
51	RW	0.52	0/911	0.63	0/1220
51	YW	0.68	0/911	0.64	0/1220
52	RX	0.52	0/739	0.60	0/993
52	YX	0.66	0/739	0.68	0/993
53	RY	0.72	4/831 (0.5%)	0.67	2/1108 (0.2%)
53	YY	0.73	1/831 (0.1%)	0.72	1/1108 (0.1%)
54	RZ	0.43	0/1493	0.89	6/2026 (0.3%)
54	YZ	0.51	0/1561	0.85	5/2119 (0.2%)
All	All	0.40	63/315379 (0.0%)	1.01	2644/471694 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	XA	1	16

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Mol	Chain	#Chirality outliers	#Planarity outliers
28	Y4	1	1
34	RA	0	1
34	YA	0	6
37	RE	0	1
37	YE	0	1
50	RV	0	2
54	RZ	0	1
54	YZ	0	1
All	All	2	30

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y4	5	ILE	CA-CB	-21.62	1.05	1.54
28	Y4	4	GLY	N-CA	-18.71	1.18	1.46
1	XA	309	G	C3'-C2'	-15.74	1.35	1.52
30	R6	16	CYS	CB-SG	14.21	2.06	1.82
30	Y6	16	CYS	CB-SG	-14.07	1.58	1.82

The worst 5 of 2644 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	617	G	C4-N9-C1'	38.95	177.13	126.50
1	XA	617	G	C8-N9-C1'	-38.89	76.44	127.00
1	XA	1505	G	C8-N9-C1'	-27.87	90.77	127.00
1	XA	625	G	C8-N9-C1'	-27.83	90.82	127.00
1	XA	1505	G	C4-N9-C1'	27.65	162.44	126.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	XA	617	G	C2'
28	Y4	5	ILE	CA

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	RA	1649	G	Sidechain
37	RE	146	THR	Peptide
50	RV	49	THR	Mainchain,Peptide
54	RZ	166	SER	Peptide
1	XA	308	C	Sidechain



## 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	32469	0	16385	1571	0
1	XA	32551	0	16418	1288	0
2	QB	1907	0	1958	99	0
2	XB	1915	0	1965	40	0
3	QC	1605	0	1667	135	0
3	XC	1605	0	1668	92	18
4	QD	1703	0	1762	108	0
4	XD	1703	0	1763	57	7
5	QE	1155	0	1213	76	0
5	XE	1155	0	1213	33	0
6	QF	843	0	857	10	5
6	XF	843	0	855	89	0
7	QG	1257	0	1296	53	18
7	XG	1257	0	1295	62	0
8	QH	1108	0	1165	52	0
8	XH	1108	0	1165	26	0
9	QI	816	0	822	51	6
9	XI	834	0	847	22	0
10	QJ	801	0	843	199	0
10	XJ	777	0	816	114	6
11	QK	885	0	904	35	0
11	XK	864	0	880	70	0
12	QL	975	0	1062	46	0
12	XL	956	0	1046	30	0
13	QM	921	0	974	137	0
13	XM	914	0	966	128	0
14	QN	492	0	528	288	0
14	XN	492	0	521	172	0
15	QO	734	0	770	57	0
15	XO	729	0	767	44	0
16	QP	705	0	725	71	0
16	XP	705	0	725	16	0
17	QQ	834	0	904	43	0
17	XQ	834	0	902	23	0
18	QR	574	0	644	8	0
18	XR	574	0	643	102	0
19	QS	665	0	678	223	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XS	674	0	695	110	0
20	QT	763	0	861	26	0
20	XT	763	0	861	40	0
21	QU	217	0	223	44	0
21	XU	217	0	234	10	0
22	QV	1452	0	736	3	0
22	XV	1452	0	736	16	0
23	QX	409	0	209	5	0
23	XX	409	0	209	23	0
24	R0	643	0	667	12	0
24	Y0	648	0	672	11	0
25	R1	746	0	826	26	0
25	Y1	729	0	802	11	0
26	R2	581	0	629	6	1
26	Y2	575	0	624	6	0
27	R3	469	0	518	13	2
27	Y3	469	0	518	12	0
28	R4	348	0	354	25	0
28	Y4	357	0	362	9	0
29	R5	459	0	477	20	0
29	Y5	459	0	476	25	1
30	R6	453	0	474	11	0
30	Y6	453	0	473	13	0
31	R7	409	0	454	12	0
31	Y7	418	0	467	18	0
32	R8	517	0	582	31	0
32	Y8	517	0	582	27	0
33	R9	307	0	335	24	0
33	Y9	307	0	336	19	0
34	RA	62070	0	31282	990	0
34	YA	62091	0	31289	1253	1
35	RB	2573	0	1306	21	0
35	YB	2573	0	1306	13	0
36	RD	2115	0	2195	53	2
36	YD	2115	0	2195	64	0
37	RE	1568	0	1634	34	0
37	YE	1568	0	1633	33	0
38	RF	1585	0	1632	33	0
38	YF	1585	0	1632	31	0
39	RG	1474	0	1535	49	0
39	YG	1474	0	1535	27	0
40	RH	1336	0	1418	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	YH	1336	0	1418	25	0
41	RI	1136	0	1223	41	0
41	YI	1136	0	1223	30	0
42	RN	1104	0	1180	13	0
42	YN	1104	0	1180	17	0
43	RO	933	0	996	23	0
43	YO	933	0	996	19	0
44	RP	1145	0	1228	37	0
44	YP	1122	0	1206	44	2
45	RQ	1122	0	1179	41	0
45	YQ	1122	0	1179	33	0
46	RR	960	0	1021	22	0
46	YR	960	0	1021	24	0
47	RS	882	0	943	19	0
47	YS	882	0	943	16	0
48	RT	1141	0	1202	19	0
48	YT	1141	0	1202	29	0
49	RU	964	0	1022	38	0
49	YU	964	0	1022	22	0
50	RV	779	0	852	17	0
50	YV	779	0	852	11	1
51	RW	900	0	964	20	0
51	YW	900	0	964	19	0
52	RX	725	0	778	11	0
52	YX	725	0	778	9	0
53	RY	818	0	911	25	0
53	YY	818	0	910	19	0
54	RZ	1461	0	1493	36	0
54	YZ	1529	0	1551	33	0
55	QA	70	0	0	0	0
55	QE	1	0	0	0	0
55	QF	1	0	0	0	0
55	QH	2	0	0	0	0
55	QL	2	0	0	0	0
55	R0	2	0	0	0	0
55	R3	1	0	0	0	0
55	R8	2	0	0	0	0
55	RA	432	0	0	0	0
55	RD	1	0	0	0	0
55	RE	4	0	0	0	0
55	RF	2	0	0	0	0
55	RN	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	RO	1	0	0	0	0
55	XA	88	0	0	2	0
55	XE	1	0	0	0	0
55	XO	1	0	0	0	0
55	Y1	1	0	0	0	0
55	Y2	1	0	0	0	0
55	Y5	1	0	0	0	0
55	Y7	1	0	0	0	0
55	Y8	2	0	0	0	0
55	YA	394	0	0	3	0
55	YB	1	0	0	0	0
55	YD	2	0	0	0	0
55	YE	4	0	0	0	0
55	YF	1	0	0	0	0
55	YP	1	0	0	0	0
55	YQ	1	0	0	0	0
55	YR	2	0	0	0	0
55	YU	1	0	0	0	0
55	YX	1	0	0	0	0
56	QD	8	0	0	2	0
56	XD	8	0	0	0	0
57	QN	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R9	1	0	0	0	0
57	RY	1	0	0	0	0
57	XN	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YY	1	0	0	1	0
All	All	291185	0	197033	6993	35

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 15.

The worst 5 of 6993 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)
10:QJ:47:PHE:CZ	14:QN:36:PHE:HB3	1.21	1.72
14:QN:24:CYS:SG	14:QN:40:CYS:HB2	1.24	1.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:980:C:C1'	14:QN:19:ARG:HG2	1.23	1.68
1:QA:1049:U:C5	14:QN:3:ARG:HB3	1.26	1.66
1:XA:1190:G:H5'	3:XC:176:HIS:CE1	1.30	1.64

The worst 5 of 35 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)
7:QG:149:ARG:NE	3:XC:81:GLY:O[4_555]	0.51	1.69
7:QG:149:ARG:NH1	3:XC:85:ARG:N[4_555]	1.02	1.18
7:QG:149:ARG:NH1	3:XC:85:ARG:CA[4_555]	1.16	1.04
7:QG:149:ARG:CZ	3:XC:85:ARG:N[4_555]	1.35	0.85
7:QG:149:ARG:NH1	3:XC:85:ARG:CB[4_555]	1.52	0.68

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	206 (88%)	27 (12%)	0	100	100
2	XB	234/256 (91%)	202 (86%)	31 (13%)	1 (0%)	30	67
3	QC	203/239 (85%)	180 (89%)	23 (11%)	0	100	100
3	XC	203/239 (85%)	182 (90%)	21 (10%)	0	100	100
4	QD	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	25	62
4	XD	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	25	62
5	QE	149/162 (92%)	134 (90%)	14 (9%)	1 (1%)	19	56
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	19	56
6	QF	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	142 (93%)	11 (7%)	0	100	100
8	QH	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
8	XH	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
9	QI	103/128 (80%)	91 (88%)	12 (12%)	0	100	100
9	XI	105/128 (82%)	97 (92%)	8 (8%)	0	100	100
10	QJ	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	13	47
10	XJ	94/105 (90%)	87 (93%)	5 (5%)	2 (2%)	5	32
11	QK	117/129 (91%)	108 (92%)	9 (8%)	0	100	100
11	XK	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
12	QL	123/132 (93%)	98 (80%)	24 (20%)	1 (1%)	16	53
12	XL	120/132 (91%)	99 (82%)	21 (18%)	0	100	100
13	QM	113/126 (90%)	96 (85%)	16 (14%)	1 (1%)	14	50
13	XM	112/126 (89%)	100 (89%)	11 (10%)	1 (1%)	14	50
14	QN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	7	37
14	XN	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	24
15	QO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	XO	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
16	QP	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
17	XQ	98/105 (93%)	94 (96%)	4 (4%)	0	100	100
18	QR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
18	XR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
19	QS	81/93 (87%)	66 (82%)	15 (18%)	0	100	100
19	XS	82/93 (88%)	65 (79%)	17 (21%)	0	100	100
20	QT	97/106 (92%)	86 (89%)	8 (8%)	3 (3%)	3	25
20	XT	97/106 (92%)	84 (87%)	10 (10%)	3 (3%)	3	25
21	QU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	XU	23/27 (85%)	23 (100%)	0	0	100	100
24	R0	79/85 (93%)	71 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	Y0	80/85 (94%)	75 (94%)	5 (6%)	0	100	100
25	R1	93/98 (95%)	76 (82%)	17 (18%)	0	100	100
25	Y1	91/98 (93%)	78 (86%)	12 (13%)	1 (1%)	12	45
26	R2	67/72 (93%)	63 (94%)	4 (6%)	0	100	100
26	Y2	66/72 (92%)	64 (97%)	2 (3%)	0	100	100
27	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	R4	43/71 (61%)	41 (95%)	2 (5%)	0	100	100
28	Y4	44/71 (62%)	28 (64%)	12 (27%)	4 (9%)	0	10
29	R5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	7	35
29	Y5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	7	35
30	R6	51/54 (94%)	46 (90%)	5 (10%)	0	100	100
30	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
31	R7	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
31	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
32	R8	62/65 (95%)	51 (82%)	9 (14%)	2 (3%)	3	25
32	Y8	62/65 (95%)	48 (77%)	14 (23%)	0	100	100
33	R9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	Y9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
36	RD	270/276 (98%)	244 (90%)	24 (9%)	2 (1%)	19	56
36	YD	270/276 (98%)	241 (89%)	28 (10%)	1 (0%)	30	67
37	RE	203/206 (98%)	159 (78%)	39 (19%)	5 (2%)	4	29
37	YE	203/206 (98%)	162 (80%)	39 (19%)	2 (1%)	13	47
38	RF	200/210 (95%)	183 (92%)	15 (8%)	2 (1%)	13	47
38	YF	200/210 (95%)	183 (92%)	16 (8%)	1 (0%)	25	62
39	RG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	22	59
39	YG	179/182 (98%)	152 (85%)	27 (15%)	0	100	100
40	RH	172/180 (96%)	145 (84%)	24 (14%)	3 (2%)	7	37
40	YH	172/180 (96%)	147 (86%)	21 (12%)	4 (2%)	5	31
41	RI	144/148 (97%)	114 (79%)	24 (17%)	6 (4%)	2	21
41	YI	144/148 (97%)	118 (82%)	22 (15%)	4 (3%)	4	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	19	56
42	YN	136/140 (97%)	123 (90%)	12 (9%)	1 (1%)	19	56
43	RO	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
43	YO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
44	RP	148/150 (99%)	114 (77%)	31 (21%)	3 (2%)	6	34
44	YP	145/150 (97%)	116 (80%)	28 (19%)	1 (1%)	19	56
45	RQ	139/141 (99%)	120 (86%)	18 (13%)	1 (1%)	19	56
45	YQ	139/141 (99%)	111 (80%)	27 (19%)	1 (1%)	19	56
46	RR	115/118 (98%)	103 (90%)	12 (10%)	0	100	100
46	YR	115/118 (98%)	104 (90%)	10 (9%)	1 (1%)	14	50
47	RS	109/112 (97%)	95 (87%)	14 (13%)	0	100	100
47	YS	109/112 (97%)	95 (87%)	13 (12%)	1 (1%)	14	50
48	RT	135/146 (92%)	116 (86%)	19 (14%)	0	100	100
48	YT	135/146 (92%)	121 (90%)	14 (10%)	0	100	100
49	RU	115/118 (98%)	106 (92%)	6 (5%)	3 (3%)	4	29
49	YU	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
50	RV	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	13	47
50	YV	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	13	47
51	RW	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
51	YW	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
52	RX	90/96 (94%)	85 (94%)	5 (6%)	0	100	100
52	YX	90/96 (94%)	84 (93%)	6 (7%)	0	100	100
53	RY	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
53	YY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
54	RZ	181/206 (88%)	139 (77%)	38 (21%)	4 (2%)	5	32
54	YZ	191/206 (93%)	145 (76%)	39 (20%)	7 (4%)	2	23
All	All	11368/12128 (94%)	10080 (89%)	1202 (11%)	86 (1%)	16	53

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	QL	105	TYR
20	QT	75	ASN

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Mol	Chain	Res	Type
32	R8	30	ARG
37	RE	147	PRO
40	RH	157	TYR

### 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	203/220 (92%)	200 (98%)	3 (2%)	60	75
2	XB	204/220 (93%)	204 (100%)	0	100	100
3	QC	159/188 (85%)	157 (99%)	2 (1%)	65	77
3	XC	159/188 (85%)	157 (99%)	2 (1%)	65	77
4	QD	180/181 (99%)	179 (99%)	1 (1%)	84	88
4	XD	180/181 (99%)	178 (99%)	2 (1%)	70	80
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	115 (99%)	1 (1%)	75	83
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	89 (99%)	1 (1%)	70	80
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	118/119 (99%)	117 (99%)	1 (1%)	79	84
8	XH	118/119 (99%)	118 (100%)	0	100	100
9	QI	79/99 (80%)	77 (98%)	2 (2%)	42	62
9	XI	81/99 (82%)	80 (99%)	1 (1%)	67	79
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	84 (98%)	2 (2%)	45	64
11	QK	90/99 (91%)	89 (99%)	1 (1%)	70	80
11	XK	88/99 (89%)	87 (99%)	1 (1%)	70	80
12	QL	104/109 (95%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	XL	103/109 (94%)	100 (97%)	3 (3%)	37	58
13	QM	93/101 (92%)	93 (100%)	0	100	100
13	XM	92/101 (91%)	92 (100%)	0	100	100
14	QN	49/50 (98%)	48 (98%)	1 (2%)	50	68
14	XN	49/50 (98%)	47 (96%)	2 (4%)	26	49
15	QO	79/80 (99%)	77 (98%)	2 (2%)	42	62
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	95 (100%)	0	100	100
17	XQ	95/97 (98%)	93 (98%)	2 (2%)	48	66
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	72 (100%)	0	100	100
19	XS	73/80 (91%)	73 (100%)	0	100	100
20	QT	76/82 (93%)	75 (99%)	1 (1%)	65	77
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	19 (95%)	1 (5%)	20	44
21	XU	20/22 (91%)	19 (95%)	1 (5%)	20	44
24	R0	65/67 (97%)	64 (98%)	1 (2%)	60	75
24	Y0	65/67 (97%)	65 (100%)	0	100	100
25	R1	80/83 (96%)	78 (98%)	2 (2%)	42	62
25	Y1	78/83 (94%)	78 (100%)	0	100	100
26	R2	64/67 (96%)	64 (100%)	0	100	100
26	Y2	64/67 (96%)	63 (98%)	1 (2%)	58	74
27	R3	51/52 (98%)	51 (100%)	0	100	100
27	Y3	51/52 (98%)	51 (100%)	0	100	100
28	R4	40/63 (64%)	40 (100%)	0	100	100
28	Y4	41/63 (65%)	40 (98%)	1 (2%)	44	63
29	R5	51/52 (98%)	50 (98%)	1 (2%)	50	68
29	Y5	51/52 (98%)	48 (94%)	3 (6%)	16	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	R6	51/52 (98%)	49 (96%)	2 (4%)	27	50
30	Y6	51/52 (98%)	49 (96%)	2 (4%)	27	50
31	R7	40/42 (95%)	40 (100%)	0	100	100
31	Y7	41/42 (98%)	41 (100%)	0	100	100
32	R8	54/55 (98%)	54 (100%)	0	100	100
32	Y8	54/55 (98%)	54 (100%)	0	100	100
33	R9	34/34 (100%)	34 (100%)	0	100	100
33	Y9	34/34 (100%)	33 (97%)	1 (3%)	37	58
36	RD	214/218 (98%)	212 (99%)	2 (1%)	75	83
36	YD	214/218 (98%)	214 (100%)	0	100	100
37	RE	165/166 (99%)	161 (98%)	4 (2%)	44	63
37	YE	165/166 (99%)	163 (99%)	2 (1%)	67	79
38	RF	161/166 (97%)	158 (98%)	3 (2%)	52	69
38	YF	161/166 (97%)	161 (100%)	0	100	100
39	RG	155/156 (99%)	155 (100%)	0	100	100
39	YG	155/156 (99%)	154 (99%)	1 (1%)	84	88
40	RH	145/148 (98%)	137 (94%)	8 (6%)	18	42
40	YH	145/148 (98%)	143 (99%)	2 (1%)	62	75
41	RI	122/124 (98%)	121 (99%)	1 (1%)	79	84
41	YI	122/124 (98%)	118 (97%)	4 (3%)	33	55
42	RN	117/119 (98%)	116 (99%)	1 (1%)	75	83
42	YN	117/119 (98%)	115 (98%)	2 (2%)	56	72
43	RO	100/100 (100%)	100 (100%)	0	100	100
43	YO	100/100 (100%)	98 (98%)	2 (2%)	50	68
44	RP	116/116 (100%)	115 (99%)	1 (1%)	75	83
44	YP	114/116 (98%)	114 (100%)	0	100	100
45	RQ	111/111 (100%)	111 (100%)	0	100	100
45	YQ	111/111 (100%)	110 (99%)	1 (1%)	75	83
46	RR	100/101 (99%)	99 (99%)	1 (1%)	73	81
46	YR	100/101 (99%)	99 (99%)	1 (1%)	73	81
47	RS	87/88 (99%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	YS	87/88 (99%)	85 (98%)	2 (2%)	45	64
48	RT	120/127 (94%)	117 (98%)	3 (2%)	42	62
48	YT	120/127 (94%)	118 (98%)	2 (2%)	56	72
49	RU	93/94 (99%)	93 (100%)	0	100	100
49	YU	93/94 (99%)	91 (98%)	2 (2%)	47	65
50	RV	82/82 (100%)	82 (100%)	0	100	100
50	YV	82/82 (100%)	80 (98%)	2 (2%)	44	63
51	RW	92/92 (100%)	91 (99%)	1 (1%)	70	80
51	YW	92/92 (100%)	92 (100%)	0	100	100
52	RX	74/78 (95%)	71 (96%)	3 (4%)	26	49
52	YX	74/78 (95%)	72 (97%)	2 (3%)	40	60
53	RY	88/91 (97%)	88 (100%)	0	100	100
53	YY	88/91 (97%)	87 (99%)	1 (1%)	70	80
54	RZ	162/179 (90%)	162 (100%)	0	100	100
54	YZ	167/179 (93%)	165 (99%)	2 (1%)	67	79
All	All	9610/10066 (96%)	9507 (99%)	103 (1%)	70	80

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	XJ	69	ASN
29	Y5	45	VAL
52	YX	66	LEU
12	XL	8	ASN
17	XQ	74	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
6	XF	100	ASN
28	Y4	6	HIS
10	XJ	62	HIS
13	XM	77	ASN
37	YE	132	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1509/1521 (99%)	531 (35%)	14 (0%)
1	XA	1514/1521 (99%)	469 (30%)	27 (1%)
22	QV	66/77 (85%)	15 (22%)	1 (1%)
22	XV	66/77 (85%)	16 (24%)	1 (1%)
23	QX	18/19 (94%)	5 (27%)	0
23	XX	18/19 (94%)	5 (27%)	0
34	RA	2878/2905 (99%)	706 (24%)	40 (1%)
34	YA	2880/2905 (99%)	754 (26%)	40 (1%)
35	RB	119/122 (97%)	20 (16%)	1 (0%)
35	YB	119/122 (97%)	23 (19%)	1 (0%)
All	All	9187/9288 (98%)	2544 (27%)	125 (1%)

5 of 2544 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	7	G
1	QA	8	A
1	QA	9	G
1	QA	15	G

5 of 125 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	266	G
34	YA	1653	G
1	XA	1304	G
34	YA	1608	A
34	YA	2566	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 1038 ligands modelled in this entry, 1036 are monoatomic - leaving 2 for Mogul analysis.

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

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	QA	1511/1521 (99%)	-0.06	20 (1%) 74 60	186, 276, 733, 884	0
1	XA	1515/1521 (99%)	-0.17	16 (1%) 77 64	158, 261, 672, 775	0
2	QB	235/256 (91%)	0.03	10 (4%) 40 32	230, 330, 393, 429	0
2	XB	236/256 (92%)	0.28	18 (7%) 21 19	237, 291, 340, 364	0
3	QC	205/239 (85%)	0.26	13 (6%) 27 24	271, 379, 421, 449	0
3	XC	205/239 (85%)	0.35	12 (5%) 29 25	275, 359, 467, 497	0
4	QD	208/209 (99%)	0.70	23 (11%) 12 12	231, 275, 325, 369	0
4	XD	208/209 (99%)	0.60	18 (8%) 17 16	216, 258, 306, 370	0
5	QE	151/162 (93%)	0.43	10 (6%) 26 23	208, 268, 318, 333	0
5	XE	151/162 (93%)	0.12	9 (5%) 29 24	174, 222, 277, 313	0
6	QF	101/101 (100%)	0.32	6 (5%) 29 25	224, 285, 333, 355	0
6	XF	101/101 (100%)	0.46	7 (6%) 24 21	278, 343, 376, 406	0
7	QG	155/156 (99%)	-0.05	4 (2%) 57 43	332, 425, 492, 522	0
7	XG	155/156 (99%)	0.08	5 (3%) 50 38	327, 458, 559, 580	0
8	QH	137/138 (99%)	1.15	27 (19%) 3 6	230, 290, 341, 368	0
8	XH	137/138 (99%)	0.61	12 (8%) 17 16	197, 259, 299, 342	0
9	QI	105/128 (82%)	0.07	1 (0%) 79 65	289, 373, 413, 449	0
9	XI	107/128 (83%)	0.21	3 (2%) 55 41	364, 448, 487, 522	0
10	QJ	99/105 (94%)	0.41	3 (3%) 52 40	354, 404, 458, 476	0
10	XJ	96/105 (91%)	0.73	9 (9%) 15 15	340, 397, 495, 509	0
11	QK	119/129 (92%)	0.45	8 (6%) 25 22	172, 269, 315, 333	0
11	XK	116/129 (89%)	0.55	9 (7%) 20 19	213, 279, 334, 364	0
12	QL	125/132 (94%)	0.79	14 (11%) 11 12	183, 237, 288, 334	0
12	XL	122/132 (92%)	0.87	21 (17%) 5 7	168, 221, 289, 338	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	QM	115/126 (91%)	0.02	2 (1%) 69 53	298, 386, 443, 469	0
13	XM	114/126 (90%)	0.34	7 (6%) 28 24	317, 414, 450, 463	0
14	QN	60/61 (98%)	0.74	7 (11%) 10 11	295, 353, 479, 493	0
14	XN	60/61 (98%)	1.00	12 (20%) 3 6	312, 556, 587, 612	0
15	QO	88/89 (98%)	0.73	13 (14%) 7 9	196, 272, 314, 335	0
15	XO	87/89 (97%)	0.57	9 (10%) 13 13	182, 221, 267, 284	0
16	QP	84/88 (95%)	0.97	14 (16%) 5 7	189, 247, 303, 348	0
16	XP	84/88 (95%)	1.56	30 (35%) 1 2	264, 358, 461, 493	0
17	QQ	100/105 (95%)	1.19	19 (19%) 4 6	199, 251, 286, 319	0
17	XQ	100/105 (95%)	0.61	16 (16%) 6 8	174, 231, 273, 307	0
18	QR	70/88 (79%)	0.20	3 (4%) 40 32	240, 297, 336, 375	0
18	XR	70/88 (79%)	0.21	3 (4%) 40 32	168, 247, 321, 337	0
19	QS	83/93 (89%)	0.81	4 (4%) 36 30	308, 459, 605, 672	0
19	XS	84/93 (90%)	0.77	6 (7%) 23 21	341, 414, 456, 474	0
20	QT	99/106 (93%)	1.29	31 (31%) 1 3	205, 271, 358, 377	0
20	XT	99/106 (93%)	1.14	19 (19%) 4 6	198, 242, 278, 302	0
21	QU	25/27 (92%)	0.81	2 (8%) 20 18	300, 347, 463, 563	0
21	XU	25/27 (92%)	1.18	5 (20%) 3 6	336, 374, 530, 549	0
22	QV	68/77 (88%)	-0.19	1 (1%) 71 57	294, 387, 435, 446	0
22	XV	68/77 (88%)	-0.34	0 100 100	281, 411, 474, 504	0
23	QX	19/19 (100%)	0.21	0 100 100	368, 432, 461, 464	0
23	XX	19/19 (100%)	0.29	0 100 100	356, 422, 471, 476	0
24	R0	81/85 (95%)	0.79	15 (18%) 4 6	166, 206, 296, 364	0
24	Y0	82/85 (96%)	0.57	6 (7%) 22 20	120, 168, 274, 329	0
25	R1	95/98 (96%)	1.23	20 (21%) 3 5	162, 201, 262, 291	0
25	Y1	93/98 (94%)	1.06	15 (16%) 5 8	117, 176, 219, 232	0
26	R2	69/72 (95%)	0.38	4 (5%) 30 25	124, 192, 238, 283	0
26	Y2	68/72 (94%)	0.88	11 (16%) 5 8	124, 171, 214, 231	0
27	R3	59/60 (98%)	0.51	7 (11%) 10 11	175, 228, 281, 338	0
27	Y3	59/60 (98%)	0.48	4 (6%) 25 22	115, 168, 241, 269	0
28	R4	45/71 (63%)	-0.29	0 100 100	237, 382, 418, 429	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
28	Y4	46/71 (64%)	-0.31	0	100	100	206, 273, 315, 322	0
29	R5	59/60 (98%)	0.19	1 (1%)	69	53	142, 193, 225, 291	0
29	Y5	59/60 (98%)	0.15	1 (1%)	69	53	122, 172, 225, 300	0
30	R6	53/54 (98%)	-0.27	1 (1%)	66	50	175, 230, 267, 357	0
30	Y6	53/54 (98%)	0.22	2 (3%)	44	35	144, 194, 248, 260	0
31	R7	47/49 (95%)	0.96	7 (14%)	7	9	138, 167, 186, 207	0
31	Y7	48/49 (97%)	0.75	9 (18%)	4	6	111, 146, 192, 224	0
32	R8	64/65 (98%)	0.75	7 (10%)	12	13	154, 201, 248, 284	0
32	Y8	64/65 (98%)	1.21	15 (23%)	2	4	120, 172, 209, 259	0
33	R9	37/37 (100%)	1.48	10 (27%)	2	4	260, 289, 340, 357	0
33	Y9	37/37 (100%)	1.25	6 (16%)	5	8	174, 205, 233, 250	0
34	RA	2882/2905 (99%)	-0.31	3 (0%)	92	89	123, 197, 357, 505	0
34	YA	2883/2905 (99%)	-0.32	13 (0%)	87	76	96, 149, 276, 493	0
35	RB	120/122 (98%)	-0.35	0	100	100	205, 256, 303, 350	0
35	YB	120/122 (98%)	-0.41	1 (0%)	82	69	135, 175, 210, 248	0
36	RD	272/276 (98%)	0.71	38 (13%)	7	10	127, 186, 231, 284	0
36	YD	272/276 (98%)	0.62	25 (9%)	16	15	107, 159, 207, 243	0
37	RE	205/206 (99%)	0.78	30 (14%)	7	9	128, 211, 265, 310	0
37	YE	205/206 (99%)	0.68	24 (11%)	10	11	102, 157, 205, 254	0
38	RF	202/210 (96%)	0.25	9 (4%)	39	31	143, 199, 272, 328	0
38	YF	202/210 (96%)	0.47	16 (7%)	20	18	101, 160, 215, 256	0
39	RG	181/182 (99%)	-0.04	5 (2%)	55	41	231, 307, 360, 388	0
39	YG	181/182 (99%)	0.06	9 (4%)	35	29	178, 226, 291, 327	0
40	RH	174/180 (96%)	0.23	12 (6%)	24	21	189, 269, 313, 358	0
40	YH	174/180 (96%)	0.36	11 (6%)	27	24	123, 175, 217, 258	0
41	RI	146/148 (98%)	0.29	11 (7%)	22	20	188, 254, 300, 327	0
41	YI	146/148 (98%)	0.06	7 (4%)	36	30	158, 226, 271, 293	0
42	RN	138/140 (98%)	0.49	14 (10%)	14	13	139, 219, 260, 268	0
42	YN	138/140 (98%)	0.71	18 (13%)	9	10	94, 160, 205, 231	0
43	RO	122/122 (100%)	0.34	8 (6%)	26	23	158, 202, 247, 286	0
43	YO	122/122 (100%)	0.11	1 (0%)	82	69	113, 159, 199, 213	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	RP	150/150 (100%)	0.72	27 (18%) 4 7	160, 228, 287, 331	0
44	YP	147/150 (98%)	0.66	16 (10%) 12 13	128, 166, 217, 255	0
45	RQ	141/141 (100%)	0.36	13 (9%) 16 15	194, 231, 267, 309	0
45	YQ	141/141 (100%)	0.37	5 (3%) 47 36	132, 174, 238, 314	0
46	RR	117/118 (99%)	0.94	19 (16%) 5 8	121, 180, 224, 257	0
46	YR	117/118 (99%)	0.98	27 (23%) 2 4	104, 155, 212, 237	0
47	RS	111/112 (99%)	0.40	10 (9%) 17 15	191, 262, 311, 357	0
47	YS	111/112 (99%)	0.70	22 (19%) 3 6	146, 196, 282, 328	0
48	RT	137/146 (93%)	0.33	11 (8%) 20 18	158, 225, 307, 320	0
48	YT	137/146 (93%)	0.46	14 (10%) 13 13	127, 185, 257, 282	0
49	RU	117/118 (99%)	0.70	13 (11%) 12 12	149, 243, 286, 304	0
49	YU	117/118 (99%)	0.56	7 (5%) 29 24	101, 147, 194, 223	0
50	RV	101/101 (100%)	0.19	10 (9%) 14 14	165, 222, 278, 288	0
50	YV	101/101 (100%)	0.35	12 (11%) 10 11	118, 170, 240, 280	0
51	RW	113/113 (100%)	0.59	10 (8%) 17 16	117, 160, 226, 339	0
51	YW	113/113 (100%)	0.62	12 (10%) 13 13	92, 137, 192, 239	0
52	RX	92/96 (95%)	0.58	6 (6%) 26 23	127, 177, 212, 235	0
52	YX	92/96 (95%)	0.76	11 (11%) 10 11	110, 146, 190, 259	0
53	RY	107/110 (97%)	0.50	6 (5%) 31 26	170, 219, 264, 315	0
53	YY	107/110 (97%)	0.29	3 (2%) 55 41	107, 170, 205, 244	0
54	RZ	183/206 (88%)	-0.07	4 (2%) 62 47	211, 258, 298, 354	0
54	YZ	193/206 (93%)	0.14	9 (4%) 37 30	124, 196, 287, 350	0
All	All	20769/21416 (96%)	0.16	1144 (5%) 32 26	92, 221, 460, 884	0

The worst 5 of 1144 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	XD	4	TYR	11.2
17	QQ	24	GLU	9.4
2	XB	101	MET	9.1
8	QH	111	ILE	9.0
12	XL	28	LYS	8.6

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	YA	3277	1/1	-0.39	0.38	213,213,213,213	0
55	MG	QA	1634	1/1	-0.27	0.29	175,175,175,175	0
55	MG	YA	3192	1/1	-0.25	0.25	219,219,219,219	0
55	MG	RA	3139	1/1	-0.24	0.42	290,290,290,290	0
55	MG	RA	3164	1/1	-0.24	0.31	199,199,199,199	0
55	MG	YA	3145	1/1	-0.17	0.29	84,84,84,84	0
55	MG	RA	3186	1/1	-0.16	0.20	205,205,205,205	0
55	MG	YA	3142	1/1	-0.14	0.38	158,158,158,158	0
55	MG	RA	3011	1/1	-0.14	0.22	129,129,129,129	0
55	MG	QE	201	1/1	-0.12	0.43	198,198,198,198	0
55	MG	QH	201	1/1	-0.11	0.17	188,188,188,188	0
55	MG	RA	3163	1/1	-0.07	0.22	165,165,165,165	0
55	MG	RA	3169	1/1	-0.06	0.38	131,131,131,131	0
55	MG	QA	1654	1/1	-0.05	0.31	189,189,189,189	0
55	MG	RA	3224	1/1	-0.04	0.24	181,181,181,181	0
55	MG	RA	3075	1/1	-0.01	0.49	147,147,147,147	0
55	MG	RA	3272	1/1	0.02	0.26	188,188,188,188	0
55	MG	YA	3091	1/1	0.02	0.29	145,145,145,145	0
55	MG	RA	2907	1/1	0.05	0.23	158,158,158,158	0
55	MG	YA	3202	1/1	0.07	0.39	164,164,164,164	0
55	MG	RA	3211	1/1	0.07	0.27	145,145,145,145	0
55	MG	YA	3254	1/1	0.08	0.22	181,181,181,181	0
55	MG	RA	3217	1/1	0.09	0.13	205,205,205,205	0
55	MG	RA	2921	1/1	0.11	0.42	136,136,136,136	0
55	MG	XA	1675	1/1	0.12	0.16	137,137,137,137	0
55	MG	RA	3078	1/1	0.13	0.43	208,208,208,208	0
55	MG	QA	1615	1/1	0.13	0.28	139,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	RA	3326	1/1	0.13	0.21	165,165,165,165	0
55	MG	XA	1651	1/1	0.13	0.25	162,162,162,162	0
55	MG	YA	3250	1/1	0.14	0.34	148,148,148,148	0
55	MG	RA	3013	1/1	0.14	0.42	143,143,143,143	0
55	MG	RA	3223	1/1	0.14	0.41	122,122,122,122	0
55	MG	YA	3126	1/1	0.15	0.52	84,84,84,84	0
55	MG	XA	1647	1/1	0.15	0.14	199,199,199,199	0
55	MG	RA	3008	1/1	0.16	0.29	150,150,150,150	0
55	MG	RA	3172	1/1	0.17	0.24	107,107,107,107	0
55	MG	RA	3275	1/1	0.17	0.26	156,156,156,156	0
55	MG	RA	3138	1/1	0.17	0.19	185,185,185,185	0
55	MG	RA	3206	1/1	0.18	0.28	101,101,101,101	0
55	MG	RA	3030	1/1	0.18	0.22	157,157,157,157	0
55	MG	YA	2962	1/1	0.20	0.41	124,124,124,124	0
55	MG	QA	1627	1/1	0.20	0.20	173,173,173,173	0
55	MG	YA	3234	1/1	0.21	0.31	123,123,123,123	0
55	MG	YA	3176	1/1	0.21	0.21	111,111,111,111	0
55	MG	XA	1620	1/1	0.22	0.23	138,138,138,138	0
55	MG	RA	3035	1/1	0.22	0.24	113,113,113,113	0
55	MG	RA	3179	1/1	0.23	0.31	121,121,121,121	0
55	MG	QA	1605	1/1	0.23	0.31	188,188,188,188	0
55	MG	QA	1647	1/1	0.24	0.23	225,225,225,225	0
55	MG	RA	2909	1/1	0.24	0.30	186,186,186,186	0
55	MG	RA	3023	1/1	0.24	0.36	98,98,98,98	0
55	MG	YA	2965	1/1	0.25	0.35	94,94,94,94	0
55	MG	RA	2937	1/1	0.26	0.29	119,119,119,119	0
55	MG	YA	3093	1/1	0.26	0.26	127,127,127,127	0
55	MG	XA	1680	1/1	0.27	0.36	144,144,144,144	0
55	MG	QA	1624	1/1	0.27	0.23	92,92,92,92	0
55	MG	RA	3005	1/1	0.27	0.31	174,174,174,174	0
55	MG	RA	3122	1/1	0.28	0.20	97,97,97,97	0
55	MG	RA	3286	1/1	0.28	0.51	126,126,126,126	0
55	MG	YA	3262	1/1	0.28	0.44	150,150,150,150	0
55	MG	YA	3015	1/1	0.28	0.25	123,123,123,123	0
55	MG	RA	2989	1/1	0.29	0.27	136,136,136,136	0
55	MG	RA	3193	1/1	0.29	0.21	141,141,141,141	0
55	MG	RA	3018	1/1	0.29	0.12	136,136,136,136	0
55	MG	YA	3175	1/1	0.29	0.49	117,117,117,117	0
55	MG	XA	1679	1/1	0.29	0.24	124,124,124,124	0
55	MG	QA	1664	1/1	0.29	0.14	156,156,156,156	0
55	MG	YA	3213	1/1	0.30	0.20	169,169,169,169	0
55	MG	YA	3117	1/1	0.30	0.83	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	XA	1676	1/1	0.31	0.34	143,143,143,143	0
55	MG	RA	2935	1/1	0.31	0.24	132,132,132,132	0
55	MG	YA	3281	1/1	0.31	0.45	151,151,151,151	0
55	MG	QA	1602	1/1	0.32	0.20	148,148,148,148	0
55	MG	RA	3294	1/1	0.32	0.14	143,143,143,143	0
55	MG	XA	1657	1/1	0.32	0.47	236,236,236,236	0
55	MG	YA	3245	1/1	0.33	0.52	84,84,84,84	0
55	MG	YA	2980	1/1	0.33	0.23	84,84,84,84	0
55	MG	YA	2956	1/1	0.33	0.32	114,114,114,114	0
55	MG	YA	3290	1/1	0.33	0.41	211,211,211,211	0
55	MG	XA	1650	1/1	0.34	0.19	189,189,189,189	0
55	MG	XA	1660	1/1	0.34	0.32	114,114,114,114	0
55	MG	RA	2963	1/1	0.34	0.20	256,256,256,256	0
55	MG	YA	2904	1/1	0.34	0.50	122,122,122,122	0
55	MG	YA	3164	1/1	0.35	0.36	84,84,84,84	0
55	MG	YA	3137	1/1	0.35	0.31	110,110,110,110	0
55	MG	QA	1662	1/1	0.35	0.30	151,151,151,151	0
55	MG	YA	3178	1/1	0.35	0.40	84,84,84,84	0
55	MG	RA	2938	1/1	0.35	0.37	159,159,159,159	0
55	MG	YA	2954	1/1	0.36	0.40	135,135,135,135	0
55	MG	RA	3083	1/1	0.36	0.69	150,150,150,150	0
55	MG	RA	2906	1/1	0.36	0.39	150,150,150,150	0
55	MG	YA	2905	1/1	0.36	0.57	175,175,175,175	0
55	MG	RA	3173	1/1	0.37	0.26	130,130,130,130	0
55	MG	RA	3140	1/1	0.37	0.38	88,88,88,88	0
55	MG	XA	1672	1/1	0.37	0.24	160,160,160,160	0
55	MG	YA	2948	1/1	0.37	0.33	84,84,84,84	0
55	MG	YA	3162	1/1	0.38	0.13	112,112,112,112	0
55	MG	RA	3127	1/1	0.38	0.15	132,132,132,132	0
55	MG	QA	1613	1/1	0.39	0.35	127,127,127,127	0
55	MG	YA	2916	1/1	0.39	0.37	121,121,121,121	0
55	MG	RA	3161	1/1	0.39	0.29	116,116,116,116	0
55	MG	YA	3120	1/1	0.39	0.40	84,84,84,84	0
55	MG	YA	3127	1/1	0.40	0.24	84,84,84,84	0
55	MG	YA	3233	1/1	0.40	0.17	153,153,153,153	0
55	MG	RA	3124	1/1	0.40	0.14	115,115,115,115	0
55	MG	YA	3141	1/1	0.40	0.32	102,102,102,102	0
55	MG	RA	3332	1/1	0.40	0.40	120,120,120,120	0
55	MG	XA	1613	1/1	0.41	0.49	171,171,171,171	0
55	MG	YA	2972	1/1	0.41	0.31	100,100,100,100	0
55	MG	YA	3279	1/1	0.41	0.21	122,122,122,122	0
55	MG	YA	3039	1/1	0.41	0.11	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	YA	3179	1/1	0.41	0.32	84,84,84,84	0
55	MG	YB	201	1/1	0.41	0.35	104,104,104,104	0
55	MG	RA	3029	1/1	0.42	0.34	100,100,100,100	0
55	MG	YA	3194	1/1	0.42	0.52	163,163,163,163	0
55	MG	YA	3148	1/1	0.42	0.18	102,102,102,102	0
55	MG	RA	3238	1/1	0.42	0.29	157,157,157,157	0
55	MG	YA	3060	1/1	0.42	0.19	177,177,177,177	0
55	MG	RA	3117	1/1	0.43	0.12	243,243,243,243	0
55	MG	YA	3068	1/1	0.43	0.20	158,158,158,158	0
55	MG	RA	2923	1/1	0.43	0.27	174,174,174,174	0
55	MG	RA	3302	1/1	0.43	0.20	116,116,116,116	0
55	MG	RA	2962	1/1	0.43	0.27	124,124,124,124	0
55	MG	RA	3028	1/1	0.43	0.23	96,96,96,96	0
55	MG	XA	1601	1/1	0.43	0.25	174,174,174,174	0
55	MG	YA	3171	1/1	0.43	0.28	84,84,84,84	0
55	MG	YA	3059	1/1	0.43	0.15	189,189,189,189	0
55	MG	RA	3170	1/1	0.44	0.17	132,132,132,132	0
55	MG	XA	1628	1/1	0.44	0.20	109,109,109,109	0
55	MG	QA	1628	1/1	0.45	0.12	238,238,238,238	0
55	MG	RA	3314	1/1	0.45	0.39	137,137,137,137	0
55	MG	RA	2943	1/1	0.46	0.37	132,132,132,132	0
55	MG	YA	3003	1/1	0.46	0.28	97,97,97,97	0
55	MG	XA	1649	1/1	0.46	0.16	123,123,123,123	0
55	MG	QA	1636	1/1	0.46	0.26	134,134,134,134	0
55	MG	XA	1634	1/1	0.46	0.27	107,107,107,107	0
55	MG	YA	2951	1/1	0.47	0.35	101,101,101,101	0
55	MG	YA	3109	1/1	0.47	0.27	95,95,95,95	0
55	MG	YA	3186	1/1	0.47	0.23	187,187,187,187	0
55	MG	QA	1655	1/1	0.47	0.16	121,121,121,121	0
55	MG	XA	1612	1/1	0.47	0.51	191,191,191,191	0
55	MG	RA	3106	1/1	0.47	0.23	90,90,90,90	0
55	MG	RA	3074	1/1	0.47	0.16	149,149,149,149	0
55	MG	RA	3213	1/1	0.47	0.13	157,157,157,157	0
55	MG	XA	1678	1/1	0.47	0.15	173,173,173,173	0
55	MG	RA	3137	1/1	0.48	0.10	177,177,177,177	0
55	MG	RA	2930	1/1	0.48	0.33	136,136,136,136	0
55	MG	RA	2947	1/1	0.48	0.24	118,118,118,118	0
55	MG	RA	2929	1/1	0.48	0.20	211,211,211,211	0
55	MG	YA	3199	1/1	0.48	0.38	186,186,186,186	0
55	MG	YA	3140	1/1	0.48	0.16	84,84,84,84	0
55	MG	XA	1630	1/1	0.49	0.24	180,180,180,180	0
55	MG	RA	3132	1/1	0.49	0.35	238,238,238,238	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	YA	3205	1/1	0.49	0.41	152,152,152,152	0
55	MG	RA	3092	1/1	0.50	0.28	98,98,98,98	0
55	MG	RA	3104	1/1	0.50	0.37	84,84,84,84	0
55	MG	RA	3293	1/1	0.50	0.13	121,121,121,121	0
55	MG	YA	3131	1/1	0.50	0.20	141,141,141,141	0
55	MG	QA	1643	1/1	0.50	0.24	180,180,180,180	0
55	MG	RA	3052	1/1	0.50	0.23	84,84,84,84	0
55	MG	RA	3034	1/1	0.50	0.19	111,111,111,111	0
55	MG	YU	201	1/1	0.50	0.14	97,97,97,97	0
55	MG	QA	1614	1/1	0.51	0.34	120,120,120,120	0
55	MG	YA	3267	1/1	0.51	0.15	84,84,84,84	0
55	MG	YA	3097	1/1	0.51	0.68	135,135,135,135	0
55	MG	XA	1606	1/1	0.51	0.14	165,165,165,165	0
55	MG	YA	3090	1/1	0.52	0.22	84,84,84,84	0
55	MG	YA	3115	1/1	0.52	0.30	148,148,148,148	0
55	MG	RA	3026	1/1	0.52	0.36	84,84,84,84	0
55	MG	RA	3059	1/1	0.52	0.37	153,153,153,153	0
55	MG	QA	1604	1/1	0.52	0.29	153,153,153,153	0
55	MG	YA	3258	1/1	0.53	0.35	88,88,88,88	0
55	MG	RA	3324	1/1	0.53	0.32	120,120,120,120	0
55	MG	YA	2940	1/1	0.53	0.22	84,84,84,84	0
55	MG	XA	1665	1/1	0.53	0.44	123,123,123,123	0
55	MG	QA	1637	1/1	0.53	0.26	126,126,126,126	0
55	MG	YA	2989	1/1	0.53	0.15	120,120,120,120	0
55	MG	XA	1618	1/1	0.53	0.28	103,103,103,103	0
55	MG	YA	3011	1/1	0.53	0.30	84,84,84,84	0
55	MG	RA	3328	1/1	0.53	0.25	145,145,145,145	0
55	MG	YA	3259	1/1	0.54	0.17	84,84,84,84	0
55	MG	XA	1652	1/1	0.54	0.09	143,143,143,143	0
55	MG	RA	3129	1/1	0.54	0.28	126,126,126,126	0
55	MG	RA	3086	1/1	0.54	0.36	84,84,84,84	0
55	MG	RA	3320	1/1	0.54	0.26	84,84,84,84	0
55	MG	QA	1625	1/1	0.54	0.22	104,104,104,104	0
55	MG	YA	2955	1/1	0.54	0.50	110,110,110,110	0
55	MG	YA	3256	1/1	0.54	0.23	94,94,94,94	0
55	MG	RA	3101	1/1	0.54	0.71	120,120,120,120	0
55	MG	QA	1670	1/1	0.55	0.19	190,190,190,190	0
55	MG	RA	2953	1/1	0.55	0.32	101,101,101,101	0
55	MG	RA	3226	1/1	0.55	0.30	84,84,84,84	0
55	MG	XA	1688	1/1	0.55	0.15	122,122,122,122	0
55	MG	XA	1632	1/1	0.55	0.19	104,104,104,104	0
55	MG	RA	3039	1/1	0.55	0.16	256,256,256,256	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	RA	3118	1/1	0.55	0.11	186,186,186,186	0
55	MG	RA	3162	1/1	0.55	0.57	139,139,139,139	0
55	MG	RA	2916	1/1	0.55	0.27	97,97,97,97	0
55	MG	YA	3048	1/1	0.56	0.38	84,84,84,84	0
55	MG	QA	1663	1/1	0.56	0.29	128,128,128,128	0
55	MG	RA	3095	1/1	0.56	0.13	258,258,258,258	0
55	MG	RA	3190	1/1	0.56	0.18	143,143,143,143	0
55	MG	RA	3057	1/1	0.56	0.72	180,180,180,180	0
55	MG	RA	3242	1/1	0.56	0.24	101,101,101,101	0
55	MG	YA	3211	1/1	0.56	0.44	101,101,101,101	0
55	MG	RA	3221	1/1	0.56	0.52	182,182,182,182	0
57	ZN	QN	101	1/1	0.56	0.17	439,439,439,439	0
55	MG	RA	3281	1/1	0.57	0.28	105,105,105,105	0
55	MG	YA	3050	1/1	0.57	0.29	84,84,84,84	0
55	MG	YA	3004	1/1	0.57	0.48	84,84,84,84	0
55	MG	RA	2913	1/1	0.57	0.15	107,107,107,107	0
55	MG	XA	1621	1/1	0.57	0.52	128,128,128,128	0
55	MG	RA	2969	1/1	0.57	0.25	104,104,104,104	0
55	MG	RA	3174	1/1	0.58	0.22	142,142,142,142	0
55	MG	RA	3208	1/1	0.58	0.29	84,84,84,84	0
55	MG	RA	2992	1/1	0.58	0.15	123,123,123,123	0
55	MG	RA	3180	1/1	0.58	0.20	168,168,168,168	0
55	MG	RA	3183	1/1	0.58	0.33	201,201,201,201	0
55	MG	RA	3220	1/1	0.58	0.78	166,166,166,166	0
55	MG	RA	3002	1/1	0.58	0.27	132,132,132,132	0
55	MG	YA	3242	1/1	0.58	0.14	84,84,84,84	0
55	MG	RA	3073	1/1	0.58	0.22	89,89,89,89	0
55	MG	YA	3049	1/1	0.58	0.28	84,84,84,84	0
55	MG	YA	3253	1/1	0.58	0.36	84,84,84,84	0
55	MG	RA	3144	1/1	0.58	0.48	126,126,126,126	0
55	MG	RA	3308	1/1	0.59	0.24	161,161,161,161	0
55	MG	RA	3289	1/1	0.59	0.30	125,125,125,125	0
55	MG	YA	2982	1/1	0.59	0.33	84,84,84,84	0
55	MG	RA	3093	1/1	0.59	0.17	131,131,131,131	0
55	MG	YA	3183	1/1	0.59	0.14	89,89,89,89	0
55	MG	XA	1642	1/1	0.59	0.37	128,128,128,128	0
55	MG	RA	2912	1/1	0.59	0.50	132,132,132,132	0
55	MG	RA	3136	1/1	0.59	0.37	84,84,84,84	0
55	MG	YA	3057	1/1	0.60	0.29	105,105,105,105	0
55	MG	RA	3088	1/1	0.60	0.29	101,101,101,101	0
55	MG	RE	304	1/1	0.60	0.53	96,96,96,96	0
55	MG	R0	101	1/1	0.60	0.26	147,147,147,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	YA	3077	1/1	0.60	0.22	87,87,87,87	0
55	MG	RA	2941	1/1	0.60	0.39	167,167,167,167	0
55	MG	YA	3044	1/1	0.60	0.31	84,84,84,84	0
55	MG	RA	3198	1/1	0.60	0.17	144,144,144,144	0
55	MG	YA	3239	1/1	0.60	0.41	84,84,84,84	0
55	MG	YA	3288	1/1	0.60	0.46	84,84,84,84	0
55	MG	XA	1674	1/1	0.60	0.16	159,159,159,159	0
55	MG	RA	2924	1/1	0.60	0.32	98,98,98,98	0
55	MG	YA	3187	1/1	0.60	0.26	117,117,117,117	0
55	MG	YA	3114	1/1	0.60	0.29	116,116,116,116	0
55	MG	RA	3076	1/1	0.61	0.26	114,114,114,114	0
55	MG	YA	2974	1/1	0.61	0.42	84,84,84,84	0
55	MG	YA	3032	1/1	0.61	0.21	84,84,84,84	0
55	MG	RA	3065	1/1	0.61	0.24	105,105,105,105	0
55	MG	RA	3252	1/1	0.61	0.30	121,121,121,121	0
55	MG	RA	3054	1/1	0.61	0.37	84,84,84,84	0
55	MG	XA	1669	1/1	0.61	0.08	187,187,187,187	0
55	MG	RA	3134	1/1	0.61	0.26	117,117,117,117	0
55	MG	YA	3128	1/1	0.61	0.38	134,134,134,134	0
55	MG	YA	3276	1/1	0.62	0.51	115,115,115,115	0
55	MG	RA	2903	1/1	0.62	0.14	100,100,100,100	0
55	MG	YA	3069	1/1	0.62	0.26	176,176,176,176	0
55	MG	RA	3167	1/1	0.62	0.28	165,165,165,165	0
55	MG	RA	2931	1/1	0.62	0.18	125,125,125,125	0
55	MG	YA	3174	1/1	0.62	0.25	94,94,94,94	0
55	MG	XA	1607	1/1	0.62	0.24	108,108,108,108	0
55	MG	YA	2961	1/1	0.62	0.27	117,117,117,117	0
55	MG	YA	3061	1/1	0.62	0.14	146,146,146,146	0
55	MG	QA	1618	1/1	0.63	0.38	176,176,176,176	0
55	MG	XA	1682	1/1	0.63	0.19	95,95,95,95	0
55	MG	RA	3304	1/1	0.63	0.28	155,155,155,155	0
55	MG	YA	3135	1/1	0.63	0.31	84,84,84,84	0
55	MG	YA	3232	1/1	0.63	0.25	91,91,91,91	0
55	MG	YA	2984	1/1	0.63	0.52	84,84,84,84	0
55	MG	RA	2965	1/1	0.63	0.20	211,211,211,211	0
55	MG	YA	3237	1/1	0.63	0.42	115,115,115,115	0
55	MG	RA	2942	1/1	0.63	0.24	109,109,109,109	0
55	MG	YA	3287	1/1	0.63	0.36	84,84,84,84	0
55	MG	RA	3064	1/1	0.63	0.47	110,110,110,110	0
55	MG	YA	3010	1/1	0.63	0.41	84,84,84,84	0
55	MG	YA	2964	1/1	0.63	0.36	115,115,115,115	0
55	MG	XA	1646	1/1	0.63	0.19	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	QA	1629	1/1	0.63	0.24	142,142,142,142	0
55	MG	YA	2981	1/1	0.64	0.31	103,103,103,103	0
55	MG	YA	3155	1/1	0.64	0.36	99,99,99,99	0
55	MG	XA	1670	1/1	0.64	0.35	136,136,136,136	0
55	MG	YA	2952	1/1	0.64	0.41	101,101,101,101	0
55	MG	YA	3122	1/1	0.64	0.42	84,84,84,84	0
55	MG	XA	1619	1/1	0.64	0.33	111,111,111,111	0
55	MG	YA	3017	1/1	0.64	0.45	107,107,107,107	0
55	MG	YA	3144	1/1	0.64	0.32	93,93,93,93	0
55	MG	QA	1619	1/1	0.64	0.28	123,123,123,123	0
55	MG	Y8	101	1/1	0.65	0.59	197,197,197,197	0
55	MG	RA	2910	1/1	0.65	0.18	149,149,149,149	0
55	MG	RA	3123	1/1	0.65	0.28	115,115,115,115	0
55	MG	RA	2952	1/1	0.65	0.16	143,143,143,143	0
55	MG	YA	3024	1/1	0.65	0.24	84,84,84,84	0
55	MG	XA	1616	1/1	0.65	0.34	291,291,291,291	0
55	MG	RA	3103	1/1	0.65	0.41	84,84,84,84	0
55	MG	QA	1669	1/1	0.65	0.26	158,158,158,158	0
55	MG	RA	3147	1/1	0.65	0.51	104,104,104,104	0
55	MG	YA	3107	1/1	0.65	0.32	204,204,204,204	0
55	MG	QA	1645	1/1	0.65	0.18	101,101,101,101	0
55	MG	RA	3295	1/1	0.65	0.28	129,129,129,129	0
55	MG	RA	2905	1/1	0.65	0.29	184,184,184,184	0
55	MG	RA	3020	1/1	0.65	0.33	126,126,126,126	0
55	MG	YA	3196	1/1	0.65	0.20	84,84,84,84	0
55	MG	YA	3151	1/1	0.66	0.30	94,94,94,94	0
55	MG	RA	3143	1/1	0.66	0.19	109,109,109,109	0
55	MG	YA	2935	1/1	0.66	0.39	84,84,84,84	0
55	MG	RA	3260	1/1	0.66	0.41	104,104,104,104	0
55	MG	QA	1632	1/1	0.66	0.11	84,84,84,84	0
55	MG	R0	102	1/1	0.66	0.11	120,120,120,120	0
55	MG	YA	3273	1/1	0.66	0.24	102,102,102,102	0
55	MG	YA	3218	1/1	0.66	0.32	84,84,84,84	0
55	MG	RA	3313	1/1	0.66	0.24	203,203,203,203	0
55	MG	YA	3035	1/1	0.66	0.28	122,122,122,122	0
55	MG	RA	3051	1/1	0.66	0.46	170,170,170,170	0
55	MG	YA	3282	1/1	0.66	0.15	116,116,116,116	0
55	MG	QA	1607	1/1	0.66	0.36	84,84,84,84	0
55	MG	QA	1617	1/1	0.66	0.36	159,159,159,159	0
55	MG	YA	2995	1/1	0.66	0.28	116,116,116,116	0
55	MG	QA	1609	1/1	0.66	0.10	120,120,120,120	0
55	MG	RA	3111	1/1	0.66	0.34	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	YA	3005	1/1	0.66	0.32	84,84,84,84	0
55	MG	RA	2939	1/1	0.67	0.14	84,84,84,84	0
55	MG	RA	3071	1/1	0.67	0.64	288,288,288,288	0
55	MG	YA	3180	1/1	0.67	0.29	90,90,90,90	0
55	MG	YA	3182	1/1	0.67	0.15	84,84,84,84	0
55	MG	XA	1633	1/1	0.67	0.26	99,99,99,99	0
55	MG	YA	3055	1/1	0.67	0.12	92,92,92,92	0
55	MG	RA	3048	1/1	0.67	0.25	168,168,168,168	0
55	MG	YA	3018	1/1	0.67	0.91	120,120,120,120	0
55	MG	YA	3224	1/1	0.67	0.34	84,84,84,84	0
55	MG	YA	2933	1/1	0.68	0.45	97,97,97,97	0
55	MG	RA	3210	1/1	0.68	0.18	121,121,121,121	0
55	MG	RA	3094	1/1	0.68	0.10	106,106,106,106	0
55	MG	YA	3085	1/1	0.68	0.30	84,84,84,84	0
55	MG	YA	3086	1/1	0.68	0.31	84,84,84,84	0
55	MG	RA	3171	1/1	0.68	0.40	115,115,115,115	0
55	MG	RA	2986	1/1	0.68	0.33	84,84,84,84	0
55	MG	RA	2920	1/1	0.68	0.17	113,113,113,113	0
55	MG	YA	2953	1/1	0.68	0.44	113,113,113,113	0
55	MG	RA	2957	1/1	0.68	0.33	95,95,95,95	0
55	MG	YA	3209	1/1	0.68	0.18	111,111,111,111	0
55	MG	QA	1601	1/1	0.68	0.26	123,123,123,123	0
55	MG	RA	3079	1/1	0.68	0.32	135,135,135,135	0
55	MG	YA	2959	1/1	0.68	0.32	84,84,84,84	0
55	MG	RA	3053	1/1	0.69	0.34	122,122,122,122	0
55	MG	YA	3095	1/1	0.69	0.15	84,84,84,84	0
55	MG	YA	3268	1/1	0.69	0.27	89,89,89,89	0
55	MG	QA	1626	1/1	0.69	0.18	104,104,104,104	0
55	MG	YA	2957	1/1	0.69	0.19	84,84,84,84	0
55	MG	RA	3222	1/1	0.69	0.39	166,166,166,166	0
55	MG	RA	2918	1/1	0.69	0.27	176,176,176,176	0
55	MG	XA	1658	1/1	0.69	0.35	179,179,179,179	0
55	MG	YA	3247	1/1	0.69	0.20	87,87,87,87	0
55	MG	RA	3182	1/1	0.69	0.12	150,150,150,150	0
55	MG	RA	3214	1/1	0.69	0.30	157,157,157,157	0
55	MG	QA	1638	1/1	0.69	0.27	84,84,84,84	0
55	MG	RA	3240	1/1	0.69	0.21	89,89,89,89	0
55	MG	XA	1623	1/1	0.69	0.19	127,127,127,127	0
55	MG	YA	3228	1/1	0.69	0.28	115,115,115,115	0
55	MG	RA	3102	1/1	0.70	0.29	102,102,102,102	0
55	MG	XA	1671	1/1	0.70	0.08	149,149,149,149	0
55	MG	YA	2944	1/1	0.70	0.19	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	QL	201	1/1	0.70	0.19	258,258,258,258	0
55	MG	RA	3157	1/1	0.70	0.20	156,156,156,156	0
55	MG	RA	3327	1/1	0.70	0.32	84,84,84,84	0
55	MG	QA	1621	1/1	0.70	0.32	159,159,159,159	0
55	MG	RA	3031	1/1	0.70	0.15	94,94,94,94	0
55	MG	YR	202	1/1	0.70	0.39	119,119,119,119	0
55	MG	YA	3189	1/1	0.70	0.20	93,93,93,93	0
55	MG	RA	3237	1/1	0.70	0.32	84,84,84,84	0
55	MG	YA	2931	1/1	0.71	0.42	84,84,84,84	0
55	MG	QA	1648	1/1	0.71	0.27	139,139,139,139	0
55	MG	R8	102	1/1	0.71	0.14	109,109,109,109	0
55	MG	YA	2936	1/1	0.71	0.42	84,84,84,84	0
55	MG	QA	1623	1/1	0.71	0.24	84,84,84,84	0
55	MG	YA	3001	1/1	0.71	0.11	84,84,84,84	0
55	MG	XA	1656	1/1	0.71	0.13	98,98,98,98	0
55	MG	YA	2963	1/1	0.71	0.35	84,84,84,84	0
55	MG	QA	1606	1/1	0.71	0.23	116,116,116,116	0
55	MG	YA	3094	1/1	0.71	0.17	104,104,104,104	0
55	MG	RA	3305	1/1	0.71	0.22	134,134,134,134	0
55	MG	QA	1642	1/1	0.71	0.07	157,157,157,157	0
55	MG	YA	3104	1/1	0.71	0.27	105,105,105,105	0
55	MG	YA	2908	1/1	0.71	0.30	84,84,84,84	0
55	MG	RA	3133	1/1	0.71	0.87	169,169,169,169	0
55	MG	YA	3156	1/1	0.72	0.25	84,84,84,84	0
55	MG	YA	3132	1/1	0.72	0.10	124,124,124,124	0
55	MG	YA	3271	1/1	0.72	0.30	92,92,92,92	0
55	MG	YA	3133	1/1	0.72	0.16	84,84,84,84	0
55	MG	YA	3134	1/1	0.72	0.16	120,120,120,120	0
55	MG	YA	3111	1/1	0.72	0.16	119,119,119,119	0
55	MG	RA	2954	1/1	0.72	0.61	306,306,306,306	0
55	MG	QA	1622	1/1	0.72	0.49	169,169,169,169	0
55	MG	RA	2904	1/1	0.72	0.29	219,219,219,219	0
55	MG	RA	3001	1/1	0.72	0.16	95,95,95,95	0
55	MG	YA	2969	1/1	0.72	0.36	84,84,84,84	0
55	MG	RA	3045	1/1	0.72	0.32	169,169,169,169	0
55	MG	YA	3291	1/1	0.72	0.34	84,84,84,84	0
55	MG	YA	3082	1/1	0.72	0.38	84,84,84,84	0
55	MG	XA	1685	1/1	0.72	0.17	113,113,113,113	0
55	MG	XA	1668	1/1	0.72	0.13	131,131,131,131	0
55	MG	YA	3265	1/1	0.72	0.34	107,107,107,107	0
55	MG	Y5	102	1/1	0.73	0.24	84,84,84,84	0
55	MG	RA	3125	1/1	0.73	0.37	174,174,174,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	RA	2936	1/1	0.73	0.11	87,87,87,87	0
55	MG	RA	2968	1/1	0.73	0.13	176,176,176,176	0
55	MG	YA	3087	1/1	0.73	0.43	84,84,84,84	0
55	MG	RA	3322	1/1	0.73	0.23	104,104,104,104	0
55	MG	RA	2917	1/1	0.73	0.15	100,100,100,100	0
55	MG	YA	2926	1/1	0.73	0.22	84,84,84,84	0
55	MG	YA	3143	1/1	0.73	0.39	84,84,84,84	0
55	MG	YA	3123	1/1	0.73	0.23	84,84,84,84	0
55	MG	XA	1602	1/1	0.73	0.20	96,96,96,96	0
55	MG	YA	3067	1/1	0.73	0.10	102,102,102,102	0
55	MG	XA	1603	1/1	0.73	0.15	189,189,189,189	0
55	MG	YA	3153	1/1	0.73	0.41	84,84,84,84	0
55	MG	RA	2998	1/1	0.73	0.18	84,84,84,84	0
55	MG	YA	3083	1/1	0.74	0.33	84,84,84,84	0
55	MG	RA	3046	1/1	0.74	0.22	150,150,150,150	0
55	MG	QA	1660	1/1	0.74	0.16	127,127,127,127	0
55	MG	YA	3173	1/1	0.74	0.28	84,84,84,84	0
55	MG	RA	2972	1/1	0.74	0.33	84,84,84,84	0
55	MG	YA	3054	1/1	0.74	0.14	93,93,93,93	0
55	MG	YA	2976	1/1	0.74	0.28	84,84,84,84	0
55	MG	RA	3311	1/1	0.74	0.26	84,84,84,84	0
55	MG	RA	3204	1/1	0.74	0.34	167,167,167,167	0
55	MG	YA	3161	1/1	0.74	0.22	132,132,132,132	0
57	ZN	XN	101	1/1	0.74	0.14	489,489,489,489	0
55	MG	YA	2915	1/1	0.75	0.28	107,107,107,107	0
55	MG	RA	2908	1/1	0.75	0.12	102,102,102,102	0
55	MG	RA	2966	1/1	0.75	0.14	149,149,149,149	0
55	MG	YA	3065	1/1	0.75	0.14	107,107,107,107	0
55	MG	RA	3115	1/1	0.75	0.10	130,130,130,130	0
55	MG	YA	3110	1/1	0.75	0.20	177,177,177,177	0
55	MG	YA	2932	1/1	0.75	0.72	84,84,84,84	0
55	MG	QA	1666	1/1	0.75	0.13	178,178,178,178	0
55	MG	YA	2983	1/1	0.75	0.55	84,84,84,84	0
55	MG	YA	2934	1/1	0.75	0.55	84,84,84,84	0
55	MG	QA	1631	1/1	0.75	0.11	110,110,110,110	0
55	MG	RA	2964	1/1	0.75	0.17	84,84,84,84	0
55	MG	XA	1664	1/1	0.75	0.31	84,84,84,84	0
55	MG	YA	3191	1/1	0.75	0.27	84,84,84,84	0
55	MG	RA	3330	1/1	0.75	0.22	84,84,84,84	0
55	MG	YA	3051	1/1	0.75	0.32	84,84,84,84	0
55	MG	YA	2907	1/1	0.75	0.47	151,151,151,151	0
55	MG	YA	2968	1/1	0.75	0.32	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	RA	3200	1/1	0.75	0.24	141,141,141,141	0
55	MG	YA	3257	1/1	0.75	0.19	84,84,84,84	0
55	MG	YA	3203	1/1	0.75	0.28	84,84,84,84	0
55	MG	RA	3152	1/1	0.76	0.46	122,122,122,122	0
55	MG	YA	3210	1/1	0.76	0.41	121,121,121,121	0
55	MG	RA	3280	1/1	0.76	0.13	84,84,84,84	0
55	MG	RA	3156	1/1	0.76	0.20	106,106,106,106	0
55	MG	RA	3285	1/1	0.76	0.17	161,161,161,161	0
55	MG	RA	2975	1/1	0.76	0.50	104,104,104,104	0
55	MG	QA	1658	1/1	0.76	0.10	84,84,84,84	0
55	MG	RA	2926	1/1	0.76	0.31	124,124,124,124	0
55	MG	YA	2912	1/1	0.76	0.30	84,84,84,84	0
55	MG	YA	3027	1/1	0.76	0.12	102,102,102,102	0
55	MG	YA	3075	1/1	0.76	0.39	84,84,84,84	0
55	MG	RA	3112	1/1	0.76	0.23	84,84,84,84	0
55	MG	YA	3286	1/1	0.76	0.32	144,144,144,144	0
55	MG	RA	3066	1/1	0.76	0.22	117,117,117,117	0
55	MG	RA	2928	1/1	0.76	0.18	138,138,138,138	0
55	MG	YA	3154	1/1	0.76	0.14	138,138,138,138	0
55	MG	YA	2930	1/1	0.76	0.41	84,84,84,84	0
55	MG	RA	3056	1/1	0.76	0.30	139,139,139,139	0
55	MG	RA	3146	1/1	0.76	0.09	84,84,84,84	0
55	MG	RA	2950	1/1	0.76	0.09	108,108,108,108	0
55	MG	YA	3002	1/1	0.76	0.28	132,132,132,132	0
55	MG	RA	3310	1/1	0.76	0.55	116,116,116,116	0
55	MG	YA	3195	1/1	0.77	0.16	84,84,84,84	0
55	MG	RA	3307	1/1	0.77	0.41	132,132,132,132	0
55	MG	YA	3158	1/1	0.77	0.31	84,84,84,84	0
55	MG	YA	3159	1/1	0.77	0.29	84,84,84,84	0
55	MG	YA	2945	1/1	0.77	0.18	86,86,86,86	0
55	MG	XA	1641	1/1	0.77	0.17	112,112,112,112	0
55	MG	YA	2922	1/1	0.77	0.22	84,84,84,84	0
55	MG	XE	201	1/1	0.77	0.21	157,157,157,157	0
55	MG	YA	2929	1/1	0.77	0.40	84,84,84,84	0
55	MG	YA	2979	1/1	0.77	0.38	95,95,95,95	0
55	MG	RA	3273	1/1	0.77	0.30	113,113,113,113	0
55	MG	QF	301	1/1	0.77	0.12	145,145,145,145	0
55	MG	RA	3199	1/1	0.77	0.26	84,84,84,84	0
55	MG	RA	2976	1/1	0.77	0.46	139,139,139,139	0
55	MG	YA	2906	1/1	0.77	0.29	84,84,84,84	0
55	MG	YA	3038	1/1	0.77	0.26	84,84,84,84	0
55	MG	RA	3282	1/1	0.77	0.28	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	YA	3042	1/1	0.77	0.34	84,84,84,84	0
55	MG	YA	3240	1/1	0.77	0.25	84,84,84,84	0
55	MG	YA	3118	1/1	0.77	0.33	84,84,84,84	0
55	MG	YA	3243	1/1	0.77	0.28	108,108,108,108	0
55	MG	YA	3119	1/1	0.77	0.39	84,84,84,84	0
55	MG	RA	3271	1/1	0.77	0.22	102,102,102,102	0
55	MG	YA	3248	1/1	0.77	0.26	134,134,134,134	0
55	MG	YA	2938	1/1	0.77	0.21	84,84,84,84	0
55	MG	RA	2999	1/1	0.77	0.39	121,121,121,121	0
55	MG	YA	3130	1/1	0.78	0.22	84,84,84,84	0
55	MG	XA	1625	1/1	0.78	0.14	190,190,190,190	0
55	MG	YA	2921	1/1	0.78	0.59	84,84,84,84	0
55	MG	QA	1665	1/1	0.78	0.17	84,84,84,84	0
55	MG	RA	3318	1/1	0.78	0.40	84,84,84,84	0
55	MG	XA	1605	1/1	0.78	0.43	161,161,161,161	0
55	MG	QA	1616	1/1	0.78	0.10	128,128,128,128	0
55	MG	YA	3272	1/1	0.78	0.26	98,98,98,98	0
55	MG	YA	3025	1/1	0.78	0.11	98,98,98,98	0
55	MG	YA	3275	1/1	0.78	0.23	112,112,112,112	0
55	MG	YA	3066	1/1	0.78	0.23	113,113,113,113	0
55	MG	RA	3299	1/1	0.78	0.10	102,102,102,102	0
55	MG	XA	1637	1/1	0.78	0.17	84,84,84,84	0
55	MG	RA	3278	1/1	0.78	0.12	113,113,113,113	0
55	MG	YA	3073	1/1	0.78	0.15	84,84,84,84	0
55	MG	YA	3284	1/1	0.78	0.11	128,128,128,128	0
55	MG	YA	2988	1/1	0.78	0.32	84,84,84,84	0
55	MG	RA	3241	1/1	0.78	0.28	84,84,84,84	0
55	MG	RA	3177	1/1	0.78	0.15	156,156,156,156	0
55	MG	RA	2970	1/1	0.78	0.52	102,102,102,102	0
55	MG	RA	3256	1/1	0.78	0.10	84,84,84,84	0
55	MG	RA	3205	1/1	0.78	0.27	100,100,100,100	0
55	MG	YE	302	1/1	0.78	0.26	131,131,131,131	0
55	MG	RA	3038	1/1	0.78	0.20	119,119,119,119	0
55	MG	YA	3088	1/1	0.78	0.25	84,84,84,84	0
55	MG	RA	3218	1/1	0.78	0.17	196,196,196,196	0
55	MG	YA	3129	1/1	0.78	0.29	84,84,84,84	0
55	MG	YA	3043	1/1	0.79	0.29	84,84,84,84	0
55	MG	RA	3036	1/1	0.79	0.07	136,136,136,136	0
55	MG	QA	1651	1/1	0.79	0.26	116,116,116,116	0
55	MG	YA	3212	1/1	0.79	0.29	84,84,84,84	0
55	MG	RA	3251	1/1	0.79	0.16	177,177,177,177	0
55	MG	RA	3022	1/1	0.79	0.30	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	YA	3188	1/1	0.79	0.14	124,124,124,124	0
55	MG	QA	1641	1/1	0.79	0.18	155,155,155,155	0
55	MG	YA	3096	1/1	0.79	0.26	92,92,92,92	0
55	MG	YA	3168	1/1	0.79	0.50	84,84,84,84	0
55	MG	YA	3053	1/1	0.79	0.22	93,93,93,93	0
55	MG	YA	3292	1/1	0.79	0.12	109,109,109,109	0
55	MG	RA	3225	1/1	0.79	0.32	93,93,93,93	0
55	MG	YD	302	1/1	0.79	0.36	99,99,99,99	0
55	MG	RA	3202	1/1	0.79	0.18	134,134,134,134	0
55	MG	RA	2933	1/1	0.79	0.16	194,194,194,194	0
55	MG	YA	3006	1/1	0.79	0.34	84,84,84,84	0
55	MG	QA	1649	1/1	0.79	0.25	109,109,109,109	0
55	MG	RA	3176	1/1	0.79	0.15	152,152,152,152	0
55	MG	YA	3150	1/1	0.80	0.68	84,84,84,84	0
55	MG	YA	2911	1/1	0.80	0.24	84,84,84,84	0
55	MG	YA	2975	1/1	0.80	0.13	97,97,97,97	0
55	MG	RA	3166	1/1	0.80	0.23	124,124,124,124	0
55	MG	YA	3026	1/1	0.80	0.28	84,84,84,84	0
55	MG	YA	3263	1/1	0.80	0.56	88,88,88,88	0
55	MG	YA	2950	1/1	0.80	0.17	111,111,111,111	0
55	MG	RA	3243	1/1	0.80	0.17	84,84,84,84	0
55	MG	RA	3017	1/1	0.80	0.18	84,84,84,84	0
55	MG	RA	2959	1/1	0.80	0.30	84,84,84,84	0
55	MG	RA	3037	1/1	0.80	0.09	145,145,145,145	0
55	MG	RA	2987	1/1	0.80	0.23	84,84,84,84	0
55	MG	YA	3167	1/1	0.80	0.19	84,84,84,84	0
55	MG	QA	1603	1/1	0.80	0.10	121,121,121,121	0
55	MG	RA	3116	1/1	0.80	0.18	89,89,89,89	0
55	MG	YA	2958	1/1	0.80	0.40	84,84,84,84	0
55	MG	YA	3231	1/1	0.80	0.19	84,84,84,84	0
55	MG	RA	3297	1/1	0.80	0.21	167,167,167,167	0
55	MG	XA	1610	1/1	0.80	0.57	237,237,237,237	0
55	MG	RA	3195	1/1	0.80	0.53	170,170,170,170	0
55	MG	YA	2903	1/1	0.80	0.18	90,90,90,90	0
55	MG	RA	3141	1/1	0.80	0.26	84,84,84,84	0
55	MG	YA	3136	1/1	0.80	0.24	84,84,84,84	0
55	MG	XA	1614	1/1	0.80	0.07	106,106,106,106	0
55	MG	YA	2967	1/1	0.80	0.08	84,84,84,84	0
55	MG	YA	3101	1/1	0.80	0.69	139,139,139,139	0
55	MG	XA	1644	1/1	0.80	0.32	235,235,235,235	0
55	MG	YA	3013	1/1	0.80	0.24	84,84,84,84	0
55	MG	RA	2982	1/1	0.80	0.15	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	YA	3062	1/1	0.80	0.20	119,119,119,119	0
55	MG	RA	3025	1/1	0.80	0.12	84,84,84,84	0
55	MG	YA	3255	1/1	0.80	0.24	84,84,84,84	0
55	MG	QA	1610	1/1	0.81	1.26	211,211,211,211	0
55	MG	YA	3270	1/1	0.81	0.26	84,84,84,84	0
55	MG	YA	3030	1/1	0.81	0.26	110,110,110,110	0
55	MG	YA	3031	1/1	0.81	0.49	84,84,84,84	0
55	MG	YA	3236	1/1	0.81	0.27	84,84,84,84	0
55	MG	YA	2999	1/1	0.81	0.19	84,84,84,84	0
55	MG	RA	3175	1/1	0.81	0.13	84,84,84,84	0
55	MG	XA	1686	1/1	0.81	0.22	108,108,108,108	0
55	MG	RA	2911	1/1	0.81	0.17	111,111,111,111	0
55	MG	RA	3207	1/1	0.81	0.13	151,151,151,151	0
55	MG	YA	3072	1/1	0.81	0.32	106,106,106,106	0
55	MG	YA	3197	1/1	0.81	0.13	84,84,84,84	0
55	MG	YA	3165	1/1	0.81	0.23	84,84,84,84	0
55	MG	Y2	101	1/1	0.81	0.20	133,133,133,133	0
55	MG	RA	3194	1/1	0.81	0.13	111,111,111,111	0
55	MG	RA	3107	1/1	0.81	0.25	94,94,94,94	0
55	MG	RA	3265	1/1	0.81	0.34	84,84,84,84	0
55	MG	RA	2995	1/1	0.81	0.29	260,260,260,260	0
55	MG	RA	2974	1/1	0.81	0.38	84,84,84,84	0
55	MG	RA	3010	1/1	0.81	0.13	138,138,138,138	0
55	MG	XA	1654	1/1	0.81	0.13	118,118,118,118	0
55	MG	YP	201	1/1	0.81	0.16	113,113,113,113	0
55	MG	QA	1620	1/1	0.81	0.21	159,159,159,159	0
55	MG	YA	3149	1/1	0.81	0.16	93,93,93,93	0
55	MG	RA	3276	1/1	0.81	0.14	138,138,138,138	0
55	MG	RA	3203	1/1	0.81	0.14	193,193,193,193	0
55	MG	YA	2985	1/1	0.82	0.48	84,84,84,84	0
55	MG	XA	1673	1/1	0.82	0.13	114,114,114,114	0
55	MG	YA	2943	1/1	0.82	0.18	93,93,93,93	0
55	MG	YA	3274	1/1	0.82	0.28	84,84,84,84	0
55	MG	YA	2919	1/1	0.82	0.36	84,84,84,84	0
55	MG	YA	2997	1/1	0.82	0.38	84,84,84,84	0
55	MG	XA	1640	1/1	0.82	0.08	101,101,101,101	0
55	MG	YA	2946	1/1	0.82	0.15	87,87,87,87	0
55	MG	RA	2983	1/1	0.82	0.30	84,84,84,84	0
55	MG	YA	3198	1/1	0.82	0.44	124,124,124,124	0
55	MG	RA	3004	1/1	0.82	0.06	205,205,205,205	0
55	MG	RA	3021	1/1	0.82	0.10	96,96,96,96	0
55	MG	QA	1657	1/1	0.82	0.38	157,157,157,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	XA	1629	1/1	0.82	0.10	135,135,135,135	0
55	MG	YA	3074	1/1	0.82	0.16	84,84,84,84	0
55	MG	YA	3112	1/1	0.82	0.34	96,96,96,96	0
55	MG	RA	3323	1/1	0.82	0.29	205,205,205,205	0
55	MG	RA	3047	1/1	0.82	0.07	139,139,139,139	0
55	MG	RA	3325	1/1	0.82	0.18	84,84,84,84	0
55	MG	RA	2901	1/1	0.82	0.14	98,98,98,98	0
55	MG	YA	2913	1/1	0.82	0.29	84,84,84,84	0
55	MG	YQ	201	1/1	0.82	0.08	111,111,111,111	0
55	MG	YA	2937	1/1	0.82	0.22	84,84,84,84	0
55	MG	RA	3120	1/1	0.82	0.27	129,129,129,129	0
55	MG	YA	3056	1/1	0.82	0.26	84,84,84,84	0
55	MG	YA	3124	1/1	0.82	0.37	84,84,84,84	0
55	MG	RA	3098	1/1	0.83	0.41	212,212,212,212	0
55	MG	RA	3003	1/1	0.83	0.17	108,108,108,108	0
55	MG	RA	3306	1/1	0.83	0.12	111,111,111,111	0
55	MG	RA	3080	1/1	0.83	0.15	108,108,108,108	0
55	MG	RA	3150	1/1	0.83	0.17	84,84,84,84	0
55	MG	RA	2914	1/1	0.83	0.15	129,129,129,129	0
55	MG	YA	3034	1/1	0.83	0.22	84,84,84,84	0
55	MG	YA	2971	1/1	0.83	0.25	84,84,84,84	0
55	MG	RE	303	1/1	0.83	0.18	109,109,109,109	0
55	MG	RA	2927	1/1	0.83	0.10	135,135,135,135	0
55	MG	YA	3252	1/1	0.83	0.31	118,118,118,118	0
55	MG	YA	3041	1/1	0.83	0.25	84,84,84,84	0
55	MG	RF	301	1/1	0.83	0.25	118,118,118,118	0
55	MG	RA	3192	1/1	0.83	0.12	105,105,105,105	0
55	MG	YA	3007	1/1	0.83	0.57	84,84,84,84	0
55	MG	RA	3058	1/1	0.83	0.31	147,147,147,147	0
55	MG	YA	3177	1/1	0.83	0.11	90,90,90,90	0
55	MG	YA	3078	1/1	0.83	0.27	140,140,140,140	0
55	MG	RA	3027	1/1	0.83	0.23	92,92,92,92	0
55	MG	YE	303	1/1	0.83	0.40	124,124,124,124	0
55	MG	RA	3228	1/1	0.83	0.21	105,105,105,105	0
55	MG	RA	3042	1/1	0.83	0.08	111,111,111,111	0
55	MG	RA	3077	1/1	0.83	0.54	185,185,185,185	0
55	MG	R8	101	1/1	0.83	0.18	111,111,111,111	0
55	MG	YA	3021	1/1	0.83	0.58	84,84,84,84	0
55	MG	YA	2942	1/1	0.83	0.26	120,120,120,120	0
55	MG	RA	3168	1/1	0.84	0.06	206,206,206,206	0
55	MG	RA	3329	1/1	0.84	0.20	93,93,93,93	0
55	MG	RA	2994	1/1	0.84	0.12	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	YA	3103	1/1	0.84	0.49	84,84,84,84	0
55	MG	YA	3070	1/1	0.84	0.23	84,84,84,84	0
55	MG	QA	1635	1/1	0.84	0.11	112,112,112,112	0
55	MG	YA	2990	1/1	0.84	0.09	84,84,84,84	0
55	MG	RA	3160	1/1	0.84	0.12	109,109,109,109	0
55	MG	YA	3022	1/1	0.84	0.27	84,84,84,84	0
55	MG	YA	3169	1/1	0.84	0.15	119,119,119,119	0
55	MG	YA	2996	1/1	0.84	0.13	84,84,84,84	0
55	MG	YA	3052	1/1	0.84	0.10	84,84,84,84	0
55	MG	XA	1687	1/1	0.84	0.55	172,172,172,172	0
55	MG	RA	2985	1/1	0.84	0.32	139,139,139,139	0
55	MG	XA	1615	1/1	0.84	0.09	162,162,162,162	0
55	MG	RA	3135	1/1	0.84	0.15	100,100,100,100	0
55	MG	RA	2961	1/1	0.84	0.15	101,101,101,101	0
55	MG	YA	2941	1/1	0.84	0.11	106,106,106,106	0
55	MG	RA	2945	1/1	0.84	0.25	84,84,84,84	0
55	MG	YA	3223	1/1	0.84	0.14	84,84,84,84	0
55	MG	YA	3181	1/1	0.84	0.14	115,115,115,115	0
55	MG	YA	3227	1/1	0.84	0.29	90,90,90,90	0
55	MG	YR	201	1/1	0.84	0.14	95,95,95,95	0
55	MG	Y8	102	1/1	0.84	0.32	123,123,123,123	0
55	MG	RA	2934	1/1	0.84	0.23	94,94,94,94	0
55	MG	QA	1608	1/1	0.84	0.18	97,97,97,97	0
55	MG	YA	3040	1/1	0.84	0.18	84,84,84,84	0
55	MG	QA	1656	1/1	0.85	0.17	105,105,105,105	0
55	MG	RA	3110	1/1	0.85	0.14	108,108,108,108	0
55	MG	RA	3151	1/1	0.85	0.12	84,84,84,84	0
55	MG	RA	3298	1/1	0.85	0.17	95,95,95,95	0
55	MG	YA	2910	1/1	0.85	0.20	84,84,84,84	0
55	MG	YA	3009	1/1	0.85	0.24	84,84,84,84	0
55	MG	RA	3012	1/1	0.85	0.13	106,106,106,106	0
55	MG	QH	202	1/1	0.85	0.32	211,211,211,211	0
55	MG	XA	1635	1/1	0.85	0.11	159,159,159,159	0
55	MG	YA	3200	1/1	0.85	0.39	142,142,142,142	0
55	MG	RA	3315	1/1	0.85	0.20	100,100,100,100	0
55	MG	RA	3119	1/1	0.85	0.11	137,137,137,137	0
55	MG	YA	3157	1/1	0.85	0.25	84,84,84,84	0
55	MG	YE	304	1/1	0.85	0.32	84,84,84,84	0
55	MG	YA	2973	1/1	0.85	0.14	90,90,90,90	0
55	MG	YA	3020	1/1	0.85	0.18	110,110,110,110	0
55	MG	RA	3201	1/1	0.85	0.34	125,125,125,125	0
55	MG	RA	3230	1/1	0.85	0.18	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	XA	1643	1/1	0.85	0.19	105,105,105,105	0
55	MG	XA	1661	1/1	0.85	0.20	105,105,105,105	0
55	MG	YA	3222	1/1	0.85	0.15	84,84,84,84	0
55	MG	YA	3206	1/1	0.86	0.11	84,84,84,84	0
55	MG	RA	2981	1/1	0.86	0.21	109,109,109,109	0
55	MG	YA	3098	1/1	0.86	0.26	174,174,174,174	0
55	MG	RA	2956	1/1	0.86	0.27	198,198,198,198	0
55	MG	RA	3283	1/1	0.86	0.42	117,117,117,117	0
55	MG	YA	2914	1/1	0.86	0.47	84,84,84,84	0
55	MG	YA	3185	1/1	0.86	0.12	87,87,87,87	0
55	MG	XA	1655	1/1	0.86	0.26	84,84,84,84	0
55	MG	YA	3108	1/1	0.86	0.12	117,117,117,117	0
55	MG	RA	3043	1/1	0.86	0.09	133,133,133,133	0
55	MG	YA	2918	1/1	0.86	0.21	84,84,84,84	0
55	MG	XA	1608	1/1	0.86	0.17	108,108,108,108	0
55	MG	RA	2967	1/1	0.86	0.10	230,230,230,230	0
55	MG	RA	3097	1/1	0.86	0.04	98,98,98,98	0
55	MG	QL	202	1/1	0.86	0.09	95,95,95,95	0
55	MG	RA	3087	1/1	0.86	0.29	164,164,164,164	0
55	MG	YA	2986	1/1	0.86	0.20	84,84,84,84	0
55	MG	YA	3063	1/1	0.86	0.19	104,104,104,104	0
55	MG	XA	1681	1/1	0.86	0.10	171,171,171,171	0
55	MG	XA	1631	1/1	0.86	0.32	167,167,167,167	0
55	MG	RA	2977	1/1	0.86	0.11	84,84,84,84	0
55	MG	YA	2970	1/1	0.86	0.45	84,84,84,84	0
55	MG	RA	3089	1/1	0.86	0.17	198,198,198,198	0
55	MG	RA	2951	1/1	0.87	0.24	255,255,255,255	0
55	MG	RA	3055	1/1	0.87	0.24	123,123,123,123	0
55	MG	RA	2919	1/1	0.87	0.10	130,130,130,130	0
55	MG	YA	2901	1/1	0.87	0.32	242,242,242,242	0
55	MG	RA	3236	1/1	0.87	0.23	84,84,84,84	0
55	MG	RA	2979	1/1	0.87	0.11	135,135,135,135	0
55	MG	RA	3303	1/1	0.87	0.20	256,256,256,256	0
55	MG	QA	1661	1/1	0.87	0.12	108,108,108,108	0
55	MG	XA	1645	1/1	0.87	0.21	106,106,106,106	0
55	MG	YA	3283	1/1	0.87	0.29	131,131,131,131	0
55	MG	YA	2939	1/1	0.87	0.11	84,84,84,84	0
55	MG	YA	3285	1/1	0.87	0.13	94,94,94,94	0
55	MG	RA	3121	1/1	0.87	0.30	177,177,177,177	0
55	MG	RA	3181	1/1	0.87	0.14	180,180,180,180	0
55	MG	QA	1646	1/1	0.87	0.07	84,84,84,84	0
55	MG	RA	3062	1/1	0.87	0.26	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	RA	3246	1/1	0.87	0.20	84,84,84,84	0
55	MG	XA	1626	1/1	0.87	0.05	112,112,112,112	0
55	MG	YA	3071	1/1	0.87	0.23	84,84,84,84	0
55	MG	RA	3250	1/1	0.87	0.21	84,84,84,84	0
55	MG	RA	3006	1/1	0.87	0.17	84,84,84,84	0
55	MG	RA	3288	1/1	0.87	0.14	99,99,99,99	0
55	MG	RA	3041	1/1	0.87	0.07	131,131,131,131	0
55	MG	RA	3292	1/1	0.87	0.14	105,105,105,105	0
55	MG	XA	1659	1/1	0.87	0.15	84,84,84,84	0
55	MG	YA	3080	1/1	0.87	0.12	94,94,94,94	0
55	MG	YA	3226	1/1	0.87	0.06	100,100,100,100	0
55	MG	YA	3081	1/1	0.87	0.18	84,84,84,84	0
55	MG	RA	3191	1/1	0.87	0.39	148,148,148,148	0
55	MG	RA	3033	1/1	0.87	0.16	95,95,95,95	0
55	MG	RA	3231	1/1	0.88	0.10	141,141,141,141	0
55	MG	QA	1639	1/1	0.88	0.08	135,135,135,135	0
55	MG	YA	3147	1/1	0.88	0.19	84,84,84,84	0
55	MG	RA	3215	1/1	0.88	0.10	102,102,102,102	0
55	MG	RA	2960	1/1	0.88	0.22	108,108,108,108	0
55	MG	XA	1627	1/1	0.88	0.41	165,165,165,165	0
55	MG	RA	3185	1/1	0.88	0.24	84,84,84,84	0
55	MG	QA	1612	1/1	0.88	0.09	141,141,141,141	0
55	MG	RA	3277	1/1	0.88	0.13	182,182,182,182	0
55	MG	RA	3301	1/1	0.88	0.17	142,142,142,142	0
55	MG	YA	3217	1/1	0.88	0.17	104,104,104,104	0
55	MG	XA	1609	1/1	0.88	0.20	96,96,96,96	0
55	MG	YA	3220	1/1	0.88	0.17	84,84,84,84	0
55	MG	QA	1659	1/1	0.88	0.04	125,125,125,125	0
55	MG	RA	3016	1/1	0.88	0.18	84,84,84,84	0
55	MG	RA	3100	1/1	0.88	0.60	165,165,165,165	0
55	MG	RA	3247	1/1	0.88	0.19	84,84,84,84	0
55	MG	YE	301	1/1	0.88	0.24	113,113,113,113	0
55	MG	YA	2966	1/1	0.88	0.28	84,84,84,84	0
55	MG	RA	3148	1/1	0.88	0.21	89,89,89,89	0
55	MG	YA	3266	1/1	0.88	0.22	102,102,102,102	0
55	MG	RA	2988	1/1	0.88	0.16	101,101,101,101	0
55	MG	QA	1652	1/1	0.88	0.09	162,162,162,162	0
55	MG	XA	1667	1/1	0.88	0.13	173,173,173,173	0
55	MG	YA	3029	1/1	0.88	0.18	84,84,84,84	0
55	MG	YA	3235	1/1	0.88	0.25	84,84,84,84	0
55	MG	RA	3044	1/1	0.88	0.38	156,156,156,156	0
57	ZN	R9	101	1/1	0.88	0.10	314,314,314,314	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	RA	3155	1/1	0.88	0.13	95,95,95,95	0
55	MG	YA	2920	1/1	0.89	0.12	84,84,84,84	0
55	MG	RA	3068	1/1	0.89	0.16	113,113,113,113	0
55	MG	YA	2993	1/1	0.89	0.19	84,84,84,84	0
55	MG	RA	3113	1/1	0.89	0.12	84,84,84,84	0
55	MG	RA	3149	1/1	0.89	0.42	85,85,85,85	0
55	MG	YA	2909	1/1	0.89	0.25	84,84,84,84	0
55	MG	YA	2998	1/1	0.89	0.33	84,84,84,84	0
55	MG	RE	302	1/1	0.89	0.25	84,84,84,84	0
55	MG	YA	2978	1/1	0.89	0.10	90,90,90,90	0
55	MG	YA	3269	1/1	0.89	0.25	84,84,84,84	0
55	MG	RA	2948	1/1	0.89	0.12	84,84,84,84	0
55	MG	RA	3209	1/1	0.89	0.14	165,165,165,165	0
55	MG	XA	1611	1/1	0.89	0.41	278,278,278,278	0
55	MG	YA	2949	1/1	0.89	0.17	84,84,84,84	0
55	MG	XA	1666	1/1	0.89	0.15	113,113,113,113	0
55	MG	RA	3165	1/1	0.89	0.13	197,197,197,197	0
55	MG	RA	2946	1/1	0.89	0.17	96,96,96,96	0
55	MG	YA	3036	1/1	0.89	0.23	84,84,84,84	0
55	MG	RA	3197	1/1	0.89	0.34	84,84,84,84	0
55	MG	YA	2987	1/1	0.89	0.23	84,84,84,84	0
55	MG	YA	3064	1/1	0.89	0.17	84,84,84,84	0
57	ZN	RY	201	1/1	0.89	0.07	344,344,344,344	0
55	MG	RA	3317	1/1	0.89	0.11	84,84,84,84	0
55	MG	YA	3201	1/1	0.90	0.36	139,139,139,139	0
55	MG	RA	3114	1/1	0.90	0.10	84,84,84,84	0
55	MG	RA	3153	1/1	0.90	0.08	117,117,117,117	0
55	MG	RA	3184	1/1	0.90	0.10	103,103,103,103	0
55	MG	YA	3246	1/1	0.90	0.10	129,129,129,129	0
55	MG	RA	3096	1/1	0.90	0.11	122,122,122,122	0
55	MG	RA	3126	1/1	0.90	0.08	137,137,137,137	0
55	MG	RA	3105	1/1	0.90	0.18	107,107,107,107	0
55	MG	RA	3032	1/1	0.90	0.20	84,84,84,84	0
55	MG	RA	3131	1/1	0.90	0.12	117,117,117,117	0
55	MG	RA	3254	1/1	0.90	0.11	130,130,130,130	0
55	MG	YA	3289	1/1	0.90	0.11	84,84,84,84	0
55	MG	RA	2993	1/1	0.90	0.07	141,141,141,141	0
55	MG	RA	3109	1/1	0.90	0.12	84,84,84,84	0
55	MG	YA	2923	1/1	0.90	0.16	84,84,84,84	0
55	MG	YA	3125	1/1	0.90	0.26	89,89,89,89	0
55	MG	YA	3037	1/1	0.90	0.26	84,84,84,84	0
55	MG	RA	3264	1/1	0.90	0.14	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	YA	2947	1/1	0.90	0.10	84,84,84,84	0
55	MG	QA	1644	1/1	0.90	0.09	84,84,84,84	0
55	MG	RA	3178	1/1	0.90	0.41	232,232,232,232	0
55	MG	YA	3230	1/1	0.90	0.20	84,84,84,84	0
55	MG	YA	3016	1/1	0.90	0.05	84,84,84,84	0
55	MG	RA	3050	1/1	0.90	0.22	110,110,110,110	0
55	MG	YA	2992	1/1	0.90	0.12	84,84,84,84	0
55	MG	YA	3045	1/1	0.90	0.23	84,84,84,84	0
55	MG	YA	3166	1/1	0.90	0.21	144,144,144,144	0
55	MG	YA	3019	1/1	0.90	0.07	84,84,84,84	0
55	MG	RA	3009	1/1	0.90	0.11	101,101,101,101	0
55	MG	RA	3040	1/1	0.90	0.12	89,89,89,89	0
55	MG	RA	3287	1/1	0.91	0.11	123,123,123,123	0
55	MG	YA	3238	1/1	0.91	0.10	129,129,129,129	0
55	MG	YA	3105	1/1	0.91	0.17	135,135,135,135	0
55	MG	RA	3099	1/1	0.91	0.29	84,84,84,84	0
55	MG	YA	3280	1/1	0.91	0.06	120,120,120,120	0
55	MG	RA	3232	1/1	0.91	0.06	99,99,99,99	0
55	MG	RA	3291	1/1	0.91	0.15	84,84,84,84	0
55	MG	YA	3138	1/1	0.91	0.17	98,98,98,98	0
55	MG	RA	3234	1/1	0.91	0.07	101,101,101,101	0
55	MG	QA	1650	1/1	0.91	0.24	108,108,108,108	0
55	MG	QA	1653	1/1	0.91	0.31	130,130,130,130	0
55	MG	XA	1662	1/1	0.91	0.10	141,141,141,141	0
55	MG	XA	1636	1/1	0.91	0.12	95,95,95,95	0
55	MG	RA	2980	1/1	0.91	0.18	84,84,84,84	0
55	MG	RA	3239	1/1	0.91	0.10	84,84,84,84	0
55	MG	YA	3216	1/1	0.91	0.16	84,84,84,84	0
55	MG	RA	3128	1/1	0.91	0.21	187,187,187,187	0
55	MG	XA	1617	1/1	0.91	0.16	84,84,84,84	0
55	MG	YA	3121	1/1	0.91	0.09	84,84,84,84	0
55	MG	RA	3262	1/1	0.91	0.26	194,194,194,194	0
55	MG	RA	3300	1/1	0.91	0.13	117,117,117,117	0
55	MG	RF	302	1/1	0.91	0.08	158,158,158,158	0
55	MG	YA	3008	1/1	0.91	0.26	84,84,84,84	0
55	MG	RA	3319	1/1	0.91	0.11	114,114,114,114	0
55	MG	XA	1622	1/1	0.91	0.11	132,132,132,132	0
55	MG	RA	2996	1/1	0.91	0.18	177,177,177,177	0
55	MG	RA	3321	1/1	0.91	0.12	88,88,88,88	0
55	MG	YA	3193	1/1	0.91	0.33	176,176,176,176	0
55	MG	YX	101	1/1	0.91	0.08	84,84,84,84	0
55	MG	YA	3160	1/1	0.91	0.09	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	XA	1604	1/1	0.91	0.12	176,176,176,176	0
55	MG	RA	3219	1/1	0.91	0.38	143,143,143,143	0
55	MG	RA	2915	1/1	0.91	0.10	84,84,84,84	0
55	MG	XA	1663	1/1	0.92	0.11	115,115,115,115	0
55	MG	XA	1684	1/1	0.92	0.13	210,210,210,210	0
55	MG	RA	3019	1/1	0.92	0.13	84,84,84,84	0
55	MG	RA	3267	1/1	0.92	0.16	143,143,143,143	0
55	MG	RA	3014	1/1	0.92	0.13	84,84,84,84	0
55	MG	XA	1648	1/1	0.92	0.05	137,137,137,137	0
55	MG	RA	2997	1/1	0.92	0.27	161,161,161,161	0
55	MG	YA	3264	1/1	0.92	0.20	84,84,84,84	0
55	MG	YA	3046	1/1	0.92	0.19	124,124,124,124	0
55	MG	YA	3047	1/1	0.92	0.15	84,84,84,84	0
55	MG	RN	201	1/1	0.92	0.13	98,98,98,98	0
55	MG	YA	3100	1/1	0.92	0.18	84,84,84,84	0
55	MG	QA	1640	1/1	0.92	0.30	101,101,101,101	0
55	MG	RA	3188	1/1	0.92	0.22	140,140,140,140	0
55	MG	YA	3028	1/1	0.92	0.20	84,84,84,84	0
55	MG	RA	3069	1/1	0.92	0.57	189,189,189,189	0
55	MG	RA	3091	1/1	0.92	0.28	132,132,132,132	0
55	MG	RA	2958	1/1	0.92	0.19	91,91,91,91	0
55	MG	RA	3257	1/1	0.92	0.19	86,86,86,86	0
55	MG	RA	3258	1/1	0.92	0.25	165,165,165,165	0
55	MG	RA	3063	1/1	0.92	0.17	84,84,84,84	0
55	MG	YA	3278	1/1	0.92	0.06	85,85,85,85	0
55	MG	YA	3190	1/1	0.92	0.28	99,99,99,99	0
55	MG	XA	1624	1/1	0.92	0.06	115,115,115,115	0
55	MG	RA	3227	1/1	0.92	0.26	123,123,123,123	0
55	MG	RA	3081	1/1	0.92	0.20	84,84,84,84	0
55	MG	RA	3284	1/1	0.93	0.10	108,108,108,108	0
55	MG	RA	2949	1/1	0.93	0.13	96,96,96,96	0
55	MG	RA	3248	1/1	0.93	0.09	105,105,105,105	0
55	MG	RA	3249	1/1	0.93	0.10	84,84,84,84	0
55	MG	YA	3139	1/1	0.93	0.07	84,84,84,84	0
55	MG	RO	201	1/1	0.93	0.35	186,186,186,186	0
55	MG	QA	1667	1/1	0.93	0.13	154,154,154,154	0
55	MG	YA	3000	1/1	0.93	0.10	93,93,93,93	0
55	MG	YA	2917	1/1	0.93	0.23	98,98,98,98	0
55	MG	RA	2978	1/1	0.93	0.22	84,84,84,84	0
55	MG	YA	3092	1/1	0.93	0.09	149,149,149,149	0
55	MG	YD	301	1/1	0.93	0.14	86,86,86,86	0
55	MG	RA	3212	1/1	0.93	0.10	170,170,170,170	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	RA	3253	1/1	0.93	0.23	84,84,84,84	0
55	MG	RA	3007	1/1	0.93	0.13	87,87,87,87	0
55	MG	RA	2944	1/1	0.93	0.11	84,84,84,84	0
55	MG	RA	3189	1/1	0.93	0.31	174,174,174,174	0
55	MG	RA	3216	1/1	0.93	0.12	122,122,122,122	0
55	MG	YA	2928	1/1	0.93	0.18	103,103,103,103	0
55	MG	RA	3259	1/1	0.93	0.19	97,97,97,97	0
55	MG	YA	3076	1/1	0.93	0.24	158,158,158,158	0
55	MG	RD	301	1/1	0.93	0.19	128,128,128,128	0
55	MG	RA	3244	1/1	0.93	0.08	144,144,144,144	0
55	MG	YA	3106	1/1	0.93	0.12	84,84,84,84	0
55	MG	YA	3079	1/1	0.93	0.12	84,84,84,84	0
55	MG	YA	3221	1/1	0.93	0.10	84,84,84,84	0
55	MG	RA	3235	1/1	0.93	0.14	84,84,84,84	0
55	MG	RA	3279	1/1	0.94	0.04	169,169,169,169	0
55	MG	XA	1677	1/1	0.94	0.05	147,147,147,147	0
55	MG	YA	3204	1/1	0.94	0.13	135,135,135,135	0
55	MG	XA	1653	1/1	0.94	0.11	84,84,84,84	0
55	MG	RA	2990	1/1	0.94	0.14	103,103,103,103	0
55	MG	RA	3268	1/1	0.94	0.13	84,84,84,84	0
55	MG	RA	3024	1/1	0.94	0.08	159,159,159,159	0
55	MG	YA	3099	1/1	0.94	0.18	84,84,84,84	0
55	MG	QA	1611	1/1	0.94	0.15	124,124,124,124	0
55	MG	RA	2922	1/1	0.94	0.15	105,105,105,105	0
55	MG	YA	3241	1/1	0.94	0.18	84,84,84,84	0
55	MG	YA	3215	1/1	0.94	0.18	84,84,84,84	0
55	MG	RA	3060	1/1	0.94	0.12	106,106,106,106	0
55	MG	RA	3061	1/1	0.94	0.18	91,91,91,91	0
55	MG	RA	3158	1/1	0.94	0.07	117,117,117,117	0
55	MG	YF	301	1/1	0.94	0.09	90,90,90,90	0
55	MG	YA	3170	1/1	0.94	0.09	84,84,84,84	0
55	MG	RE	301	1/1	0.94	0.10	84,84,84,84	0
55	MG	YA	3249	1/1	0.94	0.07	131,131,131,131	0
55	MG	YA	2991	1/1	0.94	0.10	95,95,95,95	0
55	MG	RA	3266	1/1	0.94	0.14	305,305,305,305	0
55	MG	XO	101	1/1	0.94	0.05	151,151,151,151	0
55	MG	YA	2960	1/1	0.94	0.25	84,84,84,84	0
55	MG	YA	3014	1/1	0.94	0.04	84,84,84,84	0
55	MG	Y1	101	1/1	0.94	0.07	117,117,117,117	0
55	MG	YA	3113	1/1	0.94	0.05	84,84,84,84	0
55	MG	RA	3312	1/1	0.95	0.16	115,115,115,115	0
55	MG	RA	3269	1/1	0.95	0.06	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	YA	3163	1/1	0.95	0.10	104,104,104,104	0
55	MG	YA	2924	1/1	0.95	0.12	84,84,84,84	0
55	MG	YA	3116	1/1	0.95	0.29	133,133,133,133	0
55	MG	RA	3130	1/1	0.95	0.10	119,119,119,119	0
55	MG	RA	3072	1/1	0.95	0.05	142,142,142,142	0
55	MG	RA	2925	1/1	0.95	0.18	84,84,84,84	0
55	MG	YA	3260	1/1	0.95	0.04	84,84,84,84	0
55	MG	XA	1639	1/1	0.95	0.12	84,84,84,84	0
55	MG	RA	3274	1/1	0.95	0.09	149,149,149,149	0
55	MG	YA	3293	1/1	0.95	0.09	102,102,102,102	0
55	MG	RA	3015	1/1	0.95	0.16	141,141,141,141	0
55	MG	YA	3172	1/1	0.95	0.18	84,84,84,84	0
55	MG	YA	3146	1/1	0.95	0.08	84,84,84,84	0
55	MG	RA	3142	1/1	0.95	0.19	152,152,152,152	0
55	MG	RA	3263	1/1	0.95	0.06	136,136,136,136	0
55	MG	RA	3090	1/1	0.95	0.18	138,138,138,138	0
55	MG	YA	3033	1/1	0.95	0.09	84,84,84,84	0
55	MG	Y7	101	1/1	0.95	0.26	208,208,208,208	0
55	MG	YA	3152	1/1	0.95	0.11	84,84,84,84	0
55	MG	YA	3012	1/1	0.95	0.12	84,84,84,84	0
55	MG	RA	2973	1/1	0.95	0.17	84,84,84,84	0
55	MG	RA	3000	1/1	0.95	0.04	109,109,109,109	0
55	MG	YA	2994	1/1	0.95	0.52	84,84,84,84	0
55	MG	RA	3309	1/1	0.95	0.07	120,120,120,120	0
55	MG	RA	3233	1/1	0.95	0.11	84,84,84,84	0
55	MG	YA	2977	1/1	0.95	0.09	84,84,84,84	0
55	MG	RA	2991	1/1	0.95	0.02	110,110,110,110	0
55	MG	YA	3219	1/1	0.95	0.07	91,91,91,91	0
55	MG	RA	3145	1/1	0.96	0.14	112,112,112,112	0
55	MG	RA	3261	1/1	0.96	0.07	191,191,191,191	0
55	MG	RA	2955	1/1	0.96	0.09	192,192,192,192	0
55	MG	YA	3023	1/1	0.96	0.07	84,84,84,84	0
55	MG	QA	1630	1/1	0.96	0.10	137,137,137,137	0
55	MG	YA	3225	1/1	0.96	0.14	100,100,100,100	0
55	MG	YA	3184	1/1	0.96	0.08	95,95,95,95	0
55	MG	RA	3290	1/1	0.96	0.06	95,95,95,95	0
55	MG	YA	3251	1/1	0.96	0.06	99,99,99,99	0
55	MG	YA	3058	1/1	0.96	0.05	84,84,84,84	0
55	MG	R3	101	1/1	0.96	0.10	94,94,94,94	0
55	MG	YA	3207	1/1	0.96	0.07	84,84,84,84	0
55	MG	XA	1638	1/1	0.96	0.18	84,84,84,84	0
55	MG	RA	2932	1/1	0.96	0.05	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	RA	3196	1/1	0.96	0.24	168,168,168,168	0
55	MG	RA	3159	1/1	0.96	0.12	104,104,104,104	0
55	MG	RA	3187	1/1	0.96	0.14	130,130,130,130	0
55	MG	RA	3067	1/1	0.96	0.05	101,101,101,101	0
55	MG	YA	3261	1/1	0.96	0.07	190,190,190,190	0
56	SF4	QD	301	8/8	0.96	0.06	181,237,336,420	0
55	MG	RA	3270	1/1	0.96	0.11	84,84,84,84	0
55	MG	YA	3084	1/1	0.96	0.17	84,84,84,84	0
55	MG	RA	3049	1/1	0.96	0.10	84,84,84,84	0
55	MG	RA	2984	1/1	0.96	0.07	84,84,84,84	0
57	ZN	Y9	101	1/1	0.96	0.05	162,162,162,162	0
55	MG	RA	3331	1/1	0.97	0.09	84,84,84,84	0
55	MG	QA	1633	1/1	0.97	0.05	190,190,190,190	0
55	MG	XA	1683	1/1	0.97	0.06	120,120,120,120	0
55	MG	YA	3102	1/1	0.97	0.16	178,178,178,178	0
55	MG	YA	3214	1/1	0.97	0.04	95,95,95,95	0
55	MG	RA	3082	1/1	0.97	0.10	84,84,84,84	0
55	MG	RA	3070	1/1	0.97	0.13	181,181,181,181	0
55	MG	YA	3294	1/1	0.97	0.04	103,103,103,103	0
55	MG	RA	3084	1/1	0.97	0.11	150,150,150,150	0
56	SF4	XD	301	8/8	0.97	0.05	163,216,235,295	0
55	MG	RA	3255	1/1	0.97	0.05	99,99,99,99	0
57	ZN	R5	101	1/1	0.97	0.03	268,268,268,268	0
57	ZN	R6	101	1/1	0.97	0.05	149,149,149,149	0
55	MG	YA	3244	1/1	0.97	0.12	84,84,84,84	0
55	MG	YA	2925	1/1	0.97	0.11	84,84,84,84	0
55	MG	RA	3245	1/1	0.97	0.19	93,93,93,93	0
57	ZN	Y5	101	1/1	0.97	0.07	308,308,308,308	0
55	MG	YA	2927	1/1	0.97	0.10	103,103,103,103	0
55	MG	RA	2940	1/1	0.98	0.04	84,84,84,84	0
55	MG	YA	2902	1/1	0.98	0.09	86,86,86,86	0
55	MG	RA	2902	1/1	0.98	0.04	84,84,84,84	0
55	MG	RA	3108	1/1	0.98	0.06	117,117,117,117	0
55	MG	RA	3296	1/1	0.98	0.07	121,121,121,121	0
55	MG	RA	3154	1/1	0.98	0.06	127,127,127,127	0
55	MG	YA	3229	1/1	0.98	0.07	84,84,84,84	0
55	MG	QA	1668	1/1	0.98	0.06	114,114,114,114	0
55	MG	YA	3208	1/1	0.98	0.09	100,100,100,100	0
55	MG	RA	3085	1/1	0.98	0.09	140,140,140,140	0
55	MG	YA	3089	1/1	0.98	0.07	84,84,84,84	0
55	MG	RA	3229	1/1	0.98	0.09	84,84,84,84	0
55	MG	RA	3316	1/1	0.99	0.03	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	ZN	Y6	101	1/1	0.99	0.02	144,144,144,144	0
55	MG	RA	2971	1/1	0.99	0.04	84,84,84,84	0
57	ZN	YY	201	1/1	0.99	0.02	193,193,193,193	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.