



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 11:27 AM UTC

PDB ID : 6NSH / pdb_00006nsh
Title : Modified ASL proline bound to Thermus thermophilus 70S (near-cognate)
Authors : Hoffer, E.D.; Maehigashi, T.; Subaramanian, S.; Hong, S.; Dunham, C.M.
Deposited on : 2019-01-24
Resolution : 3.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.48.1

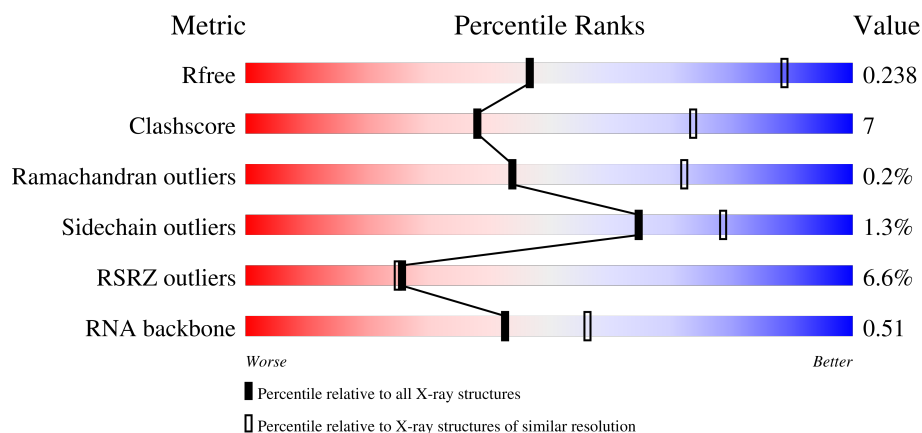
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)
RNA backbone	3690	1033 (3.80-3.00)

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 ≥ 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	RA	2915	
1	YA	2915	
2	RB	122	
2	YB	122	

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Mol	Chain	Length	Quality of chain
3	RD	276	82% 16% ..
3	YD	276	82% 14% ..
4	RE	206	76% 21% ..
4	YE	206	5% 75% 23% .
5	RF	210	2% 75% 20% ..
5	YF	210	5% 71% 24% .
6	RG	182	19% 65% 30% ..
6	YG	182	7% 70% 29% ..
7	RH	180	17% 68% 25% ..
7	YH	180	3% 80% 15% ..
8	RI	148	18% 65% 26% 6% ..
8	YI	148	9% 64% 31% ..
9	RN	140	4% 75% 23% ..
9	YN	140	3% 76% 21% .
10	RO	122	2% 73% 26% .
10	YO	122	80% 20% .
11	RP	150	7% 64% 32% ..
11	YP	150	2% 71% 25% ..
12	RQ	141	14% 62% 33% 5%
12	YQ	141	5% 82% 16% .
13	RR	118	3% 83% 14% .
13	YR	118	3% 81% 16% ..
14	RS	112	11% 74% 23% ...
14	YS	112	7% 86% 12% .
15	RT	146	5% 74% 19% 6%

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Mol	Chain	Length	Quality of chain
15	YT	146	
16	RU	118	
16	YU	118	
17	RV	101	
17	YV	101	
18	RW	113	
18	YW	113	
19	RX	96	
19	YX	96	
20	RY	110	
20	YY	110	
21	RZ	206	
21	YZ	206	
22	R0	85	
22	Y0	85	
23	R1	98	
23	Y1	98	
24	R2	72	
24	Y2	72	
25	R3	60	
25	Y3	60	
26	R4	71	
26	Y4	71	
27	R5	60	
27	Y5	60	

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Mol	Chain	Length	Quality of chain
28	R6	54	
28	Y6	54	
29	R7	49	
29	Y7	49	
30	R8	65	
30	Y8	65	
31	R9	37	
31	Y9	37	
32	QA	1521	
32	XA	1521	
33	QB	256	
33	XB	256	
34	QC	239	
34	XC	239	
35	QD	209	
35	XD	209	
36	QE	162	
36	XE	162	
37	QF	101	
37	XF	101	
38	QG	156	
38	XG	156	
39	QH	138	
39	XH	138	
40	QI	128	

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Mol	Chain	Length	Quality of chain
40	XI	128	
41	QJ	105	
41	XJ	105	
42	QK	129	
42	XK	129	
43	QL	132	
43	XL	132	
44	QM	126	
44	XM	126	
45	QN	61	
45	XN	61	
46	QO	89	
46	XO	89	
47	QP	88	
47	XP	88	
48	QQ	105	
48	XQ	105	
49	QR	88	
49	XR	88	
50	QS	93	
50	XS	93	
51	QT	106	
51	XT	106	
52	QU	27	
52	XU	27	

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Mol	Chain	Length	Quality of chain
53	QV	17	
53	XV	17	
54	QX	19	
54	XX	19	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	RA	3246	-	-	-	X
55	MG	RF	301	-	-	-	X
55	MG	YA	3193	-	-	-	X
55	MG	YA	3393	-	-	-	X
57	SF4	XD	301	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 290035 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 23S rRNA.

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

- Molecule 2 is a RNA chain called 5S rRNA.

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

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
3	YD	273	Total	C	N	O	S	0	0	0
			2126	1341	424	358	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	RP	148	Total	C	N	O	S	0	0	0
			1130	704	230	193	3			
11	YP	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	RR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	YR	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	RX	92	Total	C	N	O	S	0	0	0
			725	471	131	123				
19	YX	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	RZ	203	Total	C	N	O	S	0	0	0
			1601	1020	283	295	3			
21	YZ	201	Total	C	N	O	S	0	0	0
			1587	1012	281	291	3			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	R0	76	Total	C	N	O	S	0	0	0
			603	372	128	102	1			
22	Y0	75	Total	C	N	O	S	0	0	0
			599	370	127	101	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
24	Y2	72	Total	C	N	O	S	0	0	0
			606	375	122	107	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L31.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L32.

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

- Molecule 28 is a protein called 50S ribosomal protein L33.

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

- Molecule 29 is a protein called 50S ribosomal protein L34.

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

- Molecule 30 is a protein called 50S ribosomal protein L35.

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

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	R9	36	Total	C	N	O	S	0	0	0
			302	186	67	45	4			
31	Y9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	QA	1511	Total	C	N	O	P	0	0	0
			32469	14453	6011	10495	1510			
32	XA	1511	Total	C	N	O	P	0	0	0
			32471	14454	6014	10493	1510			

- Molecule 33 is a protein called 30S ribosomal protein S2.

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

- Molecule 34 is a protein called 30S ribosomal protein S3.

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

- Molecule 35 is a protein called 30S ribosomal protein S4.

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

- Molecule 36 is a protein called 30S ribosomal protein S5.

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

- Molecule 37 is a protein called 30S ribosomal protein S6.

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

- Molecule 38 is a protein called 30S ribosomal protein S7.

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

- Molecule 39 is a protein called 30S ribosomal protein S8.

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

- Molecule 40 is a protein called 30S ribosomal protein S9.

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

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	QJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			
41	XJ	96	Total	C	N	O	S	0	0	0
			777	487	153	136	1			

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	QK	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	XK	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 43 is a protein called 30S ribosomal protein S12.

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

- Molecule 44 is a protein called 30S ribosomal protein S13.

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

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 46 is a protein called 30S ribosomal protein S15.

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

- Molecule 47 is a protein called 30S ribosomal protein S16.

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

- Molecule 48 is a protein called 30S ribosomal protein S17.

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

- Molecule 49 is a protein called 30S ribosomal protein S18.

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

- Molecule 50 is a protein called 30S ribosomal protein S19.

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

- Molecule 51 is a protein called 30S ribosomal protein S20.

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

- Molecule 52 is a protein called 30S ribosomal protein Thx.

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

- Molecule 53 is a RNA chain called P-site ASLPro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	QV	17	Total	C	N	O	P	0	0	0
			365	163	65	120	17			
53	XV	15	Total	C	N	O	P	0	0	0
			322	144	57	106	15			

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	QX	18	Total	C	N	O	P	0	0	0
			389	174	76	121	18			
54	XX	19	Total	C	N	O	P	0	0	0
			412	184	81	128	19			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	RA	485	Total	Mg	0	0
			485	485		
55	RB	8	Total	Mg	0	0
			8	8		
55	RE	2	Total	Mg	0	0
			2	2		
55	RF	1	Total	Mg	0	0
			1	1		
55	RN	1	Total	Mg	0	0
			1	1		
55	RO	1	Total	Mg	0	0
			1	1		
55	RP	2	Total	Mg	0	0
			2	2		
55	RQ	2	Total	Mg	0	0
			2	2		
55	RT	1	Total	Mg	0	0
			1	1		
55	RX	1	Total	Mg	0	0
			1	1		
55	R0	1	Total	Mg	0	0
			1	1		
55	R1	1	Total	Mg	0	0
			1	1		
55	R5	1	Total	Mg	0	0
			1	1		
55	R8	1	Total	Mg	0	0
			1	1		

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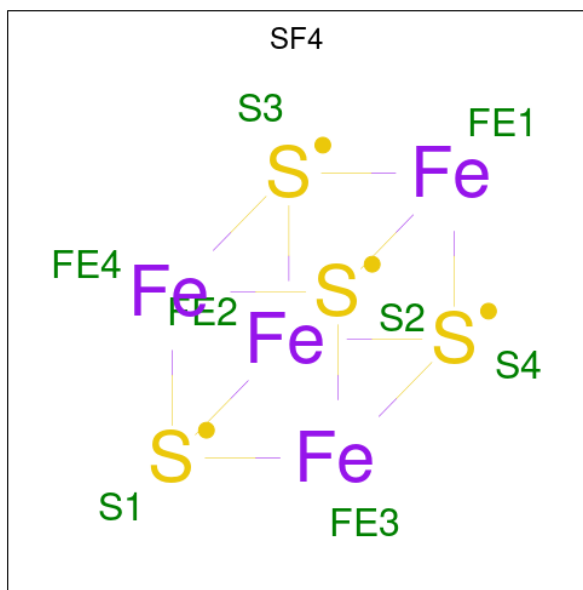
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	66	Total 66	Mg 66	0	0
55	QF	1	Total 1	Mg 1	0	0
55	YA	510	Total 510	Mg 510	0	0
55	YB	7	Total 7	Mg 7	0	0
55	YD	1	Total 1	Mg 1	0	0
55	YE	4	Total 4	Mg 4	0	0
55	YO	1	Total 1	Mg 1	0	0
55	YP	2	Total 2	Mg 2	0	0
55	YQ	1	Total 1	Mg 1	0	0
55	YR	1	Total 1	Mg 1	0	0
55	Y0	2	Total 2	Mg 2	0	0
55	Y1	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	1	Total 1	Mg 1	0	0
55	XA	87	Total 87	Mg 87	0	0
55	XE	1	Total 1	Mg 1	0	0
55	XL	1	Total 1	Mg 1	0	0
55	XQ	1	Total 1	Mg 1	0	0
55	XS	1	Total 1	Mg 1	0	0

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	RY	1	Total Zn 1 1	0	0
56	R4	1	Total Zn 1 1	0	0
56	R5	1	Total Zn 1 1	0	0
56	R6	1	Total Zn 1 1	0	0
56	R9	1	Total Zn 1 1	0	0
56	QN	1	Total Zn 1 1	0	0
56	YY	1	Total Zn 1 1	0	0
56	Y4	1	Total Zn 1 1	0	0
56	Y5	1	Total Zn 1 1	0	0
56	Y6	1	Total Zn 1 1	0	0
56	Y9	1	Total Zn 1 1	0	0
56	XN	1	Total Zn 1 1	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

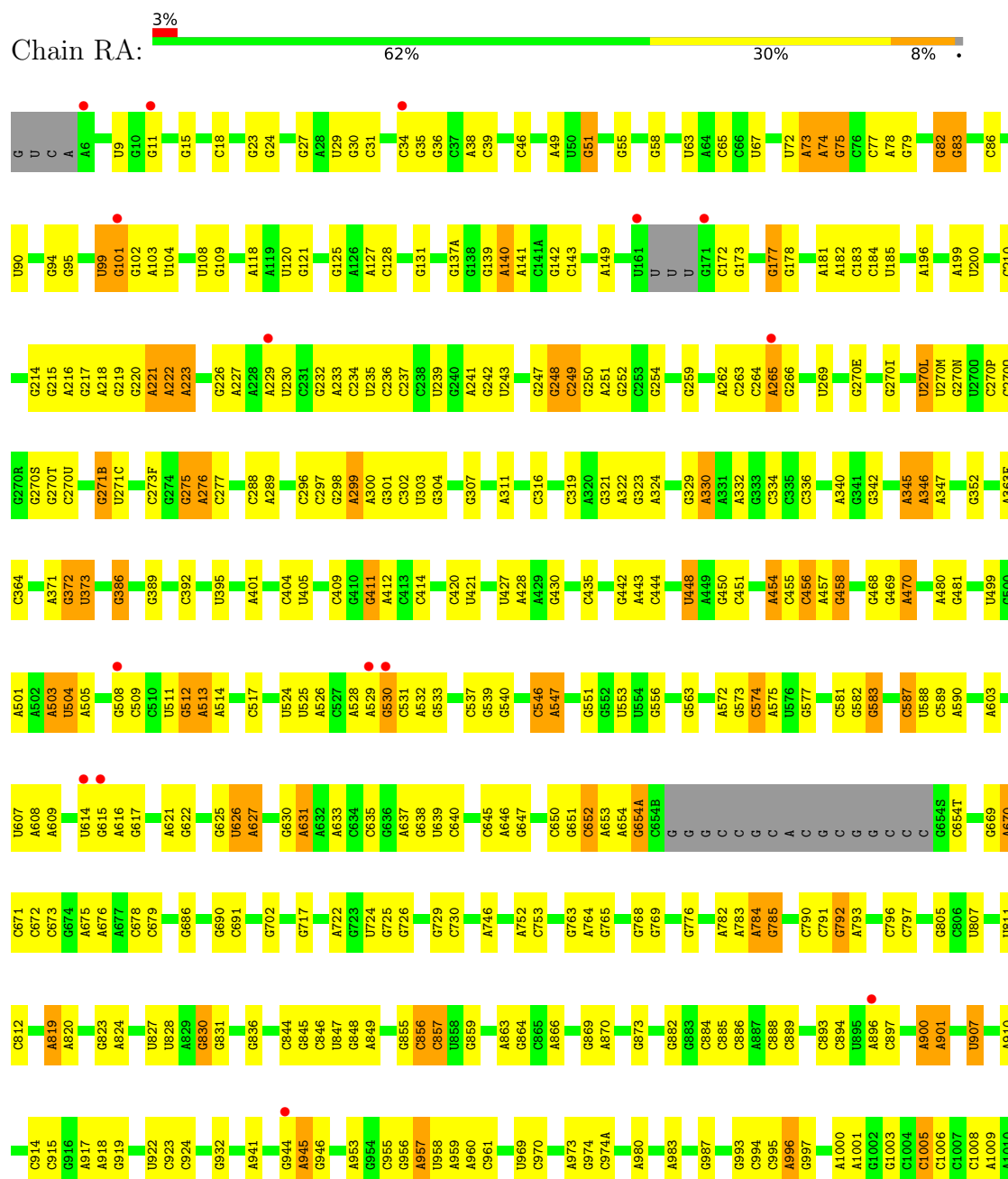


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	QD	1	Total 8	Fe 4	S 4	0	0
57	XD	1	Total 8	Fe 4	S 4	0	0

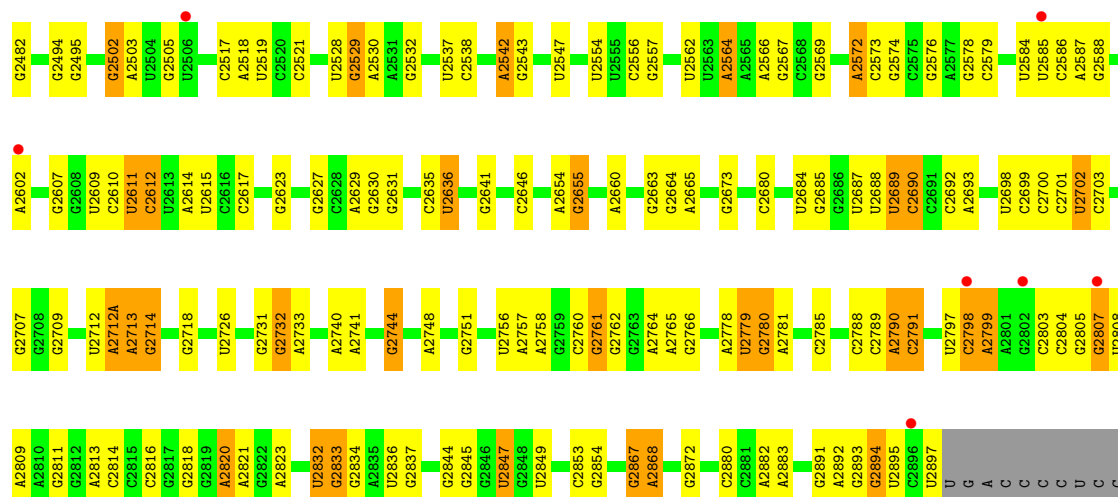
3 Residue-property plots [i](#)

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

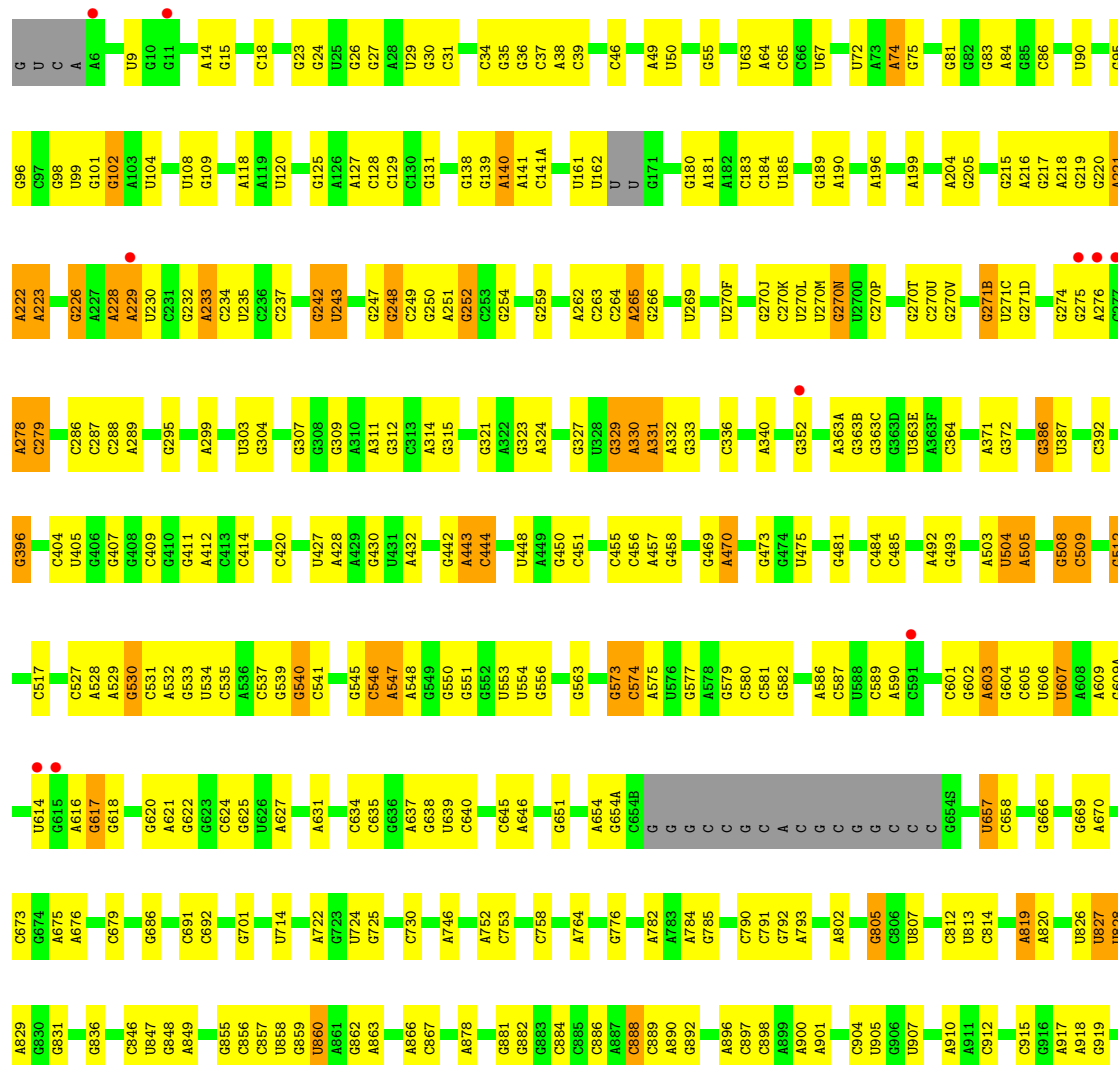
• Molecule 1: 23S rRNA



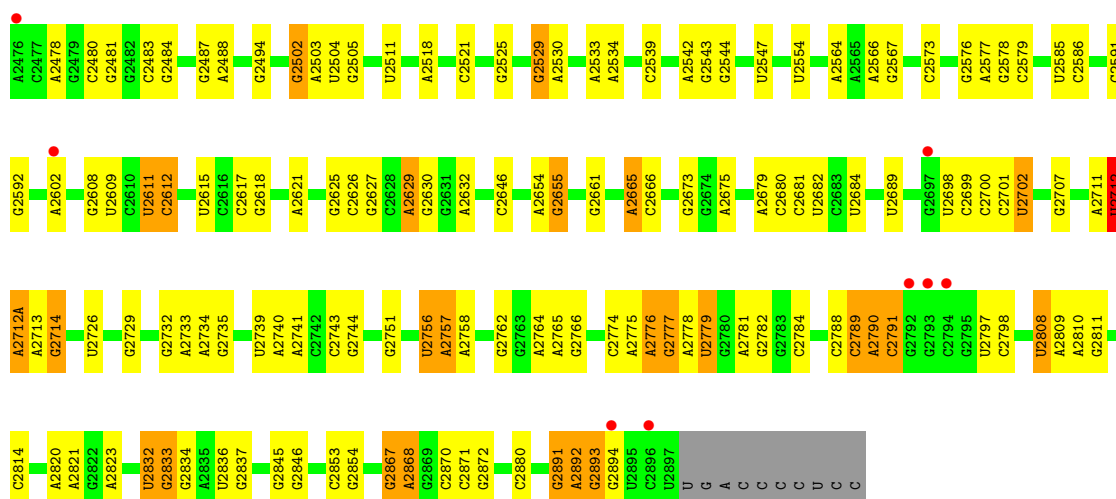
G2365	A2266	G2162	U2099	G1992	G1858	C1742	C1598	C1411	G1296	G1187	G1087	G1011
G2374	A2269	C2163	G2100	U1993	A1859	G1743	C1599	G1416	U1300	U1188	A1088	U1012
G2383	C2275	G2165	U2102	C1996	U1864	G1750	A1603	C1417	A1301	A1189	U1090	C1013
G2384	G2278	G2167	C2103	G2002	G1869	G1756	C1607	A1419	G1310	G1190	C1091	U1019
G2385	A2279	C2168	C2105	A2005	U1869	U1757	A1608	A1420	G1311	G1195	C1092	A1020
G2387	G2280	A2169	G2106	C2006	A1871	G1758	A1609	U1421	U1312	G1199	G1093	A1021
G2388	G2283	A2171	C2108	G2010	G1878	U1762	A1616	G1426	G1314	G1203	U1094	G1022
G2389	A2284	U2172	U2109	G2011	G1882	G1763	G1617	A1427	A1204	U1205	A1095	G1025
G2390	C2285	A2173	G2110	G2012	G1883	G1764	C1617	C1428	A1321	U1206	U1097	U1026
G2391	A2286	C2174	C2111	G2012	U1888	U1766	G1622	U1433	A1322	A1210	C1102	A1027
G2392	A2287	G2175	G2112	A2019	C1767	C1767	G1622	U1433	U1323	U1211	A1103	
G2395	A2288	A2114	U2113	A2020	G1889	A1773	A1634	G1441	U1329	A1214	C1109	G1031
G2403	C2178	G2115	G2116	C2021	U1915	A1773	G1635	G1442	U1338	A1220	G1110	A1033
G2406	C2179	G2117	A2117	U2022	A1900	G1776	C1636	G1444A	U1341	C1221	A1111	C1041
G2410	C2292	U2180	U2118	G2023	G1903	U1779	C1637	A1445	U1341	C1222	U1113	G1042
G2415	U2296	A2181	U2119	A2030	U1779	U1779	C1638	G1445	U1341	C1223	U1114	
G2422	G2302	G2182	G2120	A2031	A1780	C1781	U1639	G1448	A1348	G1224	G1115	A1046
G2423	G2302	G2184	G2121	G2032	C1781	C1782	C1640	U1449	A1349	G1224	G1115	A1047
G2424	G2305	G2187	U2123	A2033	U1786	A1786	C1648	G1449A	U1352	A1227	C1122	A1048
G2425	C2306	U2188	G2124	C2043	A1787	A1787	G1653	G1455	A1353	G1235	C1124	
G2426	G2307	U2189	A2125	G2049	C1788	C1788	A1654	G1456	A1354	G1236	A1129	C1053
G2427	A2308	C2190	G2126	C2055	A1916	A1789	C1657	A1460	A1359	A1237	U1130	C1054
G2428	A2310	G2191	C2127	A2051	U1917	A1790	C1658	G1461	A1359	G1238	U1130	G1055
G2429	A2311	G2192	C2128	G2052	U1917	A1791	C1658	G1464	A1365	G1248	C1135	G1056
G2430	U2312	G2193	U2129	G2053	A1918	A1791	C1658	G1464	A1365	U1249	G1136	A1057
G2431	C2313	U2197	G2130	A2054	G1929	U1796	A1668	A1471	G1368	G1250	G1137	G1058
G2435	G2315	A2198	U2132	G2056	G1930	C1797	A1669	G1478	G1369	C1251	G1138	G1059
U2438	G2319	U2208	A2134	A2059	A1936	G1799	C1670	G1479	G1371	A1252	G1139	U1060
A2439	A2320	G2209	A2135	A2060	A1937	G1800	G1674	U1482	A1379	U1253	U1141	U
C2440	G2325	G2210	C2136	A2061	A1938	G1801	G1678	G1483	A1384	U1262	U1142	G1063
C2441	A2326	A2212	C2137	A2062	U1939	G1801	G1678	G1484	G1385	U1263	A1142A	G1064
C2442	A2327	U2213	G2140	U2068	A1952	G1812	G1681	G1486	A1386	U1264	C1150	U1065
C2443	A2328	G2215	G2141	G2069	U1955	G1813	A1689	G1487	U1390	A1265	G1153	U1066
C2444	G2334	G2224	C2145	G2070	U1963	G1816	U1693	C1493	U1391	A1266	C1154	A1067
C2445	A2335	A2225	C2146	A2071	C1967	U1817	C1694	A1494	U1391	A1272	U1165	A1068
A2448	A2336	G2236	G2147	A2072	A1968	U1818	G1695	A1496	U1393	U1273	G1171	A1069
C2465	G2345	G2237	G2148	U2074	G1969	U1819	U1695	U1497	U1394	A1274	G1173	G1074
G2468	A2346	G2238	G2151	U2075	A1970	U1820	A1698	C1498	A1395	A1275	G1174	C1075
A2469	A2347	G2239	G2152	U2079	A1971	G1823	G1725	C1585	U1396	G1281	A1175	G1076
U2473	C2350	U2243	G2153	U2086	A1972	G1824	G1726	A1586	U1397	G1282	G1176	U1077
U2474	G2353	G2244	G2154	G2087	G1980	A1829	U1727	C1504	C1403	G1283	A1177	C1079
C2475	G2353	U2245	G2155	U2088	A1981	U1833	G1728	C1506	C1404	U1282	G1178	U1082
C2476	A2361	G2246	G2156	U2089	G1982	U1834	U1730	A1507	U1405	G1283	C1181	U1083
C2477	G2364	A2247	U2157	G2093	G1982	G1835	U1731	A1508	U1406	A1286	A1182	A1084
C2480	G2481	G2250	A2158	U2096	G1989	A1847	G1732	C1509	C1408	A1287	G1184	A1085
G2481			G2159	U2096	C1990	A1847	A1733	A1511		U1288		A1086
			C2161	U1991	U1991	A1848		G1512		C1295		



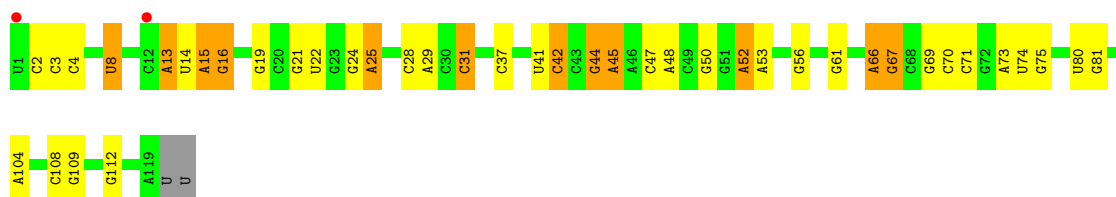
● Molecule 1: 23S rRNA



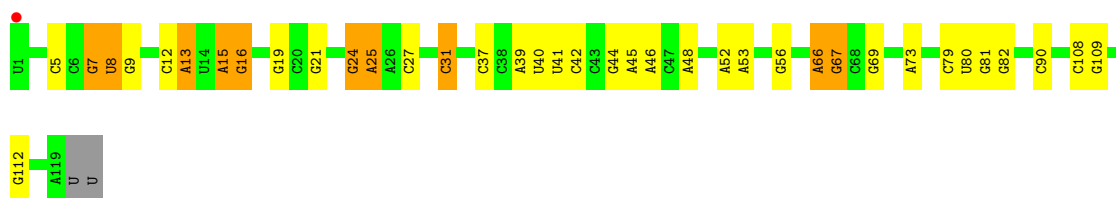
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		A2273	G2275	G2280	C2283	A2287	A2288		C2291	C2292		G2160	U2099	C1982	U1864	G1728	U1590		A1471	A1354		A103	A1020	C923
												G2161	G2100	G1989	G1869	A1729	G1869					A1021	A1021	C924
												G2162	G2101	G1990	G1870	G1730	G1592					G1022	G1022	C925
												G2163	G2102	G1991	A1871	G1731	G1593					G1024	G1024	G932
												G2164	G2103	U1993	A1872		G1594					G1025	G1025	A933
												G2165	C2104	U1994	A1873	G1743	G1595					U1026	U1026	G938
												G2166	G2105	U1995	G1878		G1596					A1027	A1027	
												G2167	G2106	C2006	C1882	C1754	G1597					G1031	G1031	A941
												G2168	G2107	G2007	G1883	A1755	A1598					U1032	U1032	A945
												G2169	G2108	A1884	G1884	G1756	C1599					U1033	U1033	A946
												A2170	G2109	A1885	G1885	G1757	C1599							
												G2173	G2110	G2010	A1603	G1758	A1603					U1045	U1045	G952
												G2174	G2111	G2011	A1607	A1759	A1607					A1046	A1046	A953
												G2175	G2112	G2012	C1607		A1496					G1047	G1047	
												A2176	G2113	A2020	A1608	G1762	A1497					A1050	A1050	G956
												G2180	U2113	G2021	A1609	G1763	U1497					U1051	U1051	A957
												G2181	G2114	U2022	A1610	G1764						G1056	G1056	A959
												G2182	G2115	G2023	G1903							A1057	A1057	C961
												G2183	G2116	G2030	G1906	A1773						G1058	G1058	C964
												G2184	U2117	A2030	C1617							G1059	G1059	
												G2185	U2118	A2031	A1618	A1784						U1060	U1060	C967
												G2186	A2119	A2032	A1619	U1779						U1061	U1061	
												G2187	G2120	G2032	A1622	A1780						G1062	G1062	G974
												G2188	G2121	G2033	G1622							G1063	G1063	C974A
												G2189	U2122	A2042	A1637	A1783						G1064	G1064	
												G2190	G2123	G2037	C1638	A1784						U1065	U1065	A980
												G2191	G2124	G2038	U1639							U1066	U1066	A983
												G2192	G2125	C2039	C1640	A1787						G1067	G1067	
												G2193	A2126	G2042	G1645	A1790						G1068	G1068	
												G2194	G2127	C2043	G1646	G1791						U1069	U1069	G987
												G2195	G2128	G2051	C1647	A1792						G1070	G1070	A988
												G2196	U2130	G2052	C1648	G1793						G1071	G1071	G989
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												G2198	U2132	G2053	C1653	U1797						A1073	A1073	
												G2199	G2133	C2055	A1936	U1798						U1074	U1074	G993
												G2200	A2134	G2056	A1937	U1799						U1075	U1075	C994
												G2201	G2135	A2059	U1938	G1799						U1076	U1076	G996
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												G2207	C2141	C2065	U1954	G1816						U1085	U1085	C1006
												G2208	G2142	G2066	A1960	G1817						G1086	G1086	A1009
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												G2211	C2145	G2069	G1963	A1819						G1091	G1091	U1012
												G2212	U2146	G2070	G1964							G1092	G1092	C1013
												G2213	G2147	A2071	C1965	G1823						U1094	U1094	U1014
												G2214		G2072	U1966	G1824						A1095	A1095	G1015
												G2215	G2151	U2074	A1967	U1833						A1096	A1096	C1018
												G2216	G2152	U2075	G1968	U1834								
												G2217	G2153	U2076	U1969	G1835								
												G2218	G2154	U2086	A1970	G1835								
												G2219	G2155	G2087	A1971									
												G2220	G2156	G2093	A1972	A1847								
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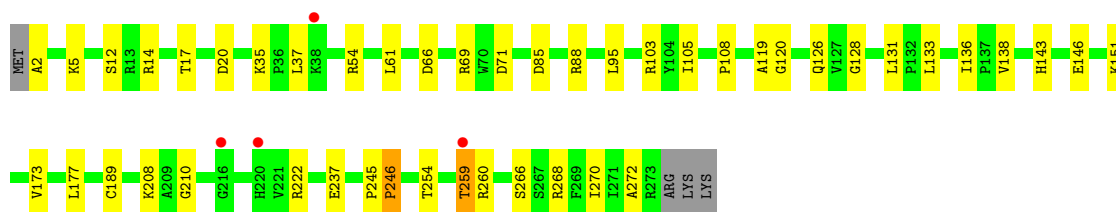
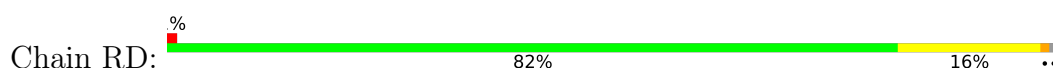
• Molecule 2: 5S rRNA



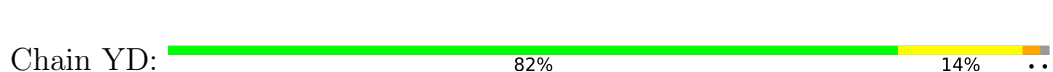
• Molecule 2: 5S rRNA

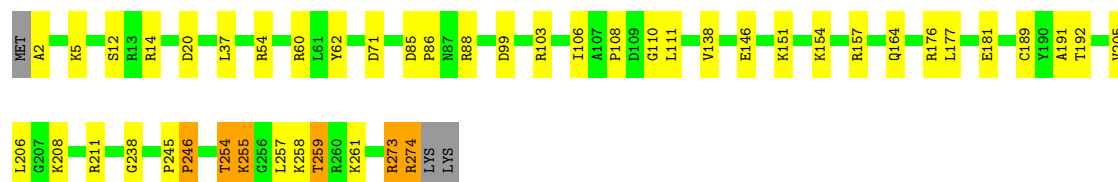


• Molecule 3: 50S ribosomal protein L2



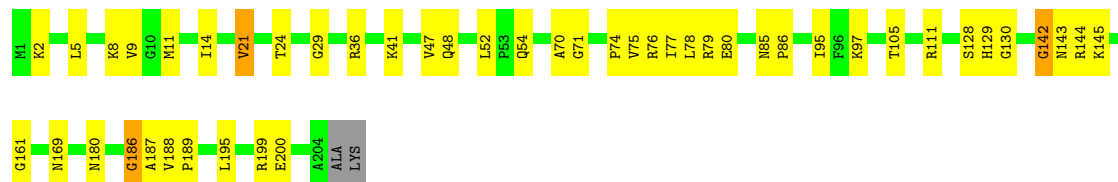
• Molecule 3: 50S ribosomal protein L2





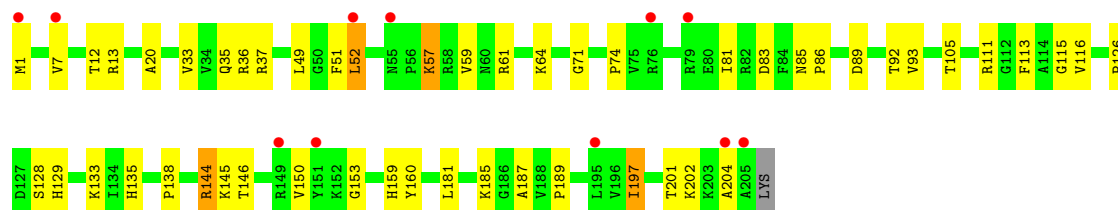
- Molecule 4: 50S ribosomal protein L3

Chain RE: 76% 21% ..



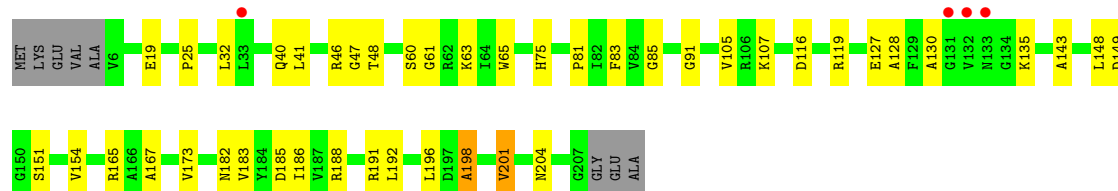
- Molecule 4: 50S ribosomal protein L3

Chain YE: 5% 75% 23% .



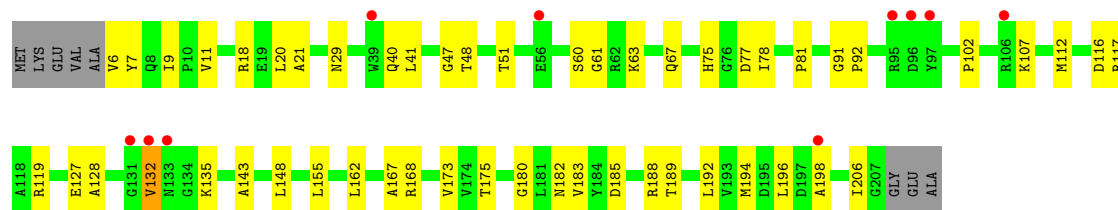
- Molecule 5: 50S ribosomal protein L4

Chain RF: 2% 75% 20% . .

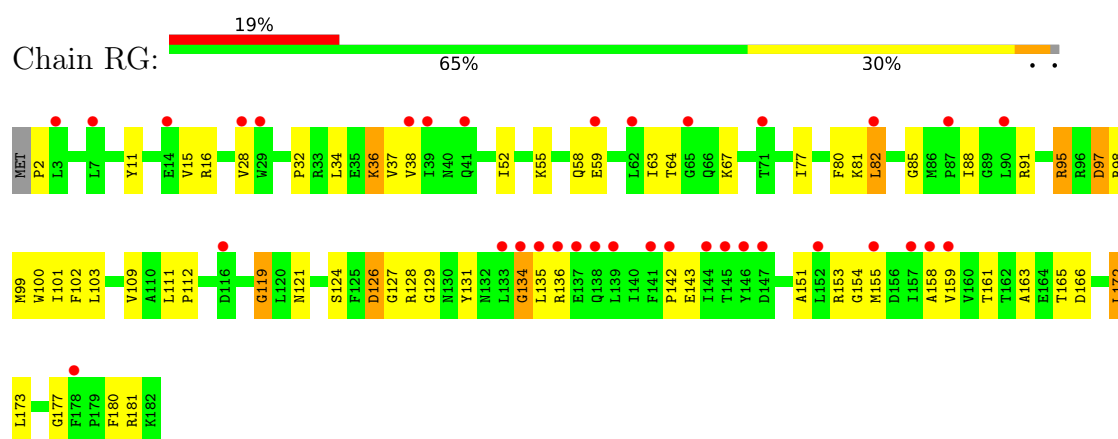


- Molecule 5: 50S ribosomal protein L4

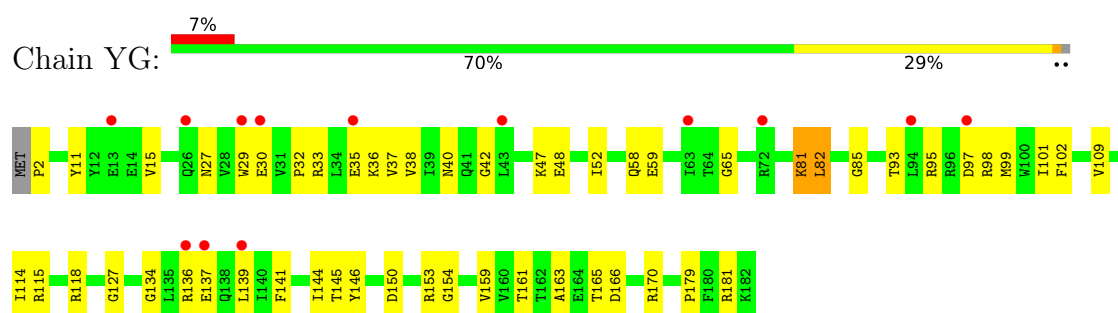
Chain YF: 5% 71% 24% .



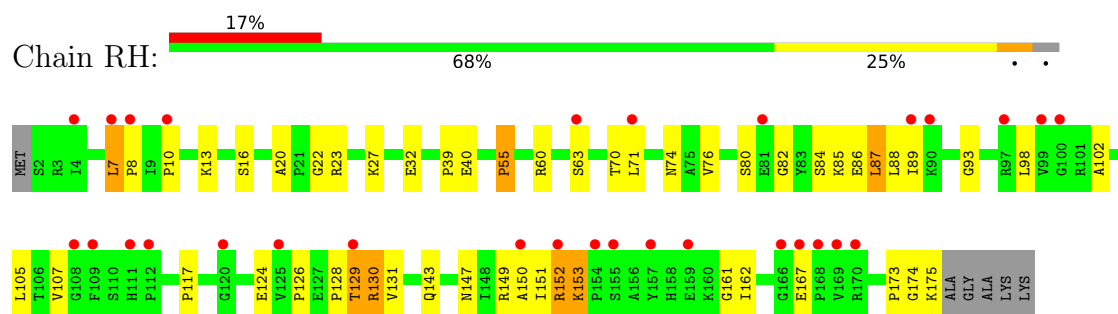
- Molecule 6: 50S ribosomal protein L5



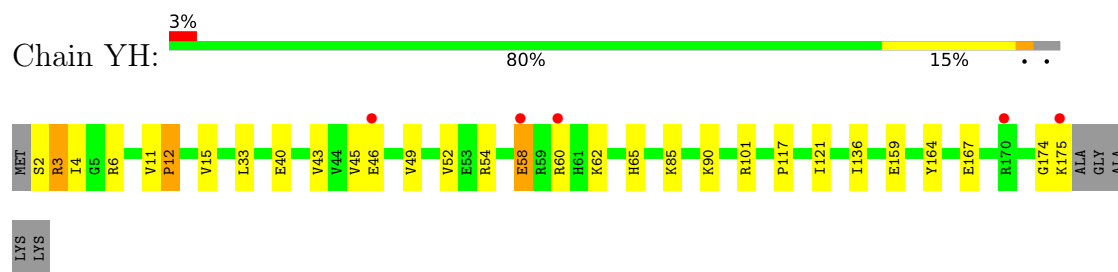
- Molecule 6: 50S ribosomal protein L5



- Molecule 7: 50S ribosomal protein L6

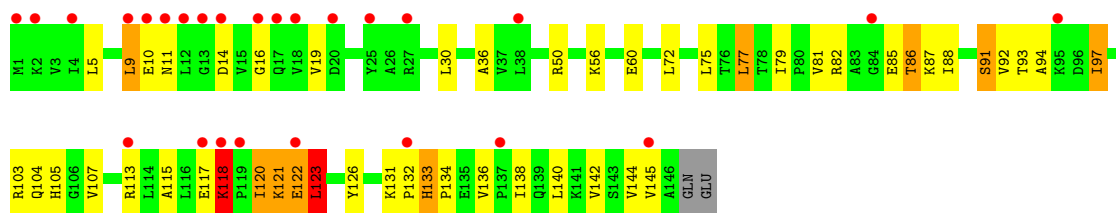


- Molecule 7: 50S ribosomal protein L6

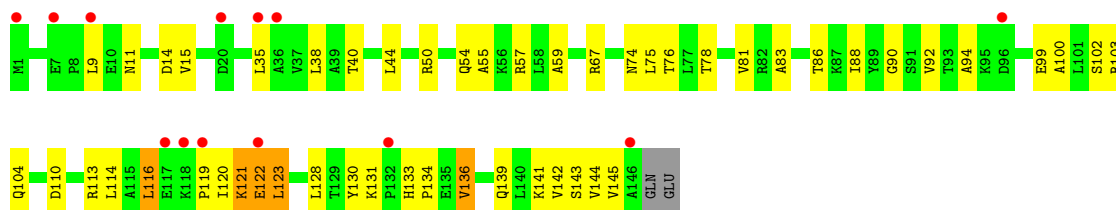


- Molecule 8: 50S ribosomal protein L9

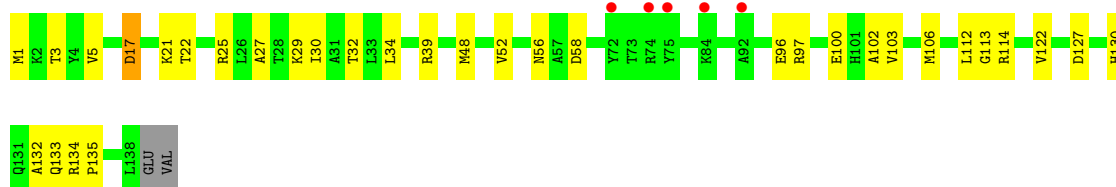
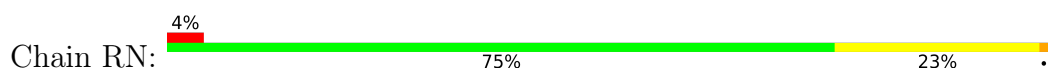




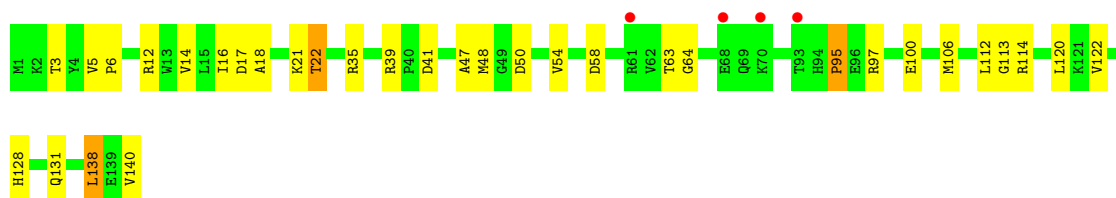
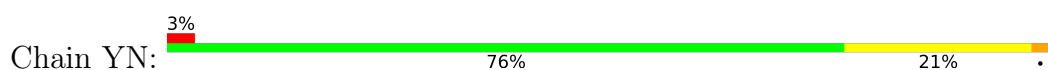
• Molecule 8: 50S ribosomal protein L9



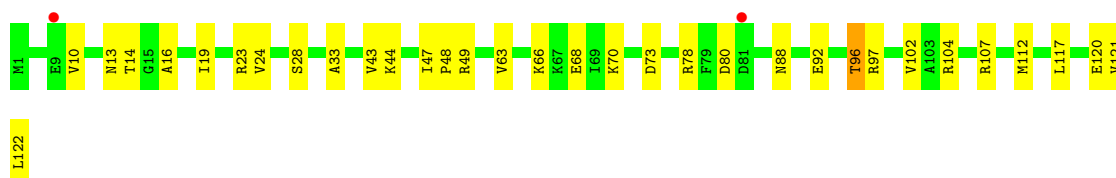
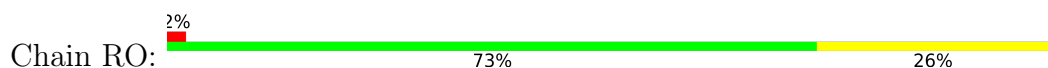
• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L14



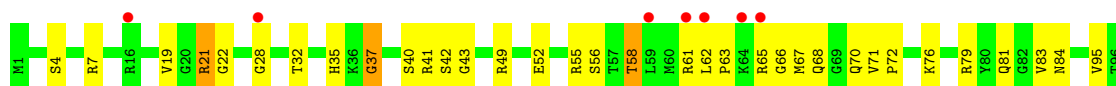
• Molecule 10: 50S ribosomal protein L14

Chain YO:  80% 20% .



• Molecule 11: 50S ribosomal protein L15

Chain RP:  7% 64% 32% . .



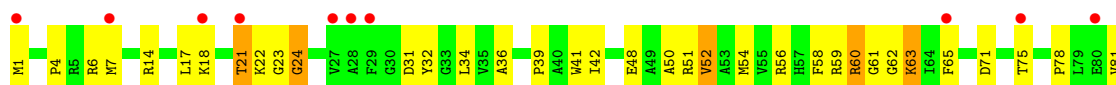
• Molecule 11: 50S ribosomal protein L15

Chain YP:  2% 71% 25% . .



• Molecule 12: 50S ribosomal protein L16

Chain RQ:  14% 62% 33% 5%



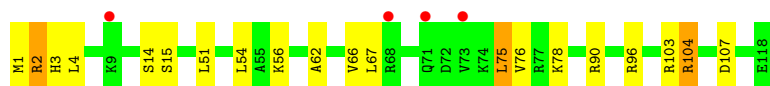
• Molecule 12: 50S ribosomal protein L16

Chain YQ:  5% 82% 16% .

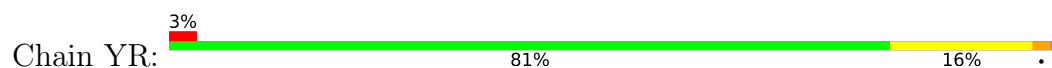


• Molecule 13: 50S ribosomal protein L17

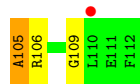
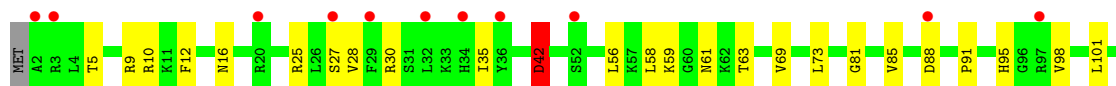
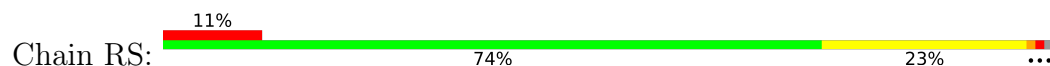
Chain RR:  3% 83% 14% .



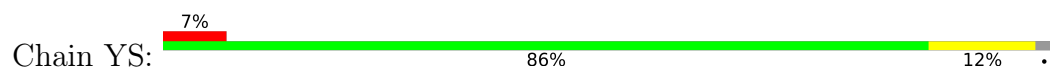
- Molecule 13: 50S ribosomal protein L17



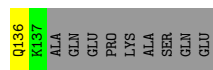
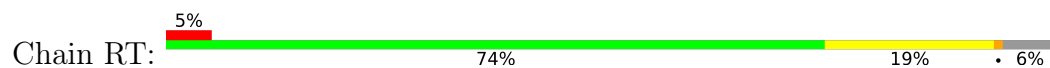
- Molecule 14: 50S ribosomal protein L18



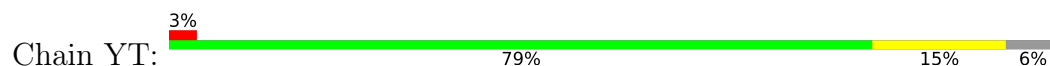
- Molecule 14: 50S ribosomal protein L18



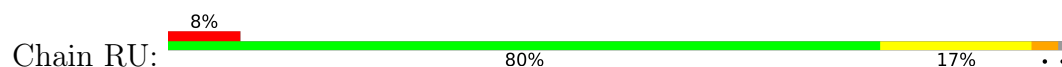
- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19

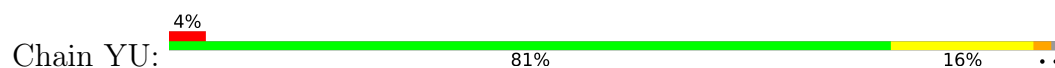


- Molecule 16: 50S ribosomal protein L20

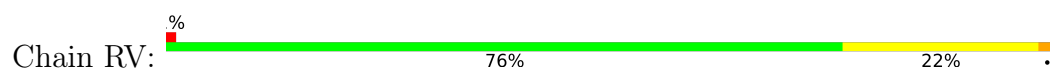




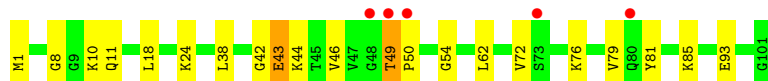
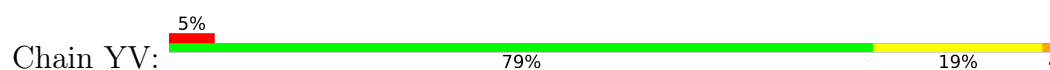
- Molecule 16: 50S ribosomal protein L20



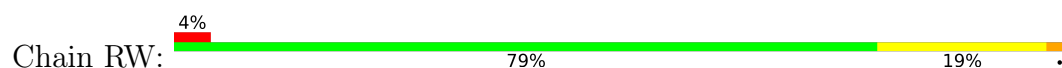
- Molecule 17: 50S ribosomal protein L21



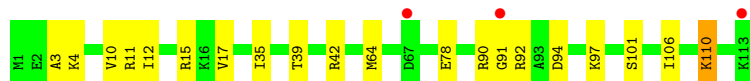
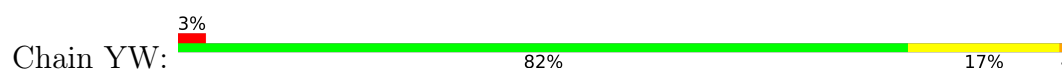
- Molecule 17: 50S ribosomal protein L21



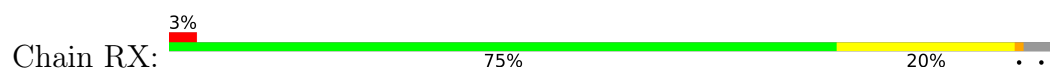
- Molecule 18: 50S ribosomal protein L22



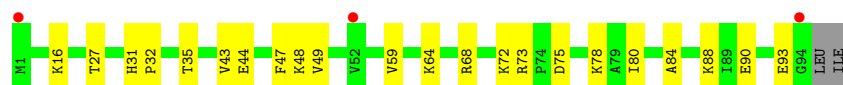
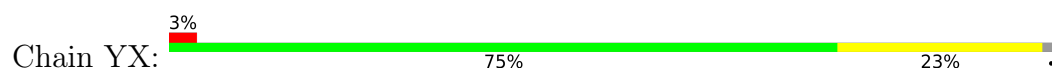
- Molecule 18: 50S ribosomal protein L22



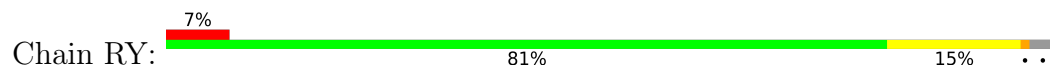
- Molecule 19: 50S ribosomal protein L23



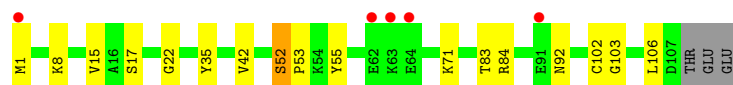
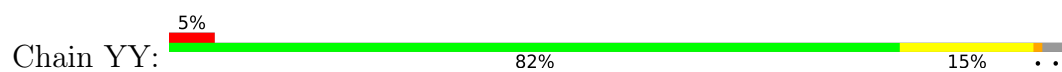
- Molecule 19: 50S ribosomal protein L23



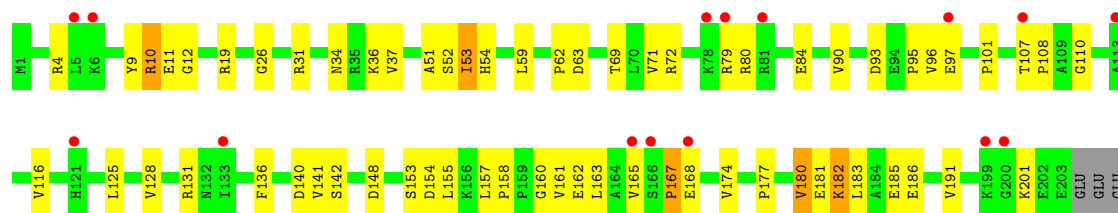
- Molecule 20: 50S ribosomal protein L24



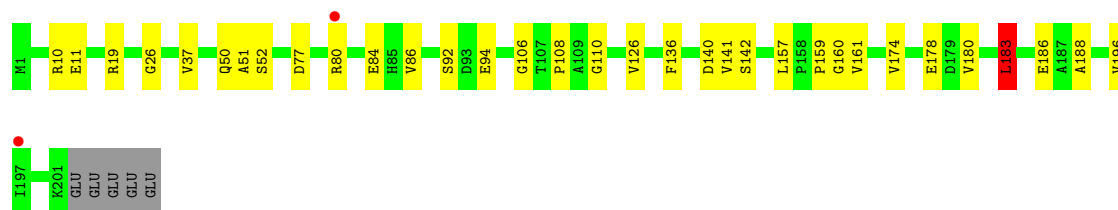
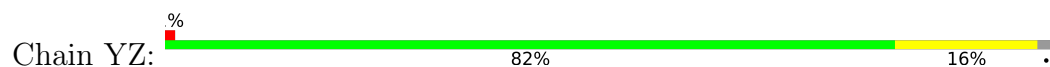
- Molecule 20: 50S ribosomal protein L24



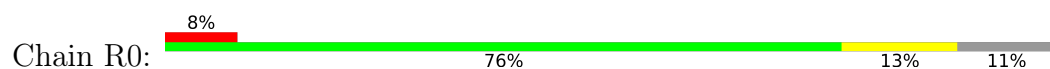
- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25



- Molecule 22: 50S ribosomal protein L27



- | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|
| MET | ALA | HIS | LYS | LYS | GLY | LEU | GLY | S9 | T10 | R11 | R14 | D15 | S16 | Q17 | A18 | K19 | R20 | Y26 | E27 | G28 | Q29 | R39 | G42 | T43 | R44 | F57 | D64 | E68 | R74 | H80 | P83 | LEU | ALA |
|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|

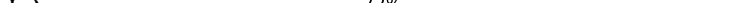
-
- | Disease | Number of Cases |
|---------|-----------------|
| MET | 10 |
| S2 | 10 |
| R11 | 10 |
| R21 | 10 |
| V30 | 10 |
| L46 | 10 |
| Q47 | 10 |
| R50 | 10 |
| V53 | 10 |
| A54 | 10 |
| I58 | 10 |
| S65 | 10 |
| H66 | 10 |
| A77 | 10 |
| K78 | 10 |
| G79 | 10 |
| L80 | 10 |
| K81 | 10 |
| L82 | 10 |
| E83 | 10 |
| G84 | 10 |
| L85 | 10 |
| S86 | 10 |
| P87 | 10 |
| I90 | 10 |
| K91 | 10 |
| K96 | 10 |
| L97 | 10 |
| I98 | 10 |

- | MET |
|-----|
| S2 |
| R11 |
| S17 |
| R26 |
| V30 |
| K39 |
| R40 |
| Y43 |
| V49 |
| R50 |
| V51 |
| R52 |
| T59 |
| F60 |
| V70 |
| E75 |
| K78 |
| L82 |
| E83 |
| G84 |
| L85 |
| S86 |
| E89 |
| L94 |
| LEU |
| LYS |
| LEU |
| LEU |

-
- | Category | Count |
|----------|-------|
| MET | 1 |
| LYS | 1 |
| LEU | 1 |
| S4 | 1 |
| R7 | 1 |
| K8 | 1 |
| Q9 | 1 |
| L10 | 1 |
| E11 | 1 |
| R14 | 1 |
| K15 | 1 |
| P18 | 1 |
| L21 | 1 |
| M33 | 1 |
| Q38 | 1 |
| I41 | 1 |
| G42 | 1 |
| Q43 | 1 |
| L44 | 1 |
| S45 | 1 |
| Q46 | 1 |
| N47 | 1 |
| D52 | 1 |
| R69 | 1 |
| Q70 | 1 |
| N71 | 1 |
| A72 | 1 |

-

-

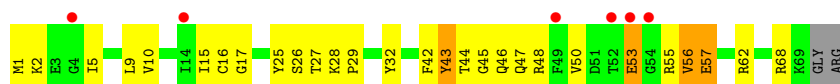
- Chain Y3:  72% 23% .



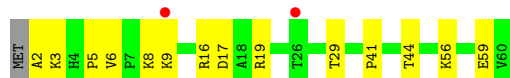
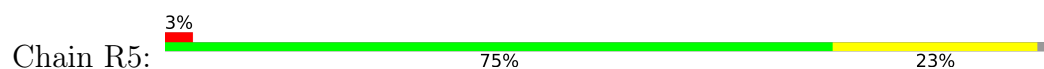
- Molecule 26: 50S ribosomal protein L31



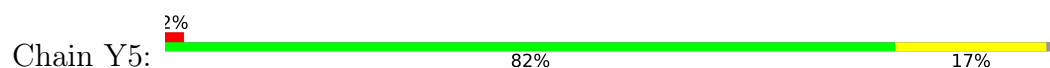
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



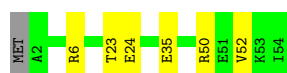
- Molecule 27: 50S ribosomal protein L32



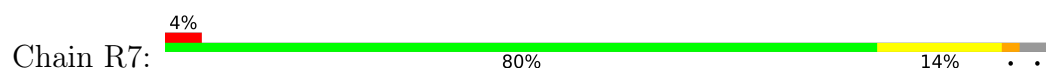
- Molecule 28: 50S ribosomal protein L33



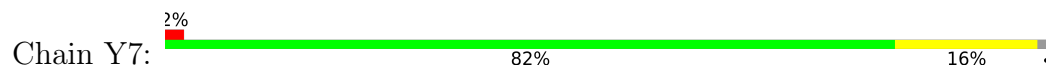
- Molecule 28: 50S ribosomal protein L33



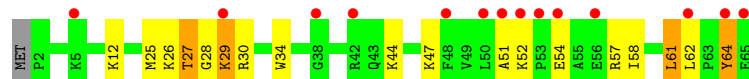
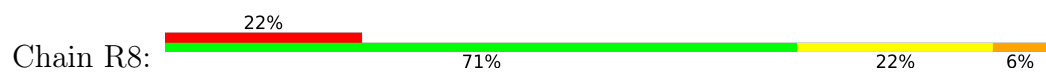
- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



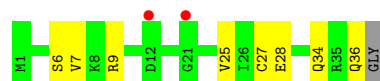
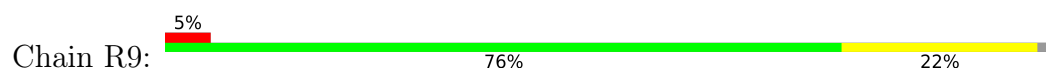
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



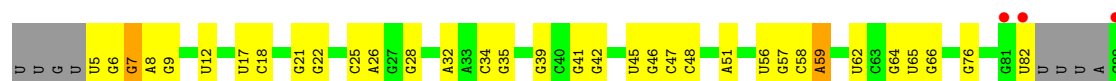
- Molecule 31: 50S ribosomal protein L36

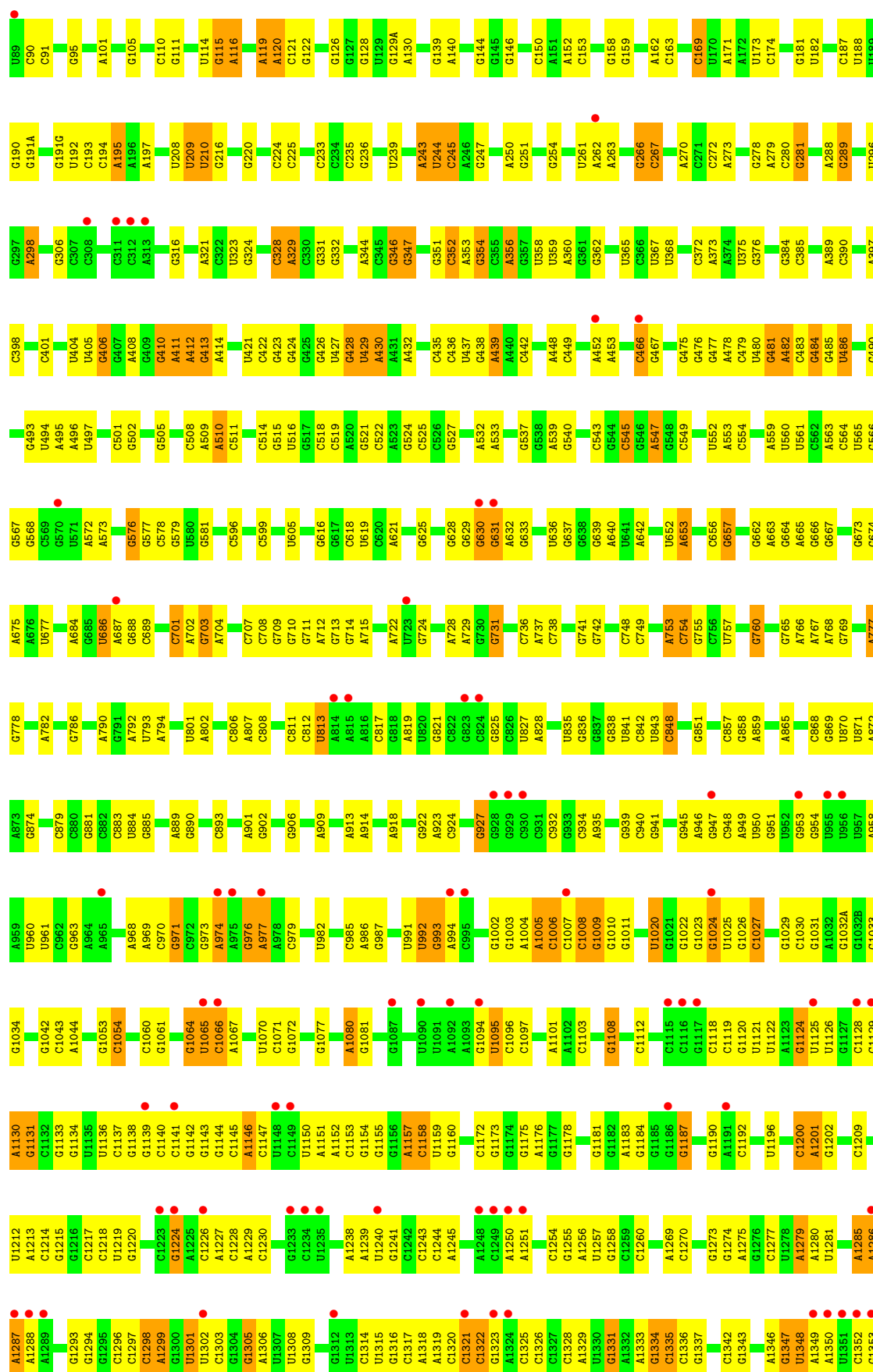


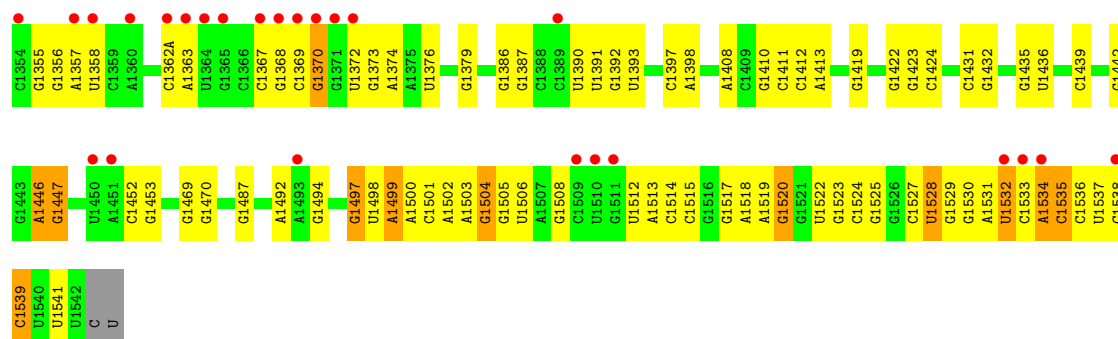
- Molecule 31: 50S ribosomal protein L36



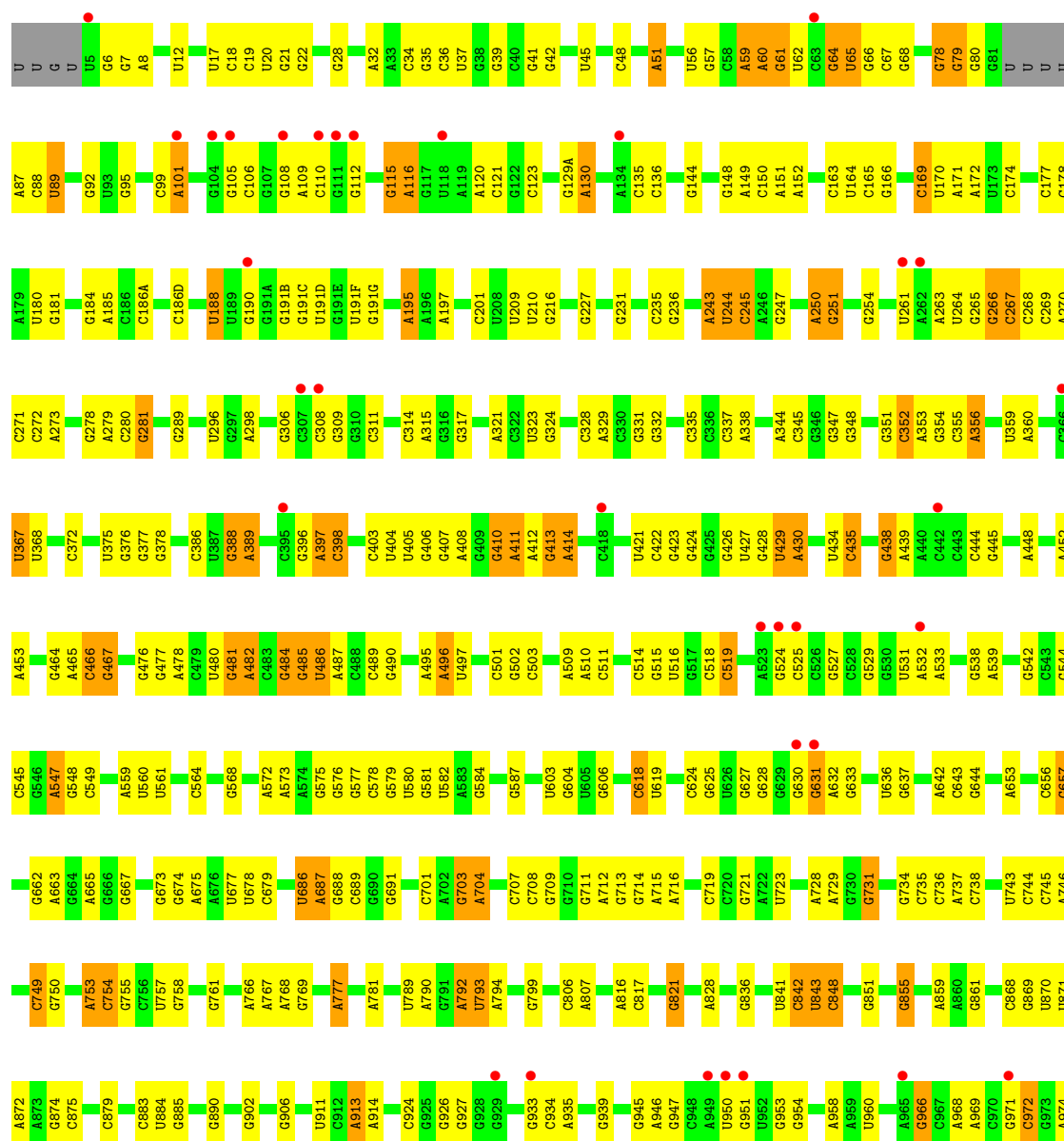
- Molecule 32: 16S rRNA

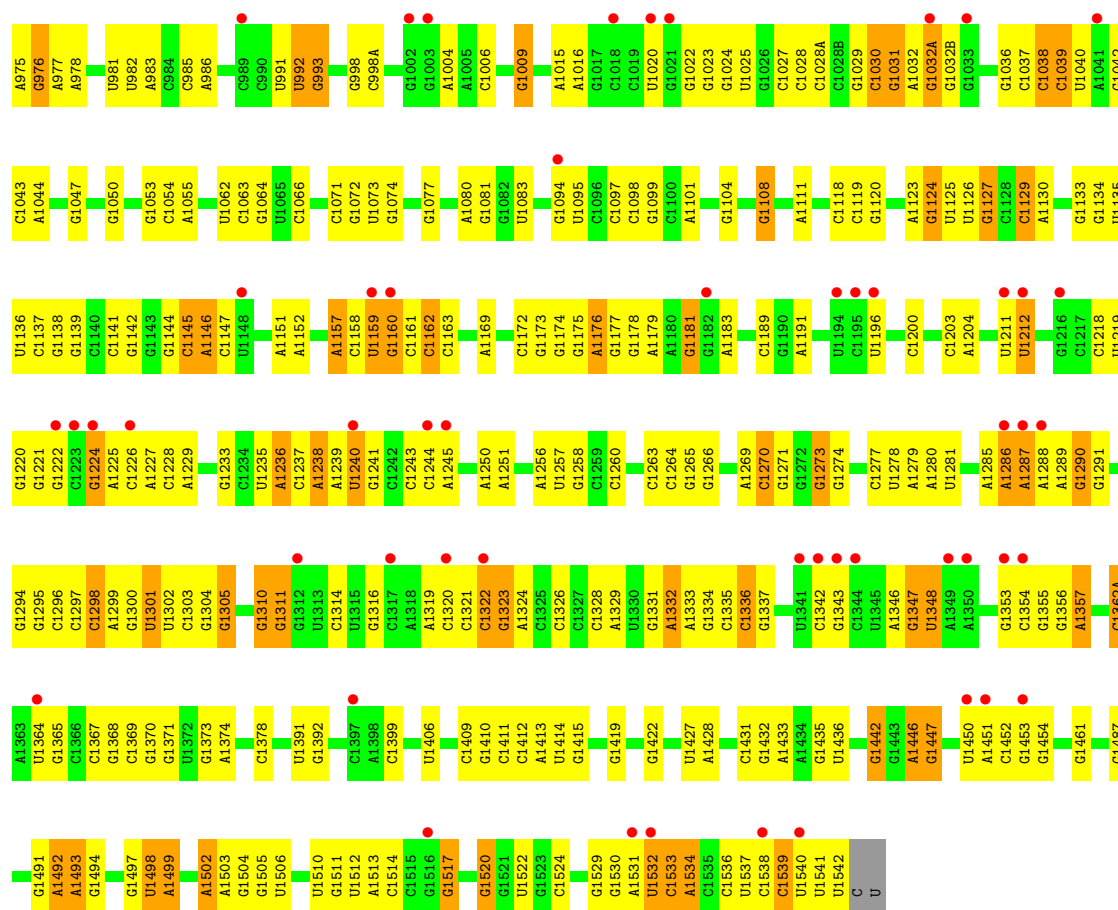


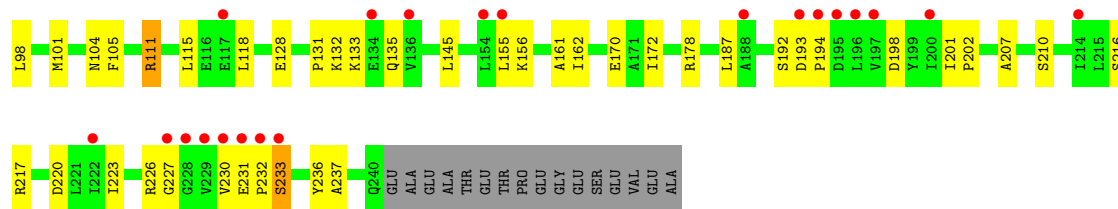




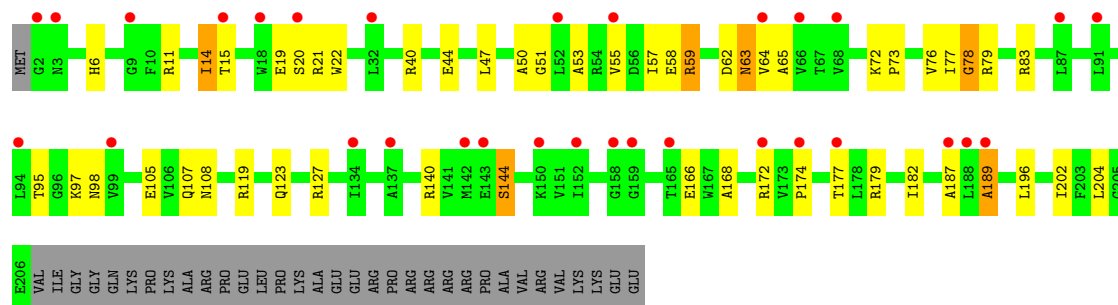
• Molecule 32: 16S rRNA



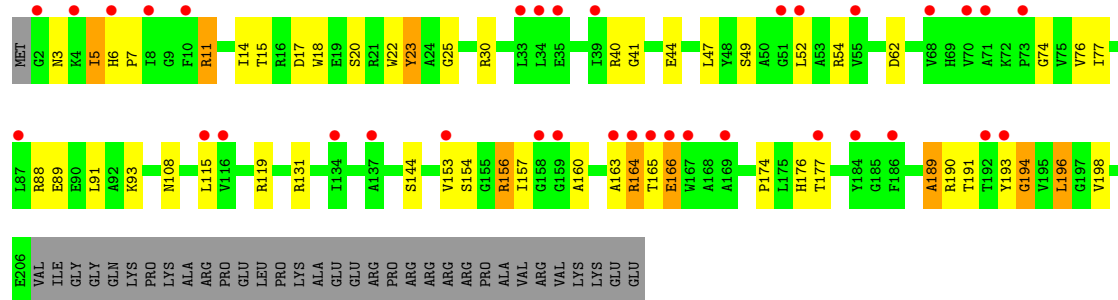




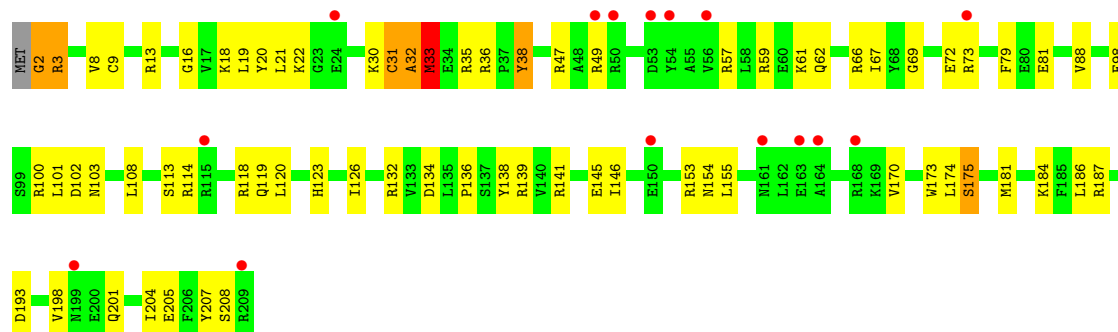
• Molecule 34: 30S ribosomal protein S3



• Molecule 34: 30S ribosomal protein S3

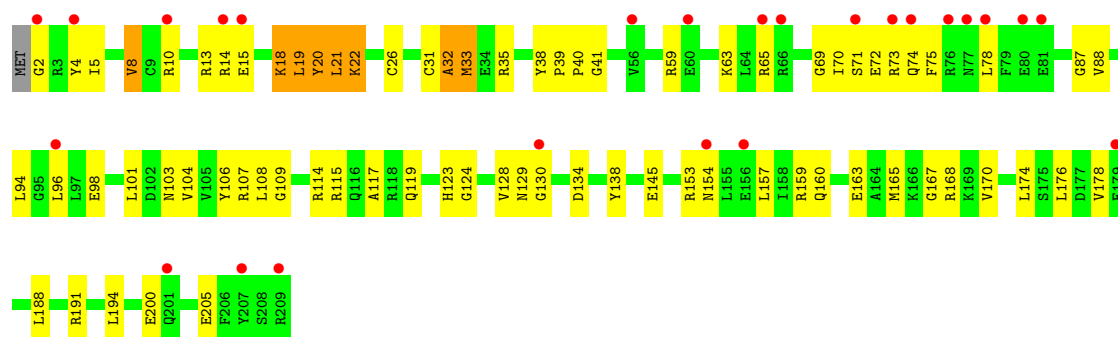


• Molecule 35: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S4

Chain XD: 



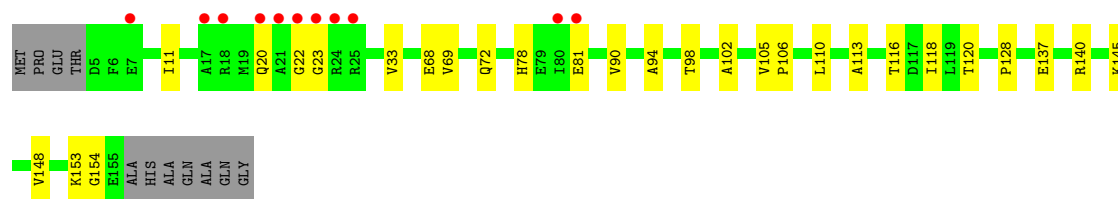
- Molecule 36: 30S ribosomal protein S5

Chain QE: 



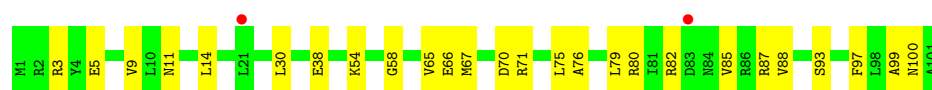
- Molecule 36: 30S ribosomal protein S5

Chain XE: 



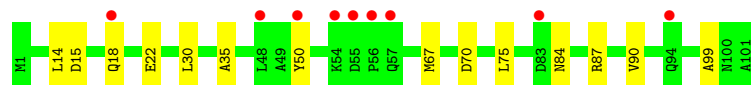
- Molecule 37: 30S ribosomal protein S6

Chain QF: 

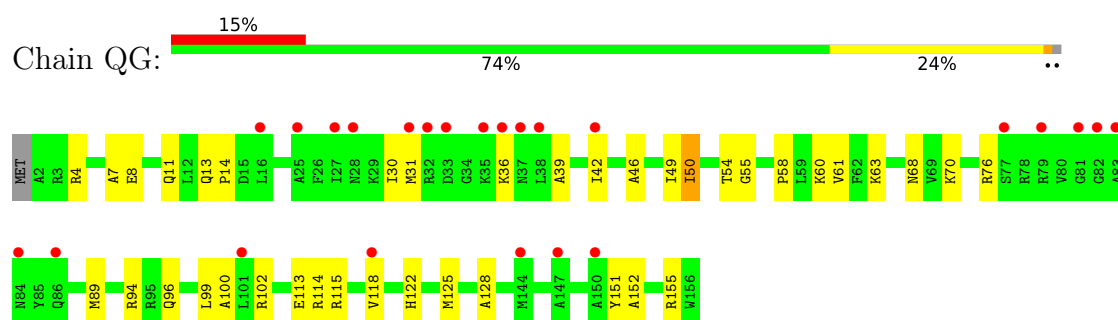


- Molecule 37: 30S ribosomal protein S6

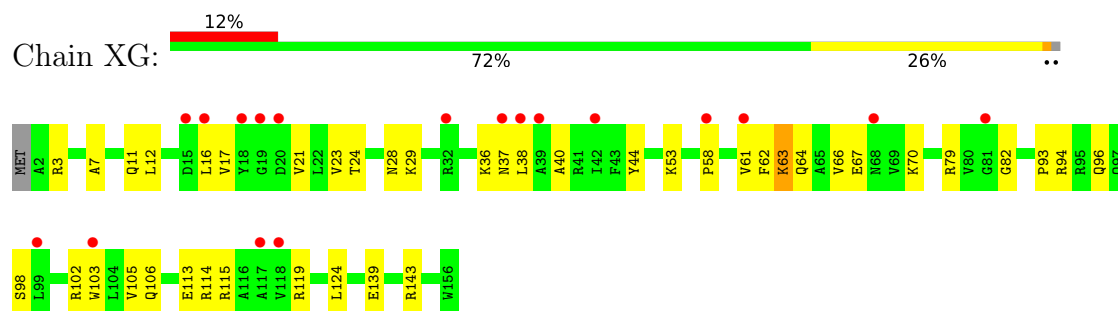
Chain XF: 



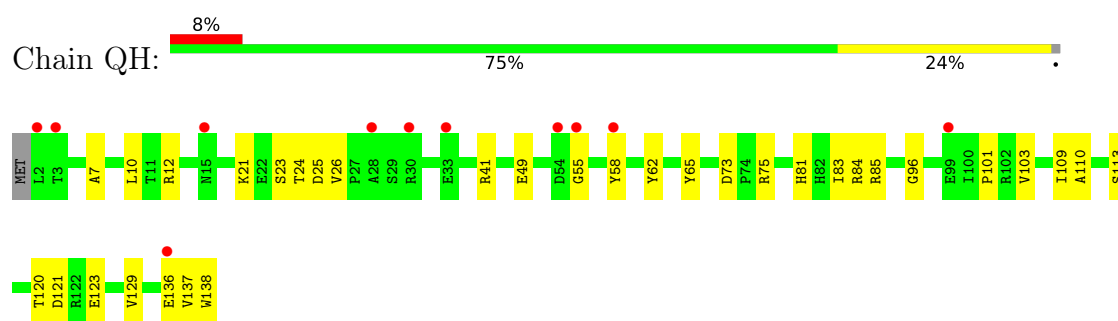
- Molecule 38: 30S ribosomal protein S7



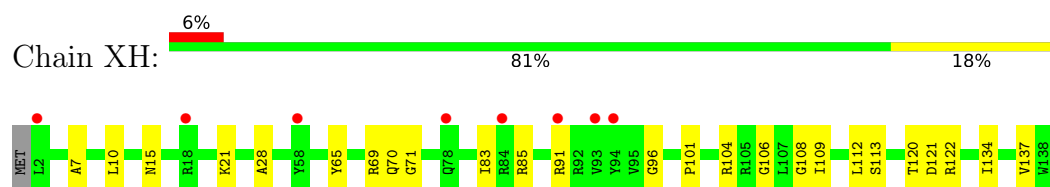
- Molecule 38: 30S ribosomal protein S7



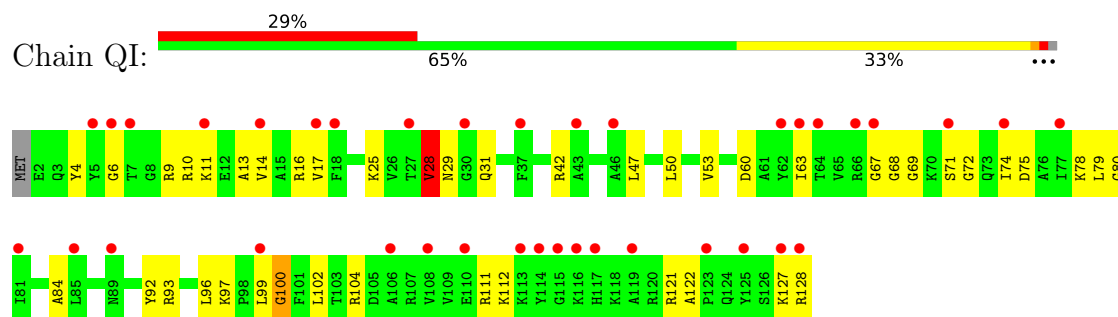
- Molecule 39: 30S ribosomal protein S8



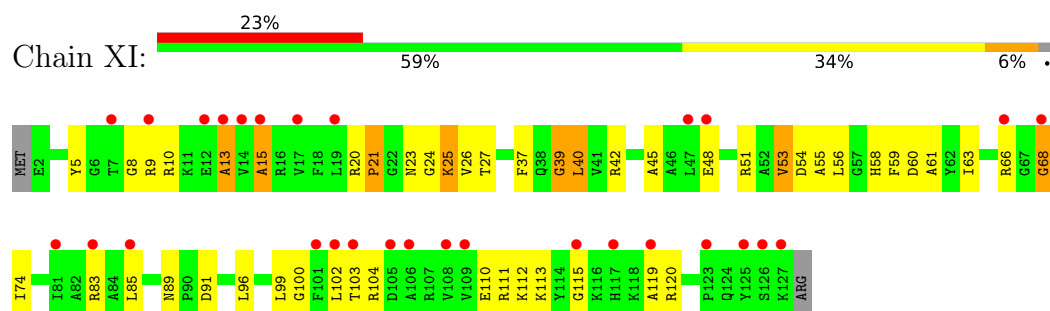
- Molecule 39: 30S ribosomal protein S8



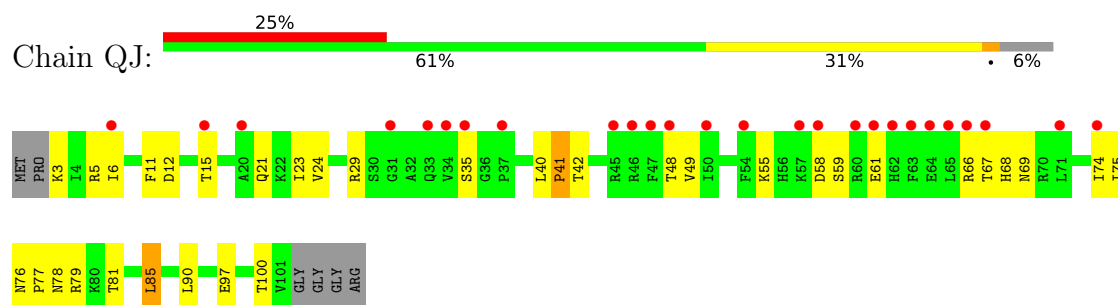
- Molecule 40: 30S ribosomal protein S9



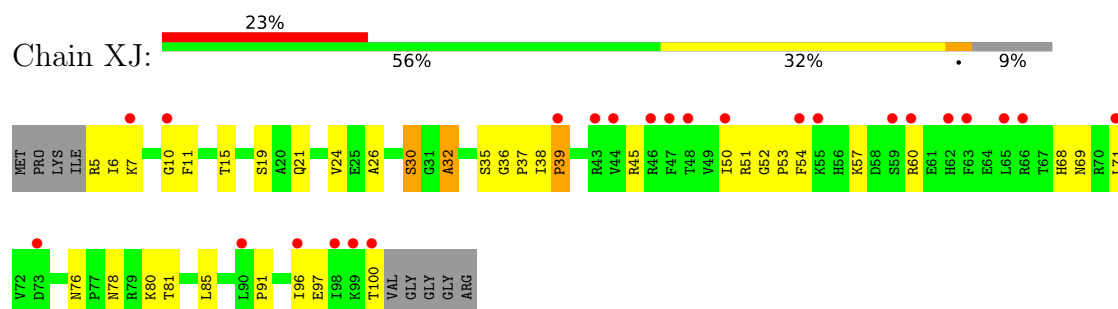
- Molecule 40: 30S ribosomal protein S9



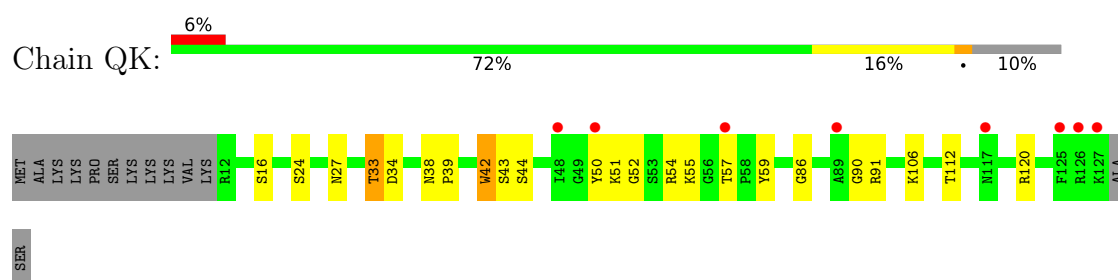
- Molecule 41: 30S ribosomal protein S10



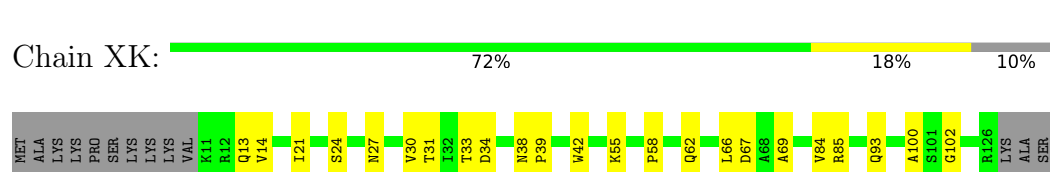
- Molecule 41: 30S ribosomal protein S10



- Molecule 42: 30S ribosomal protein S11

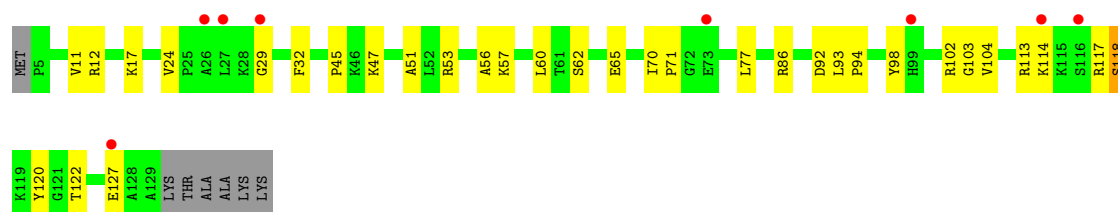


- Molecule 42: 30S ribosomal protein S11



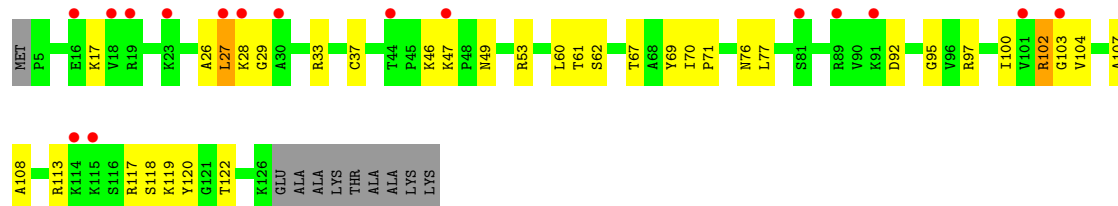
- Molecule 43: 30S ribosomal protein S12

Chain QL: 



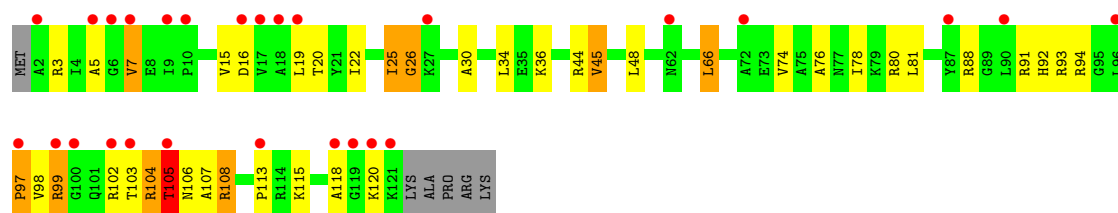
- Molecule 43: 30S ribosomal protein S12

Chain XL: 



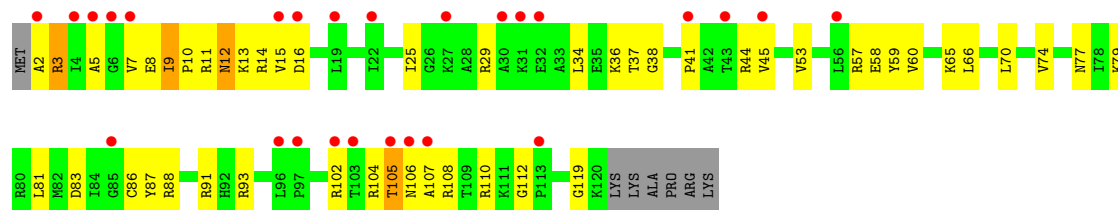
- Molecule 44: 30S ribosomal protein S13

Chain QM: 



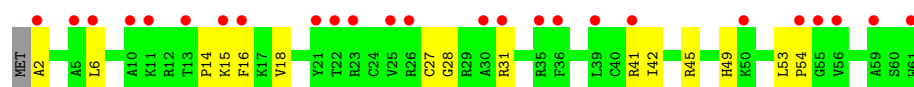
- Molecule 44: 30S ribosomal protein S13

Chain XM: 

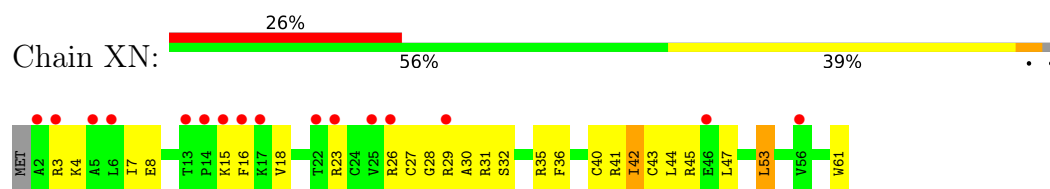


- Molecule 45: 30S ribosomal protein S14 type Z

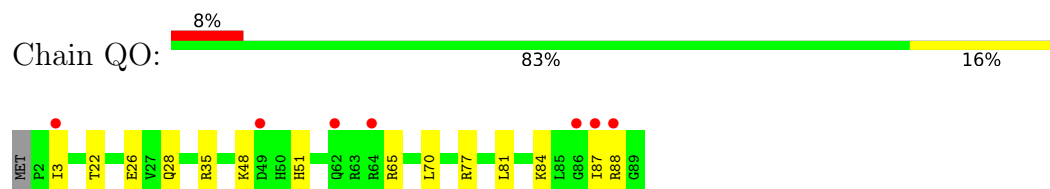
Chain QN: 



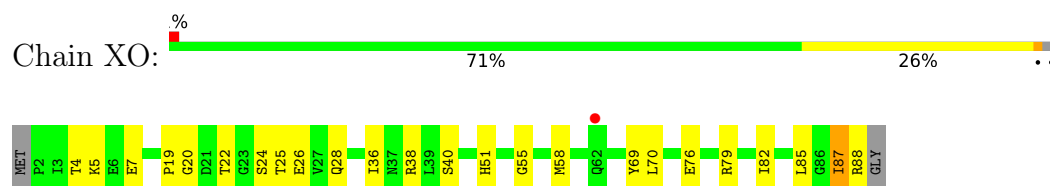
- Molecule 45: 30S ribosomal protein S14 type Z



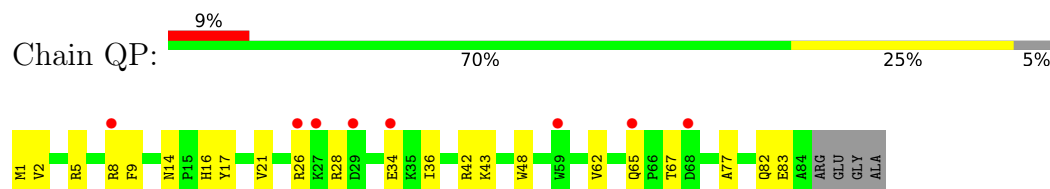
- Molecule 46: 30S ribosomal protein S15



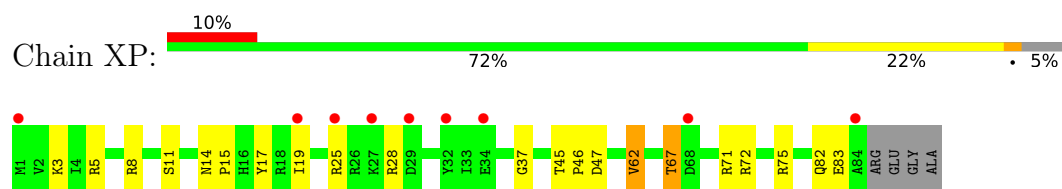
- Molecule 46: 30S ribosomal protein S15



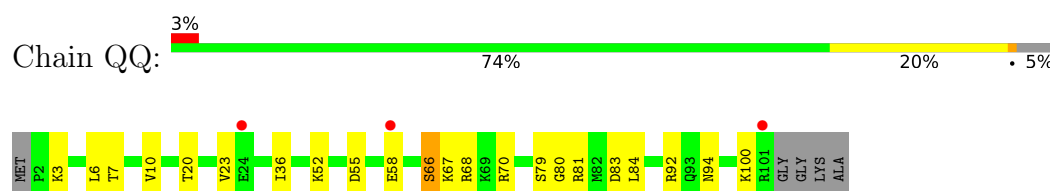
- Molecule 47: 30S ribosomal protein S16



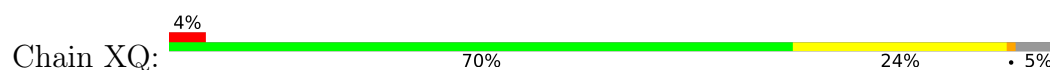
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17





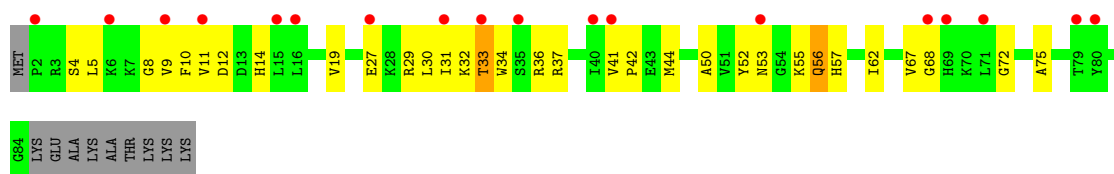
- Molecule 49: 30S ribosomal protein S18



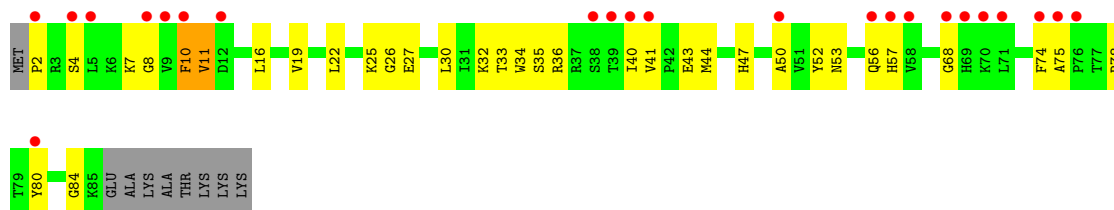
- Molecule 49: 30S ribosomal protein S18



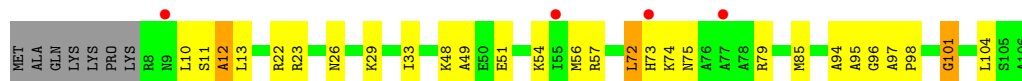
- Molecule 50: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S19

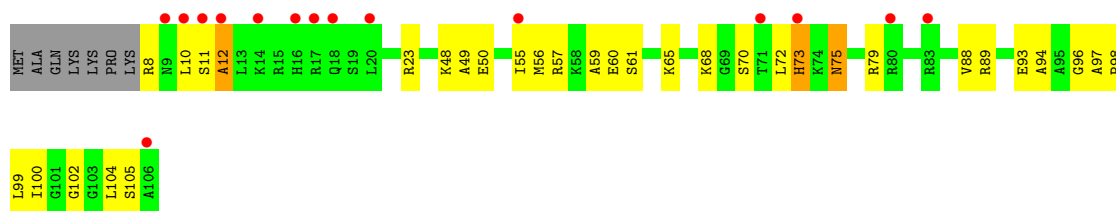


- Molecule 51: 30S ribosomal protein S20

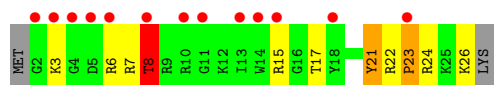


- Molecule 51: 30S ribosomal protein S20

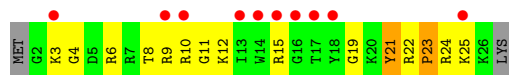




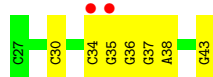
- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



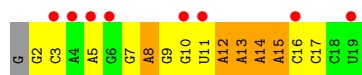
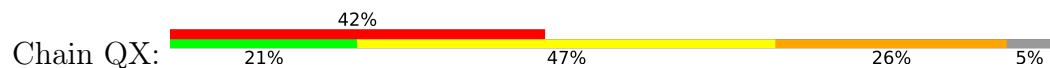
- Molecule 53: P-site ASLPro



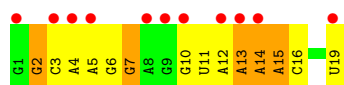
- Molecule 53: P-site ASLPro



- Molecule 54: mRNA



- Molecule 54: mRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.12Å 451.80Å 622.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	188.68 – 3.40 188.68 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (188.68-3.40) 98.8 (188.68-3.40)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.198 , 0.237 0.200 , 0.238	Depositor DCC
R_{free} test set	36729 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	79.0	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 149.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	290035	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: ZN, 1MG, SF4, MG

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	RA	0.46	0/69498	0.43	1/108491 (0.0%)
1	YA	0.56	0/69543	0.48	3/108563 (0.0%)
2	RB	0.34	0/2878	0.40	0/4490
2	YB	0.48	0/2878	0.47	0/4490
3	RD	0.66	0/2165	0.61	1/2919 (0.0%)
3	YD	0.79	0/2176	0.66	0/2933
4	RE	0.62	0/1596	0.63	0/2153
4	YE	0.75	0/1601	0.78	1/2160 (0.0%)
5	RF	0.59	0/1620	0.60	0/2194
5	YF	0.73	0/1620	0.66	0/2194
6	RG	0.33	0/1499	0.69	0/2016
6	YG	0.43	0/1499	0.67	0/2016
7	RH	0.39	0/1362	0.62	0/1841
7	YH	0.59	0/1362	0.59	0/1841
8	RI	0.56	0/1151	0.88	3/1558 (0.2%)
8	YI	0.46	0/1151	0.71	0/1558
9	RN	0.57	0/1131	0.60	0/1525
9	YN	0.72	0/1148	0.64	0/1547
10	RO	0.66	1/943 (0.1%)	0.57	0/1269
10	YO	0.76	2/943 (0.2%)	0.62	0/1269
11	RP	0.57	0/1147	0.73	0/1525
11	YP	0.74	0/1139	0.74	0/1514
12	RQ	0.55	0/1143	0.75	2/1527 (0.1%)
12	YQ	0.70	0/1143	0.63	0/1527
13	RR	0.62	0/982	0.70	0/1312
13	YR	0.74	0/974	0.74	1/1302 (0.1%)
14	RS	0.41	0/892	0.70	2/1187 (0.2%)
14	YS	0.58	0/887	0.58	0/1180
15	RT	0.56	0/1155	0.67	0/1542
15	YT	0.64	0/1155	0.59	0/1542
16	RU	0.59	0/982	0.63	0/1306
16	YU	0.78	0/982	0.68	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	RV	0.49	0/790	0.56	0/1057
17	YV	0.74	0/790	0.67	2/1057 (0.2%)
18	RW	0.63	0/911	0.57	0/1220
18	YW	0.77	0/911	0.66	1/1220 (0.1%)
19	RX	0.57	0/739	0.60	0/993
19	YX	0.71	0/756	0.66	0/1014
20	RY	0.48	0/831	0.52	0/1108
20	YY	0.64	0/831	0.58	2/1108 (0.2%)
21	RZ	0.44	0/1634	0.76	2/2216 (0.1%)
21	YZ	0.54	0/1620	0.59	0/2197
22	R0	0.54	0/611	0.58	0/814
22	Y0	0.72	0/607	0.62	0/809
23	R1	0.60	0/770	0.63	0/1022
23	Y1	0.69	0/736	0.57	0/978
24	R2	0.44	0/583	0.53	0/771
24	Y2	0.62	0/608	0.52	0/803
25	R3	0.53	0/474	0.56	0/635
25	Y3	0.71	0/474	0.70	1/635 (0.2%)
26	R4	0.30	0/578	0.65	0/776
26	Y4	0.34	0/578	0.80	0/776
27	R5	0.67	0/473	0.61	0/639
27	Y5	0.75	0/473	0.70	0/639
28	R6	0.50	0/460	0.53	0/613
28	Y6	0.64	0/460	0.56	0/613
29	R7	0.72	0/417	0.60	0/550
29	Y7	0.88	1/426 (0.2%)	0.63	0/561
30	R8	0.61	0/525	0.77	0/691
30	Y8	0.74	0/525	0.70	0/691
31	R9	0.47	0/305	0.48	0/402
31	Y9	0.67	0/310	0.48	0/407
32	QA	0.34	0/36343	0.39	0/56720
32	XA	0.35	0/36346	0.40	0/56725
33	QB	0.37	0/1942	0.67	2/2619 (0.1%)
33	XB	0.36	0/1950	0.66	0/2630
34	QC	0.30	0/1629	0.63	0/2195
34	XC	0.30	0/1629	0.62	0/2195
35	QD	0.50	0/1733	0.65	0/2318
35	XD	0.46	0/1733	0.67	0/2318
36	QE	0.43	0/1171	0.59	0/1576
36	XE	0.46	0/1171	0.57	0/1576
37	QF	0.43	0/856	0.59	0/1154
37	XF	0.42	0/856	0.52	0/1154
38	QG	0.27	0/1276	0.58	0/1709

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	XG	0.29	0/1276	0.58	0/1709
39	QH	0.46	0/1128	0.58	0/1517
39	XH	0.45	0/1128	0.57	0/1517
40	QI	0.27	0/1029	0.66	0/1379
40	XI	0.29	0/1017	0.63	1/1365 (0.1%)
41	QJ	0.30	0/814	0.65	0/1095
41	XJ	0.30	0/790	0.56	0/1063
42	QK	0.42	0/879	0.53	0/1187
42	XK	0.43	0/879	0.53	0/1187
43	QL	0.53	0/991	0.59	0/1327
43	XL	0.48	0/972	0.69	0/1301
44	QM	0.31	0/965	0.72	2/1292 (0.2%)
44	XM	0.38	0/956	0.75	2/1281 (0.2%)
45	QN	0.37	0/501	0.77	0/664
45	XN	0.33	0/501	0.67	0/664
46	QO	0.41	0/745	0.52	0/992
46	XO	0.45	0/740	0.52	0/987
47	QP	0.47	0/721	0.57	0/970
47	XP	0.41	0/721	0.63	0/970
48	QQ	0.47	0/847	0.54	0/1131
48	XQ	0.44	0/847	0.54	0/1131
49	QR	0.44	0/579	0.56	0/768
49	XR	0.45	0/579	0.56	0/768
50	QS	0.26	0/680	0.60	0/915
50	XS	0.27	0/689	0.72	0/926
51	QT	0.42	0/765	0.57	0/1007
51	XT	0.40	0/765	0.58	0/1007
52	QU	0.27	0/221	0.53	0/288
52	XU	0.31	0/221	0.59	0/288
53	QV	0.34	1/380 (0.3%)	0.25	0/590
53	XV	0.37	1/332 (0.3%)	0.31	0/515
54	QX	0.25	0/436	0.36	0/678
54	XX	0.22	0/462	0.37	0/719
All	All	0.49	6/313742 (0.0%)	0.50	29/468899 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	RD	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	YD	0	10
4	RE	0	10
4	YE	0	13
5	RF	0	13
5	YF	0	9
6	RG	0	17
6	YG	0	18
7	RH	0	24
7	YH	0	5
8	RI	0	13
8	YI	0	18
9	RN	0	10
9	YN	0	6
10	RO	0	2
10	YO	0	2
11	RP	0	19
11	YP	0	18
12	RQ	0	11
12	YQ	0	8
13	RR	0	6
13	YR	0	5
14	RS	0	8
14	YS	0	2
15	RT	0	6
15	YT	0	4
16	RU	0	3
16	YU	0	5
17	RV	0	8
17	YV	0	4
18	RW	0	5
18	YW	0	5
19	RX	0	5
19	YX	0	4
20	RY	0	5
20	YY	0	2
21	RZ	0	22
21	YZ	0	9
22	R0	0	2
22	Y0	0	3
23	R1	0	6
23	Y1	0	2
24	R2	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	R3	0	3
25	Y3	0	1
26	R4	0	10
26	Y4	0	12
27	R5	0	1
27	Y5	0	2
29	R7	0	2
30	R8	0	7
30	Y8	0	4
31	Y9	0	1
33	QB	0	21
33	XB	0	18
34	QC	0	14
34	XC	0	17
35	QD	0	13
35	XD	0	13
36	QE	0	5
36	XE	0	5
37	QF	0	2
37	XF	0	1
38	QG	0	9
38	XG	0	6
39	QH	0	4
39	XH	0	8
40	QI	0	11
40	XI	0	19
41	QJ	0	6
41	XJ	0	9
42	QK	0	4
42	XK	0	5
43	QL	0	8
43	XL	0	12
44	QM	0	17
44	XM	0	14
45	QN	0	6
45	XN	0	5
46	QO	0	2
46	XO	0	3
47	QP	0	6
47	XP	0	7
48	QQ	0	2
48	XQ	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
49	QR	0	4
49	XR	0	4
50	QS	0	11
50	XS	0	14
51	QT	0	13
51	XT	0	13
52	QU	0	3
52	XU	0	5
All	All	0	749

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	RO	14	THR	CA-C	-6.95	1.43	1.52
10	YO	70	LYS	C-N	-6.46	1.24	1.33
29	Y7	23	ARG	C-N	-6.24	1.20	1.33
10	YO	14	THR	CA-C	-5.74	1.44	1.52
53	XV	37	1MG	O3'-P	5.22	1.61	1.56

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	XM	12	ASN	N-CA-C	7.38	122.00	112.92
4	YE	144	ARG	N-CA-CB	7.13	116.78	109.51
8	RI	122	GLU	CA-C-N	6.87	131.55	121.31
8	RI	122	GLU	C-N-CA	6.87	131.55	121.31
13	YR	3	HIS	N-CA-C	-6.52	99.07	108.07

There are no chirality outliers.

5 of 749 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	RD	119	ALA	Peptide
3	RD	120	GLY	Peptide
3	RD	126	GLN	Peptide
3	RD	2	ALA	Peptide
3	RD	246	PRO	Peptide

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	RA	62051	0	31279	542	1
1	YA	62091	0	31300	505	0
2	RB	2573	0	1306	26	0
2	YB	2573	0	1306	17	0
3	RD	2115	0	2195	31	0
3	YD	2126	0	2208	42	0
4	RE	1563	0	1629	29	0
4	YE	1568	0	1633	31	0
5	RF	1585	0	1632	22	0
5	YF	1585	0	1632	30	0
6	RG	1474	0	1535	38	0
6	YG	1474	0	1535	27	0
7	RH	1336	0	1418	22	0
7	YH	1336	0	1418	23	1
8	RI	1136	0	1223	35	2
8	YI	1136	0	1223	22	0
9	RN	1104	0	1180	17	0
9	YN	1121	0	1195	18	0
10	RO	933	0	996	24	0
10	YO	933	0	996	15	0
11	RP	1130	0	1217	25	0
11	YP	1122	0	1206	23	0
12	RQ	1122	0	1179	51	0
12	YQ	1122	0	1179	16	0
13	RR	968	0	1033	10	0
13	YR	960	0	1021	10	0
14	RS	882	0	943	13	0
14	YS	877	0	938	9	0
15	RT	1141	0	1202	17	0
15	YT	1141	0	1202	13	0
16	RU	964	0	1022	20	0
16	YU	964	0	1022	20	0
17	RV	779	0	852	12	0
17	YV	779	0	852	18	0
18	RW	900	0	964	16	1
18	YW	900	0	964	11	0
19	RX	725	0	778	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	YX	742	0	803	9	0
20	RY	818	0	909	12	0
20	YY	818	0	909	9	2
21	RZ	1601	0	1630	43	0
21	YZ	1587	0	1622	16	0
22	R0	603	0	619	7	0
22	Y0	599	0	617	9	0
23	R1	763	0	848	10	0
23	Y1	729	0	802	12	0
24	R2	581	0	629	9	0
24	Y2	606	0	665	5	1
25	R3	469	0	518	6	0
25	Y3	469	0	518	12	0
26	R4	565	0	557	11	0
26	Y4	565	0	557	15	0
27	R5	459	0	476	11	0
27	Y5	459	0	476	7	0
28	R6	453	0	473	3	0
28	Y6	453	0	473	3	0
29	R7	409	0	454	6	0
29	Y7	418	0	467	4	0
30	R8	517	0	582	14	0
30	Y8	517	0	582	15	0
31	R9	302	0	332	6	0
31	Y9	307	0	335	10	0
32	QA	32469	0	16393	422	0
32	XA	32471	0	16393	441	2
33	QB	1907	0	1958	37	0
33	XB	1915	0	1969	29	0
34	QC	1605	0	1668	28	0
34	XC	1605	0	1668	30	0
35	QD	1703	0	1763	68	0
35	XD	1703	0	1764	52	0
36	QE	1155	0	1213	19	0
36	XE	1155	0	1213	11	0
37	QF	843	0	857	17	0
37	XF	843	0	857	15	0
38	QG	1257	0	1296	22	0
38	XG	1257	0	1296	25	0
39	QH	1108	0	1165	17	0
39	XH	1108	0	1165	12	0
40	QI	1010	0	1037	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	XI	998	0	1024	27	0
41	QJ	801	0	849	21	0
41	XJ	777	0	816	26	0
42	QK	864	0	881	15	0
42	XK	864	0	881	12	0
43	QL	975	0	1062	18	0
43	XL	956	0	1046	18	0
44	QM	955	0	1021	25	0
44	XM	946	0	1008	32	0
45	QN	492	0	529	10	0
45	XN	492	0	529	17	0
46	QO	734	0	771	11	0
46	XO	729	0	768	15	0
47	QP	705	0	725	12	0
47	XP	705	0	725	11	0
48	QQ	834	0	904	16	0
48	XQ	834	0	904	15	0
49	QR	574	0	644	9	0
49	XR	574	0	644	10	0
50	QS	665	0	686	16	0
50	XS	674	0	699	16	0
51	QT	763	0	861	14	0
51	XT	763	0	861	16	0
52	QU	217	0	234	10	0
52	XU	217	0	234	11	0
53	QV	365	0	186	5	0
53	XV	322	0	164	5	0
54	QX	389	0	197	27	0
54	XX	412	0	208	12	0
55	QA	66	0	0	0	0
55	QF	1	0	0	0	0
55	R0	1	0	0	0	0
55	R1	1	0	0	0	0
55	R5	1	0	0	0	0
55	R8	1	0	0	0	0
55	RA	485	0	0	0	0
55	RB	8	0	0	0	0
55	RE	2	0	0	0	0
55	RF	1	0	0	0	0
55	RN	1	0	0	0	0
55	RO	1	0	0	0	0
55	RP	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	RQ	2	0	0	0	0
55	RT	1	0	0	0	0
55	RX	1	0	0	0	0
55	XA	87	0	0	0	0
55	XE	1	0	0	0	0
55	XL	1	0	0	0	0
55	XQ	1	0	0	0	0
55	XS	1	0	0	0	0
55	Y0	2	0	0	0	0
55	Y1	1	0	0	0	0
55	Y5	1	0	0	0	0
55	Y7	1	0	0	0	0
55	Y8	1	0	0	0	0
55	YA	510	0	0	0	0
55	YB	7	0	0	0	0
55	YD	1	0	0	0	0
55	YE	4	0	0	0	0
55	YO	1	0	0	0	0
55	YP	2	0	0	0	0
55	YQ	1	0	0	0	0
55	YR	1	0	0	0	0
56	QN	1	0	0	0	0
56	R4	1	0	0	0	0
56	R5	1	0	0	0	0
56	R6	1	0	0	0	0
56	R9	1	0	0	0	0
56	RY	1	0	0	0	0
56	XN	1	0	0	0	0
56	Y4	1	0	0	0	0
56	Y5	1	0	0	0	0
56	Y6	1	0	0	0	0
56	Y9	1	0	0	0	0
56	YY	1	0	0	0	0
57	QD	8	0	0	1	0
57	XD	8	0	0	3	0
All	All	290035	0	197002	3194	5

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

The worst 5 of 3194 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)
32:QA:1535:C:N4	54:QX:9:G:C2	1.91	1.37
32:QA:1535:C:N4	54:QX:9:G:N2	1.78	1.30
17:YV:49:THR:OG1	17:YV:50:PRO:HD2	1.30	1.25
21:RZ:182:LYS:O	21:RZ:186:GLU:HG2	1.39	1.22
32:QA:1535:C:C4	54:QX:9:G:N2	2.07	1.22

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:307:G:O6	24:Y2:71:ASN:O[3_555]	1.47	0.73
7:YH:46:GLU:CB	20:YY:22:GLY:O[4_445]	1.82	0.38
8:RI:82:ARG:NH1	32:XA:56:U:O2'[4_555]	2.05	0.15
8:RI:91:SER:OG	32:XA:368:U:OP1[4_555]	2.07	0.13
18:RW:63:ASP:OD1	20:YY:92:ASN:ND2[3_555]	2.08	0.12

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	RD	270/276 (98%)	257 (95%)	13 (5%)	0	100	100
3	YD	271/276 (98%)	261 (96%)	10 (4%)	0	100	100
4	RE	202/206 (98%)	190 (94%)	12 (6%)	0	100	100
4	YE	203/206 (98%)	170 (84%)	32 (16%)	1 (0%)	25	54
5	RF	200/210 (95%)	191 (96%)	9 (4%)	0	100	100
5	YF	200/210 (95%)	182 (91%)	18 (9%)	0	100	100
6	RG	179/182 (98%)	153 (86%)	25 (14%)	1 (1%)	22	50
6	YG	179/182 (98%)	151 (84%)	27 (15%)	1 (1%)	22	50
7	RH	172/180 (96%)	149 (87%)	21 (12%)	2 (1%)	11	35
7	YH	172/180 (96%)	164 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	RI	144/148 (97%)	119 (83%)	24 (17%)	1 (1%)	19	47
8	YI	144/148 (97%)	122 (85%)	22 (15%)	0	100	100
9	RN	136/140 (97%)	121 (89%)	15 (11%)	0	100	100
9	YN	138/140 (99%)	125 (91%)	12 (9%)	1 (1%)	19	47
10	RO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	RP	146/150 (97%)	122 (84%)	24 (16%)	0	100	100
11	YP	145/150 (97%)	129 (89%)	15 (10%)	1 (1%)	19	47
12	RQ	139/141 (99%)	120 (86%)	18 (13%)	1 (1%)	19	47
12	YQ	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
13	RR	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
13	YR	115/118 (98%)	106 (92%)	9 (8%)	0	100	100
14	RS	109/112 (97%)	91 (84%)	18 (16%)	0	100	100
14	YS	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
15	RT	135/146 (92%)	121 (90%)	14 (10%)	0	100	100
15	YT	135/146 (92%)	127 (94%)	8 (6%)	0	100	100
16	RU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	41
16	YU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	41
17	RV	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
17	YV	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	13	39
18	RW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
18	YW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
19	RX	90/96 (94%)	85 (94%)	5 (6%)	0	100	100
19	YX	92/96 (96%)	84 (91%)	8 (9%)	0	100	100
20	RY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
20	YY	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
21	RZ	201/206 (98%)	180 (90%)	20 (10%)	1 (0%)	25	54
21	YZ	199/206 (97%)	188 (94%)	9 (4%)	2 (1%)	13	39
22	R0	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
22	Y0	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
23	R1	95/98 (97%)	83 (87%)	12 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	Y1	91/98 (93%)	91 (100%)	0	0	100	100
24	R2	67/72 (93%)	64 (96%)	3 (4%)	0	100	100
24	Y2	70/72 (97%)	69 (99%)	1 (1%)	0	100	100
25	R3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
25	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	R4	67/71 (94%)	56 (84%)	11 (16%)	0	100	100
26	Y4	67/71 (94%)	58 (87%)	9 (13%)	0	100	100
27	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	Y5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	R7	45/49 (92%)	45 (100%)	0	0	100	100
29	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	R8	62/65 (95%)	54 (87%)	8 (13%)	0	100	100
30	Y8	62/65 (95%)	56 (90%)	6 (10%)	0	100	100
31	R9	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
31	Y9	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
33	QB	233/256 (91%)	201 (86%)	32 (14%)	0	100	100
33	XB	234/256 (91%)	205 (88%)	29 (12%)	0	100	100
34	QC	203/239 (85%)	187 (92%)	16 (8%)	0	100	100
34	XC	203/239 (85%)	186 (92%)	17 (8%)	0	100	100
35	QD	206/209 (99%)	191 (93%)	13 (6%)	2 (1%)	13	39
35	XD	206/209 (99%)	191 (93%)	13 (6%)	2 (1%)	13	39
36	QE	149/162 (92%)	139 (93%)	10 (7%)	0	100	100
36	XE	149/162 (92%)	135 (91%)	14 (9%)	0	100	100
37	QF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
37	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
38	QG	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
38	XG	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
39	QH	135/138 (98%)	123 (91%)	12 (9%)	0	100	100
39	XH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	QI	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
40	XI	124/128 (97%)	110 (89%)	14 (11%)	0	100	100
41	QJ	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
41	XJ	94/105 (90%)	84 (89%)	10 (11%)	0	100	100
42	QK	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
42	XK	114/129 (88%)	108 (95%)	6 (5%)	0	100	100
43	QL	123/132 (93%)	108 (88%)	15 (12%)	0	100	100
43	XL	120/132 (91%)	106 (88%)	14 (12%)	0	100	100
44	QM	118/126 (94%)	104 (88%)	13 (11%)	1 (1%)	16	44
44	XM	117/126 (93%)	105 (90%)	10 (8%)	2 (2%)	7	28
45	QN	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
45	XN	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
46	QO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	XO	85/89 (96%)	82 (96%)	3 (4%)	0	100	100
47	QP	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
47	XP	82/88 (93%)	75 (92%)	7 (8%)	0	100	100
48	QQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
48	XQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
49	QR	68/88 (77%)	62 (91%)	6 (9%)	0	100	100
49	XR	68/88 (77%)	64 (94%)	4 (6%)	0	100	100
50	QS	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
50	XS	82/93 (88%)	68 (83%)	13 (16%)	1 (1%)	11	35
51	QT	97/106 (92%)	89 (92%)	8 (8%)	0	100	100
51	XT	97/106 (92%)	86 (89%)	11 (11%)	0	100	100
52	QU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
52	XU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	11486/12128 (95%)	10518 (92%)	945 (8%)	23 (0%)	44	72

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	YV	49	THR
35	XD	32	ALA

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Mol	Chain	Res	Type
21	YZ	52	SER
16	RU	93	LYS
35	QD	32	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	RD	214/218 (98%)	212 (99%)	2 (1%)	75	86
3	YD	215/218 (99%)	212 (99%)	3 (1%)	62	77
4	RE	165/166 (99%)	162 (98%)	3 (2%)	54	73
4	YE	165/166 (99%)	162 (98%)	3 (2%)	54	73
5	RF	161/166 (97%)	158 (98%)	3 (2%)	52	71
5	YF	161/166 (97%)	160 (99%)	1 (1%)	84	90
6	RG	155/156 (99%)	154 (99%)	1 (1%)	84	90
6	YG	155/156 (99%)	155 (100%)	0	100	100
7	RH	145/148 (98%)	143 (99%)	2 (1%)	62	77
7	YH	145/148 (98%)	138 (95%)	7 (5%)	21	48
8	RI	122/124 (98%)	107 (88%)	15 (12%)	4	14
8	YI	122/124 (98%)	119 (98%)	3 (2%)	42	65
9	RN	117/119 (98%)	115 (98%)	2 (2%)	56	74
9	YN	119/119 (100%)	116 (98%)	3 (2%)	42	65
10	RO	100/100 (100%)	99 (99%)	1 (1%)	73	83
10	YO	100/100 (100%)	99 (99%)	1 (1%)	73	83
11	RP	115/116 (99%)	114 (99%)	1 (1%)	75	86
11	YP	114/116 (98%)	112 (98%)	2 (2%)	54	73
12	RQ	111/111 (100%)	108 (97%)	3 (3%)	40	63
12	YQ	111/111 (100%)	109 (98%)	2 (2%)	54	73
13	RR	101/101 (100%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	YR	100/101 (99%)	99 (99%)	1 (1%)	73	83
14	RS	87/88 (99%)	86 (99%)	1 (1%)	70	81
14	YS	87/88 (99%)	86 (99%)	1 (1%)	70	81
15	RT	120/127 (94%)	118 (98%)	2 (2%)	56	74
15	YT	120/127 (94%)	120 (100%)	0	100	100
16	RU	93/94 (99%)	93 (100%)	0	100	100
16	YU	93/94 (99%)	92 (99%)	1 (1%)	70	81
17	RV	82/82 (100%)	78 (95%)	4 (5%)	21	48
17	YV	82/82 (100%)	80 (98%)	2 (2%)	44	66
18	RW	92/92 (100%)	91 (99%)	1 (1%)	70	81
18	YW	92/92 (100%)	92 (100%)	0	100	100
19	RX	74/78 (95%)	70 (95%)	4 (5%)	18	44
19	YX	76/78 (97%)	72 (95%)	4 (5%)	19	45
20	RY	88/91 (97%)	88 (100%)	0	100	100
20	YY	88/91 (97%)	88 (100%)	0	100	100
21	RZ	174/179 (97%)	170 (98%)	4 (2%)	45	67
21	YZ	173/179 (97%)	170 (98%)	3 (2%)	56	74
22	R0	61/67 (91%)	61 (100%)	0	100	100
22	Y0	61/67 (91%)	61 (100%)	0	100	100
23	R1	82/83 (99%)	82 (100%)	0	100	100
23	Y1	78/83 (94%)	78 (100%)	0	100	100
24	R2	64/67 (96%)	64 (100%)	0	100	100
24	Y2	67/67 (100%)	67 (100%)	0	100	100
25	R3	51/52 (98%)	50 (98%)	1 (2%)	50	70
25	Y3	51/52 (98%)	50 (98%)	1 (2%)	50	70
26	R4	62/63 (98%)	60 (97%)	2 (3%)	34	59
26	Y4	62/63 (98%)	62 (100%)	0	100	100
27	R5	51/52 (98%)	50 (98%)	1 (2%)	50	70
27	Y5	51/52 (98%)	50 (98%)	1 (2%)	50	70
28	R6	51/52 (98%)	51 (100%)	0	100	100
28	Y6	51/52 (98%)	50 (98%)	1 (2%)	50	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	R7	40/42 (95%)	40 (100%)	0	100	100
29	Y7	41/42 (98%)	41 (100%)	0	100	100
30	R8	54/55 (98%)	53 (98%)	1 (2%)	52	71
30	Y8	54/55 (98%)	54 (100%)	0	100	100
31	R9	34/34 (100%)	34 (100%)	0	100	100
31	Y9	34/34 (100%)	34 (100%)	0	100	100
33	QB	203/220 (92%)	201 (99%)	2 (1%)	73	83
33	XB	204/220 (93%)	203 (100%)	1 (0%)	86	91
34	QC	159/188 (85%)	158 (99%)	1 (1%)	84	90
34	XC	159/188 (85%)	158 (99%)	1 (1%)	84	90
35	QD	180/181 (99%)	178 (99%)	2 (1%)	70	81
35	XD	180/181 (99%)	174 (97%)	6 (3%)	33	58
36	QE	116/123 (94%)	114 (98%)	2 (2%)	56	74
36	XE	116/123 (94%)	113 (97%)	3 (3%)	41	64
37	QF	90/90 (100%)	90 (100%)	0	100	100
37	XF	90/90 (100%)	90 (100%)	0	100	100
38	QG	126/127 (99%)	126 (100%)	0	100	100
38	XG	126/127 (99%)	124 (98%)	2 (2%)	58	75
39	QH	118/119 (99%)	118 (100%)	0	100	100
39	XH	118/119 (99%)	118 (100%)	0	100	100
40	QI	98/99 (99%)	96 (98%)	2 (2%)	50	70
40	XI	97/99 (98%)	97 (100%)	0	100	100
41	QJ	89/92 (97%)	88 (99%)	1 (1%)	70	81
41	XJ	86/92 (94%)	86 (100%)	0	100	100
42	QK	88/99 (89%)	87 (99%)	1 (1%)	70	81
42	XK	88/99 (89%)	87 (99%)	1 (1%)	70	81
43	QL	104/109 (95%)	104 (100%)	0	100	100
43	XL	103/109 (94%)	103 (100%)	0	100	100
44	QM	96/101 (95%)	94 (98%)	2 (2%)	48	69
44	XM	95/101 (94%)	93 (98%)	2 (2%)	48	69
45	QN	49/50 (98%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	XN	49/50 (98%)	48 (98%)	1 (2%)	50	70
46	QO	79/80 (99%)	78 (99%)	1 (1%)	65	78
46	XO	79/80 (99%)	79 (100%)	0	100	100
47	QP	72/74 (97%)	71 (99%)	1 (1%)	62	77
47	XP	72/74 (97%)	71 (99%)	1 (1%)	62	77
48	QQ	95/97 (98%)	95 (100%)	0	100	100
48	XQ	95/97 (98%)	94 (99%)	1 (1%)	70	81
49	QR	61/77 (79%)	61 (100%)	0	100	100
49	XR	61/77 (79%)	61 (100%)	0	100	100
50	QS	72/80 (90%)	71 (99%)	1 (1%)	62	77
50	XS	73/80 (91%)	72 (99%)	1 (1%)	62	77
51	QT	76/82 (93%)	76 (100%)	0	100	100
51	XT	76/82 (93%)	76 (100%)	0	100	100
52	QU	20/22 (91%)	19 (95%)	1 (5%)	20	46
52	XU	20/22 (91%)	20 (100%)	0	100	100
All	All	9712/10066 (96%)	9581 (99%)	131 (1%)	65	78

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	XD	19	LEU
36	XE	11	ILE
50	XS	11	VAL
21	RZ	185	GLU
21	RZ	182	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
36	XE	141	GLN
37	XF	73	ASN
40	XI	73	GLN
38	QG	51	GLN
34	QC	118	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	RA	2877/2915 (98%)	581 (20%)	41 (1%)
1	YA	2880/2915 (98%)	558 (19%)	40 (1%)
2	RB	119/122 (97%)	19 (15%)	1 (0%)
2	YB	119/122 (97%)	23 (19%)	2 (1%)
32	QA	1510/1521 (99%)	292 (19%)	37 (2%)
32	XA	1509/1521 (99%)	277 (18%)	29 (1%)
53	QV	16/17 (94%)	1 (6%)	0
53	XV	14/17 (82%)	0	0
54	QX	17/19 (89%)	5 (29%)	1 (5%)
54	XX	18/19 (94%)	9 (50%)	1 (5%)
All	All	9079/9188 (98%)	1765 (19%)	152 (1%)

5 of 1765 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	RA	9	U
1	RA	15	G
1	RA	34	C
1	RA	35	G
1	RA	46	C

5 of 152 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	YA	2712	U
32	XA	992	U
1	YA	2867	G
32	XA	388	G
32	XA	1537	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	1MG	XV	37	53	19,26,27	0.81	0	18,39,42	1.14	2 (11%)
53	1MG	QV	37	53	19,26,27	0.83	1 (5%)	18,39,42	1.21	3 (16%)

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
53	1MG	XV	37	53	-	0/3/25/26	0/3/3/3
53	1MG	QV	37	53	-	0/3/25/26	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	QV	37	1MG	C2-N1	2.07	1.41	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	QV	37	1MG	C8-N7-C5	3.01	107.67	102.55
53	XV	37	1MG	C8-N7-C5	2.91	107.51	102.55
53	XV	37	1MG	C5-C6-N1	2.33	117.33	113.96
53	QV	37	1MG	C5-C6-N1	2.11	117.00	113.96
53	QV	37	1MG	CM1-N1-C6	2.07	120.35	117.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1213 ligands modelled in this entry, 1211 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	SF4	XD	301	35	0,12,12	-	-	-		
57	SF4	QD	301	35	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
57	SF4	XD	301	35	-	-	0/6/5/5
57	SF4	QD	301	35	-	-	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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	XD	301	SF4	3	0
57	QD	301	SF4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	RA	2881/2915 (98%)	-0.06	87 (3%)	52	45	42, 74, 214, 568	0
1	YA	2883/2915 (98%)	-0.19	68 (2%)	59	51	29, 52, 212, 440	0
2	RB	120/122 (98%)	0.20	2 (1%)	69	59	79, 127, 167, 200	0
2	YB	120/122 (98%)	-0.20	1 (0%)	82	75	51, 77, 104, 135	0
3	RD	272/276 (98%)	0.14	4 (1%)	71	62	41, 65, 98, 124	0
3	YD	273/276 (98%)	-0.02	0	100	100	32, 52, 78, 104	0
4	RE	204/206 (99%)	-0.00	0	100	100	40, 70, 108, 132	0
4	YE	205/206 (99%)	0.24	11 (5%)	32	29	31, 56, 103, 184	0
5	RF	202/210 (96%)	0.27	4 (1%)	64	55	43, 81, 139, 181	0
5	YF	202/210 (96%)	0.35	10 (4%)	35	31	26, 57, 122, 164	0
6	RG	181/182 (99%)	1.23	35 (19%)	4	6	108, 165, 236, 297	0
6	YG	181/182 (99%)	0.79	13 (7%)	23	22	77, 119, 184, 221	0
7	RH	174/180 (96%)	1.17	30 (17%)	5	7	91, 130, 171, 232	0
7	YH	174/180 (96%)	0.06	5 (2%)	54	46	38, 69, 100, 122	0
8	RI	146/148 (98%)	1.03	26 (17%)	4	7	63, 121, 154, 186	0
8	YI	146/148 (98%)	0.61	13 (8%)	17	18	59, 103, 141, 161	0
9	RN	138/140 (98%)	0.48	5 (3%)	46	39	50, 81, 123, 160	0
9	YN	140/140 (100%)	0.19	4 (2%)	54	46	37, 55, 95, 146	0
10	RO	122/122 (100%)	0.09	2 (1%)	70	61	46, 72, 105, 123	0
10	YO	122/122 (100%)	0.02	0	100	100	36, 58, 92, 109	0
11	RP	148/150 (98%)	0.65	10 (6%)	25	24	49, 91, 132, 176	0
11	YP	147/150 (98%)	0.25	3 (2%)	64	55	29, 60, 96, 129	0
12	RQ	141/141 (100%)	0.64	20 (14%)	7	10	59, 90, 135, 232	0
12	YQ	141/141 (100%)	0.21	7 (4%)	35	31	40, 60, 90, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	RR	118/118 (100%)	0.33	4 (3%) 48 41	44, 71, 102, 124	0
13	YR	117/118 (99%)	0.22	3 (2%) 57 49	33, 54, 78, 122	0
14	RS	111/112 (99%)	0.84	12 (10%) 12 15	97, 120, 175, 207	0
14	YS	110/112 (98%)	0.27	8 (7%) 22 22	51, 77, 105, 118	0
15	RT	137/146 (93%)	0.28	7 (5%) 34 30	52, 79, 139, 185	0
15	YT	137/146 (93%)	0.18	4 (2%) 54 46	36, 63, 122, 178	0
16	RU	117/118 (99%)	0.60	10 (8%) 18 19	45, 79, 129, 241	0
16	YU	117/118 (99%)	0.29	5 (4%) 40 35	29, 47, 91, 196	0
17	RV	101/101 (100%)	0.19	1 (0%) 79 71	58, 96, 129, 140	0
17	YV	101/101 (100%)	0.00	5 (4%) 35 31	31, 57, 91, 175	0
18	RW	113/113 (100%)	0.18	5 (4%) 39 35	42, 63, 103, 213	0
18	YW	113/113 (100%)	0.00	3 (2%) 56 48	33, 47, 83, 195	0
19	RX	92/96 (95%)	0.30	3 (3%) 49 42	54, 80, 111, 135	0
19	YX	94/96 (97%)	0.10	3 (3%) 50 42	35, 54, 92, 123	0
20	RY	107/110 (97%)	0.59	8 (7%) 22 21	67, 94, 130, 157	0
20	YY	107/110 (97%)	0.26	5 (4%) 37 33	42, 67, 103, 137	0
21	RZ	203/206 (98%)	0.66	15 (7%) 22 22	88, 123, 159, 219	0
21	YZ	201/206 (97%)	0.02	2 (0%) 79 71	51, 84, 126, 143	0
22	R0	76/85 (89%)	0.66	7 (9%) 16 17	66, 86, 108, 129	0
22	Y0	75/85 (88%)	0.14	2 (2%) 56 48	35, 60, 84, 93	0
23	R1	97/98 (98%)	0.70	8 (8%) 19 20	51, 77, 134, 245	0
23	Y1	93/98 (94%)	0.18	2 (2%) 62 53	35, 60, 93, 117	0
24	R2	69/72 (95%)	0.77	7 (10%) 14 16	59, 96, 143, 158	0
24	Y2	72/72 (100%)	0.40	6 (8%) 19 20	35, 61, 112, 216	0
25	R3	59/60 (98%)	0.07	1 (1%) 69 59	53, 83, 134, 175	0
25	Y3	59/60 (98%)	0.07	0 100 100	32, 57, 102, 150	0
26	R4	69/71 (97%)	0.77	4 (5%) 30 28	131, 200, 263, 278	0
26	Y4	69/71 (97%)	0.73	6 (8%) 17 18	110, 173, 242, 272	0
27	R5	59/60 (98%)	0.28	2 (3%) 48 41	42, 61, 104, 135	0
27	Y5	59/60 (98%)	-0.01	1 (1%) 69 59	34, 51, 91, 147	0
28	R6	53/54 (98%)	0.01	3 (5%) 30 28	66, 87, 115, 184	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	Y6	53/54 (98%)	0.04	0	100	100	52, 65, 88, 102	0
29	R7	47/49 (95%)	0.28	2 (4%)	40	35	40, 59, 89, 106	0
29	Y7	48/49 (97%)	0.15	1 (2%)	63	53	32, 45, 78, 125	0
30	R8	64/65 (98%)	1.25	14 (21%)	3	5	59, 81, 119, 190	0
30	Y8	64/65 (98%)	0.33	3 (4%)	37	33	40, 54, 85, 115	0
31	R9	36/37 (97%)	0.84	2 (5%)	31	29	77, 99, 123, 160	0
31	Y9	37/37 (100%)	0.38	3 (8%)	19	20	50, 68, 100, 155	0
32	QA	1511/1521 (99%)	0.34	103 (6%)	25	24	62, 108, 271, 392	0
32	XA	1511/1521 (99%)	0.38	85 (5%)	31	29	51, 119, 271, 367	0
33	QB	235/256 (91%)	0.82	20 (8%)	18	19	100, 141, 197, 229	0
33	XB	236/256 (92%)	1.01	34 (14%)	7	9	99, 142, 187, 221	0
34	QC	205/239 (85%)	1.01	31 (15%)	6	9	115, 160, 216, 243	0
34	XC	205/239 (85%)	1.03	35 (17%)	5	7	116, 167, 212, 242	0
35	QD	208/209 (99%)	0.59	15 (7%)	23	22	77, 106, 139, 163	0
35	XD	208/209 (99%)	0.81	25 (12%)	10	13	81, 118, 164, 191	0
36	QE	151/162 (93%)	0.40	9 (5%)	29	27	75, 104, 142, 174	0
36	XE	151/162 (93%)	0.39	11 (7%)	22	22	65, 105, 142, 200	0
37	QF	101/101 (100%)	0.26	2 (1%)	64	55	74, 109, 145, 189	0
37	XF	101/101 (100%)	0.48	9 (8%)	17	18	76, 106, 142, 180	0
38	QG	155/156 (99%)	1.00	24 (15%)	6	8	127, 176, 231, 274	0
38	XG	155/156 (99%)	1.00	18 (11%)	11	14	120, 164, 209, 253	0
39	QH	137/138 (99%)	0.43	11 (8%)	20	20	71, 107, 137, 154	0
39	XH	137/138 (99%)	0.48	8 (5%)	30	28	76, 110, 142, 179	0
40	QI	127/128 (99%)	1.48	37 (29%)	1	3	124, 195, 235, 268	0
40	XI	126/128 (98%)	1.36	30 (23%)	2	4	123, 184, 231, 253	0
41	QJ	99/105 (94%)	1.66	26 (26%)	2	4	161, 191, 229, 260	0
41	XJ	96/105 (91%)	1.45	24 (25%)	2	4	162, 186, 228, 245	0
42	QK	116/129 (89%)	0.46	8 (6%)	24	23	67, 117, 152, 189	0
42	XK	116/129 (89%)	0.39	0	100	100	69, 106, 141, 194	0
43	QL	125/132 (94%)	0.37	8 (6%)	27	26	63, 89, 130, 209	0
43	XL	122/132 (92%)	0.86	16 (13%)	8	11	69, 94, 123, 166	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	QM	120/126 (95%)	1.23	27 (22%) 3 5	134, 196, 241, 277	0
44	XM	119/126 (94%)	1.39	26 (21%) 3 5	136, 193, 260, 292	0
45	QN	60/61 (98%)	1.89	25 (41%) 1 1	137, 169, 213, 260	0
45	XN	60/61 (98%)	1.48	16 (26%) 2 4	133, 173, 216, 242	0
46	QO	88/89 (98%)	0.50	7 (7%) 20 20	59, 103, 138, 165	0
46	XO	87/89 (97%)	0.37	1 (1%) 77 70	65, 95, 136, 162	0
47	QP	84/88 (95%)	0.84	8 (9%) 15 17	75, 101, 140, 169	0
47	XP	84/88 (95%)	1.01	9 (10%) 12 15	78, 121, 165, 184	0
48	QQ	100/105 (95%)	0.31	3 (3%) 52 45	69, 94, 119, 171	0
48	XQ	100/105 (95%)	0.34	4 (4%) 43 37	65, 99, 138, 144	0
49	QR	70/88 (79%)	0.66	7 (10%) 14 16	68, 106, 143, 157	0
49	XR	70/88 (79%)	0.21	0 100 100	68, 102, 140, 159	0
50	QS	83/93 (89%)	1.25	18 (21%) 3 5	165, 199, 249, 272	0
50	XS	84/93 (90%)	1.47	23 (27%) 2 3	152, 199, 239, 260	0
51	QT	99/106 (93%)	0.51	4 (4%) 43 37	68, 93, 150, 184	0
51	XT	99/106 (93%)	0.84	15 (15%) 6 9	82, 113, 165, 174	0
52	QU	25/27 (92%)	2.13	13 (52%) 0 0	135, 157, 199, 211	0
52	XU	25/27 (92%)	2.08	10 (40%) 1 1	128, 175, 233, 253	0
53	QV	16/17 (94%)	0.71	2 (12%) 9 12	177, 204, 219, 223	0
53	XV	14/17 (82%)	0.75	0 100 100	176, 181, 204, 205	0
54	QX	18/19 (94%)	2.01	8 (44%) 1 1	136, 267, 324, 335	0
54	XX	19/19 (100%)	2.07	11 (57%) 0 0	125, 256, 314, 321	0
All	All	20775/21316 (97%)	0.34	1363 (6%) 26 25	26, 89, 218, 568	0

The worst 5 of 1363 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	YA	2602	A	9.0
41	QJ	48	THR	8.3
12	YQ	112	GLU	7.9
41	QJ	62	HIS	7.9
6	RG	137	GLU	7.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
53	1MG	QV	37	24/25	0.78	0.10	84,144,150,160	0
53	1MG	XV	37	24/25	0.80	0.13	171,173,175,184	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	YA	3390	1/1	0.36	0.40	86,86,86,86	0
55	MG	RA	3205	1/1	0.39	0.33	95,95,95,95	0
55	MG	RF	301	1/1	0.40	0.54	83,83,83,83	0
55	MG	RA	3246	1/1	0.44	0.46	91,91,91,91	0
55	MG	RA	3193	1/1	0.47	0.23	77,77,77,77	0
55	MG	RA	3312	1/1	0.49	0.34	80,80,80,80	0
55	MG	YA	3333	1/1	0.50	0.07	19,19,19,19	0
55	MG	RA	3147	1/1	0.55	0.21	60,60,60,60	0
55	MG	RA	3137	1/1	0.55	0.29	55,55,55,55	0
55	MG	RB	208	1/1	0.56	0.19	63,63,63,63	0
55	MG	YA	3330	1/1	0.56	0.23	58,58,58,58	0
55	MG	RA	3316	1/1	0.57	0.37	74,74,74,74	0
55	MG	YA	3449	1/1	0.58	0.24	54,54,54,54	0
55	MG	RA	3176	1/1	0.59	0.18	75,75,75,75	0
55	MG	YA	3212	1/1	0.59	0.32	62,62,62,62	0
55	MG	QA	1642	1/1	0.60	0.16	79,79,79,79	0
55	MG	RA	3440	1/1	0.60	0.31	61,61,61,61	0
55	MG	RA	3411	1/1	0.61	0.32	87,87,87,87	0
55	MG	RA	3301	1/1	0.62	0.19	72,72,72,72	0
55	MG	QA	1648	1/1	0.63	0.18	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3389	1/1	0.63	0.33	62,62,62,62	0
55	MG	RA	3315	1/1	0.63	0.31	81,81,81,81	0
55	MG	YA	3293	1/1	0.65	0.13	62,62,62,62	0
55	MG	RA	3068	1/1	0.65	0.13	66,66,66,66	0
55	MG	YA	3081	1/1	0.65	0.19	55,55,55,55	0
55	MG	RA	3111	1/1	0.65	0.22	92,92,92,92	0
55	MG	YA	3288	1/1	0.65	0.20	60,60,60,60	0
55	MG	RA	3249	1/1	0.66	0.14	60,60,60,60	0
55	MG	RA	3156	1/1	0.66	0.18	78,78,78,78	0
55	MG	YA	3402	1/1	0.67	0.21	74,74,74,74	0
55	MG	YA	3358	1/1	0.67	0.18	32,32,32,32	0
55	MG	XA	1668	1/1	0.67	0.09	77,77,77,77	0
55	MG	XA	1674	1/1	0.67	0.22	64,64,64,64	0
55	MG	YA	3464	1/1	0.68	0.21	63,63,63,63	0
55	MG	YA	3494	1/1	0.68	0.31	56,56,56,56	0
55	MG	YA	3206	1/1	0.68	0.30	64,64,64,64	0
55	MG	YA	3393	1/1	0.68	0.42	69,69,69,69	0
55	MG	RA	3432	1/1	0.69	0.26	81,81,81,81	0
55	MG	RA	3186	1/1	0.69	0.24	76,76,76,76	0
55	MG	YA	3429	1/1	0.70	0.26	82,82,82,82	0
55	MG	RA	3129	1/1	0.70	0.21	58,58,58,58	0
55	MG	YA	3380	1/1	0.70	0.29	70,70,70,70	0
55	MG	RA	3243	1/1	0.70	0.21	57,57,57,57	0
55	MG	YA	3210	1/1	0.70	0.13	59,59,59,59	0
55	MG	RA	3419	1/1	0.70	0.21	61,61,61,61	0
55	MG	XA	1681	1/1	0.70	0.20	82,82,82,82	0
55	MG	YA	3324	1/1	0.71	0.23	55,55,55,55	0
55	MG	YA	3472	1/1	0.71	0.18	68,68,68,68	0
55	MG	RA	3372	1/1	0.71	0.17	66,66,66,66	0
55	MG	YA	3321	1/1	0.72	0.17	63,63,63,63	0
55	MG	YA	3184	1/1	0.72	0.18	60,60,60,60	0
55	MG	QA	1634	1/1	0.72	0.32	65,65,65,65	0
55	MG	YA	3208	1/1	0.72	0.18	51,51,51,51	0
55	MG	RA	3308	1/1	0.72	0.24	66,66,66,66	0
55	MG	RA	3183	1/1	0.72	0.30	90,90,90,90	0
55	MG	YA	3500	1/1	0.72	0.30	79,79,79,79	0
55	MG	XA	1645	1/1	0.72	0.21	78,78,78,78	0
55	MG	YA	3382	1/1	0.72	0.32	53,53,53,53	0
55	MG	QA	1622	1/1	0.72	0.18	96,96,96,96	0
55	MG	YA	3136	1/1	0.72	0.17	43,43,43,43	0
55	MG	QA	1618	1/1	0.73	0.26	108,108,108,108	0
55	MG	YA	3342	1/1	0.73	0.36	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1640	1/1	0.73	0.20	65,65,65,65	0
55	MG	RA	3008	1/1	0.73	0.23	65,65,65,65	0
55	MG	RA	3447	1/1	0.73	0.17	55,55,55,55	0
55	MG	YA	3215	1/1	0.73	0.26	56,56,56,56	0
55	MG	YA	3229	1/1	0.73	0.25	47,47,47,47	0
55	MG	RA	3204	1/1	0.74	0.22	62,62,62,62	0
55	MG	YE	303	1/1	0.74	0.21	44,44,44,44	0
55	MG	RA	3306	1/1	0.74	0.14	51,51,51,51	0
55	MG	QA	1662	1/1	0.74	0.24	57,57,57,57	0
55	MG	RA	3361	1/1	0.74	0.12	68,68,68,68	0
55	MG	RA	3084	1/1	0.74	0.14	33,33,33,33	0
55	MG	RA	3207	1/1	0.74	0.22	81,81,81,81	0
55	MG	YA	3193	1/1	0.75	0.40	70,70,70,70	0
55	MG	RA	3053	1/1	0.75	0.19	36,36,36,36	0
55	MG	RA	3148	1/1	0.75	0.18	56,56,56,56	0
55	MG	RA	3357	1/1	0.75	0.26	73,73,73,73	0
55	MG	RA	3212	1/1	0.75	0.21	67,67,67,67	0
55	MG	YA	3366	1/1	0.75	0.12	32,32,32,32	0
55	MG	RA	3056	1/1	0.75	0.12	61,61,61,61	0
55	MG	XA	1630	1/1	0.75	0.14	39,39,39,39	0
55	MG	RA	3386	1/1	0.75	0.19	61,61,61,61	0
55	MG	RA	3387	1/1	0.75	0.14	56,56,56,56	0
55	MG	YA	3180	1/1	0.75	0.18	67,67,67,67	0
55	MG	RA	3093	1/1	0.75	0.18	57,57,57,57	0
55	MG	YA	3419	1/1	0.75	0.13	60,60,60,60	0
55	MG	R0	101	1/1	0.76	0.19	40,40,40,40	0
55	MG	RA	3211	1/1	0.76	0.17	73,73,73,73	0
55	MG	YA	3261	1/1	0.76	0.25	53,53,53,53	0
55	MG	YA	3497	1/1	0.76	0.12	51,51,51,51	0
55	MG	XA	1670	1/1	0.76	0.13	59,59,59,59	0
55	MG	RA	3167	1/1	0.76	0.17	80,80,80,80	0
55	MG	RA	3144	1/1	0.76	0.22	47,47,47,47	0
55	MG	RA	3474	1/1	0.77	0.34	58,58,58,58	0
55	MG	YA	3123	1/1	0.77	0.17	29,29,29,29	0
55	MG	RA	3300	1/1	0.77	0.26	60,60,60,60	0
55	MG	QA	1639	1/1	0.77	0.13	73,73,73,73	0
55	MG	RA	3121	1/1	0.77	0.14	59,59,59,59	0
55	MG	RA	3285	1/1	0.77	0.23	67,67,67,67	0
55	MG	RA	3457	1/1	0.77	0.25	51,51,51,51	0
55	MG	YA	3317	1/1	0.77	0.30	47,47,47,47	0
55	MG	YA	3011	1/1	0.77	0.22	40,40,40,40	0
55	MG	RA	3108	1/1	0.78	0.14	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3119	1/1	0.78	0.18	43,43,43,43	0
55	MG	RA	3145	1/1	0.78	0.10	36,36,36,36	0
55	MG	RA	3269	1/1	0.78	0.27	70,70,70,70	0
55	MG	YA	3149	1/1	0.78	0.18	36,36,36,36	0
55	MG	QA	1635	1/1	0.78	0.21	59,59,59,59	0
55	MG	RA	3466	1/1	0.78	0.34	74,74,74,74	0
55	MG	RA	3399	1/1	0.78	0.24	69,69,69,69	0
55	MG	YA	3410	1/1	0.78	0.16	40,40,40,40	0
55	MG	RA	3358	1/1	0.78	0.21	68,68,68,68	0
55	MG	RA	3200	1/1	0.78	0.25	45,45,45,45	0
55	MG	RA	3287	1/1	0.78	0.32	58,58,58,58	0
55	MG	YA	3458	1/1	0.78	0.12	47,47,47,47	0
55	MG	XA	1683	1/1	0.78	0.23	155,155,155,155	0
56	ZN	Y4	101	1/1	0.78	0.16	196,196,196,196	0
55	MG	RT	201	1/1	0.79	0.35	82,82,82,82	0
55	MG	YA	3144	1/1	0.79	0.23	41,41,41,41	0
55	MG	XA	1620	1/1	0.79	0.14	62,62,62,62	0
55	MG	RA	3413	1/1	0.79	0.19	68,68,68,68	0
55	MG	XA	1639	1/1	0.79	0.12	42,42,42,42	0
55	MG	RA	3314	1/1	0.79	0.21	51,51,51,51	0
55	MG	RA	3237	1/1	0.79	0.20	57,57,57,57	0
55	MG	RB	204	1/1	0.79	0.33	57,57,57,57	0
55	MG	YA	3462	1/1	0.79	0.14	39,39,39,39	0
55	MG	YA	3202	1/1	0.79	0.11	47,47,47,47	0
55	MG	YA	3296	1/1	0.79	0.17	48,48,48,48	0
55	MG	RA	3271	1/1	0.79	0.23	79,79,79,79	0
55	MG	RA	3181	1/1	0.79	0.18	57,57,57,57	0
55	MG	RA	3394	1/1	0.80	0.23	52,52,52,52	0
55	MG	YA	3370	1/1	0.80	0.17	44,44,44,44	0
55	MG	RA	3371	1/1	0.80	0.18	70,70,70,70	0
55	MG	RA	3340	1/1	0.80	0.18	52,52,52,52	0
55	MG	YA	3016	1/1	0.80	0.39	74,74,74,74	0
55	MG	YA	3197	1/1	0.80	0.30	58,58,58,58	0
55	MG	YA	3305	1/1	0.80	0.11	33,33,33,33	0
55	MG	RA	3379	1/1	0.80	0.22	79,79,79,79	0
55	MG	RA	3475	1/1	0.80	0.18	68,68,68,68	0
55	MG	RA	3248	1/1	0.80	0.22	45,45,45,45	0
55	MG	YA	3328	1/1	0.80	0.10	43,43,43,43	0
55	MG	YA	3132	1/1	0.80	0.19	35,35,35,35	0
55	MG	RA	3171	1/1	0.80	0.15	65,65,65,65	0
55	MG	RA	3262	1/1	0.80	0.20	63,63,63,63	0
55	MG	YA	3216	1/1	0.80	0.10	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3260	1/1	0.81	0.30	66,66,66,66	0
55	MG	YA	3178	1/1	0.81	0.24	47,47,47,47	0
55	MG	YA	3420	1/1	0.81	0.17	52,52,52,52	0
55	MG	RA	3299	1/1	0.81	0.10	35,35,35,35	0
55	MG	YA	3310	1/1	0.81	0.33	69,69,69,69	0
55	MG	QA	1641	1/1	0.81	0.18	70,70,70,70	0
55	MG	YA	3318	1/1	0.81	0.12	41,41,41,41	0
55	MG	RA	3236	1/1	0.81	0.29	48,48,48,48	0
55	MG	RA	3396	1/1	0.81	0.17	64,64,64,64	0
55	MG	QA	1654	1/1	0.81	0.14	65,65,65,65	0
55	MG	RA	3268	1/1	0.81	0.35	67,67,67,67	0
55	MG	RA	3410	1/1	0.81	0.12	39,39,39,39	0
55	MG	YA	3507	1/1	0.81	0.34	21,21,21,21	0
55	MG	RA	3201	1/1	0.81	0.25	44,44,44,44	0
55	MG	YA	3353	1/1	0.81	0.16	42,42,42,42	0
55	MG	RA	3136	1/1	0.81	0.12	57,57,57,57	0
55	MG	RA	3309	1/1	0.81	0.11	59,59,59,59	0
55	MG	RA	3310	1/1	0.81	0.27	76,76,76,76	0
55	MG	YA	3371	1/1	0.81	0.09	27,27,27,27	0
55	MG	YA	3224	1/1	0.81	0.22	30,30,30,30	0
55	MG	XA	1669	1/1	0.81	0.31	51,51,51,51	0
55	MG	RA	3276	1/1	0.81	0.24	67,67,67,67	0
55	MG	QA	1630	1/1	0.81	0.09	70,70,70,70	0
55	MG	YA	3282	1/1	0.81	0.18	44,44,44,44	0
55	MG	YA	3394	1/1	0.81	0.32	70,70,70,70	0
55	MG	XL	201	1/1	0.81	0.09	69,69,69,69	0
55	MG	XS	101	1/1	0.81	0.11	89,89,89,89	0
55	MG	RA	3250	1/1	0.81	0.18	70,70,70,70	0
55	MG	YA	3002	1/1	0.82	0.13	37,37,37,37	0
55	MG	YA	3008	1/1	0.82	0.11	32,32,32,32	0
55	MG	QA	1617	1/1	0.82	0.08	58,58,58,58	0
55	MG	RA	3338	1/1	0.82	0.17	51,51,51,51	0
55	MG	YA	3351	1/1	0.82	0.20	36,36,36,36	0
55	MG	YA	3496	1/1	0.82	0.23	72,72,72,72	0
55	MG	RA	3242	1/1	0.82	0.30	43,43,43,43	0
55	MG	YA	3110	1/1	0.82	0.15	31,31,31,31	0
55	MG	RA	3345	1/1	0.82	0.11	43,43,43,43	0
55	MG	YA	3121	1/1	0.82	0.14	16,16,16,16	0
55	MG	XA	1610	1/1	0.82	0.19	70,70,70,70	0
55	MG	RA	3352	1/1	0.82	0.24	79,79,79,79	0
55	MG	RA	3292	1/1	0.82	0.11	39,39,39,39	0
55	MG	XA	1631	1/1	0.82	0.11	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1637	1/1	0.82	0.11	106,106,106,106	0
55	MG	RA	3294	1/1	0.82	0.28	65,65,65,65	0
55	MG	RA	3175	1/1	0.82	0.23	63,63,63,63	0
55	MG	YA	3147	1/1	0.82	0.22	70,70,70,70	0
55	MG	XA	1657	1/1	0.82	0.17	59,59,59,59	0
55	MG	RA	3254	1/1	0.82	0.20	54,54,54,54	0
55	MG	YA	3170	1/1	0.82	0.20	60,60,60,60	0
55	MG	QA	1643	1/1	0.82	0.12	58,58,58,58	0
55	MG	QA	1645	1/1	0.82	0.10	81,81,81,81	0
55	MG	RA	3122	1/1	0.82	0.18	42,42,42,42	0
55	MG	RA	3376	1/1	0.82	0.16	58,58,58,58	0
55	MG	YA	3434	1/1	0.82	0.10	27,27,27,27	0
55	MG	RA	3166	1/1	0.82	0.22	61,61,61,61	0
55	MG	YA	3453	1/1	0.82	0.22	89,89,89,89	0
55	MG	YA	3498	1/1	0.83	0.22	61,61,61,61	0
55	MG	RA	3151	1/1	0.83	0.10	42,42,42,42	0
55	MG	RA	3405	1/1	0.83	0.26	64,64,64,64	0
55	MG	YE	302	1/1	0.83	0.13	51,51,51,51	0
55	MG	RA	3154	1/1	0.83	0.10	33,33,33,33	0
55	MG	YA	3403	1/1	0.83	0.28	63,63,63,63	0
55	MG	RA	3045	1/1	0.83	0.12	30,30,30,30	0
55	MG	YA	3214	1/1	0.83	0.20	34,34,34,34	0
55	MG	RA	3141	1/1	0.83	0.20	75,75,75,75	0
55	MG	YA	3161	1/1	0.83	0.16	48,48,48,48	0
55	MG	RA	3349	1/1	0.83	0.12	54,54,54,54	0
55	MG	YA	3442	1/1	0.83	0.15	52,52,52,52	0
55	MG	YA	3042	1/1	0.83	0.40	194,194,194,194	0
55	MG	RA	3103	1/1	0.83	0.27	48,48,48,48	0
55	MG	YA	3454	1/1	0.83	0.19	88,88,88,88	0
55	MG	YA	3280	1/1	0.83	0.22	54,54,54,54	0
55	MG	RA	3125	1/1	0.83	0.28	49,49,49,49	0
55	MG	YA	3186	1/1	0.83	0.21	40,40,40,40	0
55	MG	YA	3468	1/1	0.83	0.16	43,43,43,43	0
55	MG	RA	3114	1/1	0.83	0.18	43,43,43,43	0
55	MG	XE	201	1/1	0.83	0.17	72,72,72,72	0
55	MG	YA	3194	1/1	0.83	0.15	60,60,60,60	0
55	MG	RA	3119	1/1	0.83	0.15	56,56,56,56	0
55	MG	QA	1650	1/1	0.83	0.19	44,44,44,44	0
55	MG	YA	3487	1/1	0.84	0.26	53,53,53,53	0
55	MG	YA	3223	1/1	0.84	0.08	54,54,54,54	0
55	MG	YA	3166	1/1	0.84	0.21	44,44,44,44	0
55	MG	YA	3014	1/1	0.84	0.12	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3175	1/1	0.84	0.17	34,34,34,34	0
55	MG	RA	3120	1/1	0.84	0.23	32,32,32,32	0
55	MG	YA	3039	1/1	0.84	0.43	28,28,28,28	0
55	MG	RA	3206	1/1	0.84	0.27	66,66,66,66	0
55	MG	RB	203	1/1	0.84	0.08	64,64,64,64	0
55	MG	YA	3190	1/1	0.84	0.15	23,23,23,23	0
55	MG	XA	1617	1/1	0.84	0.24	43,43,43,43	0
55	MG	RA	3153	1/1	0.84	0.23	65,65,65,65	0
55	MG	RA	3127	1/1	0.84	0.22	40,40,40,40	0
55	MG	RA	3431	1/1	0.84	0.37	84,84,84,84	0
55	MG	RA	3393	1/1	0.84	0.08	63,63,63,63	0
55	MG	YA	3425	1/1	0.84	0.16	52,52,52,52	0
55	MG	RA	3187	1/1	0.84	0.14	62,62,62,62	0
55	MG	YA	3433	1/1	0.84	0.22	60,60,60,60	0
55	MG	XA	1647	1/1	0.84	0.08	133,133,133,133	0
55	MG	RA	3265	1/1	0.84	0.19	39,39,39,39	0
55	MG	YA	3440	1/1	0.84	0.21	58,58,58,58	0
55	MG	RA	3232	1/1	0.84	0.11	34,34,34,34	0
55	MG	RA	3458	1/1	0.84	0.25	63,63,63,63	0
55	MG	YA	3213	1/1	0.84	0.13	28,28,28,28	0
55	MG	YA	3339	1/1	0.84	0.31	83,83,83,83	0
55	MG	RA	3464	1/1	0.84	0.10	42,42,42,42	0
55	MG	YA	3150	1/1	0.84	0.21	35,35,35,35	0
55	MG	RA	3347	1/1	0.84	0.17	61,61,61,61	0
55	MG	YA	3218	1/1	0.84	0.26	66,66,66,66	0
55	MG	YA	3359	1/1	0.84	0.20	56,56,56,56	0
55	MG	RA	3444	1/1	0.85	0.22	82,82,82,82	0
55	MG	RA	3403	1/1	0.85	0.15	20,20,20,20	0
55	MG	RA	3178	1/1	0.85	0.16	59,59,59,59	0
55	MG	YA	3153	1/1	0.85	0.19	34,34,34,34	0
55	MG	YE	304	1/1	0.85	0.14	19,19,19,19	0
55	MG	XA	1607	1/1	0.85	0.18	44,44,44,44	0
55	MG	YA	3156	1/1	0.85	0.28	34,34,34,34	0
55	MG	RA	3077	1/1	0.85	0.14	26,26,26,26	0
55	MG	RA	3326	1/1	0.85	0.16	46,46,46,46	0
55	MG	RA	3412	1/1	0.85	0.16	73,73,73,73	0
55	MG	RA	3327	1/1	0.85	0.09	69,69,69,69	0
55	MG	YA	3075	1/1	0.85	0.20	65,65,65,65	0
55	MG	YA	3450	1/1	0.85	0.17	53,53,53,53	0
55	MG	YA	3451	1/1	0.85	0.16	35,35,35,35	0
55	MG	YA	3251	1/1	0.85	0.25	56,56,56,56	0
55	MG	YA	3360	1/1	0.85	0.14	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1653	1/1	0.85	0.10	89,89,89,89	0
55	MG	RA	3007	1/1	0.85	0.19	56,56,56,56	0
55	MG	XA	1658	1/1	0.85	0.21	55,55,55,55	0
55	MG	YA	3459	1/1	0.85	0.16	41,41,41,41	0
55	MG	YA	3101	1/1	0.85	0.22	41,41,41,41	0
55	MG	YA	3105	1/1	0.85	0.26	34,34,34,34	0
55	MG	RA	3420	1/1	0.85	0.17	54,54,54,54	0
55	MG	XA	1679	1/1	0.85	0.08	90,90,90,90	0
55	MG	RA	3423	1/1	0.85	0.12	62,62,62,62	0
55	MG	RA	3280	1/1	0.85	0.36	73,73,73,73	0
55	MG	RA	3281	1/1	0.85	0.18	54,54,54,54	0
55	MG	RQ	201	1/1	0.85	0.10	59,59,59,59	0
55	MG	RA	3435	1/1	0.85	0.11	70,70,70,70	0
55	MG	RA	3006	1/1	0.85	0.11	53,53,53,53	0
55	MG	RA	3282	1/1	0.86	0.26	57,57,57,57	0
55	MG	QA	1647	1/1	0.86	0.20	67,67,67,67	0
55	MG	RA	3049	1/1	0.86	0.13	39,39,39,39	0
55	MG	YA	3426	1/1	0.86	0.35	54,54,54,54	0
55	MG	XA	1601	1/1	0.86	0.19	45,45,45,45	0
55	MG	RA	3321	1/1	0.86	0.19	33,33,33,33	0
55	MG	XA	1608	1/1	0.86	0.15	57,57,57,57	0
55	MG	YA	3228	1/1	0.86	0.26	46,46,46,46	0
55	MG	RA	3192	1/1	0.86	0.10	60,60,60,60	0
55	MG	RA	3470	1/1	0.86	0.27	47,47,47,47	0
55	MG	YA	3259	1/1	0.86	0.20	47,47,47,47	0
55	MG	YA	3446	1/1	0.86	0.30	78,78,78,78	0
55	MG	RA	3150	1/1	0.86	0.21	33,33,33,33	0
55	MG	YA	3263	1/1	0.86	0.13	23,23,23,23	0
55	MG	YA	3004	1/1	0.86	0.11	36,36,36,36	0
55	MG	RA	3012	1/1	0.86	0.18	23,23,23,23	0
55	MG	RA	3482	1/1	0.86	0.19	45,45,45,45	0
55	MG	YA	3374	1/1	0.86	0.18	53,53,53,53	0
55	MG	YA	3375	1/1	0.86	0.15	57,57,57,57	0
55	MG	RB	202	1/1	0.86	0.08	51,51,51,51	0
55	MG	YA	3207	1/1	0.86	0.16	42,42,42,42	0
55	MG	YA	3465	1/1	0.86	0.14	31,31,31,31	0
55	MG	YA	3385	1/1	0.86	0.31	57,57,57,57	0
55	MG	YA	3471	1/1	0.86	0.13	43,43,43,43	0
55	MG	RA	3442	1/1	0.86	0.24	61,61,61,61	0
55	MG	RA	3443	1/1	0.86	0.09	76,76,76,76	0
55	MG	RA	3172	1/1	0.86	0.13	40,40,40,40	0
55	MG	YA	3399	1/1	0.86	0.29	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3165	1/1	0.86	0.12	39,39,39,39	0
55	MG	XQ	201	1/1	0.86	0.09	86,86,86,86	0
55	MG	QA	1644	1/1	0.86	0.27	62,62,62,62	0
55	MG	YA	3092	1/1	0.86	0.24	22,22,22,22	0
55	MG	YA	3376	1/1	0.87	0.17	29,29,29,29	0
55	MG	RA	3373	1/1	0.87	0.23	57,57,57,57	0
55	MG	RA	3215	1/1	0.87	0.09	71,71,71,71	0
55	MG	RA	3263	1/1	0.87	0.12	30,30,30,30	0
55	MG	YA	3192	1/1	0.87	0.21	26,26,26,26	0
55	MG	QA	1666	1/1	0.87	0.18	58,58,58,58	0
55	MG	YA	3502	1/1	0.87	0.14	30,30,30,30	0
55	MG	RA	3478	1/1	0.87	0.10	50,50,50,50	0
55	MG	QA	1631	1/1	0.87	0.11	35,35,35,35	0
55	MG	YA	3200	1/1	0.87	0.13	24,24,24,24	0
55	MG	RA	3198	1/1	0.87	0.13	42,42,42,42	0
55	MG	Y0	102	1/1	0.87	0.14	32,32,32,32	0
55	MG	YA	3405	1/1	0.87	0.14	43,43,43,43	0
55	MG	XA	1604	1/1	0.87	0.09	114,114,114,114	0
55	MG	YA	3203	1/1	0.87	0.10	49,49,49,49	0
55	MG	YA	3415	1/1	0.87	0.09	40,40,40,40	0
55	MG	YA	3312	1/1	0.87	0.22	51,51,51,51	0
55	MG	YA	3204	1/1	0.87	0.10	42,42,42,42	0
55	MG	YA	3009	1/1	0.87	0.14	40,40,40,40	0
55	MG	RA	3162	1/1	0.87	0.09	49,49,49,49	0
55	MG	YA	3427	1/1	0.87	0.10	56,56,56,56	0
55	MG	XA	1635	1/1	0.87	0.11	63,63,63,63	0
55	MG	YA	3323	1/1	0.87	0.17	48,48,48,48	0
55	MG	YA	3431	1/1	0.87	0.30	58,58,58,58	0
55	MG	RA	3018	1/1	0.87	0.11	7,7,7,7	0
55	MG	YA	3325	1/1	0.87	0.19	43,43,43,43	0
55	MG	RA	3445	1/1	0.87	0.19	53,53,53,53	0
55	MG	XA	1652	1/1	0.87	0.11	104,104,104,104	0
55	MG	YA	3017	1/1	0.87	0.17	42,42,42,42	0
55	MG	RA	3202	1/1	0.87	0.27	58,58,58,58	0
55	MG	YA	3337	1/1	0.87	0.19	80,80,80,80	0
55	MG	XA	1667	1/1	0.87	0.14	42,42,42,42	0
55	MG	RA	3337	1/1	0.87	0.07	57,57,57,57	0
55	MG	YA	3162	1/1	0.87	0.26	36,36,36,36	0
55	MG	YA	3056	1/1	0.87	0.27	41,41,41,41	0
55	MG	XA	1673	1/1	0.87	0.14	50,50,50,50	0
55	MG	YA	3167	1/1	0.87	0.26	30,30,30,30	0
55	MG	XA	1675	1/1	0.87	0.18	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3221	1/1	0.87	0.17	42,42,42,42	0
55	MG	RA	3293	1/1	0.87	0.17	75,75,75,75	0
55	MG	YA	3173	1/1	0.87	0.16	60,60,60,60	0
55	MG	YA	3225	1/1	0.87	0.27	55,55,55,55	0
55	MG	RA	3426	1/1	0.87	0.20	44,44,44,44	0
55	MG	RA	3107	1/1	0.87	0.13	35,35,35,35	0
55	MG	YA	3241	1/1	0.87	0.29	49,49,49,49	0
55	MG	QA	1613	1/1	0.87	0.13	50,50,50,50	0
55	MG	YR	201	1/1	0.88	0.34	33,33,33,33	0
55	MG	QA	1628	1/1	0.88	0.08	63,63,63,63	0
55	MG	YA	3163	1/1	0.88	0.12	47,47,47,47	0
55	MG	RA	3105	1/1	0.88	0.12	27,27,27,27	0
55	MG	RA	3115	1/1	0.88	0.26	35,35,35,35	0
55	MG	YA	3267	1/1	0.88	0.17	65,65,65,65	0
55	MG	RA	3449	1/1	0.88	0.14	55,55,55,55	0
55	MG	XA	1614	1/1	0.88	0.11	59,59,59,59	0
55	MG	RA	3046	1/1	0.88	0.12	34,34,34,34	0
55	MG	QA	1638	1/1	0.88	0.21	40,40,40,40	0
55	MG	YA	3291	1/1	0.88	0.37	74,74,74,74	0
55	MG	YA	3292	1/1	0.88	0.29	56,56,56,56	0
55	MG	YA	3372	1/1	0.88	0.25	38,38,38,38	0
55	MG	YA	3176	1/1	0.88	0.20	30,30,30,30	0
55	MG	YA	3295	1/1	0.88	0.09	29,29,29,29	0
55	MG	RA	3311	1/1	0.88	0.17	51,51,51,51	0
55	MG	YA	3299	1/1	0.88	0.43	74,74,74,74	0
55	MG	RA	3074	1/1	0.88	0.24	37,37,37,37	0
55	MG	XA	1648	1/1	0.88	0.07	61,61,61,61	0
55	MG	XA	1649	1/1	0.88	0.12	63,63,63,63	0
55	MG	YA	3383	1/1	0.88	0.27	51,51,51,51	0
55	MG	RA	3247	1/1	0.88	0.15	29,29,29,29	0
55	MG	XA	1656	1/1	0.88	0.08	59,59,59,59	0
55	MG	YA	3387	1/1	0.88	0.26	65,65,65,65	0
55	MG	RA	3406	1/1	0.88	0.22	44,44,44,44	0
55	MG	XA	1662	1/1	0.88	0.15	54,54,54,54	0
55	MG	XA	1665	1/1	0.88	0.10	53,53,53,53	0
55	MG	YA	3316	1/1	0.88	0.24	67,67,67,67	0
55	MG	YA	3486	1/1	0.88	0.25	28,28,28,28	0
55	MG	RA	3050	1/1	0.88	0.17	31,31,31,31	0
55	MG	YA	3488	1/1	0.88	0.17	19,19,19,19	0
55	MG	YA	3222	1/1	0.88	0.22	27,27,27,27	0
55	MG	RA	3283	1/1	0.88	0.21	54,54,54,54	0
55	MG	RA	3168	1/1	0.88	0.18	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3053	1/1	0.88	0.15	18,18,18,18	0
55	MG	RA	3323	1/1	0.88	0.17	60,60,60,60	0
55	MG	YA	3069	1/1	0.88	0.20	28,28,28,28	0
55	MG	QA	1624	1/1	0.88	0.09	54,54,54,54	0
55	MG	YB	205	1/1	0.88	0.10	63,63,63,63	0
55	MG	YA	3243	1/1	0.88	0.24	51,51,51,51	0
55	MG	YA	3336	1/1	0.88	0.13	23,23,23,23	0
55	MG	YA	3248	1/1	0.88	0.20	54,54,54,54	0
55	MG	QA	1649	1/1	0.89	0.10	79,79,79,79	0
55	MG	YA	3127	1/1	0.89	0.20	22,22,22,22	0
55	MG	YA	3300	1/1	0.89	0.13	55,55,55,55	0
55	MG	YA	3303	1/1	0.89	0.12	41,41,41,41	0
55	MG	YA	3304	1/1	0.89	0.32	67,67,67,67	0
55	MG	RA	3185	1/1	0.89	0.13	27,27,27,27	0
55	MG	Y1	101	1/1	0.89	0.17	41,41,41,41	0
55	MG	YA	3414	1/1	0.89	0.09	37,37,37,37	0
55	MG	RA	3094	1/1	0.89	0.08	34,34,34,34	0
55	MG	YA	3137	1/1	0.89	0.16	30,30,30,30	0
55	MG	RA	3274	1/1	0.89	0.18	43,43,43,43	0
55	MG	YA	3424	1/1	0.89	0.22	71,71,71,71	0
55	MG	RQ	202	1/1	0.89	0.09	55,55,55,55	0
55	MG	YA	3148	1/1	0.89	0.10	23,23,23,23	0
55	MG	YA	3001	1/1	0.89	0.23	39,39,39,39	0
55	MG	RA	3441	1/1	0.89	0.18	48,48,48,48	0
55	MG	YA	3151	1/1	0.89	0.17	42,42,42,42	0
55	MG	RA	3161	1/1	0.89	0.15	41,41,41,41	0
55	MG	YA	3326	1/1	0.89	0.09	64,64,64,64	0
55	MG	RA	3397	1/1	0.89	0.28	48,48,48,48	0
55	MG	YA	3220	1/1	0.89	0.12	44,44,44,44	0
55	MG	RA	3036	1/1	0.89	0.19	36,36,36,36	0
55	MG	RA	3402	1/1	0.89	0.07	62,62,62,62	0
55	MG	RA	3446	1/1	0.89	0.13	39,39,39,39	0
55	MG	RA	3140	1/1	0.89	0.23	45,45,45,45	0
55	MG	RA	3177	1/1	0.89	0.07	67,67,67,67	0
55	MG	RA	3128	1/1	0.89	0.15	49,49,49,49	0
55	MG	YA	3171	1/1	0.89	0.15	33,33,33,33	0
55	MG	RA	3407	1/1	0.89	0.08	57,57,57,57	0
55	MG	RA	3463	1/1	0.89	0.12	49,49,49,49	0
55	MG	RA	3225	1/1	0.89	0.19	36,36,36,36	0
55	MG	RA	3370	1/1	0.89	0.12	42,42,42,42	0
55	MG	YA	3466	1/1	0.89	0.13	46,46,46,46	0
55	MG	YA	3257	1/1	0.89	0.27	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3286	1/1	0.89	0.25	57,57,57,57	0
55	MG	YA	3182	1/1	0.89	0.13	55,55,55,55	0
55	MG	RA	3082	1/1	0.89	0.22	36,36,36,36	0
55	MG	YA	3185	1/1	0.89	0.10	42,42,42,42	0
55	MG	RA	3291	1/1	0.89	0.08	34,34,34,34	0
55	MG	YA	3492	1/1	0.89	0.17	25,25,25,25	0
55	MG	YA	3281	1/1	0.89	0.12	40,40,40,40	0
55	MG	XA	1682	1/1	0.89	0.12	132,132,132,132	0
55	MG	RA	3233	1/1	0.89	0.19	39,39,39,39	0
55	MG	RA	3234	1/1	0.89	0.15	33,33,33,33	0
55	MG	RA	3135	1/1	0.89	0.13	57,57,57,57	0
55	MG	RA	3428	1/1	0.89	0.17	41,41,41,41	0
55	MG	YA	3120	1/1	0.89	0.21	57,57,57,57	0
55	MG	RA	3203	1/1	0.89	0.09	59,59,59,59	0
55	MG	YA	3391	1/1	0.90	0.20	41,41,41,41	0
55	MG	RA	3229	1/1	0.90	0.24	50,50,50,50	0
55	MG	YA	3508	1/1	0.90	0.26	31,31,31,31	0
55	MG	YB	202	1/1	0.90	0.17	35,35,35,35	0
55	MG	RX	101	1/1	0.90	0.21	57,57,57,57	0
55	MG	YA	3395	1/1	0.90	0.18	43,43,43,43	0
55	MG	YA	3397	1/1	0.90	0.14	50,50,50,50	0
55	MG	RA	3332	1/1	0.90	0.21	65,65,65,65	0
55	MG	RA	3062	1/1	0.90	0.07	29,29,29,29	0
55	MG	RA	3409	1/1	0.90	0.20	56,56,56,56	0
55	MG	YA	3306	1/1	0.90	0.18	35,35,35,35	0
55	MG	Y8	101	1/1	0.90	0.14	30,30,30,30	0
55	MG	RA	3088	1/1	0.90	0.23	23,23,23,23	0
55	MG	RA	3450	1/1	0.90	0.17	37,37,37,37	0
55	MG	RA	3149	1/1	0.90	0.09	34,34,34,34	0
55	MG	RA	3344	1/1	0.90	0.20	27,27,27,27	0
55	MG	XA	1609	1/1	0.90	0.22	44,44,44,44	0
55	MG	YA	3157	1/1	0.90	0.18	33,33,33,33	0
55	MG	RA	3461	1/1	0.90	0.16	25,25,25,25	0
55	MG	RA	3252	1/1	0.90	0.18	31,31,31,31	0
55	MG	XA	1619	1/1	0.90	0.28	56,56,56,56	0
55	MG	RA	3031	1/1	0.90	0.24	21,21,21,21	0
55	MG	RA	3298	1/1	0.90	0.12	61,61,61,61	0
55	MG	YA	3065	1/1	0.90	0.10	28,28,28,28	0
55	MG	RA	3392	1/1	0.90	0.19	56,56,56,56	0
55	MG	YA	3071	1/1	0.90	0.17	28,28,28,28	0
55	MG	YA	3226	1/1	0.90	0.22	59,59,59,59	0
55	MG	YA	3438	1/1	0.90	0.15	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1642	1/1	0.90	0.13	37,37,37,37	0
55	MG	YA	3172	1/1	0.90	0.16	27,27,27,27	0
55	MG	XA	1646	1/1	0.90	0.22	47,47,47,47	0
55	MG	RA	3424	1/1	0.90	0.06	70,70,70,70	0
55	MG	YA	3444	1/1	0.90	0.25	63,63,63,63	0
55	MG	YA	3239	1/1	0.90	0.19	7,7,7,7	0
55	MG	RA	3351	1/1	0.90	0.10	55,55,55,55	0
55	MG	YA	3343	1/1	0.90	0.20	49,49,49,49	0
55	MG	XA	1654	1/1	0.90	0.14	44,44,44,44	0
55	MG	YA	3090	1/1	0.90	0.17	28,28,28,28	0
55	MG	RA	3112	1/1	0.90	0.15	36,36,36,36	0
55	MG	YA	3357	1/1	0.90	0.26	50,50,50,50	0
55	MG	YA	3096	1/1	0.90	0.14	30,30,30,30	0
55	MG	RA	3051	1/1	0.90	0.22	18,18,18,18	0
55	MG	RB	201	1/1	0.90	0.22	70,70,70,70	0
55	MG	YA	3365	1/1	0.90	0.23	47,47,47,47	0
55	MG	YA	3108	1/1	0.90	0.08	36,36,36,36	0
55	MG	RA	3029	1/1	0.90	0.12	8,8,8,8	0
55	MG	RA	3398	1/1	0.90	0.23	43,43,43,43	0
55	MG	YA	3279	1/1	0.90	0.12	51,51,51,51	0
55	MG	RA	3437	1/1	0.90	0.17	39,39,39,39	0
55	MG	XA	1676	1/1	0.90	0.16	43,43,43,43	0
55	MG	RA	3360	1/1	0.90	0.20	63,63,63,63	0
55	MG	RA	3400	1/1	0.90	0.19	55,55,55,55	0
55	MG	YA	3379	1/1	0.90	0.27	29,29,29,29	0
55	MG	YA	3195	1/1	0.90	0.13	35,35,35,35	0
55	MG	XA	1687	1/1	0.90	0.14	79,79,79,79	0
55	MG	RN	201	1/1	0.90	0.22	60,60,60,60	0
55	MG	YA	3199	1/1	0.90	0.18	56,56,56,56	0
55	MG	RA	3039	1/1	0.90	0.15	22,22,22,22	0
55	MG	YA	3135	1/1	0.90	0.28	27,27,27,27	0
55	MG	RA	3363	1/1	0.90	0.07	25,25,25,25	0
55	MG	YA	3275	1/1	0.91	0.18	31,31,31,31	0
55	MG	YA	3277	1/1	0.91	0.18	56,56,56,56	0
55	MG	YA	3504	1/1	0.91	0.11	33,33,33,33	0
55	MG	RA	3258	1/1	0.91	0.21	29,29,29,29	0
55	MG	RA	3047	1/1	0.91	0.21	24,24,24,24	0
55	MG	RA	3427	1/1	0.91	0.15	39,39,39,39	0
55	MG	RA	3472	1/1	0.91	0.18	37,37,37,37	0
55	MG	RA	3473	1/1	0.91	0.16	56,56,56,56	0
55	MG	YA	3290	1/1	0.91	0.20	22,22,22,22	0
55	MG	RA	3261	1/1	0.91	0.22	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YO	201	1/1	0.91	0.07	63,63,63,63	0
55	MG	RA	3353	1/1	0.91	0.13	60,60,60,60	0
55	MG	Y0	101	1/1	0.91	0.23	41,41,41,41	0
55	MG	RA	3354	1/1	0.91	0.10	51,51,51,51	0
55	MG	YA	3294	1/1	0.91	0.07	25,25,25,25	0
55	MG	RA	3480	1/1	0.91	0.21	55,55,55,55	0
55	MG	RA	3481	1/1	0.91	0.11	58,58,58,58	0
55	MG	YA	3111	1/1	0.91	0.22	28,28,28,28	0
55	MG	RA	3180	1/1	0.91	0.16	50,50,50,50	0
55	MG	YA	3302	1/1	0.91	0.29	36,36,36,36	0
55	MG	RA	3210	1/1	0.91	0.11	44,44,44,44	0
55	MG	RA	3401	1/1	0.91	0.12	43,43,43,43	0
55	MG	XA	1611	1/1	0.91	0.14	46,46,46,46	0
55	MG	YA	3416	1/1	0.91	0.13	47,47,47,47	0
55	MG	RA	3317	1/1	0.91	0.11	49,49,49,49	0
55	MG	RA	3319	1/1	0.91	0.08	26,26,26,26	0
55	MG	YA	3129	1/1	0.91	0.15	5,5,5,5	0
55	MG	YA	3130	1/1	0.91	0.20	24,24,24,24	0
55	MG	RB	206	1/1	0.91	0.21	36,36,36,36	0
55	MG	YA	3133	1/1	0.91	0.17	38,38,38,38	0
55	MG	RA	3146	1/1	0.91	0.17	35,35,35,35	0
55	MG	RA	3182	1/1	0.91	0.09	52,52,52,52	0
55	MG	QA	1658	1/1	0.91	0.10	49,49,49,49	0
55	MG	XA	1641	1/1	0.91	0.09	68,68,68,68	0
55	MG	QA	1660	1/1	0.91	0.23	41,41,41,41	0
55	MG	YA	3437	1/1	0.91	0.09	29,29,29,29	0
55	MG	RA	3214	1/1	0.91	0.23	27,27,27,27	0
55	MG	QA	1663	1/1	0.91	0.17	67,67,67,67	0
55	MG	RP	202	1/1	0.91	0.10	47,47,47,47	0
55	MG	RA	3164	1/1	0.91	0.20	38,38,38,38	0
55	MG	YA	3332	1/1	0.91	0.27	56,56,56,56	0
55	MG	RA	3038	1/1	0.91	0.14	13,13,13,13	0
55	MG	YA	3334	1/1	0.91	0.16	33,33,33,33	0
55	MG	RA	3228	1/1	0.91	0.09	48,48,48,48	0
55	MG	RA	3303	1/1	0.91	0.15	26,26,26,26	0
55	MG	RA	3453	1/1	0.91	0.24	52,52,52,52	0
55	MG	QA	1601	1/1	0.91	0.20	47,47,47,47	0
55	MG	XA	1663	1/1	0.91	0.17	51,51,51,51	0
55	MG	QA	1604	1/1	0.91	0.13	34,34,34,34	0
55	MG	QA	1611	1/1	0.91	0.19	26,26,26,26	0
55	MG	YA	3233	1/1	0.91	0.08	34,34,34,34	0
55	MG	YA	3356	1/1	0.91	0.11	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	QA	1612	1/1	0.91	0.10	35,35,35,35	0
55	MG	YA	3467	1/1	0.91	0.07	24,24,24,24	0
55	MG	RA	3028	1/1	0.91	0.27	38,38,38,38	0
55	MG	QA	1614	1/1	0.91	0.12	68,68,68,68	0
55	MG	YA	3045	1/1	0.91	0.16	3,3,3,3	0
55	MG	YA	3476	1/1	0.91	0.12	26,26,26,26	0
55	MG	YA	3477	1/1	0.91	0.15	24,24,24,24	0
55	MG	QA	1616	1/1	0.91	0.10	60,60,60,60	0
55	MG	YA	3255	1/1	0.91	0.21	35,35,35,35	0
55	MG	XA	1685	1/1	0.91	0.08	82,82,82,82	0
55	MG	RA	3076	1/1	0.91	0.25	34,34,34,34	0
55	MG	YA	3057	1/1	0.91	0.15	17,17,17,17	0
55	MG	RA	3253	1/1	0.91	0.28	52,52,52,52	0
55	MG	YA	3177	1/1	0.91	0.19	46,46,46,46	0
55	MG	RA	3189	1/1	0.91	0.22	31,31,31,31	0
55	MG	YA	3270	1/1	0.91	0.10	41,41,41,41	0
55	MG	YA	3091	1/1	0.92	0.10	26,26,26,26	0
55	MG	YA	3268	1/1	0.92	0.23	31,31,31,31	0
55	MG	YA	3269	1/1	0.92	0.18	39,39,39,39	0
55	MG	YA	3179	1/1	0.92	0.16	40,40,40,40	0
55	MG	RA	3418	1/1	0.92	0.09	53,53,53,53	0
55	MG	RA	3208	1/1	0.92	0.11	68,68,68,68	0
55	MG	YA	3278	1/1	0.92	0.22	49,49,49,49	0
55	MG	RA	3118	1/1	0.92	0.11	35,35,35,35	0
55	MG	YA	3506	1/1	0.92	0.15	42,42,42,42	0
55	MG	RA	3023	1/1	0.92	0.19	14,14,14,14	0
55	MG	YA	3106	1/1	0.92	0.24	21,21,21,21	0
55	MG	YA	3509	1/1	0.92	0.20	6,6,6,6	0
55	MG	YA	3510	1/1	0.92	0.13	40,40,40,40	0
55	MG	YB	201	1/1	0.92	0.11	12,12,12,12	0
55	MG	RA	3092	1/1	0.92	0.13	44,44,44,44	0
55	MG	YA	3386	1/1	0.92	0.18	47,47,47,47	0
55	MG	RA	3375	1/1	0.92	0.08	45,45,45,45	0
55	MG	YA	3388	1/1	0.92	0.19	38,38,38,38	0
55	MG	YA	3289	1/1	0.92	0.11	12,12,12,12	0
55	MG	RA	3289	1/1	0.92	0.24	46,46,46,46	0
55	MG	RA	3066	1/1	0.92	0.11	28,28,28,28	0
55	MG	RA	3381	1/1	0.92	0.13	69,69,69,69	0
55	MG	RA	3385	1/1	0.92	0.20	42,42,42,42	0
55	MG	RA	3188	1/1	0.92	0.27	62,62,62,62	0
55	MG	RA	3224	1/1	0.92	0.19	11,11,11,11	0
55	MG	YA	3401	1/1	0.92	0.14	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3439	1/1	0.92	0.10	39,39,39,39	0
55	MG	YA	3297	1/1	0.92	0.26	80,80,80,80	0
55	MG	YA	3298	1/1	0.92	0.15	59,59,59,59	0
55	MG	YA	3407	1/1	0.92	0.14	28,28,28,28	0
55	MG	RA	3333	1/1	0.92	0.13	34,34,34,34	0
55	MG	YA	3412	1/1	0.92	0.09	39,39,39,39	0
55	MG	XA	1613	1/1	0.92	0.14	63,63,63,63	0
55	MG	RA	3334	1/1	0.92	0.15	66,66,66,66	0
55	MG	XA	1616	1/1	0.92	0.14	18,18,18,18	0
55	MG	RA	3033	1/1	0.92	0.15	28,28,28,28	0
55	MG	YA	3134	1/1	0.92	0.14	23,23,23,23	0
55	MG	YA	3417	1/1	0.92	0.14	45,45,45,45	0
55	MG	RA	3169	1/1	0.92	0.07	46,46,46,46	0
55	MG	RA	3395	1/1	0.92	0.24	68,68,68,68	0
55	MG	XA	1633	1/1	0.92	0.08	49,49,49,49	0
55	MG	RA	3170	1/1	0.92	0.24	45,45,45,45	0
55	MG	YA	3142	1/1	0.92	0.12	26,26,26,26	0
55	MG	YA	3311	1/1	0.92	0.38	46,46,46,46	0
55	MG	RA	3342	1/1	0.92	0.13	45,45,45,45	0
55	MG	YA	3145	1/1	0.92	0.16	43,43,43,43	0
55	MG	YA	3430	1/1	0.92	0.20	58,58,58,58	0
55	MG	XA	1643	1/1	0.92	0.16	39,39,39,39	0
55	MG	RA	3035	1/1	0.92	0.13	44,44,44,44	0
55	MG	RA	3075	1/1	0.92	0.12	37,37,37,37	0
55	MG	RA	3024	1/1	0.92	0.19	32,32,32,32	0
55	MG	YA	3435	1/1	0.92	0.07	40,40,40,40	0
55	MG	YA	3322	1/1	0.92	0.50	96,96,96,96	0
55	MG	RA	3235	1/1	0.92	0.16	60,60,60,60	0
55	MG	YA	3030	1/1	0.92	0.23	26,26,26,26	0
55	MG	RA	3307	1/1	0.92	0.22	31,31,31,31	0
55	MG	RA	3017	1/1	0.92	0.13	3,3,3,3	0
55	MG	RA	3130	1/1	0.92	0.19	19,19,19,19	0
55	MG	YA	3158	1/1	0.92	0.13	26,26,26,26	0
55	MG	XA	1661	1/1	0.92	0.24	32,32,32,32	0
55	MG	RA	3081	1/1	0.92	0.25	24,24,24,24	0
55	MG	RA	3355	1/1	0.92	0.17	49,49,49,49	0
55	MG	YA	3452	1/1	0.92	0.20	40,40,40,40	0
55	MG	RA	3278	1/1	0.92	0.23	41,41,41,41	0
55	MG	YA	3058	1/1	0.92	0.11	13,13,13,13	0
55	MG	YA	3456	1/1	0.92	0.23	35,35,35,35	0
55	MG	RA	3467	1/1	0.92	0.20	54,54,54,54	0
55	MG	XA	1671	1/1	0.92	0.09	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3338	1/1	0.92	0.15	50,50,50,50	0
55	MG	YA	3461	1/1	0.92	0.10	45,45,45,45	0
55	MG	RA	3015	1/1	0.92	0.14	29,29,29,29	0
55	MG	YA	3070	1/1	0.92	0.24	34,34,34,34	0
55	MG	XA	1678	1/1	0.92	0.19	50,50,50,50	0
55	MG	RA	3313	1/1	0.92	0.14	60,60,60,60	0
55	MG	YA	3350	1/1	0.92	0.14	44,44,44,44	0
55	MG	YA	3252	1/1	0.92	0.17	24,24,24,24	0
55	MG	YA	3253	1/1	0.92	0.29	49,49,49,49	0
55	MG	YA	3074	1/1	0.92	0.12	28,28,28,28	0
55	MG	YA	3256	1/1	0.92	0.17	39,39,39,39	0
55	MG	YA	3174	1/1	0.92	0.19	36,36,36,36	0
55	MG	YA	3258	1/1	0.92	0.28	22,22,22,22	0
55	MG	RA	3030	1/1	0.92	0.22	29,29,29,29	0
55	MG	RA	3086	1/1	0.92	0.21	30,30,30,30	0
56	ZN	R4	101	1/1	0.92	0.08	319,319,319,319	0
55	MG	RA	3415	1/1	0.92	0.08	34,34,34,34	0
55	MG	RA	3220	1/1	0.93	0.17	41,41,41,41	0
55	MG	RA	3040	1/1	0.93	0.13	42,42,42,42	0
55	MG	RA	3422	1/1	0.93	0.14	40,40,40,40	0
55	MG	RA	3335	1/1	0.93	0.12	38,38,38,38	0
55	MG	YA	3076	1/1	0.93	0.26	23,23,23,23	0
55	MG	YA	3080	1/1	0.93	0.09	28,28,28,28	0
55	MG	YA	3183	1/1	0.93	0.16	39,39,39,39	0
55	MG	QA	1636	1/1	0.93	0.11	40,40,40,40	0
55	MG	YB	207	1/1	0.93	0.28	70,70,70,70	0
55	MG	YA	3082	1/1	0.93	0.20	21,21,21,21	0
55	MG	RA	3382	1/1	0.93	0.17	48,48,48,48	0
55	MG	RA	3336	1/1	0.93	0.21	51,51,51,51	0
55	MG	RA	3131	1/1	0.93	0.14	31,31,31,31	0
55	MG	YQ	201	1/1	0.93	0.11	42,42,42,42	0
55	MG	RA	3226	1/1	0.93	0.37	71,71,71,71	0
55	MG	YA	3100	1/1	0.93	0.22	15,15,15,15	0
55	MG	YA	3404	1/1	0.93	0.09	47,47,47,47	0
55	MG	RA	3429	1/1	0.93	0.14	64,64,64,64	0
55	MG	RA	3484	1/1	0.93	0.07	47,47,47,47	0
55	MG	YA	3408	1/1	0.93	0.11	3,3,3,3	0
55	MG	RA	3430	1/1	0.93	0.12	50,50,50,50	0
55	MG	QA	1646	1/1	0.93	0.08	56,56,56,56	0
55	MG	RA	3305	1/1	0.93	0.31	61,61,61,61	0
55	MG	RA	3010	1/1	0.93	0.14	31,31,31,31	0
55	MG	RA	3116	1/1	0.93	0.15	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3231	1/1	0.93	0.18	52,52,52,52	0
55	MG	XA	1612	1/1	0.93	0.20	36,36,36,36	0
55	MG	QA	1652	1/1	0.93	0.10	41,41,41,41	0
55	MG	RA	3191	1/1	0.93	0.13	125,125,125,125	0
55	MG	YA	3209	1/1	0.93	0.13	14,14,14,14	0
55	MG	YA	3125	1/1	0.93	0.11	27,27,27,27	0
55	MG	YA	3314	1/1	0.93	0.09	43,43,43,43	0
55	MG	YA	3315	1/1	0.93	0.13	22,22,22,22	0
55	MG	XA	1623	1/1	0.93	0.12	34,34,34,34	0
55	MG	QA	1656	1/1	0.93	0.21	25,25,25,25	0
55	MG	QA	1657	1/1	0.93	0.12	60,60,60,60	0
55	MG	RA	3157	1/1	0.93	0.21	38,38,38,38	0
55	MG	XA	1634	1/1	0.93	0.05	114,114,114,114	0
55	MG	RA	3255	1/1	0.93	0.24	50,50,50,50	0
55	MG	RA	3009	1/1	0.93	0.22	25,25,25,25	0
55	MG	XA	1638	1/1	0.93	0.15	39,39,39,39	0
55	MG	YA	3217	1/1	0.93	0.21	30,30,30,30	0
55	MG	YA	3436	1/1	0.93	0.24	58,58,58,58	0
55	MG	RA	3259	1/1	0.93	0.26	77,77,77,77	0
55	MG	RA	3101	1/1	0.93	0.14	29,29,29,29	0
55	MG	RA	3089	1/1	0.93	0.12	25,25,25,25	0
55	MG	RA	3184	1/1	0.93	0.22	43,43,43,43	0
55	MG	YA	3443	1/1	0.93	0.20	65,65,65,65	0
55	MG	YA	3139	1/1	0.93	0.16	27,27,27,27	0
55	MG	RA	3239	1/1	0.93	0.16	48,48,48,48	0
55	MG	YA	3143	1/1	0.93	0.18	68,68,68,68	0
55	MG	R1	300	1/1	0.93	0.25	46,46,46,46	0
55	MG	RA	3359	1/1	0.93	0.08	9,9,9,9	0
55	MG	YA	3010	1/1	0.93	0.10	44,44,44,44	0
55	MG	RA	3173	1/1	0.93	0.09	51,51,51,51	0
55	MG	YA	3235	1/1	0.93	0.27	34,34,34,34	0
55	MG	YA	3340	1/1	0.93	0.28	57,57,57,57	0
55	MG	XA	1659	1/1	0.93	0.07	53,53,53,53	0
55	MG	QA	1610	1/1	0.93	0.13	20,20,20,20	0
55	MG	RA	3451	1/1	0.93	0.17	37,37,37,37	0
55	MG	YA	3346	1/1	0.93	0.15	34,34,34,34	0
55	MG	XA	1664	1/1	0.93	0.14	56,56,56,56	0
55	MG	RA	3266	1/1	0.93	0.10	43,43,43,43	0
55	MG	YA	3026	1/1	0.93	0.24	13,13,13,13	0
55	MG	YA	3154	1/1	0.93	0.25	36,36,36,36	0
55	MG	YA	3354	1/1	0.93	0.15	54,54,54,54	0
55	MG	RA	3322	1/1	0.93	0.13	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3031	1/1	0.93	0.09	14,14,14,14	0
55	MG	RA	3366	1/1	0.93	0.19	49,49,49,49	0
55	MG	YA	3160	1/1	0.93	0.16	34,34,34,34	0
55	MG	YA	3473	1/1	0.93	0.33	56,56,56,56	0
55	MG	RA	3459	1/1	0.93	0.14	25,25,25,25	0
55	MG	RA	3295	1/1	0.93	0.18	29,29,29,29	0
55	MG	YA	3050	1/1	0.93	0.19	20,20,20,20	0
55	MG	XA	1680	1/1	0.93	0.09	23,23,23,23	0
55	MG	RA	3296	1/1	0.93	0.06	45,45,45,45	0
55	MG	YA	3262	1/1	0.93	0.17	40,40,40,40	0
55	MG	YA	3054	1/1	0.93	0.09	25,25,25,25	0
55	MG	QA	1619	1/1	0.93	0.07	67,67,67,67	0
55	MG	RA	3297	1/1	0.93	0.10	43,43,43,43	0
55	MG	RA	3330	1/1	0.93	0.10	27,27,27,27	0
55	MG	QA	1626	1/1	0.93	0.10	36,36,36,36	0
55	MG	YA	3499	1/1	0.93	0.07	37,37,37,37	0
55	MG	YA	3273	1/1	0.93	0.18	38,38,38,38	0
55	MG	YA	3068	1/1	0.93	0.20	32,32,32,32	0
55	MG	RA	3267	1/1	0.93	0.17	33,33,33,33	0
55	MG	QA	1603	1/1	0.94	0.23	25,25,25,25	0
55	MG	RA	3142	1/1	0.94	0.21	40,40,40,40	0
55	MG	YP	202	1/1	0.94	0.09	22,22,22,22	0
55	MG	YA	3319	1/1	0.94	0.08	33,33,33,33	0
55	MG	YA	3320	1/1	0.94	0.25	18,18,18,18	0
55	MG	YA	3159	1/1	0.94	0.08	31,31,31,31	0
55	MG	RA	3190	1/1	0.94	0.18	25,25,25,25	0
55	MG	YA	3421	1/1	0.94	0.16	68,68,68,68	0
55	MG	RA	3159	1/1	0.94	0.09	29,29,29,29	0
55	MG	RA	3364	1/1	0.94	0.04	36,36,36,36	0
55	MG	XA	1603	1/1	0.94	0.18	30,30,30,30	0
55	MG	YA	3079	1/1	0.94	0.11	10,10,10,10	0
55	MG	YA	3164	1/1	0.94	0.05	64,64,64,64	0
55	MG	YA	3247	1/1	0.94	0.27	30,30,30,30	0
55	MG	YA	3165	1/1	0.94	0.11	26,26,26,26	0
55	MG	YA	3250	1/1	0.94	0.18	40,40,40,40	0
55	MG	YA	3432	1/1	0.94	0.11	37,37,37,37	0
55	MG	RA	3160	1/1	0.94	0.13	47,47,47,47	0
55	MG	RA	3436	1/1	0.94	0.08	57,57,57,57	0
55	MG	YA	3335	1/1	0.94	0.18	44,44,44,44	0
55	MG	RA	3113	1/1	0.94	0.10	38,38,38,38	0
55	MG	RA	3476	1/1	0.94	0.17	21,21,21,21	0
55	MG	RA	3196	1/1	0.94	0.15	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	QF	201	1/1	0.94	0.08	50,50,50,50	0
55	MG	RA	3277	1/1	0.94	0.08	36,36,36,36	0
55	MG	YA	3097	1/1	0.94	0.17	27,27,27,27	0
55	MG	QA	1620	1/1	0.94	0.16	45,45,45,45	0
55	MG	YA	3345	1/1	0.94	0.06	30,30,30,30	0
55	MG	RA	3087	1/1	0.94	0.14	26,26,26,26	0
55	MG	YA	3102	1/1	0.94	0.15	16,16,16,16	0
55	MG	YA	3266	1/1	0.94	0.26	22,22,22,22	0
55	MG	YA	3104	1/1	0.94	0.19	12,12,12,12	0
55	MG	RA	3374	1/1	0.94	0.10	47,47,47,47	0
55	MG	QA	1625	1/1	0.94	0.23	55,55,55,55	0
55	MG	YA	3455	1/1	0.94	0.11	56,56,56,56	0
55	MG	RA	3199	1/1	0.94	0.23	48,48,48,48	0
55	MG	RA	3320	1/1	0.94	0.12	32,32,32,32	0
55	MG	YA	3012	1/1	0.94	0.19	42,42,42,42	0
55	MG	YA	3117	1/1	0.94	0.06	34,34,34,34	0
55	MG	RA	3377	1/1	0.94	0.12	80,80,80,80	0
55	MG	RA	3348	1/1	0.94	0.05	60,60,60,60	0
55	MG	YA	3369	1/1	0.94	0.07	61,61,61,61	0
55	MG	XA	1651	1/1	0.94	0.13	40,40,40,40	0
55	MG	QA	1633	1/1	0.94	0.11	41,41,41,41	0
55	MG	RA	3152	1/1	0.94	0.10	31,31,31,31	0
55	MG	RB	205	1/1	0.94	0.18	38,38,38,38	0
55	MG	XA	1655	1/1	0.94	0.18	40,40,40,40	0
55	MG	YA	3373	1/1	0.94	0.12	43,43,43,43	0
55	MG	YA	3284	1/1	0.94	0.09	3,3,3,3	0
55	MG	YA	3286	1/1	0.94	0.18	48,48,48,48	0
55	MG	YA	3474	1/1	0.94	0.22	65,65,65,65	0
55	MG	XA	1660	1/1	0.94	0.07	51,51,51,51	0
55	MG	RA	3448	1/1	0.94	0.20	47,47,47,47	0
55	MG	YA	3034	1/1	0.94	0.17	8,8,8,8	0
55	MG	YA	3485	1/1	0.94	0.10	3,3,3,3	0
55	MG	YA	3035	1/1	0.94	0.23	12,12,12,12	0
55	MG	YA	3131	1/1	0.94	0.08	25,25,25,25	0
55	MG	RA	3350	1/1	0.94	0.14	39,39,39,39	0
55	MG	RA	3218	1/1	0.94	0.20	33,33,33,33	0
55	MG	YA	3043	1/1	0.94	0.12	13,13,13,13	0
55	MG	YA	3495	1/1	0.94	0.17	51,51,51,51	0
55	MG	YA	3044	1/1	0.94	0.15	18,18,18,18	0
55	MG	QA	1640	1/1	0.94	0.11	46,46,46,46	0
55	MG	YA	3046	1/1	0.94	0.27	24,24,24,24	0
55	MG	RA	3240	1/1	0.94	0.23	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3174	1/1	0.94	0.18	31,31,31,31	0
55	MG	RA	3455	1/1	0.94	0.15	10,10,10,10	0
55	MG	YA	3055	1/1	0.94	0.23	33,33,33,33	0
55	MG	RA	3042	1/1	0.94	0.23	20,20,20,20	0
55	MG	YA	3146	1/1	0.94	0.17	26,26,26,26	0
55	MG	RA	3079	1/1	0.94	0.09	26,26,26,26	0
55	MG	RA	3356	1/1	0.94	0.22	49,49,49,49	0
55	MG	XA	1684	1/1	0.94	0.20	41,41,41,41	0
55	MG	YA	3062	1/1	0.94	0.22	25,25,25,25	0
55	MG	YA	3064	1/1	0.94	0.20	3,3,3,3	0
55	MG	RA	3331	1/1	0.94	0.08	42,42,42,42	0
55	MG	YB	203	1/1	0.94	0.07	36,36,36,36	0
55	MG	YA	3313	1/1	0.94	0.16	48,48,48,48	0
55	MG	YA	3066	1/1	0.94	0.24	17,17,17,17	0
55	MG	RA	3288	1/1	0.94	0.45	67,67,67,67	0
55	MG	RA	3106	1/1	0.94	0.11	16,16,16,16	0
55	MG	RA	3217	1/1	0.95	0.16	28,28,28,28	0
55	MG	YA	3489	1/1	0.95	0.21	37,37,37,37	0
55	MG	YA	3361	1/1	0.95	0.23	45,45,45,45	0
55	MG	RB	207	1/1	0.95	0.17	26,26,26,26	0
55	MG	YA	3260	1/1	0.95	0.34	64,64,64,64	0
55	MG	YA	3367	1/1	0.95	0.19	39,39,39,39	0
55	MG	RA	3195	1/1	0.95	0.06	46,46,46,46	0
55	MG	RE	302	1/1	0.95	0.14	33,33,33,33	0
55	MG	RA	3102	1/1	0.95	0.14	34,34,34,34	0
55	MG	YA	3265	1/1	0.95	0.20	25,25,25,25	0
55	MG	RA	3284	1/1	0.95	0.18	43,43,43,43	0
55	MG	YA	3503	1/1	0.95	0.14	2,2,2,2	0
55	MG	RO	201	1/1	0.95	0.05	79,79,79,79	0
55	MG	QA	1651	1/1	0.95	0.07	36,36,36,36	0
55	MG	RA	3044	1/1	0.95	0.18	24,24,24,24	0
55	MG	RA	3085	1/1	0.95	0.12	16,16,16,16	0
55	MG	YA	3272	1/1	0.95	0.13	38,38,38,38	0
55	MG	YA	3381	1/1	0.95	0.10	20,20,20,20	0
55	MG	RA	3143	1/1	0.95	0.17	40,40,40,40	0
55	MG	YA	3274	1/1	0.95	0.26	40,40,40,40	0
55	MG	YA	3384	1/1	0.95	0.10	35,35,35,35	0
55	MG	RA	3027	1/1	0.95	0.11	22,22,22,22	0
55	MG	YB	206	1/1	0.95	0.10	10,10,10,10	0
55	MG	YA	3276	1/1	0.95	0.17	16,16,16,16	0
55	MG	RA	3256	1/1	0.95	0.11	38,38,38,38	0
55	MG	YA	3089	1/1	0.95	0.06	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3124	1/1	0.95	0.23	27,27,27,27	0
55	MG	QA	1661	1/1	0.95	0.17	75,75,75,75	0
55	MG	RA	3404	1/1	0.95	0.15	56,56,56,56	0
55	MG	RA	3004	1/1	0.95	0.23	27,27,27,27	0
55	MG	RA	3324	1/1	0.95	0.18	40,40,40,40	0
55	MG	YA	3285	1/1	0.95	0.23	45,45,45,45	0
55	MG	YA	3398	1/1	0.95	0.12	36,36,36,36	0
55	MG	RA	3078	1/1	0.95	0.14	20,20,20,20	0
55	MG	YA	3400	1/1	0.95	0.23	44,44,44,44	0
55	MG	QA	1605	1/1	0.95	0.25	27,27,27,27	0
55	MG	QA	1607	1/1	0.95	0.05	37,37,37,37	0
55	MG	YA	3103	1/1	0.95	0.09	11,11,11,11	0
55	MG	XA	1606	1/1	0.95	0.13	35,35,35,35	0
55	MG	YA	3003	1/1	0.95	0.13	49,49,49,49	0
55	MG	YA	3188	1/1	0.95	0.04	28,28,28,28	0
55	MG	RA	3069	1/1	0.95	0.16	23,23,23,23	0
55	MG	RA	3080	1/1	0.95	0.13	39,39,39,39	0
55	MG	RA	3367	1/1	0.95	0.17	28,28,28,28	0
55	MG	YA	3411	1/1	0.95	0.09	61,61,61,61	0
55	MG	YA	3109	1/1	0.95	0.08	3,3,3,3	0
55	MG	RA	3072	1/1	0.95	0.15	24,24,24,24	0
55	MG	XA	1615	1/1	0.95	0.10	22,22,22,22	0
55	MG	RA	3264	1/1	0.95	0.14	34,34,34,34	0
55	MG	YA	3112	1/1	0.95	0.21	19,19,19,19	0
55	MG	XA	1618	1/1	0.95	0.31	54,54,54,54	0
55	MG	YA	3113	1/1	0.95	0.12	16,16,16,16	0
55	MG	YA	3115	1/1	0.95	0.10	18,18,18,18	0
55	MG	QA	1615	1/1	0.95	0.07	46,46,46,46	0
55	MG	XA	1627	1/1	0.95	0.20	22,22,22,22	0
55	MG	YA	3013	1/1	0.95	0.13	14,14,14,14	0
55	MG	YA	3422	1/1	0.95	0.15	54,54,54,54	0
55	MG	YA	3423	1/1	0.95	0.09	41,41,41,41	0
55	MG	RA	3060	1/1	0.95	0.12	27,27,27,27	0
55	MG	YA	3015	1/1	0.95	0.12	3,3,3,3	0
55	MG	YA	3308	1/1	0.95	0.04	39,39,39,39	0
55	MG	RA	3416	1/1	0.95	0.15	49,49,49,49	0
55	MG	YA	3428	1/1	0.95	0.25	41,41,41,41	0
55	MG	YA	3124	1/1	0.95	0.10	17,17,17,17	0
55	MG	RA	3209	1/1	0.95	0.10	25,25,25,25	0
55	MG	YA	3211	1/1	0.95	0.06	29,29,29,29	0
55	MG	YA	3126	1/1	0.95	0.17	3,3,3,3	0
55	MG	YA	3018	1/1	0.95	0.19	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3128	1/1	0.95	0.17	49,49,49,49	0
55	MG	RA	3134	1/1	0.95	0.14	33,33,33,33	0
55	MG	YA	3027	1/1	0.95	0.22	19,19,19,19	0
55	MG	RA	3095	1/1	0.95	0.14	21,21,21,21	0
55	MG	RA	3302	1/1	0.95	0.18	43,43,43,43	0
55	MG	YA	3219	1/1	0.95	0.09	49,49,49,49	0
55	MG	RA	3241	1/1	0.95	0.27	38,38,38,38	0
55	MG	RA	3339	1/1	0.95	0.13	66,66,66,66	0
55	MG	RA	3425	1/1	0.95	0.21	62,62,62,62	0
55	MG	YA	3040	1/1	0.95	0.12	3,3,3,3	0
55	MG	YA	3447	1/1	0.95	0.16	34,34,34,34	0
55	MG	YA	3041	1/1	0.95	0.15	3,3,3,3	0
55	MG	YA	3327	1/1	0.95	0.11	14,14,14,14	0
55	MG	QA	1627	1/1	0.95	0.05	51,51,51,51	0
55	MG	RA	3380	1/1	0.95	0.06	44,44,44,44	0
55	MG	RA	3477	1/1	0.95	0.14	42,42,42,42	0
55	MG	RA	3270	1/1	0.95	0.17	33,33,33,33	0
55	MG	YA	3231	1/1	0.95	0.08	23,23,23,23	0
55	MG	RA	3099	1/1	0.95	0.13	28,28,28,28	0
55	MG	YA	3457	1/1	0.95	0.13	74,74,74,74	0
55	MG	YA	3234	1/1	0.95	0.11	35,35,35,35	0
55	MG	YA	3049	1/1	0.95	0.21	3,3,3,3	0
55	MG	YA	3460	1/1	0.95	0.18	85,85,85,85	0
55	MG	YA	3237	1/1	0.95	0.14	3,3,3,3	0
55	MG	RA	3384	1/1	0.95	0.25	60,60,60,60	0
55	MG	RA	3213	1/1	0.95	0.06	36,36,36,36	0
55	MG	RA	3483	1/1	0.95	0.14	30,30,30,30	0
55	MG	YA	3246	1/1	0.95	0.15	17,17,17,17	0
55	MG	YA	3344	1/1	0.95	0.07	40,40,40,40	0
55	MG	RA	3244	1/1	0.95	0.20	39,39,39,39	0
55	MG	YA	3469	1/1	0.95	0.20	44,44,44,44	0
55	MG	RA	3346	1/1	0.95	0.11	41,41,41,41	0
55	MG	YA	3249	1/1	0.95	0.24	32,32,32,32	0
55	MG	YA	3152	1/1	0.95	0.09	30,30,30,30	0
55	MG	RA	3433	1/1	0.95	0.12	42,42,42,42	0
55	MG	RA	3245	1/1	0.95	0.17	40,40,40,40	0
55	MG	YA	3061	1/1	0.95	0.24	27,27,27,27	0
55	MG	YA	3479	1/1	0.95	0.22	3,3,3,3	0
55	MG	YA	3480	1/1	0.95	0.19	3,3,3,3	0
55	MG	YA	3481	1/1	0.95	0.18	3,3,3,3	0
55	MG	RA	3155	1/1	0.95	0.12	41,41,41,41	0
55	MG	YA	3063	1/1	0.95	0.08	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3083	1/1	0.95	0.15	5,5,5,5	0
55	MG	YA	3088	1/1	0.96	0.07	9,9,9,9	0
55	MG	Y5	102	1/1	0.96	0.07	25,25,25,25	0
55	MG	YA	3441	1/1	0.96	0.08	38,38,38,38	0
55	MG	YA	3362	1/1	0.96	0.12	27,27,27,27	0
55	MG	YA	3364	1/1	0.96	0.30	72,72,72,72	0
55	MG	YA	3020	1/1	0.96	0.09	3,3,3,3	0
55	MG	YA	3445	1/1	0.96	0.06	32,32,32,32	0
55	MG	YA	3023	1/1	0.96	0.15	3,3,3,3	0
55	MG	YA	3025	1/1	0.96	0.12	19,19,19,19	0
55	MG	RA	3064	1/1	0.96	0.14	26,26,26,26	0
55	MG	YA	3094	1/1	0.96	0.17	18,18,18,18	0
55	MG	RA	3465	1/1	0.96	0.15	61,61,61,61	0
55	MG	RA	3343	1/1	0.96	0.14	34,34,34,34	0
55	MG	RA	3090	1/1	0.96	0.11	27,27,27,27	0
55	MG	R5	101	1/1	0.96	0.10	43,43,43,43	0
55	MG	RA	3132	1/1	0.96	0.12	40,40,40,40	0
55	MG	YA	3037	1/1	0.96	0.07	3,3,3,3	0
55	MG	YA	3377	1/1	0.96	0.16	26,26,26,26	0
55	MG	YA	3378	1/1	0.96	0.16	23,23,23,23	0
55	MG	YA	3038	1/1	0.96	0.16	14,14,14,14	0
55	MG	RA	3471	1/1	0.96	0.13	20,20,20,20	0
55	MG	YA	3232	1/1	0.96	0.21	22,22,22,22	0
55	MG	XA	1625	1/1	0.96	0.05	59,59,59,59	0
55	MG	RA	3133	1/1	0.96	0.06	31,31,31,31	0
55	MG	RA	3251	1/1	0.96	0.10	30,30,30,30	0
55	MG	YA	3168	1/1	0.96	0.17	41,41,41,41	0
55	MG	XA	1632	1/1	0.96	0.17	25,25,25,25	0
55	MG	RA	3273	1/1	0.96	0.07	31,31,31,31	0
55	MG	RA	3179	1/1	0.96	0.12	54,54,54,54	0
55	MG	RA	3438	1/1	0.96	0.12	33,33,33,33	0
55	MG	XA	1636	1/1	0.96	0.05	77,77,77,77	0
55	MG	YA	3242	1/1	0.96	0.19	3,3,3,3	0
55	MG	YA	3389	1/1	0.96	0.10	39,39,39,39	0
55	MG	RA	3091	1/1	0.96	0.14	15,15,15,15	0
55	MG	YA	3245	1/1	0.96	0.25	11,11,11,11	0
55	MG	RA	3378	1/1	0.96	0.15	41,41,41,41	0
55	MG	YA	3048	1/1	0.96	0.20	3,3,3,3	0
55	MG	QA	1655	1/1	0.96	0.32	34,34,34,34	0
55	MG	RA	3479	1/1	0.96	0.09	44,44,44,44	0
55	MG	RA	3065	1/1	0.96	0.17	32,32,32,32	0
55	MG	RA	3011	1/1	0.96	0.09	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3122	1/1	0.96	0.16	1,1,1,1	0
55	MG	RA	3279	1/1	0.96	0.08	43,43,43,43	0
55	MG	RA	3019	1/1	0.96	0.16	3,3,3,3	0
55	MG	RA	3383	1/1	0.96	0.10	37,37,37,37	0
55	MG	RA	3414	1/1	0.96	0.20	45,45,45,45	0
55	MG	YA	3491	1/1	0.96	0.26	29,29,29,29	0
55	MG	YA	3060	1/1	0.96	0.13	5,5,5,5	0
55	MG	YA	3493	1/1	0.96	0.06	22,22,22,22	0
55	MG	YA	3187	1/1	0.96	0.12	10,10,10,10	0
55	MG	RA	3257	1/1	0.96	0.17	44,44,44,44	0
55	MG	RA	3238	1/1	0.96	0.08	20,20,20,20	0
55	MG	RA	3139	1/1	0.96	0.12	37,37,37,37	0
55	MG	RA	3058	1/1	0.96	0.25	12,12,12,12	0
55	MG	YA	3413	1/1	0.96	0.07	42,42,42,42	0
55	MG	YA	3264	1/1	0.96	0.23	14,14,14,14	0
55	MG	RA	3096	1/1	0.96	0.16	38,38,38,38	0
55	MG	RA	3391	1/1	0.96	0.18	65,65,65,65	0
55	MG	XA	1666	1/1	0.96	0.08	61,61,61,61	0
55	MG	QA	1629	1/1	0.96	0.14	25,25,25,25	0
55	MG	YA	3505	1/1	0.96	0.23	39,39,39,39	0
55	MG	YA	3198	1/1	0.96	0.23	28,28,28,28	0
55	MG	RA	3222	1/1	0.96	0.15	34,34,34,34	0
55	MG	RA	3223	1/1	0.96	0.21	37,37,37,37	0
55	MG	QA	1632	1/1	0.96	0.07	39,39,39,39	0
55	MG	YA	3138	1/1	0.96	0.11	14,14,14,14	0
55	MG	RA	3003	1/1	0.96	0.20	16,16,16,16	0
55	MG	YA	3205	1/1	0.96	0.14	41,41,41,41	0
55	MG	YA	3140	1/1	0.96	0.17	17,17,17,17	0
55	MG	YB	204	1/1	0.96	0.17	23,23,23,23	0
55	MG	YA	3347	1/1	0.96	0.13	40,40,40,40	0
55	MG	YA	3349	1/1	0.96	0.17	68,68,68,68	0
55	MG	RA	3100	1/1	0.96	0.18	58,58,58,58	0
55	MG	YD	301	1/1	0.96	0.10	32,32,32,32	0
55	MG	RA	3460	1/1	0.96	0.08	33,33,33,33	0
55	MG	YA	3352	1/1	0.96	0.24	42,42,42,42	0
55	MG	XA	1686	1/1	0.96	0.18	34,34,34,34	0
55	MG	YA	3078	1/1	0.96	0.18	19,19,19,19	0
55	MG	RA	3365	1/1	0.96	0.18	40,40,40,40	0
55	MG	QA	1637	1/1	0.96	0.16	31,31,31,31	0
55	MG	RA	3462	1/1	0.96	0.08	59,59,59,59	0
55	MG	RA	3041	1/1	0.96	0.12	30,30,30,30	0
55	MG	YA	3084	1/1	0.96	0.10	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3085	1/1	0.96	0.11	13,13,13,13	0
56	ZN	XN	101	1/1	0.96	0.08	184,184,184,184	0
55	MG	YA	3007	1/1	0.97	0.06	32,32,32,32	0
55	MG	QA	1623	1/1	0.97	0.06	43,43,43,43	0
55	MG	Y7	101	1/1	0.97	0.08	28,28,28,28	0
55	MG	YA	3073	1/1	0.97	0.11	3,3,3,3	0
55	MG	YA	3283	1/1	0.97	0.09	8,8,8,8	0
55	MG	RA	3043	1/1	0.97	0.10	10,10,10,10	0
55	MG	YA	3363	1/1	0.97	0.07	29,29,29,29	0
55	MG	RA	3325	1/1	0.97	0.10	30,30,30,30	0
55	MG	RA	3362	1/1	0.97	0.09	24,24,24,24	0
55	MG	YA	3287	1/1	0.97	0.14	64,64,64,64	0
55	MG	YA	3077	1/1	0.97	0.14	22,22,22,22	0
55	MG	RA	3052	1/1	0.97	0.09	27,27,27,27	0
55	MG	RA	3020	1/1	0.97	0.04	21,21,21,21	0
55	MG	RA	3329	1/1	0.97	0.24	59,59,59,59	0
55	MG	RA	3158	1/1	0.97	0.05	31,31,31,31	0
55	MG	RA	3098	1/1	0.97	0.10	28,28,28,28	0
55	MG	RA	3138	1/1	0.97	0.07	27,27,27,27	0
55	MG	RA	3408	1/1	0.97	0.09	56,56,56,56	0
55	MG	YA	3155	1/1	0.97	0.15	28,28,28,28	0
55	MG	YA	3086	1/1	0.97	0.16	3,3,3,3	0
55	MG	YA	3087	1/1	0.97	0.13	0,0,0,0	0
55	MG	YA	3019	1/1	0.97	0.12	7,7,7,7	0
55	MG	XA	1621	1/1	0.97	0.11	34,34,34,34	0
55	MG	XA	1622	1/1	0.97	0.06	40,40,40,40	0
55	MG	RA	3117	1/1	0.97	0.10	30,30,30,30	0
55	MG	YA	3463	1/1	0.97	0.25	38,38,38,38	0
55	MG	XA	1626	1/1	0.97	0.08	10,10,10,10	0
55	MG	YA	3301	1/1	0.97	0.06	31,31,31,31	0
55	MG	XA	1628	1/1	0.97	0.09	35,35,35,35	0
55	MG	YA	3021	1/1	0.97	0.10	13,13,13,13	0
55	MG	RA	3054	1/1	0.97	0.16	22,22,22,22	0
55	MG	YA	3230	1/1	0.97	0.17	16,16,16,16	0
55	MG	RA	3163	1/1	0.97	0.18	39,39,39,39	0
55	MG	RA	3070	1/1	0.97	0.13	11,11,11,11	0
55	MG	RA	3452	1/1	0.97	0.19	8,8,8,8	0
55	MG	YA	3028	1/1	0.97	0.14	6,6,6,6	0
55	MG	YA	3029	1/1	0.97	0.14	3,3,3,3	0
55	MG	RA	3071	1/1	0.97	0.15	12,12,12,12	0
55	MG	RA	3055	1/1	0.97	0.09	3,3,3,3	0
55	MG	YA	3392	1/1	0.97	0.14	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3240	1/1	0.97	0.17	3,3,3,3	0
55	MG	YA	3033	1/1	0.97	0.18	12,12,12,12	0
55	MG	RA	3456	1/1	0.97	0.07	8,8,8,8	0
55	MG	XA	1644	1/1	0.97	0.12	54,54,54,54	0
55	MG	YA	3483	1/1	0.97	0.08	3,3,3,3	0
55	MG	YA	3484	1/1	0.97	0.12	3,3,3,3	0
55	MG	YA	3396	1/1	0.97	0.08	43,43,43,43	0
55	MG	RA	3272	1/1	0.97	0.25	45,45,45,45	0
55	MG	RA	3073	1/1	0.97	0.24	25,25,25,25	0
55	MG	XA	1650	1/1	0.97	0.20	32,32,32,32	0
55	MG	RA	3417	1/1	0.97	0.18	47,47,47,47	0
55	MG	RA	3216	1/1	0.97	0.14	37,37,37,37	0
55	MG	YA	3490	1/1	0.97	0.29	23,23,23,23	0
55	MG	RA	3275	1/1	0.97	0.10	32,32,32,32	0
55	MG	RA	3123	1/1	0.97	0.15	16,16,16,16	0
55	MG	RA	3421	1/1	0.97	0.12	34,34,34,34	0
55	MG	QA	1602	1/1	0.97	0.24	39,39,39,39	0
55	MG	RA	3104	1/1	0.97	0.07	45,45,45,45	0
55	MG	YA	3406	1/1	0.97	0.13	8,8,8,8	0
55	MG	RA	3219	1/1	0.97	0.18	13,13,13,13	0
55	MG	YA	3254	1/1	0.97	0.17	4,4,4,4	0
55	MG	RA	3021	1/1	0.97	0.15	12,12,12,12	0
55	MG	YA	3329	1/1	0.97	0.09	12,12,12,12	0
55	MG	YA	3501	1/1	0.97	0.18	70,70,70,70	0
55	MG	YA	3047	1/1	0.97	0.16	16,16,16,16	0
55	MG	QA	1653	1/1	0.97	0.10	45,45,45,45	0
55	MG	RA	3194	1/1	0.97	0.14	38,38,38,38	0
55	MG	QA	1608	1/1	0.97	0.06	42,42,42,42	0
55	MG	RA	3469	1/1	0.97	0.19	22,22,22,22	0
55	MG	YA	3189	1/1	0.97	0.26	44,44,44,44	0
55	MG	RA	3022	1/1	0.97	0.05	22,22,22,22	0
55	MG	XA	1672	1/1	0.97	0.09	34,34,34,34	0
55	MG	YA	3191	1/1	0.97	0.11	27,27,27,27	0
55	MG	RA	3013	1/1	0.97	0.11	15,15,15,15	0
55	MG	QA	1659	1/1	0.97	0.06	73,73,73,73	0
55	MG	RA	3001	1/1	0.97	0.06	15,15,15,15	0
55	MG	RA	3109	1/1	0.97	0.05	33,33,33,33	0
55	MG	YA	3059	1/1	0.97	0.08	7,7,7,7	0
55	MG	RA	3227	1/1	0.97	0.22	38,38,38,38	0
55	MG	RA	3318	1/1	0.97	0.19	27,27,27,27	0
55	MG	YA	3271	1/1	0.97	0.08	25,25,25,25	0
55	MG	YA	3348	1/1	0.97	0.04	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YE	301	1/1	0.97	0.21	24,24,24,24	0
55	MG	RA	3110	1/1	0.97	0.08	39,39,39,39	0
55	MG	YA	3201	1/1	0.97	0.07	28,28,28,28	0
55	MG	RA	3063	1/1	0.97	0.10	12,12,12,12	0
55	MG	RA	3230	1/1	0.97	0.15	40,40,40,40	0
55	MG	YP	201	1/1	0.97	0.10	22,22,22,22	0
55	MG	RA	3016	1/1	0.97	0.16	23,23,23,23	0
55	MG	QA	1621	1/1	0.97	0.07	35,35,35,35	0
55	MG	YA	3355	1/1	0.97	0.10	33,33,33,33	0
55	MG	RA	3290	1/1	0.97	0.18	32,32,32,32	0
55	MG	YA	3006	1/1	0.97	0.17	40,40,40,40	0
55	MG	YA	3181	1/1	0.98	0.04	18,18,18,18	0
55	MG	QA	1664	1/1	0.98	0.20	35,35,35,35	0
55	MG	QA	1665	1/1	0.98	0.06	27,27,27,27	0
55	MG	YA	3051	1/1	0.98	0.08	3,3,3,3	0
55	MG	YA	3341	1/1	0.98	0.19	24,24,24,24	0
55	MG	YA	3478	1/1	0.98	0.15	3,3,3,3	0
55	MG	YA	3052	1/1	0.98	0.15	17,17,17,17	0
55	MG	YA	3116	1/1	0.98	0.05	19,19,19,19	0
55	MG	RA	3048	1/1	0.98	0.17	24,24,24,24	0
55	MG	YA	3482	1/1	0.98	0.19	3,3,3,3	0
55	MG	YA	3118	1/1	0.98	0.13	14,14,14,14	0
55	MG	RA	3026	1/1	0.98	0.11	5,5,5,5	0
55	MG	RA	3221	1/1	0.98	0.25	44,44,44,44	0
55	MG	YA	3227	1/1	0.98	0.09	18,18,18,18	0
55	MG	RA	3034	1/1	0.98	0.07	9,9,9,9	0
55	MG	XA	1605	1/1	0.98	0.05	33,33,33,33	0
55	MG	YA	3307	1/1	0.98	0.04	48,48,48,48	0
55	MG	YA	3439	1/1	0.98	0.07	27,27,27,27	0
55	MG	RA	3005	1/1	0.98	0.22	31,31,31,31	0
55	MG	YA	3309	1/1	0.98	0.15	35,35,35,35	0
55	MG	QA	1606	1/1	0.98	0.09	51,51,51,51	0
55	MG	YA	3005	1/1	0.98	0.18	28,28,28,28	0
55	MG	RA	3388	1/1	0.98	0.11	40,40,40,40	0
55	MG	RA	3304	1/1	0.98	0.18	29,29,29,29	0
55	MG	QA	1609	1/1	0.98	0.06	9,9,9,9	0
55	MG	RA	3390	1/1	0.98	0.14	42,42,42,42	0
55	MG	YA	3448	1/1	0.98	0.06	36,36,36,36	0
55	MG	YA	3236	1/1	0.98	0.10	9,9,9,9	0
55	MG	YA	3093	1/1	0.98	0.10	3,3,3,3	0
55	MG	YA	3238	1/1	0.98	0.14	3,3,3,3	0
55	MG	RA	3067	1/1	0.98	0.06	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3095	1/1	0.98	0.13	3,3,3,3	0
55	MG	RP	201	1/1	0.98	0.16	49,49,49,49	0
55	MG	RA	3434	1/1	0.98	0.15	40,40,40,40	0
55	MG	XA	1624	1/1	0.98	0.04	34,34,34,34	0
55	MG	YA	3067	1/1	0.98	0.24	29,29,29,29	0
55	MG	YA	3244	1/1	0.98	0.17	28,28,28,28	0
55	MG	YA	3368	1/1	0.98	0.04	33,33,33,33	0
55	MG	RA	3197	1/1	0.98	0.13	42,42,42,42	0
55	MG	XA	1629	1/1	0.98	0.10	6,6,6,6	0
55	MG	RA	3341	1/1	0.98	0.05	28,28,28,28	0
55	MG	RA	3468	1/1	0.98	0.04	33,33,33,33	0
55	MG	RA	3485	1/1	0.98	0.05	64,64,64,64	0
55	MG	YA	3072	1/1	0.98	0.06	1,1,1,1	0
55	MG	YA	3418	1/1	0.98	0.13	19,19,19,19	0
55	MG	RA	3025	1/1	0.98	0.07	3,3,3,3	0
55	MG	YA	3141	1/1	0.98	0.07	3,3,3,3	0
55	MG	YA	3107	1/1	0.98	0.18	17,17,17,17	0
55	MG	RA	3126	1/1	0.98	0.12	12,12,12,12	0
55	MG	RA	3037	1/1	0.98	0.15	1,1,1,1	0
56	ZN	QN	101	1/1	0.98	0.08	174,174,174,174	0
55	MG	YA	3470	1/1	0.98	0.21	40,40,40,40	0
55	MG	R8	101	1/1	0.98	0.32	37,37,37,37	0
57	SF4	QD	301	8/8	0.98	0.05	82,98,127,192	0
57	SF4	XD	301	8/8	0.98	0.06	82,105,120,139	0
55	MG	RA	3032	1/1	0.99	0.04	19,19,19,19	0
55	MG	XA	1602	1/1	0.99	0.06	40,40,40,40	0
55	MG	YA	3331	1/1	0.99	0.08	22,22,22,22	0
55	MG	YA	3196	1/1	0.99	0.06	53,53,53,53	0
55	MG	YA	3032	1/1	0.99	0.12	15,15,15,15	0
55	MG	YA	3169	1/1	0.99	0.06	16,16,16,16	0
55	MG	RA	3097	1/1	0.99	0.05	20,20,20,20	0
55	MG	RA	3328	1/1	0.99	0.06	16,16,16,16	0
55	MG	RA	3061	1/1	0.99	0.05	18,18,18,18	0
55	MG	YA	3036	1/1	0.99	0.12	3,3,3,3	0
55	MG	RA	3057	1/1	0.99	0.25	8,8,8,8	0
55	MG	RA	3002	1/1	0.99	0.14	36,36,36,36	0
55	MG	YA	3083	1/1	0.99	0.04	13,13,13,13	0
55	MG	RA	3369	1/1	0.99	0.05	18,18,18,18	0
55	MG	YA	3475	1/1	0.99	0.06	3,3,3,3	0
56	ZN	R5	102	1/1	0.99	0.06	117,117,117,117	0
56	ZN	R6	101	1/1	0.99	0.04	93,93,93,93	0
56	ZN	R9	101	1/1	0.99	0.06	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RE	301	1/1	0.99	0.04	12,12,12,12	0
56	ZN	YY	201	1/1	0.99	0.03	74,74,74,74	0
55	MG	YA	3098	1/1	0.99	0.05	6,6,6,6	0
56	ZN	Y5	101	1/1	0.99	0.03	74,74,74,74	0
56	ZN	Y6	101	1/1	0.99	0.02	46,46,46,46	0
56	ZN	Y9	101	1/1	0.99	0.05	63,63,63,63	0
55	MG	YA	3409	1/1	0.99	0.12	36,36,36,36	0
55	MG	RA	3454	1/1	0.99	0.07	2,2,2,2	0
55	MG	XA	1677	1/1	0.99	0.11	39,39,39,39	0
55	MG	YA	3024	1/1	1.00	0.04	3,3,3,3	0
55	MG	RA	3059	1/1	1.00	0.04	21,21,21,21	0
56	ZN	RY	201	1/1	1.00	0.04	116,116,116,116	0
55	MG	YA	3114	1/1	1.00	0.05	0,0,0,0	0
55	MG	RA	3368	1/1	1.00	0.02	13,13,13,13	0
55	MG	YA	3022	1/1	1.00	0.06	7,7,7,7	0
55	MG	RA	3014	1/1	1.00	0.06	8,8,8,8	0
55	MG	YA	3099	1/1	1.00	0.04	4,4,4,4	0

6.5 Other polymers [i](#)

There are no such residues in this entry.