



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 12:25 AM EDT

PDB ID : 8FOM / pdb_00008fom
Title : Crystal structure of tRNA^{Lys}(SUU) bound to UAA codon in the ribosomal P site
Authors : Nguyen, H.A.; Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.
Deposited on : 2023-01-02
Resolution : 3.58 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 : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

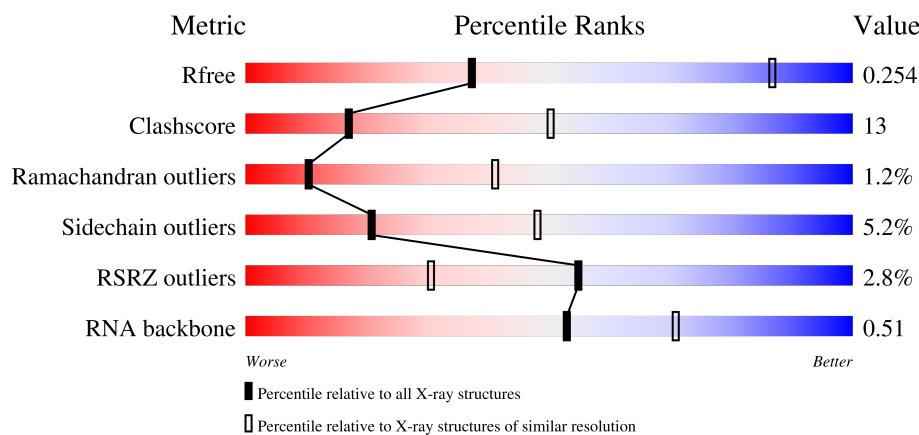
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.58 Å.

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



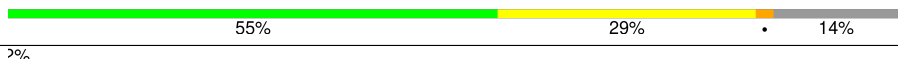
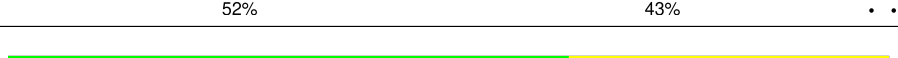
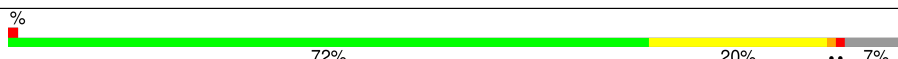
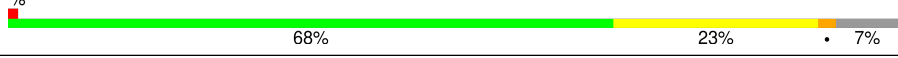
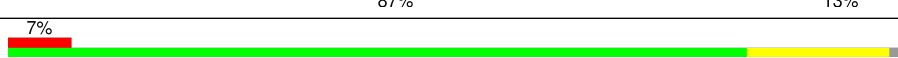
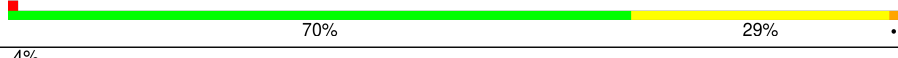
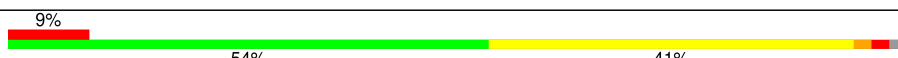
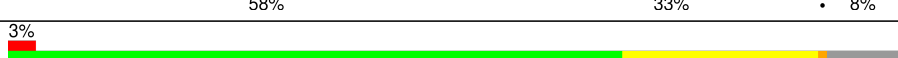
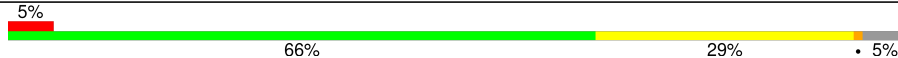
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1521 (3.66-3.50)
Clashscore	190562	1595 (3.66-3.50)
Ramachandran outliers	187476	1551 (3.66-3.50)
Sidechain outliers	187428	1551 (3.66-3.50)
RSRZ outliers	180081	1520 (3.66-3.50)
RNA backbone	3983	1013 (4.10-3.06)

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	QA	1522	
1	XA	1522	
2	QB	256	
2	XB	256	

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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	131	
12	XL	131	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	

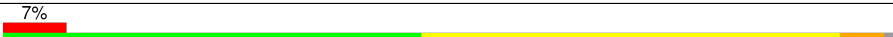
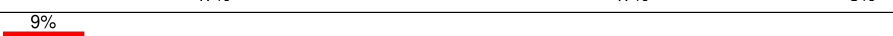
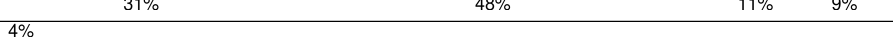
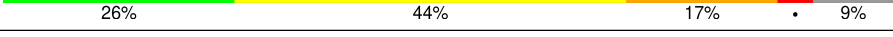
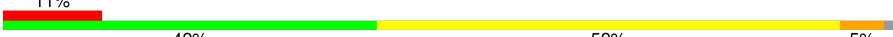
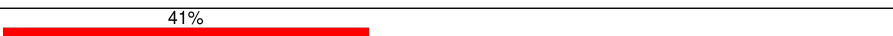
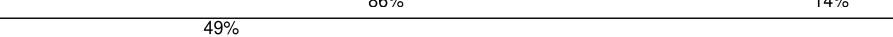
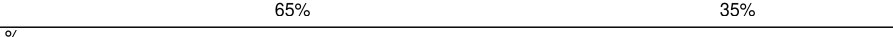
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Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	76	
22	XV	76	
23	QX	23	
23	XX	23	
24	R0	85	
24	Y0	85	
25	R1	98	
25	Y1	98	
26	R2	72	
26	Y2	72	
27	R3	60	
27	Y3	60	

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Mol	Chain	Length	Quality of chain
28	R4	71	
28	Y4	71	
29	R5	60	
29	Y5	60	
30	R6	54	
30	Y6	54	
31	R7	49	
31	Y7	49	
32	R8	65	
32	Y8	65	
33	R9	37	
33	Y9	37	
34	RA	2915	
34	YA	2915	
35	RB	122	
35	YB	122	
36	RD	276	
36	YD	276	
37	RE	206	
37	YE	206	
38	RF	210	
38	YF	210	
39	RG	182	
39	YG	182	
40	RH	180	

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

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Mol	Chain	Length	Quality of chain
53	RY	110	
53	YY	110	
54	RZ	206	
54	YZ	206	
55	XY	17	
56	Z6	3	
56	Z8	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3300	-	-	-	X
57	MG	YA	3358	-	-	-	X
58	SF4	XD	301	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 292176 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1500	Total	C	N	O	P	0	0	0
			32247	14353	5981	10414	1499			
1	XA	1511	Total	C	N	O	P	0	0	0
			32471	14454	6014	10493	1510			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
2	XB	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	XH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called P-site tRNA^{Lys}(SUU).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	74	Total	C	N	O	P	0	0	0
			1594	717	279	525	73			
22	XV	74	Total	C	N	O	P	0	0	0
			1594	717	279	525	73			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	3	Total	C	N	O	P	0	0	0
			65	29	12	21	3			
23	XX	23	Total	C	N	O	P	0	0	0
			502	224	98	157	23			

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 55 is a RNA chain called A-site ASL[^]Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	XY	17	Total	C	N	O	P	0	0	0
			362	163	68	115	16			

- Molecule 56 is a RNA chain called CC-puro.

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

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

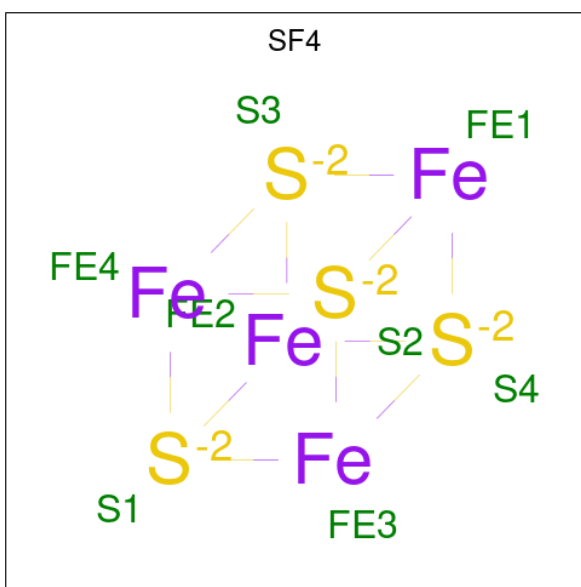
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	54	Total	Mg	0	0
			54	54		
57	QV	1	Total	Mg	0	0
			1	1		
57	R0	1	Total	Mg	0	0
			1	1		
57	R5	1	Total	Mg	0	0
			1	1		
57	R7	1	Total	Mg	0	0
			1	1		
57	R8	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	RA	333	Total 333	Mg 333	0	0
57	RB	5	Total 5	Mg 5	0	0
57	RE	1	Total 1	Mg 1	0	0
57	RF	1	Total 1	Mg 1	0	0
57	RR	2	Total 2	Mg 2	0	0
57	XA	58	Total 58	Mg 58	0	0
57	XV	2	Total 2	Mg 2	0	0
57	XX	1	Total 1	Mg 1	0	0
57	Y0	1	Total 1	Mg 1	0	0
57	Y1	1	Total 1	Mg 1	0	0
57	Y3	1	Total 1	Mg 1	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	Y7	2	Total 2	Mg 2	0	0
57	YA	361	Total 361	Mg 361	0	0
57	YB	4	Total 4	Mg 4	0	0
57	YE	2	Total 2	Mg 2	0	0
57	YP	2	Total 2	Mg 2	0	0
57	YQ	2	Total 2	Mg 2	0	0
57	YR	2	Total 2	Mg 2	0	0
57	YY	1	Total 1	Mg 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

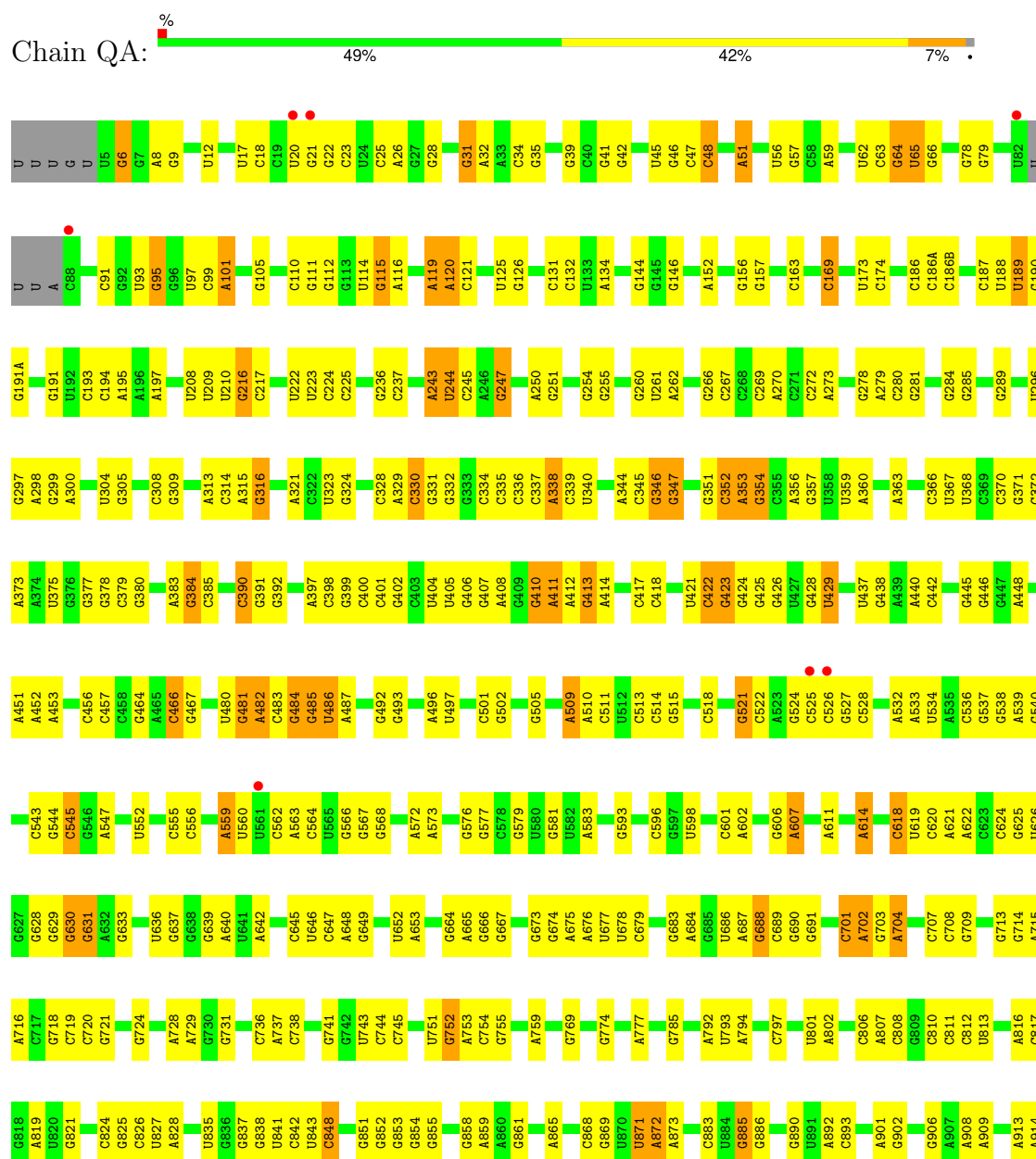
- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

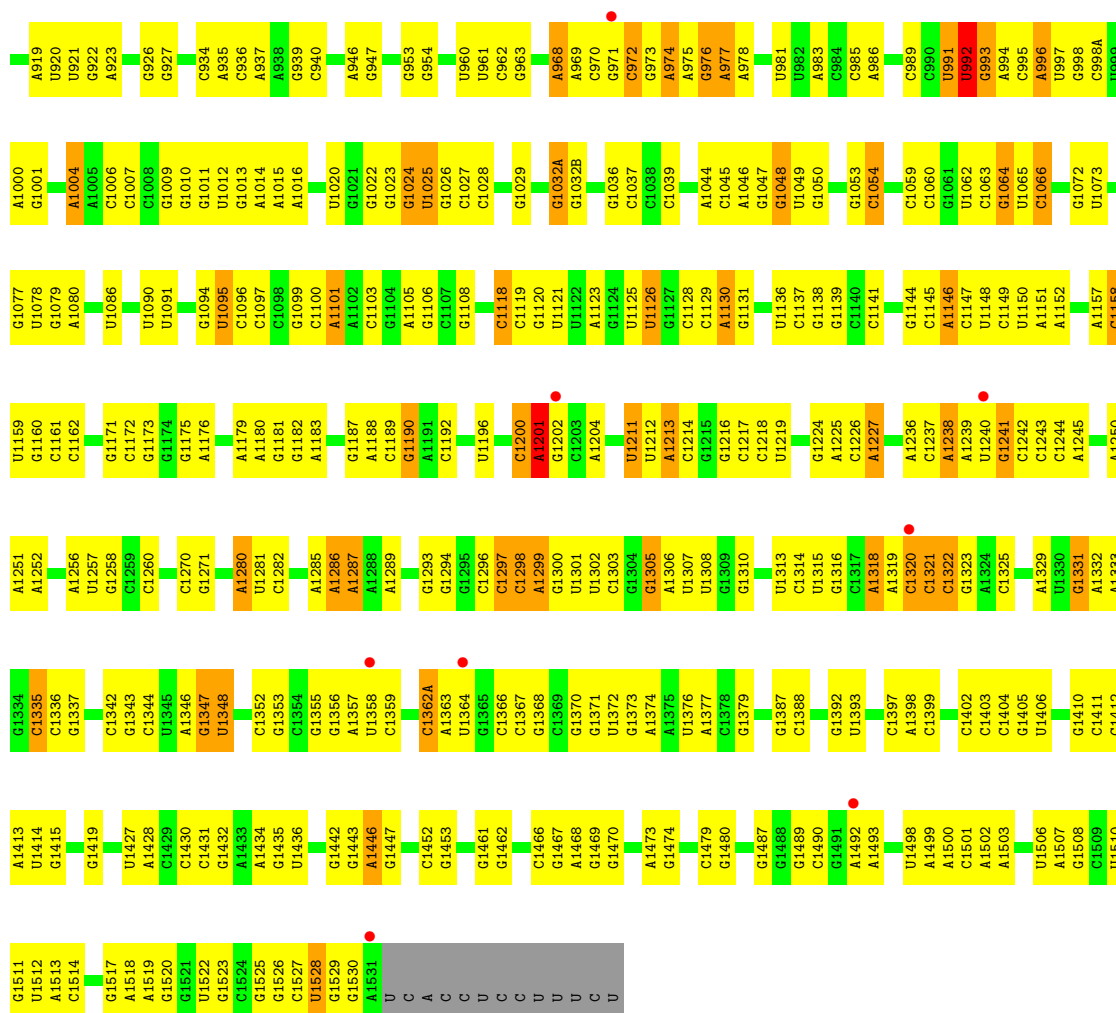
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	QN	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		

3 Residue-property plots [i](#)

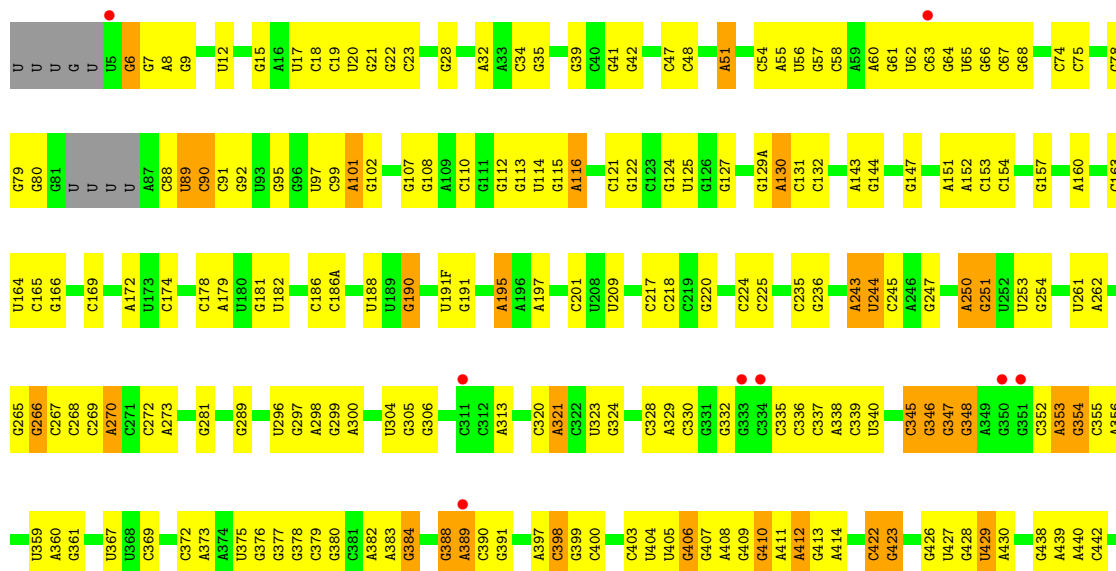
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

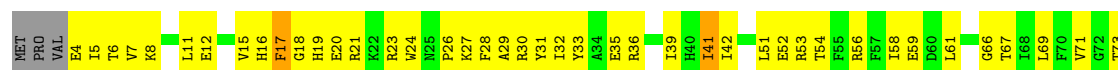
• Molecule 1: 16S rRNA

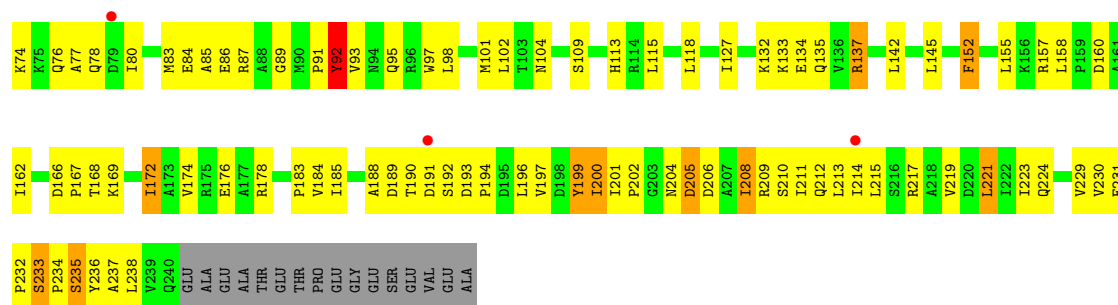




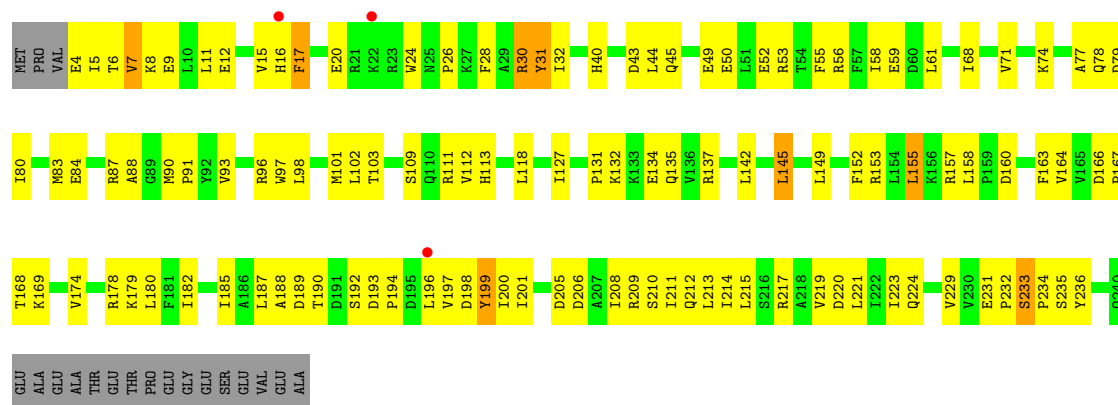
• Molecule 1: 16S rRNA



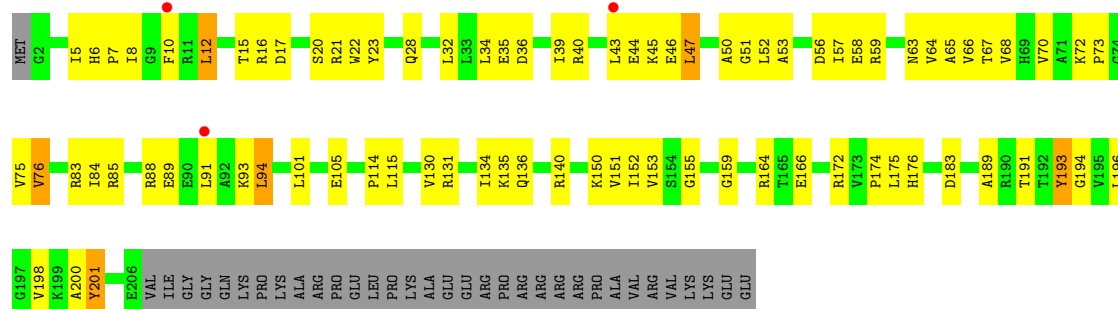




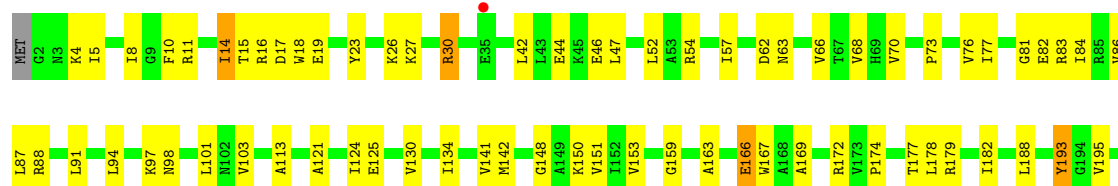
• Molecule 2: 30S ribosomal protein S2

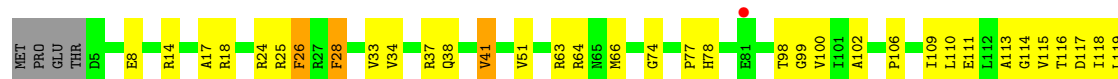


• Molecule 3: 30S ribosomal protein S3



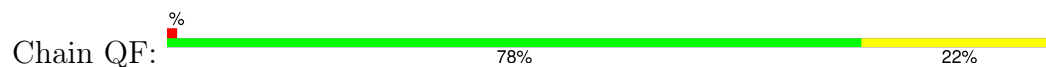
• Molecule 3: 30S ribosomal protein S3



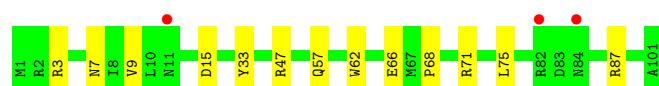
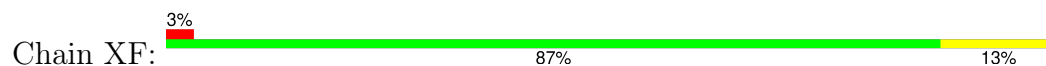




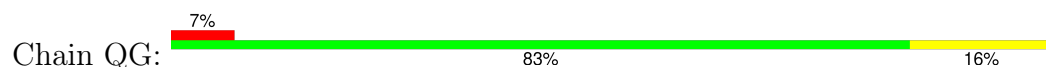
- Molecule 6: 30S ribosomal protein S6



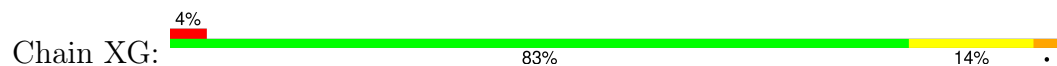
- Molecule 6: 30S ribosomal protein S6



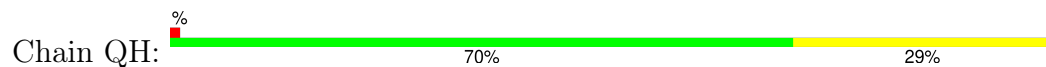
- Molecule 7: 30S ribosomal protein S7



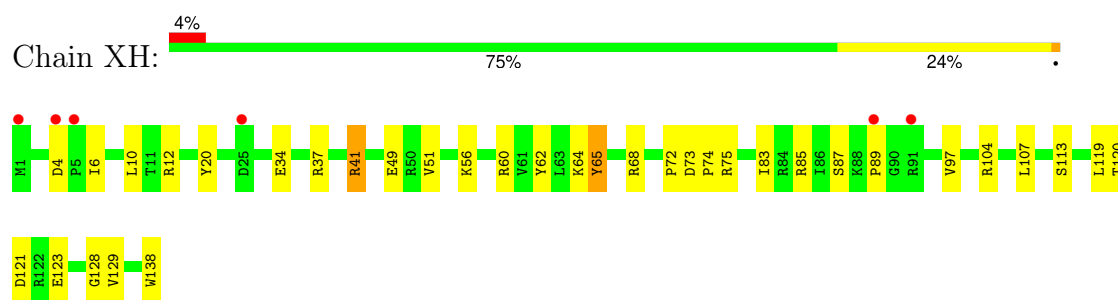
- Molecule 7: 30S ribosomal protein S7



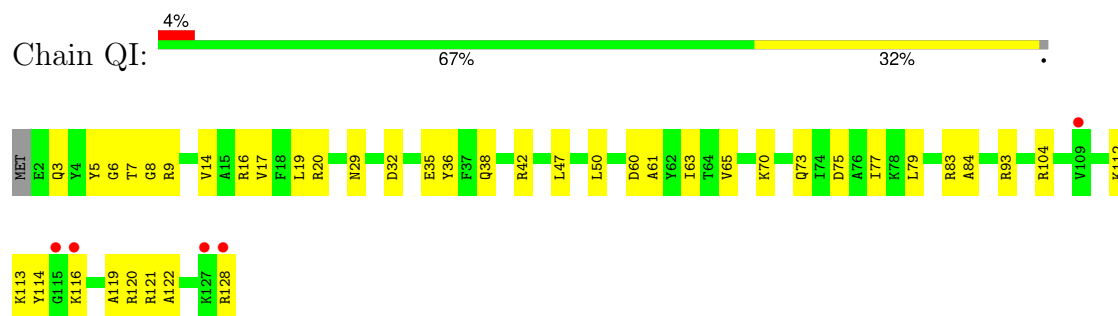
- Molecule 8: 30S ribosomal protein S8



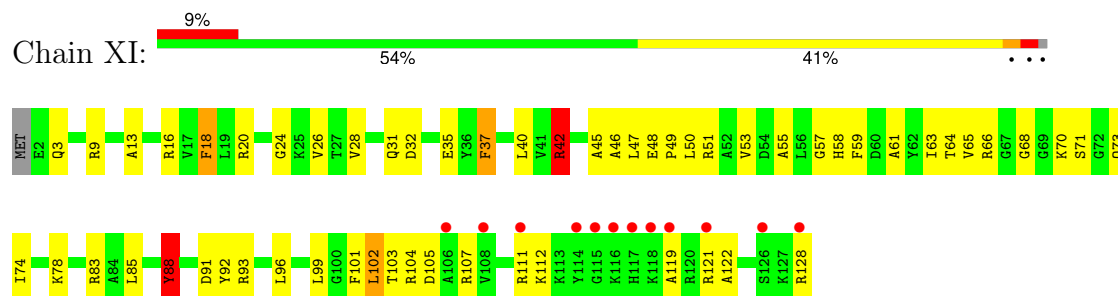
- Molecule 8: 30S ribosomal protein S8



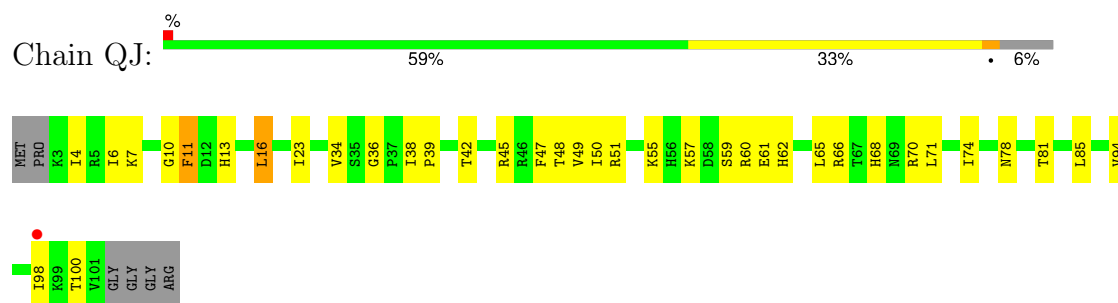
- Molecule 9: 30S ribosomal protein S9



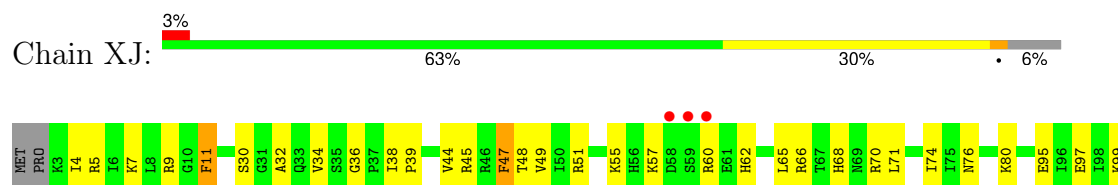
- Molecule 9: 30S ribosomal protein S9

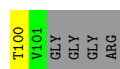


- Molecule 10: 30S ribosomal protein S10

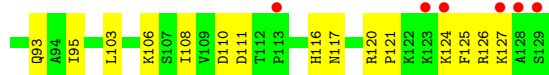


- Molecule 10: 30S ribosomal protein S10

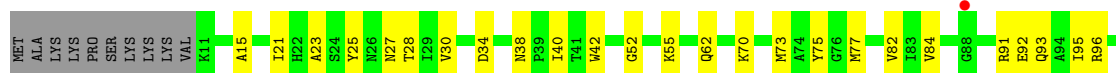




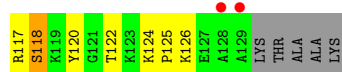
- Molecule 11: 30S ribosomal protein S11



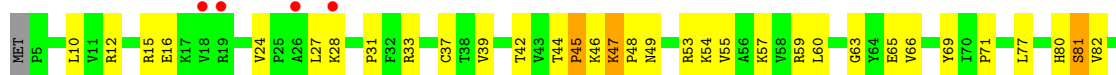
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

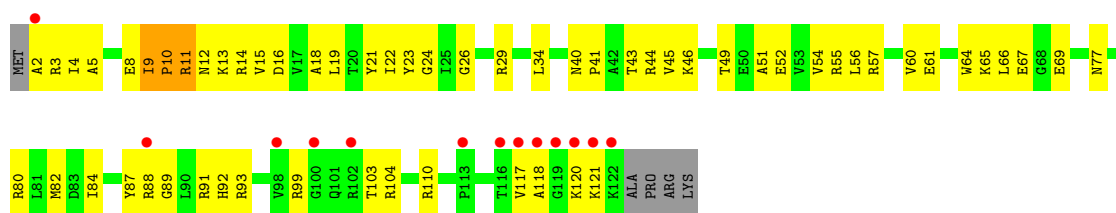


- Molecule 12: 30S ribosomal protein S12

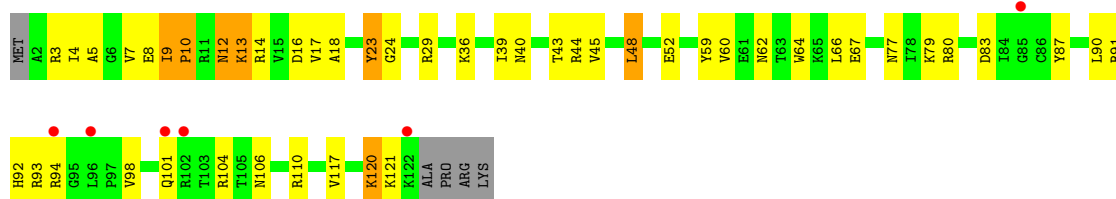


- Molecule 13: 30S ribosomal protein S13





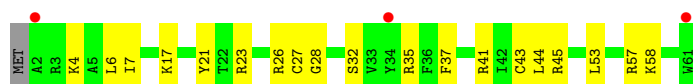
• Molecule 13: 30S ribosomal protein S13



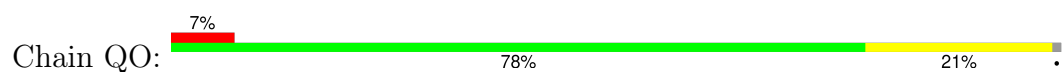
• Molecule 14: 30S ribosomal protein S14 type Z



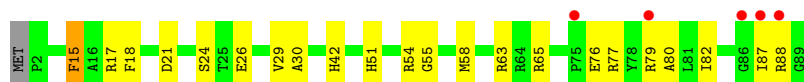
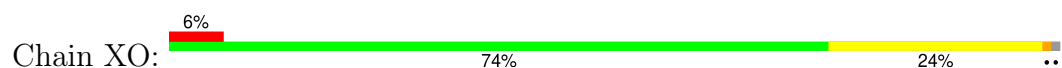
• Molecule 14: 30S ribosomal protein S14 type Z



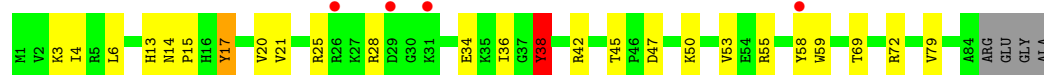
• Molecule 15: 30S ribosomal protein S15



• Molecule 15: 30S ribosomal protein S15



• Molecule 16: 30S ribosomal protein S16



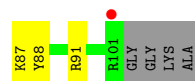
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

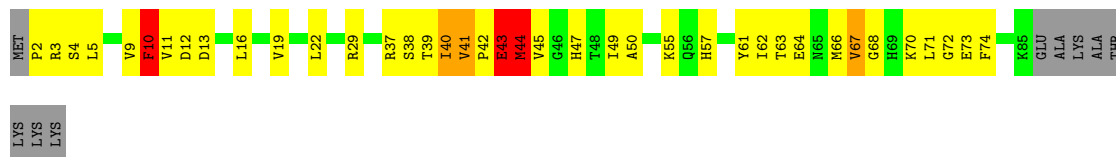


- Molecule 18: 30S ribosomal protein S18



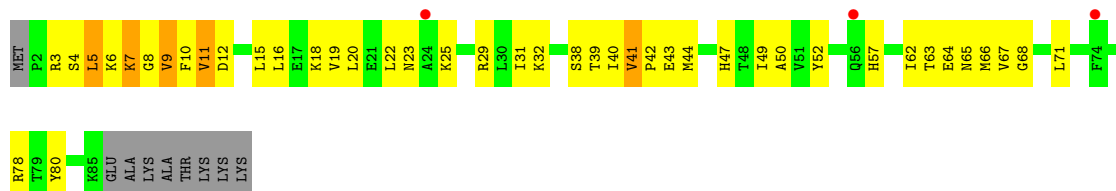
- Molecule 19: 30S ribosomal protein S19

Chain QS: 



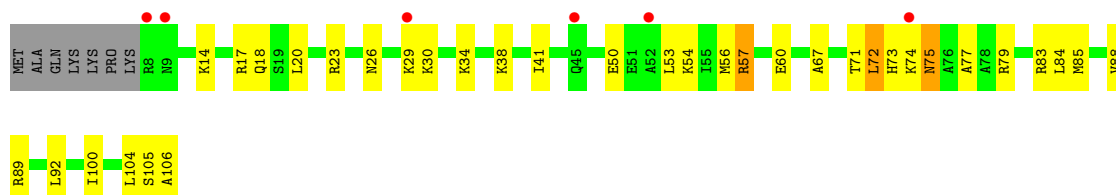
- Molecule 19: 30S ribosomal protein S19

Chain XS: 



- Molecule 20: 30S ribosomal protein S20

Chain QT: 



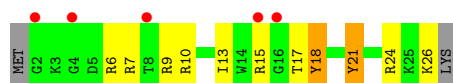
- Molecule 20: 30S ribosomal protein S20

Chain XT: 



- Molecule 21: 30S ribosomal protein Thx

Chain QU: 

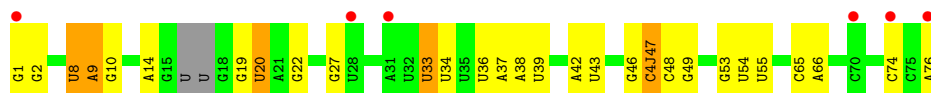


- Molecule 21: 30S ribosomal protein Thx

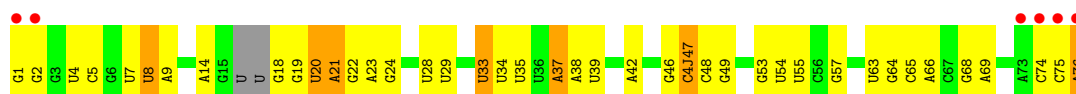
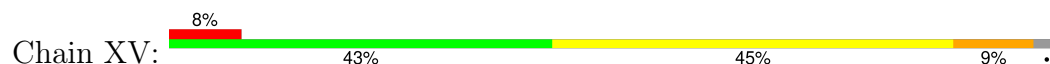
Chain XU: 



- Molecule 22: P-site tRNA^{Lys}(SUU)



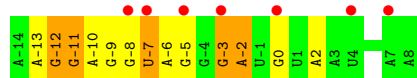
- Molecule 22: P-site tRNA^{Lys}(SUU)



- Molecule 23: mRNA



- Molecule 23: mRNA



- Molecule 24: 50S ribosomal protein L27



- Molecule 24: 50S ribosomal protein L27

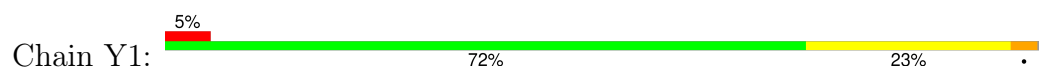


- Molecule 25: 50S ribosomal protein L28





- Molecule 25: 50S ribosomal protein L28



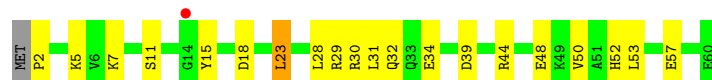
- Molecule 26: 50S ribosomal protein L29



- Molecule 26: 50S ribosomal protein L29



- Molecule 27: 50S ribosomal protein L30



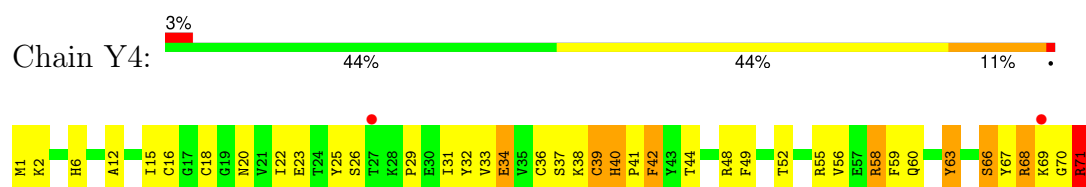
- Molecule 27: 50S ribosomal protein L30



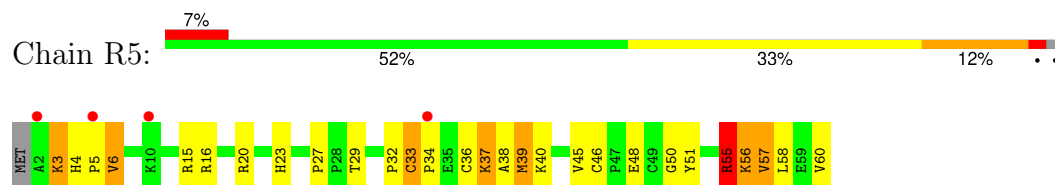
- Molecule 28: 50S ribosomal protein L31



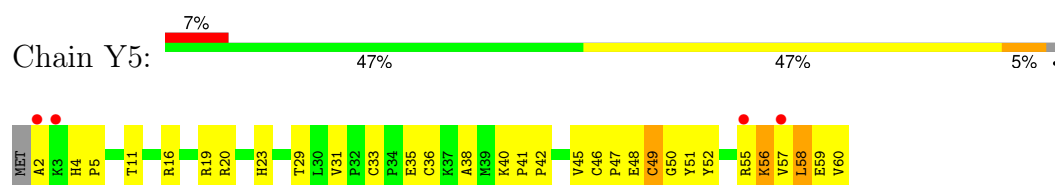
- Molecule 28: 50S ribosomal protein L31



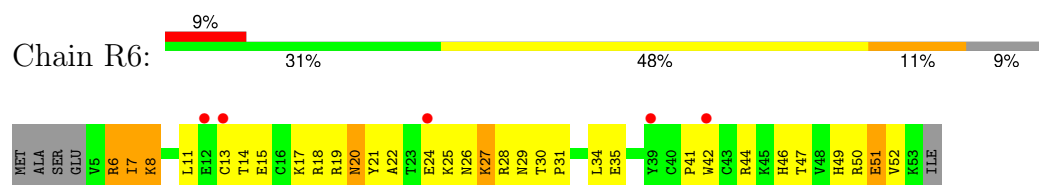
- Molecule 29: 50S ribosomal protein L32



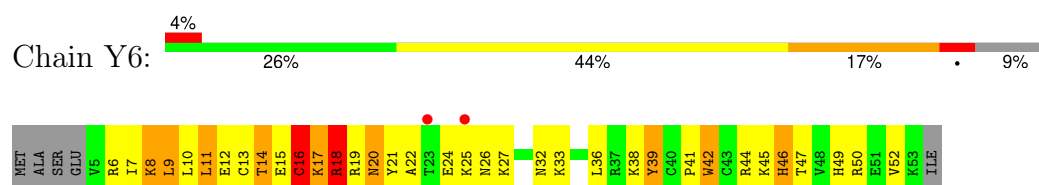
- Molecule 29: 50S ribosomal protein L32



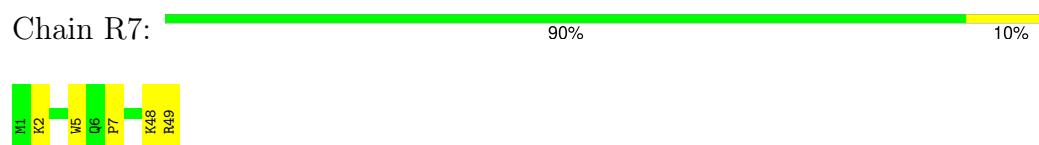
- Molecule 30: 50S ribosomal protein L33



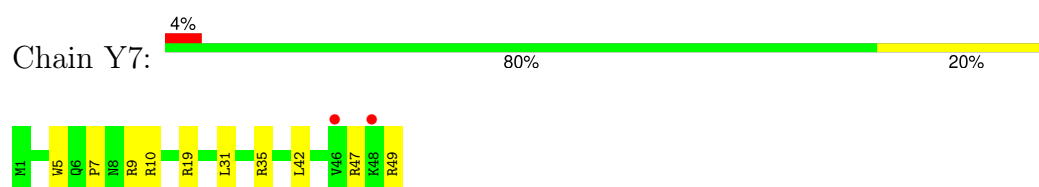
- Molecule 30: 50S ribosomal protein L33



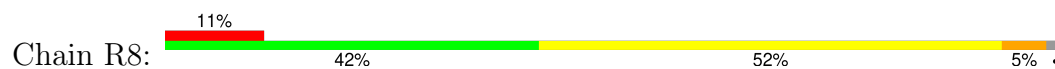
- Molecule 31: 50S ribosomal protein L34



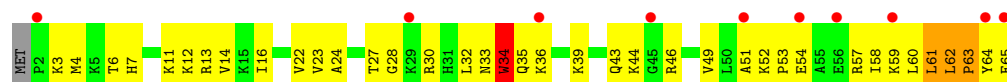
- Molecule 31: 50S ribosomal protein L34



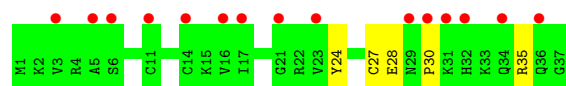
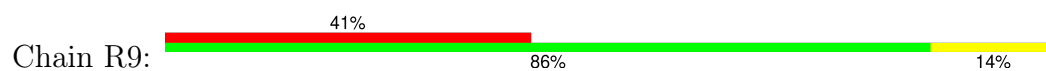
• Molecule 32: 50S ribosomal protein L35



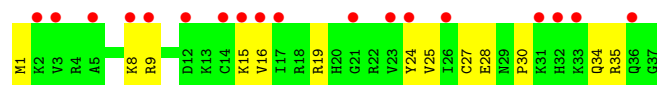
• Molecule 32: 50S ribosomal protein L35



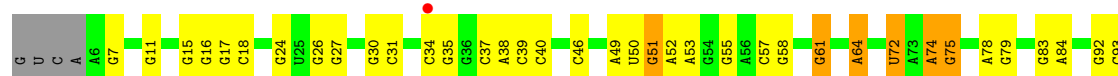
• Molecule 33: 50S ribosomal protein L36



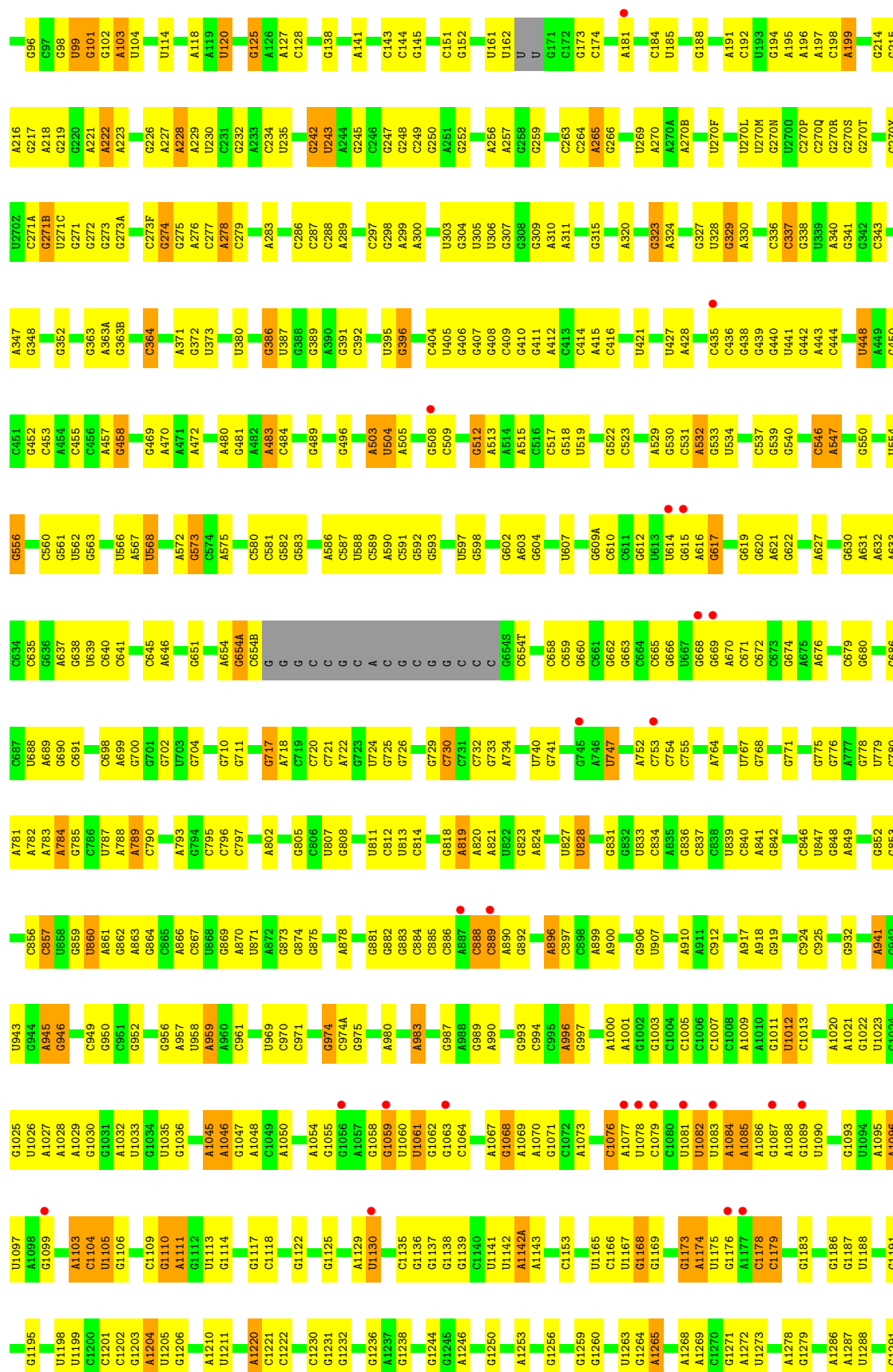
• Molecule 33: 50S ribosomal protein L36



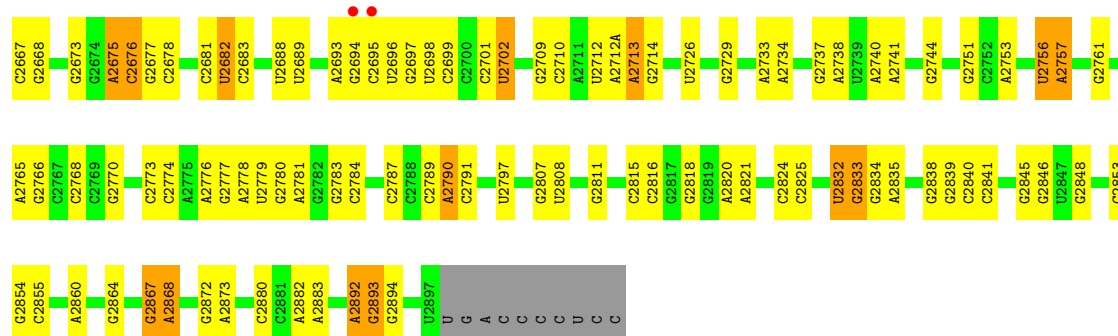
• Molecule 34: 23S rRNA



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G1674	A1567	C1476	U1288	G1193	G1093	U1022	G934	G852	A764	C654I	C517
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A1677	A1570	U1482	C1291	U1198	A1103	U1026	A941	C857	U607		G522
G1678	A1571	G1483	U1292	U1199	C1104	A1027	G942	U958	A608		C527
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G1687	A1579	U1406	C1295	C1201	G1111	U1029	A945	G863	A609A		A529
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A1689	G1581	C1408		C1203	G1112	U1034	G947	G864			C531
		C1409	G1299	A1204	U1122	U1035	G948	G869	A782		A532
C1694	A1586	U1300	A1301	U1205	G1122	U1036	G950	G872	A783		G533
G1695	C1497	G1410	A1302	G1206		C1040	G951	A872	A784		G537
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C1592	C1592	G1413	G1309	U1212	G1131		A959	G882	A621		C546
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C1711	C1505	A1419	C1314	A1220	G1139	A1050		C886	A632		G551
	C1506	U1420	C1315	G1224	C1140	G1051	U969	A887			G552
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G1728	U1729	A1427	A1321	G1230	G1149	U1060	C974A	G808	G638		U557
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G1730	G1731	G1429	C1323	G1232	C1151	U1062	A980	C812	C640		G563
A1732	A1610	U1430	U1335	G1233	C1152	G1063	A983	U813	C564		C565
G1733	C1611	C1433	G1337	G1236	C1153	U1064		C814	G642		
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G1651	A1543	G1455	G1369	C1257		C1079	C1005	A835	G725		G583
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A1654	A1545A	A1460	A1378	G1271	A1177	A1084	G1011	U839	A		U588
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		C1462	G1380	U1273	C1179	A1086	C1013	A841	C		A590
C1550	C1550		A1384	A1274	C1180	G1087	G1016	C844	C		C591
C1551	C1551	C1467	G1385	A1275	G1183	U1088	U1019	G845	G		G592
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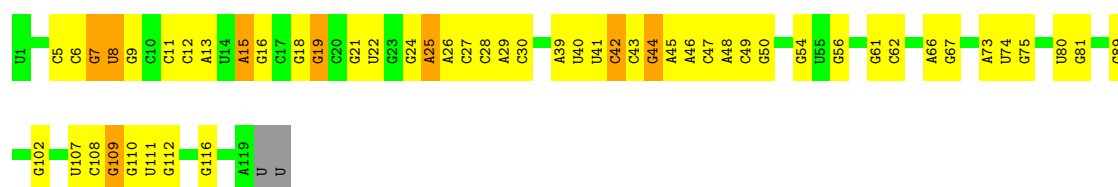


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G2576	C2471	A2392	C2293	G2184	G2112	G2024	G1813	G1695	C1585	G1491	U1405	G1296
A2577	C2475	A2393	G2303	G2185	U2113	C2025	A1918	A1698	A1586	G1492	C1407	C1297
C2578	A2476	C2394	G2306	G2186	A2114	G2026	A1919	G1699	A1587	C1493	C1408	C1298
C2579	C2477	G2395	G2307	G2187	G2115	G2027	C1920	G1699	C1588	A1494	C1409	G1299
U2584	G2484	G2396	G2308	C2188	G2116	U2028	U1818	A1700	U1589	A1495	G1410	U1300
U2585	U2189	U2189	G2309	U2189	A2117	G2029	U1819	G1709	C1589	U1497	G1411	A1301
C2586	A2402	A2310	A2309	G2190	A2118	A2031	G1824	C1710	U1591	A1498	A1412	G1309
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G2592	G2407	G2314	C2313	G2193	U2122	U2034	C1827	G1725	C1598	C1417	C1417	U1316
U2600	U2408	G2315	G2314	U2197	G2123	G2035	G1829	G1727	C1598	G1418	G1418	A1317
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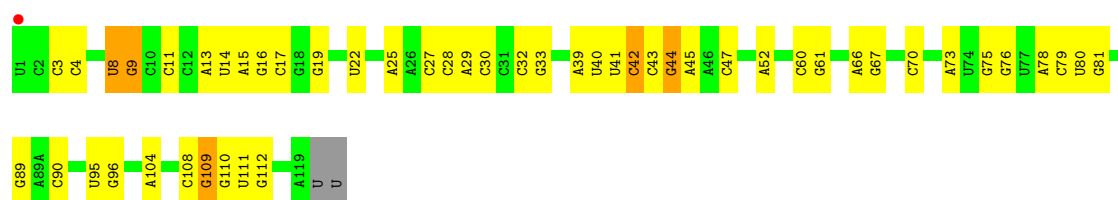
• Molecule 35: 5S rRNA

Chain RB: 55% 37% 7% .



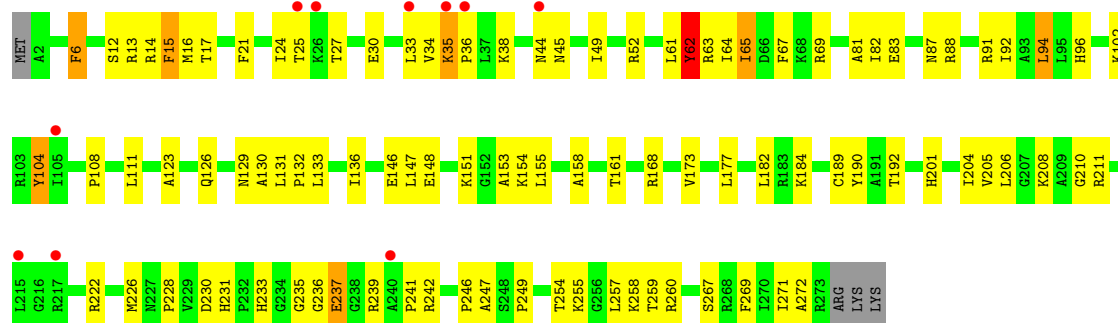
• Molecule 35: 5S rRNA

Chain YB: 57% 37% . .



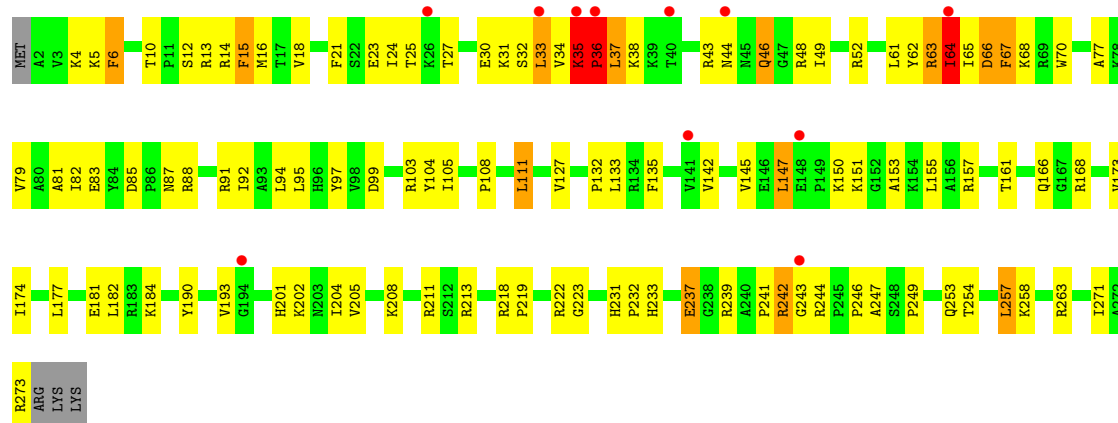
• Molecule 36: 50S ribosomal protein L2

Chain RD: 4% 63% 33% . .

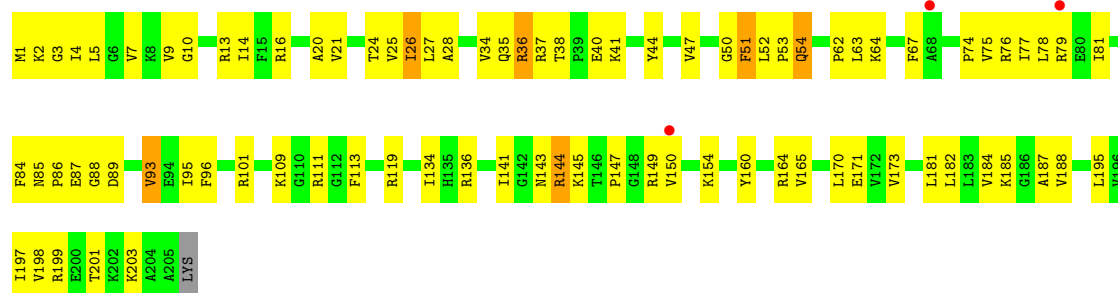


• Molecule 36: 50S ribosomal protein L2

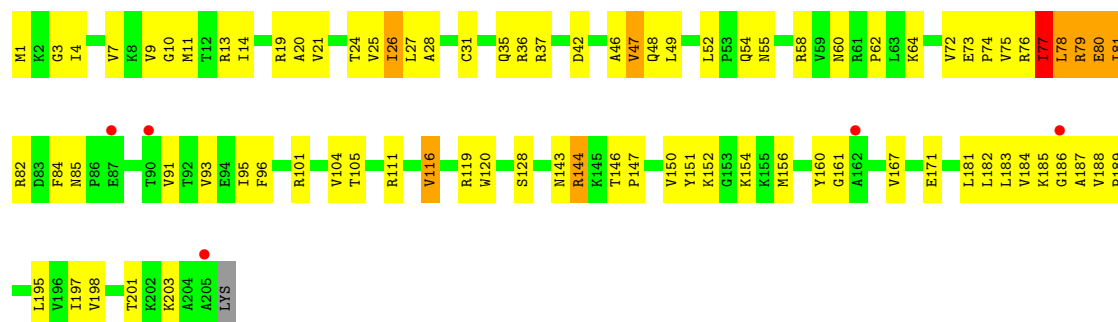
Chain YD: 4% 58% 34% 5% . .



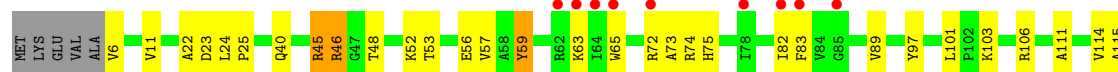
• Molecule 37: 50S ribosomal protein L3

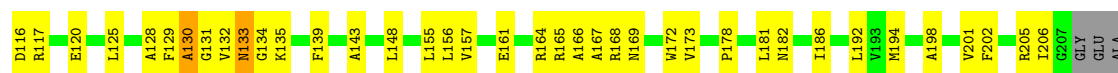


• Molecule 37: 50S ribosomal protein L3

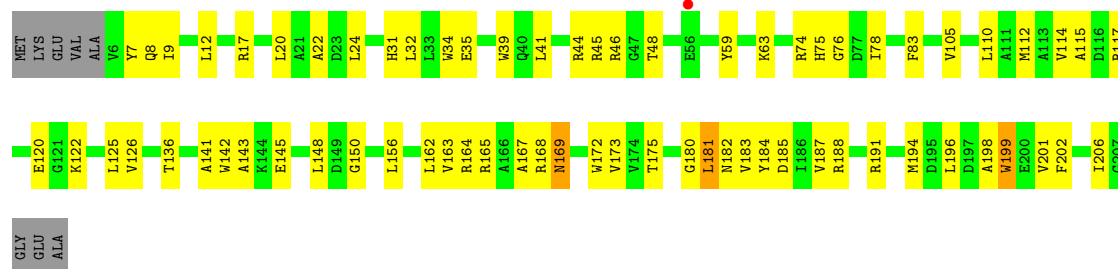


• Molecule 38: 50S ribosomal protein L4

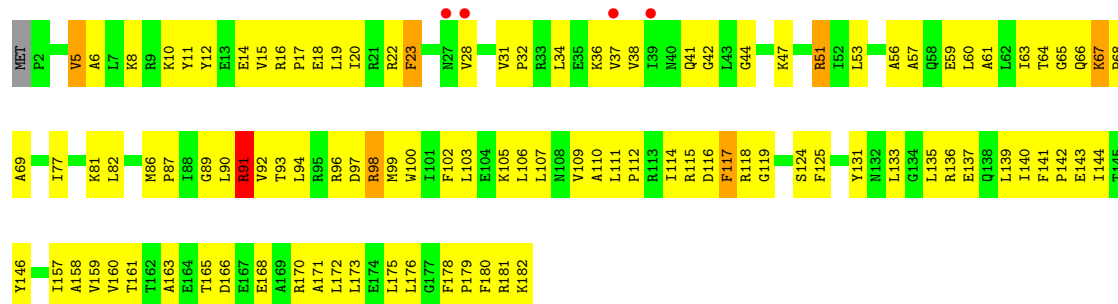




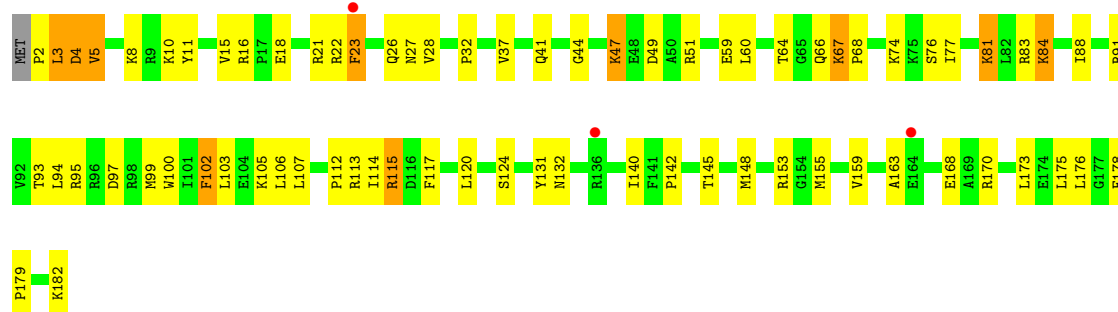
• Molecule 38: 50S ribosomal protein L4



• Molecule 39: 50S ribosomal protein L5

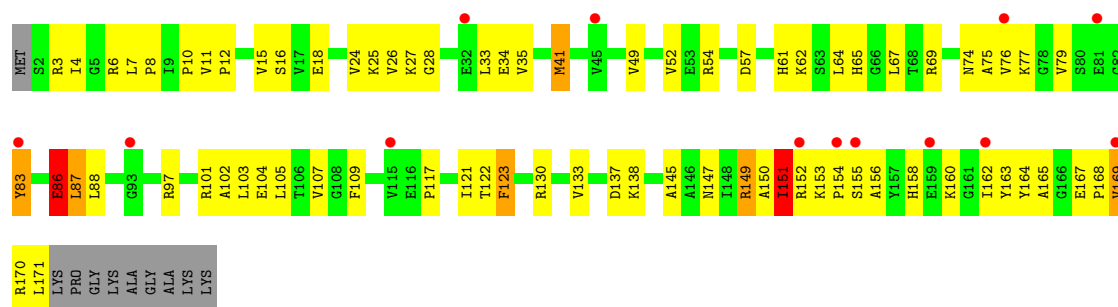


• Molecule 39: 50S ribosomal protein L5



• Molecule 40: 50S ribosomal protein L6





• Molecule 40: 50S ribosomal protein L6



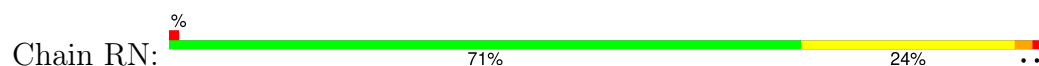
• Molecule 41: 50S ribosomal protein L9

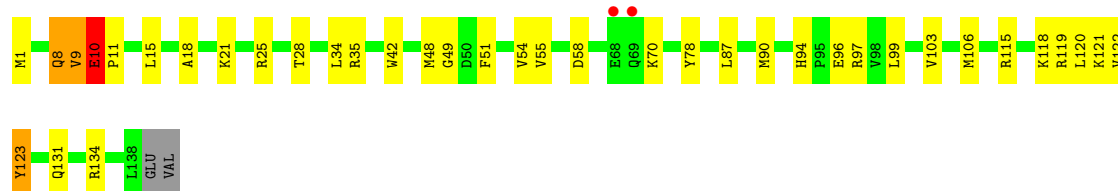


• Molecule 41: 50S ribosomal protein L9

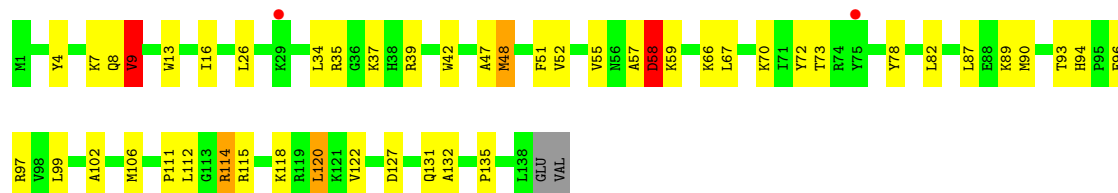


• Molecule 42: 50S ribosomal protein L13

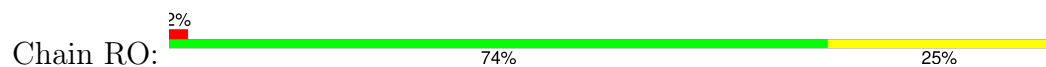




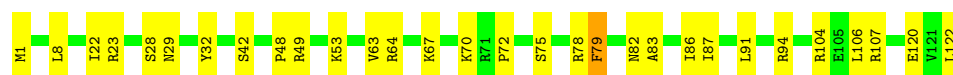
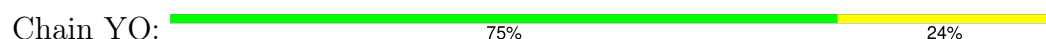
- Molecule 42: 50S ribosomal protein L13



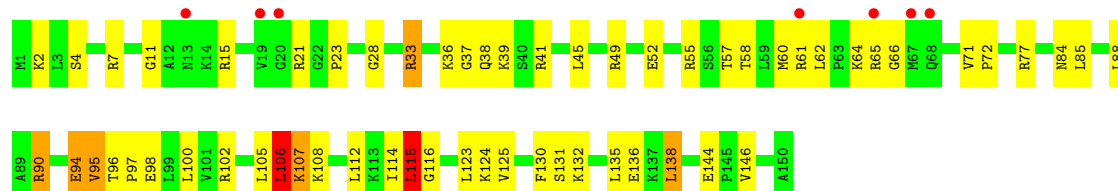
- Molecule 43: 50S ribosomal protein L14



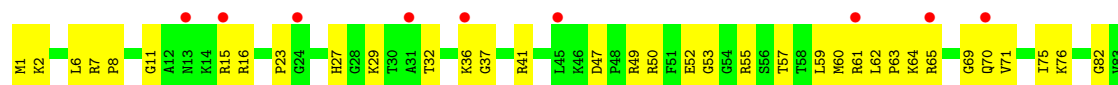
- Molecule 43: 50S ribosomal protein L14



- Molecule 44: 50S ribosomal protein L15

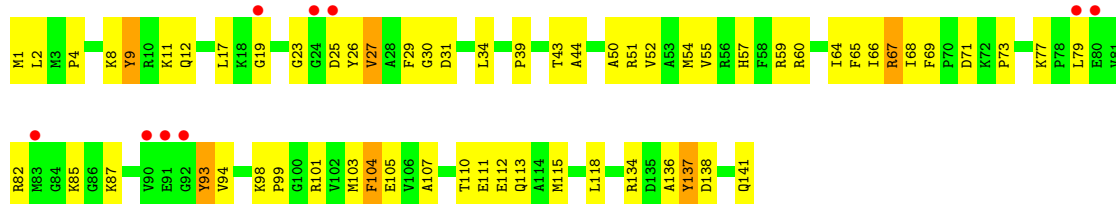


- Molecule 44: 50S ribosomal protein L15

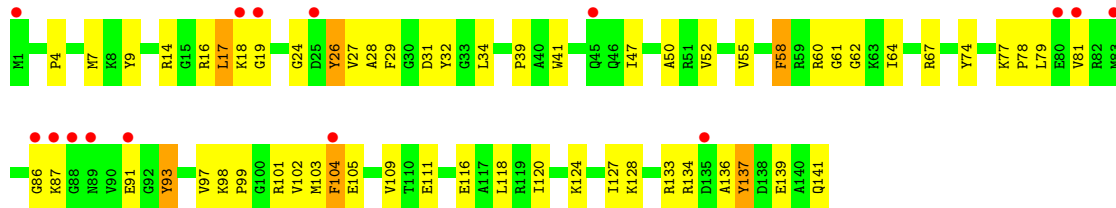




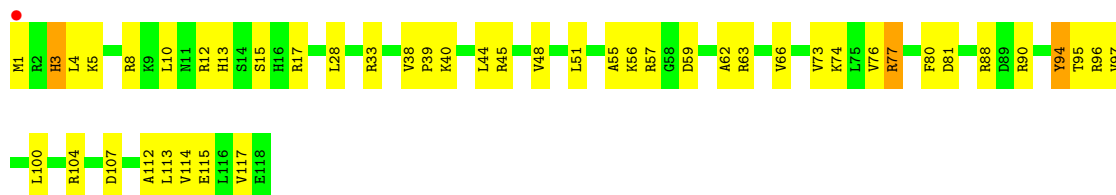
- Molecule 45: 50S ribosomal protein L16



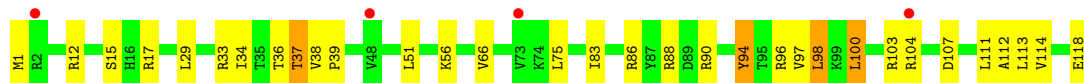
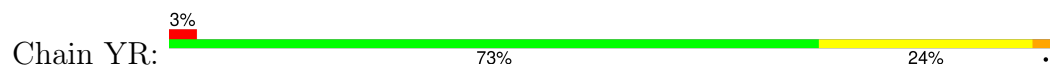
- Molecule 45: 50S ribosomal protein L16



- Molecule 46: 50S ribosomal protein L17



- Molecule 46: 50S ribosomal protein L17

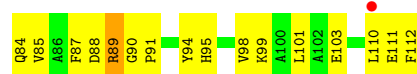


- Molecule 47: 50S ribosomal protein L18





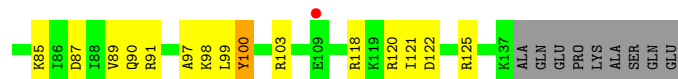
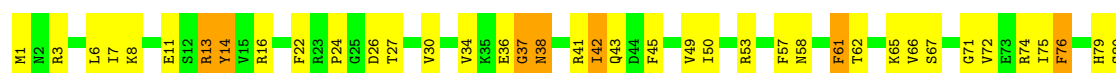
- Molecule 47: 50S ribosomal protein L18



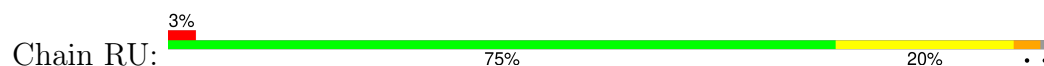
- Molecule 48: 50S ribosomal protein L19



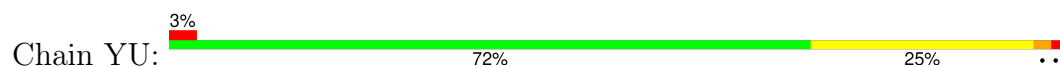
- Molecule 48: 50S ribosomal protein L19

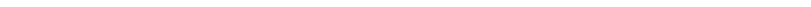


- Molecule 49: 50S ribosomal protein L20



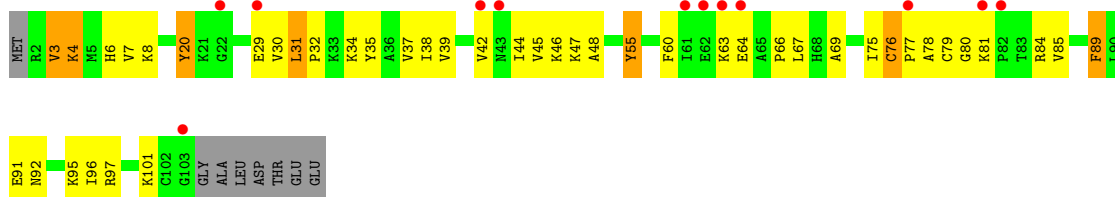
- Molecule 49: 50S ribosomal protein L20



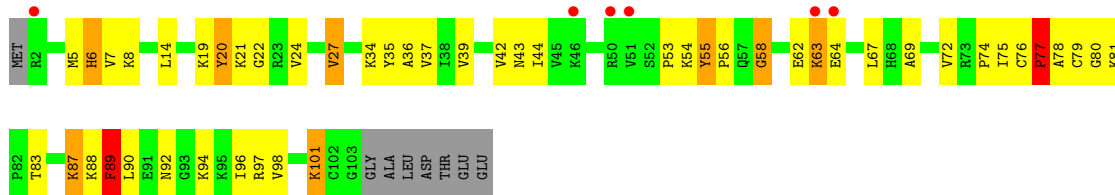
- Chain YX: 

LEU
ILE

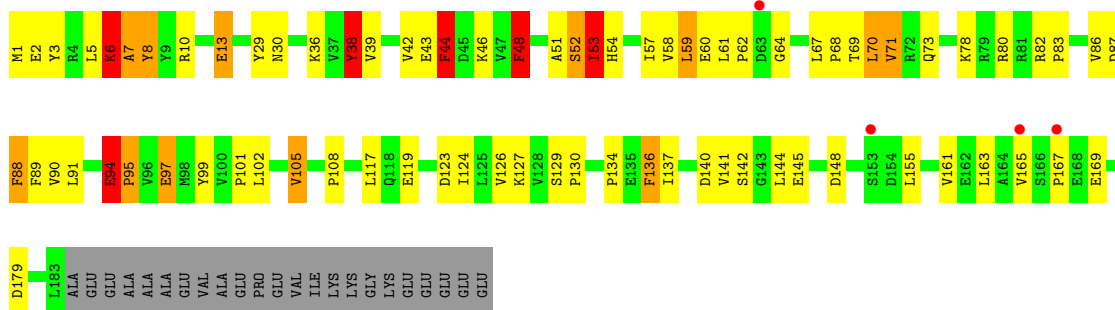
• Molecule 53: 50S ribosomal protein L24

Chain RY: 

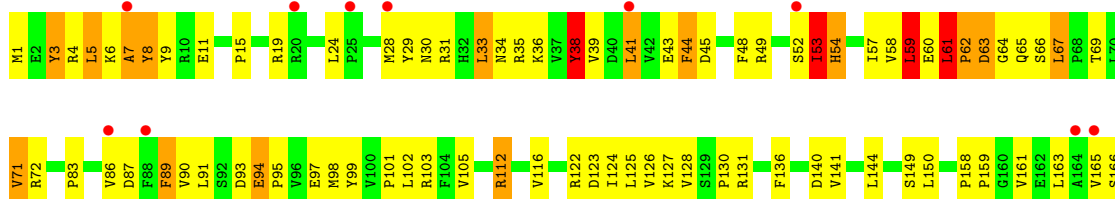
• Molecule 53: 50S ribosomal protein L24

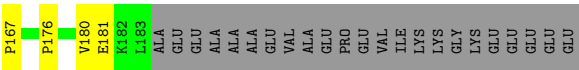
Chain YY: 

• Molecule 54: 50S ribosomal protein L25

Chain RZ: 

• Molecule 54: 50S ribosomal protein L25

Chain YZ: 



- Molecule 55: A-site ASL^Phe



- Molecule 56: CC-puro



- Molecule 56: CC-puro



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.72Å 449.48Å 617.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.33 – 3.58 153.33 – 3.58	Depositor EDS
% Data completeness (in resolution range)	98.3 (153.33-3.58) 98.3 (153.33-3.58)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.205 , 0.255 0.205 , 0.254	Depositor DCC
R_{free} test set	35613 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	96.7	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 132.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	292176	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% 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, 7MG, C4J, PSU, 5MU, SF4, T6A, MNU, H2U, MG, PPU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	QA	0.19	1/36098 (0.0%)	0.39	8/56341 (0.0%)
1	XA	0.18	0/36346	0.37	1/56725 (0.0%)
2	QB	0.31	0/1959	0.72	2/2642 (0.1%)
2	XB	0.36	0/1959	0.78	1/2642 (0.0%)
3	QC	0.22	0/1629	0.58	0/2195
3	XC	0.28	0/1629	0.67	0/2195
4	QD	0.32	0/1733	0.72	2/2318 (0.1%)
4	XD	0.26	0/1733	0.59	0/2318
5	QE	0.26	0/1171	0.57	1/1576 (0.1%)
5	XE	0.31	0/1171	0.64	1/1576 (0.1%)
6	QF	0.16	0/856	0.50	0/1154
6	XF	0.17	0/856	0.51	0/1154
7	QG	0.20	0/1276	0.55	0/1709
7	XG	0.22	0/1276	0.58	0/1709
8	QH	0.20	0/1136	0.52	0/1527
8	XH	0.41	2/1136 (0.2%)	0.73	2/1527 (0.1%)
9	QI	0.32	0/1029	0.71	2/1379 (0.1%)
9	XI	0.45	1/1029 (0.1%)	0.85	5/1379 (0.4%)
10	QJ	0.23	0/814	0.61	0/1095
10	XJ	0.31	0/814	0.69	0/1095
11	QK	0.23	0/900	0.58	0/1213
11	XK	0.23	0/900	0.56	0/1213
12	QL	0.30	0/991	0.68	1/1327 (0.1%)
12	XL	0.39	0/991	0.79	6/1327 (0.5%)
13	QM	0.38	0/974	0.76	0/1303
13	XM	0.71	2/974 (0.2%)	1.04	3/1303 (0.2%)
14	QN	0.38	0/501	0.71	1/664 (0.2%)
14	XN	0.26	0/501	0.66	0/664
15	QO	0.19	0/745	0.52	0/992
15	XO	0.20	0/745	0.55	0/992
16	QP	0.24	0/721	0.71	1/970 (0.1%)
16	XP	0.20	0/721	0.59	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.23	0/847	0.62	0/1131
17	XQ	0.21	0/847	0.57	0/1131
18	QR	0.23	0/579	0.59	0/768
18	XR	0.22	0/579	0.65	0/768
19	QS	0.57	1/689 (0.1%)	1.11	8/926 (0.9%)
19	XS	0.43	0/689	0.74	0/926
20	QT	0.35	0/765	0.76	0/1007
20	XT	0.33	0/765	0.72	0/1007
21	QU	0.28	0/221	0.72	0/288
21	XU	0.48	0/221	0.90	0/288
22	QV	0.28	0/1569	0.43	0/2437
22	XV	0.20	0/1569	0.33	0/2437
23	QX	0.09	0/72	0.19	0/110
23	XX	0.19	0/564	0.41	0/879
24	R0	0.24	0/657	0.63	0/874
24	Y0	0.29	0/657	0.69	0/874
25	R1	0.35	0/770	0.70	0/1022
25	Y1	0.31	0/770	0.67	0/1022
26	R2	0.45	0/583	0.78	0/771
26	Y2	0.35	0/600	0.78	2/793 (0.3%)
27	R3	0.22	0/474	0.56	0/635
27	Y3	0.26	0/474	0.59	0/635
28	R4	0.48	0/594	0.94	1/795 (0.1%)
28	Y4	0.71	1/594 (0.2%)	1.25	3/795 (0.4%)
29	R5	0.57	0/473	0.83	0/639
29	Y5	0.50	0/473	0.93	1/639 (0.2%)
30	R6	0.50	0/431	0.99	0/575
30	Y6	0.62	0/431	1.04	0/575
31	R7	0.21	0/438	0.57	0/575
31	Y7	0.22	0/438	0.63	0/575
32	R8	0.32	0/525	0.73	0/691
32	Y8	0.37	0/525	0.87	1/691 (0.1%)
33	R9	0.20	0/310	0.55	0/407
33	Y9	0.15	0/310	0.50	0/407
34	RA	0.18	3/69521 (0.0%)	0.39	11/108529 (0.0%)
34	YA	0.18	1/69543 (0.0%)	0.38	5/108563 (0.0%)
35	RB	0.15	0/2878	0.33	0/4490
35	YB	0.16	0/2878	0.36	0/4490
36	RD	0.30	0/2165	0.73	4/2919 (0.1%)
36	YD	0.51	3/2165 (0.1%)	0.91	7/2919 (0.2%)
37	RE	0.45	1/1601 (0.1%)	0.84	1/2160 (0.0%)
37	YE	0.43	0/1601	0.89	3/2160 (0.1%)
38	RF	0.31	0/1620	0.71	0/2194

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YF	0.25	0/1620	0.66	1/2194 (0.0%)
39	RG	0.50	2/1499 (0.1%)	0.92	8/2016 (0.4%)
39	YG	0.39	0/1499	0.79	2/2016 (0.1%)
40	RH	0.41	0/1332	0.84	5/1802 (0.3%)
40	YH	0.37	0/1332	0.85	4/1802 (0.2%)
41	RI	0.42	0/1151	0.85	2/1558 (0.1%)
41	YI	0.52	0/1151	0.94	5/1558 (0.3%)
42	RN	0.51	1/1131 (0.1%)	0.88	2/1525 (0.1%)
42	YN	0.36	0/1131	0.70	0/1525
43	RO	0.22	0/943	0.57	0/1269
43	YO	0.22	0/943	0.58	0/1269
44	RP	0.36	0/1162	0.84	4/1544 (0.3%)
44	YP	0.38	0/1162	0.85	2/1544 (0.1%)
45	RQ	0.47	0/1143	0.89	5/1527 (0.3%)
45	YQ	0.33	0/1143	0.79	0/1527
46	RR	0.27	0/982	0.73	0/1312
46	YR	0.27	0/982	0.71	4/1312 (0.3%)
47	RS	0.27	0/892	0.84	0/1187
47	YS	0.34	0/892	0.81	0/1187
48	RT	0.33	1/1155 (0.1%)	0.70	0/1542
48	YT	0.29	0/1155	0.82	2/1542 (0.1%)
49	RU	0.26	0/982	0.63	0/1306
49	YU	0.37	0/982	0.80	6/1306 (0.5%)
50	RV	0.38	0/790	0.85	0/1057
50	YV	0.37	0/790	0.84	0/1057
51	RW	0.22	0/911	0.60	0/1220
51	YW	0.21	0/911	0.58	0/1220
52	RX	0.25	0/739	0.68	0/993
52	YX	0.26	0/739	0.63	0/993
53	RY	0.59	1/798 (0.1%)	0.87	0/1064
53	YY	0.55	0/798	1.09	7/1064 (0.7%)
54	RZ	0.44	0/1493	0.89	3/2026 (0.1%)
54	YZ	0.67	2/1493 (0.1%)	1.05	5/2026 (0.2%)
55	XY	0.17	0/405	0.38	0/630
56	Z6	0.14	0/40	0.33	0/60
56	Z8	0.14	0/40	0.31	0/60
All	All	0.25	23/316100 (0.0%)	0.51	151/472551 (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
8	XH	0	1
39	RG	0	1
All	All	0	2

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	XM	10	PRO	N-CA	17.94	1.70	1.47
54	YZ	67	LEU	C-N	17.28	1.51	1.33
42	RN	10	GLU	C-N	13.71	1.50	1.33
53	RY	55	TYR	C-O	11.47	1.29	1.23
37	RE	144	ARG	CB-CG	-7.90	1.28	1.52

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	RN	10	GLU	CA-C-N	16.52	138.62	120.11
42	RN	10	GLU	C-N-CA	16.52	138.62	120.11
13	XM	9	ILE	CA-C-N	15.72	139.49	119.84
13	XM	9	ILE	C-N-CA	15.72	139.49	119.84
54	YZ	61	LEU	CA-C-N	12.72	135.74	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
39	RG	91	ARG	Sidechain
8	XH	41	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	536	0
1	XA	32471	0	16395	485	0
2	QB	1924	0	1975	113	0
2	XB	1924	0	1975	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	QC	1605	0	1668	61	0
3	XC	1605	0	1668	55	0
4	QD	1703	0	1766	96	0
4	XD	1703	0	1767	74	0
5	QE	1155	0	1213	27	0
5	XE	1155	0	1213	33	0
6	QF	843	0	857	15	0
6	XF	843	0	857	9	0
7	QG	1257	0	1296	14	0
7	XG	1257	0	1296	18	0
8	QH	1116	0	1177	30	0
8	XH	1116	0	1177	28	0
9	QI	1010	0	1037	39	0
9	XI	1010	0	1037	50	0
10	QJ	801	0	849	31	0
10	XJ	801	0	849	29	0
11	QK	885	0	904	33	0
11	XK	885	0	904	23	0
12	QL	975	0	1062	47	0
12	XL	975	0	1062	51	0
13	QM	964	0	1034	81	0
13	XM	964	0	1034	50	0
14	QN	492	0	530	32	0
14	XN	492	0	529	17	0
15	QO	734	0	771	11	0
15	XO	734	0	771	14	0
16	QP	705	0	725	21	0
16	XP	705	0	725	21	0
17	QQ	834	0	904	21	0
17	XQ	834	0	904	30	0
18	QR	574	0	644	27	0
18	XR	574	0	644	11	0
19	QS	674	0	699	89	0
19	XS	674	0	699	63	0
20	QT	763	0	861	29	0
20	XT	763	0	861	22	0
21	QU	217	0	234	11	0
21	XU	217	0	234	14	0
22	QV	1594	0	806	7	0
22	XV	1594	0	806	24	0
23	QX	65	0	33	0	0
23	XX	502	0	249	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	R0	648	0	672	18	0
24	Y0	648	0	672	20	0
25	R1	763	0	848	28	0
25	Y1	763	0	848	21	0
26	R2	581	0	629	40	0
26	Y2	598	0	653	12	0
27	R3	469	0	518	14	0
27	Y3	469	0	518	12	0
28	R4	581	0	577	75	0
28	Y4	581	0	577	93	0
29	R5	459	0	480	62	0
29	Y5	459	0	480	61	0
30	R6	424	0	450	49	0
30	Y6	424	0	450	64	0
31	R7	430	0	480	5	0
31	Y7	430	0	480	12	0
32	R8	517	0	582	36	0
32	Y8	517	0	582	68	0
33	R9	307	0	338	4	0
33	Y9	307	0	338	10	0
34	RA	62071	0	31290	723	0
34	YA	62091	0	31297	786	0
35	RB	2573	0	1306	44	0
35	YB	2573	0	1305	36	0
36	RD	2115	0	2195	95	0
36	YD	2115	0	2195	135	0
37	RE	1568	0	1634	84	0
37	YE	1568	0	1634	100	0
38	RF	1585	0	1632	71	0
38	YF	1585	0	1632	51	0
39	RG	1474	0	1535	130	0
39	YG	1474	0	1535	84	0
40	RH	1307	0	1382	88	0
40	YH	1307	0	1382	64	0
41	RI	1136	0	1223	75	0
41	YI	1136	0	1223	77	0
42	RN	1104	0	1180	38	0
42	YN	1104	0	1180	37	0
43	RO	933	0	996	29	0
43	YO	933	0	996	27	0
44	RP	1145	0	1228	57	0
44	YP	1145	0	1228	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	RQ	1122	0	1179	45	0
45	YQ	1122	0	1179	45	0
46	RR	968	0	1033	35	0
46	YR	968	0	1033	35	0
47	RS	882	0	943	27	0
47	YS	882	0	943	58	0
48	RT	1141	0	1202	36	0
48	YT	1141	0	1202	52	0
49	RU	964	0	1022	32	0
49	YU	964	0	1022	35	0
50	RV	779	0	852	42	0
50	YV	779	0	852	35	0
51	RW	900	0	964	22	0
51	YW	900	0	964	18	0
52	RX	725	0	778	27	0
52	YX	725	0	778	34	0
53	RY	785	0	878	34	0
53	YY	785	0	878	53	0
54	RZ	1461	0	1493	100	0
54	YZ	1461	0	1493	120	0
55	XY	362	0	186	3	0
56	Z6	74	0	51	0	0
56	Z8	74	0	51	2	0
57	QA	54	0	0	0	0
57	QV	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	R7	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	333	0	0	0	0
57	RB	5	0	0	0	0
57	RE	1	0	0	0	0
57	RF	1	0	0	0	0
57	RR	2	0	0	0	0
57	XA	58	0	0	0	0
57	XV	2	0	0	0	0
57	XX	1	0	0	0	0
57	Y0	1	0	0	0	0
57	Y1	1	0	0	0	0
57	Y3	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y7	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	YA	361	0	0	0	0
57	YB	4	0	0	0	0
57	YE	2	0	0	0	0
57	YP	2	0	0	0	0
57	YQ	2	0	0	0	0
57	YR	2	0	0	0	0
57	YY	1	0	0	0	0
58	QD	8	0	0	0	0
58	XD	8	0	0	2	0
59	QN	1	0	0	0	0
59	XN	1	0	0	0	0
All	All	292176	0	198335	6155	0

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 13.

The worst 5 of 6155 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)
19:QS:44:MET:SD	19:QS:49:ILE:HD11	1.50	1.48
41:RI:83:ALA:C	41:RI:144:VAL:HG13	1.33	1.48
53:RY:76:CYS:SG	53:RY:77:PRO:HD3	1.53	1.48
13:XM:10:PRO:N	13:XM:10:PRO:CA	1.70	1.46
26:R2:13:ALA:HA	26:R2:16:LEU:CD1	1.50	1.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	QB	235/256 (92%)	215 (92%)	18 (8%)	2 (1%)	14 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	XB	235/256 (92%)	213 (91%)	20 (8%)	2 (1%)	14	46
3	QC	203/239 (85%)	190 (94%)	13 (6%)	0	100	100
3	XC	203/239 (85%)	192 (95%)	11 (5%)	0	100	100
4	QD	206/209 (99%)	200 (97%)	3 (2%)	3 (2%)	8	37
4	XD	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
5	QE	149/162 (92%)	137 (92%)	12 (8%)	0	100	100
5	XE	149/162 (92%)	143 (96%)	5 (3%)	1 (1%)	18	51
6	QF	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	XF	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
7	QG	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
7	XG	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
8	QH	136/138 (99%)	125 (92%)	11 (8%)	0	100	100
8	XH	136/138 (99%)	123 (90%)	13 (10%)	0	100	100
9	QI	125/128 (98%)	117 (94%)	8 (6%)	0	100	100
9	XI	125/128 (98%)	119 (95%)	6 (5%)	0	100	100
10	QJ	97/105 (92%)	84 (87%)	13 (13%)	0	100	100
10	XJ	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
11	QK	117/129 (91%)	111 (95%)	6 (5%)	0	100	100
11	XK	117/129 (91%)	113 (97%)	4 (3%)	0	100	100
12	QL	123/131 (94%)	111 (90%)	11 (9%)	1 (1%)	16	49
12	XL	123/131 (94%)	113 (92%)	8 (6%)	2 (2%)	7	36
13	QM	119/126 (94%)	106 (89%)	12 (10%)	1 (1%)	16	49
13	XM	119/126 (94%)	105 (88%)	13 (11%)	1 (1%)	16	49
14	QN	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
14	XN	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	7	35
15	QO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	XO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
16	QP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	98 (100%)	0	0	100	100
17	XQ	98/105 (93%)	98 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	QR	68/88 (77%)	67 (98%)	1 (2%)	0	100	100
18	XR	68/88 (77%)	64 (94%)	4 (6%)	0	100	100
19	QS	82/93 (88%)	64 (78%)	13 (16%)	5 (6%)	1	13
19	XS	82/93 (88%)	73 (89%)	8 (10%)	1 (1%)	10	41
20	QT	97/106 (92%)	88 (91%)	9 (9%)	0	100	100
20	XT	97/106 (92%)	87 (90%)	10 (10%)	0	100	100
21	QU	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
21	XU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
24	R0	80/85 (94%)	74 (92%)	6 (8%)	0	100	100
24	Y0	80/85 (94%)	76 (95%)	4 (5%)	0	100	100
25	R1	95/98 (97%)	87 (92%)	6 (6%)	2 (2%)	5	31
25	Y1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	43
26	R2	67/72 (93%)	65 (97%)	2 (3%)	0	100	100
26	Y2	69/72 (96%)	64 (93%)	4 (6%)	1 (1%)	9	38
27	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	R4	69/71 (97%)	52 (75%)	13 (19%)	4 (6%)	1	13
28	Y4	69/71 (97%)	48 (70%)	19 (28%)	2 (3%)	3	25
29	R5	57/60 (95%)	48 (84%)	6 (10%)	3 (5%)	1	15
29	Y5	57/60 (95%)	50 (88%)	6 (10%)	1 (2%)	6	34
30	R6	47/54 (87%)	36 (77%)	10 (21%)	1 (2%)	5	31
30	Y6	47/54 (87%)	34 (72%)	9 (19%)	4 (8%)	0	7
31	R7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
31	Y7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
32	R8	62/65 (95%)	53 (86%)	9 (14%)	0	100	100
32	Y8	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	3	24
33	R9	35/37 (95%)	35 (100%)	0	0	100	100
33	Y9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
36	RD	270/276 (98%)	251 (93%)	18 (7%)	1 (0%)	30	60
36	YD	270/276 (98%)	246 (91%)	21 (8%)	3 (1%)	11	43
37	RE	203/206 (98%)	177 (87%)	23 (11%)	3 (2%)	8	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	YE	203/206 (98%)	174 (86%)	27 (13%)	2 (1%)	12	44
38	RF	200/210 (95%)	188 (94%)	9 (4%)	3 (2%)	8	37
38	YF	200/210 (95%)	189 (94%)	11 (6%)	0	100	100
39	RG	179/182 (98%)	159 (89%)	18 (10%)	2 (1%)	11	43
39	YG	179/182 (98%)	160 (89%)	19 (11%)	0	100	100
40	RH	168/180 (93%)	136 (81%)	26 (16%)	6 (4%)	2	22
40	YH	168/180 (93%)	145 (86%)	18 (11%)	5 (3%)	3	25
41	RI	144/148 (97%)	130 (90%)	9 (6%)	5 (4%)	3	23
41	YI	144/148 (97%)	123 (85%)	11 (8%)	10 (7%)	1	11
42	RN	136/140 (97%)	129 (95%)	6 (4%)	1 (1%)	18	51
42	YN	136/140 (97%)	126 (93%)	8 (6%)	2 (2%)	8	37
43	RO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
43	YO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
44	RP	148/150 (99%)	129 (87%)	16 (11%)	3 (2%)	6	32
44	YP	148/150 (99%)	129 (87%)	16 (11%)	3 (2%)	6	32
45	RQ	139/141 (99%)	114 (82%)	24 (17%)	1 (1%)	18	51
45	YQ	139/141 (99%)	113 (81%)	22 (16%)	4 (3%)	3	25
46	RR	116/118 (98%)	108 (93%)	6 (5%)	2 (2%)	7	35
46	YR	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
47	RS	109/112 (97%)	93 (85%)	14 (13%)	2 (2%)	6	34
47	YS	109/112 (97%)	94 (86%)	12 (11%)	3 (3%)	4	26
48	RT	135/146 (92%)	124 (92%)	9 (7%)	2 (2%)	8	37
48	YT	135/146 (92%)	127 (94%)	8 (6%)	0	100	100
49	RU	115/118 (98%)	109 (95%)	5 (4%)	1 (1%)	14	46
49	YU	115/118 (98%)	109 (95%)	5 (4%)	1 (1%)	14	46
50	RV	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	6	32
50	YV	99/101 (98%)	86 (87%)	8 (8%)	5 (5%)	1	15
51	RW	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
51	YW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
52	RX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
52	YX	90/96 (94%)	90 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	RY	100/110 (91%)	85 (85%)	13 (13%)	2 (2%)	6	32
53	YY	100/110 (91%)	77 (77%)	18 (18%)	5 (5%)	1	16
54	RZ	181/206 (88%)	158 (87%)	18 (10%)	5 (3%)	4	26
54	YZ	181/206 (88%)	159 (88%)	13 (7%)	9 (5%)	1	16
All	All	11472/12126 (95%)	10464 (91%)	874 (8%)	134 (1%)	10	41

5 of 134 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	233	SER
19	QS	67	VAL
25	R1	30	VAL
28	R4	49	PHE
28	R4	50	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	193 (94%)	12 (6%)	18	45
2	XB	205/220 (93%)	197 (96%)	8 (4%)	28	54
3	QC	159/188 (85%)	151 (95%)	8 (5%)	22	48
3	XC	159/188 (85%)	152 (96%)	7 (4%)	25	51
4	QD	180/181 (99%)	169 (94%)	11 (6%)	17	44
4	XD	180/181 (99%)	178 (99%)	2 (1%)	65	74
5	QE	116/123 (94%)	114 (98%)	2 (2%)	53	69
5	XE	116/123 (94%)	112 (97%)	4 (3%)	32	57
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	123 (98%)	3 (2%)	43	63
7	XG	126/127 (99%)	121 (96%)	5 (4%)	28	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	QH	119/119 (100%)	118 (99%)	1 (1%)	73	77
8	XH	119/119 (100%)	118 (99%)	1 (1%)	73	77
9	QI	98/99 (99%)	98 (100%)	0	100	100
9	XI	98/99 (99%)	93 (95%)	5 (5%)	21	48
10	QJ	89/92 (97%)	87 (98%)	2 (2%)	45	65
10	XJ	89/92 (97%)	87 (98%)	2 (2%)	45	65
11	QK	90/99 (91%)	89 (99%)	1 (1%)	65	74
11	XK	90/99 (91%)	87 (97%)	3 (3%)	33	58
12	QL	104/108 (96%)	100 (96%)	4 (4%)	29	55
12	XL	104/108 (96%)	99 (95%)	5 (5%)	23	49
13	QM	97/101 (96%)	95 (98%)	2 (2%)	47	65
13	XM	97/101 (96%)	92 (95%)	5 (5%)	21	48
14	QN	49/50 (98%)	45 (92%)	4 (8%)	10	35
14	XN	49/50 (98%)	48 (98%)	1 (2%)	48	66
15	QO	79/80 (99%)	78 (99%)	1 (1%)	61	72
15	XO	79/80 (99%)	78 (99%)	1 (1%)	61	72
16	QP	72/74 (97%)	68 (94%)	4 (6%)	19	46
16	XP	72/74 (97%)	71 (99%)	1 (1%)	59	71
17	QQ	95/97 (98%)	91 (96%)	4 (4%)	26	52
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	16	43
18	QR	61/77 (79%)	58 (95%)	3 (5%)	22	49
18	XR	61/77 (79%)	60 (98%)	1 (2%)	55	69
19	QS	73/80 (91%)	67 (92%)	6 (8%)	10	35
19	XS	73/80 (91%)	65 (89%)	8 (11%)	6	27
20	QT	76/82 (93%)	71 (93%)	5 (7%)	15	42
20	XT	76/82 (93%)	74 (97%)	2 (3%)	40	62
21	QU	20/22 (91%)	18 (90%)	2 (10%)	7	30
21	XU	20/22 (91%)	18 (90%)	2 (10%)	7	30
24	R0	65/67 (97%)	61 (94%)	4 (6%)	16	44
24	Y0	65/67 (97%)	61 (94%)	4 (6%)	16	44
25	R1	82/83 (99%)	79 (96%)	3 (4%)	30	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	Y1	82/83 (99%)	77 (94%)	5 (6%)	17	44
26	R2	64/67 (96%)	57 (89%)	7 (11%)	6	27
26	Y2	66/67 (98%)	60 (91%)	6 (9%)	9	33
27	R3	51/52 (98%)	49 (96%)	2 (4%)	28	54
27	Y3	51/52 (98%)	48 (94%)	3 (6%)	18	45
28	R4	63/63 (100%)	54 (86%)	9 (14%)	3	18
28	Y4	63/63 (100%)	55 (87%)	8 (13%)	4	22
29	R5	51/52 (98%)	44 (86%)	7 (14%)	3	20
29	Y5	51/52 (98%)	48 (94%)	3 (6%)	18	45
30	R6	48/52 (92%)	42 (88%)	6 (12%)	4	23
30	Y6	48/52 (92%)	37 (77%)	11 (23%)	1	6
31	R7	42/42 (100%)	42 (100%)	0	100	100
31	Y7	42/42 (100%)	42 (100%)	0	100	100
32	R8	54/55 (98%)	51 (94%)	3 (6%)	19	46
32	Y8	54/55 (98%)	50 (93%)	4 (7%)	13	38
33	R9	34/34 (100%)	34 (100%)	0	100	100
33	Y9	34/34 (100%)	34 (100%)	0	100	100
36	RD	214/218 (98%)	206 (96%)	8 (4%)	30	56
36	YD	214/218 (98%)	191 (89%)	23 (11%)	6	28
37	RE	165/166 (99%)	158 (96%)	7 (4%)	26	52
37	YE	165/166 (99%)	156 (94%)	9 (6%)	19	46
38	RF	161/166 (97%)	157 (98%)	4 (2%)	42	63
38	YF	161/166 (97%)	157 (98%)	4 (2%)	42	63
39	RG	155/156 (99%)	149 (96%)	6 (4%)	28	54
39	YG	155/156 (99%)	146 (94%)	9 (6%)	18	45
40	RH	142/148 (96%)	135 (95%)	7 (5%)	22	49
40	YH	142/148 (96%)	134 (94%)	8 (6%)	19	46
41	RI	122/124 (98%)	108 (88%)	14 (12%)	5	25
41	YI	122/124 (98%)	107 (88%)	15 (12%)	4	23
42	RN	117/119 (98%)	111 (95%)	6 (5%)	21	48
42	YN	117/119 (98%)	108 (92%)	9 (8%)	12	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	RO	100/100 (100%)	97 (97%)	3 (3%)	36	60
43	YO	100/100 (100%)	98 (98%)	2 (2%)	48	66
44	RP	116/116 (100%)	108 (93%)	8 (7%)	14	41
44	YP	116/116 (100%)	112 (97%)	4 (3%)	32	57
45	RQ	111/111 (100%)	102 (92%)	9 (8%)	11	36
45	YQ	111/111 (100%)	101 (91%)	10 (9%)	9	33
46	RR	101/101 (100%)	98 (97%)	3 (3%)	36	60
46	YR	101/101 (100%)	98 (97%)	3 (3%)	36	60
47	RS	87/88 (99%)	85 (98%)	2 (2%)	44	64
47	YS	87/88 (99%)	83 (95%)	4 (5%)	24	50
48	RT	120/127 (94%)	117 (98%)	3 (2%)	42	63
48	YT	120/127 (94%)	113 (94%)	7 (6%)	18	45
49	RU	93/94 (99%)	90 (97%)	3 (3%)	34	58
49	YU	93/94 (99%)	92 (99%)	1 (1%)	65	74
50	RV	82/82 (100%)	71 (87%)	11 (13%)	4	21
50	YV	82/82 (100%)	75 (92%)	7 (8%)	10	35
51	RW	92/92 (100%)	88 (96%)	4 (4%)	26	52
51	YW	92/92 (100%)	90 (98%)	2 (2%)	45	65
52	RX	74/78 (95%)	71 (96%)	3 (4%)	27	53
52	YX	74/78 (95%)	70 (95%)	4 (5%)	20	47
53	RY	85/91 (93%)	78 (92%)	7 (8%)	10	35
53	YY	85/91 (93%)	77 (91%)	8 (9%)	8	32
54	RZ	162/179 (90%)	145 (90%)	17 (10%)	6	29
54	YZ	162/179 (90%)	145 (90%)	17 (10%)	6	29
All	All	9704/10064 (96%)	9204 (95%)	500 (5%)	21	48

5 of 500 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
54	RZ	52	SER
45	YQ	104	PHE
13	XM	48	LEU
45	YQ	17	LEU
52	YX	28	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
11	XK	116	HIS
42	YN	128	HIS
13	XM	62	ASN
36	YD	227	ASN
48	YT	38	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	271 (18%)	40 (2%)
1	XA	1509/1522 (99%)	258 (17%)	33 (2%)
22	QV	72/76 (94%)	15 (20%)	0
22	XV	72/76 (94%)	16 (22%)	0
23	QX	2/23 (8%)	0	0
23	XX	22/23 (95%)	9 (40%)	0
34	RA	2879/2915 (98%)	556 (19%)	47 (1%)
34	YA	2880/2915 (98%)	557 (19%)	47 (1%)
35	RB	119/122 (97%)	23 (19%)	1 (0%)
35	YB	119/122 (97%)	20 (16%)	1 (0%)
55	XY	16/17 (94%)	6 (37%)	0
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9190/9339 (98%)	1731 (18%)	169 (1%)

5 of 1731 RNA backbone outliers are listed below:

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

5 of 169 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	1200	C
34	YA	1085	A
1	XA	1446	A
34	YA	404	C

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Mol	Chain	Res	Type
34	YA	1653	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	C4J	XV	47	22	25,29,30	2.79	6 (24%)	28,42,45	1.57	5 (17%)
22	H2U	QV	20	22	18,21,22	1.04	1 (5%)	19,30,33	1.36	3 (15%)
22	5MU	XV	54	22	19,22,23	1.36	5 (26%)	27,32,35	2.01	7 (25%)
22	T6A	QV	37	22	31,34,35	1.37	4 (12%)	43,49,52	2.04	12 (27%)
22	MNU	QV	34	23,22	21,24,25	1.24	3 (14%)	27,34,37	1.71	8 (29%)
22	T6A	XV	37	22	31,34,35	1.39	4 (12%)	43,49,52	1.88	12 (27%)
22	PSU	XV	39	22	18,21,22	1.39	2 (11%)	21,30,33	1.99	3 (14%)
22	PSU	QV	55	22	18,21,22	1.44	2 (11%)	21,30,33	2.09	4 (19%)
22	PSU	XV	55	22	18,21,22	1.39	2 (11%)	21,30,33	2.02	3 (14%)
22	PSU	QV	39	22	18,21,22	1.41	2 (11%)	21,30,33	2.10	4 (19%)
56	PPU	Z8	76	56,34	37,40,41	1.32	4 (10%)	47,57,60	2.02	12 (25%)
22	7MG	QV	46	22	23,26,27	1.39	5 (21%)	27,39,42	2.52	5 (18%)
22	H2U	XV	20	22	18,21,22	1.04	2 (11%)	19,30,33	1.23	3 (15%)
56	PPU	Z6	76	56,34	37,40,41	1.28	4 (10%)	47,57,60	2.03	12 (25%)
22	C4J	QV	47	22	25,29,30	2.87	7 (28%)	28,42,45	1.74	5 (17%)
22	5MU	QV	54	22	19,22,23	1.36	4 (21%)	27,32,35	2.07	8 (29%)
22	MNU	XV	34	23,22	21,24,25	1.25	4 (19%)	27,34,37	1.84	7 (25%)
22	7MG	XV	46	22	23,26,27	1.30	3 (13%)	27,39,42	2.62	7 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	C4J	XV	47	22	-	4/16/34/35	0/2/2/2
22	H2U	QV	20	22	-	5/7/38/39	0/2/2/2
22	5MU	XV	54	22	-	0/7/25/26	0/2/2/2
22	T6A	QV	37	22	-	10/23/41/42	0/3/3/3
22	MNU	QV	34	23,22	-	2/10/28/29	0/2/2/2
22	T6A	XV	37	22	-	8/23/41/42	0/3/3/3
22	PSU	XV	39	22	-	0/7/25/26	0/2/2/2
22	PSU	QV	55	22	-	0/7/25/26	0/2/2/2
22	PSU	XV	55	22	-	0/7/25/26	0/2/2/2
22	PSU	QV	39	22	-	0/7/25/26	0/2/2/2
56	PPU	Z8	76	56,34	-	3/25/43/44	0/4/4/4
22	7MG	QV	46	22	-	2/7/37/38	0/3/3/3
22	H2U	XV	20	22	-	5/7/38/39	0/2/2/2
56	PPU	Z6	76	56,34	-	3/25/43/44	0/4/4/4
22	C4J	QV	47	22	-	4/16/34/35	0/2/2/2
22	5MU	QV	54	22	-	0/7/25/26	0/2/2/2
22	MNU	XV	34	23,22	-	4/10/28/29	0/2/2/2
22	7MG	XV	46	22	-	0/7/37/38	0/3/3/3

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	47	C4J	C6-C5	10.37	1.49	1.35
22	XV	47	C4J	C6-C5	10.21	1.49	1.35
22	QV	47	C4J	C2-N3	6.56	1.50	1.38
22	XV	47	C4J	C2-N3	6.10	1.49	1.38
56	Z8	76	PPU	C5-C4	5.15	1.48	1.39

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	XV	46	7MG	N9-C4-N3	8.91	138.52	125.46
22	QV	46	7MG	N9-C4-N3	8.70	138.21	125.46
22	QV	55	PSU	N1-C2-N3	6.73	122.27	115.17
22	QV	39	PSU	N1-C2-N3	6.33	121.84	115.17
22	XV	55	PSU	N1-C2-N3	6.19	121.70	115.17

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	XV	20	H2U	C2'-C1'-N1-C2
22	QV	34	MNU	C6-C5-C7-N8
22	QV	34	MNU	C4-C5-C7-N8
22	XV	34	MNU	C6-C5-C7-N8
22	XV	34	MNU	C4-C5-C7-N8

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	XV	37	T6A	1	0
56	Z8	76	PPU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 846 ligands modelled in this entry, 844 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	$\# Z > 2$
58	SF4	QD	301	4	0,12,12	-	-	-		
58	SF4	XD	301	4	0,12,12	-	-	-		

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	XD	301	SF4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1522 (98%)	-0.02	15 (1%) 79 53	65, 123, 231, 395	0
1	XA	1511/1522 (99%)	0.08	57 (3%) 44 24	60, 122, 218, 363	0
2	QB	237/256 (92%)	0.21	3 (1%) 75 47	122, 192, 248, 311	0
2	XB	237/256 (92%)	0.26	3 (1%) 75 47	90, 152, 222, 280	0
3	QC	205/239 (85%)	-0.01	3 (1%) 72 44	95, 174, 232, 279	0
3	XC	205/239 (85%)	-0.06	1 (0%) 87 66	93, 142, 199, 231	0
4	QD	208/209 (99%)	0.43	5 (2%) 59 34	97, 139, 197, 245	0
4	XD	208/209 (99%)	0.19	1 (0%) 87 66	68, 116, 161, 186	0
5	QE	151/162 (93%)	0.24	2 (1%) 75 47	95, 143, 186, 218	0
5	XE	151/162 (93%)	-0.05	1 (0%) 84 60	68, 108, 150, 194	0
6	QF	101/101 (100%)	0.27	1 (0%) 79 53	83, 130, 181, 207	0
6	XF	101/101 (100%)	0.53	3 (2%) 52 29	74, 120, 168, 261	0
7	QG	155/156 (99%)	0.49	11 (7%) 22 13	118, 166, 226, 275	0
7	XG	155/156 (99%)	0.26	6 (3%) 43 23	103, 152, 208, 237	0
8	QH	138/138 (100%)	0.16	2 (1%) 73 45	95, 138, 183, 215	0
8	XH	138/138 (100%)	0.34	6 (4%) 40 21	76, 125, 172, 207	0
9	QI	127/128 (99%)	0.39	5 (3%) 43 23	129, 184, 234, 307	0
9	XI	127/128 (99%)	0.36	12 (9%) 14 9	107, 164, 221, 281	0
10	QJ	99/105 (94%)	0.41	1 (1%) 79 53	136, 190, 252, 301	0
10	XJ	99/105 (94%)	0.32	3 (3%) 52 29	110, 166, 215, 265	0
11	QK	119/129 (92%)	0.42	7 (5%) 28 16	98, 129, 188, 255	0
11	XK	119/129 (92%)	0.38	4 (3%) 48 27	73, 117, 190, 277	0
12	QL	125/131 (95%)	0.35	6 (4%) 35 19	74, 111, 159, 237	0
12	XL	125/131 (95%)	0.20	4 (3%) 50 28	57, 98, 155, 256	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	0.77	13 (10%) 11 8	123, 171, 219, 278	0
13	XM	121/126 (96%)	0.32	6 (4%) 34 19	103, 159, 199, 257	0
14	QN	60/61 (98%)	0.14	0 100 100	122, 169, 222, 250	0
14	XN	60/61 (98%)	0.28	3 (5%) 34 19	103, 138, 172, 195	0
15	QO	88/89 (98%)	0.50	6 (6%) 23 14	75, 124, 170, 188	0
15	XO	88/89 (98%)	0.47	5 (5%) 29 17	71, 109, 157, 184	0
16	QP	84/88 (95%)	0.51	4 (4%) 35 19	76, 108, 155, 224	0
16	XP	84/88 (95%)	0.21	1 (1%) 76 49	92, 131, 184, 200	0
17	QQ	100/105 (95%)	0.36	3 (3%) 52 29	81, 114, 149, 170	0
17	XQ	100/105 (95%)	0.38	2 (2%) 65 37	84, 123, 166, 173	0
18	QR	70/88 (79%)	-0.04	1 (1%) 73 45	100, 140, 181, 188	0
18	XR	70/88 (79%)	0.38	0 100 100	81, 120, 160, 191	0
19	QS	84/93 (90%)	0.12	0 100 100	134, 188, 256, 354	0
19	XS	84/93 (90%)	0.12	3 (3%) 46 25	127, 176, 238, 259	0
20	QT	99/106 (93%)	0.46	6 (6%) 27 15	72, 110, 169, 235	0
20	XT	99/106 (93%)	0.28	3 (3%) 52 29	107, 146, 209, 231	0
21	QU	25/27 (92%)	1.43	5 (20%) 3 3	145, 175, 223, 226	0
21	XU	25/27 (92%)	0.20	0 100 100	125, 154, 200, 213	0
22	QV	66/76 (86%)	0.70	6 (9%) 15 10	124, 253, 275, 293	0
22	XV	66/76 (86%)	0.44	6 (9%) 15 10	102, 217, 247, 262	0
23	QX	3/23 (13%)	0.37	0 100 100	99, 99, 100, 127	0
23	XX	23/23 (100%)	1.72	7 (30%) 1 1	97, 220, 268, 305	0
24	R0	82/85 (96%)	0.34	3 (3%) 45 25	68, 103, 148, 184	0
24	Y0	82/85 (96%)	0.44	4 (4%) 35 19	63, 105, 132, 169	0
25	R1	97/98 (98%)	0.65	8 (8%) 17 11	38, 92, 165, 221	0
25	Y1	97/98 (98%)	0.41	5 (5%) 33 18	54, 84, 170, 254	0
26	R2	69/72 (95%)	0.15	0 100 100	71, 116, 170, 206	0
26	Y2	71/72 (98%)	0.17	2 (2%) 55 30	56, 88, 160, 261	0
27	R3	59/60 (98%)	0.31	1 (1%) 69 40	69, 99, 170, 231	0
27	Y3	59/60 (98%)	0.20	2 (3%) 48 27	73, 100, 152, 177	0
28	R4	71/71 (100%)	0.24	0 100 100	150, 221, 299, 329	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
28	Y4	71/71 (100%)	0.26	2 (2%)	55 30	125, 199, 313, 339	0
29	R5	59/60 (98%)	0.39	4 (6%)	23 14	53, 89, 208, 249	0
29	Y5	59/60 (98%)	0.46	4 (6%)	23 14	60, 92, 216, 310	0
30	R6	49/54 (90%)	0.84	5 (10%)	12 8	191, 247, 316, 341	0
30	Y6	49/54 (90%)	0.59	2 (4%)	41 22	179, 236, 296, 337	0
31	R7	49/49 (100%)	-0.01	0	100 100	43, 62, 136, 244	0
31	Y7	49/49 (100%)	0.15	2 (4%)	41 22	44, 60, 138, 178	0
32	R8	64/65 (98%)	0.62	7 (10%)	10 8	54, 88, 134, 328	0
32	Y8	64/65 (98%)	0.98	10 (15%)	5 5	67, 92, 166, 199	0
33	R9	37/37 (100%)	1.82	15 (40%)	0 1	152, 211, 269, 297	0
33	Y9	37/37 (100%)	2.11	18 (48%)	0 1	178, 217, 280, 312	0
34	RA	2882/2915 (98%)	-0.19	17 (0%)	85 63	43, 83, 229, 398	0
34	YA	2883/2915 (98%)	-0.11	34 (1%)	76 49	41, 82, 243, 435	0
35	RB	120/122 (98%)	0.09	0	100 100	96, 165, 199, 259	0
35	YB	120/122 (98%)	-0.02	1 (0%)	82 58	94, 134, 169, 250	0
36	RD	272/276 (98%)	0.39	10 (3%)	45 25	43, 78, 113, 165	0
36	YD	272/276 (98%)	0.34	11 (4%)	42 23	38, 72, 110, 221	0
37	RE	205/206 (99%)	0.13	3 (1%)	72 44	45, 81, 146, 270	0
37	YE	205/206 (99%)	0.32	5 (2%)	59 34	46, 98, 154, 210	0
38	RF	202/210 (96%)	0.34	9 (4%)	38 20	50, 92, 160, 191	0
38	YF	202/210 (96%)	0.05	1 (0%)	87 66	39, 84, 141, 190	0
39	RG	181/182 (99%)	0.35	4 (2%)	62 35	132, 183, 256, 304	0
39	YG	181/182 (99%)	0.38	3 (1%)	69 40	102, 147, 200, 251	0
40	RH	170/180 (94%)	0.57	13 (7%)	20 12	79, 170, 240, 274	0
40	YH	170/180 (94%)	0.44	10 (5%)	28 16	70, 111, 159, 274	0
41	RI	146/148 (98%)	0.44	7 (4%)	35 19	74, 130, 184, 350	0
41	YI	146/148 (98%)	0.24	4 (2%)	56 31	68, 123, 187, 214	0
42	RN	138/140 (98%)	0.35	2 (1%)	73 45	66, 97, 153, 213	0
42	YN	138/140 (98%)	0.18	2 (1%)	73 45	58, 100, 155, 209	0
43	RO	122/122 (100%)	0.04	2 (1%)	70 42	40, 75, 113, 136	0
43	YO	122/122 (100%)	-0.02	0	100 100	48, 83, 123, 145	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RP	150/150 (100%)	0.30	7 (4%) 36 19	53, 105, 160, 276	0
44	YP	150/150 (100%)	0.61	9 (6%) 27 16	50, 101, 167, 244	0
45	RQ	141/141 (100%)	0.49	9 (6%) 25 15	67, 103, 157, 208	0
45	YQ	141/141 (100%)	0.57	15 (10%) 11 8	58, 99, 159, 242	0
46	RR	118/118 (100%)	0.02	1 (0%) 82 58	45, 74, 104, 157	0
46	YR	118/118 (100%)	0.18	4 (3%) 48 27	59, 90, 135, 188	0
47	RS	111/112 (99%)	0.25	2 (1%) 67 40	119, 147, 209, 253	0
47	YS	111/112 (99%)	0.55	2 (1%) 67 40	88, 138, 185, 278	0
48	RT	137/146 (93%)	0.34	6 (4%) 39 21	52, 91, 157, 192	0
48	YT	137/146 (93%)	0.14	1 (0%) 84 60	67, 101, 174, 238	0
49	RU	117/118 (99%)	0.29	4 (3%) 48 27	51, 90, 156, 186	0
49	YU	117/118 (99%)	0.19	3 (2%) 57 32	54, 91, 152, 204	0
50	RV	101/101 (100%)	0.31	4 (3%) 42 23	63, 110, 150, 242	0
50	YV	101/101 (100%)	0.23	2 (1%) 65 37	64, 111, 165, 252	0
51	RW	113/113 (100%)	0.01	2 (1%) 67 40	48, 71, 131, 285	0
51	YW	113/113 (100%)	-0.00	1 (0%) 81 55	43, 76, 144, 212	0
52	RX	92/96 (95%)	0.05	1 (1%) 78 51	64, 90, 128, 173	0
52	YX	92/96 (95%)	-0.17	0 100 100	45, 74, 112, 148	0
53	RY	102/110 (92%)	0.89	12 (11%) 9 7	69, 115, 172, 303	0
53	YY	102/110 (92%)	0.57	6 (5%) 28 16	52, 98, 178, 233	0
54	RZ	183/206 (88%)	0.21	4 (2%) 62 35	90, 142, 188, 229	0
54	YZ	183/206 (88%)	0.40	10 (5%) 30 17	94, 136, 200, 254	0
55	XY	17/17 (100%)	0.21	0 100 100	133, 179, 250, 263	0
56	Z6	2/3 (66%)	0.51	0 100 100	148, 148, 148, 152	0
56	Z8	2/3 (66%)	1.01	0 100 100	156, 156, 156, 156	0
All	All	20863/21465 (97%)	0.15	579 (2%) 55 30	38, 111, 222, 435	0

The worst 5 of 579 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	QM	120	LYS	9.3
11	XK	129	SER	7.4
7	XG	5	ARG	7.3

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Mol	Chain	Res	Type	RSRZ
11	XK	128	ALA	7.3
34	YA	669	G	6.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	C4J	QV	47	28/29	0.19	0.16	216,236,255,258	0
22	C4J	XV	47	28/29	0.26	0.14	216,238,248,253	0
22	H2U	QV	20	20/21	0.33	0.12	350,356,363,365	0
22	7MG	QV	46	24/25	0.55	0.10	269,282,291,313	0
22	5MU	XV	54	21/22	0.67	0.10	220,226,234,237	0
22	H2U	XV	20	20/21	0.72	0.09	264,273,283,285	0
22	PSU	XV	55	20/21	0.72	0.08	225,233,240,242	0
22	5MU	QV	54	21/22	0.73	0.09	229,235,242,243	0
22	7MG	XV	46	24/25	0.76	0.08	214,229,235,237	0
22	PSU	QV	55	20/21	0.77	0.09	234,239,249,252	0
22	T6A	QV	37	32/33	0.77	0.17	138,161,200,207	0
22	T6A	XV	37	32/33	0.88	0.14	96,111,152,158	0
22	PSU	QV	39	20/21	0.89	0.10	122,123,132,138	0
22	MNU	XV	34	23/24	0.92	0.11	95,100,117,132	0
22	PSU	XV	39	20/21	0.93	0.10	91,100,120,125	0
22	MNU	QV	34	23/24	0.94	0.10	121,122,145,148	0
56	PPU	Z8	76	37/38	0.95	0.13	74,104,122,130	0
56	PPU	Z6	76	37/38	0.96	0.12	76,109,123,127	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($\text{\AA}^2$)	Q<0.9
57	MG	Y7	102	1/1	-0.08	0.21	72,72,72,72	0
57	MG	YA	3265	1/1	0.20	0.18	254,254,254,254	0
57	MG	YA	3300	1/1	0.26	0.46	109,109,109,109	0
57	MG	YA	3359	1/1	0.30	0.20	78,78,78,78	0
57	MG	RB	202	1/1	0.33	0.10	129,129,129,129	0
57	MG	YA	3184	1/1	0.40	0.22	190,190,190,190	0
57	MG	YA	3339	1/1	0.43	0.30	132,132,132,132	0
57	MG	RA	3224	1/1	0.43	0.22	110,110,110,110	0
57	MG	QA	1642	1/1	0.46	0.27	111,111,111,111	0
57	MG	YA	3315	1/1	0.46	0.33	151,151,151,151	0
57	MG	YA	3223	1/1	0.47	0.15	71,71,71,71	0
57	MG	RA	3129	1/1	0.50	0.19	92,92,92,92	0
57	MG	RA	3203	1/1	0.53	0.25	84,84,84,84	0
57	MG	YA	3323	1/1	0.55	0.20	94,94,94,94	0
57	MG	YA	3341	1/1	0.56	0.28	122,122,122,122	0
57	MG	YA	3152	1/1	0.57	0.11	99,99,99,99	0
57	MG	RA	3209	1/1	0.59	0.14	76,76,76,76	0
57	MG	YA	3358	1/1	0.61	0.45	140,140,140,140	0
57	MG	YA	3171	1/1	0.62	0.12	136,136,136,136	0
57	MG	YA	3349	1/1	0.63	0.15	72,72,72,72	0
57	MG	YA	3354	1/1	0.63	0.19	76,76,76,76	0
57	MG	QA	1646	1/1	0.63	0.16	97,97,97,97	0
57	MG	YA	3335	1/1	0.63	0.36	129,129,129,129	0
57	MG	YA	3221	1/1	0.64	0.13	54,54,54,54	0
57	MG	YA	3340	1/1	0.65	0.08	62,62,62,62	0
57	MG	RA	3261	1/1	0.67	0.20	84,84,84,84	0
57	MG	XA	1639	1/1	0.67	0.11	138,138,138,138	0
57	MG	YR	201	1/1	0.67	0.12	81,81,81,81	0
57	MG	QA	1645	1/1	0.68	0.16	98,98,98,98	0
57	MG	Y0	101	1/1	0.69	0.22	80,80,80,80	0
57	MG	YA	3307	1/1	0.70	0.29	76,76,76,76	0
57	MG	XA	1650	1/1	0.70	0.17	65,65,65,65	0
57	MG	YA	3186	1/1	0.70	0.21	73,73,73,73	0
57	MG	RA	3149	1/1	0.71	0.12	64,64,64,64	0
57	MG	RA	3001	1/1	0.71	0.37	134,134,134,134	0
57	MG	RA	3283	1/1	0.72	0.16	65,65,65,65	0
57	MG	YA	3322	1/1	0.72	0.13	84,84,84,84	0
57	MG	YE	301	1/1	0.72	0.16	38,38,38,38	0
57	MG	YA	3266	1/1	0.72	0.14	82,82,82,82	0
57	MG	QA	1635	1/1	0.73	0.13	101,101,101,101	0
57	MG	YA	3135	1/1	0.73	0.12	51,51,51,51	0
57	MG	YA	3350	1/1	0.73	0.16	83,83,83,83	0
57	MG	YA	3214	1/1	0.73	0.17	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3344	1/1	0.74	0.20	92,92,92,92	0
57	MG	RA	3165	1/1	0.74	0.10	61,61,61,61	0
57	MG	YB	204	1/1	0.74	0.27	67,67,67,67	0
57	MG	YA	3115	1/1	0.74	0.14	88,88,88,88	0
57	MG	YA	3336	1/1	0.74	0.33	72,72,72,72	0
57	MG	XA	1654	1/1	0.75	0.15	97,97,97,97	0
57	MG	YA	3326	1/1	0.76	0.10	73,73,73,73	0
57	MG	YA	3288	1/1	0.76	0.11	112,112,112,112	0
57	MG	YA	3211	1/1	0.76	0.18	90,90,90,90	0
57	MG	YA	3181	1/1	0.77	0.12	82,82,82,82	0
57	MG	YA	3151	1/1	0.77	0.20	62,62,62,62	0
57	MG	RA	3277	1/1	0.77	0.21	54,54,54,54	0
57	MG	YA	3191	1/1	0.77	0.31	85,85,85,85	0
57	MG	YA	3282	1/1	0.77	0.26	111,111,111,111	0
57	MG	YA	3204	1/1	0.77	0.14	66,66,66,66	0
57	MG	YA	3166	1/1	0.77	0.13	79,79,79,79	0
57	MG	YA	3301	1/1	0.77	0.09	39,39,39,39	0
57	MG	RA	3274	1/1	0.77	0.17	94,94,94,94	0
57	MG	XA	1649	1/1	0.78	0.31	83,83,83,83	0
57	MG	QA	1638	1/1	0.78	0.18	104,104,104,104	0
57	MG	YB	201	1/1	0.78	0.17	47,47,47,47	0
57	MG	YA	3261	1/1	0.79	0.13	55,55,55,55	0
57	MG	YA	3263	1/1	0.79	0.33	76,76,76,76	0
57	MG	XA	1613	1/1	0.79	0.24	50,50,50,50	0
57	MG	YA	3213	1/1	0.79	0.18	79,79,79,79	0
57	MG	YA	3187	1/1	0.79	0.22	59,59,59,59	0
57	MG	RA	3326	1/1	0.79	0.09	17,17,17,17	0
57	MG	RA	3250	1/1	0.79	0.11	34,34,34,34	0
57	MG	YA	3264	1/1	0.80	0.16	91,91,91,91	0
57	MG	QA	1611	1/1	0.80	0.12	66,66,66,66	0
57	MG	YA	3338	1/1	0.80	0.15	86,86,86,86	0
57	MG	RA	3273	1/1	0.80	0.12	40,40,40,40	0
57	MG	YA	3318	1/1	0.80	0.28	120,120,120,120	0
57	MG	YA	3244	1/1	0.80	0.21	31,31,31,31	0
57	MG	XA	1622	1/1	0.80	0.14	63,63,63,63	0
57	MG	RA	3190	1/1	0.80	0.29	52,52,52,52	0
57	MG	YA	3168	1/1	0.81	0.08	70,70,70,70	0
57	MG	YA	3142	1/1	0.81	0.24	52,52,52,52	0
57	MG	RA	3010	1/1	0.81	0.12	59,59,59,59	0
57	MG	YA	3360	1/1	0.81	0.17	100,100,100,100	0
57	MG	YA	3294	1/1	0.81	0.12	63,63,63,63	0
57	MG	QA	1641	1/1	0.81	0.11	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3157	1/1	0.81	0.12	49,49,49,49	0
57	MG	RA	3246	1/1	0.81	0.17	77,77,77,77	0
57	MG	YA	3328	1/1	0.82	0.14	39,39,39,39	0
57	MG	YA	3216	1/1	0.82	0.27	85,85,85,85	0
57	MG	RA	3286	1/1	0.82	0.20	55,55,55,55	0
57	MG	RA	3211	1/1	0.82	0.16	76,76,76,76	0
57	MG	YA	3324	1/1	0.82	0.22	87,87,87,87	0
57	MG	YQ	202	1/1	0.82	0.12	88,88,88,88	0
57	MG	XA	1652	1/1	0.82	0.09	54,54,54,54	0
57	MG	YA	3331	1/1	0.83	0.07	53,53,53,53	0
57	MG	YA	3343	1/1	0.83	0.13	96,96,96,96	0
57	MG	RA	3310	1/1	0.83	0.22	76,76,76,76	0
57	MG	YA	3279	1/1	0.83	0.10	56,56,56,56	0
57	MG	XA	1614	1/1	0.83	0.11	53,53,53,53	0
57	MG	RA	3196	1/1	0.83	0.11	67,67,67,67	0
57	MG	RA	3299	1/1	0.83	0.14	68,68,68,68	0
57	MG	YA	3332	1/1	0.84	0.09	56,56,56,56	0
57	MG	YA	3190	1/1	0.84	0.11	84,84,84,84	0
57	MG	Y1	101	1/1	0.84	0.19	91,91,91,91	0
57	MG	YA	3319	1/1	0.84	0.28	63,63,63,63	0
57	MG	YA	3175	1/1	0.84	0.23	94,94,94,94	0
57	MG	YA	3257	1/1	0.84	0.17	36,36,36,36	0
57	MG	RA	3201	1/1	0.84	0.17	70,70,70,70	0
57	MG	RA	3291	1/1	0.84	0.27	37,37,37,37	0
57	MG	RA	3120	1/1	0.84	0.18	47,47,47,47	0
57	MG	RA	3303	1/1	0.84	0.07	92,92,92,92	0
57	MG	QA	1639	1/1	0.85	0.11	88,88,88,88	0
57	MG	RA	3248	1/1	0.85	0.11	33,33,33,33	0
57	MG	YA	3120	1/1	0.85	0.12	39,39,39,39	0
57	MG	YA	3345	1/1	0.85	0.14	83,83,83,83	0
57	MG	YA	3348	1/1	0.85	0.19	83,83,83,83	0
57	MG	YA	3124	1/1	0.85	0.09	56,56,56,56	0
57	MG	RA	3215	1/1	0.85	0.14	59,59,59,59	0
57	MG	RA	3210	1/1	0.85	0.20	63,63,63,63	0
57	MG	YA	3231	1/1	0.85	0.08	53,53,53,53	0
57	MG	YA	3296	1/1	0.85	0.17	47,47,47,47	0
57	MG	YA	3298	1/1	0.85	0.19	126,126,126,126	0
57	MG	RB	203	1/1	0.85	0.22	29,29,29,29	0
57	MG	RB	205	1/1	0.85	0.19	58,58,58,58	0
57	MG	YA	3302	1/1	0.85	0.16	76,76,76,76	0
57	MG	RA	3270	1/1	0.85	0.17	46,46,46,46	0
57	MG	RA	3226	1/1	0.85	0.34	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3131	1/1	0.86	0.27	39,39,39,39	0
57	MG	YA	3136	1/1	0.86	0.15	72,72,72,72	0
57	MG	QA	1619	1/1	0.86	0.07	63,63,63,63	0
57	MG	YA	3193	1/1	0.86	0.18	95,95,95,95	0
57	MG	YA	3281	1/1	0.86	0.24	84,84,84,84	0
57	MG	RA	3012	1/1	0.86	0.12	17,17,17,17	0
57	MG	RA	3170	1/1	0.86	0.11	71,71,71,71	0
57	MG	XA	1643	1/1	0.86	0.06	56,56,56,56	0
57	MG	YA	3162	1/1	0.86	0.17	56,56,56,56	0
57	MG	RA	3053	1/1	0.87	0.24	31,31,31,31	0
57	MG	XA	1604	1/1	0.87	0.10	56,56,56,56	0
57	MG	YA	3205	1/1	0.87	0.19	104,104,104,104	0
57	MG	RA	3009	1/1	0.87	0.23	75,75,75,75	0
57	MG	RA	3267	1/1	0.87	0.09	60,60,60,60	0
57	MG	YA	3295	1/1	0.87	0.16	31,31,31,31	0
57	MG	YA	3106	1/1	0.87	0.17	156,156,156,156	0
57	MG	QA	1630	1/1	0.87	0.20	72,72,72,72	0
57	MG	YA	3299	1/1	0.87	0.19	73,73,73,73	0
57	MG	YA	3218	1/1	0.87	0.17	67,67,67,67	0
57	MG	YA	3169	1/1	0.87	0.11	17,17,17,17	0
57	MG	YA	3170	1/1	0.87	0.11	86,86,86,86	0
57	MG	RA	3003	1/1	0.87	0.10	34,34,34,34	0
57	MG	YA	3121	1/1	0.87	0.24	44,44,44,44	0
57	MG	YA	3123	1/1	0.87	0.33	45,45,45,45	0
57	MG	YA	3260	1/1	0.87	0.08	85,85,85,85	0
57	MG	RA	3138	1/1	0.87	0.17	47,47,47,47	0
57	MG	RA	3333	1/1	0.87	0.23	55,55,55,55	0
57	MG	RA	3014	1/1	0.87	0.29	30,30,30,30	0
57	MG	RA	3154	1/1	0.87	0.12	94,94,94,94	0
57	MG	YA	3146	1/1	0.87	0.11	66,66,66,66	0
57	MG	YA	3268	1/1	0.87	0.22	42,42,42,42	0
57	MG	YR	202	1/1	0.87	0.30	82,82,82,82	0
57	MG	YA	3161	1/1	0.88	0.28	47,47,47,47	0
57	MG	RA	3315	1/1	0.88	0.14	48,48,48,48	0
57	MG	YA	3164	1/1	0.88	0.24	47,47,47,47	0
57	MG	RA	3322	1/1	0.88	0.09	68,68,68,68	0
57	MG	YA	3247	1/1	0.88	0.23	81,81,81,81	0
57	MG	YA	3252	1/1	0.88	0.12	139,139,139,139	0
57	MG	RA	3200	1/1	0.88	0.12	74,74,74,74	0
57	MG	RA	3130	1/1	0.88	0.26	52,52,52,52	0
57	MG	RA	3163	1/1	0.88	0.18	28,28,28,28	0
57	MG	YA	3070	1/1	0.88	0.12	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3083	1/1	0.88	0.18	68,68,68,68	0
57	MG	YA	3105	1/1	0.88	0.25	38,38,38,38	0
57	MG	YA	3182	1/1	0.88	0.11	56,56,56,56	0
57	MG	RA	3011	1/1	0.88	0.15	92,92,92,92	0
57	MG	RA	3124	1/1	0.88	0.24	28,28,28,28	0
57	MG	RR	202	1/1	0.88	0.22	62,62,62,62	0
57	MG	XA	1603	1/1	0.88	0.13	63,63,63,63	0
57	MG	RA	3290	1/1	0.88	0.16	69,69,69,69	0
57	MG	YA	3291	1/1	0.88	0.10	47,47,47,47	0
57	MG	RA	3251	1/1	0.88	0.26	53,53,53,53	0
57	MG	YA	3202	1/1	0.88	0.06	52,52,52,52	0
57	MG	RA	3296	1/1	0.88	0.18	55,55,55,55	0
57	MG	QA	1621	1/1	0.88	0.19	67,67,67,67	0
57	MG	YA	3210	1/1	0.88	0.12	87,87,87,87	0
57	MG	RA	3153	1/1	0.88	0.23	45,45,45,45	0
57	MG	YA	3212	1/1	0.88	0.11	126,126,126,126	0
57	MG	RA	3307	1/1	0.88	0.14	60,60,60,60	0
57	MG	YP	201	1/1	0.88	0.31	89,89,89,89	0
57	MG	XA	1647	1/1	0.88	0.19	39,39,39,39	0
57	MG	RA	3220	1/1	0.88	0.15	53,53,53,53	0
57	MG	RA	3312	1/1	0.88	0.11	49,49,49,49	0
57	MG	YA	3287	1/1	0.89	0.09	32,32,32,32	0
57	MG	YA	3178	1/1	0.89	0.10	69,69,69,69	0
57	MG	YA	3290	1/1	0.89	0.15	88,88,88,88	0
57	MG	YA	3180	1/1	0.89	0.16	81,81,81,81	0
57	MG	YA	3292	1/1	0.89	0.28	85,85,85,85	0
57	MG	YA	3220	1/1	0.89	0.17	68,68,68,68	0
57	MG	YA	3139	1/1	0.89	0.19	92,92,92,92	0
57	MG	RA	3281	1/1	0.89	0.15	46,46,46,46	0
57	MG	Y7	101	1/1	0.89	0.15	55,55,55,55	0
57	MG	XA	1625	1/1	0.89	0.13	59,59,59,59	0
57	MG	XA	1627	1/1	0.89	0.19	43,43,43,43	0
57	MG	RA	3171	1/1	0.89	0.17	62,62,62,62	0
57	MG	RB	204	1/1	0.89	0.34	58,58,58,58	0
57	MG	XA	1644	1/1	0.89	0.06	65,65,65,65	0
57	MG	RA	3186	1/1	0.89	0.23	60,60,60,60	0
57	MG	YA	3203	1/1	0.89	0.12	64,64,64,64	0
57	MG	RA	3070	1/1	0.89	0.16	28,28,28,28	0
57	MG	YA	3361	1/1	0.89	0.14	41,41,41,41	0
57	MG	RA	3249	1/1	0.89	0.26	116,116,116,116	0
57	MG	YB	202	1/1	0.89	0.24	199,199,199,199	0
57	MG	YB	203	1/1	0.89	0.07	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1651	1/1	0.89	0.10	43,43,43,43	0
57	MG	RA	3293	1/1	0.89	0.07	45,45,45,45	0
57	MG	RA	3205	1/1	0.89	0.15	61,61,61,61	0
57	MG	YA	3327	1/1	0.89	0.11	59,59,59,59	0
57	MG	YA	3173	1/1	0.89	0.17	54,54,54,54	0
57	MG	RA	3140	1/1	0.89	0.18	87,87,87,87	0
57	MG	XA	1624	1/1	0.90	0.07	70,70,70,70	0
57	MG	QA	1654	1/1	0.90	0.21	41,41,41,41	0
57	MG	YA	3179	1/1	0.90	0.13	46,46,46,46	0
57	MG	XA	1626	1/1	0.90	0.07	55,55,55,55	0
57	MG	QA	1623	1/1	0.90	0.08	87,87,87,87	0
57	MG	YA	3222	1/1	0.90	0.16	64,64,64,64	0
57	MG	XA	1633	1/1	0.90	0.26	46,46,46,46	0
57	MG	RA	3216	1/1	0.90	0.05	46,46,46,46	0
57	MG	YA	3009	1/1	0.90	0.10	47,47,47,47	0
57	MG	YA	3245	1/1	0.90	0.09	13,13,13,13	0
57	MG	YA	3010	1/1	0.90	0.20	11,11,11,11	0
57	MG	YA	3188	1/1	0.90	0.13	47,47,47,47	0
57	MG	YA	3022	1/1	0.90	0.30	11,11,11,11	0
57	MG	YA	3067	1/1	0.90	0.16	44,44,44,44	0
57	MG	YA	3192	1/1	0.90	0.14	55,55,55,55	0
57	MG	RA	3141	1/1	0.90	0.16	77,77,77,77	0
57	MG	QA	1624	1/1	0.90	0.08	84,84,84,84	0
57	MG	RA	3132	1/1	0.90	0.07	55,55,55,55	0
57	MG	XA	1648	1/1	0.90	0.14	61,61,61,61	0
57	MG	YA	3114	1/1	0.90	0.12	50,50,50,50	0
57	MG	RA	3271	1/1	0.90	0.15	56,56,56,56	0
57	MG	YA	3118	1/1	0.90	0.06	33,33,33,33	0
57	MG	RA	3189	1/1	0.90	0.11	70,70,70,70	0
57	MG	YA	3283	1/1	0.90	0.24	71,71,71,71	0
57	MG	RA	3134	1/1	0.90	0.16	62,62,62,62	0
57	MG	YA	3098	1/1	0.91	0.10	45,45,45,45	0
57	MG	XA	1631	1/1	0.91	0.12	44,44,44,44	0
57	MG	RA	3085	1/1	0.91	0.22	32,32,32,32	0
57	MG	RA	3319	1/1	0.91	0.11	27,27,27,27	0
57	MG	RA	3225	1/1	0.91	0.12	15,15,15,15	0
57	MG	YA	3116	1/1	0.91	0.13	30,30,30,30	0
57	MG	RA	3197	1/1	0.91	0.15	44,44,44,44	0
57	MG	YA	3119	1/1	0.91	0.14	60,60,60,60	0
57	MG	YA	3333	1/1	0.91	0.40	107,107,107,107	0
57	MG	RA	3329	1/1	0.91	0.15	34,34,34,34	0
57	MG	RA	3331	1/1	0.91	0.14	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3161	1/1	0.91	0.17	62,62,62,62	0
57	MG	RA	3088	1/1	0.91	0.17	28,28,28,28	0
57	MG	RA	3109	1/1	0.91	0.18	40,40,40,40	0
57	MG	QA	1629	1/1	0.91	0.28	71,71,71,71	0
57	MG	YA	3197	1/1	0.91	0.09	53,53,53,53	0
57	MG	YA	3199	1/1	0.91	0.10	35,35,35,35	0
57	MG	YA	3200	1/1	0.91	0.09	41,41,41,41	0
57	MG	RA	3292	1/1	0.91	0.08	80,80,80,80	0
57	MG	XA	1657	1/1	0.91	0.15	91,91,91,91	0
57	MG	XX	101	1/1	0.91	0.08	47,47,47,47	0
57	MG	QA	1613	1/1	0.91	0.06	56,56,56,56	0
57	MG	YA	3207	1/1	0.91	0.09	76,76,76,76	0
57	MG	YA	3208	1/1	0.91	0.09	60,60,60,60	0
57	MG	RA	3254	1/1	0.91	0.17	72,72,72,72	0
57	MG	Y3	101	1/1	0.91	0.17	66,66,66,66	0
57	MG	RA	3182	1/1	0.91	0.20	70,70,70,70	0
57	MG	RA	3300	1/1	0.91	0.09	57,57,57,57	0
57	MG	RA	3125	1/1	0.91	0.20	42,42,42,42	0
57	MG	RA	3305	1/1	0.91	0.06	52,52,52,52	0
57	MG	QA	1632	1/1	0.91	0.06	71,71,71,71	0
57	MG	RA	3309	1/1	0.91	0.14	47,47,47,47	0
57	MG	QA	1628	1/1	0.91	0.10	62,62,62,62	0
57	MG	YA	3080	1/1	0.91	0.15	51,51,51,51	0
57	MG	RA	3192	1/1	0.91	0.21	100,100,100,100	0
57	MG	YA	3217	1/1	0.92	0.06	63,63,63,63	0
57	MG	RA	3214	1/1	0.92	0.16	51,51,51,51	0
57	MG	YA	3303	1/1	0.92	0.13	51,51,51,51	0
57	MG	RA	3059	1/1	0.92	0.23	35,35,35,35	0
57	MG	YA	3308	1/1	0.92	0.11	41,41,41,41	0
57	MG	YA	3314	1/1	0.92	0.21	48,48,48,48	0
57	MG	YA	3092	1/1	0.92	0.15	86,86,86,86	0
57	MG	RA	3144	1/1	0.92	0.14	36,36,36,36	0
57	MG	YA	3176	1/1	0.92	0.14	53,53,53,53	0
57	MG	YA	3227	1/1	0.92	0.17	66,66,66,66	0
57	MG	YA	3228	1/1	0.92	0.18	72,72,72,72	0
57	MG	XA	1638	1/1	0.92	0.10	54,54,54,54	0
57	MG	YA	3233	1/1	0.92	0.07	47,47,47,47	0
57	MG	YA	3242	1/1	0.92	0.14	35,35,35,35	0
57	MG	RA	3318	1/1	0.92	0.23	50,50,50,50	0
57	MG	YA	3329	1/1	0.92	0.19	46,46,46,46	0
57	MG	YA	3112	1/1	0.92	0.12	40,40,40,40	0
57	MG	RA	3066	1/1	0.92	0.20	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3320	1/1	0.92	0.09	36,36,36,36	0
57	MG	YA	3253	1/1	0.92	0.29	87,87,87,87	0
57	MG	QA	1627	1/1	0.92	0.06	62,62,62,62	0
57	MG	YA	3337	1/1	0.92	0.30	66,66,66,66	0
57	MG	RA	3278	1/1	0.92	0.22	63,63,63,63	0
57	MG	QA	1610	1/1	0.92	0.07	51,51,51,51	0
57	MG	RA	3158	1/1	0.92	0.15	26,26,26,26	0
57	MG	RA	3236	1/1	0.92	0.17	30,30,30,30	0
57	MG	RB	201	1/1	0.92	0.06	93,93,93,93	0
57	MG	RA	3160	1/1	0.92	0.09	48,48,48,48	0
57	MG	YA	3267	1/1	0.92	0.11	52,52,52,52	0
57	MG	YA	3346	1/1	0.92	0.15	50,50,50,50	0
57	MG	YA	3347	1/1	0.92	0.14	61,61,61,61	0
57	MG	YA	3129	1/1	0.92	0.14	86,86,86,86	0
57	MG	RA	3033	1/1	0.92	0.19	11,11,11,11	0
57	MG	RA	3107	1/1	0.92	0.18	78,78,78,78	0
57	MG	QA	1637	1/1	0.92	0.10	48,48,48,48	0
57	MG	YA	3357	1/1	0.92	0.10	27,27,27,27	0
57	MG	RA	3168	1/1	0.92	0.22	40,40,40,40	0
57	MG	RA	3298	1/1	0.92	0.15	61,61,61,61	0
57	MG	RA	3114	1/1	0.92	0.21	40,40,40,40	0
57	MG	RA	3257	1/1	0.92	0.07	21,21,21,21	0
57	MG	YA	3154	1/1	0.92	0.07	37,37,37,37	0
57	MG	RA	3301	1/1	0.92	0.18	41,41,41,41	0
57	MG	YA	3293	1/1	0.92	0.11	54,54,54,54	0
57	MG	RA	3258	1/1	0.92	0.12	47,47,47,47	0
57	MG	RA	3058	1/1	0.92	0.24	16,16,16,16	0
57	MG	YE	302	1/1	0.92	0.13	24,24,24,24	0
57	MG	YA	3037	1/1	0.92	0.22	9,9,9,9	0
57	MG	YP	202	1/1	0.92	0.13	25,25,25,25	0
57	MG	YA	3042	1/1	0.92	0.17	32,32,32,32	0
57	MG	RA	3176	1/1	0.92	0.13	29,29,29,29	0
57	MG	RA	3268	1/1	0.92	0.14	47,47,47,47	0
57	MG	QA	1653	1/1	0.93	0.05	65,65,65,65	0
57	MG	YA	3109	1/1	0.93	0.09	31,31,31,31	0
57	MG	YA	3177	1/1	0.93	0.13	47,47,47,47	0
57	MG	YA	3234	1/1	0.93	0.13	32,32,32,32	0
57	MG	RA	3256	1/1	0.93	0.18	30,30,30,30	0
57	MG	XA	1611	1/1	0.93	0.18	28,28,28,28	0
57	MG	RA	3316	1/1	0.93	0.06	31,31,31,31	0
57	MG	XA	1655	1/1	0.93	0.12	39,39,39,39	0
57	MG	QA	1622	1/1	0.93	0.09	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1658	1/1	0.93	0.15	83,83,83,83	0
57	MG	XV	102	1/1	0.93	0.09	29,29,29,29	0
57	MG	XA	1616	1/1	0.93	0.15	18,18,18,18	0
57	MG	XA	1618	1/1	0.93	0.18	57,57,57,57	0
57	MG	YA	3262	1/1	0.93	0.17	38,38,38,38	0
57	MG	RA	3157	1/1	0.93	0.13	25,25,25,25	0
57	MG	YA	3125	1/1	0.93	0.28	91,91,91,91	0
57	MG	RA	3202	1/1	0.93	0.15	48,48,48,48	0
57	MG	YA	3133	1/1	0.93	0.13	46,46,46,46	0
57	MG	YA	3196	1/1	0.93	0.05	73,73,73,73	0
57	MG	RA	3321	1/1	0.93	0.07	34,34,34,34	0
57	MG	YA	3278	1/1	0.93	0.09	20,20,20,20	0
57	MG	RA	3062	1/1	0.93	0.05	53,53,53,53	0
57	MG	YA	3006	1/1	0.93	0.17	24,24,24,24	0
57	MG	RA	3229	1/1	0.93	0.07	18,18,18,18	0
57	MG	YA	3144	1/1	0.93	0.07	32,32,32,32	0
57	MG	XA	1628	1/1	0.93	0.09	46,46,46,46	0
57	MG	RA	3185	1/1	0.93	0.07	61,61,61,61	0
57	MG	YA	3206	1/1	0.93	0.09	53,53,53,53	0
57	MG	YA	3353	1/1	0.93	0.48	74,74,74,74	0
57	MG	YA	3029	1/1	0.93	0.07	35,35,35,35	0
57	MG	RA	3237	1/1	0.93	0.10	23,23,23,23	0
57	MG	YA	3156	1/1	0.93	0.17	45,45,45,45	0
57	MG	RA	3243	1/1	0.93	0.15	76,76,76,76	0
57	MG	YA	3158	1/1	0.93	0.13	37,37,37,37	0
57	MG	YA	3159	1/1	0.93	0.10	51,51,51,51	0
57	MG	YA	3062	1/1	0.93	0.20	78,78,78,78	0
57	MG	R7	101	1/1	0.93	0.10	26,26,26,26	0
57	MG	QA	1615	1/1	0.93	0.07	52,52,52,52	0
57	MG	QA	1647	1/1	0.93	0.10	109,109,109,109	0
57	MG	XA	1645	1/1	0.93	0.11	45,45,45,45	0
57	MG	QA	1648	1/1	0.93	0.22	49,49,49,49	0
57	MG	RA	3089	1/1	0.93	0.12	15,15,15,15	0
57	MG	YA	3103	1/1	0.93	0.24	39,39,39,39	0
57	MG	YA	3310	1/1	0.93	0.13	41,41,41,41	0
57	MG	YA	3313	1/1	0.93	0.09	37,37,37,37	0
57	MG	RA	3311	1/1	0.93	0.10	50,50,50,50	0
57	MG	YY	201	1/1	0.93	0.09	41,41,41,41	0
57	MG	RA	3074	1/1	0.94	0.14	37,37,37,37	0
57	MG	YA	3306	1/1	0.94	0.21	54,54,54,54	0
57	MG	RA	3151	1/1	0.94	0.12	26,26,26,26	0
57	MG	YA	3160	1/1	0.94	0.13	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3077	1/1	0.94	0.14	20,20,20,20	0
57	MG	XA	1646	1/1	0.94	0.04	43,43,43,43	0
57	MG	RA	3218	1/1	0.94	0.06	35,35,35,35	0
57	MG	YA	3084	1/1	0.94	0.17	17,17,17,17	0
57	MG	YA	3224	1/1	0.94	0.15	43,43,43,43	0
57	MG	QA	1626	1/1	0.94	0.06	98,98,98,98	0
57	MG	YA	3097	1/1	0.94	0.18	40,40,40,40	0
57	MG	YA	3229	1/1	0.94	0.14	46,46,46,46	0
57	MG	RF	301	1/1	0.94	0.18	77,77,77,77	0
57	MG	YA	3101	1/1	0.94	0.08	51,51,51,51	0
57	MG	YA	3172	1/1	0.94	0.20	49,49,49,49	0
57	MG	RA	3223	1/1	0.94	0.11	11,11,11,11	0
57	MG	YA	3174	1/1	0.94	0.11	25,25,25,25	0
57	MG	RA	3155	1/1	0.94	0.17	48,48,48,48	0
57	MG	QA	1605	1/1	0.94	0.17	34,34,34,34	0
57	MG	YA	3249	1/1	0.94	0.07	44,44,44,44	0
57	MG	RA	3272	1/1	0.94	0.10	31,31,31,31	0
57	MG	R5	101	1/1	0.94	0.14	58,58,58,58	0
57	MG	YA	3256	1/1	0.94	0.24	47,47,47,47	0
57	MG	RA	3093	1/1	0.94	0.11	25,25,25,25	0
57	MG	RA	3105	1/1	0.94	0.10	32,32,32,32	0
57	MG	RA	3022	1/1	0.94	0.28	28,28,28,28	0
57	MG	QA	1652	1/1	0.94	0.08	61,61,61,61	0
57	MG	RA	3042	1/1	0.94	0.09	17,17,17,17	0
57	MG	RA	3204	1/1	0.94	0.16	66,66,66,66	0
57	MG	RA	3115	1/1	0.94	0.08	22,22,22,22	0
57	MG	RA	3119	1/1	0.94	0.12	34,34,34,34	0
57	MG	RA	3146	1/1	0.94	0.09	63,63,63,63	0
57	MG	RA	3327	1/1	0.94	0.23	50,50,50,50	0
57	MG	YA	3270	1/1	0.94	0.14	58,58,58,58	0
57	MG	YA	3274	1/1	0.94	0.10	26,26,26,26	0
57	MG	YA	3352	1/1	0.94	0.21	74,74,74,74	0
57	MG	RA	3253	1/1	0.94	0.15	40,40,40,40	0
57	MG	YA	3131	1/1	0.94	0.12	21,21,21,21	0
57	MG	YA	3132	1/1	0.94	0.14	56,56,56,56	0
57	MG	XA	1634	1/1	0.94	0.14	45,45,45,45	0
57	MG	YA	3017	1/1	0.94	0.15	32,32,32,32	0
57	MG	XA	1635	1/1	0.94	0.05	23,23,23,23	0
57	MG	YA	3138	1/1	0.94	0.14	34,34,34,34	0
57	MG	RA	3178	1/1	0.94	0.07	28,28,28,28	0
57	MG	YA	3032	1/1	0.94	0.32	29,29,29,29	0
57	MG	YA	3033	1/1	0.94	0.12	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3297	1/1	0.94	0.27	50,50,50,50	0
57	MG	YA	3147	1/1	0.94	0.19	45,45,45,45	0
57	MG	YA	3148	1/1	0.94	0.18	50,50,50,50	0
57	MG	YA	3039	1/1	0.94	0.21	18,18,18,18	0
57	MG	YA	3040	1/1	0.94	0.17	24,24,24,24	0
57	MG	XA	1640	1/1	0.94	0.22	26,26,26,26	0
57	MG	YA	3049	1/1	0.94	0.14	47,47,47,47	0
57	MG	YA	3051	1/1	0.94	0.17	21,21,21,21	0
57	MG	YA	3215	1/1	0.94	0.15	15,15,15,15	0
57	MG	YA	3078	1/1	0.95	0.14	8,8,8,8	0
57	MG	YA	3079	1/1	0.95	0.08	44,44,44,44	0
57	MG	YA	3284	1/1	0.95	0.30	86,86,86,86	0
57	MG	YA	3285	1/1	0.95	0.18	50,50,50,50	0
57	MG	QA	1650	1/1	0.95	0.08	14,14,14,14	0
57	MG	YA	3183	1/1	0.95	0.07	45,45,45,45	0
57	MG	YA	3289	1/1	0.95	0.12	52,52,52,52	0
57	MG	RA	3110	1/1	0.95	0.11	21,21,21,21	0
57	MG	RA	3112	1/1	0.95	0.12	74,74,74,74	0
57	MG	YA	3087	1/1	0.95	0.14	41,41,41,41	0
57	MG	RA	3054	1/1	0.95	0.11	20,20,20,20	0
57	MG	RA	3008	1/1	0.95	0.14	11,11,11,11	0
57	MG	QA	1651	1/1	0.95	0.12	34,34,34,34	0
57	MG	QA	1612	1/1	0.95	0.13	46,46,46,46	0
57	MG	QA	1618	1/1	0.95	0.07	39,39,39,39	0
57	MG	YA	3194	1/1	0.95	0.22	22,22,22,22	0
57	MG	RA	3235	1/1	0.95	0.06	14,14,14,14	0
57	MG	RA	3302	1/1	0.95	0.07	23,23,23,23	0
57	MG	YA	3107	1/1	0.95	0.05	9,9,9,9	0
57	MG	QA	1609	1/1	0.95	0.07	62,62,62,62	0
57	MG	YA	3305	1/1	0.95	0.07	60,60,60,60	0
57	MG	RA	3174	1/1	0.95	0.08	38,38,38,38	0
57	MG	RA	3306	1/1	0.95	0.07	44,44,44,44	0
57	MG	RA	3126	1/1	0.95	0.09	54,54,54,54	0
57	MG	YA	3309	1/1	0.95	0.05	52,52,52,52	0
57	MG	RA	3128	1/1	0.95	0.10	20,20,20,20	0
57	MG	YA	3311	1/1	0.95	0.20	46,46,46,46	0
57	MG	YA	3312	1/1	0.95	0.06	22,22,22,22	0
57	MG	RA	3072	1/1	0.95	0.18	25,25,25,25	0
57	MG	R0	101	1/1	0.95	0.08	19,19,19,19	0
57	MG	QA	1620	1/1	0.95	0.10	41,41,41,41	0
57	MG	YA	3316	1/1	0.95	0.09	49,49,49,49	0
57	MG	RA	3313	1/1	0.95	0.08	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3188	1/1	0.95	0.13	50,50,50,50	0
57	MG	YA	3320	1/1	0.95	0.12	15,15,15,15	0
57	MG	RA	3081	1/1	0.95	0.16	49,49,49,49	0
57	MG	RA	3317	1/1	0.95	0.07	45,45,45,45	0
57	MG	RA	3027	1/1	0.95	0.11	16,16,16,16	0
57	MG	YA	3130	1/1	0.95	0.20	21,21,21,21	0
57	MG	QA	1625	1/1	0.95	0.20	27,27,27,27	0
57	MG	RA	3194	1/1	0.95	0.09	55,55,55,55	0
57	MG	RA	3195	1/1	0.95	0.10	35,35,35,35	0
57	MG	RA	3259	1/1	0.95	0.20	43,43,43,43	0
57	MG	RA	3323	1/1	0.95	0.15	30,30,30,30	0
57	MG	RA	3325	1/1	0.95	0.13	27,27,27,27	0
57	MG	RA	3260	1/1	0.95	0.18	35,35,35,35	0
57	MG	RA	3139	1/1	0.95	0.06	16,16,16,16	0
57	MG	RA	3262	1/1	0.95	0.12	58,58,58,58	0
57	MG	RA	3330	1/1	0.95	0.05	32,32,32,32	0
57	MG	RA	3266	1/1	0.95	0.15	22,22,22,22	0
57	MG	RA	3332	1/1	0.95	0.12	103,103,103,103	0
57	MG	YA	3149	1/1	0.95	0.18	85,85,85,85	0
57	MG	RA	3034	1/1	0.95	0.19	24,24,24,24	0
57	MG	YA	3239	1/1	0.95	0.10	32,32,32,32	0
57	MG	RA	3090	1/1	0.95	0.15	43,43,43,43	0
57	MG	RA	3142	1/1	0.95	0.09	62,62,62,62	0
57	MG	RA	3092	1/1	0.95	0.18	15,15,15,15	0
57	MG	RA	3145	1/1	0.95	0.08	34,34,34,34	0
57	MG	RA	3039	1/1	0.95	0.22	21,21,21,21	0
57	MG	RA	3148	1/1	0.95	0.20	74,74,74,74	0
57	MG	RR	201	1/1	0.95	0.13	21,21,21,21	0
57	MG	YA	3038	1/1	0.95	0.22	39,39,39,39	0
57	MG	RA	3276	1/1	0.95	0.05	35,35,35,35	0
57	MG	RA	3208	1/1	0.95	0.09	22,22,22,22	0
57	MG	RA	3099	1/1	0.95	0.11	59,59,59,59	0
57	MG	YA	3046	1/1	0.95	0.14	43,43,43,43	0
57	MG	RA	3102	1/1	0.95	0.07	33,33,33,33	0
57	MG	YA	3050	1/1	0.95	0.14	40,40,40,40	0
57	MG	RA	3040	1/1	0.95	0.13	27,27,27,27	0
57	MG	YA	3052	1/1	0.95	0.10	16,16,16,16	0
57	MG	YA	3061	1/1	0.95	0.25	31,31,31,31	0
57	MG	QA	1640	1/1	0.95	0.07	84,84,84,84	0
57	MG	YA	3065	1/1	0.95	0.19	32,32,32,32	0
57	MG	YA	3271	1/1	0.95	0.21	56,56,56,56	0
57	MG	YA	3273	1/1	0.95	0.05	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3288	1/1	0.95	0.16	48,48,48,48	0
57	MG	YA	3276	1/1	0.95	0.26	89,89,89,89	0
57	MG	RA	3108	1/1	0.95	0.09	63,63,63,63	0
57	MG	YA	3074	1/1	0.95	0.16	12,12,12,12	0
57	MG	YA	3076	1/1	0.95	0.16	17,17,17,17	0
57	MG	YA	3201	1/1	0.96	0.07	46,46,46,46	0
57	MG	RA	3308	1/1	0.96	0.12	58,58,58,58	0
57	MG	YA	3019	1/1	0.96	0.16	16,16,16,16	0
57	MG	XA	1615	1/1	0.96	0.24	37,37,37,37	0
57	MG	RA	3265	1/1	0.96	0.21	44,44,44,44	0
57	MG	XA	1617	1/1	0.96	0.22	28,28,28,28	0
57	MG	RA	3180	1/1	0.96	0.10	63,63,63,63	0
57	MG	XA	1620	1/1	0.96	0.21	24,24,24,24	0
57	MG	YA	3137	1/1	0.96	0.07	38,38,38,38	0
57	MG	RA	3181	1/1	0.96	0.13	22,22,22,22	0
57	MG	RA	3050	1/1	0.96	0.14	29,29,29,29	0
57	MG	YA	3140	1/1	0.96	0.11	43,43,43,43	0
57	MG	RA	3183	1/1	0.96	0.19	75,75,75,75	0
57	MG	YA	3143	1/1	0.96	0.09	67,67,67,67	0
57	MG	RA	3094	1/1	0.96	0.17	13,13,13,13	0
57	MG	RA	3097	1/1	0.96	0.13	21,21,21,21	0
57	MG	YA	3048	1/1	0.96	0.16	13,13,13,13	0
57	MG	RA	3150	1/1	0.96	0.05	20,20,20,20	0
57	MG	RA	3071	1/1	0.96	0.14	27,27,27,27	0
57	MG	YA	3150	1/1	0.96	0.07	49,49,49,49	0
57	MG	RA	3231	1/1	0.96	0.20	40,40,40,40	0
57	MG	RA	3051	1/1	0.96	0.05	25,25,25,25	0
57	MG	YA	3053	1/1	0.96	0.13	12,12,12,12	0
57	MG	YA	3317	1/1	0.96	0.18	40,40,40,40	0
57	MG	RA	3030	1/1	0.96	0.16	42,42,42,42	0
57	MG	XA	1636	1/1	0.96	0.20	56,56,56,56	0
57	MG	RA	3280	1/1	0.96	0.34	57,57,57,57	0
57	MG	RA	3076	1/1	0.96	0.08	25,25,25,25	0
57	MG	RA	3324	1/1	0.96	0.11	8,8,8,8	0
57	MG	YA	3238	1/1	0.96	0.11	27,27,27,27	0
57	MG	XA	1641	1/1	0.96	0.04	77,77,77,77	0
57	MG	YA	3240	1/1	0.96	0.14	7,7,7,7	0
57	MG	RA	3239	1/1	0.96	0.11	30,30,30,30	0
57	MG	RA	3285	1/1	0.96	0.17	49,49,49,49	0
57	MG	YA	3330	1/1	0.96	0.09	28,28,28,28	0
57	MG	YA	3165	1/1	0.96	0.06	49,49,49,49	0
57	MG	RA	3002	1/1	0.96	0.33	294,294,294,294	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3248	1/1	0.96	0.13	11,11,11,11	0
57	MG	RA	3287	1/1	0.96	0.14	45,45,45,45	0
57	MG	RA	3244	1/1	0.96	0.19	52,52,52,52	0
57	MG	RA	3133	1/1	0.96	0.11	39,39,39,39	0
57	MG	YA	3085	1/1	0.96	0.08	23,23,23,23	0
57	MG	YA	3086	1/1	0.96	0.08	48,48,48,48	0
57	MG	YA	3258	1/1	0.96	0.07	16,16,16,16	0
57	MG	RA	3247	1/1	0.96	0.09	46,46,46,46	0
57	MG	RA	3159	1/1	0.96	0.10	30,30,30,30	0
57	MG	YA	3096	1/1	0.96	0.05	27,27,27,27	0
57	MG	QA	1608	1/1	0.96	0.09	49,49,49,49	0
57	MG	RA	3135	1/1	0.96	0.11	76,76,76,76	0
57	MG	RA	3137	1/1	0.96	0.07	11,11,11,11	0
57	MG	QA	1604	1/1	0.96	0.07	51,51,51,51	0
57	MG	RA	3166	1/1	0.96	0.04	53,53,53,53	0
57	MG	RA	3087	1/1	0.96	0.25	30,30,30,30	0
57	MG	YA	3269	1/1	0.96	0.08	32,32,32,32	0
57	MG	QA	1601	1/1	0.96	0.08	36,36,36,36	0
57	MG	RA	3064	1/1	0.96	0.26	16,16,16,16	0
57	MG	XA	1601	1/1	0.96	0.17	28,28,28,28	0
57	MG	YA	3185	1/1	0.96	0.17	54,54,54,54	0
57	MG	RA	3116	1/1	0.96	0.06	49,49,49,49	0
57	MG	YA	3277	1/1	0.96	0.13	34,34,34,34	0
57	MG	QA	1634	1/1	0.96	0.10	50,50,50,50	0
57	MG	XA	1605	1/1	0.96	0.05	51,51,51,51	0
57	MG	YA	3280	1/1	0.96	0.23	86,86,86,86	0
57	MG	XA	1607	1/1	0.96	0.17	22,22,22,22	0
57	MG	YA	3005	1/1	0.96	0.07	25,25,25,25	0
57	MG	XA	1610	1/1	0.96	0.06	40,40,40,40	0
57	MG	RA	3177	1/1	0.96	0.05	35,35,35,35	0
57	MG	YA	3122	1/1	0.96	0.14	22,22,22,22	0
57	MG	RA	3069	1/1	0.96	0.06	46,46,46,46	0
57	MG	YA	3014	1/1	0.96	0.15	49,49,49,49	0
57	MG	YA	3198	1/1	0.96	0.18	39,39,39,39	0
57	MG	YA	3015	1/1	0.96	0.06	14,14,14,14	0
57	MG	YA	3128	1/1	0.96	0.14	41,41,41,41	0
57	MG	Y5	101	1/1	0.97	0.05	23,23,23,23	0
57	MG	YA	3141	1/1	0.97	0.07	19,19,19,19	0
57	MG	RA	3083	1/1	0.97	0.10	22,22,22,22	0
57	MG	RA	3127	1/1	0.97	0.14	1,1,1,1	0
57	MG	RA	3044	1/1	0.97	0.11	32,32,32,32	0
57	MG	YA	3145	1/1	0.97	0.14	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3047	1/1	0.97	0.15	20,20,20,20	0
57	MG	YA	3007	1/1	0.97	0.06	22,22,22,22	0
57	MG	QA	1631	1/1	0.97	0.04	39,39,39,39	0
57	MG	RA	3013	1/1	0.97	0.08	17,17,17,17	0
57	MG	QA	1602	1/1	0.97	0.23	33,33,33,33	0
57	MG	RA	3091	1/1	0.97	0.13	30,30,30,30	0
57	MG	RA	3187	1/1	0.97	0.04	55,55,55,55	0
57	MG	YA	3153	1/1	0.97	0.05	2,2,2,2	0
57	MG	RA	3019	1/1	0.97	0.11	26,26,26,26	0
57	MG	QA	1616	1/1	0.97	0.10	40,40,40,40	0
57	MG	YA	3023	1/1	0.97	0.18	20,20,20,20	0
57	MG	YA	3024	1/1	0.97	0.05	34,34,34,34	0
57	MG	YA	3025	1/1	0.97	0.09	22,22,22,22	0
57	MG	RA	3026	1/1	0.97	0.15	13,13,13,13	0
57	MG	YA	3031	1/1	0.97	0.10	13,13,13,13	0
57	MG	RA	3263	1/1	0.97	0.07	53,53,53,53	0
57	MG	RA	3264	1/1	0.97	0.17	31,31,31,31	0
57	MG	RA	3095	1/1	0.97	0.08	15,15,15,15	0
57	MG	RA	3096	1/1	0.97	0.12	14,14,14,14	0
57	MG	RA	3060	1/1	0.97	0.15	18,18,18,18	0
57	MG	RA	3004	1/1	0.97	0.16	21,21,21,21	0
57	MG	RA	3269	1/1	0.97	0.05	29,29,29,29	0
57	MG	YA	3043	1/1	0.97	0.12	11,11,11,11	0
57	MG	RA	3100	1/1	0.97	0.07	14,14,14,14	0
57	MG	YA	3047	1/1	0.97	0.07	7,7,7,7	0
57	MG	RA	3198	1/1	0.97	0.10	30,30,30,30	0
57	MG	RA	3199	1/1	0.97	0.21	41,41,41,41	0
57	MG	RA	3101	1/1	0.97	0.05	53,53,53,53	0
57	MG	XA	1606	1/1	0.97	0.04	30,30,30,30	0
57	MG	RA	3028	1/1	0.97	0.08	17,17,17,17	0
57	MG	YA	3297	1/1	0.97	0.20	36,36,36,36	0
57	MG	RA	3275	1/1	0.97	0.10	51,51,51,51	0
57	MG	YA	3055	1/1	0.97	0.16	30,30,30,30	0
57	MG	YA	3060	1/1	0.97	0.05	26,26,26,26	0
57	MG	RA	3104	1/1	0.97	0.07	17,17,17,17	0
57	MG	XA	1612	1/1	0.97	0.21	46,46,46,46	0
57	MG	YA	3063	1/1	0.97	0.09	26,26,26,26	0
57	MG	RA	3005	1/1	0.97	0.13	16,16,16,16	0
57	MG	RA	3106	1/1	0.97	0.06	23,23,23,23	0
57	MG	YA	3068	1/1	0.97	0.14	17,17,17,17	0
57	MG	RA	3031	1/1	0.97	0.13	22,22,22,22	0
57	MG	YA	3189	1/1	0.97	0.17	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3006	1/1	0.97	0.17	11,11,11,11	0
57	MG	RA	3152	1/1	0.97	0.09	48,48,48,48	0
57	MG	RA	3284	1/1	0.97	0.07	34,34,34,34	0
57	MG	QA	1617	1/1	0.97	0.08	43,43,43,43	0
57	MG	RA	3037	1/1	0.97	0.09	22,22,22,22	0
57	MG	YA	3195	1/1	0.97	0.10	44,44,44,44	0
57	MG	YA	3081	1/1	0.97	0.14	11,11,11,11	0
57	MG	XA	1623	1/1	0.97	0.22	61,61,61,61	0
57	MG	RA	3212	1/1	0.97	0.14	27,27,27,27	0
57	MG	RA	3111	1/1	0.97	0.11	35,35,35,35	0
57	MG	RA	3289	1/1	0.97	0.05	53,53,53,53	0
57	MG	YA	3321	1/1	0.97	0.06	48,48,48,48	0
57	MG	RA	3073	1/1	0.97	0.08	40,40,40,40	0
57	MG	YA	3090	1/1	0.97	0.10	17,17,17,17	0
57	MG	RA	3113	1/1	0.97	0.06	32,32,32,32	0
57	MG	YA	3093	1/1	0.97	0.12	11,11,11,11	0
57	MG	YA	3095	1/1	0.97	0.04	41,41,41,41	0
57	MG	RA	3217	1/1	0.97	0.08	48,48,48,48	0
57	MG	XA	1632	1/1	0.97	0.12	20,20,20,20	0
57	MG	QA	1607	1/1	0.97	0.14	26,26,26,26	0
57	MG	YA	3209	1/1	0.97	0.08	43,43,43,43	0
57	MG	RA	3295	1/1	0.97	0.17	36,36,36,36	0
57	MG	RA	3219	1/1	0.97	0.12	44,44,44,44	0
57	MG	YA	3334	1/1	0.97	0.05	17,17,17,17	0
57	MG	QA	1644	1/1	0.97	0.09	40,40,40,40	0
57	MG	RA	3221	1/1	0.97	0.19	21,21,21,21	0
57	MG	RA	3041	1/1	0.97	0.10	20,20,20,20	0
57	MG	RA	3162	1/1	0.97	0.04	34,34,34,34	0
57	MG	YA	3111	1/1	0.97	0.14	12,12,12,12	0
57	MG	RA	3117	1/1	0.97	0.07	49,49,49,49	0
57	MG	XA	1642	1/1	0.97	0.21	41,41,41,41	0
57	MG	YA	3342	1/1	0.97	0.06	53,53,53,53	0
57	MG	RA	3078	1/1	0.97	0.08	42,42,42,42	0
57	MG	RA	3228	1/1	0.97	0.05	21,21,21,21	0
57	MG	RA	3079	1/1	0.97	0.07	6,6,6,6	0
57	MG	RA	3167	1/1	0.97	0.05	36,36,36,36	0
57	MG	RA	3232	1/1	0.97	0.13	30,30,30,30	0
57	MG	YA	3226	1/1	0.97	0.15	46,46,46,46	0
57	MG	RA	3233	1/1	0.97	0.12	34,34,34,34	0
57	MG	RA	3234	1/1	0.97	0.22	23,23,23,23	0
57	MG	YA	3351	1/1	0.97	0.24	76,76,76,76	0
57	MG	RA	3121	1/1	0.97	0.14	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3230	1/1	0.97	0.14	14,14,14,14	0
57	MG	RA	3169	1/1	0.97	0.05	35,35,35,35	0
57	MG	YA	3355	1/1	0.97	0.06	27,27,27,27	0
57	MG	RA	3122	1/1	0.97	0.13	33,33,33,33	0
57	MG	YA	3127	1/1	0.97	0.16	18,18,18,18	0
57	MG	YA	3235	1/1	0.97	0.05	16,16,16,16	0
57	MG	YA	3236	1/1	0.97	0.13	13,13,13,13	0
57	MG	XA	1653	1/1	0.97	0.09	56,56,56,56	0
57	MG	RA	3123	1/1	0.97	0.15	54,54,54,54	0
57	MG	RA	3314	1/1	0.97	0.04	58,58,58,58	0
57	MG	YA	3241	1/1	0.97	0.16	13,13,13,13	0
57	MG	XA	1656	1/1	0.97	0.06	74,74,74,74	0
57	MG	RA	3241	1/1	0.97	0.07	26,26,26,26	0
57	MG	RA	3172	1/1	0.97	0.05	26,26,26,26	0
57	MG	YA	3134	1/1	0.97	0.03	53,53,53,53	0
57	MG	RA	3173	1/1	0.97	0.04	30,30,30,30	0
57	MG	YQ	201	1/1	0.97	0.13	25,25,25,25	0
57	MG	RA	3245	1/1	0.97	0.11	23,23,23,23	0
57	MG	R8	101	1/1	0.97	0.23	49,49,49,49	0
57	MG	RA	3175	1/1	0.97	0.07	35,35,35,35	0
57	MG	RA	3082	1/1	0.97	0.09	9,9,9,9	0
59	ZN	QN	100	1/1	0.97	0.05	136,136,136,136	0
57	MG	XA	1602	1/1	0.98	0.24	43,43,43,43	0
57	MG	YA	3088	1/1	0.98	0.10	44,44,44,44	0
57	MG	YA	3089	1/1	0.98	0.04	9,9,9,9	0
57	MG	QA	1643	1/1	0.98	0.08	38,38,38,38	0
57	MG	YA	3091	1/1	0.98	0.05	9,9,9,9	0
57	MG	RA	3052	1/1	0.98	0.09	11,11,11,11	0
57	MG	QV	101	1/1	0.98	0.08	54,54,54,54	0
57	MG	RA	3252	1/1	0.98	0.05	66,66,66,66	0
57	MG	RA	3086	1/1	0.98	0.09	31,31,31,31	0
57	MG	XA	1608	1/1	0.98	0.07	49,49,49,49	0
57	MG	XA	1609	1/1	0.98	0.21	42,42,42,42	0
57	MG	YA	3099	1/1	0.98	0.11	33,33,33,33	0
57	MG	YA	3100	1/1	0.98	0.06	12,12,12,12	0
57	MG	YA	3001	1/1	0.98	0.12	52,52,52,52	0
57	MG	YA	3002	1/1	0.98	0.09	18,18,18,18	0
57	MG	RA	3029	1/1	0.98	0.12	16,16,16,16	0
57	MG	RA	3255	1/1	0.98	0.14	52,52,52,52	0
57	MG	RA	3143	1/1	0.98	0.09	15,15,15,15	0
57	MG	YA	3008	1/1	0.98	0.11	35,35,35,35	0
57	MG	YA	3110	1/1	0.98	0.12	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1649	1/1	0.98	0.05	60,60,60,60	0
57	MG	RA	3304	1/1	0.98	0.18	75,75,75,75	0
57	MG	YA	3113	1/1	0.98	0.07	36,36,36,36	0
57	MG	QA	1614	1/1	0.98	0.03	76,76,76,76	0
57	MG	RA	3032	1/1	0.98	0.16	7,7,7,7	0
57	MG	YA	3304	1/1	0.98	0.32	40,40,40,40	0
57	MG	YA	3016	1/1	0.98	0.10	10,10,10,10	0
57	MG	RA	3179	1/1	0.98	0.13	74,74,74,74	0
57	MG	YA	3018	1/1	0.98	0.10	11,11,11,11	0
57	MG	RA	3147	1/1	0.98	0.13	36,36,36,36	0
57	MG	YA	3021	1/1	0.98	0.13	28,28,28,28	0
57	MG	XA	1619	1/1	0.98	0.11	33,33,33,33	0
57	MG	RA	3118	1/1	0.98	0.11	26,26,26,26	0
57	MG	XA	1621	1/1	0.98	0.18	12,12,12,12	0
57	MG	QA	1636	1/1	0.98	0.07	68,68,68,68	0
57	MG	YA	3026	1/1	0.98	0.09	28,28,28,28	0
57	MG	YA	3027	1/1	0.98	0.09	19,19,19,19	0
57	MG	RA	3015	1/1	0.98	0.04	2,2,2,2	0
57	MG	YA	3030	1/1	0.98	0.14	13,13,13,13	0
57	MG	RA	3222	1/1	0.98	0.13	11,11,11,11	0
57	MG	YA	3219	1/1	0.98	0.11	38,38,38,38	0
57	MG	RA	3184	1/1	0.98	0.07	21,21,21,21	0
57	MG	RA	3065	1/1	0.98	0.10	27,27,27,27	0
57	MG	YA	3034	1/1	0.98	0.21	15,15,15,15	0
57	MG	YA	3036	1/1	0.98	0.04	15,15,15,15	0
57	MG	RA	3036	1/1	0.98	0.06	15,15,15,15	0
57	MG	YA	3325	1/1	0.98	0.10	20,20,20,20	0
57	MG	RA	3067	1/1	0.98	0.10	18,18,18,18	0
57	MG	XA	1629	1/1	0.98	0.09	58,58,58,58	0
57	MG	XA	1630	1/1	0.98	0.06	70,70,70,70	0
57	MG	YA	3041	1/1	0.98	0.21	32,32,32,32	0
57	MG	RA	3227	1/1	0.98	0.10	21,21,21,21	0
57	MG	RA	3016	1/1	0.98	0.06	4,4,4,4	0
57	MG	YA	3232	1/1	0.98	0.10	25,25,25,25	0
57	MG	RA	3017	1/1	0.98	0.05	22,22,22,22	0
57	MG	RA	3230	1/1	0.98	0.15	23,23,23,23	0
57	MG	RA	3156	1/1	0.98	0.08	36,36,36,36	0
57	MG	RA	3191	1/1	0.98	0.05	52,52,52,52	0
57	MG	YA	3237	1/1	0.98	0.21	18,18,18,18	0
57	MG	XA	1637	1/1	0.98	0.03	45,45,45,45	0
57	MG	RA	3007	1/1	0.98	0.10	8,8,8,8	0
57	MG	RA	3193	1/1	0.98	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3020	1/1	0.98	0.10	21,21,21,21	0
57	MG	RA	3279	1/1	0.98	0.21	33,33,33,33	0
57	MG	YA	3057	1/1	0.98	0.12	11,11,11,11	0
57	MG	YA	3058	1/1	0.98	0.13	19,19,19,19	0
57	MG	YA	3246	1/1	0.98	0.09	6,6,6,6	0
57	MG	YA	3059	1/1	0.98	0.06	19,19,19,19	0
57	MG	QA	1633	1/1	0.98	0.04	28,28,28,28	0
57	MG	RA	3328	1/1	0.98	0.12	36,36,36,36	0
57	MG	YA	3250	1/1	0.98	0.18	20,20,20,20	0
57	MG	YA	3251	1/1	0.98	0.19	68,68,68,68	0
57	MG	RA	3043	1/1	0.98	0.09	21,21,21,21	0
57	MG	RA	3282	1/1	0.98	0.12	22,22,22,22	0
57	MG	YA	3255	1/1	0.98	0.07	28,28,28,28	0
57	MG	YA	3064	1/1	0.98	0.09	11,11,11,11	0
57	MG	RA	3238	1/1	0.98	0.11	37,37,37,37	0
57	MG	RA	3103	1/1	0.98	0.05	20,20,20,20	0
57	MG	YA	3259	1/1	0.98	0.09	25,25,25,25	0
57	MG	YA	3163	1/1	0.98	0.13	18,18,18,18	0
57	MG	RA	3240	1/1	0.98	0.22	26,26,26,26	0
57	MG	RA	3075	1/1	0.98	0.03	44,44,44,44	0
57	MG	YA	3072	1/1	0.98	0.08	36,36,36,36	0
57	MG	YA	3073	1/1	0.98	0.04	16,16,16,16	0
57	MG	RA	3242	1/1	0.98	0.04	21,21,21,21	0
57	MG	RA	3023	1/1	0.98	0.06	40,40,40,40	0
57	MG	YA	3077	1/1	0.98	0.10	19,19,19,19	0
57	MG	RA	3045	1/1	0.98	0.11	16,16,16,16	0
57	MG	RA	3025	1/1	0.98	0.05	27,27,27,27	0
57	MG	RE	301	1/1	0.98	0.07	7,7,7,7	0
57	MG	RA	3048	1/1	0.98	0.08	17,17,17,17	0
57	MG	RA	3136	1/1	0.98	0.06	9,9,9,9	0
57	MG	QA	1603	1/1	0.98	0.11	72,72,72,72	0
57	MG	YA	3275	1/1	0.98	0.13	34,34,34,34	0
57	MG	RA	3294	1/1	0.98	0.07	46,46,46,46	0
58	SF4	QD	301	8/8	0.98	0.05	71,100,181,225	0
58	SF4	XD	301	8/8	0.98	0.07	70,85,155,236	0
57	MG	XV	101	1/1	0.98	0.07	64,64,64,64	0
59	ZN	XN	101	1/1	0.98	0.04	149,149,149,149	0
57	MG	YA	3056	1/1	0.99	0.06	13,13,13,13	0
57	MG	YA	3003	1/1	0.99	0.05	27,27,27,27	0
57	MG	YA	3028	1/1	0.99	0.12	1,1,1,1	0
57	MG	YA	3094	1/1	0.99	0.05	30,30,30,30	0
57	MG	YA	3004	1/1	0.99	0.07	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3046	1/1	0.99	0.05	30,30,30,30	0
57	MG	RA	3021	1/1	0.99	0.07	15,15,15,15	0
57	MG	RA	3084	1/1	0.99	0.04	11,11,11,11	0
57	MG	RA	3098	1/1	0.99	0.04	3,3,3,3	0
57	MG	RA	3061	1/1	0.99	0.15	15,15,15,15	0
57	MG	YA	3035	1/1	0.99	0.07	18,18,18,18	0
57	MG	YA	3102	1/1	0.99	0.11	21,21,21,21	0
57	MG	RA	3024	1/1	0.99	0.12	11,11,11,11	0
57	MG	YA	3104	1/1	0.99	0.14	11,11,11,11	0
57	MG	YA	3011	1/1	0.99	0.10	1,1,1,1	0
57	MG	YA	3012	1/1	0.99	0.05	12,12,12,12	0
57	MG	YA	3013	1/1	0.99	0.04	11,11,11,11	0
57	MG	RA	3063	1/1	0.99	0.23	16,16,16,16	0
57	MG	YA	3225	1/1	0.99	0.03	24,24,24,24	0
57	MG	RA	3049	1/1	0.99	0.04	7,7,7,7	0
57	MG	YA	3075	1/1	0.99	0.03	17,17,17,17	0
57	MG	YA	3356	1/1	0.99	0.09	38,38,38,38	0
57	MG	RA	3055	1/1	0.99	0.06	14,14,14,14	0
57	MG	RA	3056	1/1	0.99	0.06	12,12,12,12	0
57	MG	YA	3272	1/1	0.99	0.06	67,67,67,67	0
57	MG	YA	3044	1/1	0.99	0.07	17,17,17,17	0
57	MG	YA	3045	1/1	0.99	0.07	11,11,11,11	0
57	MG	RA	3206	1/1	0.99	0.02	68,68,68,68	0
57	MG	YA	3117	1/1	0.99	0.05	13,13,13,13	0
57	MG	YA	3155	1/1	0.99	0.07	9,9,9,9	0
57	MG	RA	3207	1/1	0.99	0.02	51,51,51,51	0
57	MG	YA	3082	1/1	0.99	0.05	12,12,12,12	0
57	MG	YA	3020	1/1	0.99	0.04	3,3,3,3	0
57	MG	RA	3057	1/1	0.99	0.08	13,13,13,13	0
57	MG	RA	3068	1/1	0.99	0.11	21,21,21,21	0
57	MG	RA	3080	1/1	0.99	0.03	16,16,16,16	0
57	MG	RA	3164	1/1	0.99	0.06	26,26,26,26	0
57	MG	QA	1606	1/1	0.99	0.18	12,12,12,12	0
57	MG	YA	3286	1/1	0.99	0.13	33,33,33,33	0
57	MG	YA	3243	1/1	0.99	0.14	13,13,13,13	0
57	MG	YA	3126	1/1	0.99	0.03	31,31,31,31	0
57	MG	YA	3054	1/1	0.99	0.07	11,11,11,11	0
57	MG	RA	3213	1/1	0.99	0.04	45,45,45,45	0
57	MG	YA	3167	1/1	0.99	0.09	35,35,35,35	0
57	MG	RA	3038	1/1	1.00	0.04	11,11,11,11	0
57	MG	YA	3069	1/1	1.00	0.02	15,15,15,15	0
57	MG	RA	3018	1/1	1.00	0.07	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3254	1/1	1.00	0.04	12,12,12,12	0
57	MG	YA	3071	1/1	1.00	0.06	22,22,22,22	0
57	MG	YA	3108	1/1	1.00	0.04	19,19,19,19	0
57	MG	YA	3066	1/1	1.00	0.03	4,4,4,4	0
57	MG	RA	3035	1/1	1.00	0.03	5,5,5,5	0

6.5 Other polymers [i](#)

There are no such residues in this entry.