



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 07:49 am BST

PDB ID : 5VPO  
Title : The 70S P-site ASL SufA6 complex  
Authors : Hong, S.; Sunita, S.; Dunkle, J.A.; Maehigashi, T.; Dunham, C.M.  
Deposited on : 2017-05-05  
Resolution : 3.34 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11



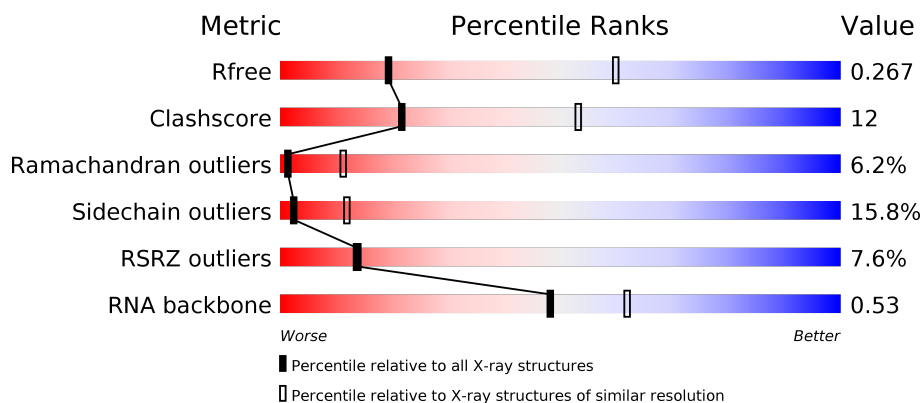
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.34 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))
$R_{free}$	130704	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)
RNA backbone	3102	1129 (3.78-2.90)

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

Mol	Chain	Length	Quality of chain
1	QX	19	<div> <div>11%</div> <div> <div>16%</div> <div>5%</div> <div>79%</div> </div> </div>
1	XX	19	<div> <div>5%</div> <div> <div>16%</div> <div>5%</div> <div>79%</div> </div> </div>
2	QA	1521	<div> <div>8%</div> <div> <div>57%</div> <div>33%</div> <div>8%</div> <div>..</div> </div> </div>
2	XA	1521	<div> <div>7%</div> <div> <div>55%</div> <div>34%</div> <div>8%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	QB	256	
3	XB	256	
4	QC	239	
4	XC	239	
5	QD	209	
5	XD	209	
6	QE	162	
6	XE	162	
7	QF	101	
7	XF	101	
8	QG	156	
8	XG	156	
9	QH	138	
9	XH	138	
10	QI	128	
10	XI	128	
11	QJ	105	
11	XJ	105	
12	QK	129	
12	XK	129	
13	QL	132	
13	XL	132	
14	QM	126	
14	XM	126	
15	QN	61	

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Mol	Chain	Length	Quality of chain
15	XN	61	
16	QO	89	
16	XO	89	
17	QP	88	
17	XP	88	
18	QQ	105	
18	XQ	105	
19	QR	88	
19	XR	88	
20	QS	93	
20	XS	93	
21	QT	106	
21	XT	106	
22	QU	27	
22	XU	27	
23	RA	2915	
23	YA	2915	
24	RB	122	
24	YB	122	
25	RD	276	
25	YD	276	
26	RE	206	
26	YE	206	
27	RF	210	
27	YF	210	

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Mol	Chain	Length	Quality of chain
28	RG	182	
28	YG	182	
29	RH	180	
29	YH	180	
30	RI	148	
30	YI	148	
31	RN	140	
31	YN	140	
32	RO	122	
32	YO	122	
33	RP	150	
33	YP	150	
34	RQ	141	
34	YQ	141	
35	RR	118	
35	YR	118	
36	RS	112	
36	YS	112	
37	RT	146	
37	YT	146	
38	RU	118	
38	YU	118	
39	RV	101	
39	YV	101	
40	RW	113	

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Mol	Chain	Length	Quality of chain
40	YW	113	
41	RX	96	
41	YX	96	
42	RY	110	
42	YY	110	
43	RZ	206	
43	YZ	206	
44	R0	85	
44	Y0	85	
45	R1	98	
45	Y1	98	
46	R2	72	
46	Y2	72	
47	R3	60	
47	Y3	60	
48	R4	71	
48	Y4	71	
49	R5	60	
49	Y5	60	
50	R6	54	
50	Y6	54	
51	R7	49	
51	Y7	49	
52	R8	65	
52	Y8	65	

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Mol	Chain	Length	Quality of chain
53	R9	37	
53	Y9	37	
54	QV	18	
54	XV	18	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	QA	1605	-	-	-	X
55	MG	QA	1619	-	-	-	X
55	MG	QA	1622	-	-	-	X
55	MG	QA	1623	-	-	-	X
55	MG	QA	1624	-	-	-	X
55	MG	QA	1629	-	-	-	X
55	MG	QA	1631	-	-	-	X
55	MG	QA	1639	-	-	-	X
55	MG	QA	1647	-	-	-	X
55	MG	QA	1651	-	-	-	X
55	MG	QA	1657	-	-	-	X
55	MG	QA	1661	-	-	-	X
55	MG	QA	1662	-	-	-	X
55	MG	QA	1666	-	-	-	X
55	MG	RA	3004	-	-	-	X
55	MG	RA	3009	-	-	-	X
55	MG	RA	3156	-	-	-	X
55	MG	RA	3184	-	-	-	X
55	MG	RA	3223	-	-	-	X
55	MG	RA	3225	-	-	-	X
55	MG	RA	3230	-	-	-	X
55	MG	XA	1623	-	-	-	X
55	MG	XA	1624	-	-	-	X
55	MG	XA	1629	-	-	-	X
55	MG	XA	1634	-	-	-	X
55	MG	XA	1644	-	-	-	X
55	MG	XA	1648	-	-	-	X
55	MG	XA	1652	-	-	-	X
55	MG	XA	1655	-	-	-	X
55	MG	XA	1660	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	XA	1661	-	-	-	X
55	MG	XA	1662	-	-	-	X
55	MG	XA	1663	-	-	-	X
55	MG	XA	1665	-	-	-	X
55	MG	XA	1671	-	-	-	X
55	MG	XB	301	-	-	-	X
55	MG	XL	201	-	-	-	X
55	MG	XM	201	-	-	-	X
55	MG	YA	3122	-	-	-	X
55	MG	YA	3143	-	-	-	X
55	MG	YA	3144	-	-	-	X
55	MG	YA	3198	-	-	-	X
55	MG	YP	202	-	-	-	X



## 2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 288423 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 messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QX	4	Total	C	N	O	P	0	0	0
			80	36	11	29	4			
1	XX	4	Total	C	N	O	P	0	0	0
			80	36	11	29	4			

- Molecule 2 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QA	1500	Total	C	N	O	P	0	0	0
			32247	14353	5981	10414	1499			
2	XA	1500	Total	C	N	O	P	0	0	0
			32249	14354	5984	10412	1499			

- Molecule 3 is a protein called 30S ribosomal protein S2.

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

- Molecule 4 is a protein called 30S ribosomal protein S3.

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

- Molecule 5 is a protein called 30S ribosomal protein S4.



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

- Molecule 6 is a protein called 30S ribosomal protein S5.

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

- Molecule 7 is a protein called 30S ribosomal protein S6.

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

- Molecule 8 is a protein called 30S ribosomal protein S7.

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

- Molecule 9 is a protein called 30S ribosomal protein S8.

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

- Molecule 10 is a protein called 30S ribosomal protein S9.

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

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

- Molecule 11 is a protein called 30S ribosomal protein S10.

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

- Molecule 12 is a protein called 30S ribosomal protein S11.

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

- Molecule 13 is a protein called 30S ribosomal protein S12.

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

- Molecule 14 is a protein called 30S ribosomal protein S13.

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

- Molecule 15 is a protein called 30S ribosomal protein S14 type Z.

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



- Molecule 16 is a protein called 30S ribosomal protein S15.

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

- Molecule 17 is a protein called 30S ribosomal protein S16.

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

- Molecule 18 is a protein called 30S ribosomal protein S17.

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

- Molecule 19 is a protein called 30S ribosomal protein S18.

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

- Molecule 20 is a protein called 30S ribosomal protein S19.

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

- Molecule 21 is a protein called 30S ribosomal protein S20.



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

- Molecule 22 is a protein called 30S ribosomal protein Thx.

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

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

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

- Molecule 24 is a RNA chain called 5S rRNA.

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

- Molecule 25 is a protein called 50S ribosomal protein L2.

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

- Molecule 26 is a protein called 50S ribosomal protein L3.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L4.

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

- Molecule 28 is a protein called 50S ribosomal protein L5.

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

- Molecule 29 is a protein called 50S ribosomal protein L6.

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

- Molecule 30 is a protein called 50S ribosomal protein L9.

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

- Molecule 31 is a protein called 50S ribosomal protein L13.

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



- Molecule 32 is a protein called 50S ribosomal protein L14.

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

- Molecule 33 is a protein called 50S ribosomal protein L15.

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

- Molecule 34 is a protein called 50S ribosomal protein L16.

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

- Molecule 35 is a protein called 50S ribosomal protein L17.

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

- Molecule 36 is a protein called 50S ribosomal protein L18.

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

- Molecule 37 is a protein called 50S ribosomal protein L19.



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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

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

- Molecule 42 is a protein called 50S ribosomal protein L24.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

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

- Molecule 45 is a protein called 50S ribosomal protein L28.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

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

- Molecule 47 is a protein called 50S ribosomal protein L30.

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



- Molecule 48 is a protein called 50S ribosomal protein L31.

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

- Molecule 49 is a protein called 50S ribosomal protein L32.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L34.

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

- Molecule 52 is a protein called 50S ribosomal protein L35.

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

- Molecule 53 is a protein called 50S ribosomal protein L36.



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

- Molecule 54 is a RNA chain called P-site ASL SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	XV	18	Total	C	N	O	P	0	0	0
			385	173	70	125	17			
54	QV	18	Total	C	N	O	P	0	0	0
			385	173	70	125	17			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	66	Total	Mg	0	0
			66	66		
55	RP	2	Total	Mg	0	0
			2	2		
55	YA	267	Total	Mg	0	0
			267	267		
55	QM	1	Total	Mg	0	0
			1	1		
55	YD	2	Total	Mg	0	0
			2	2		
55	XA	71	Total	Mg	0	0
			71	71		
55	R0	1	Total	Mg	0	0
			1	1		
55	QH	1	Total	Mg	0	0
			1	1		
55	R8	1	Total	Mg	0	0
			1	1		
55	YX	1	Total	Mg	0	0
			1	1		
55	RR	1	Total	Mg	0	0
			1	1		
55	RD	1	Total	Mg	0	0
			1	1		
55	XB	1	Total	Mg	0	0
			1	1		
55	QF	1	Total	Mg	0	0
			1	1		

*Continued on next page...*



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	R5	1	Total 1	Mg 1	0	0
55	RA	243	Total 243	Mg 243	0	0
55	YP	2	Total 2	Mg 2	0	0
55	Y5	1	Total 1	Mg 1	0	0
55	RE	2	Total 2	Mg 2	0	0
55	XL	1	Total 1	Mg 1	0	0
55	YB	4	Total 4	Mg 4	0	0
55	RB	2	Total 2	Mg 2	0	0
55	R3	1	Total 1	Mg 1	0	0
55	RF	1	Total 1	Mg 1	0	0
55	XM	1	Total 1	Mg 1	0	0
55	YE	1	Total 1	Mg 1	0	0

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

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



### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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.

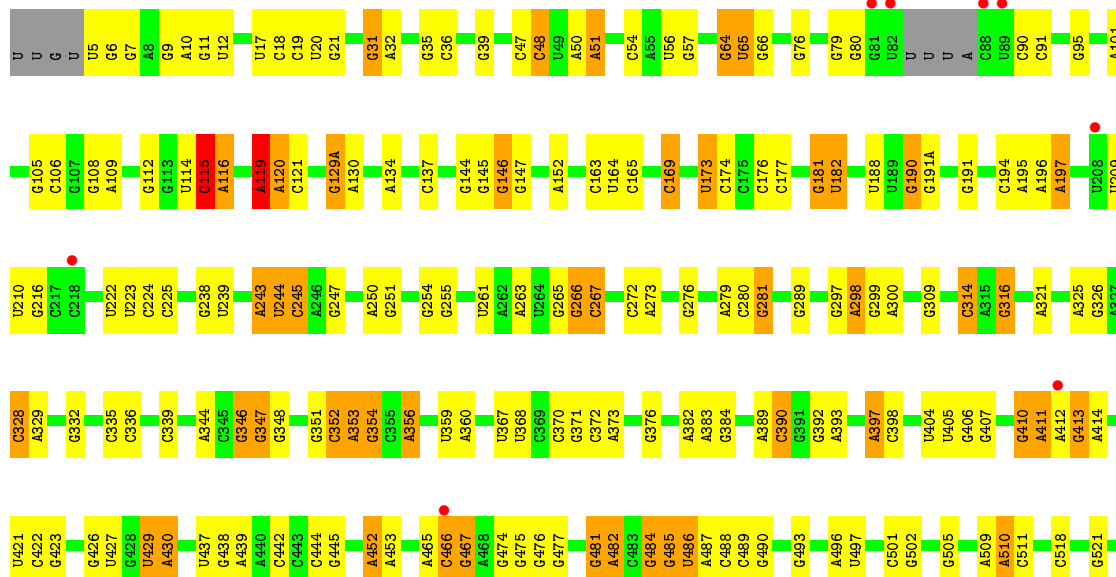
- Molecule 1: messenger RNA



- Molecule 1: messenger RNA



- Molecule 2: 16S rRNA



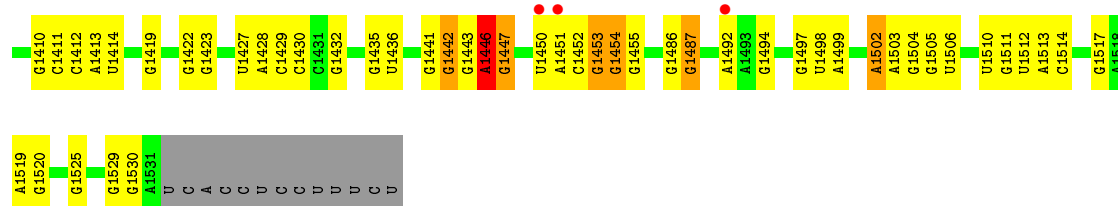




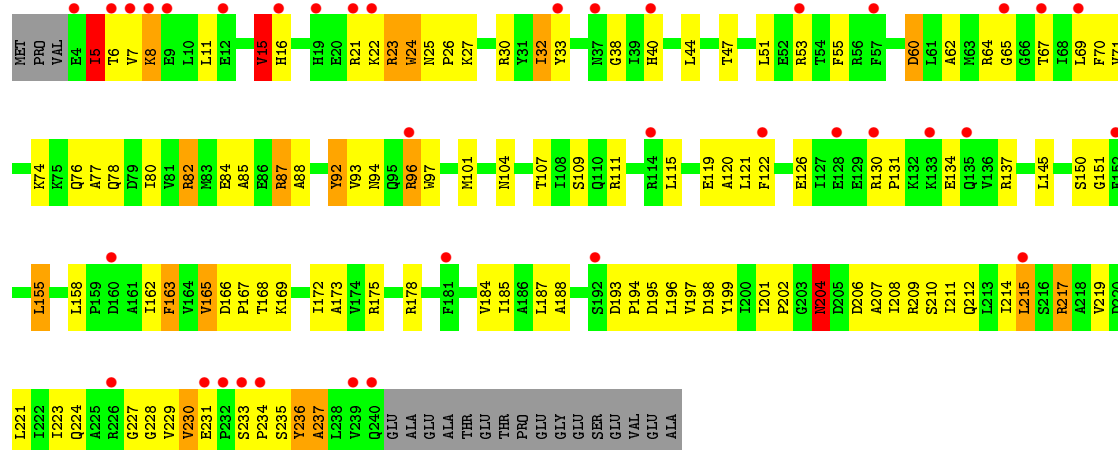




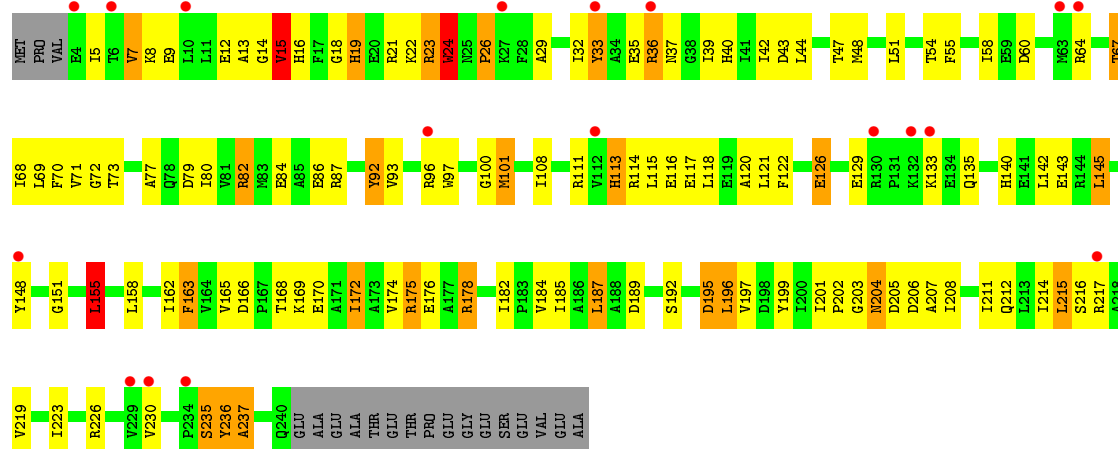




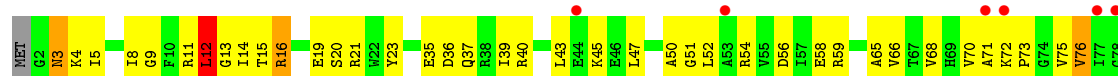
• Molecule 3: 30S ribosomal protein S2



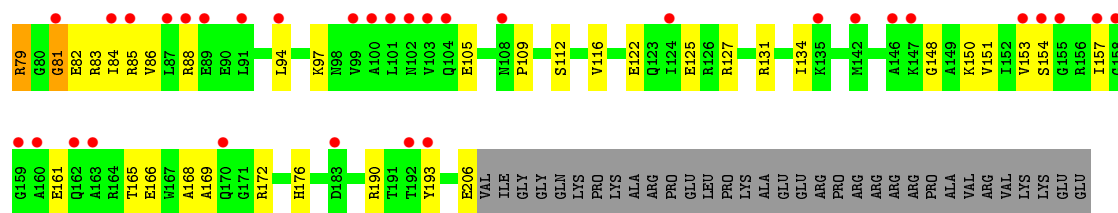
• Molecule 3: 30S ribosomal protein S2



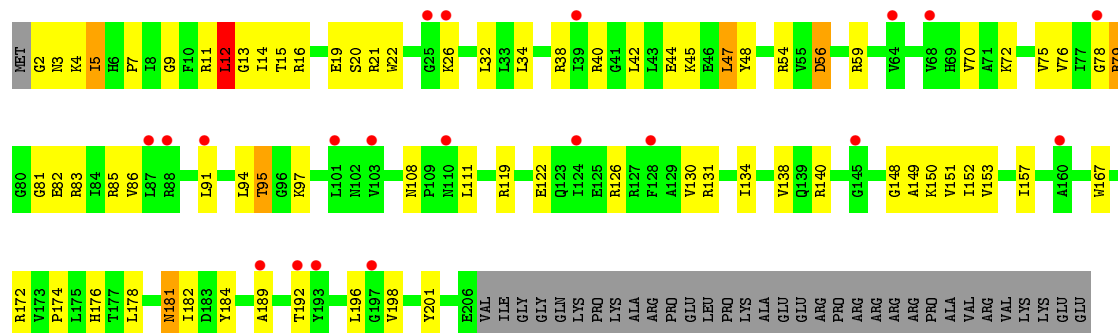
• Molecule 4: 30S ribosomal protein S3



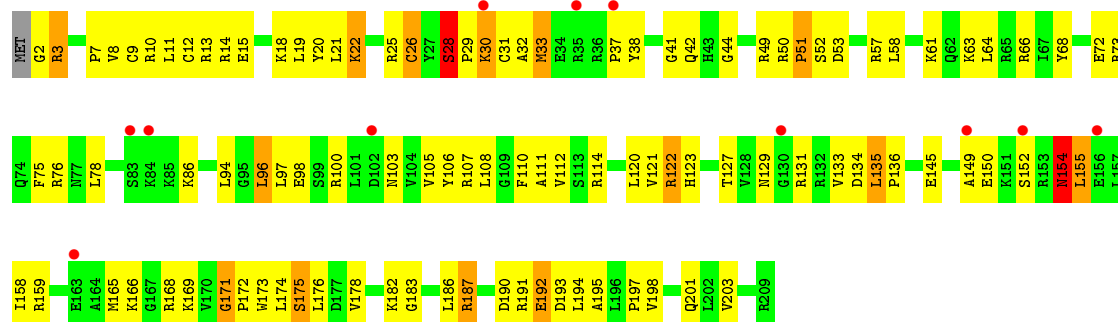




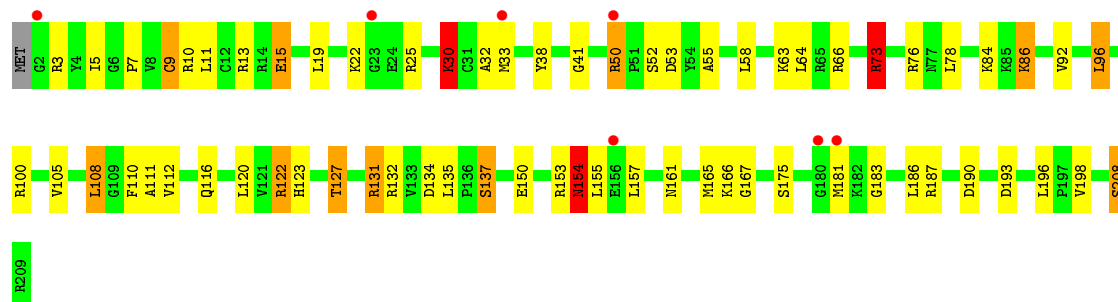
• Molecule 4: 30S ribosomal protein S3



• Molecule 5: 30S ribosomal protein S4

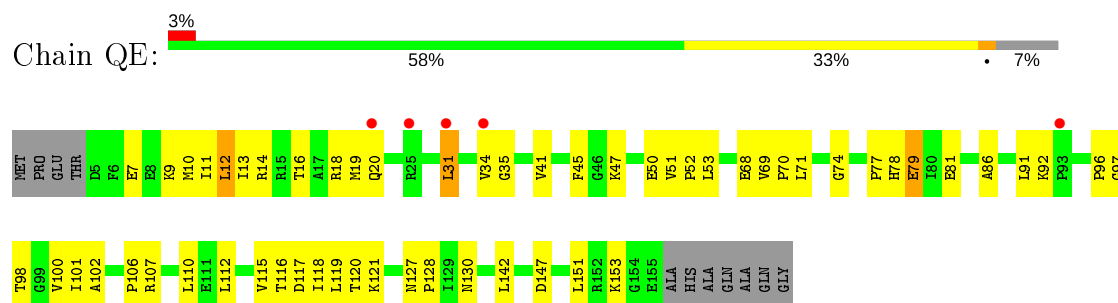


• Molecule 5: 30S ribosomal protein S4





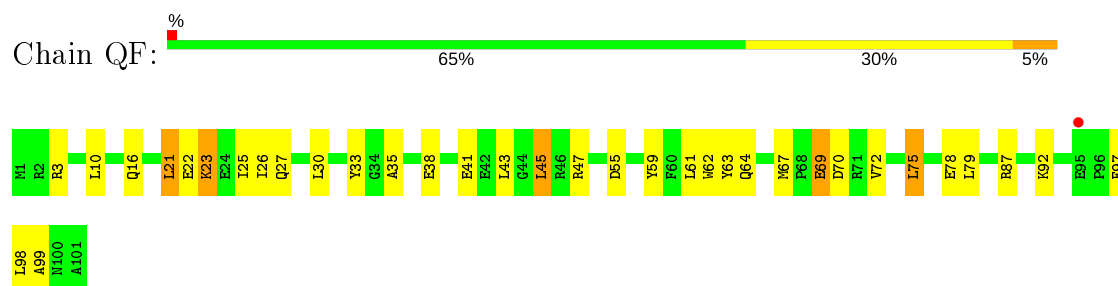
- Molecule 6: 30S ribosomal protein S5



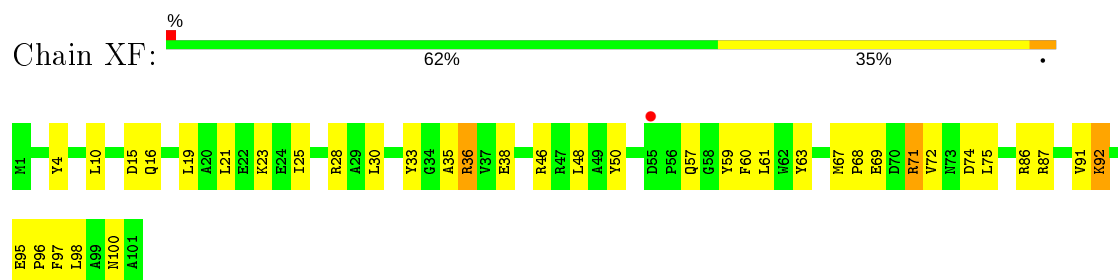
- Molecule 6: 30S ribosomal protein S5



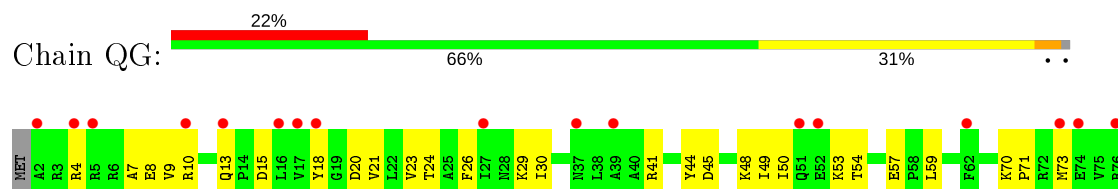
- Molecule 7: 30S ribosomal protein S6



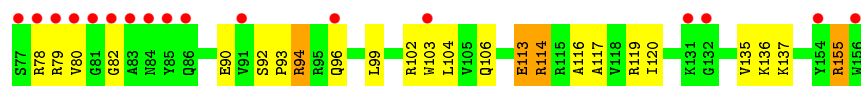
- Molecule 7: 30S ribosomal protein S6



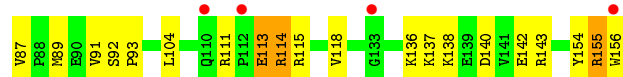
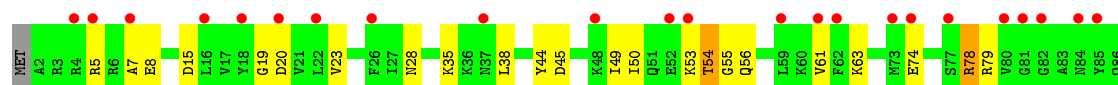
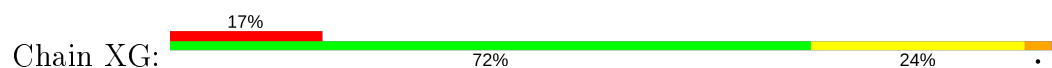
- Molecule 8: 30S ribosomal protein S7







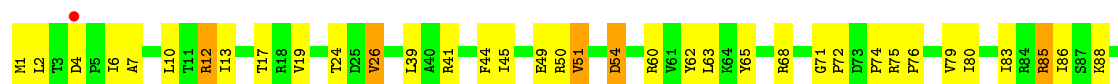
- Molecule 8: 30S ribosomal protein S7



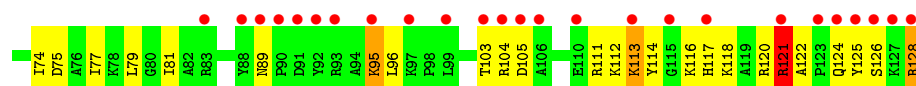
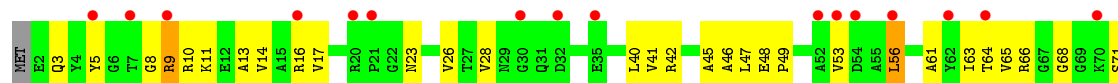
- Molecule 9: 30S ribosomal protein S8



- Molecule 9: 30S ribosomal protein S8



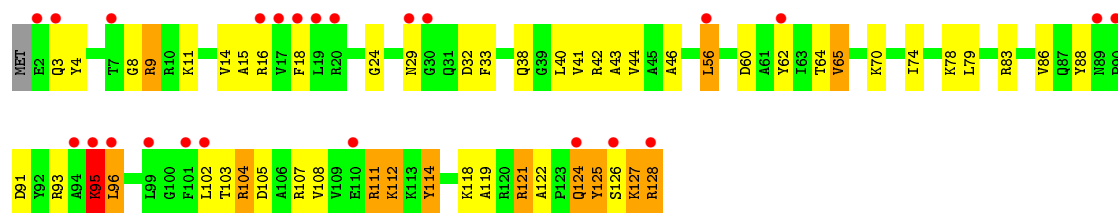
- Molecule 10: 30S ribosomal protein S9



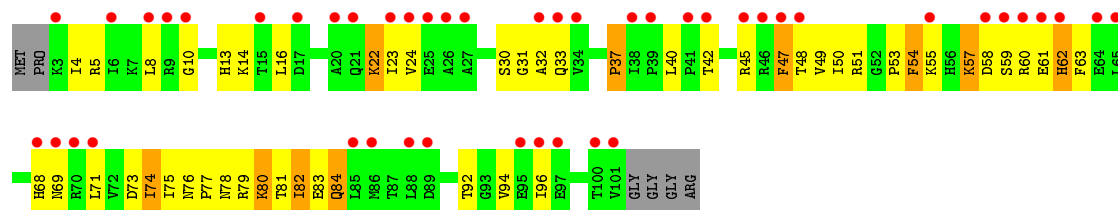
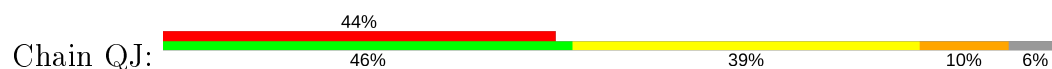
- Molecule 10: 30S ribosomal protein S9



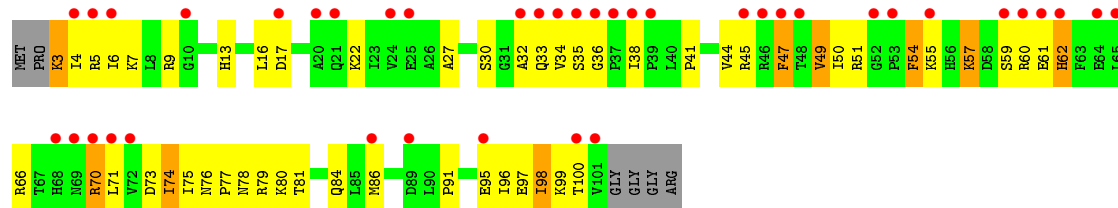
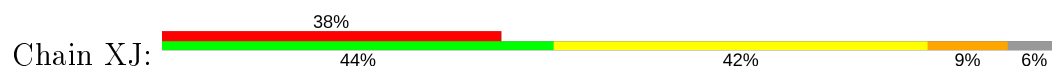




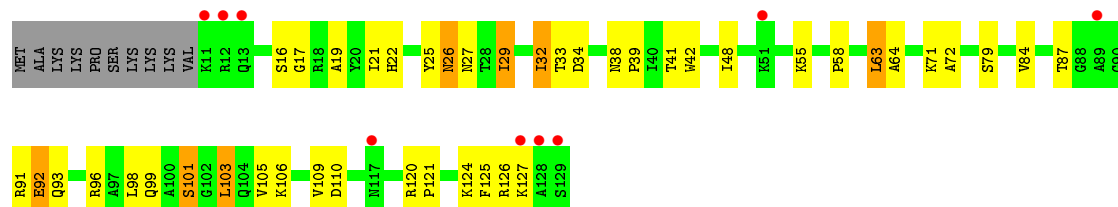
• Molecule 11: 30S ribosomal protein S10



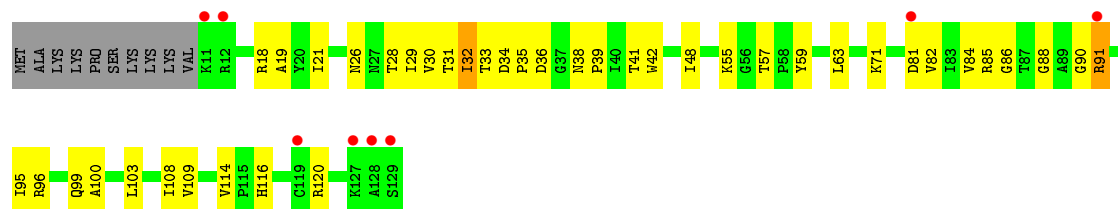
• Molecule 11: 30S ribosomal protein S10



• Molecule 12: 30S ribosomal protein S11

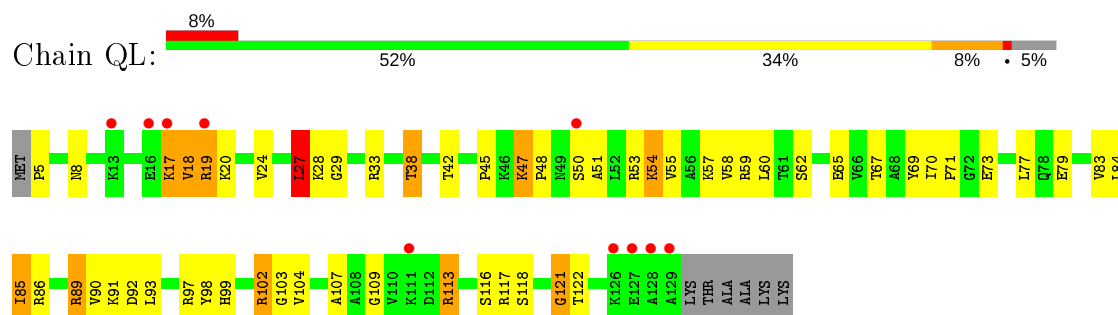


• Molecule 12: 30S ribosomal protein S11

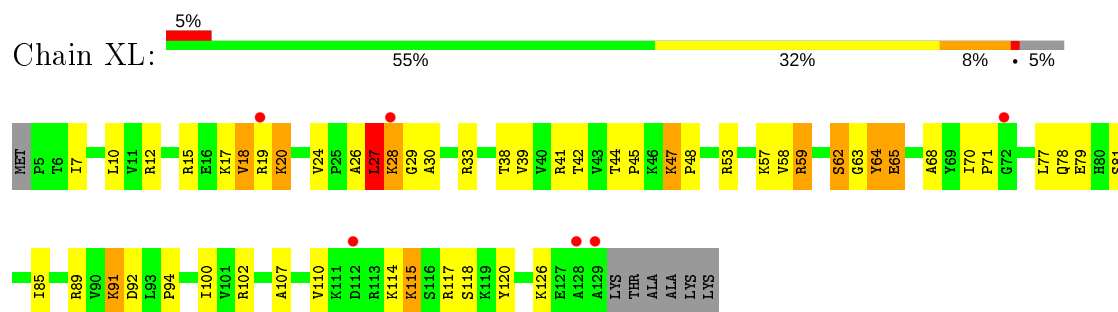




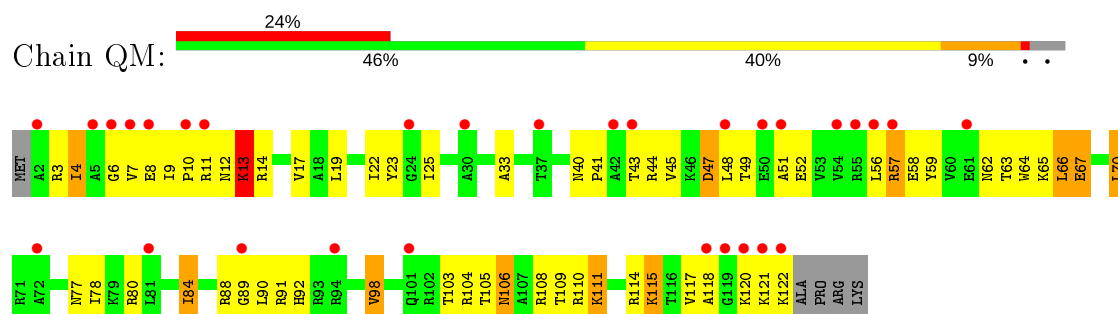
- Molecule 13: 30S ribosomal protein S12



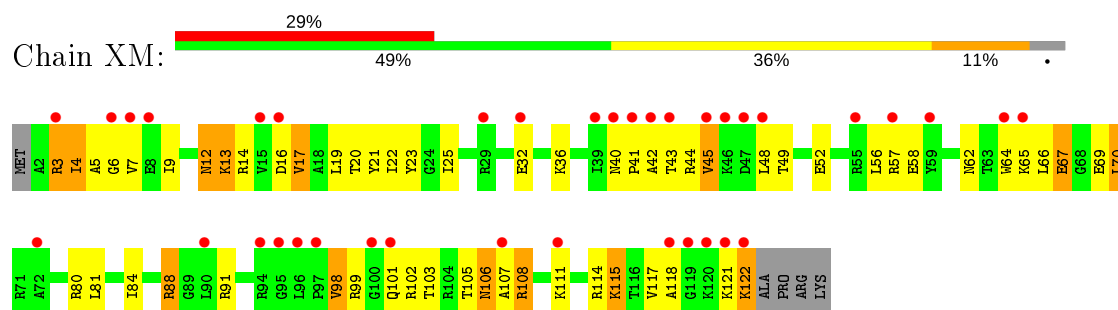
- Molecule 13: 30S ribosomal protein S12



- Molecule 14: 30S ribosomal protein S13



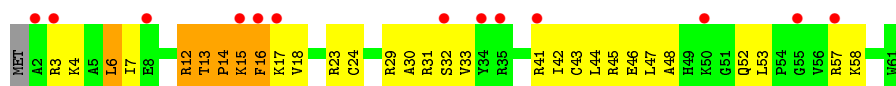
- Molecule 14: 30S ribosomal protein S13



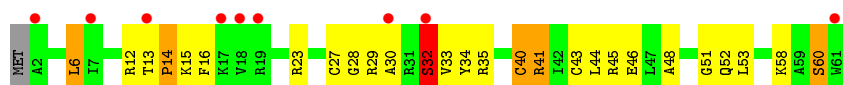
- Molecule 15: 30S ribosomal protein S14 type Z







- Molecule 15: 30S ribosomal protein S14 type Z



- Molecule 16: 30S ribosomal protein S15



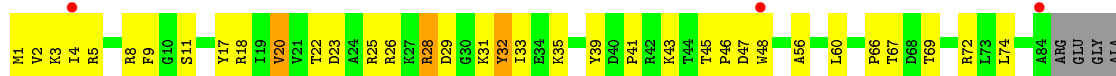
- Molecule 16: 30S ribosomal protein S15



- Molecule 17: 30S ribosomal protein S16



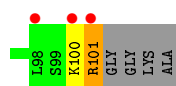
- Molecule 17: 30S ribosomal protein S16



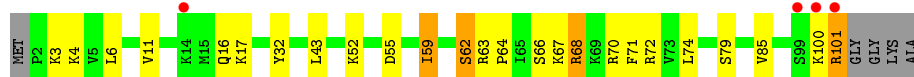
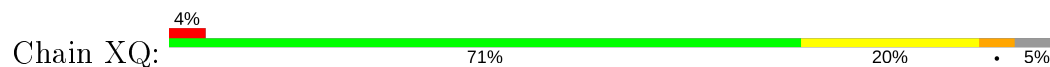
- Molecule 18: 30S ribosomal protein S17







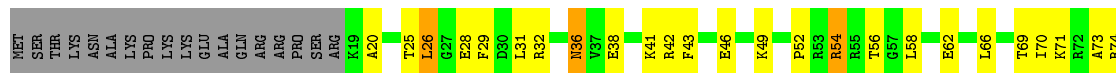
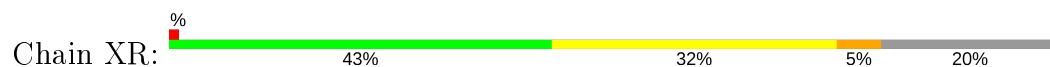
- Molecule 18: 30S ribosomal protein S17



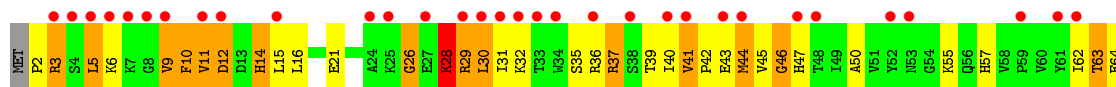
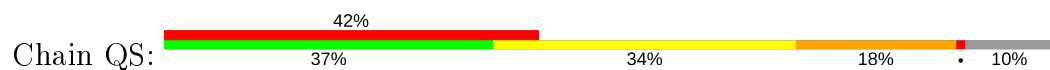
- Molecule 19: 30S ribosomal protein S18



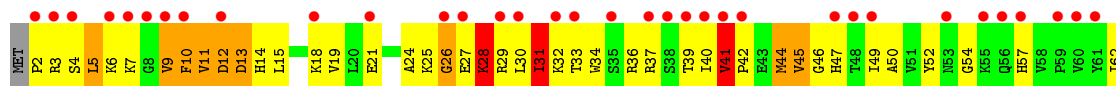
- Molecule 19: 30S ribosomal protein S18



- Molecule 20: 30S ribosomal protein S19



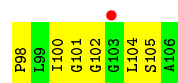
- Molecule 20: 30S ribosomal protein S19



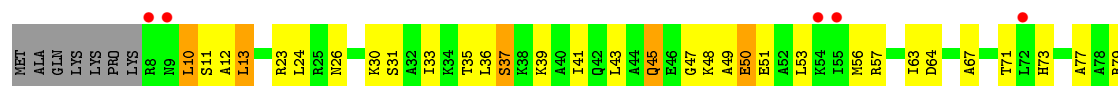




- Molecule 21: 30S ribosomal protein S20



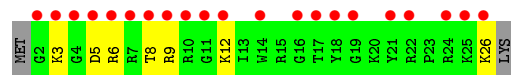
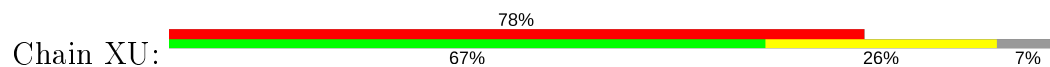
- Molecule 21: 30S ribosomal protein S20



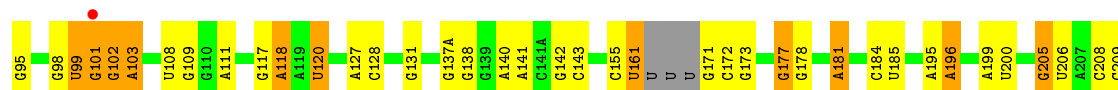
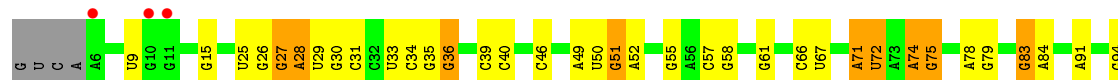
- Molecule 22: 30S ribosomal protein Thx



- Molecule 22: 30S ribosomal protein Thx



- Molecule 23: 23S rRNA



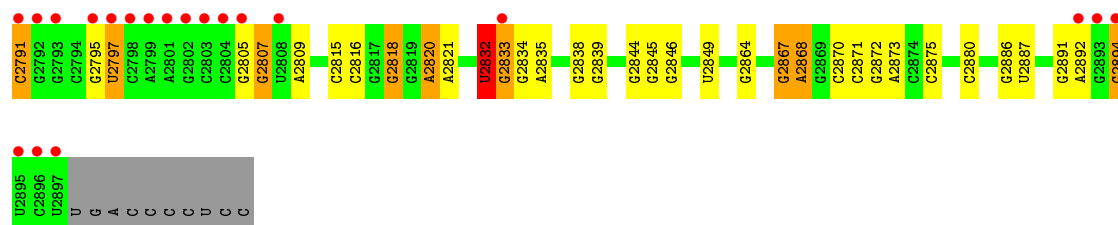




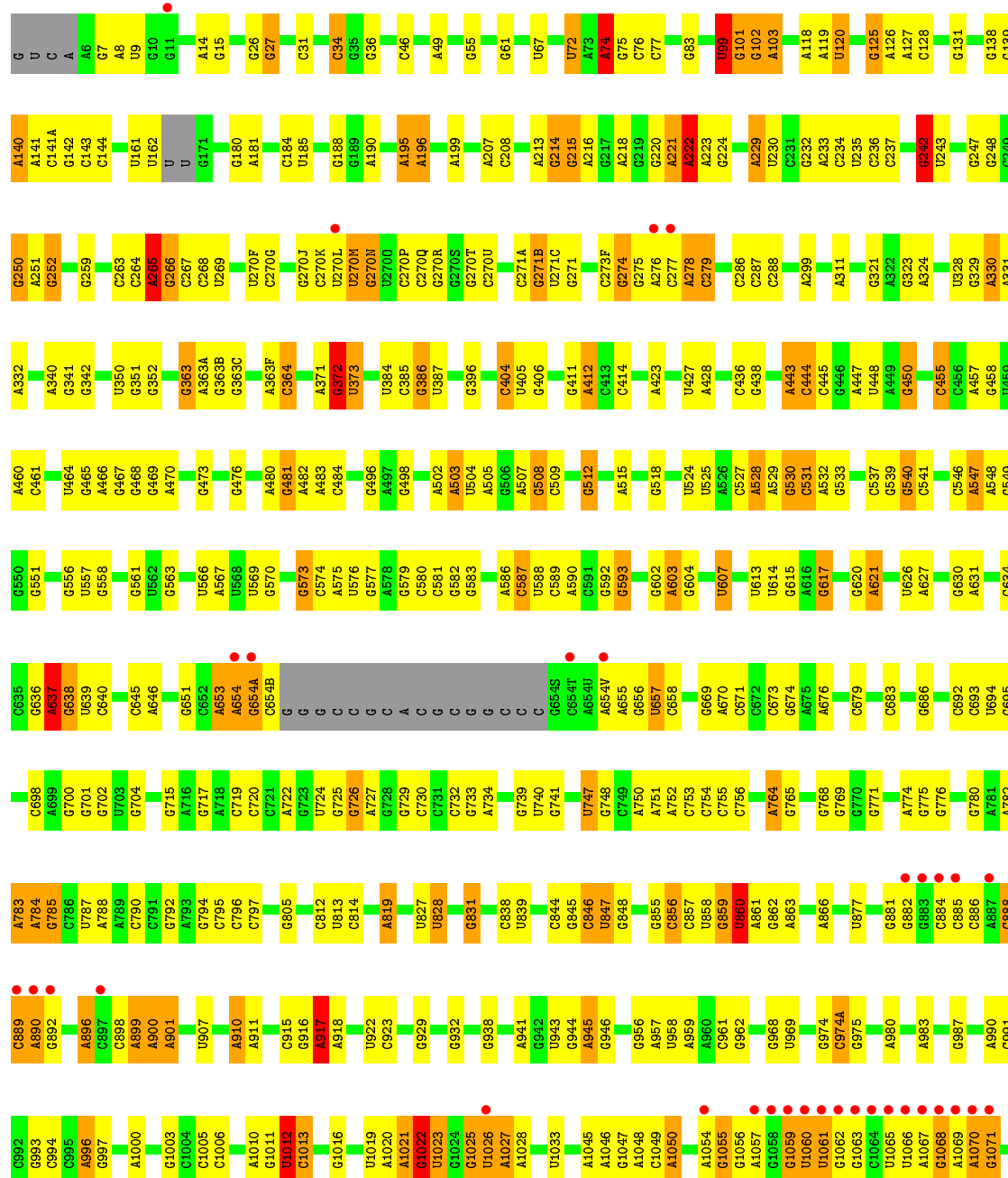


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G2611	G2389	G2611	G2389	C2293	G2189	G2129	C2040	A1913	U1798	G1667	G1542	U1454
G2612	U2390	G2612	U2390	G2296	G2190	U2130	A2041	G1929	G1799	G1674	A1543	G1455
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C2394	C2394	G2394	C2394	G2300	A2198	A2134	A2055	G1936	C1804	G1681	A1559	A1459
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A2411	A2411	U2312	A2411	U2312	A2226	C2145			A1698	A1698	A1583	A1471
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G2429	G2429	G2335	G2429	G2335	U2244	G2156	G2093	C1974	A1847	G1733	C1598	
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U2438	U2438	G2342	U2438	G2342	A2247	C2161	G2101	C1982	G1857	G1755	C1506	C1506
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• Molecule 23: 23S rRNA



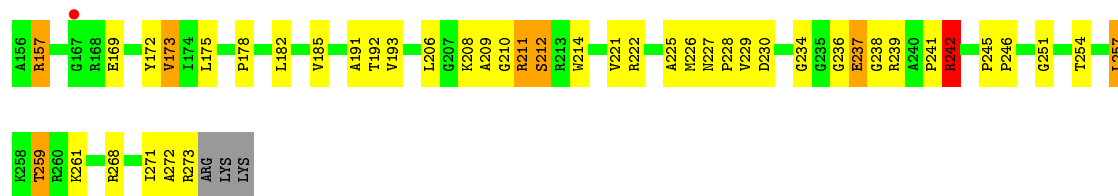


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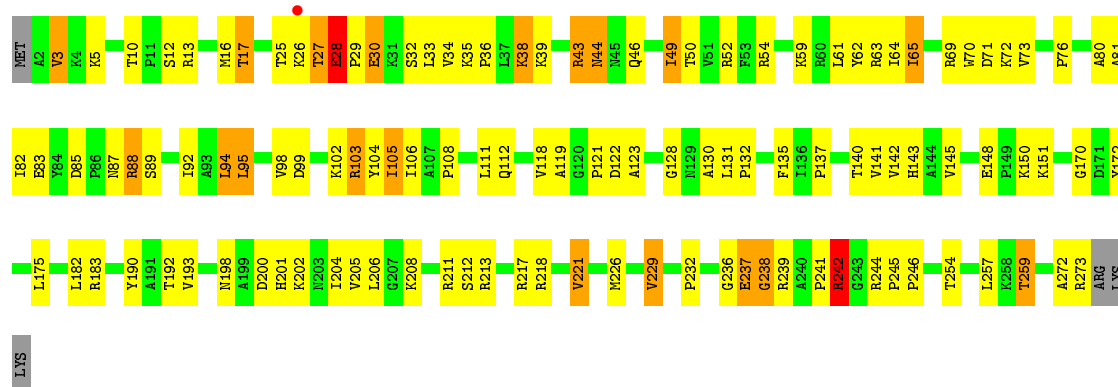






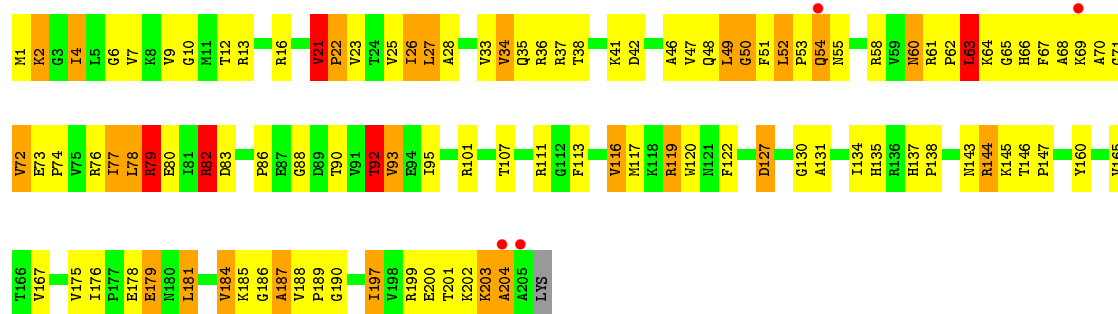
• Molecule 25: 50S ribosomal protein L2

Chain YD: 56% 35% 7% ..



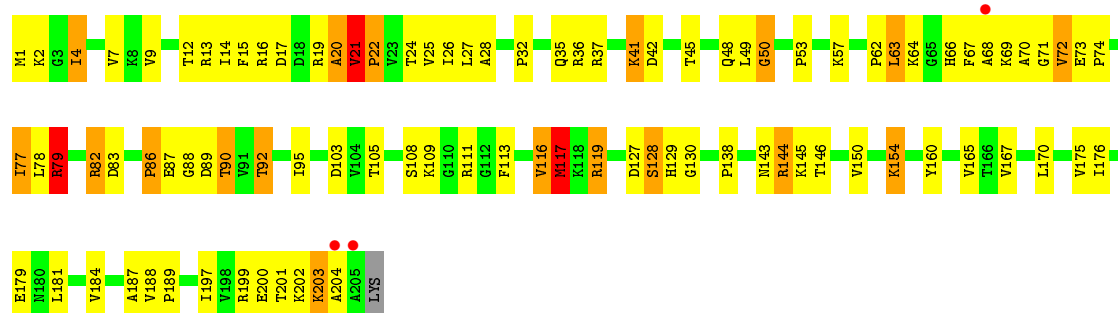
• Molecule 26: 50S ribosomal protein L3

Chain RE: 2% 48% 37% 13% .



• Molecule 26: 50S ribosomal protein L3

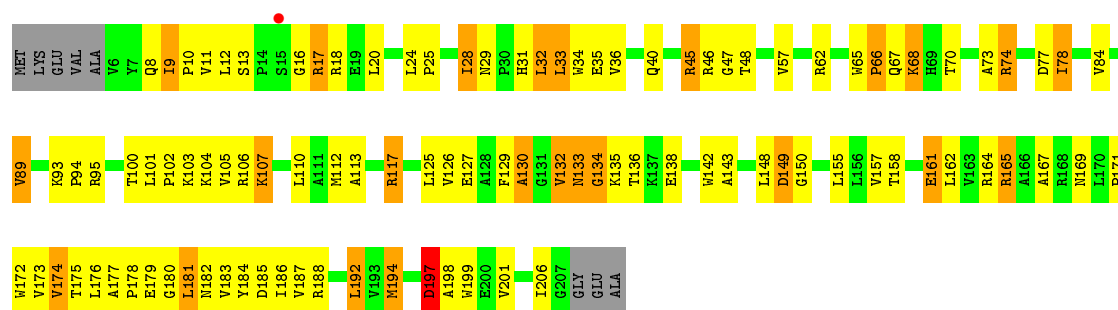
Chain YE: % 53% 36% 9% .





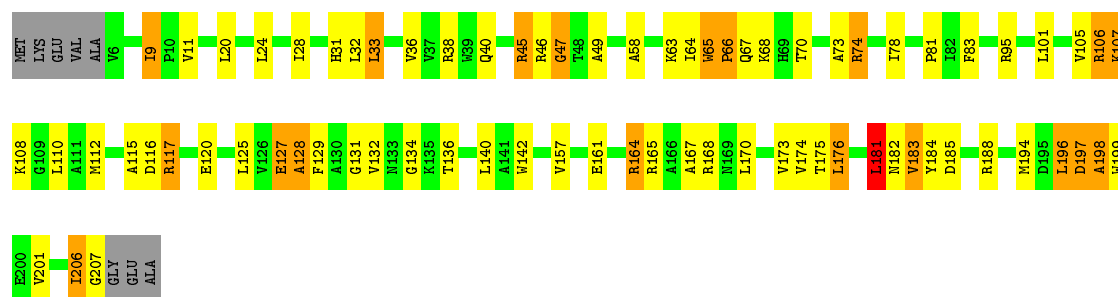
- Molecule 27: 50S ribosomal protein L4

Chain RF: 



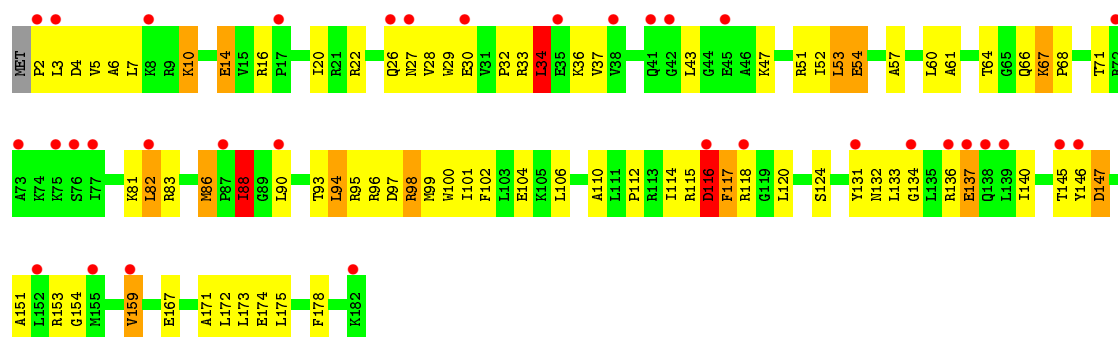
- Molecule 27: 50S ribosomal protein L4

Chain YF: 



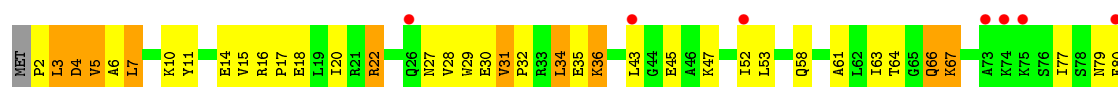
- Molecule 28: 50S ribosomal protein L5

Chain RG: 

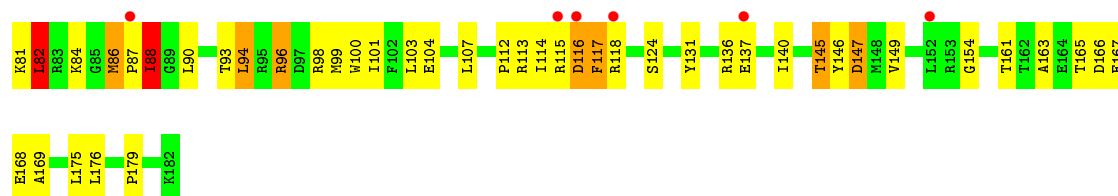


- Molecule 28: 50S ribosomal protein L5

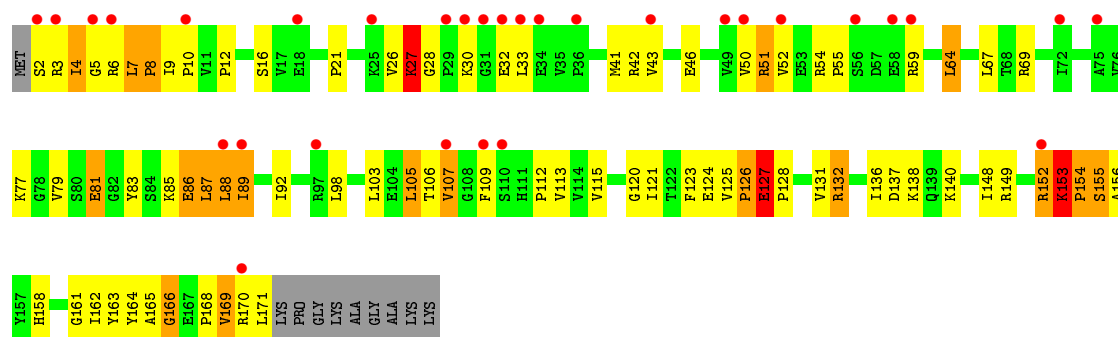
Chain YG: 



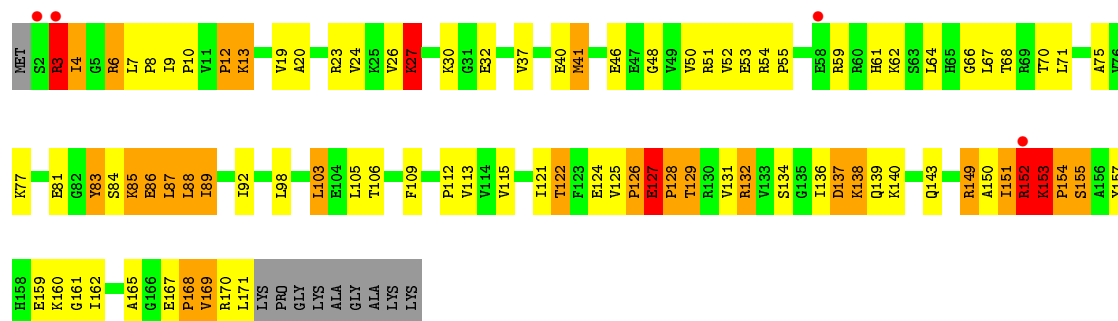




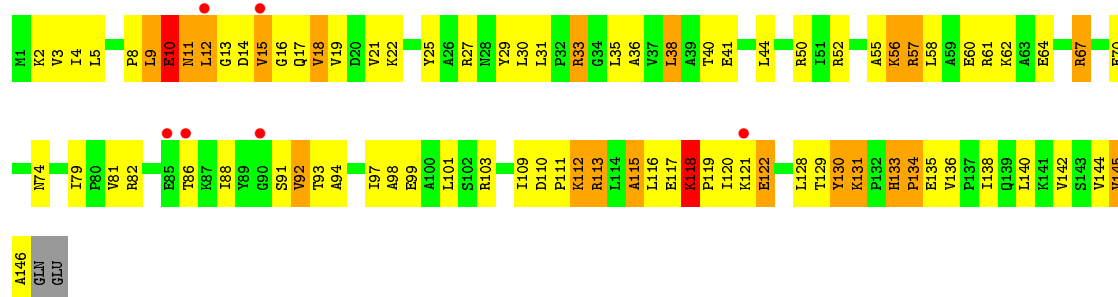
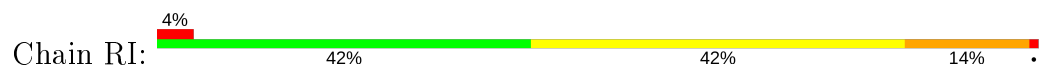
• Molecule 29: 50S ribosomal protein L6



• Molecule 29: 50S ribosomal protein L6

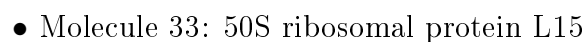


• Molecule 30: 50S ribosomal protein L9

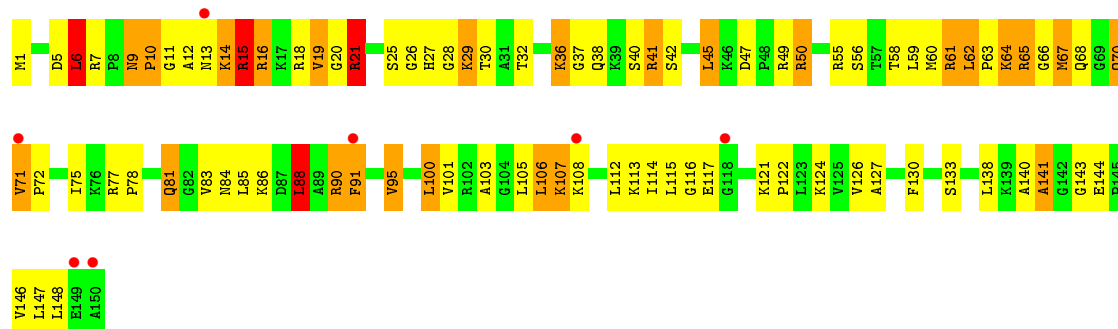
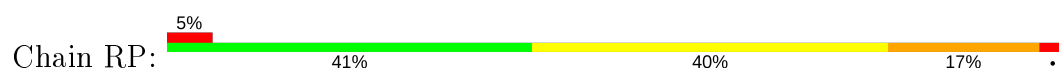


• Molecule 30: 50S ribosomal protein L9

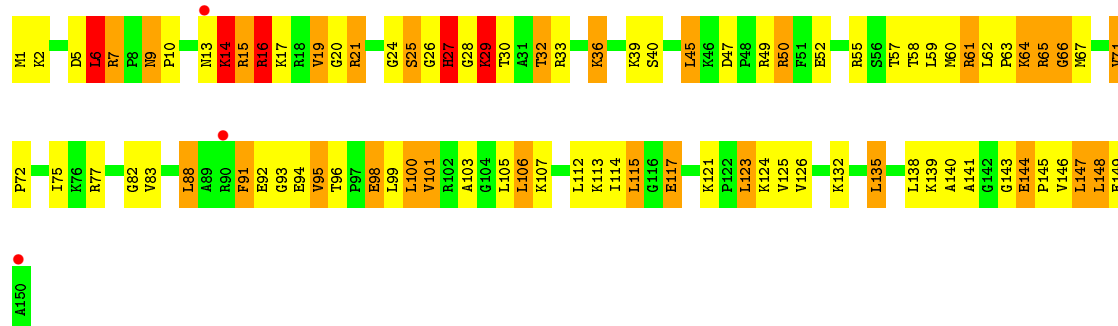
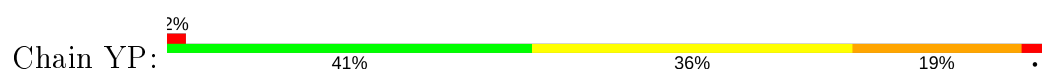




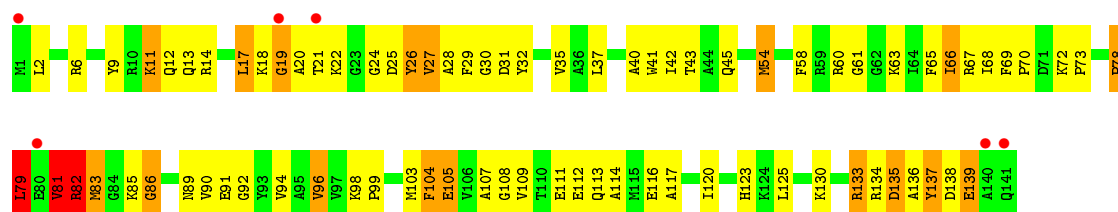




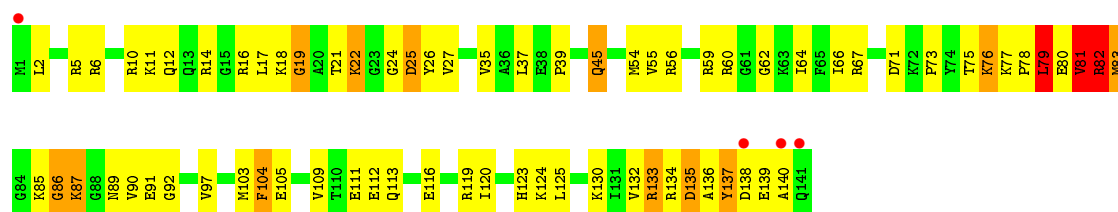
- Molecule 33: 50S ribosomal protein L15



- Molecule 34: 50S ribosomal protein L16



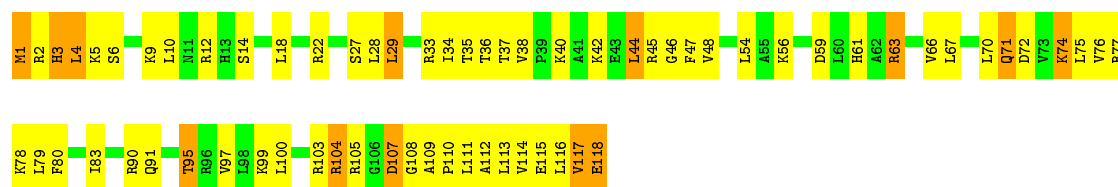
- Molecule 34: 50S ribosomal protein L16



- Molecule 35: 50S ribosomal protein L17

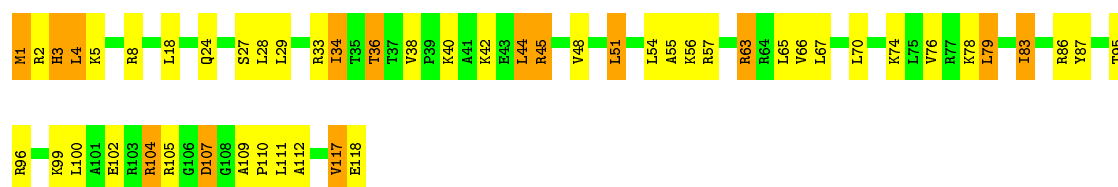


Chain RR: 



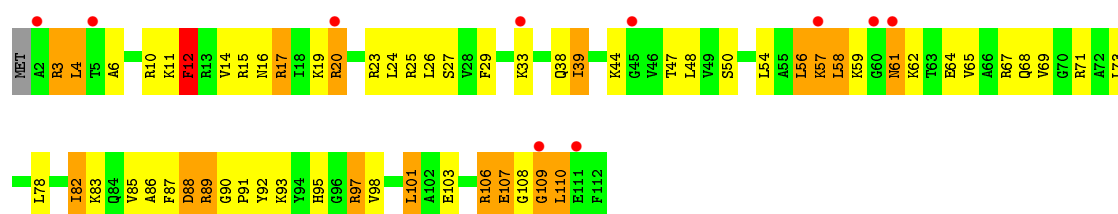
- Molecule 35: 50S ribosomal protein L17

Chain YR: 



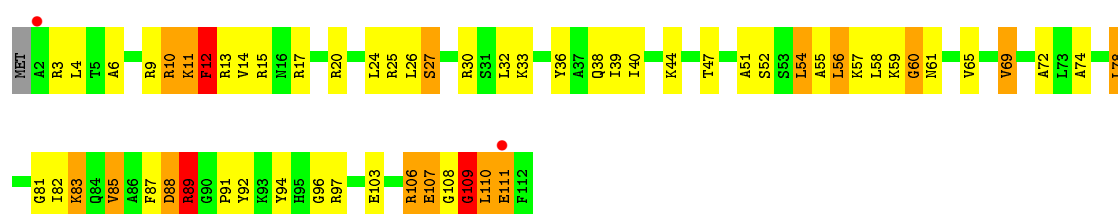
- Molecule 36: 50S ribosomal protein L18

Chain RS: 



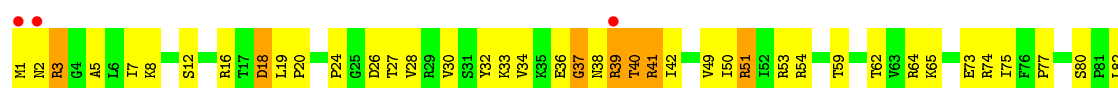
- Molecule 36: 50S ribosomal protein L18

Chain YS: 



- Molecule 37: 50S ribosomal protein L19

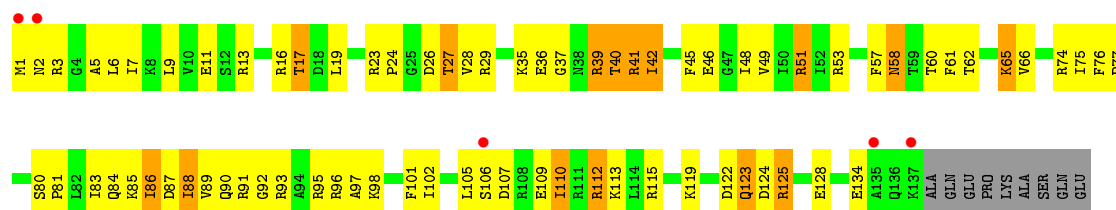
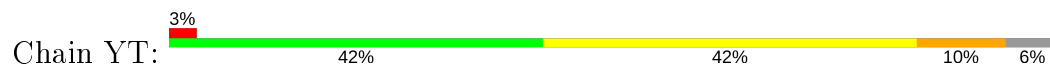
Chain RT: 



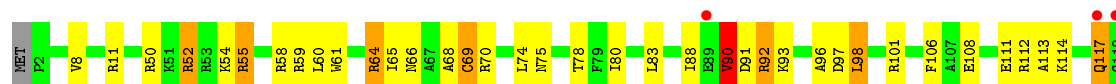




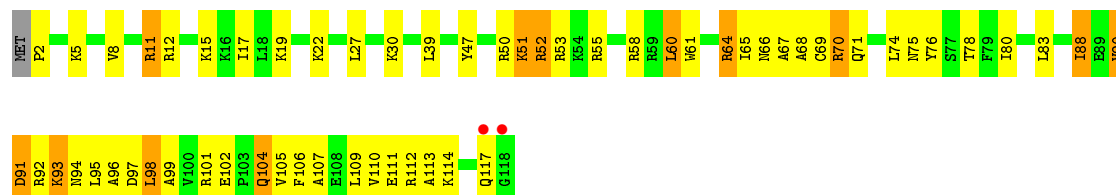
- Molecule 37: 50S ribosomal protein L19



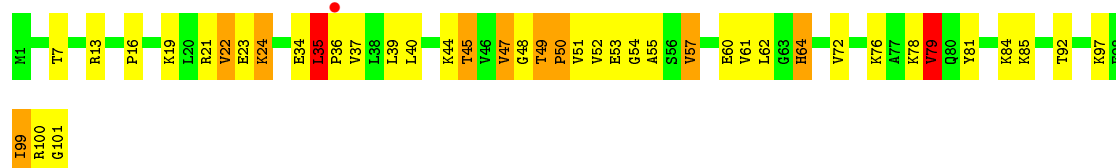
- Molecule 38: 50S ribosomal protein L20



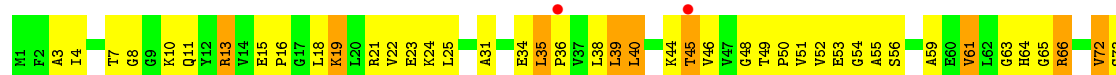
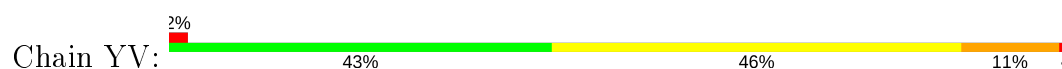
- Molecule 38: 50S ribosomal protein L20



- Molecule 39: 50S ribosomal protein L21



- Molecule 39: 50S ribosomal protein L21







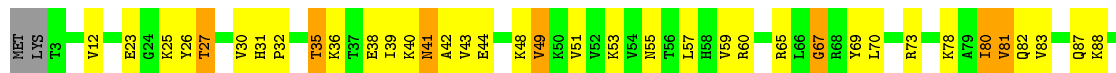
- Molecule 40: 50S ribosomal protein L22



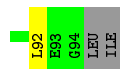
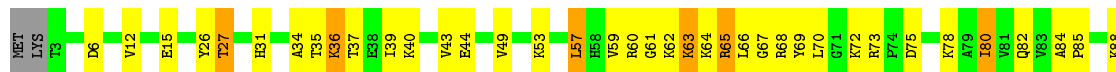
- Molecule 40: 50S ribosomal protein L22



- Molecule 41: 50S ribosomal protein L23



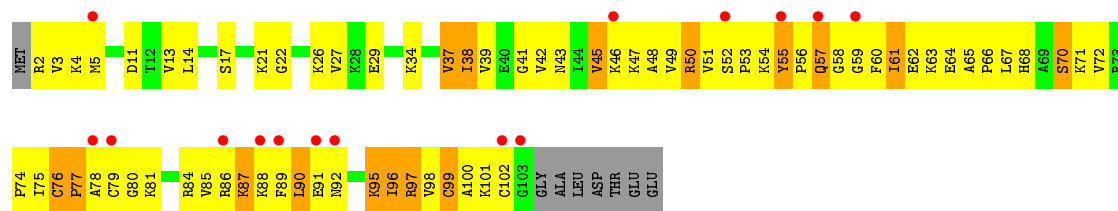
- Molecule 41: 50S ribosomal protein L23



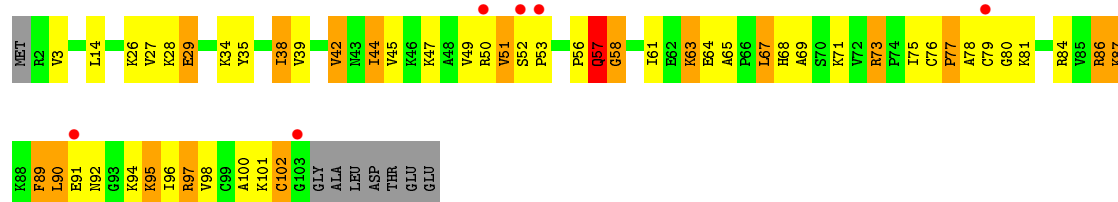
- Molecule 42: 50S ribosomal protein L24



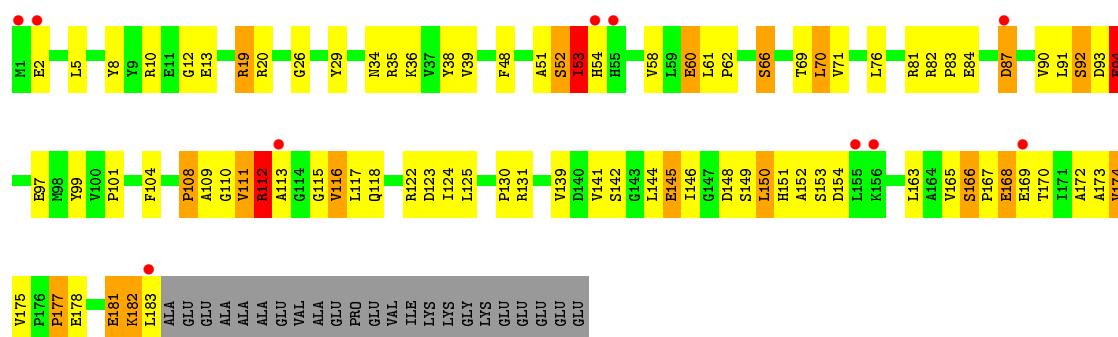




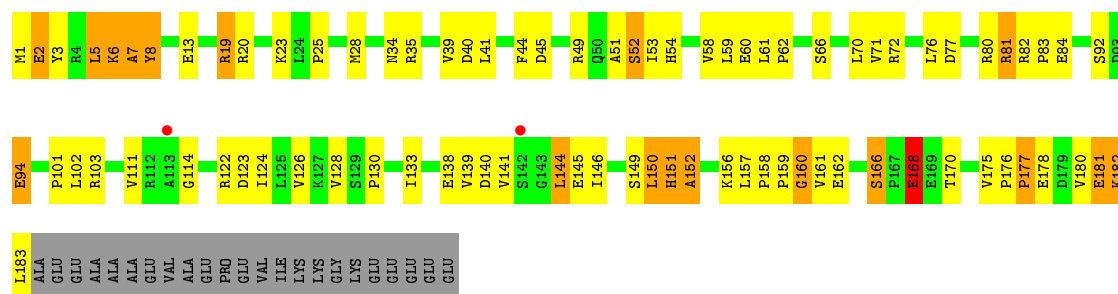
• Molecule 42: 50S ribosomal protein L24



• Molecule 43: 50S ribosomal protein L25



• Molecule 43: 50S ribosomal protein L25



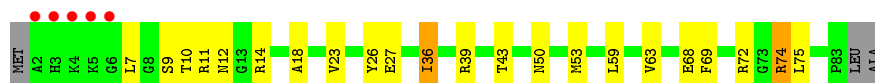
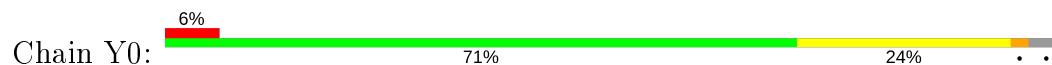
• Molecule 44: 50S ribosomal protein L27



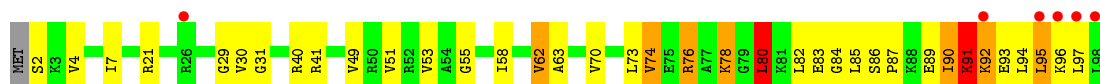




- Molecule 44: 50S ribosomal protein L27



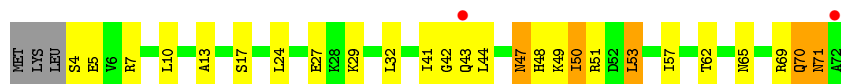
- Molecule 45: 50S ribosomal protein L28



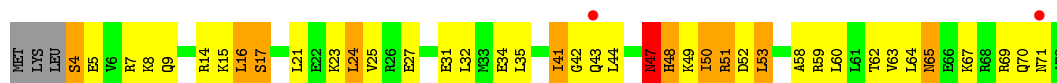
- Molecule 45: 50S ribosomal protein L28



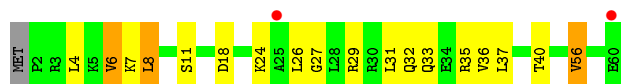
- Molecule 46: 50S ribosomal protein L29



- Molecule 46: 50S ribosomal protein L29

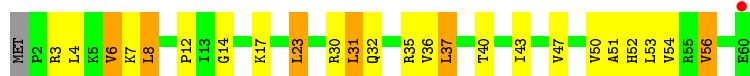


- Molecule 47: 50S ribosomal protein L30

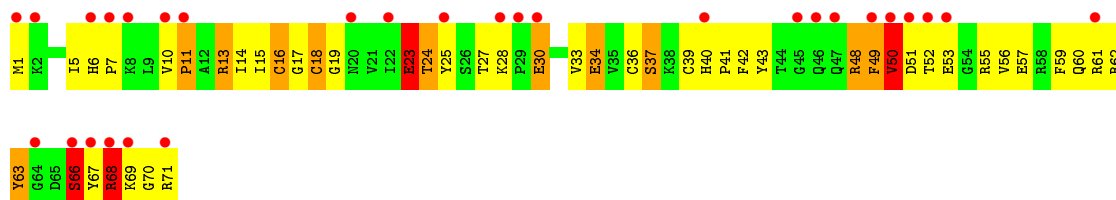
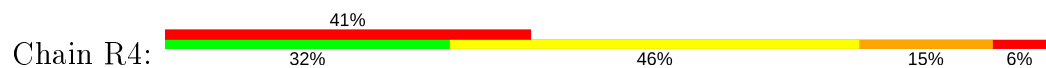


- Molecule 47: 50S ribosomal protein L30

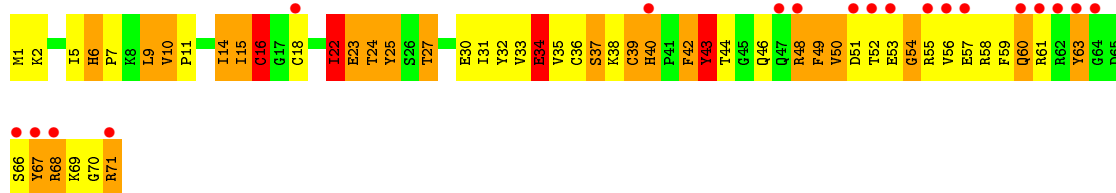
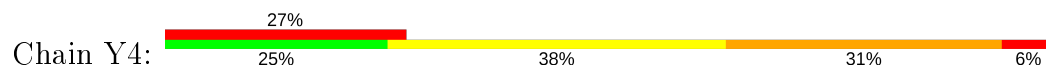




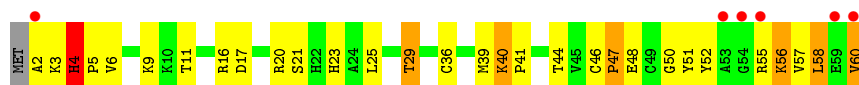
- Molecule 48: 50S ribosomal protein L31



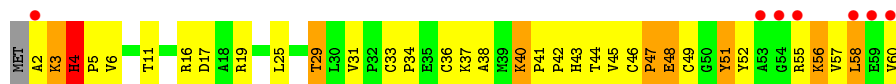
- Molecule 48: 50S ribosomal protein L31



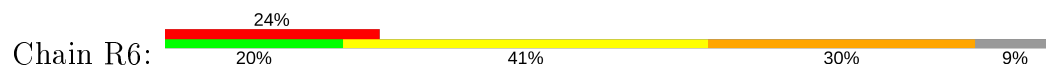
- Molecule 49: 50S ribosomal protein L32



- Molecule 49: 50S ribosomal protein L32



- Molecule 50: 50S ribosomal protein L33

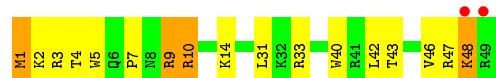


- Molecule 50: 50S ribosomal protein L33





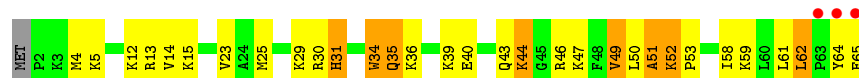
- Molecule 51: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L34



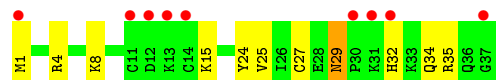
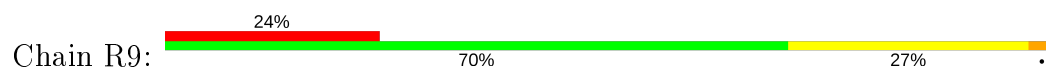
- Molecule 52: 50S ribosomal protein L35



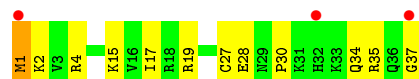
- Molecule 52: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L36



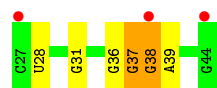
- Molecule 53: 50S ribosomal protein L36





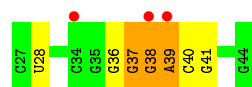
## ● Molecule 54: P-site ASL SufA6

Chain XV: 



## ● Molecule 54: P-site ASL SufA6

Chain QV: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.12Å 448.51Å 621.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.99 – 3.34 34.99 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.5 (34.99-3.34) 96.6 (34.99-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 3.18Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.237 , 0.267 0.237 , 0.267	Depositor DCC
$R_{free}$ test set	43433 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.9	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 51.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	288423	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	QX	0.52	0/87	1.10	0/132
1	XX	0.47	0/87	1.10	0/132
2	QA	0.29	0/36098	0.81	32/56341 (0.1%)
2	XA	0.31	0/36101	0.82	31/56346 (0.1%)
3	QB	0.31	0/1959	0.52	0/2642
3	XB	0.32	0/1959	0.54	0/2642
4	QC	0.31	0/1629	0.53	0/2195
4	XC	0.36	0/1629	0.56	0/2195
5	QD	0.38	0/1733	0.59	1/2318 (0.0%)
5	XD	0.40	0/1733	0.60	0/2318
6	QE	0.35	0/1171	0.56	0/1576
6	XE	0.39	0/1171	0.59	0/1576
7	QF	0.38	0/856	0.54	0/1154
7	XF	0.39	0/856	0.58	0/1154
8	QG	0.33	0/1276	0.50	0/1709
8	XG	0.34	0/1276	0.50	0/1709
9	QH	0.33	0/1136	0.55	0/1527
9	XH	0.38	0/1136	0.58	0/1527
10	QI	0.31	0/1029	0.55	0/1379
10	XI	0.34	0/1029	0.58	0/1379
11	QJ	0.33	0/814	0.54	0/1095
11	XJ	0.35	0/814	0.59	0/1095
12	QK	0.36	0/900	0.57	0/1213
12	XK	0.39	0/900	0.58	0/1213
13	QL	0.37	0/991	0.61	0/1327
13	XL	0.45	0/991	0.74	1/1327 (0.1%)
14	QM	0.32	0/974	0.59	0/1303
14	XM	0.37	0/974	0.63	0/1303
15	QN	0.41	0/501	0.60	0/664
15	XN	0.42	0/501	0.66	0/664
16	QO	0.35	0/745	0.53	0/992
16	XO	0.39	0/745	0.54	0/992



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	QP	0.36	0/721	0.57	0/970
17	XP	0.35	0/721	0.57	0/970
18	QQ	0.35	0/847	0.53	0/1131
18	XQ	0.35	0/847	0.54	0/1131
19	QR	0.35	0/579	0.64	1/768 (0.1%)
19	XR	0.37	0/579	0.59	0/768
20	QS	0.33	0/689	0.61	0/926
20	XS	0.38	0/689	0.69	1/926 (0.1%)
21	QT	0.36	0/765	0.64	0/1007
21	XT	0.31	0/765	0.59	0/1007
22	QU	0.30	0/221	0.54	0/288
22	XU	0.31	0/221	0.62	0/288
23	RA	0.37	0/69521	0.86	56/108529 (0.1%)
23	YA	0.48	1/69543 (0.0%)	0.93	97/108563 (0.1%)
24	RB	0.30	0/2878	0.82	0/4490
24	YB	0.37	0/2878	0.86	2/4490 (0.0%)
25	RD	0.50	0/2165	0.70	0/2919
25	YD	0.58	0/2165	0.78	1/2919 (0.0%)
26	RE	0.43	0/1601	0.73	3/2160 (0.1%)
26	YE	0.46	0/1601	0.75	2/2160 (0.1%)
27	RF	0.42	0/1620	0.62	0/2194
27	YF	0.48	0/1620	0.71	1/2194 (0.0%)
28	RG	0.31	0/1499	0.57	1/2016 (0.0%)
28	YG	0.39	0/1499	0.60	0/2016
29	RH	0.29	0/1332	0.58	0/1802
29	YH	0.45	0/1332	0.73	0/1802
30	RI	0.32	0/1151	0.57	0/1558
30	YI	0.30	0/1151	0.57	0/1558
31	RN	0.41	0/1131	0.62	0/1525
31	YN	0.43	0/1131	0.64	0/1525
32	RO	0.41	0/943	0.62	1/1269 (0.1%)
32	YO	0.50	0/943	0.65	0/1269
33	RP	0.43	0/1162	0.81	1/1544 (0.1%)
33	YP	0.49	0/1162	0.90	2/1544 (0.1%)
34	RQ	0.47	0/1143	0.73	2/1527 (0.1%)
34	YQ	0.57	0/1143	0.80	1/1527 (0.1%)
35	RR	0.42	0/982	0.69	0/1312
35	YR	0.45	0/982	0.73	0/1312
36	RS	0.36	0/892	0.64	0/1187
36	YS	0.40	0/892	0.75	1/1187 (0.1%)
37	RT	0.42	0/1155	0.63	0/1542
37	YT	0.44	0/1155	0.67	0/1542
38	RU	0.39	0/982	0.65	0/1306



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	YU	0.50	0/982	0.69	0/1306
39	RV	0.38	0/790	0.61	1/1057 (0.1%)
39	YV	0.45	0/790	0.73	1/1057 (0.1%)
40	RW	0.49	0/911	0.67	0/1220
40	YW	0.45	0/911	0.67	0/1220
41	RX	0.47	0/739	0.62	0/993
41	YX	0.50	0/739	0.66	0/993
42	RY	0.44	0/798	0.68	0/1064
42	YY	0.46	0/798	0.70	0/1064
43	RZ	0.34	0/1493	0.54	0/2026
43	YZ	0.33	0/1493	0.56	0/2026
44	R0	0.32	0/657	0.53	0/874
44	Y0	0.38	0/657	0.55	0/874
45	R1	0.44	0/770	0.66	0/1022
45	Y1	0.46	0/770	0.69	0/1022
46	R2	0.39	0/583	0.65	0/771
46	Y2	0.52	0/583	0.73	0/771
47	R3	0.35	0/474	0.57	0/635
47	Y3	0.41	0/474	0.59	0/635
48	R4	0.33	0/594	0.68	0/795
48	Y4	0.37	0/594	0.68	0/795
49	R5	0.43	0/473	0.74	0/639
49	Y5	0.43	0/473	0.77	1/639 (0.2%)
50	R6	0.35	0/431	0.69	0/575
50	Y6	0.37	0/431	0.67	0/575
51	R7	0.49	0/438	0.68	0/575
51	Y7	0.57	0/438	0.71	0/575
52	R8	0.55	0/525	0.79	0/691
52	Y8	0.58	0/525	0.82	0/691
53	R9	0.27	0/310	0.46	0/407
53	Y9	0.32	0/310	0.48	0/407
54	QV	0.38	0/403	0.86	0/627
54	XV	0.35	0/403	0.83	0/627
All	All	0.39	1/312559 (0.0%)	0.81	241/467055 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	QL	0	1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
13	XL	0	1
26	RE	0	1
26	YE	0	1
27	YF	0	1
29	RH	0	2
29	YH	0	2
36	YS	0	1
43	YZ	0	1
46	Y2	0	1
52	R8	0	2
52	Y8	0	2
All	All	0	16

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	YA	528	A	N9-C4	-5.51	1.34	1.37

The worst 5 of 241 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	YA	2031	A	O4'-C1'-N9	8.08	114.67	108.20
23	YA	265	A	O4'-C1'-N9	7.83	114.46	108.20
2	QA	1158	C	C2-N1-C1'	7.62	127.18	118.80
2	QA	1301	U	C2-N1-C1'	7.49	126.69	117.70
23	RA	2420	C	O5'-P-OP1	-7.46	98.99	105.70

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	QL	47	LYS	Peptide
52	R8	30	ARG	Peptide
26	RE	21	VAL	Peptide
29	RH	127	GLU	Peptide
29	RH	153	LYS	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen



atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QX	80	0	44	1	0
1	XX	80	0	44	1	0
2	QA	32247	0	16278	439	0
2	XA	32249	0	16279	454	1
3	QB	1924	0	1975	78	0
3	XB	1924	0	1975	93	0
4	QC	1605	0	1668	59	0
4	XC	1605	0	1668	56	0
5	QD	1703	0	1763	74	0
5	XD	1703	0	1763	45	0
6	QE	1155	0	1213	38	0
6	XE	1155	0	1213	42	0
7	QF	843	0	857	21	0
7	XF	843	0	857	27	0
8	QG	1257	0	1296	38	0
8	XG	1257	0	1296	26	0
9	QH	1116	0	1177	52	0
9	XH	1116	0	1177	37	0
10	QI	1010	0	1037	34	0
10	XI	1010	0	1037	43	0
11	QJ	801	0	849	47	0
11	XJ	801	0	849	44	0
12	QK	885	0	904	28	0
12	XK	885	0	904	44	0
13	QL	975	0	1062	33	0
13	XL	975	0	1062	38	0
14	QM	964	0	1034	64	0
14	XM	964	0	1034	57	0
15	QN	492	0	529	23	0
15	XN	492	0	529	20	0
16	QO	734	0	771	21	0
16	XO	734	0	771	18	0
17	QP	705	0	725	16	0
17	XP	705	0	725	22	0
18	QQ	834	0	904	19	0
18	XQ	834	0	904	17	0
19	QR	574	0	644	14	0
19	XR	574	0	644	22	0
20	QS	674	0	698	150	0
20	XS	674	0	698	146	0
21	QT	763	0	860	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	XT	763	0	861	41	0
22	QU	217	0	234	10	0
22	XU	217	0	234	4	0
23	RA	62071	0	31291	765	0
23	YA	62091	0	31298	741	0
24	RB	2573	0	1306	38	0
24	YB	2573	0	1306	29	0
25	RD	2115	0	2195	102	0
25	YD	2115	0	2195	96	0
26	RE	1568	0	1634	68	0
26	YE	1568	0	1634	58	0
27	RF	1585	0	1632	77	0
27	YF	1585	0	1632	66	0
28	RG	1474	0	1535	56	0
28	YG	1474	0	1535	57	0
29	RH	1307	0	1382	61	0
29	YH	1307	0	1382	67	0
30	RI	1136	0	1223	55	1
30	YI	1136	0	1223	46	0
31	RN	1104	0	1180	36	0
31	YN	1104	0	1180	50	0
32	RO	933	0	996	21	0
32	YO	933	0	996	27	0
33	RP	1145	0	1227	82	0
33	YP	1145	0	1228	86	0
34	RQ	1122	0	1179	55	0
34	YQ	1122	0	1179	44	0
35	RR	968	0	1033	48	0
35	YR	968	0	1033	36	0
36	RS	882	0	943	49	0
36	YS	882	0	943	40	0
37	RT	1141	0	1202	52	0
37	YT	1141	0	1202	53	0
38	RU	964	0	1022	29	0
38	YU	964	0	1022	55	0
39	RV	779	0	852	21	0
39	YV	779	0	852	43	0
40	RW	900	0	964	29	0
40	YW	900	0	964	26	0
41	RX	725	0	778	28	0
41	YX	725	0	778	22	0
42	RY	785	0	878	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	YY	785	0	878	40	0
43	RZ	1461	0	1493	53	0
43	YZ	1461	0	1493	46	0
44	R0	648	0	672	19	0
44	Y0	648	0	672	20	0
45	R1	763	0	848	27	0
45	Y1	763	0	848	31	0
46	R2	581	0	629	17	0
46	Y2	581	0	629	25	0
47	R3	469	0	518	8	0
47	Y3	469	0	518	15	0
48	R4	581	0	574	158	0
48	Y4	581	0	569	163	0
49	R5	459	0	480	26	0
49	Y5	459	0	480	33	0
50	R6	424	0	450	26	0
50	Y6	424	0	450	29	0
51	R7	430	0	480	14	0
51	Y7	430	0	480	19	0
52	R8	517	0	582	31	0
52	Y8	517	0	582	46	0
53	R9	307	0	338	8	0
53	Y9	307	0	338	10	0
54	QV	385	0	198	6	0
54	XV	385	0	198	5	0
55	QA	66	0	0	0	0
55	QF	1	0	0	0	0
55	QH	1	0	0	0	0
55	QM	1	0	0	0	0
55	R0	1	0	0	0	0
55	R3	1	0	0	0	0
55	R5	1	0	0	0	0
55	R8	1	0	0	0	0
55	RA	243	0	0	0	0
55	RB	2	0	0	0	0
55	RD	1	0	0	0	0
55	RE	2	0	0	0	0
55	RF	1	0	0	0	0
55	RP	2	0	0	0	0
55	RR	1	0	0	0	0
55	XA	71	0	0	0	0
55	XB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	XL	1	0	0	0	0
55	XM	1	0	0	0	0
55	Y5	1	0	0	0	0
55	YA	267	0	0	0	0
55	YB	4	0	0	0	0
55	YD	2	0	0	0	0
55	YE	1	0	0	0	0
55	YP	2	0	0	0	0
55	YX	1	0	0	0	0
56	QD	1	0	0	0	0
56	QN	1	0	0	0	0
56	XD	1	0	0	0	0
56	XN	1	0	0	0	0
All	All	288423	0	196477	5647	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 5647 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)
20:XS:68:GLY:CA	48:Y4:68:ARG:HB2	1.22	1.67
20:XS:68:GLY:HA2	48:Y4:68:ARG:CB	1.19	1.60
14:QM:80:ARG:HD3	48:R4:71:ARG:CZ	1.26	1.59
20:QS:67:VAL:N	48:R4:59:PHE:CZ	1.71	1.55
14:XM:80:ARG:HD3	48:Y4:71:ARG:CZ	1.09	1.53

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:RI:91:SER:OG	2:XA:368:U:OP1[4_555]	2.13	0.07

## 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	
3	QB	235/256 (92%)	173 (74%)	45 (19%)	17 (7%)	1	8
3	XB	235/256 (92%)	178 (76%)	42 (18%)	15 (6%)	1	10
4	QC	203/239 (85%)	163 (80%)	34 (17%)	6 (3%)	4	27
4	XC	203/239 (85%)	171 (84%)	29 (14%)	3 (2%)	10	40
5	QD	206/209 (99%)	175 (85%)	25 (12%)	6 (3%)	4	27
5	XD	206/209 (99%)	177 (86%)	24 (12%)	5 (2%)	6	31
6	QE	149/162 (92%)	136 (91%)	8 (5%)	5 (3%)	3	24
6	XE	149/162 (92%)	133 (89%)	13 (9%)	3 (2%)	7	34
7	QF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
7	XF	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
8	QG	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	12	43
8	XG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	12	43
9	QH	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	22	57
9	XH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	4	27
10	QI	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	3	20
10	XI	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	4	25
11	QJ	97/105 (92%)	75 (77%)	19 (20%)	3 (3%)	4	26
11	XJ	97/105 (92%)	78 (80%)	14 (14%)	5 (5%)	2	14
12	QK	117/129 (91%)	100 (86%)	14 (12%)	3 (3%)	5	29
12	XK	117/129 (91%)	100 (86%)	15 (13%)	2 (2%)	9	37
13	QL	123/132 (93%)	98 (80%)	18 (15%)	7 (6%)	1	12
13	XL	123/132 (93%)	98 (80%)	15 (12%)	10 (8%)	1	6
14	QM	119/126 (94%)	95 (80%)	15 (13%)	9 (8%)	1	7
14	XM	119/126 (94%)	94 (79%)	16 (13%)	9 (8%)	1	7
15	QN	58/61 (95%)	48 (83%)	6 (10%)	4 (7%)	1	9
15	XN	58/61 (95%)	46 (79%)	6 (10%)	6 (10%)	0	3
16	QO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	13	45
16	XO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	6	32
17	QP	82/88 (93%)	73 (89%)	8 (10%)	1 (1%)	13	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	XP	82/88 (93%)	71 (87%)	10 (12%)	1 (1%)	13	45
18	QQ	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	7	34
18	XQ	98/105 (93%)	88 (90%)	10 (10%)	0	100	100
19	QR	68/88 (77%)	56 (82%)	9 (13%)	3 (4%)	2	18
19	XR	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	10	40
20	QS	82/93 (88%)	55 (67%)	16 (20%)	11 (13%)	0	1
20	XS	82/93 (88%)	54 (66%)	17 (21%)	11 (13%)	0	1
21	QT	97/106 (92%)	76 (78%)	15 (16%)	6 (6%)	1	11
21	XT	97/106 (92%)	75 (77%)	16 (16%)	6 (6%)	1	11
22	QU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	2	19
22	XU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	2	19
25	RD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	2	18
25	YD	270/276 (98%)	227 (84%)	34 (13%)	9 (3%)	4	24
26	RE	203/206 (98%)	147 (72%)	36 (18%)	20 (10%)	0	4
26	YE	203/206 (98%)	142 (70%)	41 (20%)	20 (10%)	0	4
27	RF	200/210 (95%)	167 (84%)	20 (10%)	13 (6%)	1	10
27	YF	200/210 (95%)	167 (84%)	25 (12%)	8 (4%)	3	20
28	RG	179/182 (98%)	139 (78%)	26 (14%)	14 (8%)	1	7
28	YG	179/182 (98%)	142 (79%)	25 (14%)	12 (7%)	1	9
29	RH	168/180 (93%)	114 (68%)	33 (20%)	21 (12%)	0	2
29	YH	168/180 (93%)	121 (72%)	23 (14%)	24 (14%)	0	1
30	RI	144/148 (97%)	107 (74%)	25 (17%)	12 (8%)	1	6
30	YI	144/148 (97%)	108 (75%)	23 (16%)	13 (9%)	1	5
31	RN	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	1	5
31	YN	136/140 (97%)	105 (77%)	17 (12%)	14 (10%)	0	3
32	RO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	9	37
32	YO	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	9	37
33	RP	148/150 (99%)	107 (72%)	27 (18%)	14 (10%)	0	4
33	YP	148/150 (99%)	108 (73%)	23 (16%)	17 (12%)	0	3
34	RQ	139/141 (99%)	99 (71%)	22 (16%)	18 (13%)	0	1
34	YQ	139/141 (99%)	98 (70%)	22 (16%)	19 (14%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	RR	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	2	19
35	YR	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	2	14
36	RS	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	0	3
36	YS	109/112 (97%)	78 (72%)	18 (16%)	13 (12%)	0	2
37	RT	135/146 (92%)	106 (78%)	17 (13%)	12 (9%)	1	5
37	YT	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	1	8
38	RU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	3	24
38	YU	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	3	24
39	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	1	11
39	YV	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	6
40	RW	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	3	23
40	YW	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	8	37
41	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	6	33
41	YX	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	6	33
42	RY	100/110 (91%)	71 (71%)	13 (13%)	16 (16%)	0	1
42	YY	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	0	2
43	RZ	181/206 (88%)	127 (70%)	37 (20%)	17 (9%)	0	4
43	YZ	181/206 (88%)	133 (74%)	31 (17%)	17 (9%)	0	4
44	R0	80/85 (94%)	70 (88%)	10 (12%)	0	100	100
44	Y0	80/85 (94%)	73 (91%)	7 (9%)	0	100	100
45	R1	95/98 (97%)	75 (79%)	11 (12%)	9 (10%)	0	4
45	Y1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	1	11
46	R2	67/72 (93%)	53 (79%)	9 (13%)	5 (8%)	1	8
46	Y2	67/72 (93%)	55 (82%)	6 (9%)	6 (9%)	1	5
47	R3	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	3	24
47	Y3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	8	37
48	R4	69/71 (97%)	35 (51%)	18 (26%)	16 (23%)	0	0
48	Y4	69/71 (97%)	35 (51%)	15 (22%)	19 (28%)	0	0
49	R5	57/60 (95%)	44 (77%)	11 (19%)	2 (4%)	3	24
49	Y5	57/60 (95%)	46 (81%)	9 (16%)	2 (4%)	3	24
50	R6	47/54 (87%)	23 (49%)	14 (30%)	10 (21%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	Y6	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0	1
51	R7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	7	34
51	Y7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	7	34
52	R8	62/65 (95%)	51 (82%)	6 (10%)	5 (8%)	1	6
52	Y8	62/65 (95%)	48 (77%)	10 (16%)	4 (6%)	1	10
53	R9	35/37 (95%)	35 (100%)	0	0	100	100
53	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11470/12128 (95%)	9239 (80%)	1524 (13%)	707 (6%)	1	11

5 of 707 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	QB	236	TYR
4	QC	12	LEU
4	QC	190	ARG
5	QD	28	SER
14	QM	67	GLU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	QB	205/220 (93%)	172 (84%)	33 (16%)	2	11
3	XB	205/220 (93%)	180 (88%)	25 (12%)	5	20
4	QC	159/188 (85%)	145 (91%)	14 (9%)	10	36
4	XC	159/188 (85%)	146 (92%)	13 (8%)	11	39
5	QD	180/181 (99%)	157 (87%)	23 (13%)	4	18
5	XD	180/181 (99%)	154 (86%)	26 (14%)	3	15
6	QE	116/123 (94%)	104 (90%)	12 (10%)	7	28
6	XE	116/123 (94%)	104 (90%)	12 (10%)	7	28
7	QF	90/90 (100%)	78 (87%)	12 (13%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	XF	90/90 (100%)	82 (91%)	8 (9%)	9	35
8	QG	126/127 (99%)	114 (90%)	12 (10%)	8	32
8	XG	126/127 (99%)	114 (90%)	12 (10%)	8	32
9	QH	119/119 (100%)	109 (92%)	10 (8%)	11	38
9	XH	119/119 (100%)	106 (89%)	13 (11%)	6	26
10	QI	98/99 (99%)	81 (83%)	17 (17%)	2	9
10	XI	98/99 (99%)	80 (82%)	18 (18%)	1	7
11	QJ	89/92 (97%)	77 (86%)	12 (14%)	4	17
11	XJ	89/92 (97%)	74 (83%)	15 (17%)	2	9
12	QK	90/99 (91%)	81 (90%)	9 (10%)	7	29
12	XK	90/99 (91%)	81 (90%)	9 (10%)	7	29
13	QL	104/109 (95%)	87 (84%)	17 (16%)	2	10
13	XL	104/109 (95%)	93 (89%)	11 (11%)	6	27
14	QM	97/101 (96%)	73 (75%)	24 (25%)	0	2
14	XM	97/101 (96%)	78 (80%)	19 (20%)	1	6
15	QN	49/50 (98%)	40 (82%)	9 (18%)	1	7
15	XN	49/50 (98%)	42 (86%)	7 (14%)	3	15
16	QO	79/80 (99%)	72 (91%)	7 (9%)	9	35
16	XO	79/80 (99%)	69 (87%)	10 (13%)	4	19
17	QP	72/74 (97%)	63 (88%)	9 (12%)	4	19
17	XP	72/74 (97%)	64 (89%)	8 (11%)	6	25
18	QQ	95/97 (98%)	87 (92%)	8 (8%)	11	38
18	XQ	95/97 (98%)	89 (94%)	6 (6%)	18	49
19	QR	61/77 (79%)	50 (82%)	11 (18%)	1	8
19	XR	61/77 (79%)	52 (85%)	9 (15%)	3	14
20	QS	73/80 (91%)	59 (81%)	14 (19%)	1	6
20	XS	73/80 (91%)	57 (78%)	16 (22%)	1	4
21	QT	76/82 (93%)	67 (88%)	9 (12%)	5	22
21	XT	76/82 (93%)	66 (87%)	10 (13%)	4	18
22	QU	20/22 (91%)	20 (100%)	0	100	100
22	XU	20/22 (91%)	19 (95%)	1 (5%)	24	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	RD	214/218 (98%)	175 (82%)	39 (18%)	1	7
25	YD	214/218 (98%)	181 (85%)	33 (15%)	2	13
26	RE	165/166 (99%)	126 (76%)	39 (24%)	1	3
26	YE	165/166 (99%)	137 (83%)	28 (17%)	2	9
27	RF	161/166 (97%)	132 (82%)	29 (18%)	1	8
27	YF	161/166 (97%)	137 (85%)	24 (15%)	3	13
28	RG	155/156 (99%)	134 (86%)	21 (14%)	4	17
28	YG	155/156 (99%)	133 (86%)	22 (14%)	3	16
29	RH	142/148 (96%)	121 (85%)	21 (15%)	3	14
29	YH	142/148 (96%)	115 (81%)	27 (19%)	1	6
30	RI	122/124 (98%)	98 (80%)	24 (20%)	1	6
30	YI	122/124 (98%)	96 (79%)	26 (21%)	1	4
31	RN	117/119 (98%)	97 (83%)	20 (17%)	2	9
31	YN	117/119 (98%)	96 (82%)	21 (18%)	2	8
32	RO	100/100 (100%)	90 (90%)	10 (10%)	7	29
32	YO	100/100 (100%)	88 (88%)	12 (12%)	5	21
33	RP	116/116 (100%)	85 (73%)	31 (27%)	0	2
33	YP	116/116 (100%)	82 (71%)	34 (29%)	0	1
34	RQ	111/111 (100%)	95 (86%)	16 (14%)	3	15
34	YQ	111/111 (100%)	92 (83%)	19 (17%)	2	9
35	RR	101/101 (100%)	83 (82%)	18 (18%)	2	8
35	YR	101/101 (100%)	81 (80%)	20 (20%)	1	5
36	RS	87/88 (99%)	69 (79%)	18 (21%)	1	4
36	YS	87/88 (99%)	68 (78%)	19 (22%)	1	4
37	RT	120/127 (94%)	102 (85%)	18 (15%)	3	13
37	YT	120/127 (94%)	98 (82%)	22 (18%)	1	7
38	RU	93/94 (99%)	79 (85%)	14 (15%)	3	13
38	YU	93/94 (99%)	77 (83%)	16 (17%)	2	9
39	RV	82/82 (100%)	66 (80%)	16 (20%)	1	6
39	YV	82/82 (100%)	67 (82%)	15 (18%)	1	7
40	RW	92/92 (100%)	73 (79%)	19 (21%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	YW	92/92 (100%)	76 (83%)	16 (17%)	2	8
41	RX	74/78 (95%)	64 (86%)	10 (14%)	4	17
41	YX	74/78 (95%)	60 (81%)	14 (19%)	1	6
42	RY	85/91 (93%)	63 (74%)	22 (26%)	0	2
42	YY	85/91 (93%)	64 (75%)	21 (25%)	0	2
43	RZ	162/179 (90%)	137 (85%)	25 (15%)	2	13
43	YZ	162/179 (90%)	137 (85%)	25 (15%)	2	13
44	R0	65/67 (97%)	57 (88%)	8 (12%)	4	20
44	Y0	65/67 (97%)	62 (95%)	3 (5%)	27	60
45	R1	82/83 (99%)	73 (89%)	9 (11%)	6	25
45	Y1	82/83 (99%)	70 (85%)	12 (15%)	3	14
46	R2	64/67 (96%)	57 (89%)	7 (11%)	6	26
46	Y2	64/67 (96%)	47 (73%)	17 (27%)	0	2
47	R3	51/52 (98%)	45 (88%)	6 (12%)	5	22
47	Y3	51/52 (98%)	43 (84%)	8 (16%)	2	12
48	R4	63/63 (100%)	45 (71%)	18 (29%)	0	1
48	Y4	63/63 (100%)	43 (68%)	20 (32%)	0	1
49	R5	51/52 (98%)	37 (72%)	14 (28%)	0	1
49	Y5	51/52 (98%)	37 (72%)	14 (28%)	0	1
50	R6	48/52 (92%)	35 (73%)	13 (27%)	0	1
50	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	4
51	R7	42/42 (100%)	34 (81%)	8 (19%)	1	6
51	Y7	42/42 (100%)	35 (83%)	7 (17%)	2	10
52	R8	54/55 (98%)	44 (82%)	10 (18%)	1	7
52	Y8	54/55 (98%)	41 (76%)	13 (24%)	0	3
53	R9	34/34 (100%)	32 (94%)	2 (6%)	19	52
53	Y9	34/34 (100%)	32 (94%)	2 (6%)	19	52
All	All	9702/10066 (96%)	8167 (84%)	1535 (16%)	2	12

5 of 1535 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	R2	53	LEU

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Mol	Chain	Res	Type
8	XG	114	ARG
43	YZ	139	VAL
48	R4	61	ARG
3	XB	113	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
43	RZ	34	ASN
48	R4	60	GLN
7	XF	16	GLN
36	RS	34	HIS
11	XJ	78	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QX	3/19 (15%)	1 (33%)	0
1	XX	3/19 (15%)	0	0
2	QA	1499/1521 (98%)	274 (18%)	46 (3%)
2	XA	1499/1521 (98%)	272 (18%)	40 (2%)
23	RA	2879/2915 (98%)	580 (20%)	62 (2%)
23	YA	2880/2915 (98%)	586 (20%)	62 (2%)
24	RB	119/122 (97%)	22 (18%)	2 (1%)
24	YB	119/122 (97%)	25 (21%)	2 (1%)
54	QV	17/18 (94%)	4 (23%)	1 (5%)
54	XV	17/18 (94%)	4 (23%)	1 (5%)
All	All	9035/9190 (98%)	1768 (19%)	216 (2%)

5 of 1768 RNA backbone outliers are listed below:

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

5 of 216 RNA pucker outliers are listed below:



Mol	Chain	Res	Type
23	RA	2405	G
2	XA	250	A
23	YA	2126	A
23	RA	2518	A
24	RB	66	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
54	1MG	XV	37	54	18,26,27	1.49	2 (11%)	19,39,42	1.70	1 (5%)
54	1MG	QV	37	54	18,26,27	1.49	3 (16%)	19,39,42	1.68	2 (10%)

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
54	1MG	XV	37	54	-	2/3/25/26	0/3/3/3
54	1MG	QV	37	54	-	2/3/25/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	XV	37	1MG	C6-C5	4.60	1.48	1.41
54	QV	37	1MG	C6-C5	4.48	1.48	1.41
54	XV	37	1MG	C5-C4	3.01	1.48	1.40
54	QV	37	1MG	C5-C4	2.98	1.48	1.40
54	QV	37	1MG	C6-N1	2.12	1.41	1.38

All (3) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	QV	37	1MG	C2-N3-C4	5.59	121.75	115.36
54	XV	37	1MG	C2-N3-C4	5.53	121.68	115.36
54	QV	37	1MG	C3'-C2'-C1'	2.01	104.01	100.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	XV	37	1MG	3	0
54	QV	37	1MG	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 681 ligands modelled in this entry, 681 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	QX	4/19 (21%)	1.36	2 (50%) 0 0	111, 112, 113, 116	0
1	XX	4/19 (21%)	1.45	1 (25%) 0 0	97, 97, 99, 102	0
2	QA	1500/1521 (98%)	0.47	128 (8%) 10 11	68, 108, 190, 262	0
2	XA	1500/1521 (98%)	0.35	105 (7%) 16 17	54, 105, 188, 260	0
3	QB	237/256 (92%)	0.97	37 (15%) 2 1	139, 160, 171, 173	0
3	XB	237/256 (92%)	0.61	18 (7%) 13 14	123, 144, 157, 164	0
4	QC	205/239 (85%)	1.00	39 (19%) 1 1	136, 150, 164, 168	0
4	XC	205/239 (85%)	0.71	20 (9%) 7 7	129, 140, 155, 160	0
5	QD	208/209 (99%)	0.43	11 (5%) 26 27	106, 117, 124, 127	0
5	XD	208/209 (99%)	0.30	7 (3%) 45 44	96, 110, 119, 122	0
6	QE	151/162 (93%)	0.35	5 (3%) 46 45	99, 113, 122, 125	0
6	XE	151/162 (93%)	0.32	6 (3%) 38 37	88, 104, 117, 127	0
7	QF	101/101 (100%)	0.10	1 (0%) 82 83	97, 104, 109, 120	0
7	XF	101/101 (100%)	0.19	1 (0%) 82 83	89, 98, 108, 114	0
8	QG	155/156 (99%)	1.37	34 (21%) 0 0	137, 158, 164, 166	0
8	XG	155/156 (99%)	0.87	27 (17%) 1 1	124, 150, 160, 163	0
9	QH	138/138 (100%)	0.37	8 (5%) 23 24	97, 115, 130, 139	0
9	XH	138/138 (100%)	0.12	1 (0%) 87 90	87, 105, 116, 124	0
10	QI	127/128 (99%)	1.40	41 (32%) 0 0	138, 176, 181, 183	0
10	XI	127/128 (99%)	1.16	24 (18%) 1 1	129, 167, 174, 177	0
11	QJ	99/105 (94%)	1.99	46 (46%) 0 0	148, 174, 179, 181	0
11	XJ	99/105 (94%)	1.74	40 (40%) 0 0	140, 166, 173, 174	0
12	QK	119/129 (92%)	0.60	9 (7%) 13 14	86, 113, 124, 142	0
12	XK	119/129 (92%)	0.48	8 (6%) 17 19	75, 101, 116, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
13	QL	125/132 (94%)	0.59	10 (8%)	12 12	86, 94, 105, 125	0
13	XL	125/132 (94%)	0.37	6 (4%)	30 31	78, 92, 99, 125	0
14	QM	121/126 (96%)	1.53	30 (24%)	0 0	153, 176, 181, 183	0
14	XM	121/126 (96%)	1.54	37 (30%)	0 0	155, 177, 180, 184	0
15	QN	60/61 (98%)	1.23	13 (21%)	0 0	154, 160, 174, 177	0
15	XN	60/61 (98%)	1.04	9 (15%)	2 2	145, 152, 171, 172	0
16	QO	88/89 (98%)	0.20	2 (2%)	60 60	90, 109, 117, 118	0
16	XO	88/89 (98%)	0.07	1 (1%)	80 81	79, 95, 102, 103	0
17	QP	84/88 (95%)	0.27	1 (1%)	79 79	93, 102, 117, 139	0
17	XP	84/88 (95%)	0.46	3 (3%)	42 41	96, 112, 126, 151	0
18	QQ	100/105 (95%)	0.38	7 (7%)	16 17	90, 99, 105, 106	0
18	XQ	100/105 (95%)	0.30	4 (4%)	38 37	83, 98, 104, 105	0
19	QR	70/88 (79%)	0.42	5 (7%)	16 17	99, 109, 118, 121	0
19	XR	70/88 (79%)	0.24	1 (1%)	75 75	90, 101, 111, 113	0
20	QS	84/93 (90%)	2.05	39 (46%)	0 0	159, 181, 184, 185	0
20	XS	84/93 (90%)	2.61	45 (53%)	0 0	165, 185, 190, 191	0
21	QT	99/106 (93%)	0.24	2 (2%)	65 64	91, 104, 115, 118	0
21	XT	99/106 (93%)	0.56	8 (8%)	12 12	101, 117, 128, 131	0
22	QU	25/27 (92%)	2.88	16 (64%)	0 0	164, 170, 171, 173	0
22	XU	25/27 (92%)	3.72	21 (84%)	0 0	164, 169, 172, 173	0
23	RA	2882/2915 (98%)	0.23	202 (7%)	16 17	45, 71, 200, 279	0
23	YA	2883/2915 (98%)	-0.01	150 (5%)	27 27	29, 49, 175, 271	0
24	RB	120/122 (98%)	0.26	1 (0%)	86 87	82, 117, 139, 156	0
24	YB	120/122 (98%)	-0.27	0	100 100	50, 71, 89, 104	0
25	RD	272/276 (98%)	0.03	2 (0%)	87 90	46, 67, 79, 83	0
25	YD	272/276 (98%)	-0.12	1 (0%)	92 94	33, 53, 65, 73	0
26	RE	205/206 (99%)	0.02	4 (1%)	65 64	47, 76, 96, 102	0
26	YE	205/206 (99%)	-0.05	3 (1%)	73 72	34, 59, 80, 91	0
27	RF	202/210 (96%)	-0.06	1 (0%)	91 91	48, 89, 108, 118	0
27	YF	202/210 (96%)	-0.19	0	100 100	31, 58, 82, 95	0
28	RG	181/182 (99%)	1.18	34 (18%)	1 1	134, 164, 177, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	YG	181/182 (99%)	0.36	13 (7%) 15 16	79, 114, 136, 149	0
29	RH	170/180 (94%)	1.00	31 (18%) 1 1	113, 136, 151, 182	0
29	YH	170/180 (94%)	0.23	4 (2%) 59 57	64, 75, 84, 135	0
30	RI	146/148 (98%)	0.23	6 (4%) 37 36	80, 117, 131, 133	0
30	YI	146/148 (98%)	0.09	4 (2%) 54 53	65, 108, 118, 121	0
31	RN	138/140 (98%)	-0.00	1 (0%) 87 90	59, 82, 101, 108	0
31	YN	138/140 (98%)	-0.24	0 100 100	40, 54, 77, 82	0
32	RO	122/122 (100%)	-0.29	0 100 100	57, 71, 81, 84	0
32	YO	122/122 (100%)	-0.25	0 100 100	44, 57, 72, 77	0
33	RP	150/150 (100%)	0.22	7 (4%) 31 32	53, 85, 108, 123	0
33	YP	150/150 (100%)	0.00	3 (2%) 65 64	33, 59, 83, 104	0
34	RQ	141/141 (100%)	0.19	6 (4%) 35 36	66, 89, 105, 117	0
34	YQ	141/141 (100%)	-0.01	4 (2%) 53 52	45, 59, 74, 86	0
35	RR	118/118 (100%)	-0.10	0 100 100	55, 68, 77, 80	0
35	YR	118/118 (100%)	-0.18	0 100 100	41, 54, 62, 66	0
36	RS	111/112 (99%)	0.45	10 (9%) 9 10	99, 115, 123, 126	0
36	YS	111/112 (99%)	-0.06	2 (1%) 68 67	64, 73, 80, 84	0
37	RT	137/146 (93%)	0.11	8 (5%) 23 24	68, 79, 123, 139	0
37	YT	137/146 (93%)	0.01	5 (3%) 42 41	51, 64, 108, 131	0
38	RU	117/118 (99%)	0.18	3 (2%) 56 54	57, 78, 95, 108	0
38	YU	117/118 (99%)	-0.09	2 (1%) 70 69	35, 46, 63, 75	0
39	RV	101/101 (100%)	0.06	1 (0%) 82 83	56, 96, 104, 108	0
39	YV	101/101 (100%)	-0.19	2 (1%) 65 64	33, 63, 74, 80	0
40	RW	113/113 (100%)	-0.09	4 (3%) 44 43	49, 62, 83, 105	0
40	YW	113/113 (100%)	-0.28	1 (0%) 84 85	37, 45, 63, 93	0
41	RX	92/96 (95%)	-0.08	0 100 100	63, 74, 84, 88	0
41	YX	92/96 (95%)	-0.27	0 100 100	43, 49, 60, 62	0
42	RY	102/110 (92%)	0.62	15 (14%) 2 2	79, 89, 108, 115	0
42	YY	102/110 (92%)	0.26	6 (5%) 22 23	55, 63, 85, 93	0
43	RZ	183/206 (88%)	0.49	10 (5%) 25 26	98, 118, 129, 133	0
43	YZ	183/206 (88%)	-0.00	2 (1%) 80 81	64, 83, 100, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	R0	82/85 (96%)	0.36	7 (8%) 10 11	66, 80, 88, 93	0
44	Y0	82/85 (96%)	-0.09	5 (6%) 21 22	44, 52, 62, 65	0
45	R1	97/98 (98%)	0.33	6 (6%) 20 21	55, 71, 105, 108	0
45	Y1	97/98 (98%)	0.27	4 (4%) 37 36	40, 53, 90, 94	0
46	R2	69/72 (95%)	0.18	2 (2%) 51 51	81, 88, 95, 103	0
46	Y2	69/72 (95%)	0.10	2 (2%) 51 51	52, 59, 66, 78	0
47	R3	59/60 (98%)	0.21	2 (3%) 45 44	68, 81, 97, 104	0
47	Y3	59/60 (98%)	-0.15	1 (1%) 70 69	42, 53, 70, 78	0
48	R4	71/71 (100%)	1.97	29 (40%) 0 0	154, 183, 185, 185	0
48	Y4	71/71 (100%)	1.46	19 (26%) 0 0	106, 147, 190, 191	0
49	R5	59/60 (98%)	0.29	6 (10%) 6 7	48, 72, 95, 106	0
49	Y5	59/60 (98%)	0.50	7 (11%) 4 3	32, 59, 84, 87	0
50	R6	49/54 (90%)	1.25	13 (26%) 0 0	84, 95, 102, 105	0
50	Y6	49/54 (90%)	1.24	10 (20%) 1 1	63, 74, 83, 88	0
51	R7	49/49 (100%)	0.04	2 (4%) 37 36	47, 52, 59, 70	0
51	Y7	49/49 (100%)	-0.08	2 (4%) 37 36	33, 36, 46, 55	0
52	R8	64/65 (98%)	0.33	3 (4%) 31 32	63, 72, 80, 92	0
52	Y8	64/65 (98%)	0.09	1 (1%) 72 71	40, 49, 57, 66	0
53	R9	37/37 (100%)	1.61	9 (24%) 0 0	83, 96, 106, 108	0
53	Y9	37/37 (100%)	0.74	3 (8%) 12 12	54, 61, 67, 71	0
54	QV	17/18 (94%)	1.36	3 (17%) 1 1	124, 139, 156, 157	0
54	XV	17/18 (94%)	1.22	3 (17%) 1 1	112, 131, 151, 152	0
All	All	20713/21318 (97%)	0.33	1566 (7%) 13 14	29, 88, 176, 279	0

The worst 5 of 1566 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	YA	2175	C	23.2
23	YA	2116	G	19.7
23	RA	1059	G	18.9
23	YA	2112	G	17.7
23	RA	2113	U	16.6



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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	1MG	QV	37	24/25	0.77	0.28	127,127,127,127	0
54	1MG	XV	37	24/25	0.80	0.30	117,117,117,117	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	XA	1644	1/1	-0.22	0.69	155,155,155,155	0
55	MG	XM	201	1/1	0.28	0.82	168,168,168,168	0
55	MG	QA	1662	1/1	0.29	0.48	118,118,118,118	0
55	MG	XA	1661	1/1	0.33	0.81	108,108,108,108	0
55	MG	QA	1619	1/1	0.36	1.15	146,146,146,146	0
55	MG	QA	1647	1/1	0.41	1.42	156,156,156,156	0
55	MG	XA	1665	1/1	0.44	0.52	70,70,70,70	0
55	MG	QA	1623	1/1	0.45	0.56	140,140,140,140	0
55	MG	QA	1631	1/1	0.47	1.54	124,124,124,124	0
55	MG	XA	1663	1/1	0.49	0.64	103,103,103,103	0
55	MG	XA	1652	1/1	0.49	0.60	101,101,101,101	0
55	MG	XA	1671	1/1	0.49	0.92	94,94,94,94	0
55	MG	XB	301	1/1	0.49	0.66	119,119,119,119	0
55	MG	QA	1651	1/1	0.51	0.40	81,81,81,81	0
55	MG	RA	3223	1/1	0.56	0.44	76,76,76,76	0
55	MG	XA	1636	1/1	0.56	0.31	165,165,165,165	0
55	MG	QA	1666	1/1	0.56	0.92	100,100,100,100	0
55	MG	XA	1629	1/1	0.57	0.46	129,129,129,129	0
55	MG	QA	1657	1/1	0.59	0.42	160,160,160,160	0
55	MG	XA	1648	1/1	0.60	0.52	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	XA	1660	1/1	0.61	0.71	66,66,66,66	0
55	MG	XL	201	1/1	0.61	0.56	97,97,97,97	0
55	MG	QA	1607	1/1	0.62	0.17	101,101,101,101	0
55	MG	XA	1628	1/1	0.64	0.27	66,66,66,66	0
55	MG	XA	1623	1/1	0.65	0.87	121,121,121,121	0
55	MG	QA	1629	1/1	0.66	0.95	80,80,80,80	0
55	MG	QA	1644	1/1	0.66	0.28	108,108,108,108	0
55	MG	XA	1662	1/1	0.67	0.65	85,85,85,85	0
55	MG	XA	1655	1/1	0.68	0.80	69,69,69,69	0
55	MG	YA	3143	1/1	0.69	0.58	43,43,43,43	0
55	MG	YA	3169	1/1	0.69	0.16	61,61,61,61	0
55	MG	YA	3122	1/1	0.69	1.05	40,40,40,40	0
55	MG	QM	201	1/1	0.69	0.23	170,170,170,170	0
55	MG	XA	1624	1/1	0.69	0.55	133,133,133,133	0
55	MG	QA	1609	1/1	0.70	0.39	104,104,104,104	0
55	MG	RA	3230	1/1	0.70	0.74	72,72,72,72	0
55	MG	YA	3198	1/1	0.71	0.55	29,29,29,29	0
55	MG	RA	3156	1/1	0.72	0.44	57,57,57,57	0
55	MG	XA	1651	1/1	0.72	0.37	89,89,89,89	0
55	MG	YA	3207	1/1	0.73	0.28	55,55,55,55	0
55	MG	RA	3184	1/1	0.73	0.57	54,54,54,54	0
55	MG	RA	3181	1/1	0.73	0.26	60,60,60,60	0
55	MG	YA	3250	1/1	0.74	0.38	40,40,40,40	0
55	MG	QA	1605	1/1	0.74	1.02	71,71,71,71	0
55	MG	RA	3204	1/1	0.74	0.18	61,61,61,61	0
55	MG	QA	1622	1/1	0.74	0.69	140,140,140,140	0
55	MG	XA	1637	1/1	0.75	0.29	85,85,85,85	0
55	MG	RA	3009	1/1	0.75	0.47	53,53,53,53	0
55	MG	YP	202	1/1	0.76	0.79	38,38,38,38	0
55	MG	RA	3117	1/1	0.76	0.27	43,43,43,43	0
55	MG	RA	3200	1/1	0.76	0.21	65,65,65,65	0
55	MG	RA	3174	1/1	0.76	0.17	75,75,75,75	0
55	MG	RA	3178	1/1	0.76	0.37	47,47,47,47	0
55	MG	XA	1634	1/1	0.77	1.29	154,154,154,154	0
55	MG	RA	3010	1/1	0.77	0.24	64,64,64,64	0
55	MG	RA	3228	1/1	0.77	0.37	69,69,69,69	0
55	MG	QA	1635	1/1	0.77	0.36	142,142,142,142	0
55	MG	RA	3225	1/1	0.77	0.52	61,61,61,61	0
55	MG	QA	1624	1/1	0.77	0.50	95,95,95,95	0
55	MG	QA	1661	1/1	0.78	0.88	103,103,103,103	0
55	MG	RA	3205	1/1	0.78	0.27	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	YA	3144	1/1	0.78	0.44	38,38,38,38	0
55	MG	QA	1639	1/1	0.78	1.07	103,103,103,103	0
55	MG	QA	1658	1/1	0.79	0.33	82,82,82,82	0
55	MG	XA	1669	1/1	0.79	0.38	73,73,73,73	0
55	MG	RA	3160	1/1	0.79	0.30	61,61,61,61	0
55	MG	XA	1609	1/1	0.79	0.34	66,66,66,66	0
55	MG	RA	3004	1/1	0.79	1.03	68,68,68,68	0
55	MG	QA	1663	1/1	0.79	0.17	105,105,105,105	0
55	MG	QA	1603	1/1	0.80	1.55	83,83,83,83	0
55	MG	RA	3185	1/1	0.80	0.48	75,75,75,75	0
55	MG	RA	3149	1/1	0.80	0.39	60,60,60,60	0
55	MG	YA	3135	1/1	0.81	0.14	48,48,48,48	0
55	MG	RA	3111	1/1	0.81	0.46	77,77,77,77	0
55	MG	QA	1618	1/1	0.81	0.68	95,95,95,95	0
55	MG	YA	3164	1/1	0.82	0.40	59,59,59,59	0
55	MG	RA	3176	1/1	0.82	0.29	63,63,63,63	0
55	MG	XA	1618	1/1	0.82	0.34	72,72,72,72	0
55	MG	XA	1666	1/1	0.82	0.73	85,85,85,85	0
55	MG	QA	1632	1/1	0.82	0.30	90,90,90,90	0
55	MG	XA	1664	1/1	0.82	0.75	166,166,166,166	0
55	MG	QA	1656	1/1	0.82	0.59	79,79,79,79	0
55	MG	RA	3224	1/1	0.82	0.34	61,61,61,61	0
55	MG	QA	1638	1/1	0.82	0.45	78,78,78,78	0
55	MG	XA	1608	1/1	0.83	0.27	105,105,105,105	0
55	MG	QA	1621	1/1	0.83	0.35	84,84,84,84	0
55	MG	RA	3199	1/1	0.83	0.28	70,70,70,70	0
55	MG	YA	3182	1/1	0.83	0.21	38,38,38,38	0
55	MG	RA	3202	1/1	0.83	0.52	53,53,53,53	0
55	MG	RA	3221	1/1	0.83	0.43	56,56,56,56	0
55	MG	RA	3168	1/1	0.83	0.28	59,59,59,59	0
55	MG	YA	3249	1/1	0.83	0.52	26,26,26,26	0
55	MG	XA	1643	1/1	0.84	0.79	125,125,125,125	0
55	MG	RA	3130	1/1	0.84	0.14	69,69,69,69	0
55	MG	RA	3142	1/1	0.84	0.32	72,72,72,72	0
55	MG	RA	3203	1/1	0.84	0.56	58,58,58,58	0
55	MG	YA	3126	1/1	0.84	0.81	61,61,61,61	0
55	MG	YB	203	1/1	0.84	0.37	45,45,45,45	0
55	MG	YA	3216	1/1	0.84	0.28	51,51,51,51	0
55	MG	YA	3223	1/1	0.84	0.21	55,55,55,55	0
55	MG	RA	3177	1/1	0.84	0.39	61,61,61,61	0
55	MG	YA	3158	1/1	0.84	0.31	43,43,43,43	0
55	MG	R3	101	1/1	0.84	0.48	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	XA	1633	1/1	0.84	0.34	72,72,72,72	0
55	MG	QA	1637	1/1	0.84	0.35	71,71,71,71	0
55	MG	RA	3118	1/1	0.84	0.29	55,55,55,55	0
55	MG	QA	1653	1/1	0.85	0.36	108,108,108,108	0
55	MG	YA	3214	1/1	0.85	0.35	42,42,42,42	0
55	MG	RA	3238	1/1	0.85	0.41	51,51,51,51	0
55	MG	RA	3211	1/1	0.85	0.28	67,67,67,67	0
55	MG	RA	3188	1/1	0.85	0.24	50,50,50,50	0
55	MG	RA	3167	1/1	0.85	0.19	56,56,56,56	0
55	MG	QA	1613	1/1	0.85	0.85	76,76,76,76	0
55	MG	YA	3059	1/1	0.85	0.35	50,50,50,50	0
55	MG	RA	3060	1/1	0.85	0.40	45,45,45,45	0
55	MG	RA	3210	1/1	0.85	0.17	85,85,85,85	0
55	MG	QA	1652	1/1	0.85	1.35	152,152,152,152	0
55	MG	RA	3063	1/1	0.86	0.29	91,91,91,91	0
55	MG	YA	3151	1/1	0.86	0.55	29,29,29,29	0
55	MG	QA	1665	1/1	0.86	0.85	93,93,93,93	0
55	MG	XA	1649	1/1	0.86	0.83	72,72,72,72	0
55	MG	XA	1606	1/1	0.86	0.41	68,68,68,68	0
55	MG	RA	3195	1/1	0.86	0.25	52,52,52,52	0
55	MG	RA	3147	1/1	0.86	0.25	49,49,49,49	0
55	MG	XA	1602	1/1	0.86	0.97	133,133,133,133	0
55	MG	RA	3103	1/1	0.86	0.17	58,58,58,58	0
55	MG	YA	3231	1/1	0.86	0.24	38,38,38,38	0
55	MG	RA	3182	1/1	0.86	0.32	49,49,49,49	0
55	MG	RE	302	1/1	0.86	0.26	42,42,42,42	0
55	MG	RA	3216	1/1	0.86	0.50	70,70,70,70	0
55	MG	RA	3150	1/1	0.86	0.36	63,63,63,63	0
55	MG	YA	3131	1/1	0.87	0.43	62,62,62,62	0
55	MG	YA	3242	1/1	0.87	0.25	49,49,49,49	0
55	MG	QA	1616	1/1	0.87	0.16	108,108,108,108	0
55	MG	RA	3193	1/1	0.87	0.46	77,77,77,77	0
55	MG	YX	101	1/1	0.87	0.22	53,53,53,53	0
55	MG	RA	3081	1/1	0.87	0.47	68,68,68,68	0
55	MG	YA	3106	1/1	0.87	0.36	40,40,40,40	0
55	MG	YA	3152	1/1	0.87	0.25	44,44,44,44	0
55	MG	RA	3165	1/1	0.87	0.23	80,80,80,80	0
55	MG	RA	3113	1/1	0.87	0.57	70,70,70,70	0
55	MG	YA	3021	1/1	0.87	0.27	28,28,28,28	0
55	MG	QA	1660	1/1	0.87	0.83	146,146,146,146	0
55	MG	YA	3217	1/1	0.87	0.18	39,39,39,39	0
55	MG	RA	3132	1/1	0.87	0.62	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	QA	1620	1/1	0.87	0.26	76,76,76,76	0
55	MG	RA	3217	1/1	0.88	0.43	78,78,78,78	0
55	MG	XA	1635	1/1	0.88	0.58	79,79,79,79	0
55	MG	QA	1626	1/1	0.88	0.13	102,102,102,102	0
55	MG	RA	3173	1/1	0.88	0.17	46,46,46,46	0
55	MG	RA	3187	1/1	0.88	0.30	59,59,59,59	0
55	MG	YA	3227	1/1	0.88	0.20	37,37,37,37	0
55	MG	YA	3190	1/1	0.88	0.24	43,43,43,43	0
55	MG	XA	1650	1/1	0.88	0.78	166,166,166,166	0
55	MG	XA	1639	1/1	0.88	0.68	66,66,66,66	0
55	MG	RA	3242	1/1	0.88	0.47	52,52,52,52	0
55	MG	XA	1631	1/1	0.88	0.44	63,63,63,63	0
55	MG	YA	3056	1/1	0.88	0.30	32,32,32,32	0
55	MG	YA	3235	1/1	0.88	0.51	60,60,60,60	0
56	ZN	QN	101	1/1	0.89	0.11	158,158,158,158	0
55	MG	YA	3194	1/1	0.89	0.51	44,44,44,44	0
55	MG	YA	3176	1/1	0.89	0.23	59,59,59,59	0
55	MG	RA	3158	1/1	0.89	0.27	51,51,51,51	0
55	MG	RA	3214	1/1	0.89	0.25	71,71,71,71	0
55	MG	R0	101	1/1	0.89	0.22	62,62,62,62	0
55	MG	RA	3101	1/1	0.89	0.36	46,46,46,46	0
56	ZN	XN	101	1/1	0.89	0.11	152,152,152,152	0
55	MG	YA	3159	1/1	0.89	0.33	36,36,36,36	0
55	MG	YA	3162	1/1	0.89	0.38	39,39,39,39	0
55	MG	XA	1641	1/1	0.89	0.72	146,146,146,146	0
55	MG	YA	3165	1/1	0.89	0.60	50,50,50,50	0
55	MG	XA	1627	1/1	0.89	0.25	63,63,63,63	0
55	MG	YA	3180	1/1	0.89	0.19	48,48,48,48	0
55	MG	YA	3171	1/1	0.89	0.17	48,48,48,48	0
55	MG	YA	3192	1/1	0.89	0.47	48,48,48,48	0
55	MG	YA	3228	1/1	0.89	0.18	41,41,41,41	0
55	MG	RA	3172	1/1	0.89	0.19	54,54,54,54	0
55	MG	RA	3028	1/1	0.89	0.59	73,73,73,73	0
55	MG	YA	3243	1/1	0.89	0.24	50,50,50,50	0
55	MG	RA	3051	1/1	0.89	0.49	52,52,52,52	0
55	MG	YA	3099	1/1	0.89	0.48	32,32,32,32	0
55	MG	YA	3200	1/1	0.89	0.26	37,37,37,37	0
55	MG	XA	1642	1/1	0.89	0.30	134,134,134,134	0
55	MG	RA	3110	1/1	0.90	0.15	50,50,50,50	0
55	MG	RA	3055	1/1	0.90	0.34	47,47,47,47	0
55	MG	YA	3184	1/1	0.90	0.28	53,53,53,53	0
55	MG	YA	3264	1/1	0.90	0.53	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	RA	3227	1/1	0.90	0.51	68,68,68,68	0
55	MG	XA	1607	1/1	0.90	0.17	86,86,86,86	0
55	MG	QA	1643	1/1	0.90	0.48	72,72,72,72	0
55	MG	XA	1668	1/1	0.90	0.15	91,91,91,91	0
55	MG	RA	3112	1/1	0.90	0.78	73,73,73,73	0
55	MG	RP	201	1/1	0.90	1.03	60,60,60,60	0
55	MG	RA	3179	1/1	0.90	0.24	45,45,45,45	0
55	MG	RD	301	1/1	0.90	0.31	47,47,47,47	0
55	MG	RA	3239	1/1	0.90	0.34	47,47,47,47	0
55	MG	QA	1601	1/1	0.90	0.45	88,88,88,88	0
55	MG	QA	1649	1/1	0.90	0.47	96,96,96,96	0
55	MG	QA	1615	1/1	0.90	0.44	70,70,70,70	0
55	MG	RA	3126	1/1	0.90	0.91	61,61,61,61	0
55	MG	YA	3113	1/1	0.90	0.33	31,31,31,31	0
55	MG	RA	3139	1/1	0.90	0.50	68,68,68,68	0
55	MG	RA	3229	1/1	0.90	0.14	61,61,61,61	0
55	MG	YA	3139	1/1	0.90	0.36	34,34,34,34	0
55	MG	XA	1604	1/1	0.90	0.98	75,75,75,75	0
55	MG	YA	3210	1/1	0.90	0.39	38,38,38,38	0
55	MG	RA	3135	1/1	0.90	0.21	45,45,45,45	0
55	MG	YA	3071	1/1	0.90	0.20	47,47,47,47	0
55	MG	YA	3156	1/1	0.90	0.50	51,51,51,51	0
55	MG	QA	1646	1/1	0.90	0.17	94,94,94,94	0
55	MG	QA	1627	1/1	0.90	0.18	87,87,87,87	0
55	MG	XA	1611	1/1	0.90	0.52	79,79,79,79	0
55	MG	YA	3153	1/1	0.90	0.34	54,54,54,54	0
55	MG	XA	1659	1/1	0.90	0.28	98,98,98,98	0
55	MG	XA	1658	1/1	0.91	0.21	88,88,88,88	0
55	MG	QA	1625	1/1	0.91	0.94	92,92,92,92	0
55	MG	QA	1611	1/1	0.91	0.53	67,67,67,67	0
55	MG	RA	3234	1/1	0.91	0.38	56,56,56,56	0
55	MG	YA	3004	1/1	0.91	0.31	30,30,30,30	0
55	MG	RA	3161	1/1	0.91	0.27	67,67,67,67	0
55	MG	XA	1647	1/1	0.91	0.28	101,101,101,101	0
55	MG	XA	1654	1/1	0.91	0.76	69,69,69,69	0
55	MG	RA	3114	1/1	0.91	0.28	76,76,76,76	0
55	MG	QA	1642	1/1	0.91	0.49	84,84,84,84	0
55	MG	QF	201	1/1	0.91	0.55	98,98,98,98	0
55	MG	RA	3226	1/1	0.91	0.24	62,62,62,62	0
55	MG	QA	1630	1/1	0.91	0.24	80,80,80,80	0
55	MG	QA	1602	1/1	0.91	0.78	74,74,74,74	0
55	MG	RA	3233	1/1	0.91	0.51	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	RA	3133	1/1	0.91	0.15	67,67,67,67	0
55	MG	YA	3155	1/1	0.91	0.55	58,58,58,58	0
55	MG	XA	1621	1/1	0.91	0.09	77,77,77,77	0
55	MG	RA	3219	1/1	0.91	0.62	79,79,79,79	0
55	MG	RA	3220	1/1	0.91	0.88	57,57,57,57	0
55	MG	YA	3065	1/1	0.91	0.27	43,43,43,43	0
55	MG	RA	3041	1/1	0.91	0.42	44,44,44,44	0
55	MG	RA	3026	1/1	0.91	0.27	45,45,45,45	0
55	MG	RA	3039	1/1	0.91	0.37	45,45,45,45	0
55	MG	YA	3258	1/1	0.91	0.40	42,42,42,42	0
55	MG	XA	1625	1/1	0.91	0.77	143,143,143,143	0
55	MG	RA	3191	1/1	0.91	0.29	72,72,72,72	0
55	MG	QA	1614	1/1	0.91	0.44	81,81,81,81	0
55	MG	RA	3106	1/1	0.91	0.31	46,46,46,46	0
55	MG	QA	1659	1/1	0.91	0.19	69,69,69,69	0
55	MG	RA	3215	1/1	0.91	0.27	52,52,52,52	0
55	MG	XA	1613	1/1	0.91	0.18	75,75,75,75	0
55	MG	YA	3202	1/1	0.91	0.09	44,44,44,44	0
55	MG	RA	3053	1/1	0.92	0.55	40,40,40,40	0
55	MG	RA	3020	1/1	0.92	0.35	42,42,42,42	0
55	MG	RA	3002	1/1	0.92	0.53	45,45,45,45	0
55	MG	RA	3092	1/1	0.92	0.52	50,50,50,50	0
55	MG	YA	3172	1/1	0.92	0.24	67,67,67,67	0
55	MG	YA	3263	1/1	0.92	0.32	48,48,48,48	0
55	MG	RA	3011	1/1	0.92	0.58	54,54,54,54	0
55	MG	YA	3115	1/1	0.92	0.27	35,35,35,35	0
55	MG	RA	3008	1/1	0.92	0.41	60,60,60,60	0
55	MG	RA	3090	1/1	0.92	0.73	47,47,47,47	0
55	MG	RA	3192	1/1	0.92	0.15	103,103,103,103	0
55	MG	RA	3122	1/1	0.92	0.71	65,65,65,65	0
55	MG	RA	3057	1/1	0.92	0.85	40,40,40,40	0
55	MG	QA	1664	1/1	0.92	0.11	111,111,111,111	0
55	MG	RB	202	1/1	0.92	0.14	123,123,123,123	0
55	MG	RA	3164	1/1	0.92	0.97	47,47,47,47	0
55	MG	XA	1622	1/1	0.92	0.23	130,130,130,130	0
55	MG	YA	3142	1/1	0.92	0.14	32,32,32,32	0
55	MG	RA	3052	1/1	0.92	0.34	54,54,54,54	0
55	MG	YA	3261	1/1	0.92	0.42	34,34,34,34	0
55	MG	RA	3213	1/1	0.92	0.08	61,61,61,61	0
55	MG	RA	3196	1/1	0.92	0.51	72,72,72,72	0
55	MG	YA	3234	1/1	0.92	0.34	66,66,66,66	0
55	MG	YA	3125	1/1	0.92	0.46	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	XA	1605	1/1	0.93	0.52	76,76,76,76	0
55	MG	YA	3038	1/1	0.93	0.21	32,32,32,32	0
55	MG	QA	1640	1/1	0.93	0.26	85,85,85,85	0
55	MG	XA	1614	1/1	0.93	0.57	54,54,54,54	0
55	MG	RA	3201	1/1	0.93	0.62	58,58,58,58	0
55	MG	YA	3187	1/1	0.93	0.28	41,41,41,41	0
55	MG	RA	3209	1/1	0.93	0.10	58,58,58,58	0
55	MG	RA	3197	1/1	0.93	0.13	67,67,67,67	0
55	MG	XA	1630	1/1	0.93	0.46	68,68,68,68	0
55	MG	RA	3145	1/1	0.93	0.52	56,56,56,56	0
55	MG	XA	1670	1/1	0.93	0.58	77,77,77,77	0
55	MG	YA	3074	1/1	0.93	0.28	38,38,38,38	0
55	MG	YA	3029	1/1	0.93	0.43	26,26,26,26	0
55	MG	YA	3052	1/1	0.93	0.31	33,33,33,33	0
55	MG	RA	3162	1/1	0.93	0.43	55,55,55,55	0
55	MG	XA	1667	1/1	0.93	0.21	127,127,127,127	0
55	MG	YA	3179	1/1	0.93	0.49	33,33,33,33	0
55	MG	YA	3247	1/1	0.93	0.18	39,39,39,39	0
55	MG	RA	3129	1/1	0.93	0.43	50,50,50,50	0
55	MG	YA	3177	1/1	0.93	0.20	45,45,45,45	0
55	MG	RA	3136	1/1	0.93	0.16	46,46,46,46	0
55	MG	YA	3149	1/1	0.93	0.28	40,40,40,40	0
55	MG	YA	3146	1/1	0.93	0.31	34,34,34,34	0
55	MG	XA	1619	1/1	0.93	0.46	76,76,76,76	0
55	MG	YA	3239	1/1	0.93	0.11	51,51,51,51	0
55	MG	RA	3208	1/1	0.93	0.23	73,73,73,73	0
55	MG	RA	3194	1/1	0.93	0.22	80,80,80,80	0
55	MG	YA	3112	1/1	0.93	0.45	44,44,44,44	0
55	MG	QA	1655	1/1	0.93	0.36	91,91,91,91	0
55	MG	RA	3046	1/1	0.93	0.48	42,42,42,42	0
55	MG	YA	3178	1/1	0.93	0.36	59,59,59,59	0
55	MG	YA	3236	1/1	0.93	0.14	53,53,53,53	0
55	MG	RA	3056	1/1	0.93	0.35	47,47,47,47	0
55	MG	RA	3089	1/1	0.93	0.65	55,55,55,55	0
55	MG	YA	3121	1/1	0.93	0.41	49,49,49,49	0
55	MG	RA	3044	1/1	0.93	0.34	49,49,49,49	0
55	MG	RA	3171	1/1	0.93	0.60	61,61,61,61	0
55	MG	RA	3071	1/1	0.93	0.52	49,49,49,49	0
55	MG	XA	1638	1/1	0.93	0.21	101,101,101,101	0
55	MG	RA	3099	1/1	0.94	0.67	40,40,40,40	0
55	MG	YA	3117	1/1	0.94	0.28	36,36,36,36	0
55	MG	RA	3091	1/1	0.94	0.67	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	RP	202	1/1	0.94	0.30	62,62,62,62	0
55	MG	XA	1646	1/1	0.94	0.40	52,52,52,52	0
55	MG	YA	3260	1/1	0.94	0.22	40,40,40,40	0
55	MG	RA	3218	1/1	0.94	0.29	68,68,68,68	0
55	MG	R8	101	1/1	0.94	0.36	57,57,57,57	0
55	MG	YB	202	1/1	0.94	0.33	49,49,49,49	0
55	MG	YA	3030	1/1	0.94	0.60	42,42,42,42	0
55	MG	RA	3222	1/1	0.94	0.34	53,53,53,53	0
55	MG	YA	3082	1/1	0.94	0.32	31,31,31,31	0
55	MG	YA	3157	1/1	0.94	0.43	45,45,45,45	0
55	MG	RA	3006	1/1	0.94	0.55	46,46,46,46	0
55	MG	YA	3108	1/1	0.94	0.31	28,28,28,28	0
55	MG	YA	3092	1/1	0.94	0.40	35,35,35,35	0
55	MG	RA	3231	1/1	0.94	0.24	54,54,54,54	0
55	MG	YA	3170	1/1	0.94	0.58	34,34,34,34	0
55	MG	YA	3133	1/1	0.94	0.59	49,49,49,49	0
55	MG	RA	3241	1/1	0.94	0.75	48,48,48,48	0
55	MG	YA	3047	1/1	0.94	0.35	30,30,30,30	0
55	MG	RA	3080	1/1	0.94	0.50	53,53,53,53	0
55	MG	YA	3241	1/1	0.94	0.52	47,47,47,47	0
55	MG	QA	1628	1/1	0.94	0.16	71,71,71,71	0
55	MG	YA	3266	1/1	0.94	0.49	39,39,39,39	0
55	MG	YA	3203	1/1	0.94	0.24	34,34,34,34	0
55	MG	RA	3035	1/1	0.94	0.48	49,49,49,49	0
55	MG	YA	3018	1/1	0.94	0.56	28,28,28,28	0
55	MG	RA	3127	1/1	0.94	0.52	77,77,77,77	0
55	MG	YA	3085	1/1	0.94	0.47	29,29,29,29	0
55	MG	YA	3116	1/1	0.94	0.29	44,44,44,44	0
55	MG	YA	3185	1/1	0.94	0.30	37,37,37,37	0
55	MG	YA	3238	1/1	0.94	0.25	36,36,36,36	0
55	MG	RA	3183	1/1	0.94	0.34	59,59,59,59	0
55	MG	XA	1626	1/1	0.94	0.21	53,53,53,53	0
55	MG	QA	1650	1/1	0.94	0.39	78,78,78,78	0
55	MG	YA	3132	1/1	0.94	0.12	60,60,60,60	0
55	MG	YA	3119	1/1	0.94	0.34	45,45,45,45	0
55	MG	YA	3253	1/1	0.94	0.25	35,35,35,35	0
55	MG	RA	3066	1/1	0.94	0.26	51,51,51,51	0
55	MG	RA	3151	1/1	0.94	0.22	56,56,56,56	0
55	MG	RA	3100	1/1	0.94	0.16	53,53,53,53	0
55	MG	RA	3159	1/1	0.94	0.56	54,54,54,54	0
55	MG	RA	3097	1/1	0.94	0.46	48,48,48,48	0
55	MG	RA	3140	1/1	0.94	0.40	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	QA	1634	1/1	0.94	0.59	69,69,69,69	0
55	MG	RA	3180	1/1	0.94	0.30	61,61,61,61	0
55	MG	RA	3058	1/1	0.94	0.51	52,52,52,52	0
55	MG	RA	3074	1/1	0.94	0.34	51,51,51,51	0
55	MG	YA	3221	1/1	0.94	0.21	53,53,53,53	0
55	MG	QA	1648	1/1	0.94	0.21	83,83,83,83	0
55	MG	YA	3226	1/1	0.94	0.39	40,40,40,40	0
55	MG	YA	3076	1/1	0.94	0.43	21,21,21,21	0
55	MG	RA	3243	1/1	0.94	0.33	51,51,51,51	0
55	MG	YA	3244	1/1	0.94	0.49	39,39,39,39	0
55	MG	YA	3077	1/1	0.94	0.23	32,32,32,32	0
55	MG	YA	3078	1/1	0.94	0.41	31,31,31,31	0
55	MG	RA	3189	1/1	0.94	0.21	58,58,58,58	0
55	MG	RA	3131	1/1	0.94	0.24	51,51,51,51	0
55	MG	YA	3006	1/1	0.94	0.53	36,36,36,36	0
55	MG	YA	3075	1/1	0.94	0.22	37,37,37,37	0
55	MG	RA	3138	1/1	0.94	0.39	44,44,44,44	0
55	MG	YA	3224	1/1	0.94	0.26	25,25,25,25	0
55	MG	RA	3084	1/1	0.94	0.58	56,56,56,56	0
55	MG	RA	3095	1/1	0.94	0.55	47,47,47,47	0
55	MG	RA	3025	1/1	0.94	0.32	43,43,43,43	0
55	MG	RA	3048	1/1	0.95	0.57	46,46,46,46	0
55	MG	QA	1604	1/1	0.95	0.62	74,74,74,74	0
55	MG	RA	3141	1/1	0.95	1.03	72,72,72,72	0
55	MG	RA	3137	1/1	0.95	0.43	46,46,46,46	0
55	MG	YA	3015	1/1	0.95	0.17	28,28,28,28	0
55	MG	YA	3145	1/1	0.95	0.26	44,44,44,44	0
55	MG	YA	3068	1/1	0.95	0.54	45,45,45,45	0
55	MG	YA	3240	1/1	0.95	0.30	40,40,40,40	0
55	MG	RA	3152	1/1	0.95	0.68	62,62,62,62	0
55	MG	RA	3001	1/1	0.95	0.69	58,58,58,58	0
55	MG	RA	3128	1/1	0.95	0.29	53,53,53,53	0
55	MG	YA	3023	1/1	0.95	0.54	27,27,27,27	0
55	MG	RA	3007	1/1	0.95	0.81	39,39,39,39	0
55	MG	YA	3233	1/1	0.95	0.45	42,42,42,42	0
55	MG	RA	3175	1/1	0.95	0.41	48,48,48,48	0
55	MG	QA	1617	1/1	0.95	0.34	98,98,98,98	0
55	MG	RA	3134	1/1	0.95	0.27	52,52,52,52	0
55	MG	RA	3032	1/1	0.95	0.35	47,47,47,47	0
55	MG	YA	3041	1/1	0.95	0.29	30,30,30,30	0
55	MG	QA	1645	1/1	0.95	0.25	70,70,70,70	0
55	MG	RA	3232	1/1	0.95	0.71	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	YA	3097	1/1	0.95	0.32	35,35,35,35	0
55	MG	RA	3143	1/1	0.95	0.12	51,51,51,51	0
55	MG	RA	3169	1/1	0.95	0.41	50,50,50,50	0
55	MG	XA	1616	1/1	0.95	0.48	68,68,68,68	0
55	MG	RA	3237	1/1	0.95	0.58	56,56,56,56	0
55	MG	YA	3129	1/1	0.95	0.31	44,44,44,44	0
55	MG	YA	3033	1/1	0.95	0.36	31,31,31,31	0
55	MG	QA	1606	1/1	0.95	0.26	89,89,89,89	0
55	MG	YA	3195	1/1	0.95	0.22	54,54,54,54	0
55	MG	YA	3218	1/1	0.95	0.46	38,38,38,38	0
55	MG	YA	3138	1/1	0.95	0.17	39,39,39,39	0
55	MG	YA	3206	1/1	0.95	0.42	45,45,45,45	0
55	MG	QA	1636	1/1	0.95	0.26	87,87,87,87	0
55	MG	YA	3181	1/1	0.95	0.38	32,32,32,32	0
55	MG	RA	3088	1/1	0.95	0.52	42,42,42,42	0
55	MG	YA	3134	1/1	0.95	0.22	42,42,42,42	0
55	MG	YA	3237	1/1	0.95	0.20	34,34,34,34	0
55	MG	QA	1641	1/1	0.95	0.47	87,87,87,87	0
55	MG	RA	3119	1/1	0.95	0.46	70,70,70,70	0
55	MG	YA	3048	1/1	0.95	0.34	36,36,36,36	0
55	MG	RA	3102	1/1	0.95	0.23	51,51,51,51	0
55	MG	YA	3026	1/1	0.95	0.66	59,59,59,59	0
55	MG	YA	3094	1/1	0.95	0.55	39,39,39,39	0
55	MG	YA	3007	1/1	0.95	0.41	28,28,28,28	0
55	MG	QA	1610	1/1	0.95	0.38	75,75,75,75	0
55	MG	RA	3073	1/1	0.95	0.28	51,51,51,51	0
55	MG	YA	3229	1/1	0.95	0.50	38,38,38,38	0
55	MG	YA	3186	1/1	0.95	0.20	65,65,65,65	0
55	MG	RA	3034	1/1	0.95	0.63	38,38,38,38	0
55	MG	YA	3070	1/1	0.95	0.10	36,36,36,36	0
55	MG	YA	3205	1/1	0.95	0.22	40,40,40,40	0
55	MG	RA	3061	1/1	0.95	0.45	42,42,42,42	0
55	MG	RA	3236	1/1	0.95	0.52	49,49,49,49	0
55	MG	XA	1617	1/1	0.95	0.51	60,60,60,60	0
55	MG	RA	3036	1/1	0.95	0.62	47,47,47,47	0
55	MG	YB	204	1/1	0.95	0.18	71,71,71,71	0
55	MG	YA	3054	1/1	0.95	0.28	41,41,41,41	0
55	MG	YA	3201	1/1	0.95	0.12	46,46,46,46	0
55	MG	QA	1608	1/1	0.95	0.30	91,91,91,91	0
55	MG	YA	3034	1/1	0.95	0.43	31,31,31,31	0
55	MG	YA	3222	1/1	0.95	0.27	56,56,56,56	0
55	MG	YA	3014	1/1	0.95	0.59	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	XA	1657	1/1	0.95	0.33	78,78,78,78	0
55	MG	YA	3150	1/1	0.95	0.14	61,61,61,61	0
55	MG	R5	101	1/1	0.95	0.42	45,45,45,45	0
55	MG	YA	3104	1/1	0.95	0.47	30,30,30,30	0
55	MG	YA	3215	1/1	0.95	0.24	40,40,40,40	0
55	MG	YD	301	1/1	0.95	0.59	34,34,34,34	0
55	MG	YA	3101	1/1	0.95	0.60	38,38,38,38	0
55	MG	RA	3235	1/1	0.95	0.59	53,53,53,53	0
55	MG	YA	3013	1/1	0.95	0.55	27,27,27,27	0
55	MG	YA	3160	1/1	0.95	0.27	37,37,37,37	0
55	MG	YA	3248	1/1	0.96	0.33	42,42,42,42	0
55	MG	YA	3137	1/1	0.96	0.37	41,41,41,41	0
55	MG	YA	3057	1/1	0.96	0.69	38,38,38,38	0
55	MG	YA	3069	1/1	0.96	0.37	34,34,34,34	0
55	MG	RA	3155	1/1	0.96	0.15	60,60,60,60	0
55	MG	YA	3095	1/1	0.96	0.39	40,40,40,40	0
55	MG	YA	3089	1/1	0.96	0.50	28,28,28,28	0
55	MG	RA	3005	1/1	0.96	0.58	35,35,35,35	0
55	MG	YA	3130	1/1	0.96	0.24	31,31,31,31	0
55	MG	RA	3027	1/1	0.96	0.61	44,44,44,44	0
55	MG	YA	3002	1/1	0.96	0.53	30,30,30,30	0
55	MG	RA	3014	1/1	0.96	0.41	39,39,39,39	0
55	MG	YA	3140	1/1	0.96	0.42	38,38,38,38	0
55	MG	RA	3096	1/1	0.96	0.54	39,39,39,39	0
55	MG	YA	3166	1/1	0.96	0.18	41,41,41,41	0
55	MG	XA	1632	1/1	0.96	0.38	96,96,96,96	0
55	MG	RA	3085	1/1	0.96	0.30	49,49,49,49	0
55	MG	RA	3115	1/1	0.96	0.21	45,45,45,45	0
55	MG	RA	3186	1/1	0.96	0.59	78,78,78,78	0
55	MG	RA	3078	1/1	0.96	0.49	43,43,43,43	0
55	MG	YA	3168	1/1	0.96	0.32	38,38,38,38	0
55	MG	YA	3183	1/1	0.96	0.34	53,53,53,53	0
55	MG	YA	3105	1/1	0.96	0.40	32,32,32,32	0
55	MG	YA	3043	1/1	0.96	0.46	32,32,32,32	0
55	MG	RF	301	1/1	0.96	0.49	84,84,84,84	0
55	MG	RA	3240	1/1	0.96	0.19	51,51,51,51	0
55	MG	XA	1645	1/1	0.96	0.41	92,92,92,92	0
55	MG	YA	3255	1/1	0.96	0.41	30,30,30,30	0
55	MG	RA	3146	1/1	0.96	0.41	69,69,69,69	0
55	MG	XA	1603	1/1	0.96	0.51	49,49,49,49	0
56	ZN	QD	301	1/1	0.96	0.19	116,116,116,116	0
55	MG	YA	3019	1/1	0.96	0.65	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	YA	3090	1/1	0.96	0.33	39,39,39,39	0
55	MG	RA	3075	1/1	0.96	0.24	62,62,62,62	0
55	MG	YA	3103	1/1	0.96	0.40	24,24,24,24	0
55	MG	YA	3259	1/1	0.96	0.44	32,32,32,32	0
55	MG	RA	3023	1/1	0.96	0.67	45,45,45,45	0
55	MG	RA	3047	1/1	0.96	0.35	52,52,52,52	0
55	MG	YA	3173	1/1	0.96	0.12	45,45,45,45	0
55	MG	RA	3003	1/1	0.96	0.89	47,47,47,47	0
55	MG	RA	3029	1/1	0.96	0.35	50,50,50,50	0
55	MG	RA	3108	1/1	0.96	0.23	49,49,49,49	0
55	MG	XA	1601	1/1	0.96	0.60	55,55,55,55	0
55	MG	YA	3147	1/1	0.96	0.19	36,36,36,36	0
55	MG	YA	3039	1/1	0.96	0.35	30,30,30,30	0
55	MG	RA	3121	1/1	0.96	0.41	55,55,55,55	0
55	MG	YA	3040	1/1	0.96	0.43	25,25,25,25	0
55	MG	YA	3093	1/1	0.96	0.48	26,26,26,26	0
55	MG	YA	3197	1/1	0.96	0.50	36,36,36,36	0
55	MG	RA	3012	1/1	0.96	0.32	42,42,42,42	0
55	MG	RA	3166	1/1	0.96	0.28	54,54,54,54	0
55	MG	RA	3093	1/1	0.96	0.51	46,46,46,46	0
55	MG	RA	3154	1/1	0.96	0.30	65,65,65,65	0
55	MG	YA	3204	1/1	0.96	0.20	43,43,43,43	0
55	MG	XA	1610	1/1	0.96	0.36	63,63,63,63	0
55	MG	YA	3098	1/1	0.96	0.37	29,29,29,29	0
55	MG	XA	1620	1/1	0.96	0.69	68,68,68,68	0
55	MG	RA	3018	1/1	0.96	0.24	50,50,50,50	0
55	MG	YE	301	1/1	0.96	0.28	32,32,32,32	0
55	MG	RA	3124	1/1	0.96	0.41	56,56,56,56	0
55	MG	YA	3188	1/1	0.96	0.16	43,43,43,43	0
55	MG	RA	3163	1/1	0.96	0.19	62,62,62,62	0
55	MG	YA	3208	1/1	0.96	0.23	36,36,36,36	0
55	MG	RA	3076	1/1	0.96	0.31	42,42,42,42	0
55	MG	RR	201	1/1	0.96	0.32	52,52,52,52	0
55	MG	RA	3104	1/1	0.96	0.38	43,43,43,43	0
55	MG	RA	3072	1/1	0.96	0.39	61,61,61,61	0
55	MG	YA	3001	1/1	0.96	0.48	27,27,27,27	0
55	MG	RA	3042	1/1	0.96	0.60	46,46,46,46	0
55	MG	YB	201	1/1	0.96	0.17	63,63,63,63	0
55	MG	RA	3094	1/1	0.96	0.42	45,45,45,45	0
55	MG	RA	3148	1/1	0.96	0.52	55,55,55,55	0
55	MG	RA	3070	1/1	0.97	0.21	56,56,56,56	0
55	MG	YA	3136	1/1	0.97	0.34	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	XA	1653	1/1	0.97	0.82	91,91,91,91	0
55	MG	YA	3254	1/1	0.97	0.48	35,35,35,35	0
55	MG	RA	3086	1/1	0.97	0.33	49,49,49,49	0
55	MG	YA	3042	1/1	0.97	0.29	35,35,35,35	0
55	MG	YA	3265	1/1	0.97	0.34	35,35,35,35	0
55	MG	RA	3017	1/1	0.97	0.52	44,44,44,44	0
55	MG	QA	1612	1/1	0.97	0.58	62,62,62,62	0
55	MG	RA	3049	1/1	0.97	0.66	41,41,41,41	0
55	MG	RA	3212	1/1	0.97	0.26	55,55,55,55	0
55	MG	RA	3040	1/1	0.97	0.33	45,45,45,45	0
55	MG	YA	3045	1/1	0.97	0.54	29,29,29,29	0
55	MG	YA	3046	1/1	0.97	0.48	24,24,24,24	0
55	MG	RA	3050	1/1	0.97	0.50	47,47,47,47	0
55	MG	YA	3245	1/1	0.97	0.16	39,39,39,39	0
55	MG	RA	3077	1/1	0.97	0.49	46,46,46,46	0
55	MG	YA	3079	1/1	0.97	0.34	34,34,34,34	0
55	MG	YA	3191	1/1	0.97	0.38	42,42,42,42	0
55	MG	RA	3107	1/1	0.97	0.31	52,52,52,52	0
55	MG	RA	3079	1/1	0.97	0.41	60,60,60,60	0
55	MG	YA	3154	1/1	0.97	0.13	31,31,31,31	0
55	MG	RA	3190	1/1	0.97	0.50	64,64,64,64	0
55	MG	RA	3030	1/1	0.97	0.55	41,41,41,41	0
55	MG	RA	3065	1/1	0.97	0.65	47,47,47,47	0
55	MG	YA	3003	1/1	0.97	0.32	29,29,29,29	0
55	MG	YA	3096	1/1	0.97	0.29	30,30,30,30	0
55	MG	YA	3110	1/1	0.97	0.36	54,54,54,54	0
55	MG	YA	3084	1/1	0.97	0.24	29,29,29,29	0
55	MG	RA	3083	1/1	0.97	0.46	44,44,44,44	0
55	MG	YA	3124	1/1	0.97	0.42	27,27,27,27	0
55	MG	YA	3267	1/1	0.97	0.43	37,37,37,37	0
55	MG	YA	3109	1/1	0.97	0.28	33,33,33,33	0
55	MG	RA	3033	1/1	0.97	0.55	61,61,61,61	0
55	MG	RA	3198	1/1	0.97	0.23	49,49,49,49	0
55	MG	YA	3114	1/1	0.97	0.39	38,38,38,38	0
55	MG	YA	3196	1/1	0.97	0.20	52,52,52,52	0
56	ZN	XD	301	1/1	0.97	0.30	99,99,99,99	0
55	MG	YA	3220	1/1	0.97	0.27	37,37,37,37	0
55	MG	YA	3005	1/1	0.97	0.29	37,37,37,37	0
55	MG	YA	3167	1/1	0.97	0.23	52,52,52,52	0
55	MG	QA	1633	1/1	0.97	0.08	110,110,110,110	0
55	MG	YA	3209	1/1	0.97	0.24	38,38,38,38	0
55	MG	YA	3009	1/1	0.97	0.68	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	RA	3031	1/1	0.97	0.38	44,44,44,44	0
55	MG	RA	3087	1/1	0.97	0.39	75,75,75,75	0
55	MG	YA	3123	1/1	0.97	0.25	36,36,36,36	0
55	MG	YA	3212	1/1	0.97	0.26	40,40,40,40	0
55	MG	YA	3062	1/1	0.97	0.37	30,30,30,30	0
55	MG	YA	3083	1/1	0.97	0.60	35,35,35,35	0
55	MG	YA	3141	1/1	0.97	0.49	31,31,31,31	0
55	MG	YA	3032	1/1	0.97	0.46	39,39,39,39	0
55	MG	YA	3189	1/1	0.97	0.20	47,47,47,47	0
55	MG	YA	3022	1/1	0.97	0.53	30,30,30,30	0
55	MG	YA	3060	1/1	0.97	0.34	39,39,39,39	0
55	MG	YA	3073	1/1	0.97	0.53	35,35,35,35	0
55	MG	RA	3144	1/1	0.97	0.57	45,45,45,45	0
55	MG	RA	3021	1/1	0.97	0.62	44,44,44,44	0
55	MG	RA	3067	1/1	0.97	0.52	43,43,43,43	0
55	MG	RA	3125	1/1	0.97	0.41	75,75,75,75	0
55	MG	XA	1615	1/1	0.97	0.51	56,56,56,56	0
55	MG	YA	3120	1/1	0.97	0.41	29,29,29,29	0
55	MG	YA	3066	1/1	0.97	0.48	34,34,34,34	0
55	MG	RA	3022	1/1	0.97	0.40	42,42,42,42	0
55	MG	YA	3232	1/1	0.97	0.10	45,45,45,45	0
55	MG	RA	3120	1/1	0.97	0.41	48,48,48,48	0
55	MG	YA	3025	1/1	0.97	0.58	24,24,24,24	0
55	MG	YA	3163	1/1	0.97	0.31	43,43,43,43	0
55	MG	YA	3049	1/1	0.97	0.49	37,37,37,37	0
55	MG	YA	3102	1/1	0.97	0.35	52,52,52,52	0
55	MG	RA	3043	1/1	0.97	0.50	42,42,42,42	0
55	MG	RB	201	1/1	0.97	0.17	125,125,125,125	0
55	MG	YA	3008	1/1	0.98	0.39	36,36,36,36	0
55	MG	RA	3082	1/1	0.98	0.85	72,72,72,72	0
55	MG	RA	3024	1/1	0.98	0.43	50,50,50,50	0
55	MG	Y5	101	1/1	0.98	0.27	33,33,33,33	0
55	MG	QA	1654	1/1	0.98	0.10	98,98,98,98	0
55	MG	YP	201	1/1	0.98	0.10	56,56,56,56	0
55	MG	YA	3161	1/1	0.98	0.33	47,47,47,47	0
55	MG	RE	301	1/1	0.98	0.28	37,37,37,37	0
55	MG	YA	3257	1/1	0.98	0.53	28,28,28,28	0
55	MG	YA	3086	1/1	0.98	0.47	30,30,30,30	0
55	MG	YA	3017	1/1	0.98	0.54	31,31,31,31	0
55	MG	RA	3098	1/1	0.98	0.51	43,43,43,43	0
55	MG	RA	3062	1/1	0.98	0.35	41,41,41,41	0
55	MG	YA	3091	1/1	0.98	0.42	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	YA	3055	1/1	0.98	0.38	31,31,31,31	0
55	MG	YA	3020	1/1	0.98	0.45	26,26,26,26	0
55	MG	YA	3011	1/1	0.98	0.37	27,27,27,27	0
55	MG	XA	1640	1/1	0.98	0.39	56,56,56,56	0
55	MG	RA	3206	1/1	0.98	0.47	46,46,46,46	0
55	MG	YA	3053	1/1	0.98	0.32	25,25,25,25	0
55	MG	YA	3100	1/1	0.98	0.48	26,26,26,26	0
55	MG	YA	3225	1/1	0.98	0.36	27,27,27,27	0
55	MG	YA	3051	1/1	0.98	0.32	32,32,32,32	0
55	MG	YA	3199	1/1	0.98	0.37	44,44,44,44	0
55	MG	RA	3157	1/1	0.98	0.33	43,43,43,43	0
55	MG	YA	3219	1/1	0.98	0.37	52,52,52,52	0
55	MG	YA	3036	1/1	0.98	0.36	32,32,32,32	0
55	MG	YA	3174	1/1	0.98	0.36	47,47,47,47	0
55	MG	YA	3211	1/1	0.98	0.23	29,29,29,29	0
55	MG	YA	3128	1/1	0.98	0.38	42,42,42,42	0
55	MG	YA	3016	1/1	0.98	0.38	30,30,30,30	0
55	MG	YA	3230	1/1	0.98	0.15	39,39,39,39	0
55	MG	XA	1656	1/1	0.98	0.64	67,67,67,67	0
55	MG	RA	3064	1/1	0.98	0.65	32,32,32,32	0
55	MG	RA	3016	1/1	0.98	0.65	41,41,41,41	0
55	MG	YA	3063	1/1	0.98	0.41	35,35,35,35	0
55	MG	YD	302	1/1	0.98	0.20	30,30,30,30	0
55	MG	RA	3105	1/1	0.98	0.32	50,50,50,50	0
55	MG	YA	3246	1/1	0.98	0.51	32,32,32,32	0
55	MG	YA	3087	1/1	0.98	0.36	39,39,39,39	0
55	MG	YA	3107	1/1	0.98	0.50	32,32,32,32	0
55	MG	YA	3010	1/1	0.98	0.46	35,35,35,35	0
55	MG	QH	201	1/1	0.98	0.49	92,92,92,92	0
55	MG	RA	3045	1/1	0.98	0.44	61,61,61,61	0
55	MG	XA	1612	1/1	0.98	0.33	75,75,75,75	0
55	MG	YA	3252	1/1	0.98	0.51	23,23,23,23	0
55	MG	YA	3035	1/1	0.98	0.46	26,26,26,26	0
55	MG	RA	3116	1/1	0.98	0.58	53,53,53,53	0
55	MG	RA	3037	1/1	0.98	0.42	41,41,41,41	0
55	MG	YA	3127	1/1	0.98	0.49	32,32,32,32	0
55	MG	YA	3072	1/1	0.98	0.20	55,55,55,55	0
55	MG	RA	3019	1/1	0.98	0.41	40,40,40,40	0
55	MG	YA	3262	1/1	0.98	0.39	27,27,27,27	0
55	MG	YA	3193	1/1	0.98	0.23	39,39,39,39	0
55	MG	YA	3044	1/1	0.98	0.31	28,28,28,28	0
55	MG	RA	3015	1/1	0.98	0.38	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	YA	3148	1/1	0.98	0.30	32,32,32,32	0
55	MG	YA	3081	1/1	0.98	0.50	26,26,26,26	0
55	MG	YA	3028	1/1	0.98	0.21	29,29,29,29	0
55	MG	RA	3054	1/1	0.98	0.36	44,44,44,44	0
55	MG	YA	3050	1/1	0.98	0.46	27,27,27,27	0
55	MG	RA	3153	1/1	0.98	0.37	79,79,79,79	0
55	MG	YA	3027	1/1	0.98	0.29	32,32,32,32	0
55	MG	YA	3064	1/1	0.98	0.33	38,38,38,38	0
55	MG	YA	3037	1/1	0.98	0.45	25,25,25,25	0
55	MG	YA	3118	1/1	0.98	0.47	33,33,33,33	0
55	MG	RA	3170	1/1	0.98	0.16	66,66,66,66	0
55	MG	YA	3111	1/1	0.99	0.15	38,38,38,38	0
55	MG	YA	3031	1/1	0.99	0.61	33,33,33,33	0
55	MG	RA	3069	1/1	0.99	0.57	56,56,56,56	0
55	MG	RA	3109	1/1	0.99	0.25	48,48,48,48	0
55	MG	RA	3059	1/1	0.99	0.36	43,43,43,43	0
55	MG	YA	3080	1/1	0.99	0.49	28,28,28,28	0
55	MG	YA	3012	1/1	0.99	0.58	20,20,20,20	0
55	MG	YA	3256	1/1	0.99	0.54	28,28,28,28	0
55	MG	RA	3068	1/1	0.99	0.47	44,44,44,44	0
55	MG	RA	3038	1/1	0.99	0.42	39,39,39,39	0
55	MG	RA	3123	1/1	0.99	0.45	63,63,63,63	0
55	MG	YA	3067	1/1	0.99	0.33	37,37,37,37	0
55	MG	YA	3058	1/1	0.99	0.47	29,29,29,29	0
55	MG	YA	3061	1/1	0.99	0.33	35,35,35,35	0
55	MG	YA	3024	1/1	0.99	0.46	36,36,36,36	0
55	MG	YA	3175	1/1	0.99	0.41	30,30,30,30	0
55	MG	YA	3088	1/1	0.99	0.41	34,34,34,34	0
55	MG	YA	3213	1/1	0.99	0.21	37,37,37,37	0
55	MG	YA	3251	1/1	0.99	0.52	31,31,31,31	0
55	MG	RA	3013	1/1	0.99	0.23	47,47,47,47	0
55	MG	RA	3207	1/1	1.00	0.23	48,48,48,48	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.