wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 7, 2023 – 09:29 AM EST

PDB ID	:	5J3C
Title	:	Thermus thermophilus 70S termination complex containing E. coli RF1
Authors	:	Hoffer, E.D.; Dunham, C.M.
Deposited on	:	2016-03-30
Resolution	:	3.04 Å(reported)

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

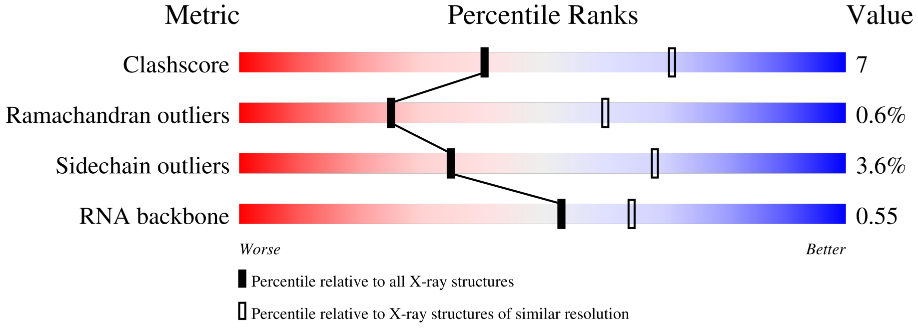
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.04 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))
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RNA backbone	3102	1034 (3.30-2.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	RA	2915	
1	YA	2915	
2	RB	122	
2	YB	122	
3	RD	276	
3	YD	276	

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Mol	Chain	Length	Quality of chain
4	RE	206	
4	YE	206	
5	RF	210	
5	YF	210	
6	RG	182	
6	YG	182	
7	RH	180	
7	YH	180	
8	RI	148	
8	YI	148	
9	RN	140	
9	YN	140	
10	RO	122	
10	YO	122	
11	RP	150	
11	YP	150	
12	RQ	141	
12	YQ	141	
13	RR	118	
13	YR	118	
14	RS	112	
14	YS	112	
15	RT	146	
15	YT	146	
16	RU	118	

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Mol	Chain	Length	Quality of chain
16	YU	118	83% 15% •
17	RV	101	83% 15% •
17	YV	101	79% 19% ••
18	RW	113	84% 14% ••
18	YW	113	81% 18% ••
19	RX	96	76% 23% •
19	YX	96	88% 11% •
20	RY	110	76% 20% • •
20	YY	110	75% 21% • •
21	RZ	206	83% 14% ••
21	YZ	206	85% 12% •
22	R0	85	74% 14% • 9%
22	Y0	85	73% 16% • 9%
23	R1	98	81% 17% ••
23	Y1	98	76% 21% • •
24	R2	72	75% 22% •
24	Y2	72	79% 18% •
25	R3	60	87% 12% •
25	Y3	60	78% 18% • •
26	R4	71	58% 35% • • •
26	Y4	71	63% 30% • • •
27	R5	60	73% 22% • •
27	Y5	60	83% 13% • •
28	R6	54	76% 22% •
28	Y6	54	80% 19% •

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Mol	Chain	Length	Quality of chain
29	R7	49	
29	Y7	49	
30	R8	65	
30	Y8	65	
31	R9	37	
31	Y9	37	
32	QA	1521	
32	XA	1521	
33	QB	256	
33	XB	256	
34	QC	239	
34	XC	239	
35	QD	209	
35	XD	209	
36	QE	162	
36	XE	162	
37	QF	101	
37	XF	101	
38	QG	156	
38	XG	156	
39	QH	138	
39	XH	138	
40	QI	128	
40	XI	128	
41	QJ	105	

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Mol	Chain	Length	Quality of chain
41	XJ	105	 68% 24% 9%
42	QK	129	 72% 16% 12%
42	XK	129	 71% 15% • 12%
43	QL	132	 77% 16% 8%
43	XL	132	 70% 20% •• 8%
44	QM	126	 70% 21% • 8%
44	XM	126	 62% 27% • 10%
45	QN	61	 77% 20% • •
45	XN	61	 77% 20% • •
46	QO	89	 78% 20% ••
46	XO	89	 79% 19% ••
47	QP	88	 67% 23% • 7%
47	XP	88	 63% 27% • 7%
48	QQ	105	 84% 10% • 6%
48	XQ	105	 83% 11% 6%
49	QR	88	 64% 13% • 23%
49	XR	88	 64% 13% • 23%
50	QS	93	 67% 18% • 11%
50	XS	93	 72% 17% 11%
51	QT	106	 68% 21% • 9%
51	XT	106	 74% 17% •• 8%
52	QU	27	 70% 15% 15%
52	XU	27	 74% 11% 15%
53	QV	77	 62% 32% 5%
53	XV	77	 64% 26% 9% •

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Mol	Chain	Length	Quality of chain
54	QX	25	
54	XX	25	
55	QY	360	
55	XY	360	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 294929 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	RA	2867	61758	27491	11552	19850	2865	0	0	0
1	YA	2867	61758	27491	11552	19850	2865	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	RB	120	2572	1145	476	832	119	0	0	0
2	YB	120	2573	1146	476	832	119	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	RD	275	2131	1346	422	360	3	0	0	0
3	YD	275	2136	1349	423	361	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	RE	204	1559	985	298	270	6	0	0	0
4	YE	204	1559	985	298	270	6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	RF	203	Total 1584	C 1009	N 298	O 275	S 2	0	0	1
5	YF	203	Total 1580	C 1007	N 297	O 274	S 2	0	0	1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	RG	181	Total 1426	C 916	N 253	O 253	S 4	0	0	0
6	YG	181	Total 1424	C 912	N 259	O 249	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	RH	174	Total 1330	C 845	N 248	O 236	S 1	0	0	0
7	YH	173	Total 1324	C 842	N 247	O 234	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	RI	147	Total 1094	C 699	N 191	O 203	S 1	0	0	0
8	YI	146	Total 1076	C 687	N 186	O 202	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	RN	140	Total 1121	C 722	N 208	O 187	S 4	0	0	0
9	YN	140	Total 1117	C 719	N 207	O 187	S 4	0	0	0

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	RP	149	1135	706	230	196	3	0	0	0
			Total	C	N	O	S			
11	YP	149	1135	706	230	196	3	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	RS	110	877	553	175	149	0	0	0
			Total	C	N	O			
14	YS	110	870	549	173	148	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	RT	131	1091	680	225	185	1	0	0	0
			Total	C	N	O	S			
15	YT	131	1083	675	224	183	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	RU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	YU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	RV	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
17	YV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	RW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
18	YW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	RX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	YX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	RY	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
20	YY	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	RZ	203	Total C N O S 1587 1011 282 292 2	0	0	0
21	YZ	201	Total C N O S 1557 995 274 286 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	R0	77	Total C N O S 608 375 129 103 1	0	0	0
22	Y0	77	Total C N O S 608 375 129 103 1	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	R1	97	Total C N O S 754 475 148 130 1	0	0	0
23	Y1	97	Total C N O S 759 478 149 131 1	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	R2	70	Total C N O S 588 365 118 103 2	0	0	0
24	Y2	70	Total C N O S 592 368 119 103 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	R3	59	Total C N O 469 298 90 81	0	0	0
25	Y3	59	Total C N O 464 296 90 78	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	R4	69	Total C N O S 546 346 96 99 5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y4	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	Y5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	Y6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	QA	1500	Total 32246	C 14358	N 5975	O 10413	P 1500	0	0	0
32	XA	1504	Total 32331	C 14396	N 5990	O 10441	P 1504	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	QB	231	Total 1842	C 1175	N 330	O 332	S 5	0	0	0
33	XB	231	Total 1825	C 1167	N 326	O 327	S 5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	QC	206	Total 1558	C 979	N 305	O 273	S 1	0	0	0
34	XC	206	Total 1542	C 968	N 300	O 273	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	QD	208	Total 1665	C 1043	N 329	O 286	S 7	0	0	0
35	XD	208	Total 1668	C 1047	N 330	O 284	S 7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	QE	148	Total 1133	C 716	N 214	O 199	S 4	0	0	0
36	XE	148	Total 1133	C 716	N 214	O 199	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	QF	100	Total 814	C 516	N 144	O 151	S 3	0	0	0
37	XF	100	Total 816	C 516	N 146	O 151	S 3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	QG	155	Total 1235	C 769	N 244	O 216	S 6	0	0	0
38	XG	155	Total 1229	C 766	N 241	O 216	S 6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	QH	137	Total 1098	C 694	N 210	O 192	S 2	0	0	0
39	XH	137	Total 1088	C 689	N 206	O 191	S 2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	QI	127	Total 986	C 625	N 193	O 168	0	0	0
40	XI	126	Total 966	C 613	N 186	O 167	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	QJ	97	Total 719	C 446	N 142	O 131	0	0	0
41	XJ	96	Total 710	C 442	N 137	O 131	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	QK	114	Total 834	C 520	N 156	O 155	S 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	XK	114	Total 833	C 519	N 156	O 155	S 3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	QL	122	Total 932	C 586	N 185	O 159	S 2	0	0	0
43	XL	122	Total 932	C 586	N 185	O 159	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	QM	116	Total 914	C 564	N 189	O 159	S 2	0	0	0
44	XM	114	Total 895	C 550	N 186	O 157	S 2	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	QO	88	Total 728	C 456	N 144	O 126	S 2	0	0	0
46	XO	88	Total 728	C 456	N 144	O 126	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	QP	82	Total 681	C 433	N 134	O 113	S 1	0	0	0
47	XP	82	Total 677	C 430	N 133	O 113	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	QQ	99	823	528	151	142	2	0	0	0
			Total	C	N	O	S			
48	XQ	99	823	528	151	142	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
49	QR	68	555	355	108	92	0	0	0
			Total	C	N	O			
49	XR	68	555	355	108	92	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	QS	83	648	415	120	111	2	0	0	0
			Total	C	N	O	S			
50	XS	83	645	410	118	115	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	QT	96	732	449	157	124	2	0	0	0
			Total	C	N	O	S			
51	XT	98	733	451	154	126	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
52	QU	23	199	122	48	29	0	0	0
			Total	C	N	O			
52	XU	23	199	122	48	29	0	0	0

- Molecule 53 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
53	QV	77	Total C N O P 1640 732 297 535 76	0	0	0
53	XV	77	Total C N O P 1644 732 297 538 77	0	0	0

- Molecule 54 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
54	QX	9	Total C N O P 193 87 37 60 9	0	0	0
54	XX	10	Total C N O P 215 97 42 66 10	0	0	0

- Molecule 55 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
55	QY	259	Total C N O S 2014 1235 382 389 8	0	0	0
55	XY	260	Total C N O S 2022 1241 383 390 8	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	RA	1032	Total Mg 1032 1032	0	0
56	RB	22	Total Mg 22 22	0	0
56	RD	15	Total Mg 15 15	0	0
56	RE	7	Total Mg 7 7	0	0
56	RF	11	Total Mg 11 11	0	0
56	RG	4	Total Mg 4 4	0	0
56	RN	2	Total Mg 2 2	0	0
56	RO	1	Total Mg 1 1	0	0
56	RP	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	RQ	5	Total Mg 5 5	0	0
56	RR	4	Total Mg 4 4	0	0
56	RS	1	Total Mg 1 1	0	0
56	RT	3	Total Mg 3 3	0	0
56	RU	3	Total Mg 3 3	0	0
56	RV	3	Total Mg 3 3	0	0
56	RW	2	Total Mg 2 2	0	0
56	RX	1	Total Mg 1 1	0	0
56	RY	1	Total Mg 1 1	0	0
56	R0	7	Total Mg 7 7	0	0
56	R1	5	Total Mg 5 5	0	0
56	R3	2	Total Mg 2 2	0	0
56	R5	1	Total Mg 1 1	0	0
56	R7	3	Total Mg 3 3	0	0
56	R9	1	Total Mg 1 1	0	0
56	QA	262	Total Mg 262 262	0	0
56	QB	1	Total Mg 1 1	0	0
56	QD	2	Total Mg 2 2	0	0
56	QE	2	Total Mg 2 2	0	0
56	QF	1	Total Mg 1 1	0	0
56	QG	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	QH	1	Total Mg 1 1	0	0
56	QI	1	Total Mg 1 1	0	0
56	QJ	1	Total Mg 1 1	0	0
56	QL	2	Total Mg 2 2	0	0
56	QN	1	Total Mg 1 1	0	0
56	QO	1	Total Mg 1 1	0	0
56	QQ	1	Total Mg 1 1	0	0
56	QR	1	Total Mg 1 1	0	0
56	QT	1	Total Mg 1 1	0	0
56	QV	6	Total Mg 6 6	0	0
56	YA	749	Total Mg 749 749	0	0
56	YB	20	Total Mg 20 20	0	0
56	YD	9	Total Mg 9 9	0	0
56	YE	6	Total Mg 6 6	0	0
56	YF	2	Total Mg 2 2	0	0
56	YG	2	Total Mg 2 2	0	0
56	YI	1	Total Mg 1 1	0	0
56	YN	1	Total Mg 1 1	0	0
56	YO	1	Total Mg 1 1	0	0
56	YP	1	Total Mg 1 1	0	0
56	YQ	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	YR	1	Total Mg 1 1	0	0
56	YT	3	Total Mg 3 3	0	0
56	YV	1	Total Mg 1 1	0	0
56	YW	2	Total Mg 2 2	0	0
56	YX	1	Total Mg 1 1	0	0
56	Y0	1	Total Mg 1 1	0	0
56	Y1	1	Total Mg 1 1	0	0
56	Y5	2	Total Mg 2 2	0	0
56	Y7	1	Total Mg 1 1	0	0
56	Y8	2	Total Mg 2 2	0	0
56	XA	187	Total Mg 187 187	0	0
56	XE	2	Total Mg 2 2	0	0
56	XF	4	Total Mg 4 4	0	0
56	XJ	1	Total Mg 1 1	0	0
56	XL	1	Total Mg 1 1	0	0
56	XT	1	Total Mg 1 1	0	0
56	XV	4	Total Mg 4 4	0	0
56	XY	1	Total Mg 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	RY	1	Total Zn 1 1	0	0

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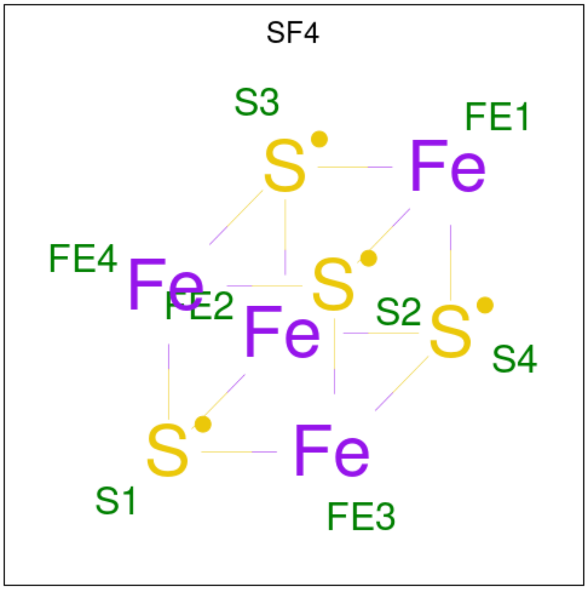
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	R4	1	Total Zn 1 1	0	0
57	R5	1	Total Zn 1 1	0	0
57	R6	1	Total Zn 1 1	0	0
57	R9	1	Total Zn 1 1	0	0
57	QN	1	Total Zn 1 1	0	0
57	YY	1	Total Zn 1 1	0	0
57	Y4	1	Total Zn 1 1	0	0
57	Y5	1	Total Zn 1 1	0	0
57	Y6	1	Total Zn 1 1	0	0
57	Y9	1	Total Zn 1 1	0	0
57	XN	1	Total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

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



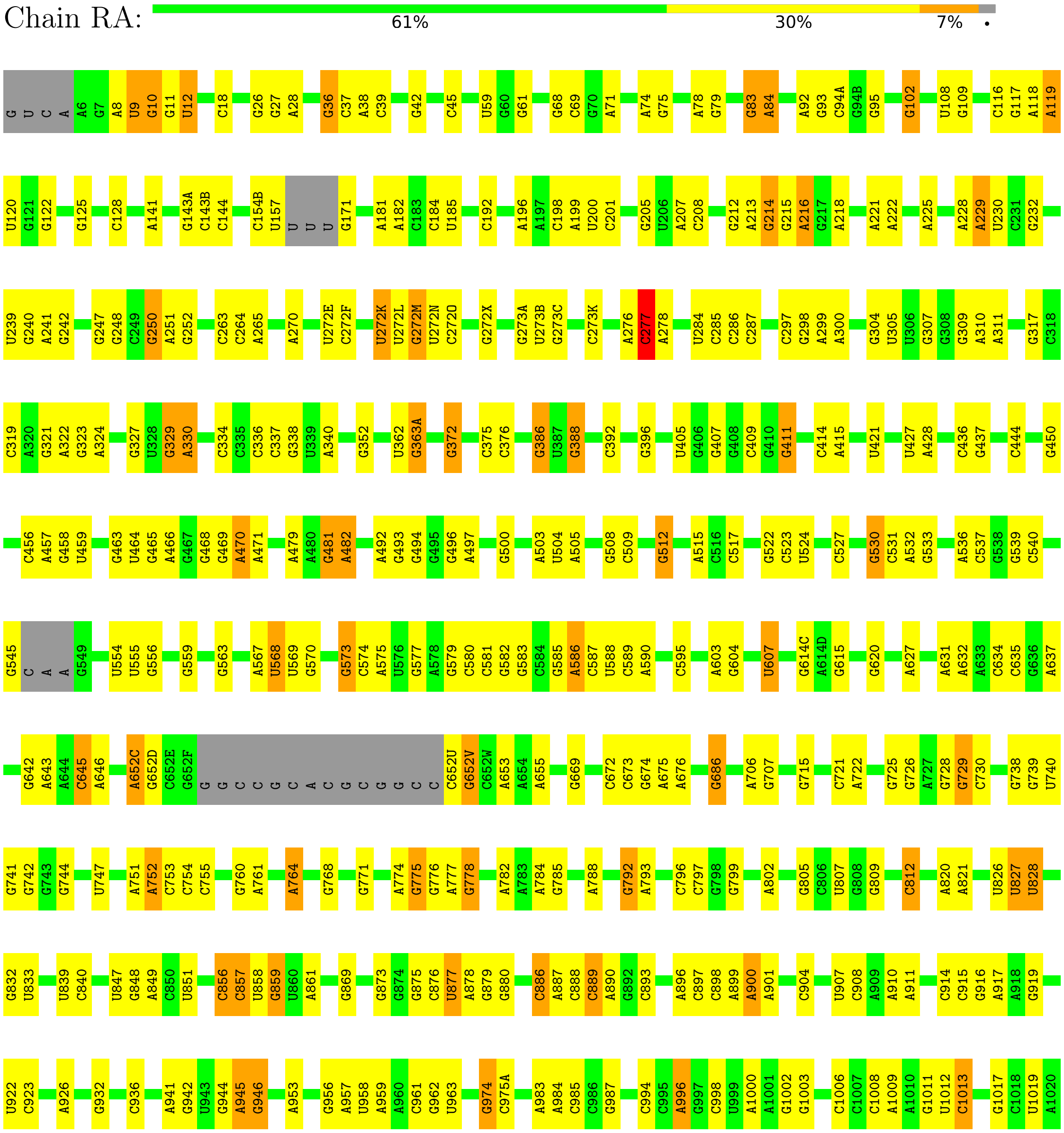
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	QD	1	Total Fe S 8 4 4	0	0
58	XD	1	Total Fe S 8 4 4	0	0

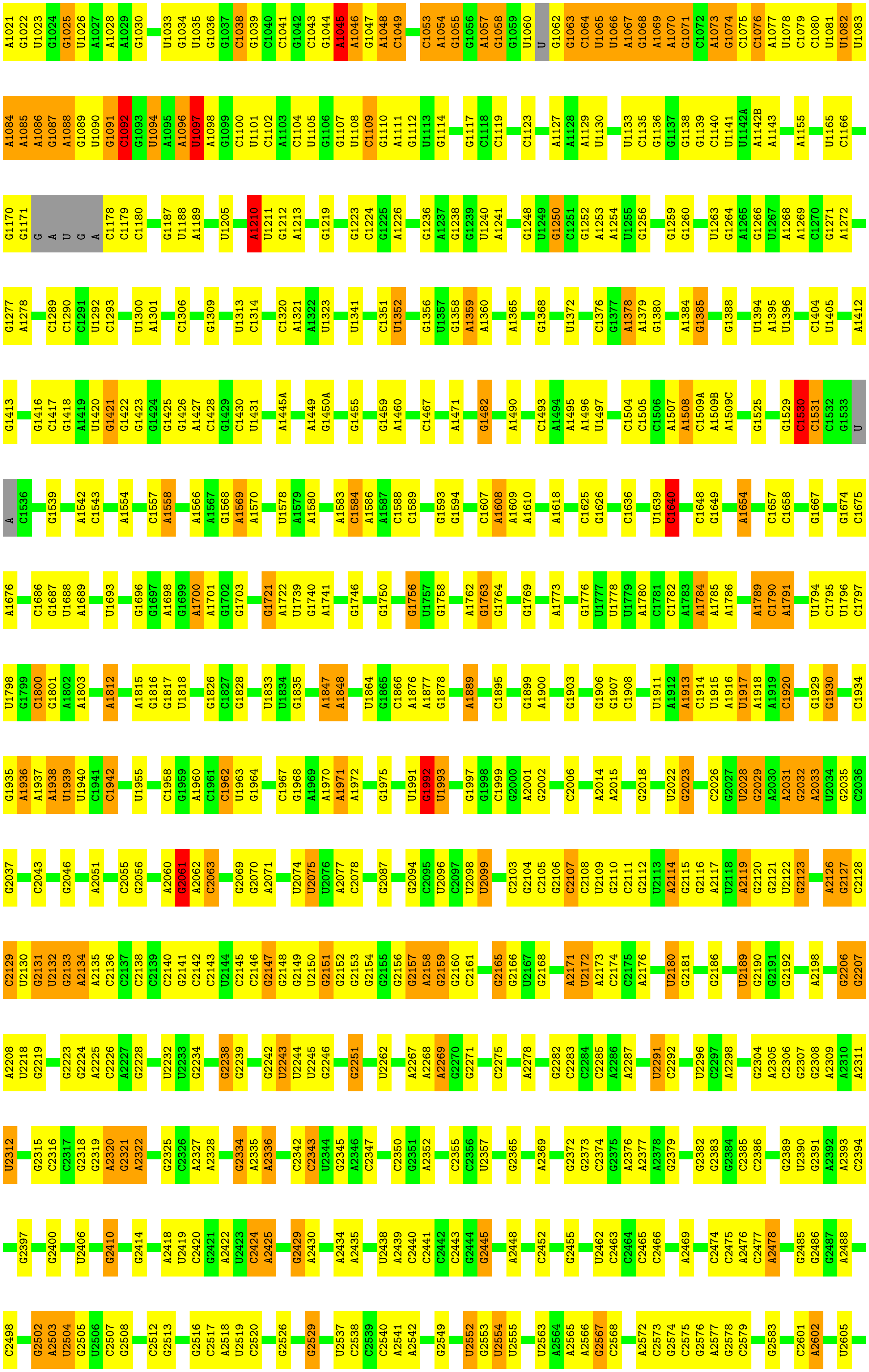
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS failed to run properly.

- Molecule 1: 23S rRNA

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A1084 A1085 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 G1110 A1111 G1112 U1113 G1114 G1117 C1118 C1119 C1123 A1127 A1128 A1129 U1130 U1133 C1135 G1136 G1137 G1138 G1139 C1140 U1141 U1142A A1142B A1143 A1155 U1165 C1166
G1170 G1171 G A U G A C1178 C1179 C1180 G1187 U1188 A1189 U1205 A1210 U1211 G1212 A1213 G1219 G1223 C1224 G1225 A1226 G1236 A1237 G1238 G1239 U1240 A1241 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 G1259 G1260 U1263 G1264 A1265 C1266 U1267 A1268 A1269 C1270 G1271 A1272
G1277 A1278 C1289 C1290 C1291 U1292 C1293 U1300 A1301 C1306 G1309 U1313 C1314 C1320 A1321 A1322 U1323 U1341 C1351 U1352 G1356 U1357 G1358 A1359 A1360 A1365 G1368 U1372 C1376 G1377 A1378 A1379 G1380 A1384 G1385 G1388 U1394 A1395 U1396 C1404 U1405 A1412
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G1935 A1936 A1937 A1938 U1939 U1940 C1941 C1942 U1955 C1958 G1959 A1960 C1961 C1962 U1963 G1964 C1967 G1968 A1969 A1970 A1971 A1972 G1975 U1991 G1992 U1993 G1997 G1998 C1999 G2000 A2001 G2002 C2006 A2014 A2015 G2018 U2022 G2023 C2026 G2027 U2028 G2029 A2030 A2031 G2032 A2033 U2034 G2035 C2036
G2037 C2043 G2046 A2051 C2055 G2056 A2060 G2061 A2062 C2063 G2069 G2070 A2071 U2074 U2075 U2076 A2077 C2078 G2087 G2094 C2095 U2096 C2097 U2098 U2099 C2103 G2104 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 A2126 G2127 C2128
C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 G2143 U2144 C2145 C2146 G2147 G2148 G2149 U2150 G2151 G2152 G2153 C2154 G2155 G2156 G2157 A2158 C2159 G2160 C2161 G2165 G2166 U2167 G2168 A2171 U2172 A2173 C2174 C2175 A2176 U2180 G2181 G2186 U2189 G2190 G2191 G2192 A2198 G2206 G2207
A2208 U2218 G2219 G2223 G2224 A2225 C2226 A2227 G2228 U2232 U2233 G2234 G2238 G2239 G2242 U2243 U2244 U2245 G2246 G2251 U2262 A2267 A2268 A2269 G2270 G2271 C2275 A2278 G2282 C2283 C2284 C2285 A2286 A2287 U2291 C2292 U2296 C2297 A2298 G2304 A2305 C2306 G2307 G2308 A2309 A2310 A2311
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G2397 G2400 U2406 G2410 G2414 A2418 U2419 C2420 G2421 A2422 U2423 C2424 A2425 G2429 A2430 A2434 A2435 U2438 A2439 C2440 C2441 C2442 C2443 G2444 G2445 A2448 C2452 G2455 U2462 C2463 C2464 C2465 C2466 A2469 C2474 C2475 A2476 C2477 A2478 G2485 G2486 G2487 A2488
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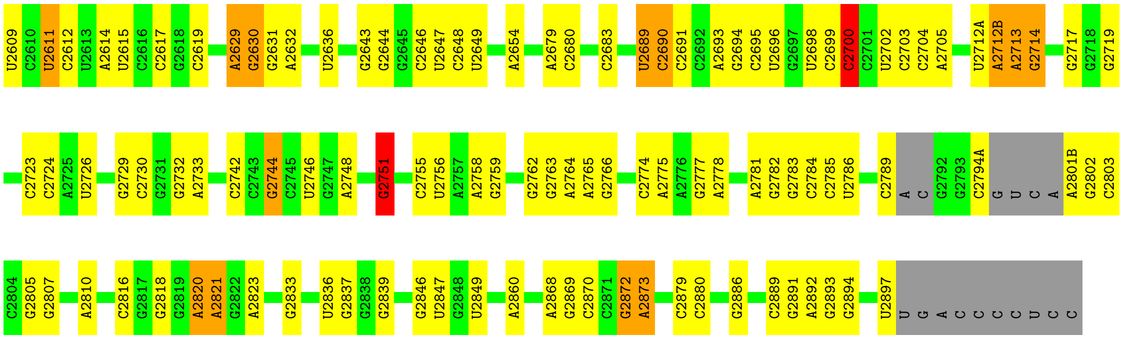
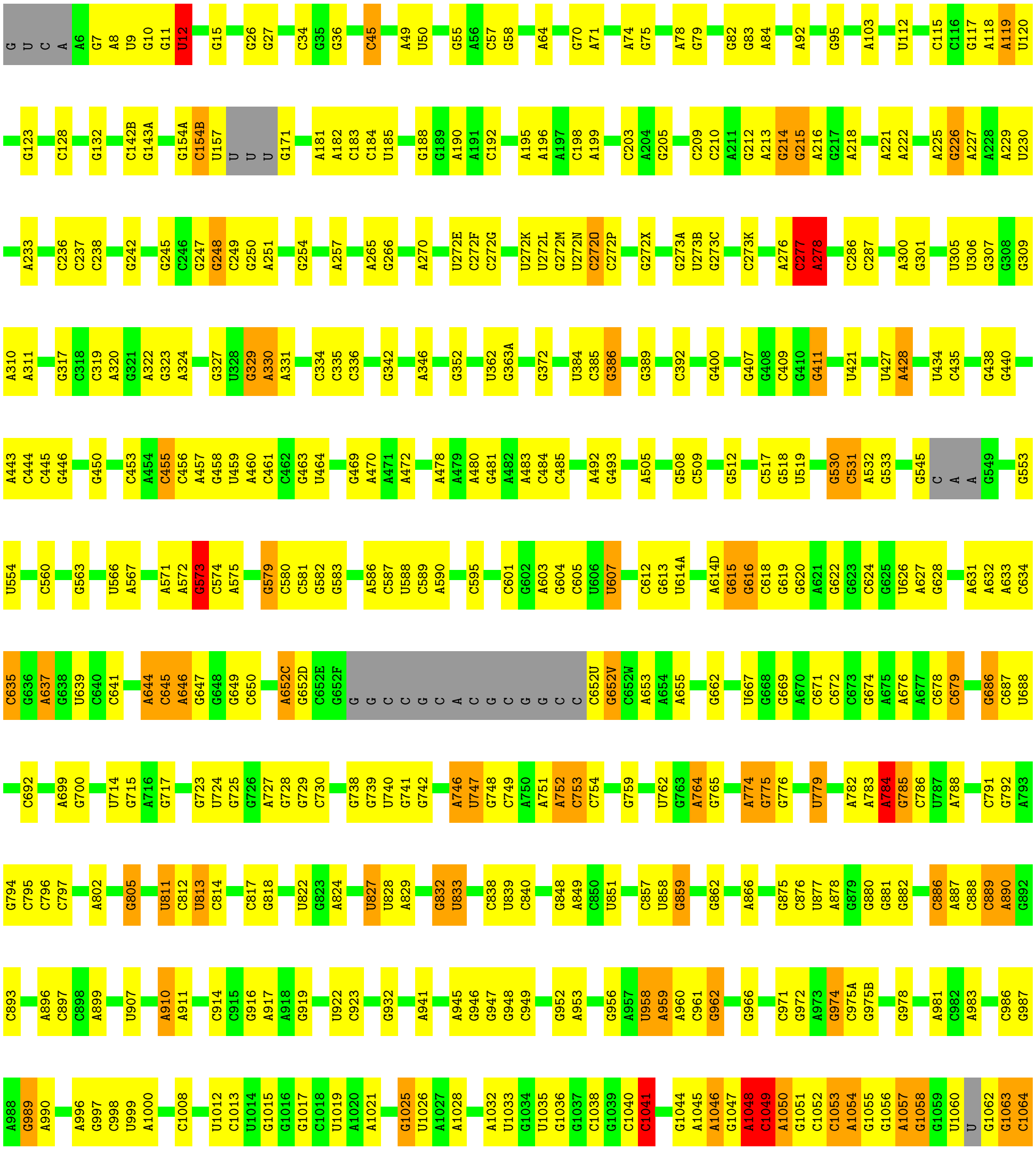
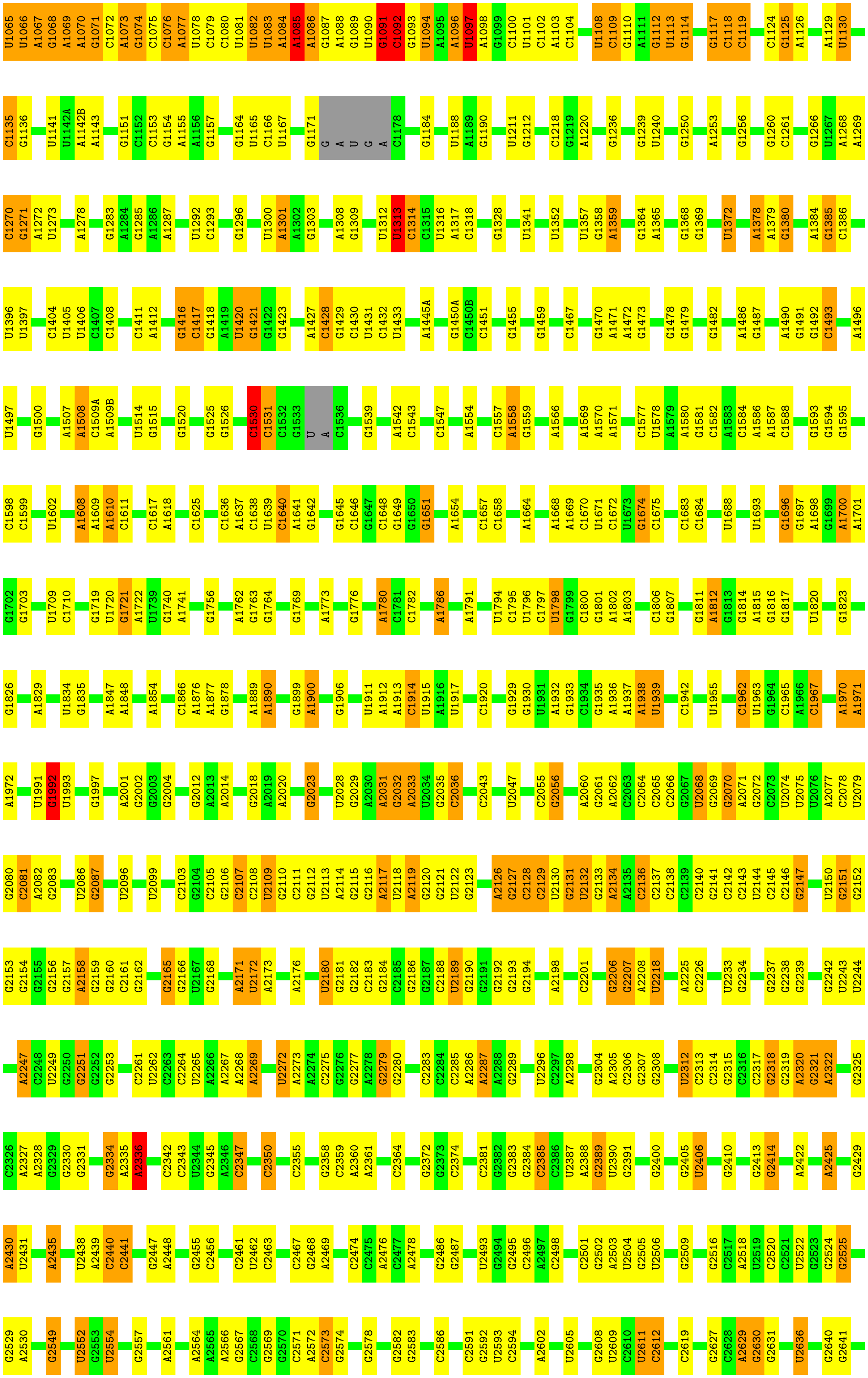


- Molecule 1: 23S rRNA

Chain YA:

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C1135 G1136 U1141 U1142A A1142B A1143 G1151 C1152 C1153 G1154 A1155 A1156 G1157 G1164 U1165 C1166 U1167 G1171 G A U G A C1178 G1184 U1188 A1189 G1190 U1211 G1212 C1218 G1219 A1220 G1236 G1239 U1240 G1250 A1253 G1256 G1260 C1261 G1266 U1267 A1268 A1269
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G2080 C2081 A2082 G2083 U2086 G2087 U2096 U2099 C2103 G2104 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 G2146 G2147 U2150 G2151 G2152
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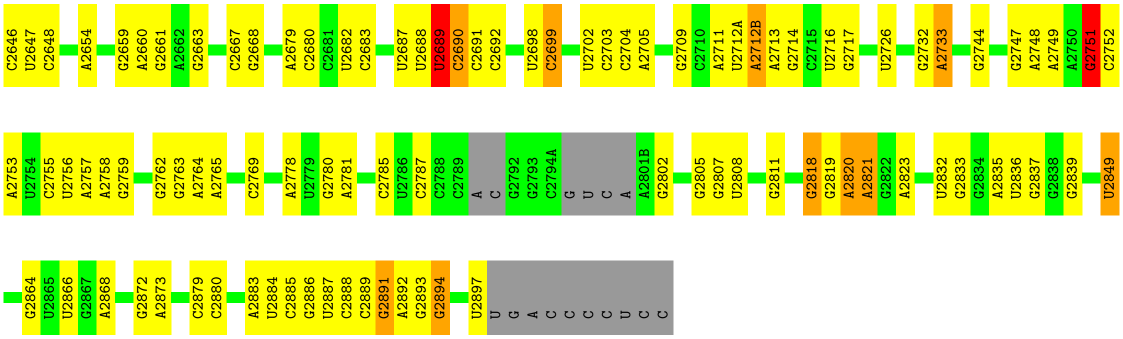
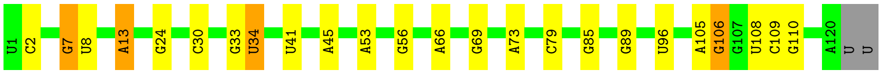


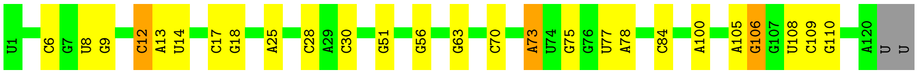
- Molecule 2: 5S rRNA

Chain RB:



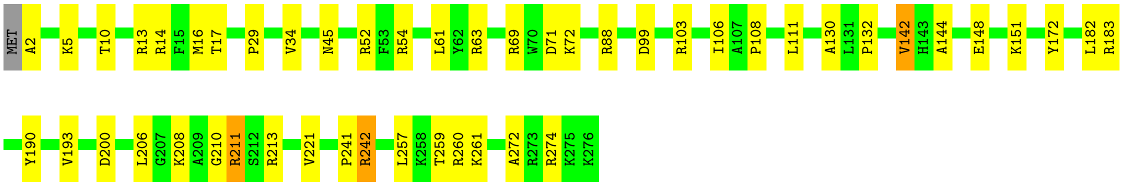
- Molecule 2: 5S rRNA

Chain YB:



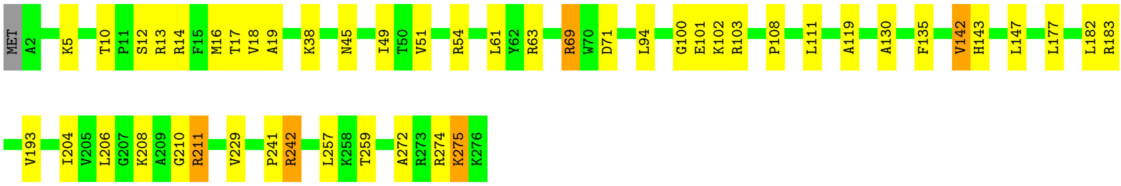
- Molecule 3: 50S ribosomal protein L2

Chain RD:



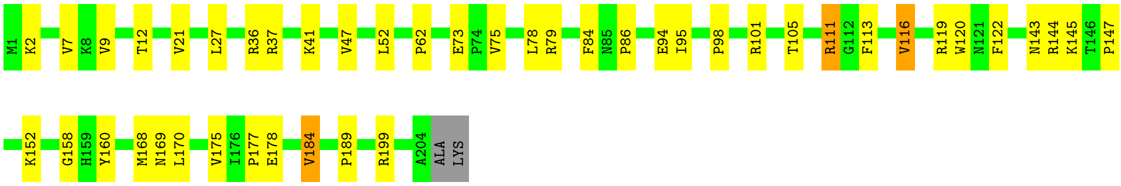
- Molecule 3: 50S ribosomal protein L2

Chain YD:



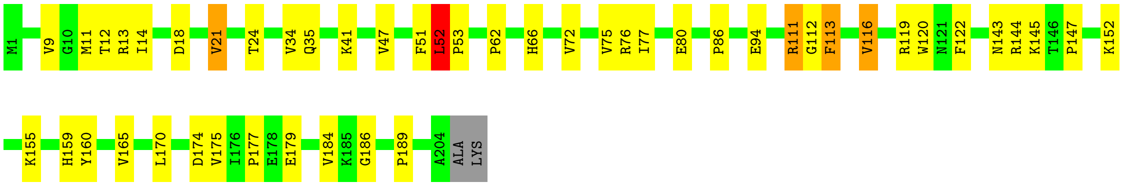
- Molecule 4: 50S ribosomal protein L3

Chain RE:



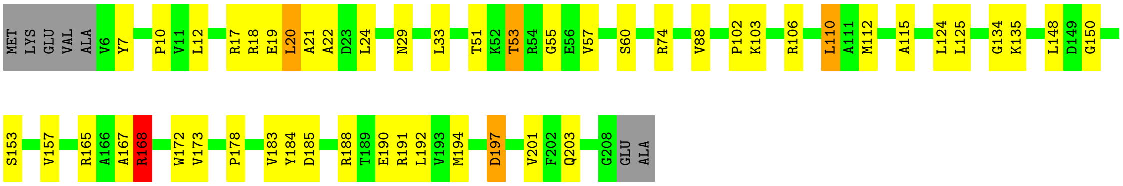
- Molecule 4: 50S ribosomal protein L3

Chain YE:



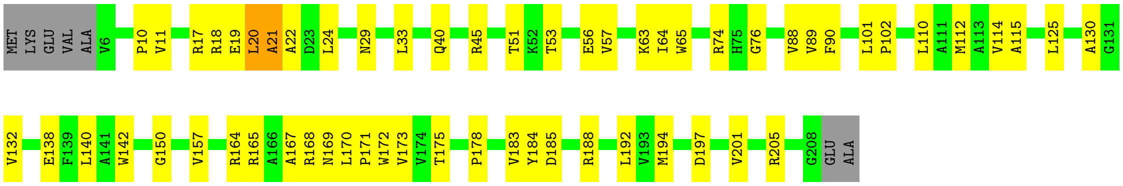
- Molecule 5: 50S ribosomal protein L4

Chain RF:



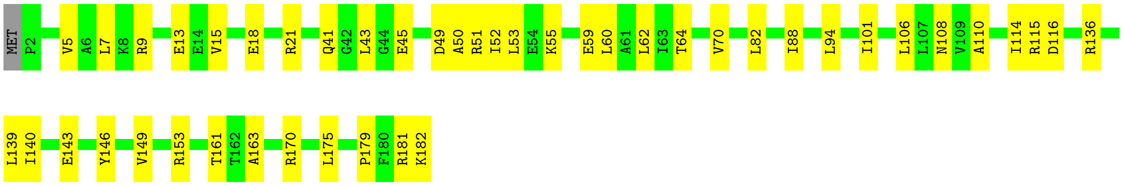
- Molecule 5: 50S ribosomal protein L4

Chain YF:



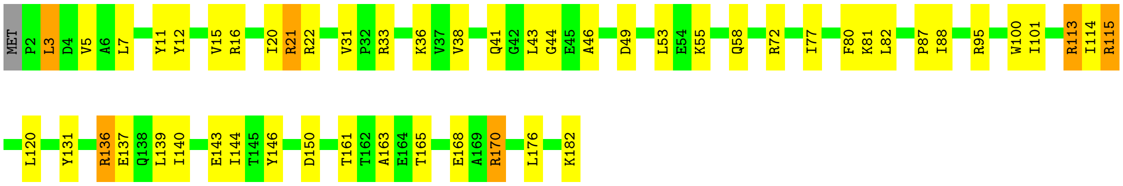
- Molecule 6: 50S ribosomal protein L5

Chain RG:



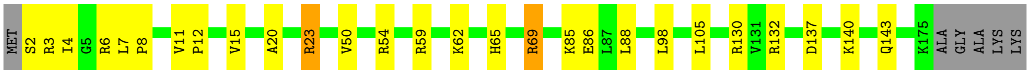
- Molecule 6: 50S ribosomal protein L5

Chain YG:



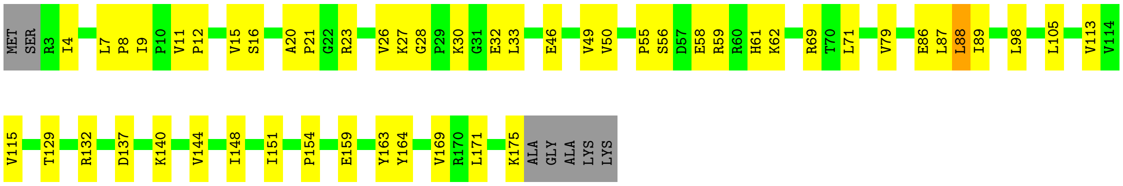
- Molecule 7: 50S ribosomal protein L6

Chain RH:



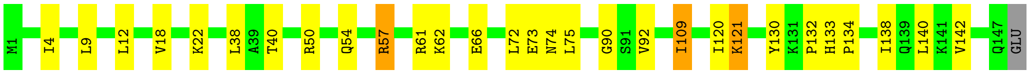
- Molecule 7: 50S ribosomal protein L6

Chain YH:



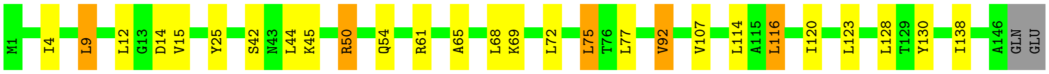
- Molecule 8: 50S ribosomal protein L9

Chain RI:



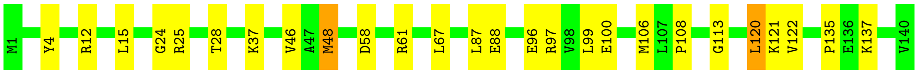
- Molecule 8: 50S ribosomal protein L9

Chain YI:



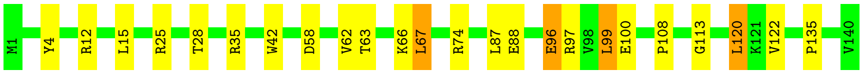
- Molecule 9: 50S ribosomal protein L13

Chain RN:



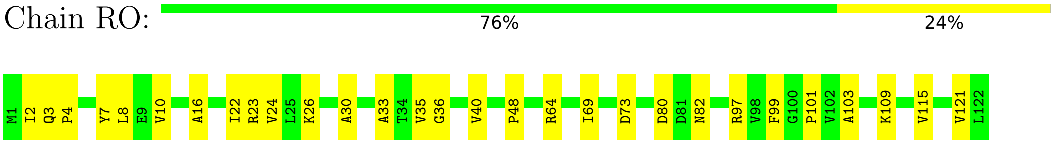
- Molecule 9: 50S ribosomal protein L13

Chain YN:



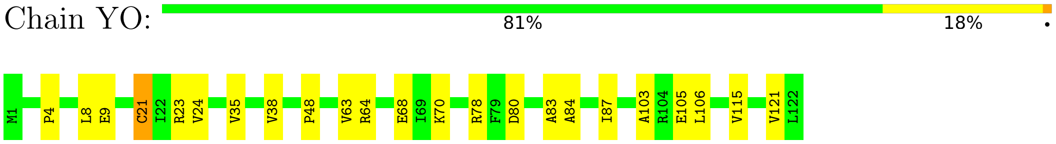
- Molecule 10: 50S ribosomal protein L14

Chain RO:



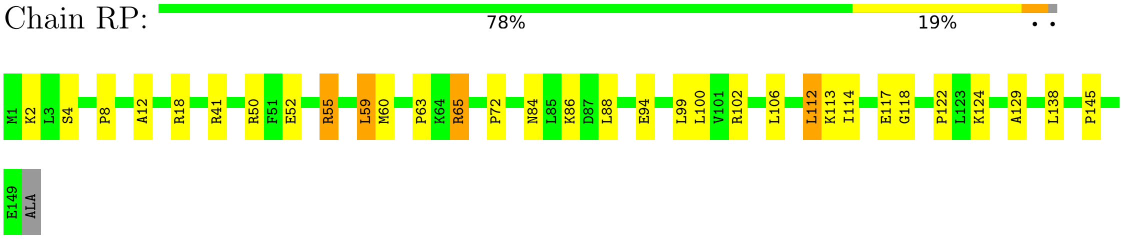
- Molecule 10: 50S ribosomal protein L14

Chain YO:



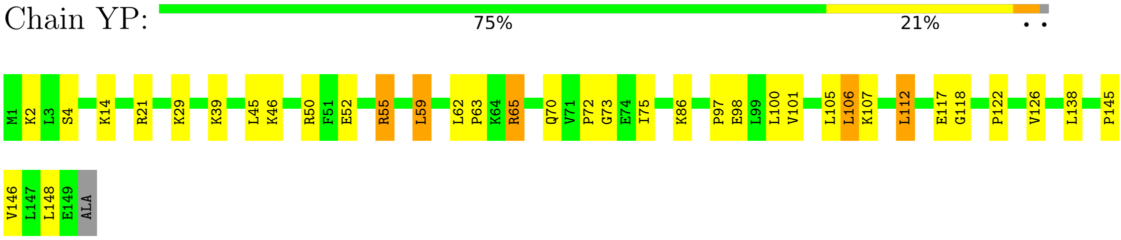
- Molecule 11: 50S ribosomal protein L15

Chain RP:



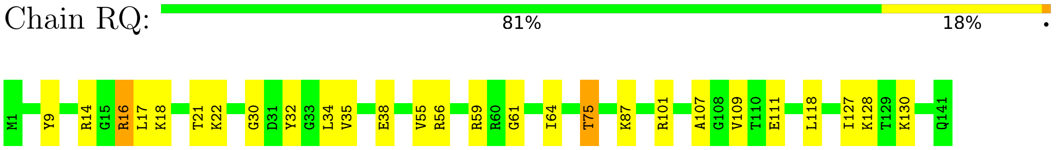
- Molecule 11: 50S ribosomal protein L15

Chain YP:



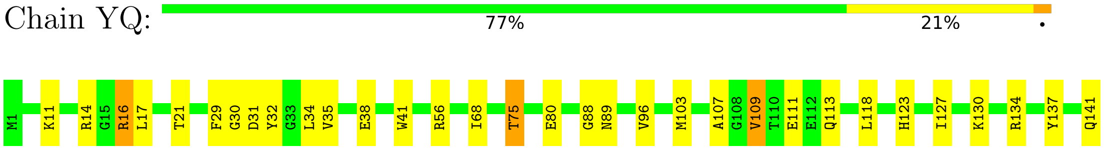
- Molecule 12: 50S ribosomal protein L16

Chain RQ:



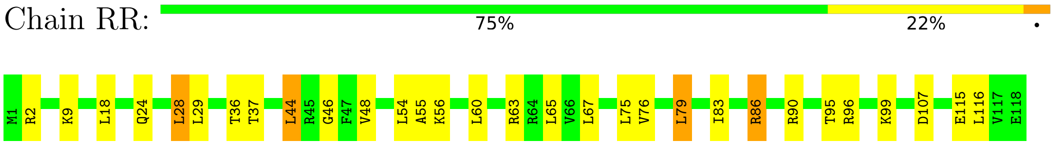
- Molecule 12: 50S ribosomal protein L16

Chain YQ:



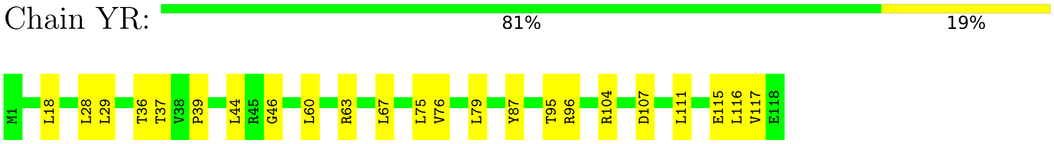
- Molecule 13: 50S ribosomal protein L17

Chain RR:



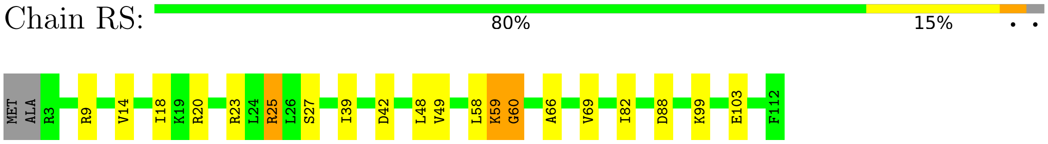
- Molecule 13: 50S ribosomal protein L17

Chain YR:



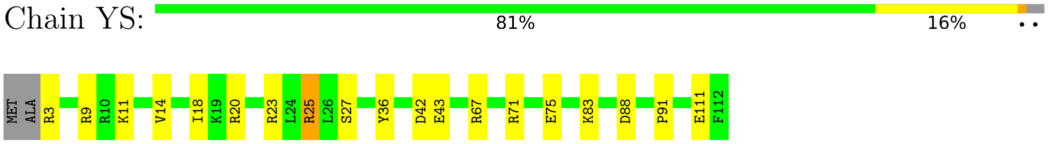
- Molecule 14: 50S ribosomal protein L18

Chain RS:



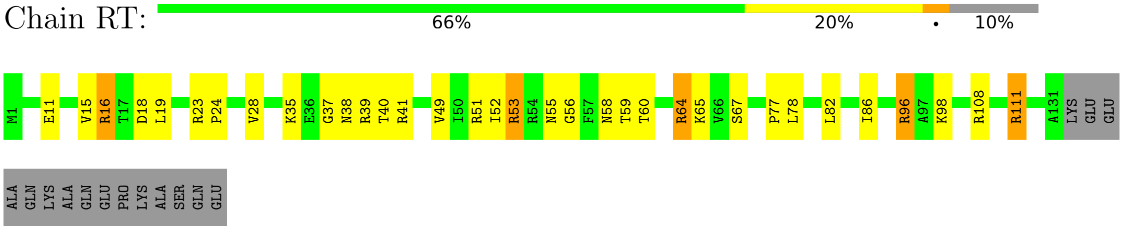
- Molecule 14: 50S ribosomal protein L18

Chain YS:



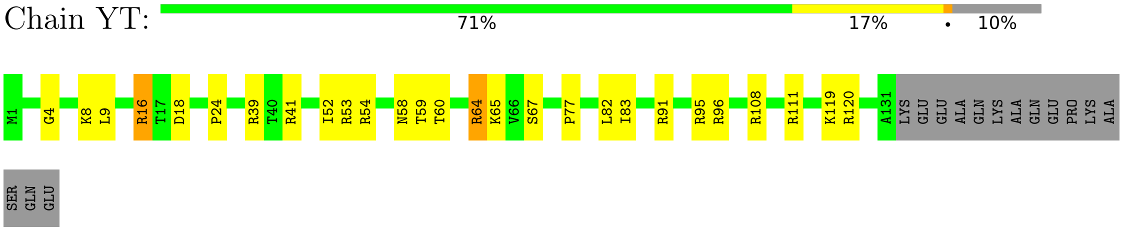
- Molecule 15: 50S ribosomal protein L19

Chain RT:



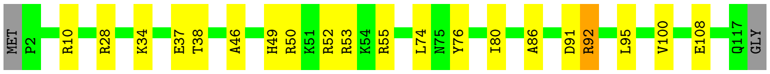
- Molecule 15: 50S ribosomal protein L19

Chain YT:



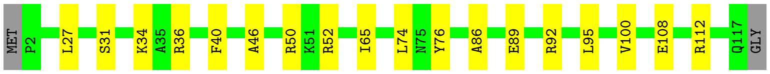
- Molecule 16: 50S ribosomal protein L20

Chain RU:



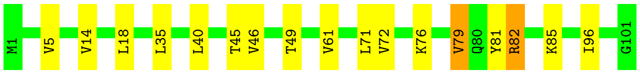
- Molecule 16: 50S ribosomal protein L20

Chain YU:



- Molecule 17: 50S ribosomal protein L21

Chain RV:

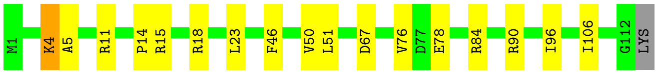


- Molecule 17: 50S ribosomal protein L21

Chain YV:

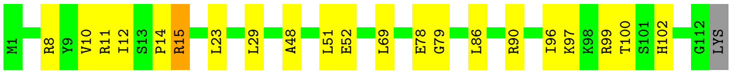
- Molecule 18: 50S ribosomal protein L22

Chain RW:



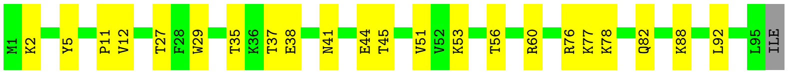
- Molecule 18: 50S ribosomal protein L22

Chain YW:



- Molecule 19: 50S ribosomal protein L23

Chain RX:

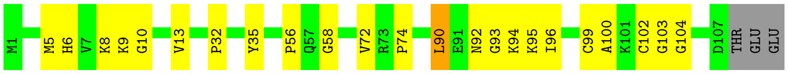


- Molecule 19: 50S ribosomal protein L23

Chain YX:

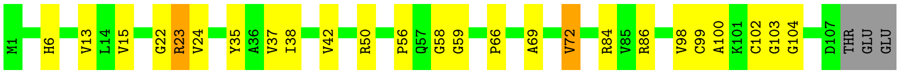
- Molecule 20: 50S ribosomal protein L24

Chain RY:



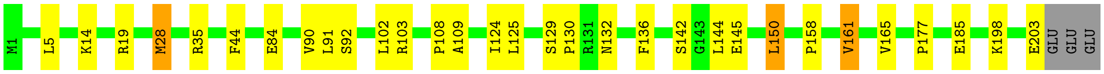
- Molecule 20: 50S ribosomal protein L24

Chain YY:



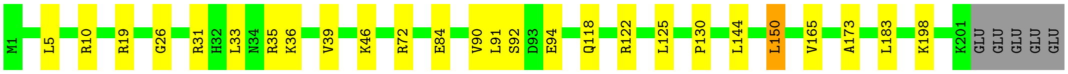
- Molecule 21: 50S ribosomal protein L25

Chain RZ:



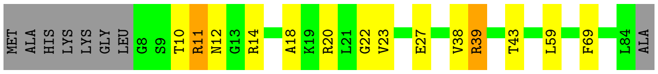
- Molecule 21: 50S ribosomal protein L25

Chain YZ:



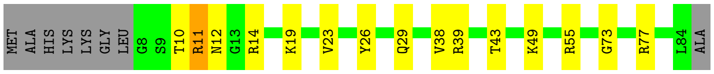
- Molecule 22: 50S ribosomal protein L27

Chain R0:



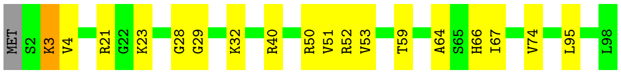
- Molecule 22: 50S ribosomal protein L27

Chain Y0:



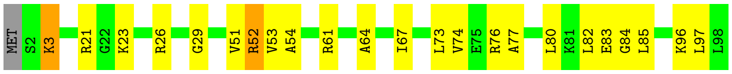
- Molecule 23: 50S ribosomal protein L28

Chain R1:



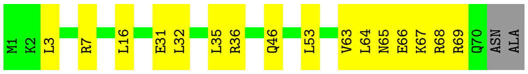
- Molecule 23: 50S ribosomal protein L28

Chain Y1:



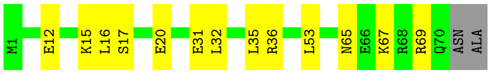
- Molecule 24: 50S ribosomal protein L29

Chain R2:



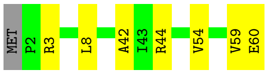
- Molecule 24: 50S ribosomal protein L29

Chain Y2:



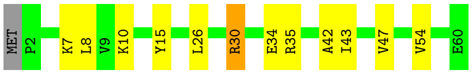
- Molecule 25: 50S ribosomal protein L30

Chain R3:



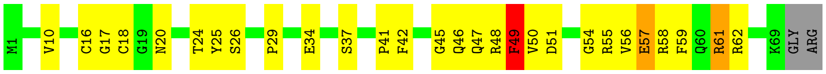
- Molecule 25: 50S ribosomal protein L30

Chain Y3:



- Molecule 26: 50S ribosomal protein L31

Chain R4:

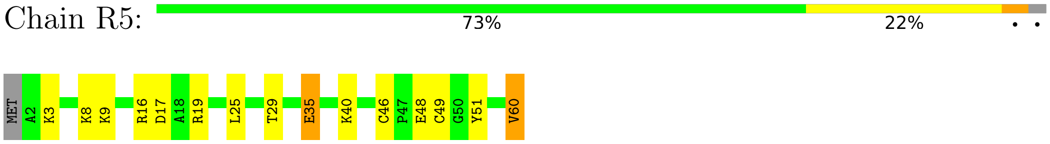


- Molecule 26: 50S ribosomal protein L31

Chain Y4:

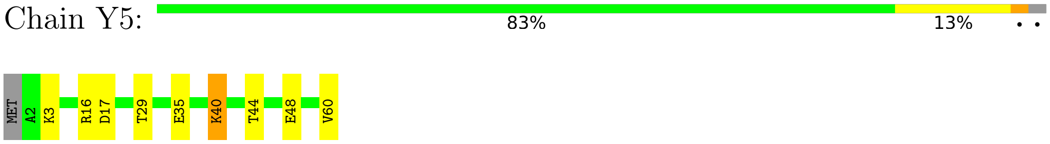
- Molecule 27: 50S ribosomal protein L32

Chain R5:



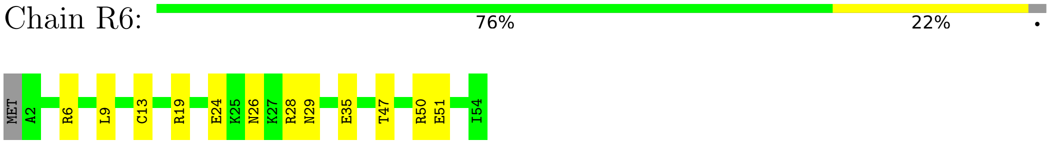
- Molecule 27: 50S ribosomal protein L32

Chain Y5:



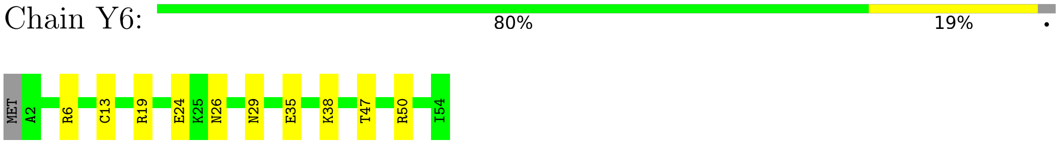
- Molecule 28: 50S ribosomal protein L33

Chain R6:



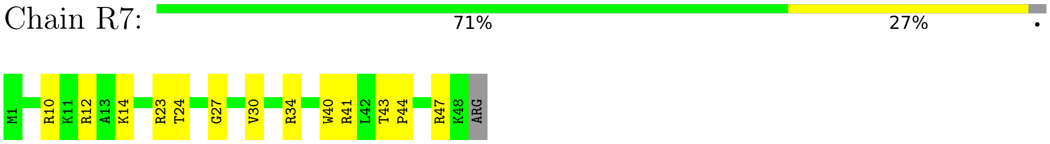
- Molecule 28: 50S ribosomal protein L33

Chain Y6:



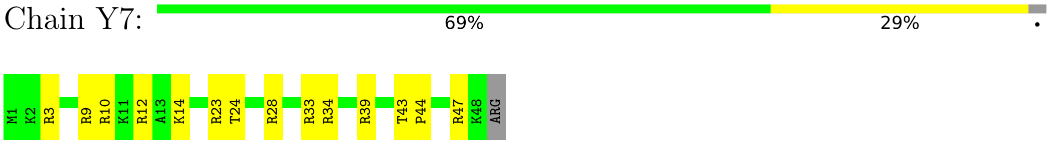
- Molecule 29: 50S ribosomal protein L34

Chain R7:



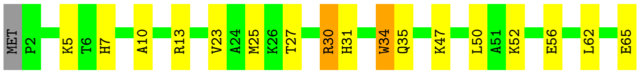
- Molecule 29: 50S ribosomal protein L34

Chain Y7:

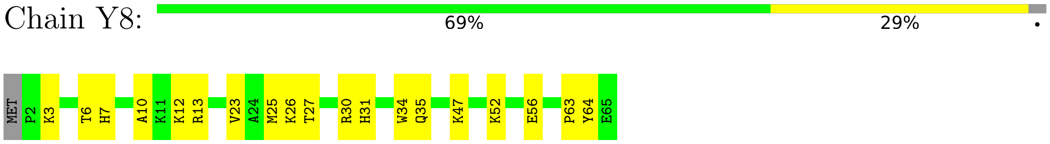


- Molecule 30: 50S ribosomal protein L35

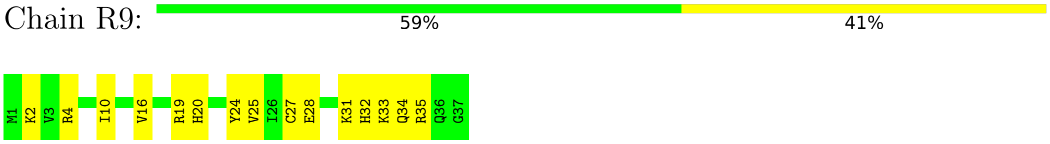
Chain R8:



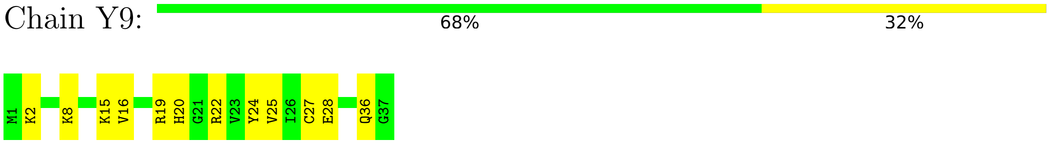
- Molecule 30: 50S ribosomal protein L35



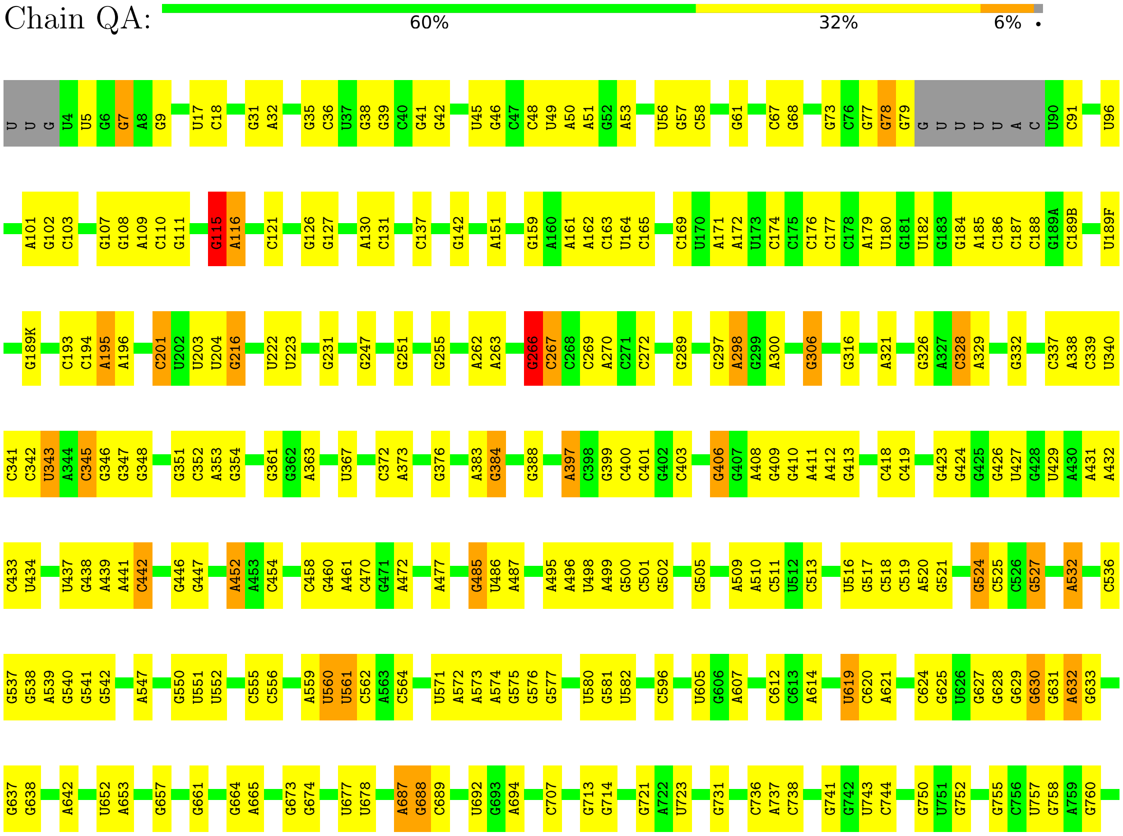
- Molecule 31: 50S ribosomal protein L36

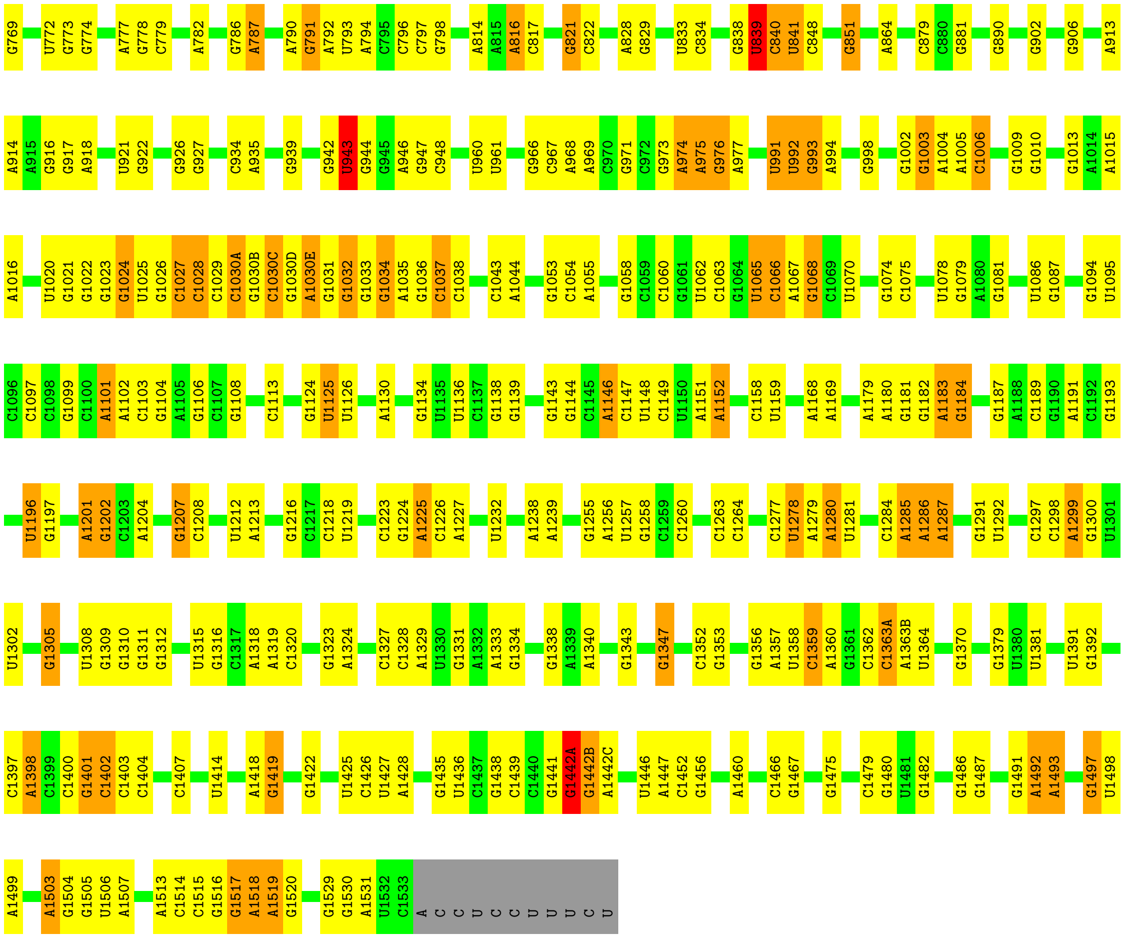


- Molecule 31: 50S ribosomal protein L36



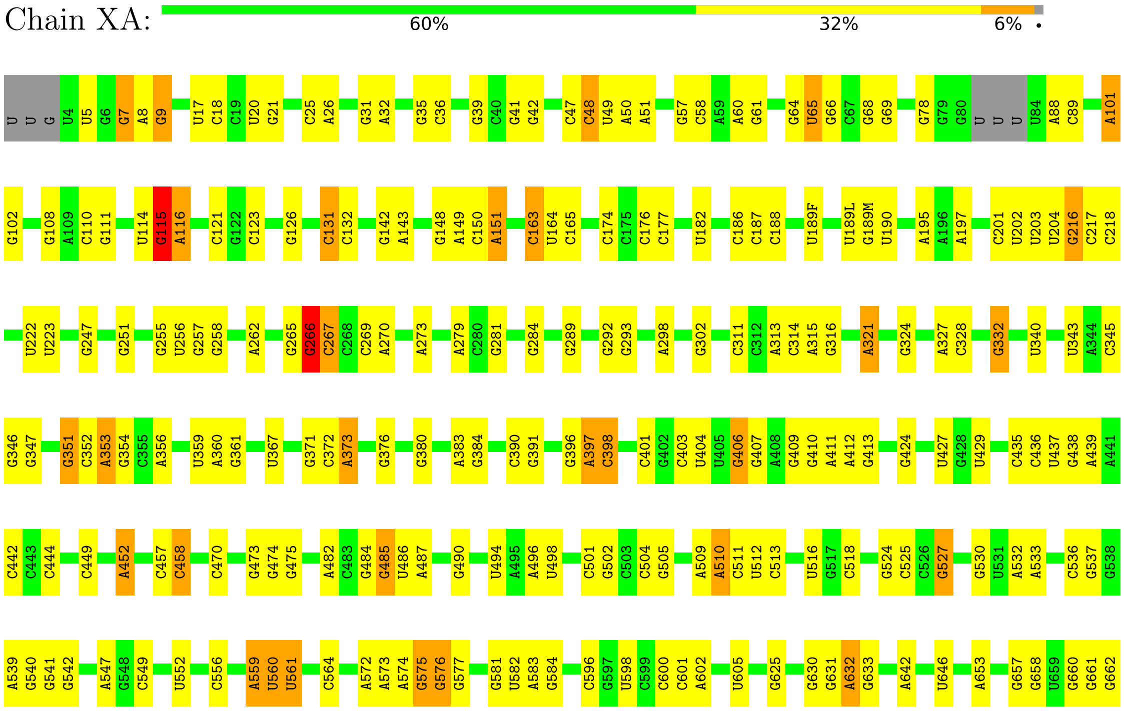
- Molecule 32: 16S rRNA

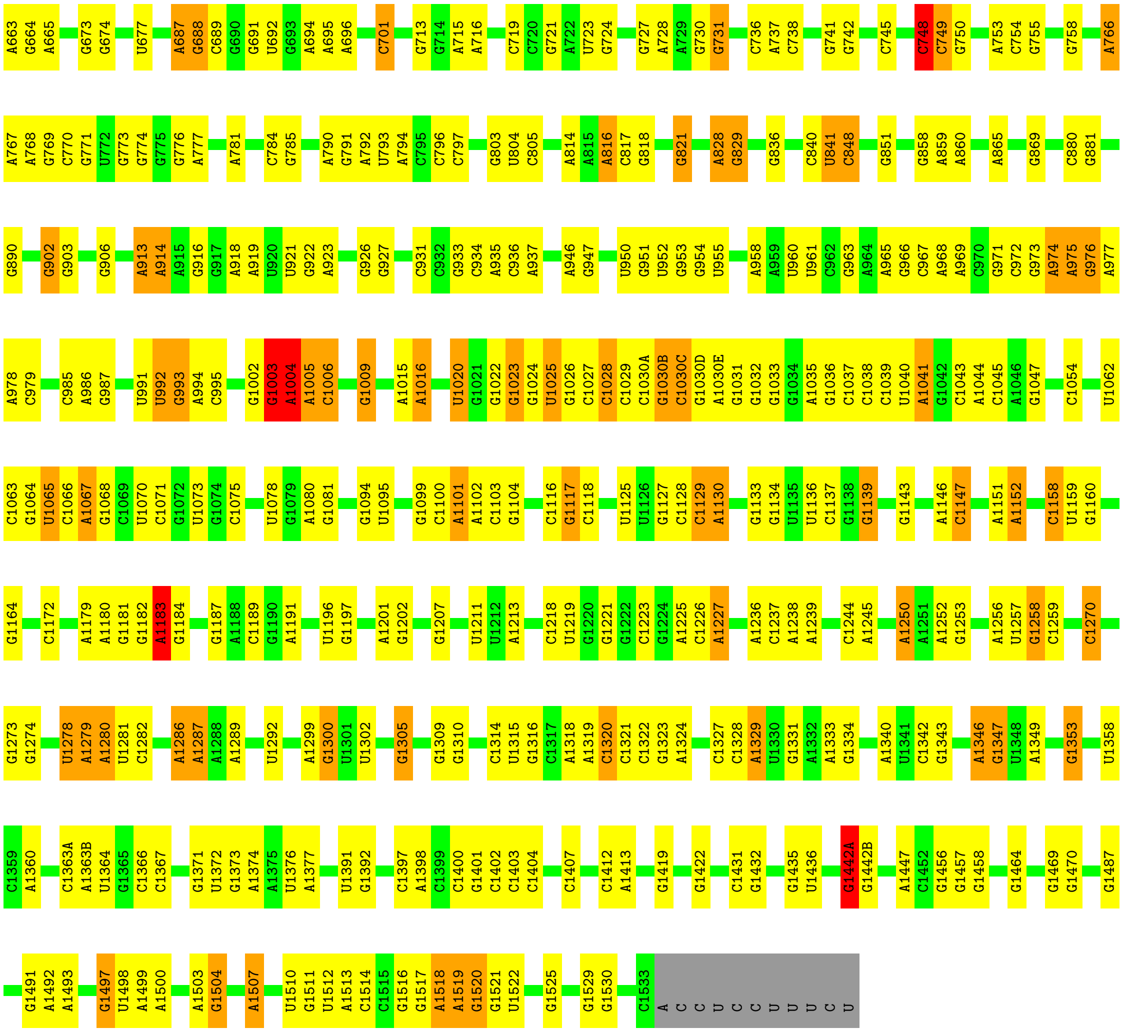




- Molecule 32: 16S rRNA

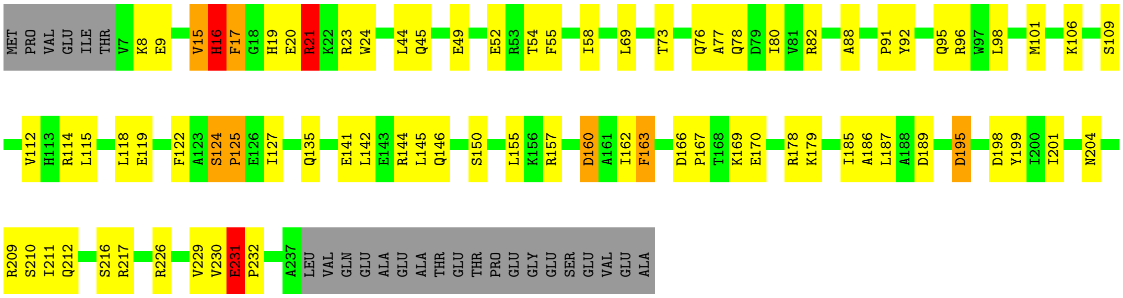
Chain XA:





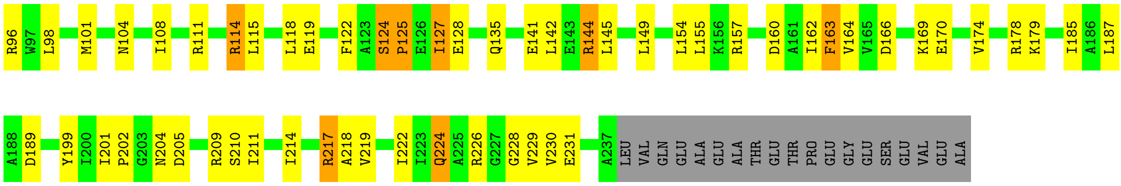
- Molecule 33: 30S ribosomal protein S2

Chain QB:

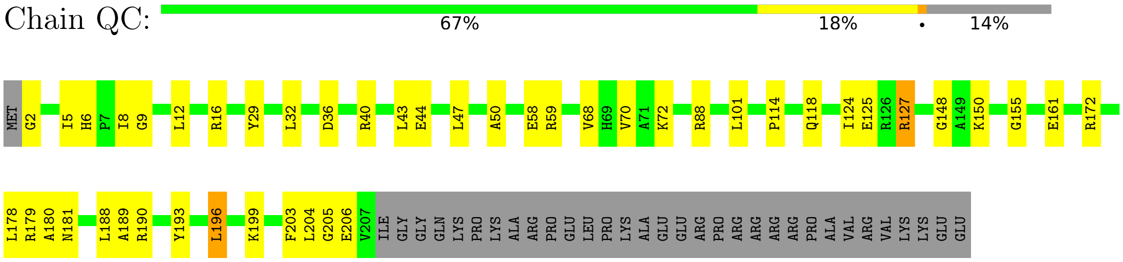


- Molecule 33: 30S ribosomal protein S2

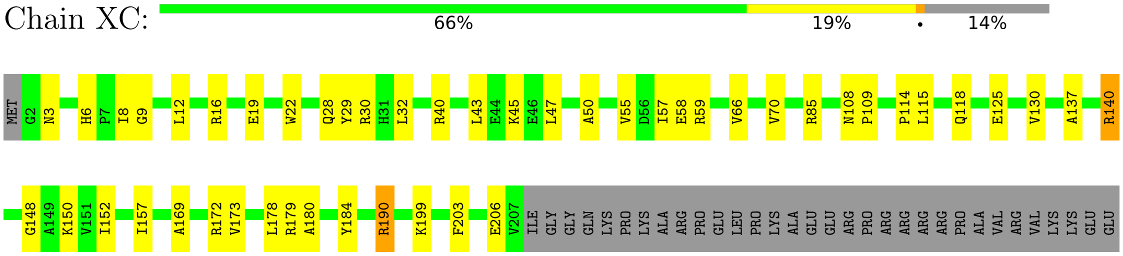
Chain XB:



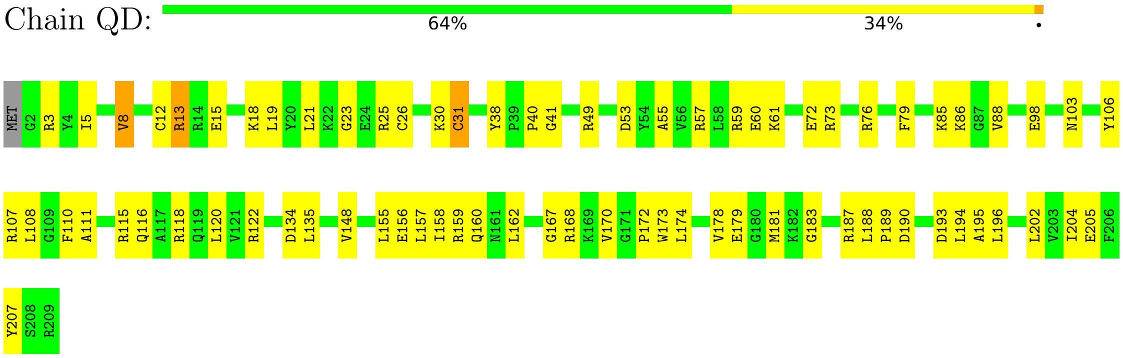
- Molecule 34: 30S ribosomal protein S3



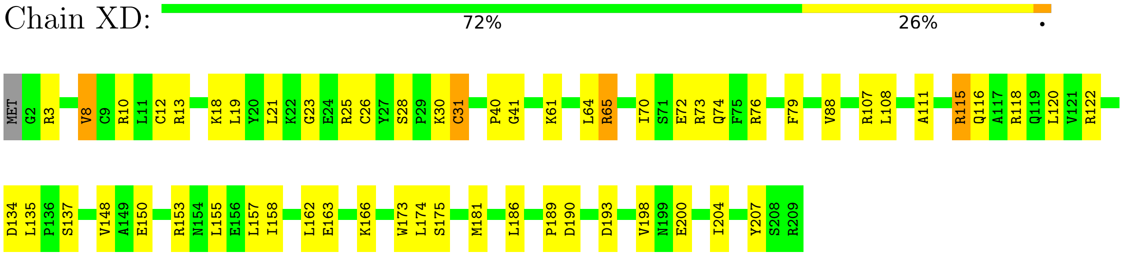
- Molecule 34: 30S ribosomal protein S3



- Molecule 35: 30S ribosomal protein S4

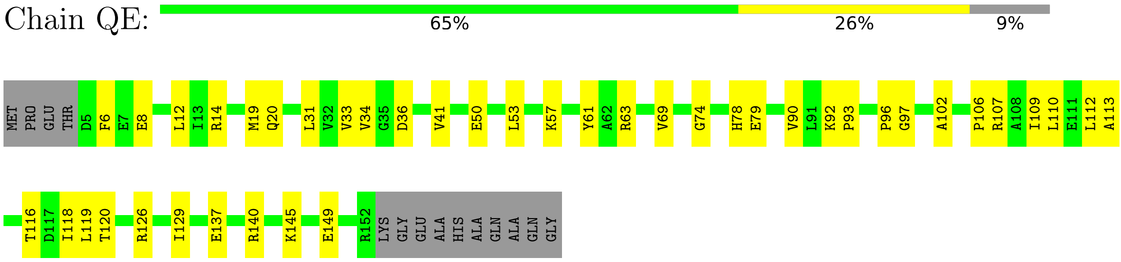


- Molecule 35: 30S ribosomal protein S4



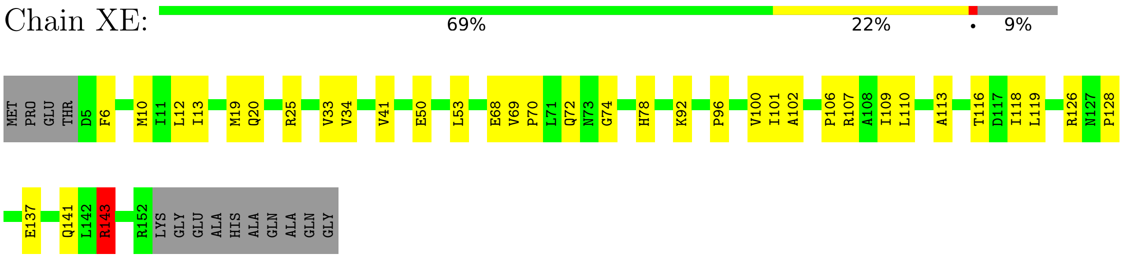
- Molecule 36: 30S ribosomal protein S5

Chain QE:



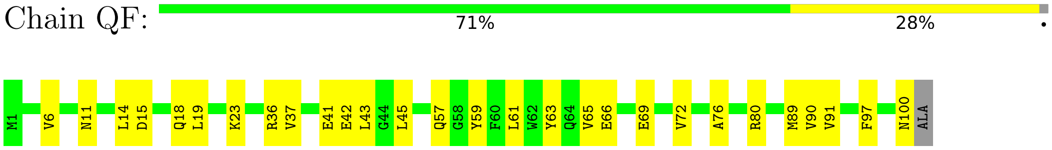
- Molecule 36: 30S ribosomal protein S5

Chain XE:



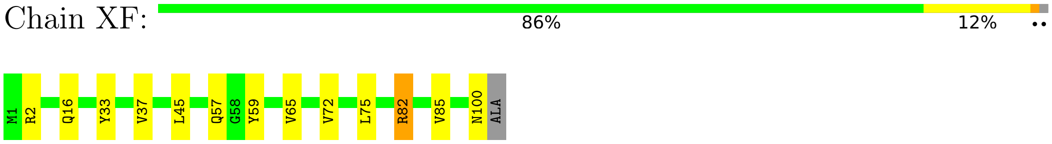
- Molecule 37: 30S ribosomal protein S6

Chain QF:



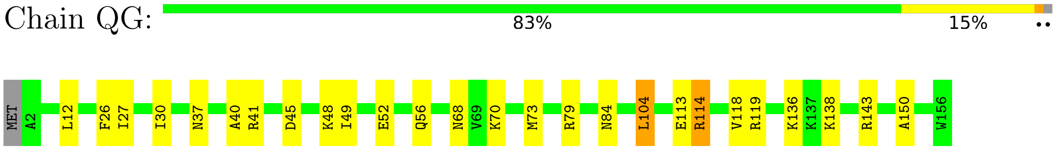
- Molecule 37: 30S ribosomal protein S6

Chain XF:



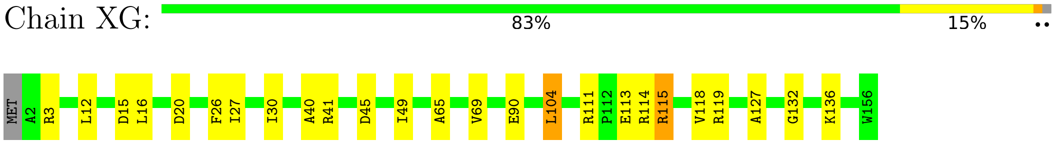
- Molecule 38: 30S ribosomal protein S7

Chain QG:



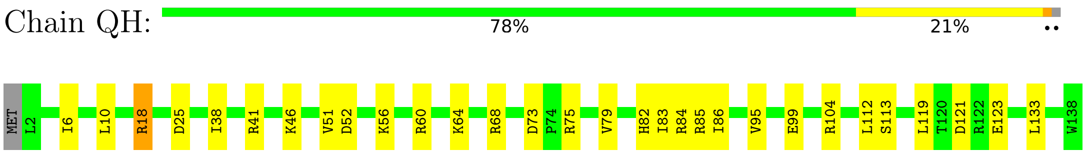
- Molecule 38: 30S ribosomal protein S7

Chain XG:



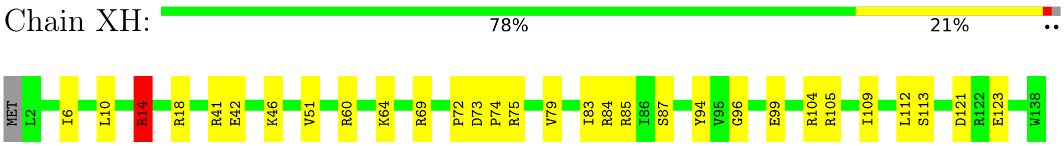
- Molecule 39: 30S ribosomal protein S8

Chain QH:



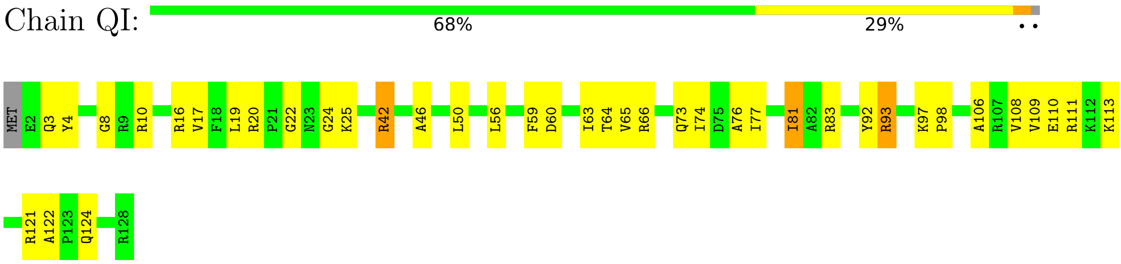
- Molecule 39: 30S ribosomal protein S8

Chain XH:



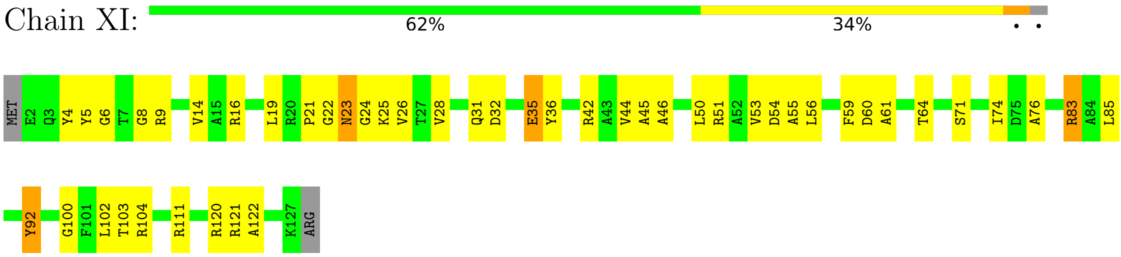
- Molecule 40: 30S ribosomal protein S9

Chain QI:



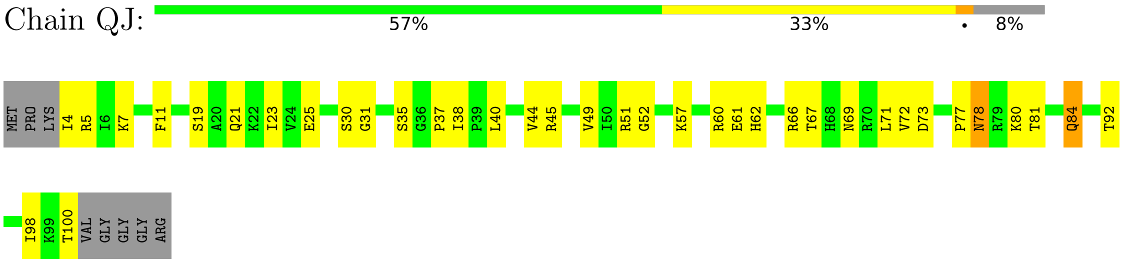
- Molecule 40: 30S ribosomal protein S9

Chain XI:



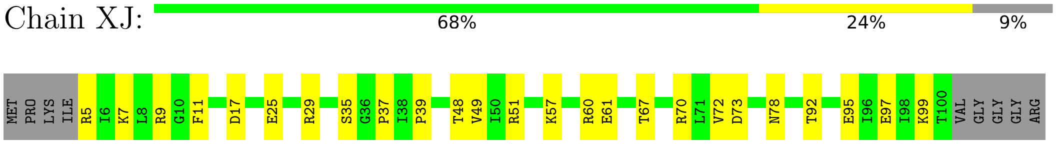
- Molecule 41: 30S ribosomal protein S10

Chain QJ:



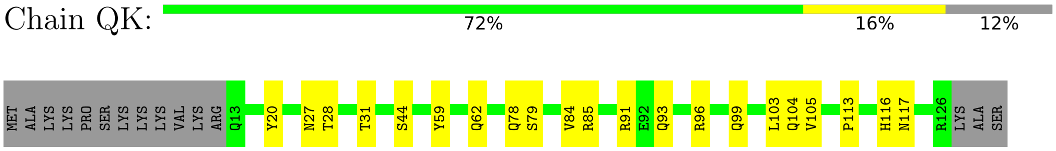
- Molecule 41: 30S ribosomal protein S10

Chain XJ:



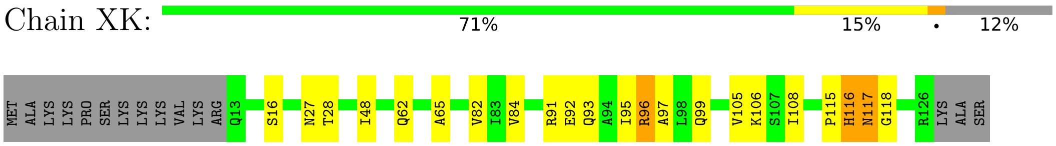
- Molecule 42: 30S ribosomal protein S11

Chain QK:



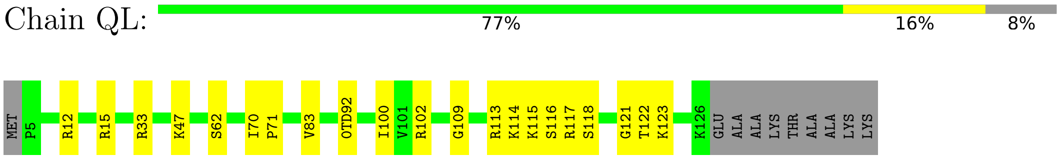
- Molecule 42: 30S ribosomal protein S11

Chain XK:



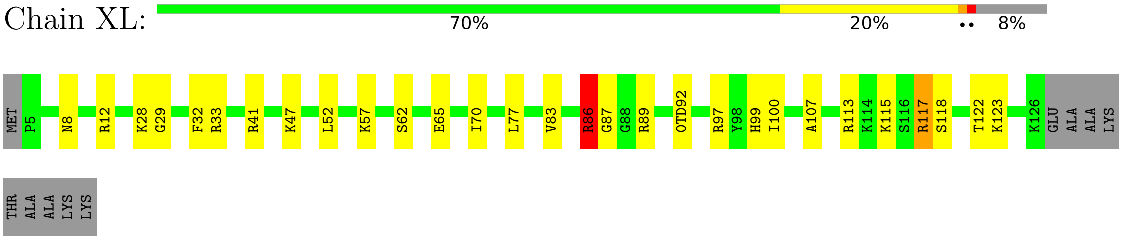
- Molecule 43: 30S ribosomal protein S12

Chain QL:



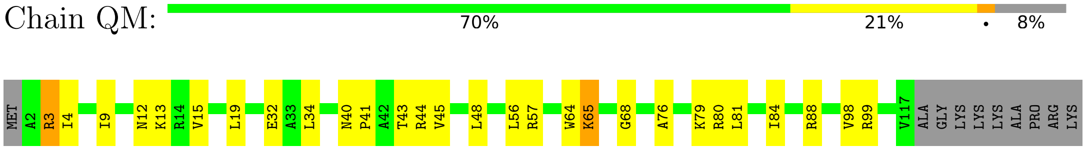
- Molecule 43: 30S ribosomal protein S12

Chain XL:



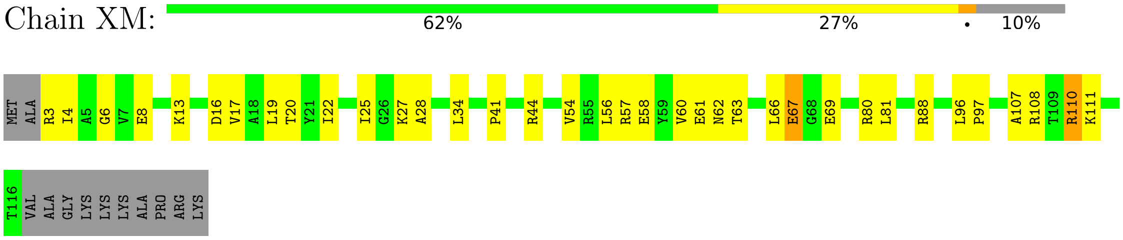
- Molecule 44: 30S ribosomal protein S13

Chain QM:



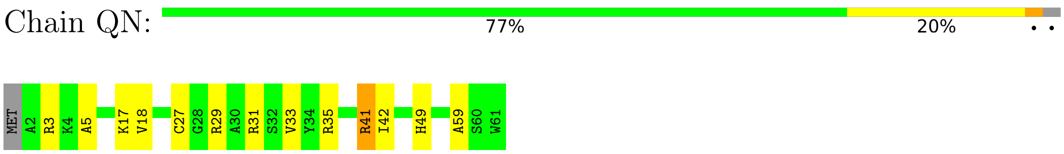
- Molecule 44: 30S ribosomal protein S13

Chain XM:



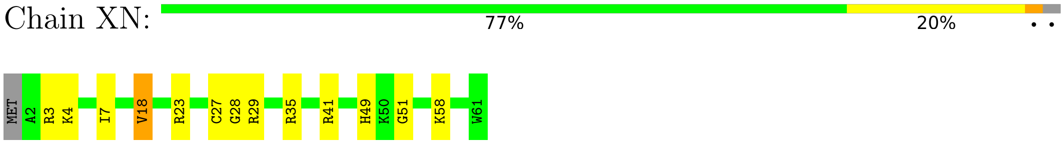
- Molecule 45: 30S ribosomal protein S14 type Z

Chain QN:



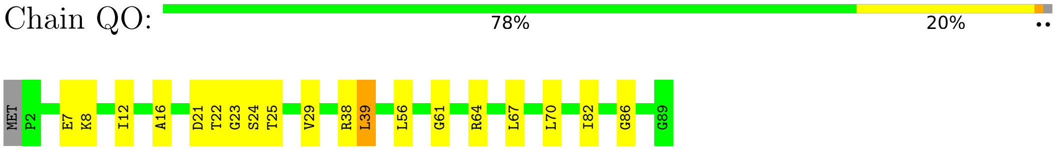
- Molecule 45: 30S ribosomal protein S14 type Z

Chain XN:



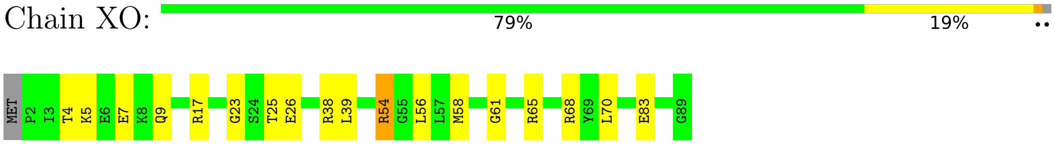
- Molecule 46: 30S ribosomal protein S15

Chain QO:



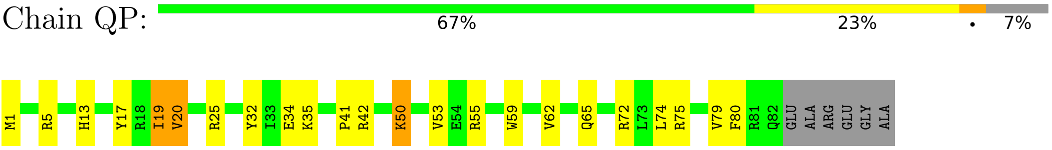
- Molecule 46: 30S ribosomal protein S15

Chain XO:



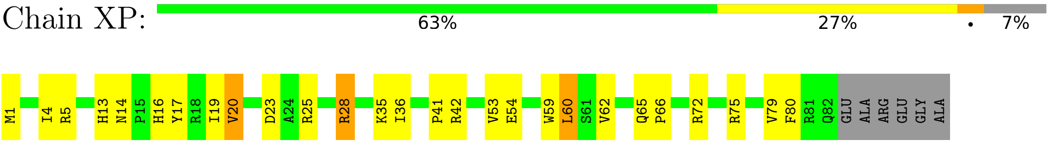
- Molecule 47: 30S ribosomal protein S16

Chain QP:



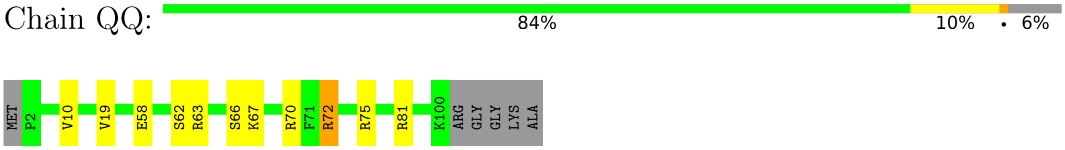
- Molecule 47: 30S ribosomal protein S16

Chain XP:

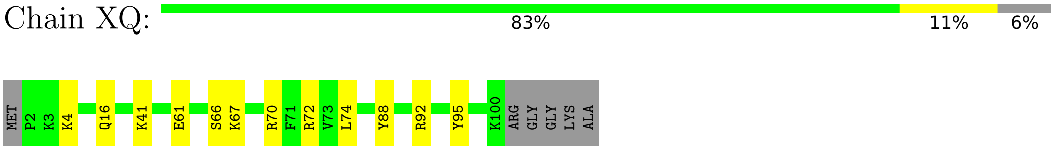


- Molecule 48: 30S ribosomal protein S17

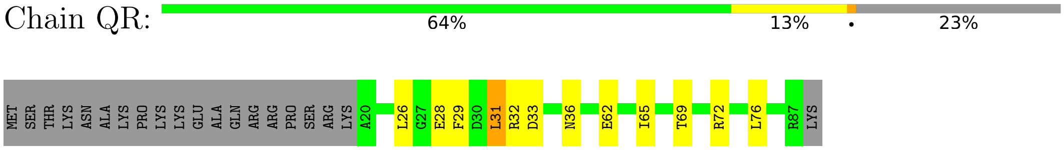
Chain QQ:



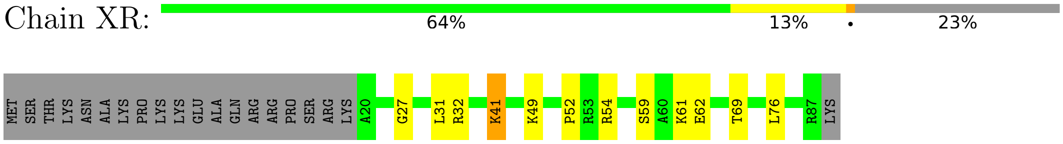
- Molecule 48: 30S ribosomal protein S17



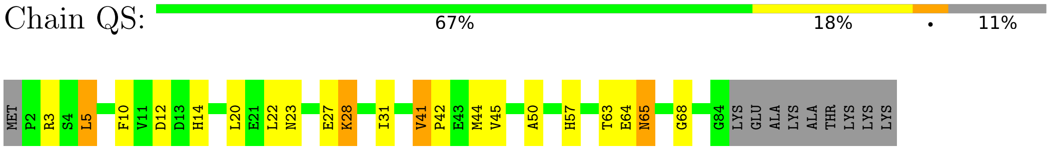
- Molecule 49: 30S ribosomal protein S18



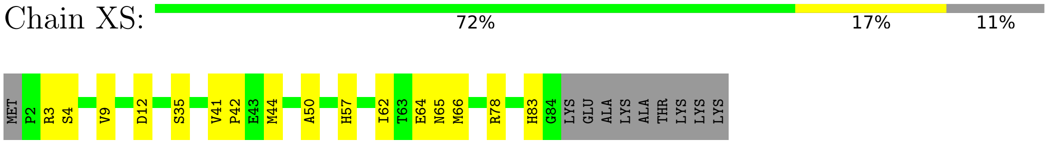
- Molecule 49: 30S ribosomal protein S18



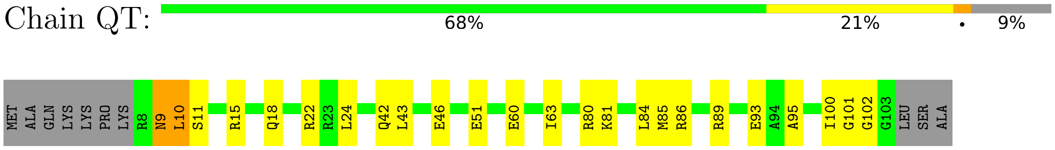
- Molecule 50: 30S ribosomal protein S19



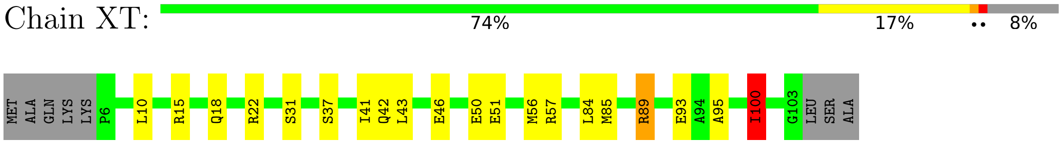
- Molecule 50: 30S ribosomal protein S19



- Molecule 51: 30S ribosomal protein S20

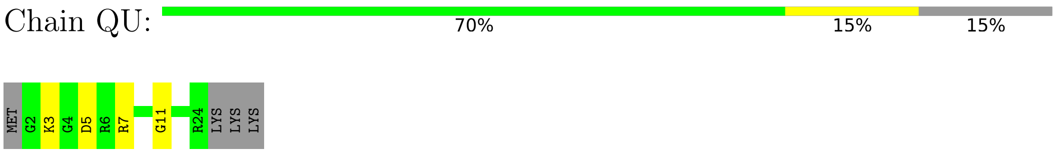


- Molecule 51: 30S ribosomal protein S20



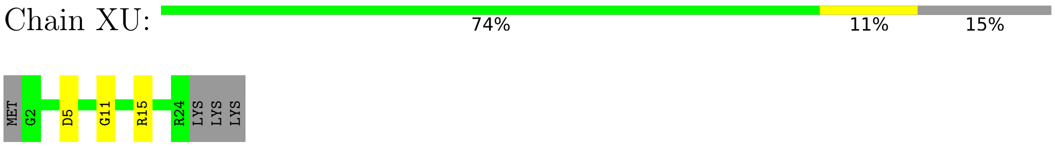
- Molecule 52: 30S ribosomal protein Thx

Chain QU:



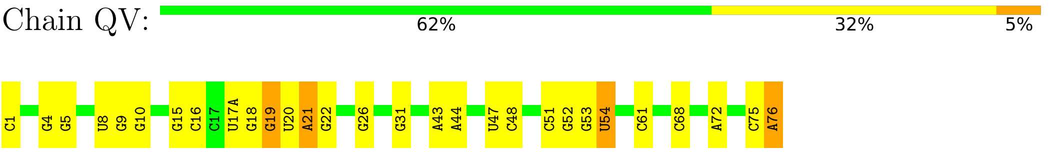
- Molecule 52: 30S ribosomal protein Thx

Chain XU:



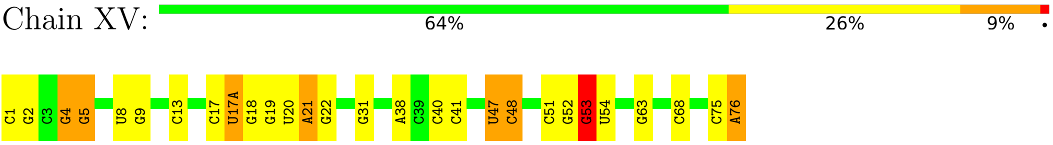
- Molecule 53: P-site tRNA fMet

Chain QV:



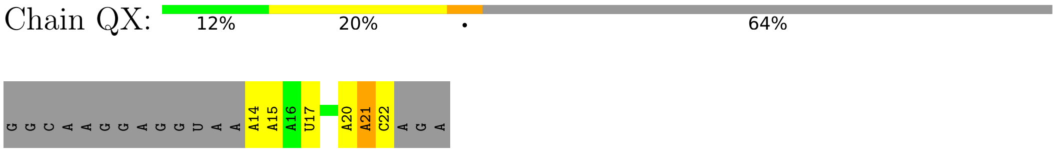
- Molecule 53: P-site tRNA fMet

Chain XV:



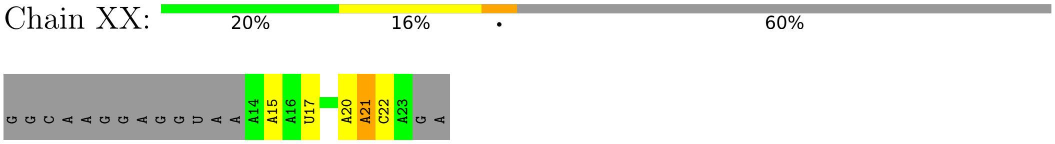
- Molecule 54: messenger RNA

Chain QX:



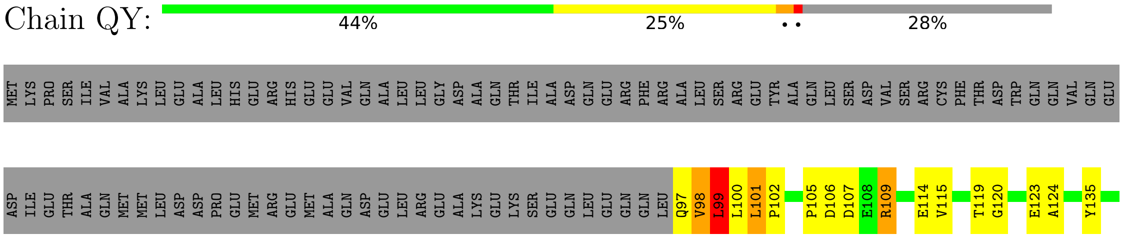
- Molecule 54: messenger RNA

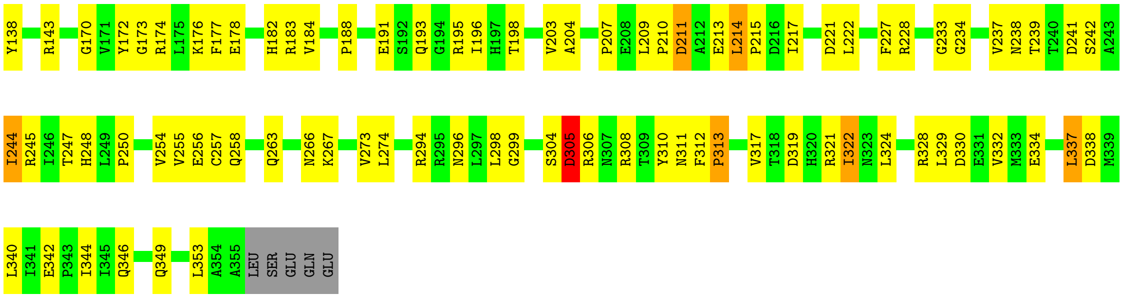
Chain XX:



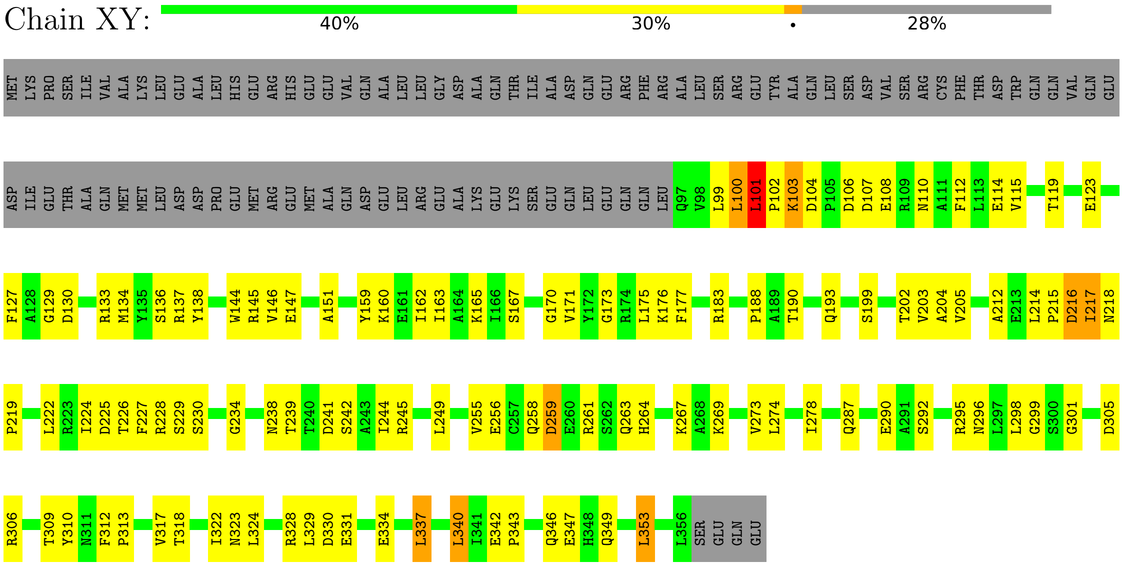
- Molecule 55: Peptide chain release factor 1

Chain QY:





- Molecule 55: Peptide chain release factor 1



4 Data and refinement statistics ⓘ

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.51Å 450.89Å 622.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.86 – 3.04	Depositor
% Data completeness (in resolution range)	99.3 (49.86-3.04)	Depositor
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 3.07Å)	Xtriage
Refinement program	PHENIX, PHENIX	Depositor
R, R_{free}	0.246 , 0.279	Depositor
Wilson B-factor (Å^2)	65.2	Xtriage
Anisotropy	0.225	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	294929	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: UR3, 5MU, 2MG, ZN, OMG, MG, PSU, 0TD, 2MA, 2MU, 4OC, 5MC, MA6, M2G, 7MG, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	RA	0.43	0/68901	1.00	55/107544 (0.1%)
1	YA	0.51	1/68901 (0.0%)	1.10	180/107544 (0.2%)
2	RB	0.35	0/2876	0.90	0/4486
2	YB	0.43	0/2878	1.00	1/4490 (0.0%)
3	RD	0.38	0/2181	0.64	1/2940 (0.0%)
3	YD	0.40	0/2186	0.66	1/2944 (0.0%)
4	RE	0.37	0/1592	0.60	0/2149
4	YE	0.38	0/1592	0.65	1/2149 (0.0%)
5	RF	0.36	0/1619	0.61	2/2193 (0.1%)
5	YF	0.42	0/1615	0.61	0/2188
6	RG	0.29	0/1451	0.54	0/1961
6	YG	0.34	0/1449	0.57	0/1957
7	RH	0.31	0/1356	0.54	1/1834 (0.1%)
7	YH	0.35	0/1350	0.57	1/1826 (0.1%)
8	RI	0.29	0/1109	0.57	0/1512
8	YI	0.34	0/1091	0.60	1/1490 (0.1%)
9	RN	0.36	0/1148	0.56	0/1547
9	YN	0.35	0/1144	0.55	0/1543
10	RO	0.34	0/943	0.58	0/1269
10	YO	0.42	1/943 (0.1%)	0.61	0/1269
11	RP	0.35	0/1152	0.60	0/1533
11	YP	0.41	0/1152	0.66	0/1533
12	RQ	0.35	0/1143	0.62	0/1527
12	YQ	0.40	0/1143	0.66	0/1527
13	RR	0.34	0/982	0.62	0/1312
13	YR	0.34	0/982	0.62	0/1312
14	RS	0.35	0/887	0.59	0/1180
14	YS	0.37	0/880	0.62	0/1172
15	RT	0.36	0/1105	0.67	1/1477 (0.1%)
15	YT	0.35	0/1097	0.63	1/1468 (0.1%)
16	RU	0.32	0/977	0.55	0/1301
16	YU	0.37	0/977	0.54	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	RV	0.35	0/786	0.57	0/1053
17	YV	0.37	0/782	0.61	0/1049
18	RW	0.35	0/897	0.57	0/1205
18	YW	0.37	0/897	0.57	0/1205
19	RX	0.39	0/764	0.59	0/1025
19	YX	0.39	0/764	0.61	0/1025
20	RY	0.34	0/823	0.64	0/1099
20	YY	0.39	0/823	0.63	0/1100
21	RZ	0.33	0/1620	0.55	0/2200
21	YZ	0.35	0/1590	0.59	0/2162
22	R0	0.39	0/616	0.70	1/821 (0.1%)
22	Y0	0.42	0/616	0.77	2/821 (0.2%)
23	R1	0.37	0/761	0.59	0/1013
23	Y1	0.38	0/766	0.64	0/1018
24	R2	0.29	0/590	0.50	0/781
24	Y2	0.35	0/594	0.54	0/785
25	R3	0.35	0/474	0.59	0/635
25	Y3	0.36	0/469	0.58	0/630
26	R4	0.37	0/559	0.70	0/754
26	Y4	0.40	0/549	0.70	1/741 (0.1%)
27	R5	0.44	0/473	0.64	0/639
27	Y5	0.41	0/469	0.60	0/635
28	R6	0.30	0/460	0.54	0/613
28	Y6	0.30	0/456	0.53	0/608
29	R7	0.40	0/426	0.67	0/561
29	Y7	0.42	0/426	0.69	0/561
30	R8	0.38	0/525	0.61	0/691
30	Y8	0.39	0/525	0.61	0/691
31	R9	0.32	0/310	0.68	0/407
31	Y9	0.33	0/310	0.68	0/407
32	QA	0.34	0/35795	0.88	12/55864 (0.0%)
32	XA	0.36	1/35890 (0.0%)	0.90	29/56012 (0.1%)
33	QB	0.34	0/1876	0.59	0/2533
33	XB	0.34	0/1860	0.60	1/2518 (0.0%)
34	QC	0.30	0/1582	0.53	0/2137
34	XC	0.36	1/1566 (0.1%)	0.61	0/2119
35	QD	0.33	0/1695	0.59	1/2274 (0.0%)
35	XD	0.32	0/1698	0.57	0/2277
36	QE	0.34	0/1149	0.55	0/1548
36	XE	0.32	0/1149	0.57	1/1548 (0.1%)
37	QF	0.31	0/827	0.55	0/1120
37	XF	0.33	0/829	0.64	1/1123 (0.1%)
38	QG	0.31	0/1254	0.46	0/1683

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
38	XG	0.31	0/1248	0.51	0/1676
39	QH	0.30	0/1118	0.53	0/1506
39	XH	0.32	0/1108	0.58	1/1494 (0.1%)
40	QI	0.32	0/1005	0.60	1/1351 (0.1%)
40	XI	0.31	0/985	0.54	0/1329
41	QJ	0.28	0/732	0.51	0/993
41	XJ	0.29	0/723	0.52	0/984
42	QK	0.30	0/849	0.55	0/1150
42	XK	0.30	0/848	0.57	0/1149
43	QL	0.39	0/937	0.61	0/1260
43	XL	0.36	0/937	0.67	0/1260
44	QM	0.30	0/924	0.57	0/1242
44	XM	0.31	0/905	0.55	0/1217
45	QN	0.34	0/501	0.59	1/664 (0.2%)
45	XN	0.35	0/501	0.58	0/664
46	QO	0.32	0/739	0.52	0/985
46	XO	0.35	0/739	0.56	0/985
47	QP	0.32	0/697	0.54	0/939
47	XP	0.30	0/693	0.57	0/935
48	QQ	0.33	0/836	0.55	0/1117
48	XQ	0.32	0/836	0.54	0/1117
49	QR	0.31	0/560	0.54	0/746
49	XR	0.32	0/560	0.59	0/746
50	QS	0.29	0/663	0.58	1/895 (0.1%)
50	XS	0.27	0/660	0.54	0/893
51	QT	0.31	0/734	0.51	0/969
51	XT	0.29	0/736	0.47	0/976
52	QU	0.30	0/203	0.58	0/266
52	XU	0.31	0/203	0.70	0/266
53	QV	0.34	0/1832	0.92	0/2855
53	XV	0.42	1/1836 (0.1%)	0.91	2/2859 (0.1%)
54	QX	0.39	0/216	0.83	0/334
54	XX	0.46	0/241	0.92	0/373
55	QY	0.36	0/2046	0.65	1/2759 (0.0%)
55	XY	0.40	0/2054	0.69	2/2770 (0.1%)
All	All	0.41	5/316497 (0.0%)	0.90	304/472893 (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
14	RS	0	1
33	QB	0	1
43	XL	0	1
55	QY	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	XV	1	C	OP3-P	-10.47	1.48	1.61
32	XA	68	G	O3'-P	-6.54	1.53	1.61
34	XC	173	VAL	C-N	6.47	1.46	1.34
10	YO	21	CYS	CB-SG	-5.52	1.72	1.81
1	YA	1046	A	N3-C4	-5.10	1.31	1.34

The worst 5 of 304 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	YA	277	C	N1-C2-O2	17.75	129.55	118.90
1	YA	210	C	C6-N1-C2	12.43	125.27	120.30
1	YA	277	C	N3-C2-O2	-11.59	113.79	121.90
1	YA	277	C	N3-C4-N4	-11.48	109.96	118.00
1	YA	277	C	C5-C4-N4	10.97	127.88	120.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	QB	231	GLU	Peptide
55	QY	305	ASP	Peptide
14	RS	58	LEU	Peptide
43	XL	86	ARG	Peptide

5.2 Too-close contacts (i)

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.

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	RA	61758	0	31144	585	0
1	YA	61758	0	31147	606	1
2	RB	2572	0	1305	11	0
2	YB	2573	0	1306	12	0
3	RD	2131	0	2207	49	0
3	YD	2136	0	2218	49	0
4	RE	1559	0	1618	34	0
4	YE	1559	0	1618	40	0
5	RF	1584	0	1625	37	0
5	YF	1580	0	1619	46	0
6	RG	1426	0	1445	30	0
6	YG	1424	0	1441	38	0
7	RH	1330	0	1407	20	0
7	YH	1324	0	1402	33	0
8	RI	1094	0	1127	22	0
8	YI	1076	0	1093	14	0
9	RN	1121	0	1195	16	0
9	YN	1117	0	1184	16	0
10	RO	933	0	996	17	0
10	YO	933	0	996	14	0
11	RP	1135	0	1212	22	0
11	YP	1135	0	1212	32	0
12	RQ	1122	0	1179	20	0
12	YQ	1122	0	1179	20	0
13	RR	968	0	1033	21	0
13	YR	968	0	1033	13	0
14	RS	877	0	938	12	0
14	YS	870	0	923	13	0
15	RT	1091	0	1151	25	0
15	YT	1083	0	1136	19	0
16	RU	959	0	1019	16	0
16	YU	959	0	1019	18	0
17	RV	775	0	841	13	0
17	YV	771	0	830	13	0
18	RW	886	0	940	12	0
18	YW	886	0	940	12	0
19	RX	750	0	814	16	0
19	YX	750	0	814	6	0
20	RY	810	0	894	15	0
20	YY	810	0	891	17	0
21	RZ	1587	0	1598	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	YZ	1557	0	1564	24	0
22	R0	608	0	622	12	0
22	Y0	608	0	622	15	0
23	R1	754	0	823	10	0
23	Y1	759	0	837	18	0
24	R2	588	0	643	11	1
24	Y2	592	0	654	7	0
25	R3	469	0	518	5	0
25	Y3	464	0	514	6	0
26	R4	546	0	523	27	0
26	Y4	536	0	516	26	0
27	R5	459	0	477	12	0
27	Y5	455	0	467	5	0
28	R6	453	0	475	7	0
28	Y6	449	0	471	7	0
29	R7	418	0	467	11	0
29	Y7	418	0	467	8	0
30	R8	517	0	582	17	0
30	Y8	517	0	582	19	0
31	R9	307	0	336	14	0
31	Y9	307	0	336	11	0
32	QA	32246	0	16294	307	0
32	XA	32331	0	16338	343	0
33	QB	1842	0	1862	54	0
33	XB	1825	0	1828	62	0
34	QC	1558	0	1557	33	0
34	XC	1542	0	1517	32	0
35	QD	1665	0	1690	60	0
35	XD	1668	0	1706	44	0
36	QE	1133	0	1191	28	0
36	XE	1133	0	1191	25	0
37	QF	814	0	808	20	0
37	XF	816	0	807	8	0
38	QG	1235	0	1249	18	0
38	XG	1229	0	1238	15	0
39	QH	1098	0	1143	20	0
39	XH	1088	0	1126	21	0
40	QI	986	0	990	28	0
40	XI	966	0	953	35	0
41	QJ	719	0	672	27	0
41	XJ	710	0	661	20	0
42	QK	834	0	838	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	XK	833	0	836	13	0
43	QL	932	0	981	18	0
43	XL	932	0	981	26	0
44	QM	914	0	954	23	0
44	XM	895	0	920	24	0
45	QN	492	0	529	11	0
45	XN	492	0	529	14	0
46	QO	728	0	760	12	0
46	XO	728	0	760	13	0
47	QP	681	0	697	19	0
47	XP	677	0	686	19	0
48	QQ	823	0	891	8	0
48	XQ	823	0	891	9	0
49	QR	555	0	618	11	0
49	XR	555	0	618	9	0
50	QS	648	0	658	17	0
50	XS	645	0	635	19	0
51	QT	732	0	809	15	0
51	XT	733	0	795	13	0
52	QU	199	0	208	3	0
52	XU	199	0	208	1	0
53	QV	1640	0	837	15	0
53	XV	1644	0	836	15	0
54	QX	193	0	98	5	0
54	XX	215	0	108	2	0
55	QY	2014	0	1980	73	0
55	XY	2022	0	1991	85	0
56	QA	262	0	0	0	0
56	QB	1	0	0	0	0
56	QD	2	0	0	0	0
56	QE	2	0	0	0	0
56	QF	1	0	0	0	0
56	QG	3	0	0	0	0
56	QH	1	0	0	0	0
56	QI	1	0	0	0	0
56	QJ	1	0	0	0	0
56	QL	2	0	0	0	0
56	QN	1	0	0	0	0
56	QO	1	0	0	0	0
56	QQ	1	0	0	0	0
56	QR	1	0	0	0	0
56	QT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	QV	6	0	0	0	0
56	R0	7	0	0	0	0
56	R1	5	0	0	0	0
56	R3	2	0	0	0	0
56	R5	1	0	0	0	0
56	R7	3	0	0	0	0
56	R9	1	0	0	0	0
56	RA	1032	0	0	0	0
56	RB	22	0	0	0	0
56	RD	15	0	0	0	0
56	RE	7	0	0	0	0
56	RF	11	0	0	0	0
56	RG	4	0	0	0	0
56	RN	2	0	0	0	0
56	RO	1	0	0	0	0
56	RP	2	0	0	0	0
56	RQ	5	0	0	0	0
56	RR	4	0	0	0	0
56	RS	1	0	0	0	0
56	RT	3	0	0	0	0
56	RU	3	0	0	0	0
56	RV	3	0	0	0	0
56	RW	2	0	0	0	0
56	RX	1	0	0	0	0
56	RY	1	0	0	0	0
56	XA	187	0	0	0	0
56	XE	2	0	0	0	0
56	XF	4	0	0	0	0
56	XJ	1	0	0	0	0
56	XL	1	0	0	0	0
56	XT	1	0	0	0	0
56	XV	4	0	0	0	0
56	XY	1	0	0	0	0
56	Y0	1	0	0	0	0
56	Y1	1	0	0	0	0
56	Y5	2	0	0	0	0
56	Y7	1	0	0	0	0
56	Y8	2	0	0	0	0
56	YA	749	0	0	0	0
56	YB	20	0	0	0	0
56	YD	9	0	0	0	0
56	YE	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	YF	2	0	0	0	0
56	YG	2	0	0	0	0
56	YI	1	0	0	0	0
56	YN	1	0	0	0	0
56	YO	1	0	0	0	0
56	YP	1	0	0	0	0
56	YQ	3	0	0	0	0
56	YR	1	0	0	0	0
56	YT	3	0	0	0	0
56	YV	1	0	0	0	0
56	YW	2	0	0	0	0
56	YX	1	0	0	0	0
57	QN	1	0	0	0	0
57	R4	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R9	1	0	0	0	0
57	RY	1	0	0	0	0
57	XN	1	0	0	0	0
57	Y4	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YY	1	0	0	0	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
All	All	294929	0	198658	3416	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 7.

The worst 5 of 3416 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)
1:RA:2552:2MU:C5	1:RA:2552:2MU:C4	1.74	1.65
1:YA:2552:2MU:C4	1:YA:2552:2MU:C5	1.75	1.56
32:XA:1003:G:H2’	32:XA:1004:A:H4’	1.40	1.03
1:YA:2131:G:H5”	1:YA:2132:U:H5’	1.46	0.98
26:Y4:59:PHE:HA	26:Y4:61:ARG:H	1.26	0.97

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)
24:R2:46:GLN:OE1	1:YA:277:C:O2'[3_555]	2.02	0.18

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	RD	273/276 (99%)	263 (96%)	10 (4%)	0	100	100
3	YD	273/276 (99%)	262 (96%)	11 (4%)	0	100	100
4	RE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	65
4	YE	202/206 (98%)	194 (96%)	8 (4%)	0	100	100
5	RF	201/210 (96%)	196 (98%)	5 (2%)	0	100	100
5	YF	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	29	65
6	RG	179/182 (98%)	168 (94%)	9 (5%)	2 (1%)	14	47
6	YG	179/182 (98%)	169 (94%)	9 (5%)	1 (1%)	25	60
7	RH	172/180 (96%)	164 (95%)	8 (5%)	0	100	100
7	YH	171/180 (95%)	163 (95%)	8 (5%)	0	100	100
8	RI	145/148 (98%)	134 (92%)	10 (7%)	1 (1%)	22	57
8	YI	144/148 (97%)	136 (94%)	8 (6%)	0	100	100
9	RN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	YN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
10	RO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	YO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
11	RP	147/150 (98%)	141 (96%)	5 (3%)	1 (1%)	22	57
11	YP	147/150 (98%)	141 (96%)	5 (3%)	1 (1%)	22	57
12	RQ	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
12	YQ	139/141 (99%)	136 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	RR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
13	YR	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	RS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	17	52
14	YS	108/112 (96%)	105 (97%)	3 (3%)	0	100	100
15	RT	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
15	YT	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
16	RU	114/118 (97%)	114 (100%)	0	0	100	100
16	YU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	RV	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
17	YV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	49
18	RW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	YW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	RX	93/96 (97%)	92 (99%)	1 (1%)	0	100	100
19	YX	93/96 (97%)	92 (99%)	0	1 (1%)	14	47
20	RY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
20	YY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
21	RZ	201/206 (98%)	196 (98%)	5 (2%)	0	100	100
21	YZ	199/206 (97%)	194 (98%)	5 (2%)	0	100	100
22	R0	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
22	Y0	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
23	R1	95/98 (97%)	94 (99%)	0	1 (1%)	14	47
23	Y1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	47
24	R2	68/72 (94%)	68 (100%)	0	0	100	100
24	Y2	68/72 (94%)	68 (100%)	0	0	100	100
25	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	R4	67/71 (94%)	55 (82%)	7 (10%)	5 (8%)	1	4
26	Y4	67/71 (94%)	56 (84%)	9 (13%)	2 (3%)	4	21
27	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	Y5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	R7	46/49 (94%)	46 (100%)	0	0	100	100
29	Y7	46/49 (94%)	46 (100%)	0	0	100	100
30	R8	62/65 (95%)	62 (100%)	0	0	100	100
30	Y8	62/65 (95%)	62 (100%)	0	0	100	100
31	R9	35/37 (95%)	35 (100%)	0	0	100	100
31	Y9	35/37 (95%)	35 (100%)	0	0	100	100
33	QB	229/256 (90%)	204 (89%)	17 (7%)	8 (4%)	3	18
33	XB	229/256 (90%)	203 (89%)	21 (9%)	5 (2%)	6	28
34	QC	204/239 (85%)	191 (94%)	13 (6%)	0	100	100
34	XC	204/239 (85%)	189 (93%)	14 (7%)	1 (0%)	29	65
35	QD	206/209 (99%)	196 (95%)	10 (5%)	0	100	100
35	XD	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
36	QE	146/162 (90%)	145 (99%)	1 (1%)	0	100	100
36	XE	146/162 (90%)	145 (99%)	1 (1%)	0	100	100
37	QF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	XF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	QG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
38	XG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
39	QH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
39	XH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
40	QI	125/128 (98%)	116 (93%)	9 (7%)	0	100	100
40	XI	124/128 (97%)	113 (91%)	9 (7%)	2 (2%)	9	37
41	QJ	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	4	20
41	XJ	94/105 (90%)	83 (88%)	10 (11%)	1 (1%)	14	47
42	QK	112/129 (87%)	105 (94%)	7 (6%)	0	100	100
42	XK	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	17	52
43	QL	119/132 (90%)	118 (99%)	1 (1%)	0	100	100
43	XL	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
44	QM	114/126 (90%)	105 (92%)	8 (7%)	1 (1%)	17	52
44	XM	112/126 (89%)	104 (93%)	7 (6%)	1 (1%)	17	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	QN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	XN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
46	QO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
46	XO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
47	QP	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
47	XP	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
48	QQ	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
48	XQ	97/105 (92%)	95 (98%)	2 (2%)	0	100	100
49	QR	66/88 (75%)	66 (100%)	0	0	100	100
49	XR	66/88 (75%)	66 (100%)	0	0	100	100
50	QS	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
50	XS	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
51	QT	94/106 (89%)	90 (96%)	3 (3%)	1 (1%)	14	47
51	XT	96/106 (91%)	90 (94%)	4 (4%)	2 (2%)	7	30
52	QU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	XU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
55	QY	257/360 (71%)	218 (85%)	21 (8%)	18 (7%)	1	5
55	XY	258/360 (72%)	215 (83%)	30 (12%)	13 (5%)	2	11
All	All	11955/12848 (93%)	11397 (95%)	481 (4%)	77 (1%)	25	60

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	R4	47	GLN
26	R4	49	PHE
33	QB	16	HIS
55	QY	98	VAL
55	QY	210	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	RD	214/218 (98%)	210 (98%)	4 (2%)	57	82
3	YD	215/218 (99%)	209 (97%)	6 (3%)	43	75
4	RE	164/166 (99%)	157 (96%)	7 (4%)	29	63
4	YE	164/166 (99%)	157 (96%)	7 (4%)	29	63
5	RF	160/166 (96%)	151 (94%)	9 (6%)	21	54
5	YF	159/166 (96%)	153 (96%)	6 (4%)	33	67
6	RG	144/156 (92%)	139 (96%)	5 (4%)	36	69
6	YG	142/156 (91%)	134 (94%)	8 (6%)	21	54
7	RH	144/148 (97%)	141 (98%)	3 (2%)	53	80
7	YH	143/148 (97%)	138 (96%)	5 (4%)	36	69
8	RI	111/124 (90%)	106 (96%)	5 (4%)	27	62
8	YI	108/124 (87%)	99 (92%)	9 (8%)	11	37
9	RN	119/119 (100%)	113 (95%)	6 (5%)	24	58
9	YN	118/119 (99%)	111 (94%)	7 (6%)	19	51
10	RO	100/100 (100%)	99 (99%)	1 (1%)	76	91
10	YO	100/100 (100%)	100 (100%)	0	100	100
11	RP	115/116 (99%)	110 (96%)	5 (4%)	29	63
11	YP	115/116 (99%)	109 (95%)	6 (5%)	23	57
12	RQ	111/111 (100%)	108 (97%)	3 (3%)	44	75
12	YQ	111/111 (100%)	107 (96%)	4 (4%)	35	68
13	RR	101/101 (100%)	95 (94%)	6 (6%)	19	51
13	YR	101/101 (100%)	95 (94%)	6 (6%)	19	51
14	RS	87/88 (99%)	84 (97%)	3 (3%)	37	70
14	YS	85/88 (97%)	82 (96%)	3 (4%)	36	69
15	RT	115/127 (91%)	110 (96%)	5 (4%)	29	63
15	YT	113/127 (89%)	109 (96%)	4 (4%)	36	69
16	RU	93/94 (99%)	91 (98%)	2 (2%)	52	79
16	YU	93/94 (99%)	92 (99%)	1 (1%)	73	90
17	RV	81/82 (99%)	77 (95%)	4 (5%)	25	59
17	YV	80/82 (98%)	76 (95%)	4 (5%)	24	58
18	RW	90/92 (98%)	86 (96%)	4 (4%)	28	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	YW	90/92 (98%)	86 (96%)	4 (4%)	28	63
19	RX	77/78 (99%)	76 (99%)	1 (1%)	69	88
19	YX	77/78 (99%)	76 (99%)	1 (1%)	69	88
20	RY	86/91 (94%)	85 (99%)	1 (1%)	71	89
20	YY	86/91 (94%)	84 (98%)	2 (2%)	50	78
21	RZ	169/179 (94%)	165 (98%)	4 (2%)	49	78
21	YZ	165/179 (92%)	163 (99%)	2 (1%)	71	89
22	R0	61/67 (91%)	59 (97%)	2 (3%)	38	71
22	Y0	61/67 (91%)	61 (100%)	0	100	100
23	R1	79/83 (95%)	76 (96%)	3 (4%)	33	67
23	Y1	81/83 (98%)	77 (95%)	4 (5%)	25	59
24	R2	65/67 (97%)	65 (100%)	0	100	100
24	Y2	66/67 (98%)	66 (100%)	0	100	100
25	R3	51/52 (98%)	48 (94%)	3 (6%)	19	51
25	Y3	50/52 (96%)	47 (94%)	3 (6%)	19	51
26	R4	58/63 (92%)	56 (97%)	2 (3%)	37	70
26	Y4	54/63 (86%)	50 (93%)	4 (7%)	13	42
27	R5	51/52 (98%)	48 (94%)	3 (6%)	19	51
27	Y5	50/52 (96%)	47 (94%)	3 (6%)	19	51
28	R6	51/52 (98%)	49 (96%)	2 (4%)	32	66
28	Y6	50/52 (96%)	49 (98%)	1 (2%)	55	81
29	R7	41/42 (98%)	39 (95%)	2 (5%)	25	59
29	Y7	41/42 (98%)	39 (95%)	2 (5%)	25	59
30	R8	54/55 (98%)	51 (94%)	3 (6%)	21	54
30	Y8	54/55 (98%)	51 (94%)	3 (6%)	21	54
31	R9	34/34 (100%)	34 (100%)	0	100	100
31	Y9	34/34 (100%)	34 (100%)	0	100	100
33	QB	191/220 (87%)	177 (93%)	14 (7%)	14	42
33	XB	187/220 (85%)	173 (92%)	14 (8%)	13	41
34	QC	144/188 (77%)	138 (96%)	6 (4%)	30	64
34	XC	140/188 (74%)	133 (95%)	7 (5%)	24	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	QD	171/181 (94%)	166 (97%)	5 (3%)	42	74
35	XD	172/181 (95%)	163 (95%)	9 (5%)	23	57
36	QE	114/123 (93%)	112 (98%)	2 (2%)	59	83
36	XE	114/123 (93%)	110 (96%)	4 (4%)	36	69
37	QF	85/90 (94%)	85 (100%)	0	100	100
37	XF	85/90 (94%)	84 (99%)	1 (1%)	71	89
38	QG	120/127 (94%)	115 (96%)	5 (4%)	30	64
38	XG	119/127 (94%)	116 (98%)	3 (2%)	47	77
39	QH	116/119 (98%)	112 (97%)	4 (3%)	37	70
39	XH	114/119 (96%)	111 (97%)	3 (3%)	46	76
40	QI	91/99 (92%)	85 (93%)	6 (7%)	16	47
40	XI	88/99 (89%)	83 (94%)	5 (6%)	20	53
41	QJ	68/92 (74%)	67 (98%)	1 (2%)	65	86
41	XJ	68/92 (74%)	68 (100%)	0	100	100
42	QK	83/99 (84%)	80 (96%)	3 (4%)	35	68
42	XK	83/99 (84%)	80 (96%)	3 (4%)	35	68
43	QL	96/108 (89%)	96 (100%)	0	100	100
43	XL	96/108 (89%)	92 (96%)	4 (4%)	30	64
44	QM	90/101 (89%)	88 (98%)	2 (2%)	52	79
44	XM	87/101 (86%)	84 (97%)	3 (3%)	37	70
45	QN	49/50 (98%)	45 (92%)	4 (8%)	11	37
45	XN	49/50 (98%)	48 (98%)	1 (2%)	55	81
46	QO	78/80 (98%)	77 (99%)	1 (1%)	69	88
46	XO	78/80 (98%)	76 (97%)	2 (3%)	46	76
47	QP	69/74 (93%)	66 (96%)	3 (4%)	29	63
47	XP	68/74 (92%)	64 (94%)	4 (6%)	19	51
48	QQ	94/97 (97%)	93 (99%)	1 (1%)	73	90
48	XQ	94/97 (97%)	92 (98%)	2 (2%)	53	80
49	QR	59/77 (77%)	57 (97%)	2 (3%)	37	70
49	XR	59/77 (77%)	58 (98%)	1 (2%)	60	84
50	QS	68/80 (85%)	65 (96%)	3 (4%)	28	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	XS	67/80 (84%)	67 (100%)	0	100	100
51	QT	71/82 (87%)	67 (94%)	4 (6%)	21	54
51	XT	70/82 (85%)	67 (96%)	3 (4%)	29	63
52	QU	18/22 (82%)	18 (100%)	0	100	100
52	XU	18/22 (82%)	17 (94%)	1 (6%)	21	54
55	QY	210/300 (70%)	206 (98%)	4 (2%)	57	82
55	XY	211/300 (70%)	202 (96%)	9 (4%)	29	63
All	All	9784/10664 (92%)	9432 (96%)	352 (4%)	35	68

5 of 352 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	YR	111	LEU
33	XB	226	ARG
15	YT	96	ARG
26	Y4	8	LYS
35	XD	118	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
20	YY	6	HIS
33	XB	78	GLN
47	XP	16	HIS
47	XP	14	ASN
50	QS	65	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	RA	2855/2915 (97%)	494 (17%)	22 (0%)
1	YA	2855/2915 (97%)	484 (16%)	24 (0%)
2	RB	119/122 (97%)	14 (11%)	0
2	YB	119/122 (97%)	13 (10%)	0
32	QA	1494/1521 (98%)	257 (17%)	15 (1%)
32	XA	1498/1521 (98%)	234 (15%)	16 (1%)
53	QV	76/77 (98%)	16 (21%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	XV	76/77 (98%)	16 (21%)	1 (1%)
54	QX	8/25 (32%)	4 (50%)	0
54	XX	9/25 (36%)	4 (44%)	0
All	All	9109/9320 (97%)	1536 (16%)	78 (0%)

5 of 1536 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	RA	10	G
1	RA	12	U
1	RA	36	G
1	RA	45	C
1	RA	59	U

5 of 78 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	YA	2172	U
32	XA	992	U
1	YA	2430	A
32	XA	560	U
32	XA	1256	A

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

48 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	$\#\|Z\| > 2$
1	5MC	YA	1942	1	18,22,23	3.71	6 (33%)	26,32,35	1.56	5 (19%)
32	2MG	XA	1207	32	18,26,27	2.84	6 (33%)	16,38,41	2.32	4 (25%)
1	OMG	YA	2251	53,56,1	18,26,27	2.74	7 (38%)	19,38,41	2.59	7 (36%)
32	5MC	QA	1404	32	18,22,23	3.91	6 (33%)	26,32,35	1.51	3 (11%)
1	2MU	YA	2552	56,1	19,22,24	6.01	13 (68%)	26,31,36	3.26	9 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
32	5MC	QA	1407	32	18,22,23	3.88	6 (33%)	26,32,35	1.46	3 (11%)
32	MA6	QA	1518	32	19,26,27	1.27	2 (10%)	18,38,41	3.29	2 (11%)
32	MA6	QA	1519	32	19,26,27	1.28	3 (15%)	18,38,41	3.53	2 (11%)
1	PSU	YA	1917	1	18,21,22	0.96	1 (5%)	22,30,33	1.69	4 (18%)
32	M2G	QA	966	32	20,27,28	3.94	6 (30%)	22,40,43	1.84	5 (22%)
32	7MG	XA	527	56,32	22,26,27	5.95	10 (45%)	29,39,42	3.61	12 (41%)
32	4OC	QA	1402	32	20,23,24	3.23	7 (35%)	26,32,35	1.20	2 (7%)
1	PSU	YA	2605	1	18,21,22	1.01	1 (5%)	22,30,33	1.42	3 (13%)
1	2MU	RA	2552	56,1	19,22,24	5.97	12 (63%)	26,31,36	3.11	10 (38%)
32	5MC	QA	1400	32	18,22,23	3.82	6 (33%)	26,32,35	1.36	3 (11%)
32	UR3	QA	1498	32	19,22,23	3.09	6 (31%)	26,32,35	1.71	5 (19%)
1	PSU	YA	1911	1	18,21,22	1.06	1 (5%)	22,30,33	1.61	5 (22%)
32	5MC	XA	1404	32	18,22,23	3.79	6 (33%)	26,32,35	1.55	4 (15%)
32	5MC	XA	1407	32	18,22,23	3.94	6 (33%)	26,32,35	1.76	6 (23%)
1	5MU	RA	1939	1	19,22,23	4.79	5 (26%)	28,32,35	3.71	8 (28%)
1	PSU	RA	1911	1	18,21,22	1.01	1 (5%)	22,30,33	1.52	4 (18%)
32	4OC	XA	1402	32	20,23,24	3.09	7 (35%)	26,32,35	1.34	4 (15%)
1	PSU	RA	2605	1	18,21,22	1.07	1 (5%)	22,30,33	1.82	3 (13%)
32	PSU	XA	516	32	18,21,22	1.02	1 (5%)	22,30,33	1.57	4 (18%)
32	UR3	XA	1498	56,32	19,22,23	3.03	6 (31%)	26,32,35	1.61	3 (11%)
1	PSU	RA	1917	1	18,21,22	1.07	1 (5%)	22,30,33	1.50	4 (18%)
32	7MG	QA	527	56,32	22,26,27	6.10	10 (45%)	29,39,42	3.77	12 (41%)
43	0TD	XL	92	43	7,9,10	1.14	0	6,11,13	2.67	4 (66%)
32	MA6	XA	1518	32	19,26,27	1.16	2 (10%)	18,38,41	3.42	2 (11%)
32	5MC	QA	967	32	18,22,23	3.92	6 (33%)	26,32,35	1.46	4 (15%)
32	2MG	QA	1207	32	18,26,27	2.92	6 (33%)	16,38,41	2.43	4 (25%)
1	4OC	YA	1920	1	19,22,24	3.10	7 (36%)	26,31,35	1.21	3 (11%)
1	5MC	YA	1962	56,1	18,22,23	3.57	6 (33%)	26,32,35	1.32	4 (15%)
32	5MC	XA	1400	32	18,22,23	3.85	6 (33%)	26,32,35	1.67	4 (15%)
1	4OC	RA	1920	1	19,22,24	3.26	7 (36%)	26,31,35	1.26	3 (11%)
1	5MU	YA	1915	1	19,22,23	5.14	6 (31%)	28,32,35	3.54	11 (39%)
1	5MU	YA	1939	56,1	19,22,23	4.86	5 (26%)	28,32,35	4.07	9 (32%)
32	PSU	QA	516	56,32	18,21,22	1.15	1 (5%)	22,30,33	1.49	5 (22%)
43	0TD	QL	92	43	7,9,10	1.21	0	6,11,13	3.24	4 (66%)
32	M2G	XA	966	32	20,27,28	3.74	6 (30%)	22,40,43	1.88	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
32	5MC	XA	967	32	18,22,23	3.90	6 (33%)	26,32,35	1.54	5 (19%)
1	5MU	RA	1915	1	19,22,23	5.09	6 (31%)	28,32,35	3.43	10 (35%)
32	MA6	XA	1519	32	19,26,27	1.44	2 (10%)	18,38,41	4.11	2 (11%)
1	5MC	RA	1962	56,1	18,22,23	3.66	6 (33%)	26,32,35	1.27	3 (11%)
1	5MC	RA	1942	56,1	18,22,23	3.78	6 (33%)	26,32,35	1.32	3 (11%)
1	2MA	YA	2503	56,1	17,25,26	2.65	5 (29%)	17,37,40	2.35	4 (23%)
1	OMG	RA	2251	53,56,1	18,26,27	2.72	6 (33%)	19,38,41	2.71	6 (31%)
1	2MA	RA	2503	56,1	17,25,26	2.75	5 (29%)	17,37,40	2.33	4 (23%)

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
1	5MC	YA	1942	1	-	0/7/25/26	0/2/2/2
32	2MG	XA	1207	32	-	0/5/27/28	0/3/3/3
1	OMG	YA	2251	53,56,1	-	0/5/27/28	0/3/3/3
32	5MC	QA	1404	32	-	0/7/25/26	0/2/2/2
1	2MU	YA	2552	56,1	-	0/9/27/28	0/2/2/2
32	5MC	QA	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	QA	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	QA	1519	32	-	3/7/29/30	0/3/3/3
1	PSU	YA	1917	1	-	0/7/25/26	0/2/2/2
32	M2G	QA	966	32	-	0/7/29/30	0/3/3/3
32	7MG	XA	527	56,32	-	2/7/37/38	0/3/3/3
32	4OC	QA	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	YA	2605	1	-	0/7/25/26	0/2/2/2
1	2MU	RA	2552	56,1	-	0/9/27/28	0/2/2/2
32	5MC	QA	1400	32	-	2/7/25/26	0/2/2/2
32	UR3	QA	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	YA	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	XA	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	XA	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	RA	1939	1	-	2/7/25/26	0/2/2/2
1	PSU	RA	1911	1	-	0/7/25/26	0/2/2/2
32	4OC	XA	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	RA	2605	1	-	0/7/25/26	0/2/2/2
32	PSU	XA	516	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	XA	1498	56,32	-	0/7/25/26	0/2/2/2
1	PSU	RA	1917	1	-	0/7/25/26	0/2/2/2
32	7MG	QA	527	56,32	-	2/7/37/38	0/3/3/3
43	0TD	XL	92	43	-	3/7/12/14	-
32	MA6	XA	1518	32	-	1/7/29/30	0/3/3/3
32	5MC	QA	967	32	-	0/7/25/26	0/2/2/2
32	2MG	QA	1207	32	-	0/5/27/28	0/3/3/3
1	4OC	YA	1920	1	-	1/9/27/30	0/2/2/2
1	5MC	YA	1962	56,1	-	0/7/25/26	0/2/2/2
32	5MC	XA	1400	32	-	2/7/25/26	0/2/2/2
1	4OC	RA	1920	1	-	0/9/27/30	0/2/2/2
1	5MU	YA	1915	1	-	2/7/25/26	0/2/2/2
1	5MU	YA	1939	56,1	-	0/7/25/26	0/2/2/2
32	PSU	QA	516	56,32	-	0/7/25/26	0/2/2/2
43	0TD	QL	92	43	-	1/7/12/14	-
32	M2G	XA	966	32	-	0/7/29/30	0/3/3/3
32	5MC	XA	967	32	-	0/7/25/26	0/2/2/2
1	5MU	RA	1915	1	-	2/7/25/26	0/2/2/2
32	MA6	XA	1519	32	-	3/7/29/30	0/3/3/3
1	5MC	RA	1962	56,1	-	0/7/25/26	0/2/2/2
1	5MC	RA	1942	56,1	-	0/7/25/26	0/2/2/2
1	2MA	YA	2503	56,1	-	2/3/25/26	0/3/3/3
1	OMG	RA	2251	53,56,1	-	0/5/27/28	0/3/3/3
1	2MA	RA	2503	56,1	-	1/3/25/26	0/3/3/3

The worst 5 of 243 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	QA	527	7MG	C8-N9	19.67	1.56	1.46
32	XA	527	7MG	C8-N9	18.81	1.56	1.46
1	YA	2552	2MU	C5-C4	14.17	1.75	1.43
1	RA	2552	2MU	C5-C4	14.11	1.74	1.43
32	QA	966	M2G	C2-N3	13.73	1.47	1.30

The worst 5 of 235 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	XA	1519	MA6	N1-C6-N6	-16.79	99.39	117.06
1	YA	1939	5MU	C5-C4-N3	14.60	127.77	115.31
32	QA	1519	MA6	N1-C6-N6	-13.43	102.92	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	RA	1939	5MU	C5-C4-N3	13.26	126.63	115.31
32	XA	1518	MA6	N1-C6-N6	-13.13	103.24	117.06

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	RA	1915	5MU	O4'-C1'-N1-C2
1	RA	1915	5MU	O4'-C1'-N1-C6
32	QA	527	7MG	C3'-C4'-C5'-O5'
32	QA	1402	4OC	O4'-C4'-C5'-O5'
32	QA	1519	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

16 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	YA	2251	OMG	1	0
1	YA	2552	2MU	3	0
32	QA	1518	MA6	1	0
32	QA	1519	MA6	2	0
32	QA	1402	4OC	1	0
1	RA	2552	2MU	3	0
1	RA	1917	PSU	1	0
32	XA	1518	MA6	5	0
1	YA	1962	5MC	2	0
1	RA	1920	4OC	1	0
1	YA	1939	5MU	1	0
32	XA	1519	MA6	4	0
1	RA	1962	5MC	1	0
1	RA	1942	5MC	1	0
1	RA	2251	OMG	1	0
1	RA	2503	2MA	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2450 ligands modelled in this entry, 2448 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	SF4	QD	302	35	0,12,12	-	-	-		
58	SF4	XD	301	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	QD	302	35	-	-	0/6/5/5
58	SF4	XD	301	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.