



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 6, 2020 – 06:06 am BST

PDB ID : 6OXI  
Title : Dimeric E.coli YoeB bound to Thermus thermophilus 70S post-cleavage (UAA)  
Authors : Pavelich, I.J.; Hoffer, E.D.; Maehigashi, T.; Dunham, C.M.  
Deposited on : 2019-05-13  
Resolution : 3.50 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 : **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) : 2.11

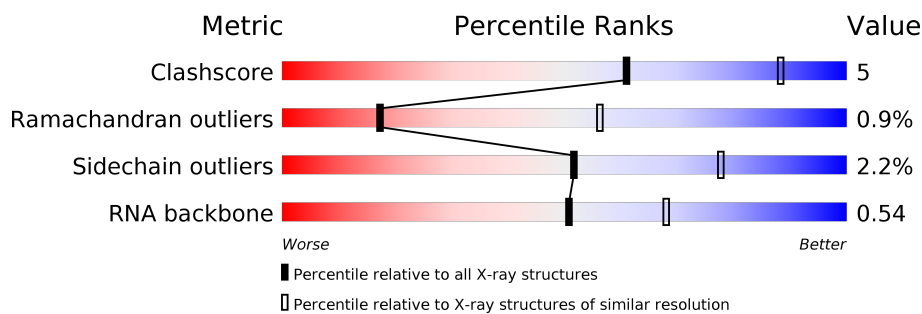
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RNA backbone	3102	1002 (4.00-3.00)


























The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	QA	1521	61% 31% 7% ..
1	XA	1521	63% 28% 8% .
2	QB	256	70% 19% . . 8%
2	XB	256	76% 15% . 8%
3	QC	239	75% 10% 14%
3	XC	239	72% 13% . 14%
4	QD	209	76% 22% .













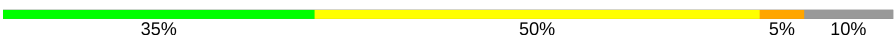












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Mol	Chain	Length	Quality of chain
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	
15	XO	89	
16	QP	88	
16	XP	88	















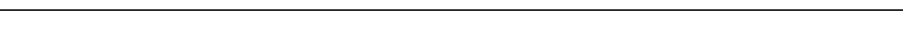




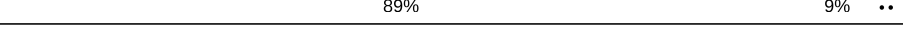





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Mol	Chain	Length	Quality of chain
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	20	
23	XX	20	
24	QY	84	
24	QZ	84	
24	XY	84	
24	XZ	84	
25	R0	85	
25	Y0	85	
26	R1	98	
26	Y1	98	
27	R2	72	
27	Y2	72	
28	R3	60	

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Mol	Chain	Length	Quality of chain
28	Y3	60	 83% 15% .
29	R4	71	 59% 30% 6% . .
29	Y4	71	 76% 18% . .
30	R5	60	 72% 27% .
30	Y5	60	 85% 13% .
31	R6	54	 72% 22% . .
31	Y6	54	 85% 13% .
32	R7	49	 88% 8% .
32	Y7	49	 84% 14% .
33	R8	65	 74% 17% 6% . .
33	Y8	65	 71% 23% 5% .
34	R9	37	 70% 30%
34	Y9	37	 81% 19%
35	RA	2915	 61% 31% 6% . .
35	YA	2915	 64% 29% 6% . .
36	RB	124	 57% 33% . . .
36	YB	124	 63% 24% 9% . .
37	RD	276	 76% 20% . .
37	YD	276	 89% 9% . .
38	RE	206	 73% 25% . .
38	YE	206	 81% 18% .
39	RF	210	 87% 9% .
39	YF	210	 78% 17% . .
40	RG	182	 80% 18% . . .
40	YG	182	 80% 18% . . .

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

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Mol	Chain	Length	Quality of chain
53	YX	96	
54	RY	110	
54	YY	110	
55	RZ	206	
55	YZ	206	
56	ZA	3	
56	ZB	3	

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 295153 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1510	Total	C	N	O	P	0	0	0
			32452	14444	6009	10489	1510			
1	XA	1507	Total	C	N	O	P	0	0	0
			32389	14416	5999	10467	1507			

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	XS	83	Total	C	N	O	S	0	0	0
			656	418	123	113	2			

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

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

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

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

- Molecule 22 is a RNA chain called P-site tRNA-fMet.

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

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	18	Total	C	N	O	P	0	0	0
			394	176	79	121	18			
23	XX	18	Total	C	N	O	P	0	0	0
			394	176	79	121	18			

- Molecule 24 is a protein called Addiction module toxin, Txe/YoeB family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
24	QZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
24	XY	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
24	XZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			

- Molecule 25 is a protein called 50S ribosomal protein L27.

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

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R1	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			
26	Y1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 27 is a protein called 50S ribosomal protein L29.

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

- Molecule 28 is a protein called 50S ribosomal protein L30.

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

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	R4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			
29	Y4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			

- Molecule 30 is a protein called 50S ribosomal protein L32.

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

- Molecule 31 is a protein called 50S ribosomal protein L33.

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

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

- Molecule 32 is a protein called 50S ribosomal protein L34.

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

- Molecule 33 is a protein called 50S ribosomal protein L35.

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

- Molecule 34 is a protein called 50S ribosomal protein L36.

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

- Molecule 35 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RA	2891	Total	C	N	O	P	0	0	0
			62266	27713	11649	20014	2890			
35	YA	2878	Total	C	N	O	P	0	0	0
			61981	27587	11589	19928	2877			

- Molecule 36 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			
36	YB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			

- Molecule 37 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
37	YD	274	Total	C	N	O	S	0	0	0
			2135	1347	426	359	3			

- Molecule 38 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
38	YE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 39 is a protein called 50S ribosomal protein L4.

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

- Molecule 40 is a protein called 50S ribosomal protein L5.

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

- Molecule 41 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
41	YH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 42 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RI	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
42	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 43 is a protein called 50S ribosomal protein L13.

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

- Molecule 44 is a protein called 50S ribosomal protein L14.

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

- Molecule 45 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
45	YP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 46 is a protein called 50S ribosomal protein L16.

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

- Molecule 47 is a protein called 50S ribosomal protein L17.

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

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

- Molecule 48 is a protein called 50S ribosomal protein L18.

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

- Molecule 49 is a protein called 50S ribosomal protein L19.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L21.

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

- Molecule 52 is a protein called 50S ribosomal protein L22.

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

- Molecule 53 is a protein called 50S ribosomal protein L23.

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

- Molecule 54 is a protein called 50S ribosomal protein L24.

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

- Molecule 55 is a protein called 50S ribosomal protein L25.

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

- Molecule 56 is a RNA chain called CCPuro.

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

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	93	Total	Mg	0	0
			93	93		
57	YV	1	Total	Mg	0	0
			1	1		
57	RP	1	Total	Mg	0	0
			1	1		
57	YA	335	Total	Mg	0	0
			335	335		

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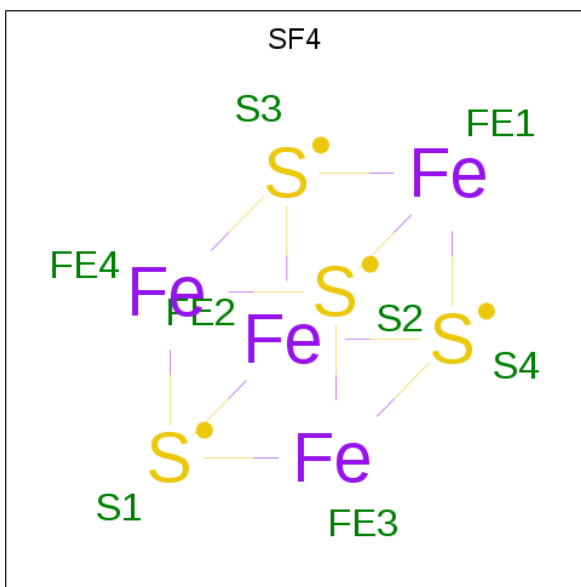
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y5	1	Total 1	Mg 1	0	0
57	YR	1	Total 1	Mg 1	0	0
57	Y9	1	Total 1	Mg 1	0	0
57	QD	1	Total 1	Mg 1	0	0
57	RN	1	Total 1	Mg 1	0	0
57	XE	1	Total 1	Mg 1	0	0
57	Y1	1	Total 1	Mg 1	0	0
57	YD	4	Total 4	Mg 4	0	0
57	QV	3	Total 3	Mg 3	0	0
57	YO	1	Total 1	Mg 1	0	0
57	XA	99	Total 99	Mg 99	0	0
57	RQ	4	Total 4	Mg 4	0	0
57	R0	2	Total 2	Mg 2	0	0
57	RO	1	Total 1	Mg 1	0	0
57	Y0	2	Total 2	Mg 2	0	0
57	YG	1	Total 1	Mg 1	0	0
57	YQ	5	Total 5	Mg 5	0	0
57	RY	1	Total 1	Mg 1	0	0
57	XF	1	Total 1	Mg 1	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RD	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	RA	302	Total 302	Mg 302	0	0
57	Y3	1	Total 1	Mg 1	0	0
57	YF	1	Total 1	Mg 1	0	0
57	YP	1	Total 1	Mg 1	0	0
57	RE	1	Total 1	Mg 1	0	0
57	XL	1	Total 1	Mg 1	0	0
57	YB	3	Total 3	Mg 3	0	0
57	QY	1	Total 1	Mg 1	0	0
57	XV	4	Total 4	Mg 4	0	0
57	RB	3	Total 3	Mg 3	0	0
57	R3	1	Total 1	Mg 1	0	0
57	QE	1	Total 1	Mg 1	0	0
57	XM	1	Total 1	Mg 1	0	0
57	YE	5	Total 5	Mg 5	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

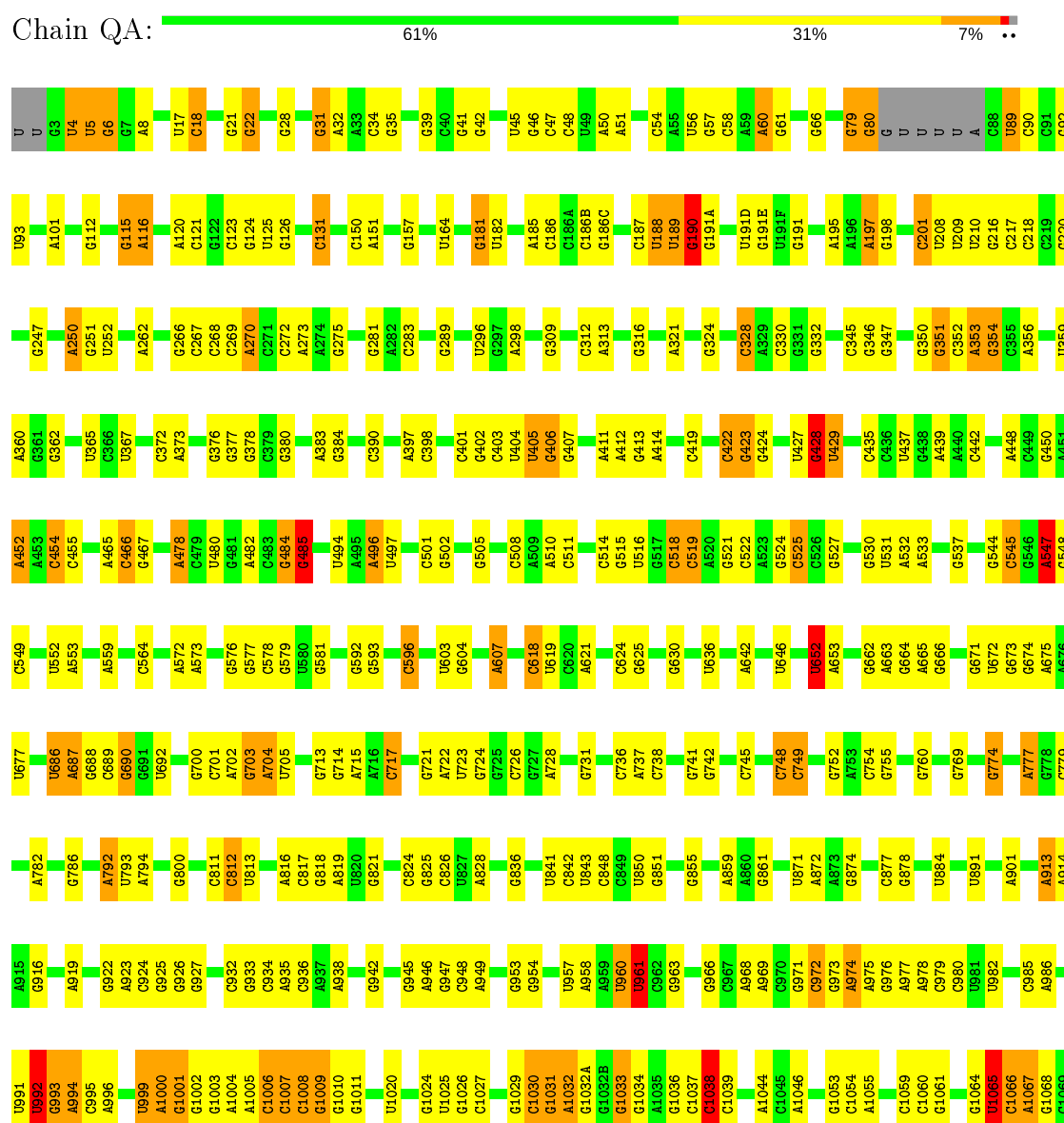
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Y6	1	Total	Zn	0	0
			1	1		
59	QN	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		
59	Y4	1	Total	Zn	0	0
			1	1		
59	R6	1	Total	Zn	0	0
			1	1		
59	R5	1	Total	Zn	0	0
			1	1		
59	R4	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		

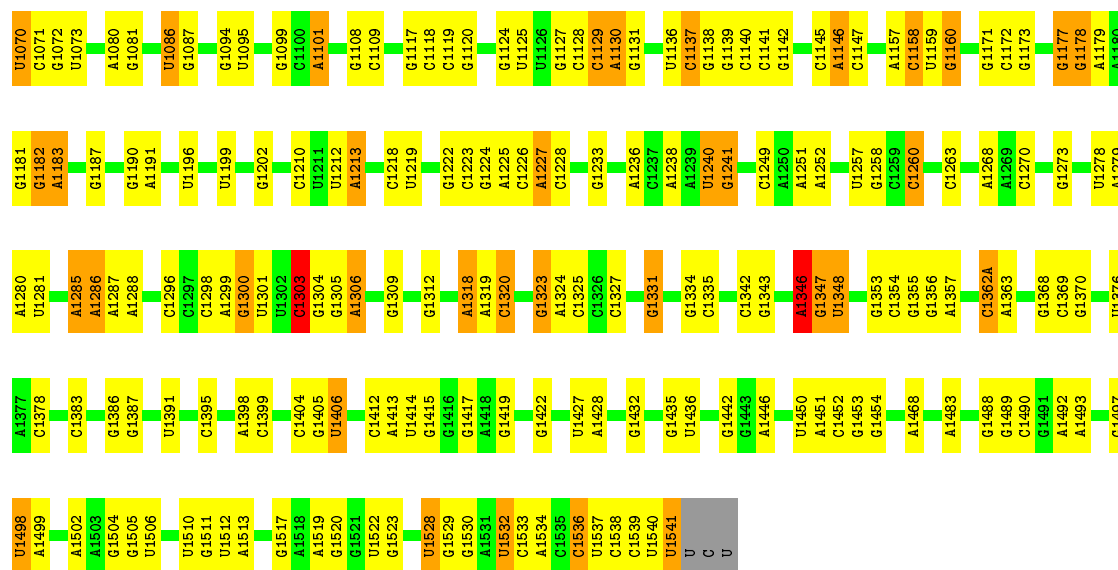
### 3 Residue-property plots

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. 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.

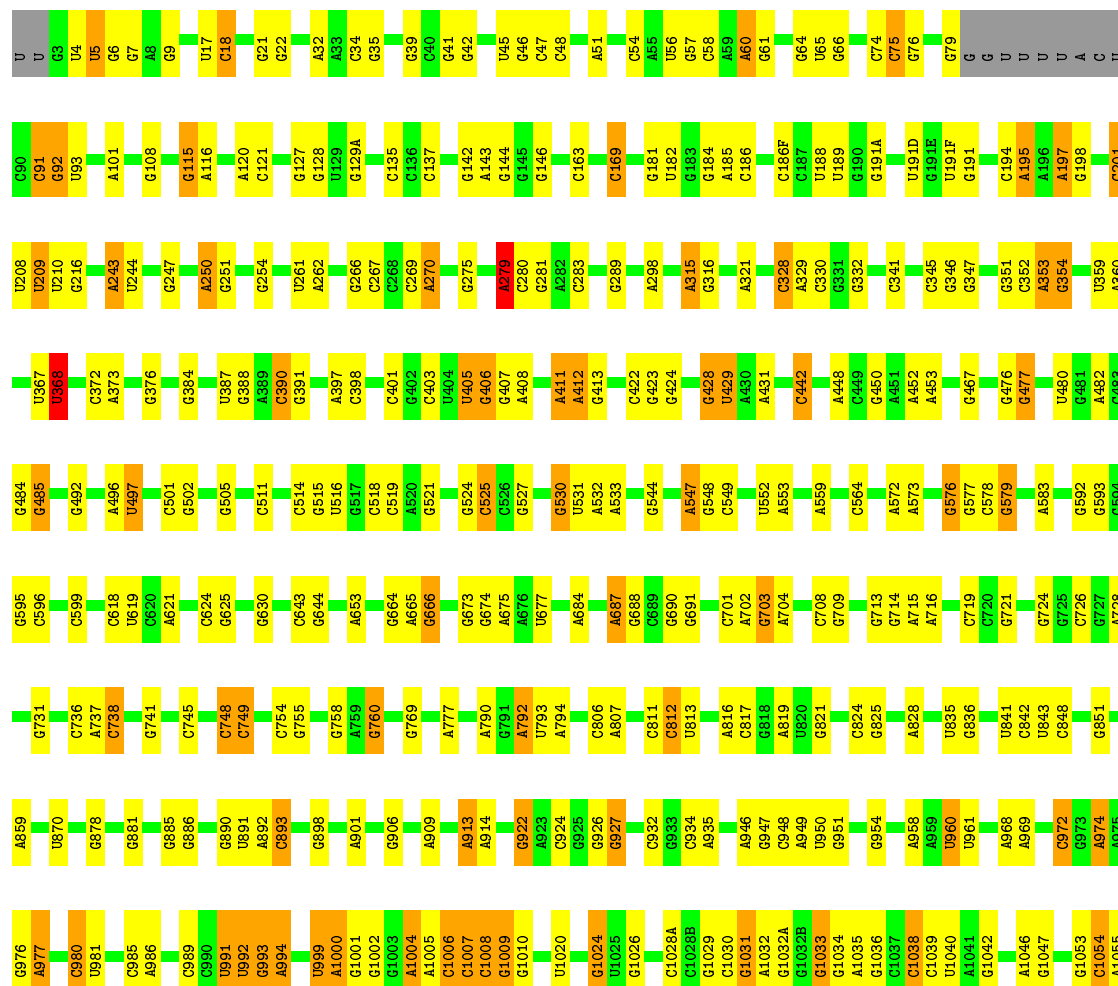
#### • Molecule 1: 16S rRNA

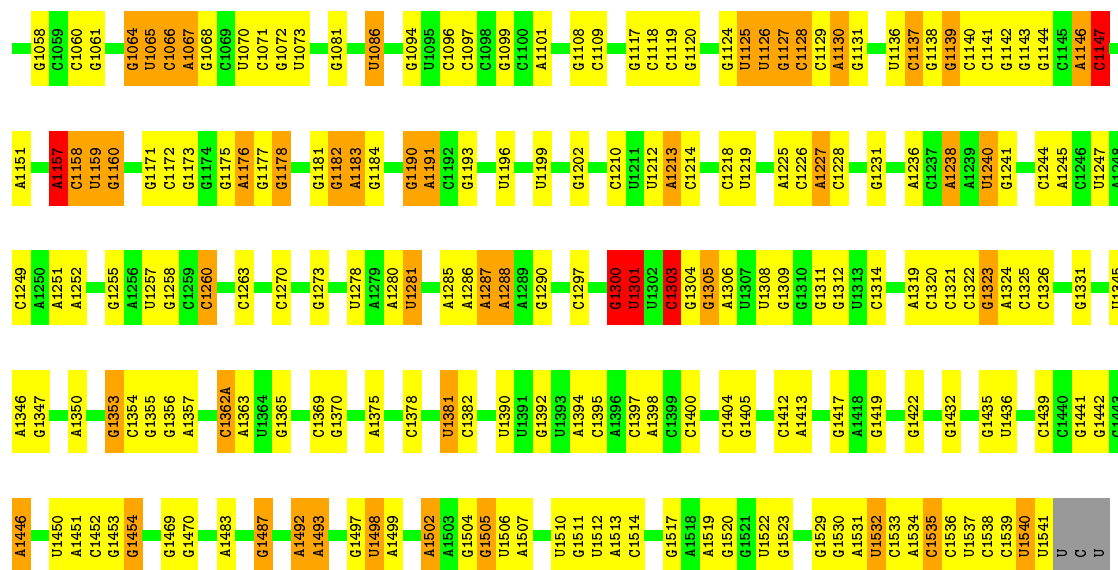




• Molecule 1: 16S rRNA

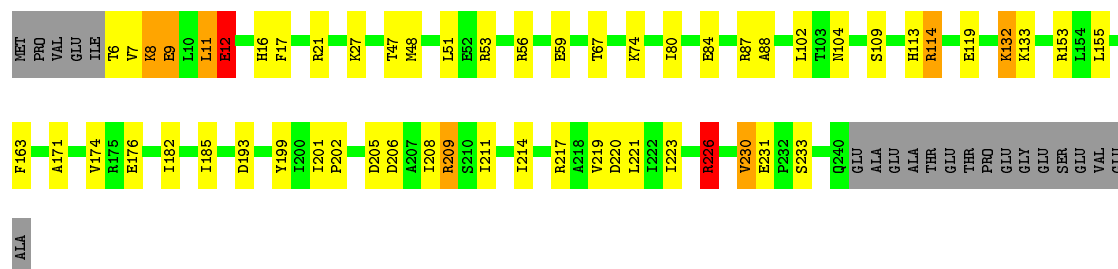
Chain XA: 63% 28% 8% •





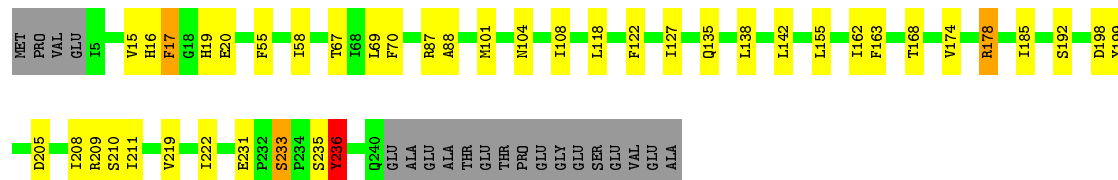
- Molecule 2: 30S ribosomal protein S2

Chain QB: 70% 19% 8%



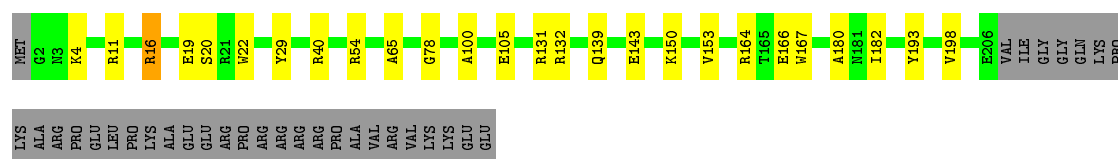
- Molecule 2: 30S ribosomal protein S2

Chain XB: 76% 15% 8%



- Molecule 3: 30S ribosomal protein S3

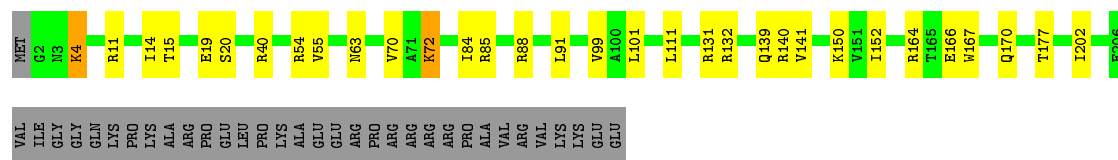
Chain QC: 75% 10% 14%






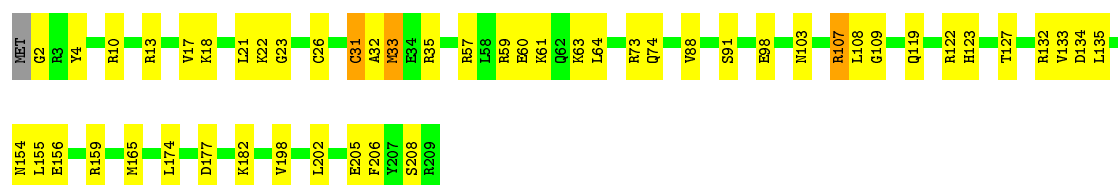
- Molecule 3: 30S ribosomal protein S3

Chain XC: 




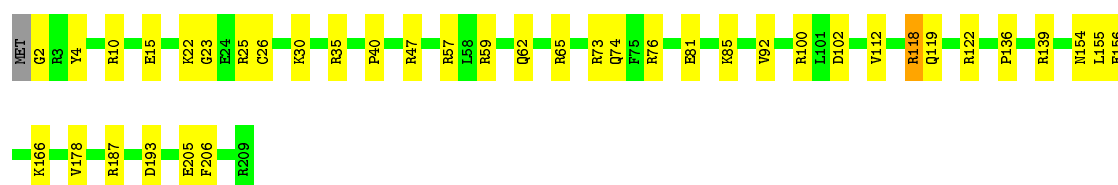
- Molecule 4: 30S ribosomal protein S4

Chain QD: 




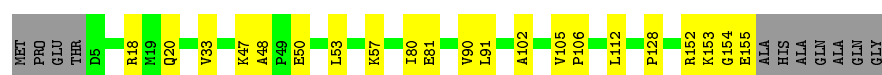
- Molecule 4: 30S ribosomal protein S4

Chain XD: 




- Molecule 5: 30S ribosomal protein S5

Chain QE: 




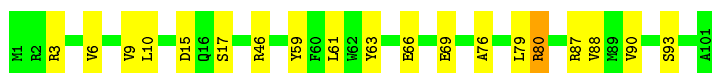
- Molecule 5: 30S ribosomal protein S5

Chain XE: 



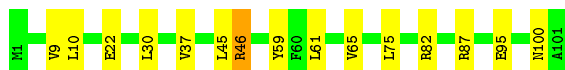
- Molecule 6: 30S ribosomal protein S6

Chain QF: 



- Molecule 6: 30S ribosomal protein S6

Chain XF: 85% 14%



- Molecule 7: 30S ribosomal protein S7

Chain QG: 88% 11%



- Molecule 7: 30S ribosomal protein S7

Chain XG: 83% 15%



- Molecule 8: 30S ribosomal protein S8

Chain QH: 75% 23%



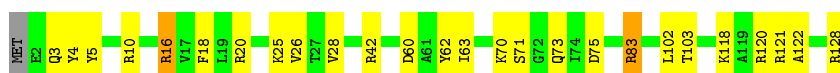
- Molecule 8: 30S ribosomal protein S8

Chain XH: 86% 13%



- Molecule 9: 30S ribosomal protein S9

Chain QI: 79% 19%

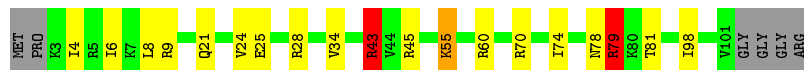
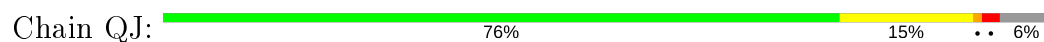


- Molecule 9: 30S ribosomal protein S9

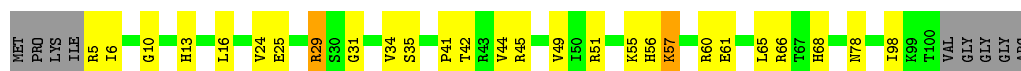
Chain XI: 78% 20%



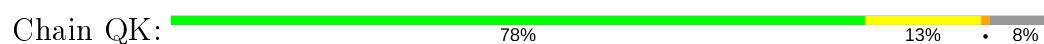
- Molecule 10: 30S ribosomal protein S10



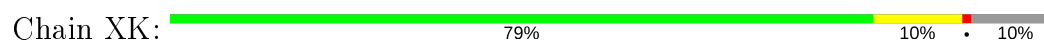
- Molecule 10: 30S ribosomal protein S10



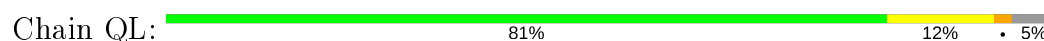
- Molecule 11: 30S ribosomal protein S11



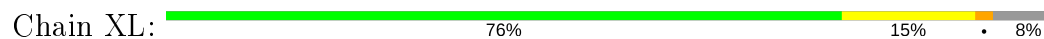
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

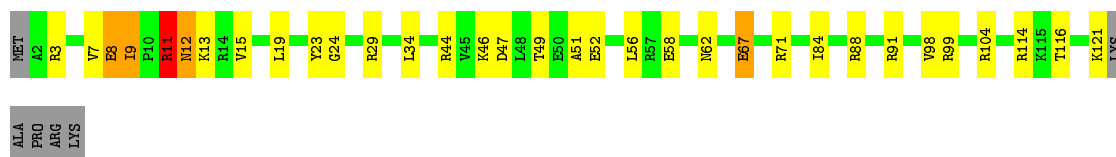


- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13





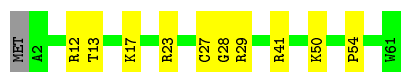
- Molecule 13: 30S ribosomal protein S13

Chain XM: 75% 17% 6%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN: 82% 16%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN: 75% 23%



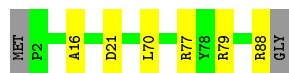
- Molecule 15: 30S ribosomal protein S15

Chain QO: 92% 7%



- Molecule 15: 30S ribosomal protein S15

Chain XO: 91% 7%




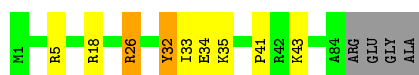
- Molecule 16: 30S ribosomal protein S16

Chain QP: 78% 17% 5%



- Molecule 16: 30S ribosomal protein S16

Chain XP:  85% 8% • 5%




- Molecule 17: 30S ribosomal protein S17

Chain QQ:  84% 10% • 5%



- Molecule 17: 30S ribosomal protein S17

Chain XQ:  78% 16% • 5%



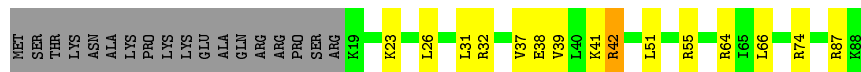
- Molecule 18: 30S ribosomal protein S18

Chain QR:  59% 19% • 20%



- Molecule 18: 30S ribosomal protein S18

Chain XR:  63% 16% • 20%



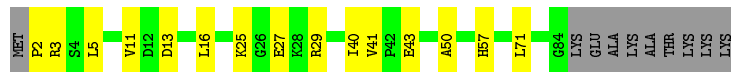
- Molecule 19: 30S ribosomal protein S19

Chain QS:  68% 18% • 11%




- Molecule 19: 30S ribosomal protein S19

Chain XS:  73% 16% 11%



- Molecule 20: 30S ribosomal protein S20

Chain QT:  82% 11% 7%



- Molecule 20: 30S ribosomal protein S20

Chain XT:  70% 23% 7%



- Molecule 21: 30S ribosomal protein Thx

Chain QU:  67% 22% 7%




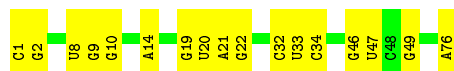
- Molecule 21: 30S ribosomal protein Thx

Chain XU:  70% 22% 7%




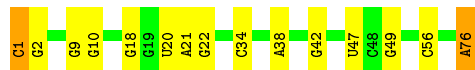
- Molecule 22: P-site tRNA-fMet

Chain QV:  78% 22%




- Molecule 22: P-site tRNA-fMet

Chain XV:  81% 17%



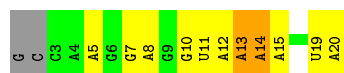
- Molecule 23: mRNA

Chain QX:  35% 50% 5% 10%




- Molecule 23: mRNA

Chain XX:  35% 45% 10% 10%



- Molecule 24: Addiction module toxin, Txe/YoeB family

Chain QY:  77% 23%




- Molecule 24: Addiction module toxin, Txe/YoeB family

Chain QZ:  74% 23%




- Molecule 24: Addiction module toxin, Txe/YoeB family

Chain XY:  79% 21%




- Molecule 24: Addiction module toxin, Txe/YoeB family

Chain XZ:  81% 18%



- Molecule 25: 50S ribosomal protein L27

Chain R0:  74% 20% 5%




- Molecule 25: 50S ribosomal protein L27

Chain Y0:  75% 20%




- Molecule 26: 50S ribosomal protein L28

Chain R1:  85% 9% . .



- Molecule 26: 50S ribosomal protein L28

Chain Y1:  77% 22% .




- Molecule 27: 50S ribosomal protein L29

Chain R2:  68% 26% . .




- Molecule 27: 50S ribosomal protein L29

Chain Y2:  85% 11% .




- Molecule 28: 50S ribosomal protein L30

Chain R3:  82% 17% .



- Molecule 28: 50S ribosomal protein L30

Chain Y3:  83% 15% .




- Molecule 29: 50S ribosomal protein L31

Chain R4:  59% 30% 6% . .



- Molecule 29: 50S ribosomal protein L31



Chain Y4:  76% 18% . .




- Molecule 30: 50S ribosomal protein L32

Chain R5:  72% 27% .



- Molecule 30: 50S ribosomal protein L32

Chain Y5:  85% 13% .




- Molecule 31: 50S ribosomal protein L33

Chain R6:  72% 22% . .



- Molecule 31: 50S ribosomal protein L33

Chain Y6:  85% 13% .




- Molecule 32: 50S ribosomal protein L34

Chain R7:  88% 8% .



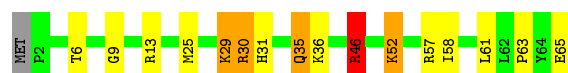
- Molecule 32: 50S ribosomal protein L34

Chain Y7:  84% 14% .



- Molecule 33: 50S ribosomal protein L35

Chain R8: 



- Molecule 33: 50S ribosomal protein L35

Chain Y8: 




- Molecule 34: 50S ribosomal protein L36

Chain R9: 



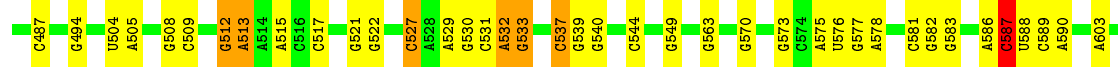
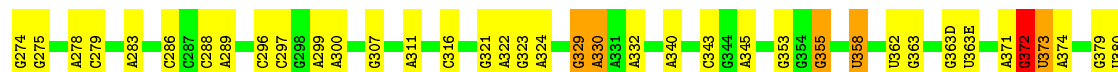
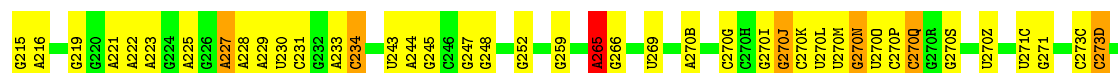
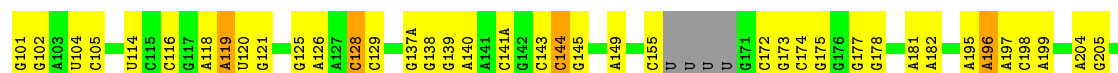
- Molecule 34: 50S ribosomal protein L36

Chain Y9: 

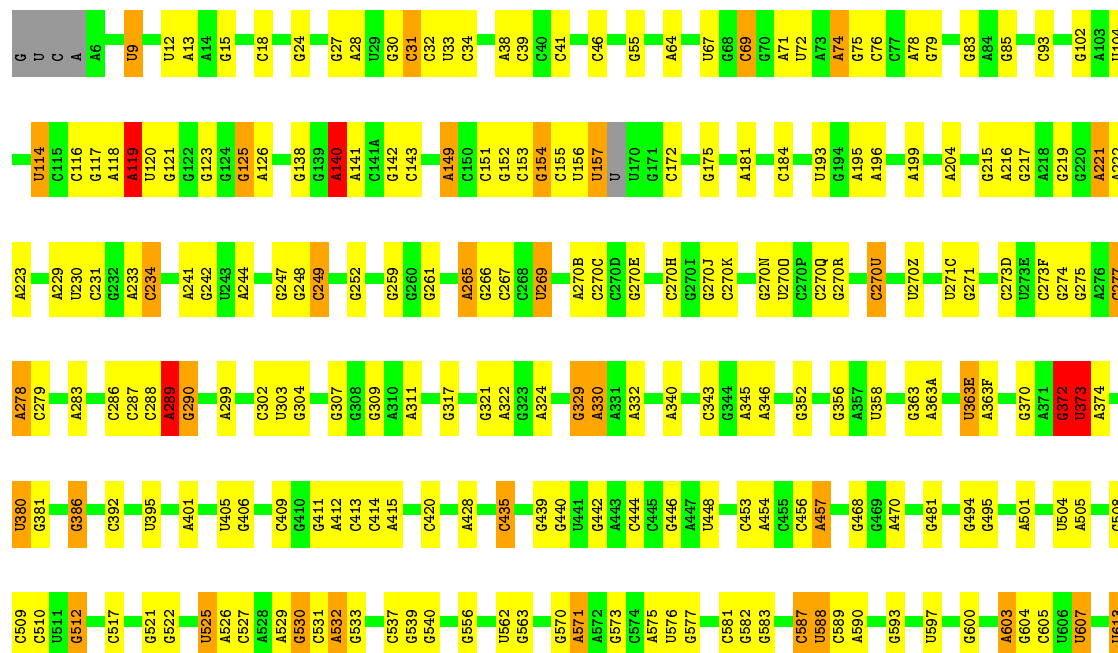


- Molecule 35: 23S rRNA

Chain RA: 



A2013	U1911	C1788	G1674	C1550	C1467	A1384	A1265	G1171	C1053	G956	A866	A784	U667
U2016	A1912	A1791	G1678	A1554	A1471	G1385	A1272	G1173	A1057	A957	A872	G785	G668
A2019	A1913	G1792	U1679	A1558	A1474	G1388	A1275	U1174	U1061	U958	G873	A788	U613
A2020	C1920	C1800	U1680	G1559	C1475	U1391	A1278	U1175	G1064	A959	U877	A789	U614
C2021	A1927	G1801	G1681	C1560	C1476	U1394	A1279	A1177	U1065	A960	A878	G792	A615
U2022	A1928	A1802	A1477	C1565	A1478	A1395	G1280	C1178	G1066	G961	G882	A793	A616
G2023	G1929	G1811	U1688	A1566	G1478	U1396	G1281	C1179	U1066	G968	G883	C797	G617
C2026	A1930	A1812	A1689	A1567	U1482	U1399	G1286	A1181	A1067	A973	C884	G797	A621
A2030	U1931	C1694	G1694	G1568	G1483	C1399	A1286	A1183	G1068	G974	C885	G805	A627
A2031	C1934	G1695	U1695	A1568	G1487	G1401	U1294	G1184	A1070	C886	C886	C906	G628
A2032	G1935	G1696	G1696	A1570	G1487	G1401	U1294	G1184	G1071	C887	A887	U807	G629
G2033	A1936	U1818	G1697	A1571	U1488	C1402	U1300	U1188	C1072	C888	C888	G808	G630
A2033	G1937	A1819	A1698	A1572	A1489	C1403	A1301	G1191	G1074	A983	A890	C812	A631
U2034	A1938	U1820	G1699	A1572	A1490	U1406	A1304	G1195	C1075	C884	C893	C814	A632
G2035	U1939	A1700	A1700	U1578	C1493	C1407	C1304	G1195	G1079	C885	C894	C814	A633
C2036	C1941	G1824	A1701	A1579	C1493	C1407	C1304	G1195	G1079	C885	C894	C814	A634
G2037	C1947	C1827	G1725	A1580	U1497	C1408	C1306	G1203	C1079	C886	C894	C814	A635
G2038	G1948	G1828	U1728	C1585	U1497	C1408	C1306	G1203	C1079	C886	C894	C814	A636
U2041	G1949	A1829	G1728	A1586	C1498	G1410	A1307	U1204	U1083	A990	U895	G708	A637
A2042	G1950	C1830	A1729	A1587	C1499	G1416	A1308	A1205	C991	A990	A896	A716	A638
C2043	U1951	G1831	U1730	C1588	C1502	G1417	G1309	G1206	A1085	C992	C898	A717	U639
G2052	A1952	G1832	G1731	C1588	C1502	G1418	G1310	A1210	A1086	C993	A900	G717	U639
U1955	U1955	G1842	A1732	C1592	C1505	A1419	U1312	U1211	G992	C994	A900	G717	U639
U1956	U1956	G1843	G1733	C1592	C1505	A1419	U1312	U1211	G992	C994	A900	G717	U639
U1957	U1957	A1847	C1734	C1599	C1509	G1421	C1314	G1212	A1095	C995	C904	A727	G650
U1958	U1958	C1853	G1735	C1599	C1509	G1422	C1315	A1220	A1096	C996	U907	A829	G651
U1959	U1959	A1854	A1755	C1600	A1510	G1423	C1316	G1221	A1096	C997	U907	A829	G651
U1960	U1960	G1857	C1742	A1603	C1518	G1424	C1317	G1224	A1096	C998	U907	A829	G651
U1961	U1961	G1858	G1743	C1607	U1519	A1427	C1318	G1225	A1096	C999	U907	A829	G651
U1962	U1962	A1864	C1754	A1608	U1520	C1428	G1319	C1225	A1096	C999	U907	A829	G651
U1963	U1963	G1863	A1755	C1607	U1520	C1428	G1319	C1225	A1096	C999	U907	A829	G651
U1964	U1964	U1864	G1756	A1608	U1520	C1428	G1319	C1225	A1096	C999	U907	A829	G651
U1965	U1965	G1869	A1756	C1622	U1523	U1431	G1329	G1230	A1111	G1011	C915	A734	G654
U1966	U1966	A1872	A1762	A1632	G1524	A1434	C1332	G1231	A1111	G1012	C915	A734	G654
U1967	U1967	G1878	G1763	A1632	G1524	A1434	C1332	G1231	A1111	G1013	C915	A734	G654
U1968	U1968	A1881	G1764	C1636	G1526	C1437	G1337	G1236	A1111	G1014	C915	A734	G654
U1969	U1969	G1882	G1769	A1637	G1527	C1437	G1338	A1237	A1111	G1015	C915	A734	G654
U1970	U1970	C1883	C1771	C1640	U1529	A1444	U1340	G1247	A1111	G1016	C915	A734	G654
U1971	U1971	A1884	A1772	C1644	U1535	A1449	U1341	G1248	A1111	G1017	C915	A734	G654
U1972	U1972	A1885	A1773	C1644	U1535	A1449	U1341	G1248	A1111	G1018	C915	A734	G654
U1973	U1973	A1886	C1774	C1648	A1536	G1450	U1249	U1249	A1111	G1019	C915	A734	G654
U1974	U1974	G1888	U1775	C1648	A1537	C1451	G1250	G1250	A1111	G1020	C915	A734	G654
U1975	U1975	A1889	G1776	C1648	A1538	A1453	G1251	U1141	A1142	G1021	C915	A734	G654
U1976	U1976	A1890	G1776	C1651	G1539	U1454	A1253	A1142	A1143	U1022	C915	A734	G654
U1977	U1977	A1891	U1779	A1652	G1540	G1455	A1254	U1254	A1143	U1023	C915	A734	G654
U1978	U1978	A1892	A1780	A1653	U1541	G1456	U1255	G1256	A1143	U1024	C915	A734	G654
U1979	U1979	C1893	C1781	A1654	U1542	A1457	A1256	G1256	A1143	U1025	C915	A734	G654
U1980	U1980	G1903	A1782	A1654	U1543	C1458	G1259	G1259	A1143	U1026	C915	A734	G654
U1981	U1981	G1904	A1783	C1657	C1544	G1461	G1260	G1260	A1143	U1027	C915	A734	G654
U1982	U1982	G1905	A1784	C1658	A1545	C1462	G1261	G1261	A1143	U1028	C915	A734	G654
U1983	U1983	G1906	A1785	C1658	A1545	C1462	G1261	G1261	A1143	U1029	C915	A734	G654
U1984	U1984	C1909	A1786	G1667	C1547	G1466	G1264	G1264	A1143	U1030	C915	A734	G654
U1985	U1985	G1910	A1787	G1667	C1547	G1466	G1264	G1264	A1143	U1031	C915	A734	G654
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U1988	U1988	G1913	A1790	G1667	C1547	G1466	G1264	G1264	A1143	U1034	C915	A734	G654
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U2004	U2004	G1929	A1806	G1667	C1547	G1466	G1264	G1264	A1143	U1050	C915	A734	G654
U2005	U2005	G1930	A1807	G1667	C1547	G1466	G1264	G1264	A1143	U1051	C915	A734	G654
U2006	U2006	G1931	A1808	G1667	C1547	G1466	G1264	G1264	A1143	U1052	C915	A734	G654
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U2008	U2008	G1933	A1810	G1667	C1547	G1466	G1264	G1264	A1143	U1054	C915	A734	G654
U2009	U2009	G1934	A1811	G1667	C1547	G1466	G1264	G1264	A1143	U1055	C915	A734	G654
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U2012	U2012	G1937	A1814	G1667	C1547	G1466	G1264	G1264	A1143	U1058	C915	A734	G654
U2013	U2013	G1938	A1815	G1667	C1547	G1466	G1264	G1264	A1143	U1059	C915	A734	G654
U2014	U2014	G1939	A1816	G1667	C1547	G1466	G1264	G1264	A1143	U1060	C915	A734	G654
U2015	U2015	G1940	A1817	G1667	C1547	G1466	G1264	G1264	A1143	U1061	C915	A734	G654
U2016	U2016	G1941	A1818	G1667	C1547	G1466	G1264	G1264	A1143	U1062	C915	A734	G654
U2017	U2017	G1942	A1819	G1667	C1547	G1466	G1264	G1264	A1143	U1063	C915	A734	G654
U2018	U2018	G1943	A1820	G1667	C1547	G1466	G1264	G1264	A1143	U1064	C915	A734	G654
U2019	U2019	G1944	A1821	G1667	C1547	G1466	G1264	G1264	A1143	U1065	C915	A734	G654
U2020	U2020	G1945	A1822	G1667	C1547	G1466	G1264	G1264	A1143	U1066	C915	A734	G654
U2021	U2021	G1946	A1823	G1667	C1547	G1466	G1264	G1264	A1143	U1067	C915	A734	G654
U2022	U2022	G1947	A1824	G1667	C1547	G1466	G1264	G1264	A1143	U1068	C915	A734	G654
U2023	U2023	G1948	A1825	G1667	C1547	G1466	G1264	G1264	A1143	U1069	C915	A734	G654
U2024	U2024	G1949	A1826	G1667	C1547	G1466	G1264	G1264	A1143	U1070	C915	A734	G654
U2025	U2025	G1950	A1827	G1667	C1547	G1466	G1264	G1264	A1143	U1071	C915	A734	G654
U2026	U2026	G1951	A1828	G1667	C1547	G1466	G1264	G1264	A1143	U1072	C915	A734	G654
U2027	U2027	G1952	A1829	G1667	C1547	G1466	G1264						



A2117	A2020	A1901	G1763	A1632	U1516	G1418	A1301	G1187	A1088	C992	A896	C812	6669	U614
U2118	C2021	C1902	G1764	G1633	U1516	G1419	A1308	U1188	A1089	C993	C897	6613	6670	G615
A2119	U2022	G1903	A1634	G1635	G1522	U1421	G1309	G1191	G1093	C994	C904	C814	6674	A616
G2120	G2023	G1906	G1636	G1523	G1524	G1422	G1311	G1195	A1094	A996	U906	C817	6675	6617
G2123	G2024	A1637	G1637	G1525	G1525	G1424	U1312	C1196	A1096	C998	U907	A819	6676	A621
A2126	C2025	G1640	G1640	A1528	A1528	A1427	U1313	A1204	G1099	U999	A910	A820	6679	G622
G2127	C2026	C1644	C1644	C1428	C1428	G1429	U1314	U1205	A1000	A999	U822	A821	6680	6624
C2128	U2028	A1912	A1780	U1535	U1535	G1429	U1316	C1315	C1102	C1005	G915	G823	6681	A627
C2129	G2029	A1913	C1781	A1536	A1536	G1430	A1317	A1210	A1103	A1009	A917	U827	6686	G628
U2130	A2030	C1914	A1782	C1537	C1537	U1431	U1329	U1211	G1106	A1010	G916	U828	6628	G629
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U2132	G2032	A1682	A1784	U1539	U1539	U1432	U1331	A1213	G1110	G1012	G919	U831	A633	A633
G2133	A2033	G1683	C1788	G1540	G1540	U1433	A1342	A1214	G1114	U1012	U832	U832	C634	C634
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A2135	G2035	A1685	G1437	G1437	G1437	G1437	U1352	C1225	G1122	A1020	G931	A835	6636	6636
C2136	C2036	C1656	A1543	C1544	C1544	A1444	A1353	G1226	G1126	A1021	G932	U836	U639	U639
G2137	G2037	C1657	A1545	A1545	A1545	C1445	A1354	A1227	G1126	G1024	A933	U837	C640	C640
G2138	G2038	G1688	A1547	A1547	A1547	A1449	A1359	G1228	A1126	U1023	G938	U838	6641	6641
C2141	U2041	G1667	A1554	A1554	A1554	G1449A	A1360	C1233	A1127	G1025	A941	U839	6642	6642
C2145	A2042	A1688	A1558	A1558	A1558	G1455	C1363	C1236	A1129	A1026	A945	U845	6645	6645
C2146	C2043	A1689	G1559	G1559	G1559	G1455	G1368	A1237	U1130	U1027	A949	U848	A646	A646
G2147	G2052	G1674	G1560	G1560	G1560	G1459	G1369	G1243	G1131	A1028	G946	C950	6652	6652
G2148	C2055	C1675	A1566	A1566	A1566	G1461	A1460	G1243	A1136	U1033	A953	U851	A653	A653
G2149	G2056	U1679	C1567	C1567	C1567	G1462	A1370	G1243	U1136	U1033	A953	U851	A653	A653
U2150	U1956	G1816	A1571	A1571	A1571	C1467	G1380	G1243	U1136	U1033	A953	U851	A653	A653
G2156	A2059	A1819	A1572	A1572	A1572	A1471	A1384	G1243	U1136	U1033	A953	U851	A653	A653
G2157	A2060	U1820	A1578	A1578	A1578	A1471	A1385	G1243	U1136	U1033	A953	U851	A653	A653
A2158	G2061	G1828	A1579	A1579	A1579	A1471	A1385	G1243	U1136	U1033	A953	U851	A653	A653
C2161	A2062	G1829	A1580	A1580	A1580	A1471	A1385	G1243	U1136	U1033	A953	U851	A653	A653
G2162	C2063	A1966	A1581	A1581	A1581	A1471	A1385	G1243	U1136	U1033	A953	U851	A653	A653
G2166	G2064	C1967	A1582	A1582	A1582	A1471	A1385	G1243	U1136	U1033	A953	U851	A653	A653
U2167	A2065	A1970	A1583	A1583	A1583	A1471	A1385	G1243	U1136	U1033	A953	U851	A653	A653
G2168	G2069	A1971	A1584	A1584	A1584	A1471	A1385	G1243	U1136	U1033	A953	U851	A653	A653
A2169	C2073	A1972	A1585	A1585	A1585	A1471	A1385	G1243	U1136	U1033	A953	U851	A653	A653
U2170	U2074	A1973	A1586	A1586	A1586	A1471	A1385	G1243	U1136	U1033	A953	U851	A653	A653
A2171	U2075	C1979	A1587	A1587	A1587	A1471	A1385	G1243	U1136	U1033	A953	U851	A653	A653
U2172	U2086	G1980	A1588	A1588	A1588	A1471	A1385	G1243	U1136	U1033	A953	U851	A653	A653
A2173	G2093	A1981	A1589	A1589	A1589	A1471	A1385	G1243	U1136	U1033	A953	U851	A653	A653
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C2177	U2096	U1983	A1591	A1591	A1591	A1471	A1385	G1243	U1136	U1033	A953	U851	A653	A653
C2178	U2096	U1983	A1592	A1592	A1592	A1471	A1385	G1243	U1136	U1033	A953	U851	A653	A653
G2187	U2099	C1996	A1593	A1593	A1593	A1471	A1385	G1243	U1136	U1033	A953	U851	A653	A653
C2188	C2103	A2001	C1881	C1881	C1881	A1499	U1406	A1272	A1175	A1073	G972	C885	6792	A654V
U2189	G2103	G2002	C1882	C1882	C1882	G1500	C1407	A1278	G1176	G1074	A980	C886	A793	A654V
G2190	C2111	C2006	G1883	G1883	G1883	G1505	C1408	A1279	G1177	C1075	A980	C887	A793	A654V
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G2192	U2113	C2006	G1885	G1885	G1885	G1505	C1408	A1279	G1177	C1075	A980	C887	A793	A654V
A2198	G2115	U2011	G1886	G1886	G1886	G1505	C1408	A1279	G1177	C1075	A980	C887	A793	A654V
A2199	G2115	U2011	G1887	G1887	G1887	G1505	C1408	A1279	G1177	C1075	A980	C887	A793	A654V
C2205	G2116	G2012	G1888	G1888	G1888	G1505	C1408	A1279	G1177	C1075	A980	C887	A793	A654V





- Molecule 37: 50S ribosomal protein L2

Chain YD: 89% 9% ..



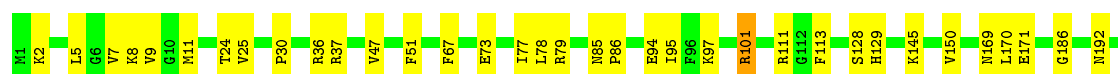
- Molecule 38: 50S ribosomal protein L3

Chain RE: 73% 25% ..



- Molecule 38: 50S ribosomal protein L3

Chain YE: 81% 18% .



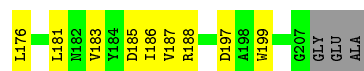
- Molecule 39: 50S ribosomal protein L4

Chain RF: 87% 9% .




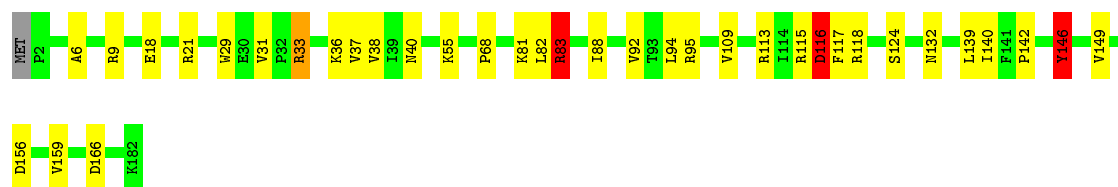
- Molecule 39: 50S ribosomal protein L4

Chain YF: 78% 17% . .




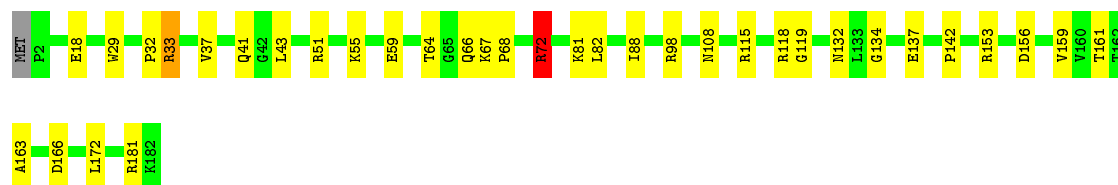
- Molecule 40: 50S ribosomal protein L5

Chain RG:  80% 18% ...




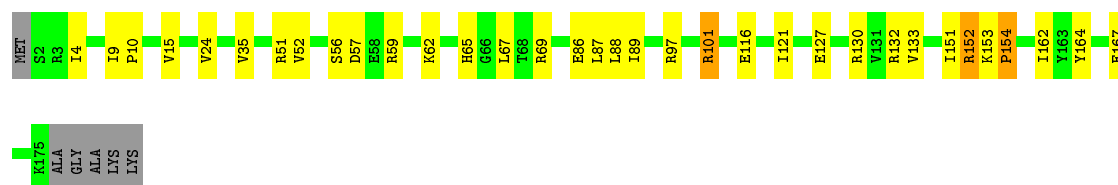
- Molecule 40: 50S ribosomal protein L5

Chain YG:  80% 18% ...




- Molecule 41: 50S ribosomal protein L6

Chain RH:  78% 17% ..



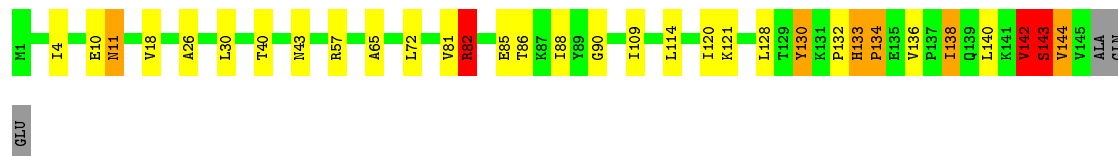
- Molecule 41: 50S ribosomal protein L6

Chain YH:  84% 12% ..




- Molecule 42: 50S ribosomal protein L9

Chain RI:  76% 16% ...



- Molecule 42: 50S ribosomal protein L9

Chain YI:  86% 9% ...





- Molecule 43: 50S ribosomal protein L13

Chain RN: 79% 17% ...



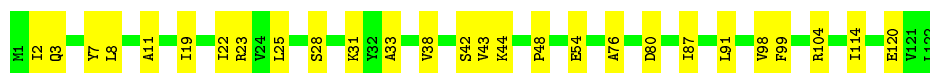
- Molecule 43: 50S ribosomal protein L13

Chain YN: 83% 14% ..



- Molecule 44: 50S ribosomal protein L14

Chain RO: 78% 22%



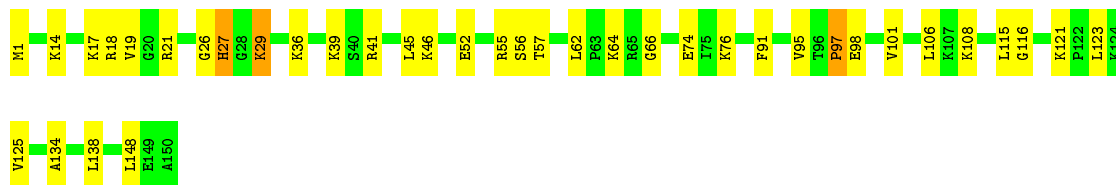
- Molecule 44: 50S ribosomal protein L14

Chain YO: 80% 20%



- Molecule 45: 50S ribosomal protein L15

Chain RP: 75% 23% .



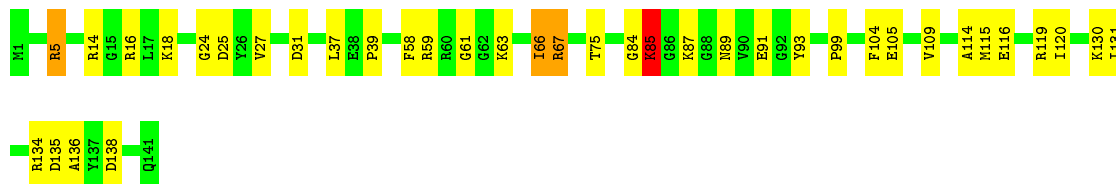
- Molecule 45: 50S ribosomal protein L15

Chain YP: 81% 19% .




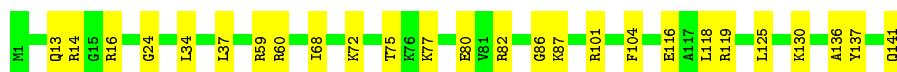
- Molecule 46: 50S ribosomal protein L16

Chain RQ:  73% 24% ..




- Molecule 46: 50S ribosomal protein L16

Chain YQ:  82% 18%




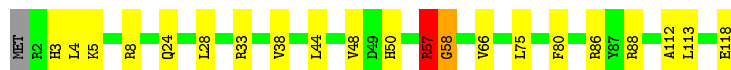
- Molecule 47: 50S ribosomal protein L17

Chain RR:  81% 16% ..




- Molecule 47: 50S ribosomal protein L17

Chain YR:  81% 16% ...




- Molecule 48: 50S ribosomal protein L18

Chain RS:  78% 21% .



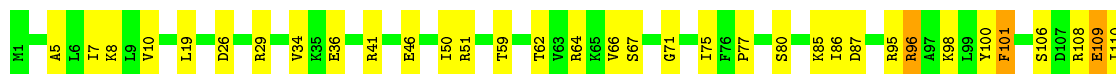
- Molecule 48: 50S ribosomal protein L18

Chain YS:  79% 20% ..



- Molecule 49: 50S ribosomal protein L19

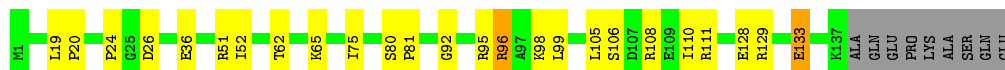
Chain RT:  69% 23% . 6%





- Molecule 49: 50S ribosomal protein L19

Chain YT: 77% 16% 6%



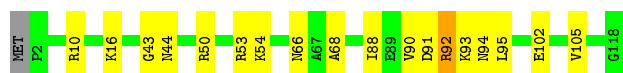
- Molecule 50: 50S ribosomal protein L20

Chain RU: 82% 15% ...



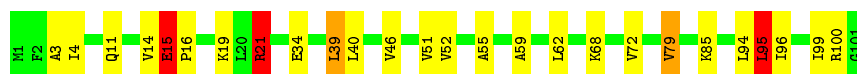
- Molecule 50: 50S ribosomal protein L20

Chain YU: 84% 14% ..



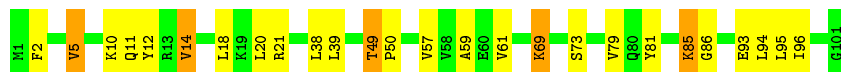
- Molecule 51: 50S ribosomal protein L21

Chain RV: 74% 21% . .



- Molecule 51: 50S ribosomal protein L21

Chain YV: 74% 21% 5%



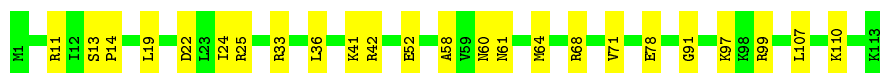
- Molecule 52: 50S ribosomal protein L22

Chain RW: 88% 11% .

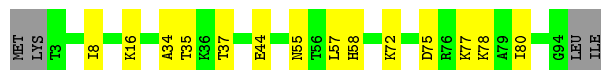
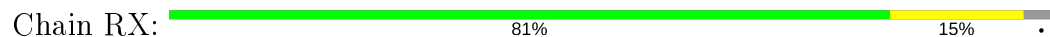


- Molecule 52: 50S ribosomal protein L22

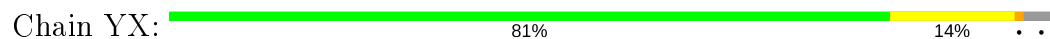
Chain YW: 79% 21%



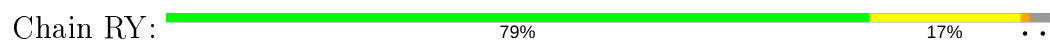
- Molecule 53: 50S ribosomal protein L23



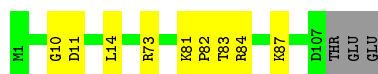
- Molecule 53: 50S ribosomal protein L23



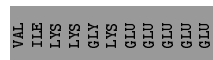
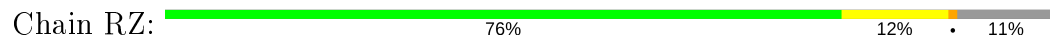
- Molecule 54: 50S ribosomal protein L24



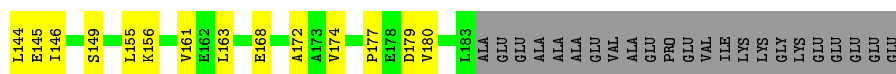
- Molecule 54: 50S ribosomal protein L24



- Molecule 55: 50S ribosomal protein L25



- Molecule 55: 50S ribosomal protein L25



- Molecule 56: CCPuro

Chain ZA:  33% 67%

 C1 C2 A3

- Molecule 56: CCPuro

Chain ZB:  67% 33%

 C1 C2 A3

## 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, $\alpha$ , $\beta$ , $\gamma$	214.68Å 453.51Å 609.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.72 – 3.50	Depositor
% Data completeness (in resolution range)	98.0 (146.72-3.50)	Depositor
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.216 , 0.246	Depositor
Wilson B-factor (Å <sup>2</sup> )	89.9	Xtriage
Anisotropy	0.032	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	295153	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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: MG, A3P, ZN, PPU, 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	QA	0.35	1/36324 (0.0%)	1.07	174/56690 (0.3%)
1	XA	1.32	6/36254 (0.0%)	1.08	179/56581 (0.3%)
2	QB	0.57	4/1942 (0.2%)	0.84	4/2619 (0.2%)
2	XB	0.39	0/1950	0.77	4/2630 (0.2%)
3	QC	0.38	0/1629	0.76	1/2195 (0.0%)
3	XC	0.38	0/1629	0.79	4/2195 (0.2%)
4	QD	0.38	0/1733	0.73	2/2318 (0.1%)
4	XD	0.38	0/1733	0.78	4/2318 (0.2%)
5	QE	0.36	0/1171	0.71	0/1576
5	XE	0.33	0/1171	0.67	0/1576
6	QF	0.32	0/856	0.67	0/1154
6	XF	0.33	0/856	0.70	1/1154 (0.1%)
7	QG	0.38	0/1276	0.75	0/1709
7	XG	0.36	0/1276	0.66	1/1709 (0.1%)
8	QH	0.32	0/1128	0.70	0/1517
8	XH	0.31	0/1128	0.72	3/1517 (0.2%)
9	QI	0.47	0/1029	0.87	2/1379 (0.1%)
9	XI	0.37	0/1017	0.79	2/1365 (0.1%)
10	QJ	0.44	1/814 (0.1%)	0.96	7/1095 (0.6%)
10	XJ	0.41	1/790 (0.1%)	0.81	2/1063 (0.2%)
11	QK	0.40	1/900 (0.1%)	0.71	0/1213
11	XK	0.38	0/879	0.73	2/1187 (0.2%)
12	QL	0.34	0/991	0.81	0/1327
12	XL	0.39	0/972	0.82	1/1301 (0.1%)
13	QM	0.42	0/965	0.92	4/1292 (0.3%)
13	XM	0.40	0/956	0.82	2/1281 (0.2%)
14	QN	0.43	0/501	0.82	1/664 (0.2%)
14	XN	0.32	0/501	0.72	1/664 (0.2%)
15	QO	0.34	0/745	0.66	1/992 (0.1%)
15	XO	0.28	0/740	0.55	0/987
16	QP	0.36	0/721	0.80	2/970 (0.2%)
16	XP	0.34	0/721	0.77	1/970 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	QQ	0.37	0/847	0.77	4/1131 (0.4%)
17	XQ	0.33	0/847	0.66	0/1131
18	QR	0.41	1/579 (0.2%)	0.81	0/768
18	XR	0.38	0/579	0.77	1/768 (0.1%)
19	QS	0.45	0/680	0.93	1/915 (0.1%)
19	XS	0.32	0/671	0.78	1/904 (0.1%)
20	QT	0.36	0/765	0.81	0/1007
20	XT	0.35	0/765	0.81	2/1007 (0.2%)
21	QU	0.43	0/221	0.89	1/288 (0.3%)
21	XU	0.31	0/221	0.83	0/288
22	QV	0.33	0/1832	1.01	4/2855 (0.1%)
22	XV	0.33	0/1832	1.02	3/2855 (0.1%)
23	QX	0.33	0/414	0.96	2/645 (0.3%)
23	XX	0.30	0/414	0.92	2/645 (0.3%)
24	QY	0.40	0/743	0.78	1/1002 (0.1%)
24	QZ	0.61	2/743 (0.3%)	0.99	2/1002 (0.2%)
24	XY	0.35	0/743	0.74	1/1002 (0.1%)
24	XZ	0.45	0/743	0.90	2/1002 (0.2%)
25	R0	0.39	0/652	0.87	2/867 (0.2%)
25	Y0	0.35	0/657	0.76	0/874
26	R1	0.43	1/744 (0.1%)	0.78	2/989 (0.2%)
26	Y1	0.36	0/770	0.73	0/1022
27	R2	0.43	0/583	0.90	4/771 (0.5%)
27	Y2	0.31	0/583	0.65	0/771
28	R3	0.31	0/474	0.67	0/635
28	Y3	0.33	0/474	0.73	0/635
29	R4	0.63	0/578	1.13	3/776 (0.4%)
29	Y4	0.40	0/578	0.93	3/776 (0.4%)
30	R5	0.37	0/473	0.72	1/639 (0.2%)
30	Y5	0.46	0/473	0.74	0/639
31	R6	0.38	0/460	0.85	1/613 (0.2%)
31	Y6	0.39	0/460	0.74	0/613
32	R7	0.31	0/417	0.64	0/550
32	Y7	0.33	0/426	0.64	0/561
33	R8	0.48	0/525	0.97	4/691 (0.6%)
33	Y8	0.51	0/525	0.80	0/691
34	R9	0.41	0/310	0.80	0/407
34	Y9	0.38	0/310	0.85	1/407 (0.2%)
35	RA	0.37	0/69739	1.11	428/108870 (0.4%)
35	YA	0.38	0/69419	1.11	379/108369 (0.3%)
36	RB	0.40	0/2881	1.13	17/4494 (0.4%)
36	YB	0.47	1/2881 (0.0%)	1.21	31/4494 (0.7%)
37	RD	0.40	0/2165	0.86	6/2919 (0.2%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	YD	0.35	0/2185	0.74	4/2944 (0.1%)
38	RE	0.48	0/1601	0.93	4/2160 (0.2%)
38	YE	0.39	0/1592	0.86	4/2149 (0.2%)
39	RF	0.33	0/1620	0.70	2/2194 (0.1%)
39	YF	0.37	1/1620 (0.1%)	0.72	3/2194 (0.1%)
40	RG	0.38	0/1499	0.88	5/2016 (0.2%)
40	YG	0.50	3/1499 (0.2%)	0.82	2/2016 (0.1%)
41	RH	0.47	0/1362	1.04	5/1841 (0.3%)
41	YH	0.39	0/1356	0.77	3/1834 (0.2%)
42	RI	2.84	2/1146 (0.2%)	1.40	9/1551 (0.6%)
42	YI	0.44	0/1151	0.92	4/1558 (0.3%)
43	RN	0.43	0/1131	0.83	3/1525 (0.2%)
43	YN	0.33	0/1131	0.72	3/1525 (0.2%)
44	RO	0.33	0/943	0.70	0/1269
44	YO	0.35	0/943	0.72	0/1269
45	RP	0.45	0/1162	0.96	4/1544 (0.3%)
45	YP	0.36	0/1152	0.86	3/1533 (0.2%)
46	RQ	0.50	2/1143 (0.2%)	0.89	3/1527 (0.2%)
46	YQ	0.34	0/1143	0.73	1/1527 (0.1%)
47	RR	0.32	0/974	0.76	3/1302 (0.2%)
47	YR	0.35	0/974	0.84	4/1302 (0.3%)
48	RS	0.38	0/892	0.83	1/1187 (0.1%)
48	YS	0.43	0/892	0.85	2/1187 (0.2%)
49	RT	0.45	0/1155	0.87	1/1542 (0.1%)
49	YT	0.45	1/1155 (0.1%)	0.83	4/1542 (0.3%)
50	RU	0.38	0/982	0.68	1/1306 (0.1%)
50	YU	0.37	0/982	0.64	0/1306
51	RV	0.72	2/790 (0.3%)	1.15	6/1057 (0.6%)
51	YV	1.42	8/790 (1.0%)	1.02	4/1057 (0.4%)
52	RW	0.33	0/911	0.70	0/1220
52	YW	0.33	0/911	0.69	0/1220
53	RX	0.34	0/739	0.68	0/993
53	YX	0.35	0/739	0.66	0/993
54	RY	0.38	0/831	0.75	1/1108 (0.1%)
54	YY	0.35	0/831	0.76	0/1108
55	RZ	0.39	0/1493	0.84	3/2026 (0.1%)
55	YZ	0.36	0/1493	0.77	0/2026
56	ZA	0.52	0/40	1.41	1/60 (1.7%)
56	ZB	0.58	0/40	1.53	0/60
All	All	0.60	38/319487 (0.0%)	1.03	1407/477274 (0.3%)

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
2	QB	0	1
7	XG	0	1
8	XH	0	1
10	QJ	0	1
11	XK	0	1
24	QZ	0	1
37	RD	0	2
37	YD	0	1
38	RE	0	1
40	RG	0	2
40	YG	0	1
41	RH	0	2
41	YH	0	1
42	RI	0	4
47	RR	0	1
47	YR	0	1
51	RV	0	1
All	All	0	23

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	XA	368	U	C2-N3	131.42	2.29	1.37
1	XA	368	U	N3-C4	105.69	2.33	1.38
42	RI	82	ARG	CZ-NH1	93.68	2.54	1.33
1	XA	368	U	N1-C2	92.50	2.21	1.38
1	XA	368	U	N1-C6	90.74	2.19	1.38

The worst 5 of 1407 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	RI	82	ARG	NE-CZ-NH2	-27.28	106.66	120.30
42	RI	82	ARG	NE-CZ-NH1	20.23	130.42	120.30
42	RI	82	ARG	CD-NE-CZ	15.62	145.47	123.60
51	YV	85	LYS	CD-CE-NZ	15.45	147.22	111.70
51	RV	21	ARG	NE-CZ-NH1	14.43	127.52	120.30

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	12	GLU	Sidechain
10	QJ	79	ARG	Sidechain
24	QZ	50	HIS	Peptide
37	RD	33	LEU	Peptide
37	RD	35	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	QA	32452	0	16383	236	0
1	XA	32389	0	16350	215	0
2	QB	1907	0	1958	31	0
2	XB	1915	0	1969	26	0
3	QC	1605	0	1668	13	0
3	XC	1605	0	1668	16	0
4	QD	1703	0	1767	31	0
4	XD	1703	0	1767	23	0
5	QE	1155	0	1213	12	0
5	XE	1155	0	1213	13	0
6	QF	843	0	857	13	0
6	XF	843	0	857	10	0
7	QG	1257	0	1296	7	0
7	XG	1257	0	1296	17	0
8	QH	1108	0	1165	23	0
8	XH	1108	0	1165	13	0
9	QI	1010	0	1037	16	0
9	XI	998	0	1024	18	0
10	QJ	801	0	849	11	0
10	XJ	777	0	816	18	0
11	QK	885	0	904	12	0
11	XK	864	0	881	9	0
12	QL	975	0	1062	11	0
12	XL	956	0	1046	13	0
13	QM	955	0	1021	26	0
13	XM	946	0	1008	15	0
14	QN	492	0	529	5	0
14	XN	492	0	529	11	0
15	QO	734	0	771	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	XO	729	0	768	3	0
16	QP	705	0	725	12	0
16	XP	705	0	725	6	0
17	QQ	834	0	904	7	0
17	XQ	834	0	904	11	0
18	QR	574	0	644	9	0
18	XR	574	0	644	12	0
19	QS	665	0	686	15	0
19	XS	656	0	666	9	0
20	QT	763	0	861	8	0
20	XT	763	0	861	15	0
21	QU	217	0	234	5	0
21	XU	217	0	234	6	0
22	QV	1640	0	837	4	0
22	XV	1640	0	837	3	0
23	QX	394	0	196	2	0
23	XX	394	0	196	4	0
24	QY	723	0	713	10	0
24	QZ	723	0	712	11	0
24	XY	723	0	713	9	0
24	XZ	723	0	713	7	0
25	R0	643	0	667	13	0
25	Y0	648	0	672	15	0
26	R1	737	0	813	6	0
26	Y1	763	0	848	18	0
27	R2	581	0	629	9	0
27	Y2	581	0	629	3	0
28	R3	469	0	518	5	0
28	Y3	469	0	518	5	0
29	R4	565	0	561	24	0
29	Y4	565	0	559	10	0
30	R5	459	0	476	12	0
30	Y5	459	0	480	6	0
31	R6	453	0	474	10	0
31	Y6	453	0	474	4	0
32	R7	409	0	454	3	0
32	Y7	418	0	467	6	0
33	R8	517	0	582	10	0
33	Y8	517	0	582	12	0
34	R9	307	0	337	9	0
34	Y9	307	0	336	4	0
35	RA	62266	0	31392	344	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	YA	61981	0	31243	331	0
36	RB	2576	0	1303	27	0
36	YB	2576	0	1305	19	0
37	RD	2115	0	2194	39	0
37	YD	2135	0	2221	20	0
38	RE	1568	0	1634	40	0
38	YE	1559	0	1617	23	0
39	RF	1585	0	1632	14	0
39	YF	1585	0	1632	26	0
40	RG	1474	0	1535	23	0
40	YG	1474	0	1535	20	0
41	RH	1336	0	1418	12	0
41	YH	1330	0	1407	18	0
42	RI	1131	0	1216	16	0
42	YI	1136	0	1223	9	0
43	RN	1104	0	1180	16	0
43	YN	1104	0	1180	14	0
44	RO	933	0	996	17	0
44	YO	933	0	996	16	0
45	RP	1145	0	1228	28	0
45	YP	1135	0	1212	16	0
46	RQ	1122	0	1179	26	0
46	YQ	1122	0	1179	20	0
47	RR	960	0	1021	12	0
47	YR	960	0	1021	11	0
48	RS	882	0	943	14	0
48	YS	882	0	943	15	0
49	RT	1141	0	1202	21	0
49	YT	1141	0	1202	13	0
50	RU	964	0	1022	19	0
50	YU	964	0	1022	22	0
51	RV	779	0	852	16	0
51	YV	779	0	852	25	0
52	RW	900	0	964	8	0
52	YW	900	0	964	16	0
53	RX	725	0	778	11	0
53	YX	725	0	778	8	0
54	RY	818	0	913	12	0
54	YY	818	0	913	5	0
55	RZ	1461	0	1493	17	0
55	YZ	1461	0	1493	28	0
56	ZA	74	0	51	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	ZB	74	0	51	7	0
57	QA	93	0	0	0	0
57	QD	1	0	0	0	0
57	QE	1	0	0	0	0
57	QV	3	0	0	0	0
57	QY	1	0	0	0	0
57	R0	2	0	0	0	0
57	R3	1	0	0	0	0
57	RA	302	0	0	0	0
57	RB	3	0	0	0	0
57	RD	2	0	0	0	0
57	RE	1	0	0	0	0
57	RN	1	0	0	0	0
57	RO	1	0	0	0	0
57	RP	1	0	0	0	0
57	RQ	4	0	0	0	0
57	RR	1	0	0	0	0
57	RY	1	0	0	0	0
57	XA	99	0	0	0	0
57	XE	1	0	0	0	0
57	XF	1	0	0	0	0
57	XL	1	0	0	0	0
57	XM	1	0	0	0	0
57	XV	4	0	0	0	0
57	Y0	2	0	0	0	0
57	Y1	1	0	0	0	0
57	Y3	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YA	335	0	0	0	0
57	YB	3	0	0	0	0
57	YD	4	0	0	0	0
57	YE	5	0	0	0	0
57	YF	1	0	0	0	0
57	YG	1	0	0	0	0
57	YO	1	0	0	0	0
57	YP	1	0	0	0	0
57	YQ	5	0	0	0	0
57	YR	1	0	0	0	0
57	YV	1	0	0	0	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	QN	1	0	0	0	0
59	R4	1	0	0	0	0
59	R5	1	0	0	0	0
59	R6	1	0	0	0	0
59	R9	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y4	1	0	0	0	0
59	Y6	1	0	0	0	0
All	All	295153	0	201053	2175	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 2175 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)
51:YV:85:LYS:CG	51:YV:85:LYS:CD	1.86	1.53
51:YV:85:LYS:CG	51:YV:85:LYS:CB	1.82	1.50
1:XA:368:U:C5	1:XA:368:U:C6	2.05	1.45
51:YV:85:LYS:CE	51:YV:85:LYS:NZ	1.87	1.36
51:YV:85:LYS:CE	51:YV:85:LYS:CD	2.10	1.30

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	202 (87%)	27 (12%)	4 (2%)	9	42
2	XB	234/256 (91%)	211 (90%)	21 (9%)	2 (1%)	17	56
3	QC	203/239 (85%)	186 (92%)	17 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	XC	203/239 (85%)	188 (93%)	14 (7%)	1 (0%)	29	68
4	QD	206/209 (99%)	193 (94%)	11 (5%)	2 (1%)	15	54
4	XD	206/209 (99%)	187 (91%)	17 (8%)	2 (1%)	15	54
5	QE	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
5	XE	149/162 (92%)	142 (95%)	7 (5%)	0	100	100
6	QF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
6	XF	99/101 (98%)	99 (100%)	0	0	100	100
7	QG	153/156 (98%)	144 (94%)	8 (5%)	1 (1%)	22	61
7	XG	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
8	QH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
8	XH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
9	QI	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
9	XI	124/128 (97%)	113 (91%)	11 (9%)	0	100	100
10	QJ	97/105 (92%)	85 (88%)	12 (12%)	0	100	100
10	XJ	94/105 (90%)	80 (85%)	13 (14%)	1 (1%)	14	52
11	QK	117/129 (91%)	107 (92%)	10 (8%)	0	100	100
11	XK	114/129 (88%)	105 (92%)	9 (8%)	0	100	100
12	QL	123/132 (93%)	110 (89%)	11 (9%)	2 (2%)	9	43
12	XL	120/132 (91%)	103 (86%)	16 (13%)	1 (1%)	19	58
13	QM	118/126 (94%)	102 (86%)	13 (11%)	3 (2%)	5	34
13	XM	117/126 (93%)	96 (82%)	21 (18%)	0	100	100
14	QN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9	42
14	XN	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	42
15	QO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	XO	85/89 (96%)	84 (99%)	1 (1%)	0	100	100
16	QP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
17	XQ	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	QR	68/88 (77%)	64 (94%)	4 (6%)	0	100	100
18	XR	68/88 (77%)	64 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	QS	81/93 (87%)	69 (85%)	11 (14%)	1 (1%)	13	50
19	XS	81/93 (87%)	75 (93%)	6 (7%)	0	100	100
20	QT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
20	XT	97/106 (92%)	88 (91%)	6 (6%)	3 (3%)	4	30
21	QU	23/27 (85%)	20 (87%)	2 (9%)	1 (4%)	2	22
21	XU	23/27 (85%)	22 (96%)	0	1 (4%)	2	22
24	QY	82/84 (98%)	70 (85%)	10 (12%)	2 (2%)	6	35
24	QZ	82/84 (98%)	72 (88%)	10 (12%)	0	100	100
24	XY	82/84 (98%)	71 (87%)	8 (10%)	3 (4%)	3	26
24	XZ	82/84 (98%)	70 (85%)	11 (13%)	1 (1%)	13	50
25	R0	79/85 (93%)	72 (91%)	6 (8%)	1 (1%)	12	48
25	Y0	80/85 (94%)	72 (90%)	8 (10%)	0	100	100
26	R1	92/98 (94%)	82 (89%)	10 (11%)	0	100	100
26	Y1	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	14	52
27	R2	67/72 (93%)	61 (91%)	5 (8%)	1 (2%)	10	45
27	Y2	67/72 (93%)	63 (94%)	2 (3%)	2 (3%)	4	30
28	R3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
28	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
29	R4	67/71 (94%)	46 (69%)	17 (25%)	4 (6%)	1	15
29	Y4	67/71 (94%)	54 (81%)	12 (18%)	1 (2%)	10	45
30	R5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
30	Y5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
31	R6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
31	Y6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
32	R7	45/49 (92%)	45 (100%)	0	0	100	100
32	Y7	46/49 (94%)	46 (100%)	0	0	100	100
33	R8	62/65 (95%)	54 (87%)	6 (10%)	2 (3%)	4	29
33	Y8	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	4	29
34	R9	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
34	Y9	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
37	RD	270/276 (98%)	244 (90%)	22 (8%)	4 (2%)	10	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	YD	272/276 (99%)	263 (97%)	9 (3%)	0	100	100
38	RE	203/206 (98%)	179 (88%)	20 (10%)	4 (2%)	7	39
38	YE	202/206 (98%)	191 (95%)	9 (4%)	2 (1%)	15	54
39	RF	200/210 (95%)	195 (98%)	5 (2%)	0	100	100
39	YF	200/210 (95%)	184 (92%)	14 (7%)	2 (1%)	15	54
40	RG	179/182 (98%)	152 (85%)	24 (13%)	3 (2%)	9	42
40	YG	179/182 (98%)	151 (84%)	26 (14%)	2 (1%)	14	52
41	RH	172/180 (96%)	137 (80%)	29 (17%)	6 (4%)	3	27
41	YH	172/180 (96%)	164 (95%)	8 (5%)	0	100	100
42	RI	143/148 (97%)	117 (82%)	20 (14%)	6 (4%)	3	23
42	YI	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	11	46
43	RN	136/140 (97%)	117 (86%)	17 (12%)	2 (2%)	10	45
43	YN	136/140 (97%)	118 (87%)	16 (12%)	2 (2%)	10	45
44	RO	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
44	YO	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	19	58
45	RP	148/150 (99%)	125 (84%)	19 (13%)	4 (3%)	5	33
45	YP	147/150 (98%)	138 (94%)	7 (5%)	2 (1%)	11	46
46	RQ	139/141 (99%)	121 (87%)	13 (9%)	5 (4%)	3	26
46	YQ	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
47	RR	115/118 (98%)	108 (94%)	6 (5%)	1 (1%)	17	56
47	YR	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	17	56
48	RS	109/112 (97%)	93 (85%)	15 (14%)	1 (1%)	17	56
48	YS	109/112 (97%)	93 (85%)	16 (15%)	0	100	100
49	RT	135/146 (92%)	119 (88%)	15 (11%)	1 (1%)	22	61
49	YT	135/146 (92%)	119 (88%)	16 (12%)	0	100	100
50	RU	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	17	56
50	YU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	56
51	RV	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
51	YV	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15	54
52	RW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
52	YW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	RX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
53	YX	90/96 (94%)	86 (96%)	3 (3%)	1 (1%)	14	52
54	RY	105/110 (96%)	94 (90%)	11 (10%)	0	100	100
54	YY	105/110 (96%)	101 (96%)	3 (3%)	1 (1%)	15	54
55	RZ	181/206 (88%)	166 (92%)	13 (7%)	2 (1%)	14	52
55	YZ	181/206 (88%)	168 (93%)	13 (7%)	0	100	100
All	All	11789/12464 (95%)	10734 (91%)	950 (8%)	105 (1%)	17	56

5 of 105 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	208	ILE
14	QN	17	LYS
21	QU	3	LYS
24	QY	82	TYR
27	R2	47	ASN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	203/220 (92%)	196 (97%)	7 (3%)	37	68
2	XB	204/220 (93%)	201 (98%)	3 (2%)	65	84
3	QC	159/188 (85%)	154 (97%)	5 (3%)	40	70
3	XC	159/188 (85%)	155 (98%)	4 (2%)	47	75
4	QD	180/181 (99%)	175 (97%)	5 (3%)	43	72
4	XD	180/181 (99%)	178 (99%)	2 (1%)	73	88
5	QE	116/123 (94%)	115 (99%)	1 (1%)	78	90
5	XE	116/123 (94%)	112 (97%)	4 (3%)	37	68
6	QF	90/90 (100%)	89 (99%)	1 (1%)	73	88
6	XF	90/90 (100%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	QG	126/127 (99%)	121 (96%)	5 (4%)	31	64
7	XG	126/127 (99%)	121 (96%)	5 (4%)	31	64
8	QH	118/119 (99%)	115 (98%)	3 (2%)	47	75
8	XH	118/119 (99%)	117 (99%)	1 (1%)	81	91
9	QI	98/99 (99%)	92 (94%)	6 (6%)	18	51
9	XI	97/99 (98%)	96 (99%)	1 (1%)	76	88
10	QJ	89/92 (97%)	84 (94%)	5 (6%)	21	54
10	XJ	86/92 (94%)	85 (99%)	1 (1%)	71	87
11	QK	90/99 (91%)	88 (98%)	2 (2%)	52	78
11	XK	88/99 (89%)	87 (99%)	1 (1%)	73	88
12	QL	104/109 (95%)	102 (98%)	2 (2%)	57	80
12	XL	103/109 (94%)	101 (98%)	2 (2%)	57	80
13	QM	96/101 (95%)	95 (99%)	1 (1%)	76	88
13	XM	95/101 (94%)	91 (96%)	4 (4%)	30	63
14	QN	49/50 (98%)	47 (96%)	2 (4%)	30	63
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	78 (99%)	1 (1%)	69	86
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	70 (97%)	2 (3%)	43	72
17	QQ	95/97 (98%)	94 (99%)	1 (1%)	73	88
17	XQ	95/97 (98%)	93 (98%)	2 (2%)	53	79
18	QR	61/77 (79%)	58 (95%)	3 (5%)	25	59
18	XR	61/77 (79%)	60 (98%)	1 (2%)	62	83
19	QS	72/80 (90%)	69 (96%)	3 (4%)	30	63
19	XS	69/80 (86%)	69 (100%)	0	100	100
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
24	QY	78/78 (100%)	74 (95%)	4 (5%)	24	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	QZ	78/78 (100%)	73 (94%)	5 (6%)	17	50
24	XY	78/78 (100%)	78 (100%)	0	100	100
24	XZ	78/78 (100%)	74 (95%)	4 (5%)	24	57
25	R0	65/67 (97%)	64 (98%)	1 (2%)	65	84
25	Y0	65/67 (97%)	62 (95%)	3 (5%)	27	61
26	R1	79/83 (95%)	78 (99%)	1 (1%)	69	86
26	Y1	82/83 (99%)	82 (100%)	0	100	100
27	R2	64/67 (96%)	63 (98%)	1 (2%)	62	83
27	Y2	64/67 (96%)	63 (98%)	1 (2%)	62	83
28	R3	51/52 (98%)	50 (98%)	1 (2%)	55	79
28	Y3	51/52 (98%)	50 (98%)	1 (2%)	55	79
29	R4	62/63 (98%)	54 (87%)	8 (13%)	4	22
29	Y4	62/63 (98%)	60 (97%)	2 (3%)	39	69
30	R5	51/52 (98%)	51 (100%)	0	100	100
30	Y5	51/52 (98%)	50 (98%)	1 (2%)	55	79
31	R6	51/52 (98%)	49 (96%)	2 (4%)	32	64
31	Y6	51/52 (98%)	49 (96%)	2 (4%)	32	64
32	R7	40/42 (95%)	40 (100%)	0	100	100
32	Y7	41/42 (98%)	41 (100%)	0	100	100
33	R8	54/55 (98%)	50 (93%)	4 (7%)	13	44
33	Y8	54/55 (98%)	52 (96%)	2 (4%)	34	65
34	R9	34/34 (100%)	33 (97%)	1 (3%)	42	71
34	Y9	34/34 (100%)	34 (100%)	0	100	100
37	RD	214/218 (98%)	209 (98%)	5 (2%)	50	77
37	YD	216/218 (99%)	214 (99%)	2 (1%)	78	90
38	RE	165/166 (99%)	160 (97%)	5 (3%)	41	71
38	YE	164/166 (99%)	163 (99%)	1 (1%)	86	94
39	RF	161/166 (97%)	160 (99%)	1 (1%)	86	94
39	YF	161/166 (97%)	160 (99%)	1 (1%)	86	94
40	RG	155/156 (99%)	149 (96%)	6 (4%)	32	64
40	YG	155/156 (99%)	150 (97%)	5 (3%)	39	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	RH	145/148 (98%)	140 (97%)	5 (3%)	37	68
41	YH	144/148 (97%)	142 (99%)	2 (1%)	67	85
42	RI	122/124 (98%)	117 (96%)	5 (4%)	30	63
42	YI	122/124 (98%)	119 (98%)	3 (2%)	47	75
43	RN	117/119 (98%)	114 (97%)	3 (3%)	46	74
43	YN	117/119 (98%)	117 (100%)	0	100	100
44	RO	100/100 (100%)	99 (99%)	1 (1%)	76	88
44	YO	100/100 (100%)	98 (98%)	2 (2%)	55	79
45	RP	116/116 (100%)	114 (98%)	2 (2%)	60	82
45	YP	115/116 (99%)	114 (99%)	1 (1%)	78	90
46	RQ	111/111 (100%)	107 (96%)	4 (4%)	35	66
46	YQ	111/111 (100%)	111 (100%)	0	100	100
47	RR	100/101 (99%)	100 (100%)	0	100	100
47	YR	100/101 (99%)	98 (98%)	2 (2%)	55	79
48	RS	87/88 (99%)	83 (95%)	4 (5%)	27	61
48	YS	87/88 (99%)	84 (97%)	3 (3%)	37	68
49	RT	120/127 (94%)	114 (95%)	6 (5%)	24	58
49	YT	120/127 (94%)	117 (98%)	3 (2%)	47	75
50	RU	93/94 (99%)	92 (99%)	1 (1%)	73	88
50	YU	93/94 (99%)	92 (99%)	1 (1%)	73	88
51	RV	82/82 (100%)	76 (93%)	6 (7%)	14	45
51	YV	82/82 (100%)	80 (98%)	2 (2%)	49	76
52	RW	92/92 (100%)	90 (98%)	2 (2%)	52	78
52	YW	92/92 (100%)	90 (98%)	2 (2%)	52	78
53	RX	74/78 (95%)	74 (100%)	0	100	100
53	YX	74/78 (95%)	72 (97%)	2 (3%)	44	73
54	RY	88/91 (97%)	88 (100%)	0	100	100
54	YY	88/91 (97%)	87 (99%)	1 (1%)	73	88
55	RZ	162/179 (90%)	160 (99%)	2 (1%)	71	87
55	YZ	162/179 (90%)	159 (98%)	3 (2%)	57	80
All	All	10001/10378 (96%)	9777 (98%)	224 (2%)	52	78

5 of 224 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	RH	154	PRO
49	RT	109	GLU
48	YS	23	ARG
42	RI	130	TYR
46	RQ	5	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
37	RD	46	GLN
40	YG	132	ASN
55	RZ	151	HIS
9	QI	3	GLN
13	XM	101	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1508/1521 (99%)	293 (19%)	33 (2%)
1	XA	1505/1521 (98%)	301 (20%)	40 (2%)
22	QV	77/77 (100%)	8 (10%)	1 (1%)
22	XV	77/77 (100%)	9 (11%)	1 (1%)
23	QX	16/20 (80%)	7 (43%)	2 (12%)
23	XX	16/20 (80%)	8 (50%)	0
35	RA	2888/2915 (99%)	623 (21%)	37 (1%)
35	YA	2875/2915 (98%)	578 (20%)	28 (0%)
36	RB	119/124 (95%)	24 (20%)	1 (0%)
36	YB	119/124 (95%)	17 (14%)	1 (0%)
56	ZA	1/3 (33%)	0	0
56	ZB	1/3 (33%)	0	0
All	All	9202/9320 (98%)	1868 (20%)	144 (1%)

5 of 1868 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	4	U
1	QA	5	U
1	QA	6	G
1	QA	22	G
1	QA	32	A

5 of 144 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	RA	2211	G
1	XA	201	C
35	YA	2211	G
35	RA	2447	G
36	RB	66	A

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

4 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
23	A3P	XX	20	23	23,28,29	5.22	7 (30%)	23,42,45	1.53	3 (13%)
23	A3P	QX	20	23	23,28,29	5.26	7 (30%)	23,42,45	1.49	4 (17%)
56	PPU	ZB	3	56,35	32,40,41	0.85	2 (6%)	33,57,60	1.87	10 (30%)
56	PPU	ZA	3	56,35	32,40,41	0.90	0	33,57,60	1.80	7 (21%)

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
23	A3P	XX	20	23	-	1/8/30/31	0/3/3/3
23	A3P	QX	20	23	-	2/8/30/31	0/3/3/3
56	PPU	ZB	3	56,35	-	14/21/43/44	0/4/4/4
56	PPU	ZA	3	56,35	-	6/21/43/44	0/4/4/4

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	QX	20	A3P	O4'-C1'	18.93	1.67	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	XX	20	A3P	O4'-C1'	18.45	1.66	1.41
23	XX	20	A3P	C2'-C1'	-13.73	1.32	1.53
23	QX	20	A3P	C2'-C1'	-13.44	1.33	1.53
23	XX	20	A3P	O4'-C4'	-5.92	1.31	1.45

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	XX	20	A3P	N3-C2-N1	-4.92	120.98	128.68
56	ZA	3	PPU	N1-C6-N6	4.77	122.08	117.06
56	ZB	3	PPU	CG-CB-CA	-4.38	105.02	114.13
23	QX	20	A3P	N3-C2-N1	-4.07	122.32	128.68
56	ZB	3	PPU	N1-C6-N6	3.96	121.22	117.06

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	XX	20	A3P	C3'-O3'-P1-O1P
56	ZB	3	PPU	N3'-C-CA-N
56	ZB	3	PPU	O-C-CA-CB
56	ZB	3	PPU	N3'-C-CA-CB
56	ZB	3	PPU	CA-C-N3'-C3'

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	XX	20	A3P	2	0
23	QX	20	A3P	1	0
56	ZB	3	PPU	7	0
56	ZA	3	PPU	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 900 ligands modelled in this entry, 898 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	XD	301	4	0,12,12	0.00	-	-		
58	SF4	QD	302	4	0,12,12	0.00	-	-		

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	XD	301	4	-	-	0/6/5/5
58	SF4	QD	302	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 [i](#)

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.