



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 15, 2023 – 12:45 PM EDT

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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

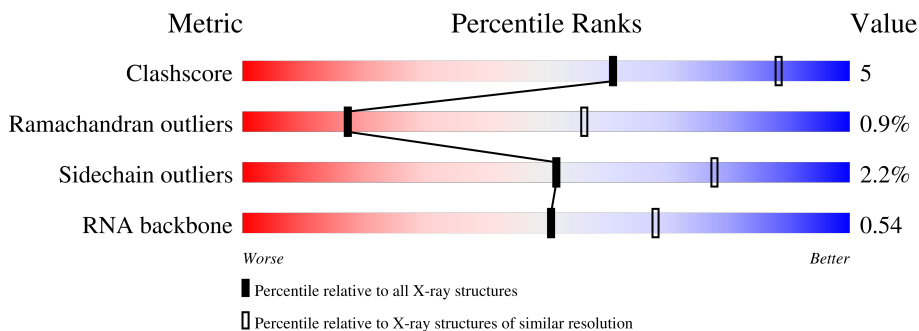
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

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%

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Mol	Chain	Length	Quality of chain
4	QD	209	76% 22%
4	XD	209	81% 18%
5	QE	162	80% 13% 7%
5	XE	162	78% 15% 7%
6	QF	101	81% 18%
6	XF	101	85% 14%
7	QG	156	88% 11%
7	XG	156	83% 15%
8	QH	138	75% 23%
8	XH	138	86% 13%
9	QI	128	79% 19%
9	XI	128	78% 20%
10	QJ	105	76% 15% 6%
10	XJ	105	66% 24% 9%
11	QK	129	78% 13% 8%
11	XK	129	79% 10% 10%
12	QL	132	81% 12% 5%
12	XL	132	76% 15% 8%
13	QM	126	69% 22% 5%
13	XM	126	75% 17% 6%
14	QN	61	82% 16%
14	XN	61	75% 23%
15	QO	89	92% 7%
15	XO	89	91% 7%
16	QP	88	78% 17% 5%









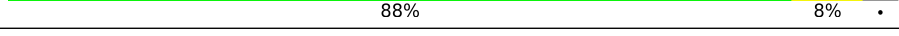

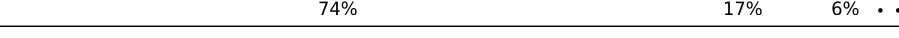
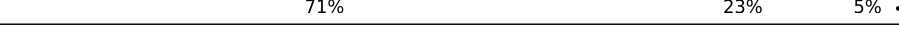

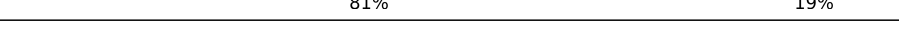


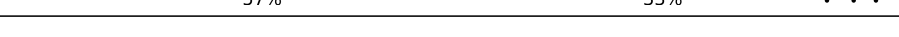

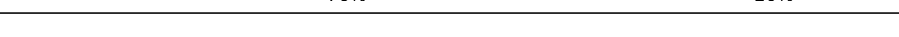






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Mol	Chain	Length	Quality of chain
16	XP	88	85% 8% • 5%
17	QQ	105	84% 10% • 5%
17	XQ	105	78% 16% • 5%
18	QR	88	59% 19% • 20%
18	XR	88	63% 16% • 20%
19	QS	93	68% 18% •• 11%
19	XS	93	73% 16% 11%
20	QT	106	82% 11% 7%
20	XT	106	70% 23% • 7%
21	QU	27	67% 22% • 7%
21	XU	27	70% 22% 7%
22	QV	77	78% 22%
22	XV	77	81% 17% •
23	QX	20	35% 45% 10% 10%
23	XX	20	35% 40% 15% 10%
24	QY	84	77% 23%
24	QZ	84	74% 23% •
24	XY	84	79% 21%
24	XZ	84	81% 18% •
25	R0	85	74% 20% • 5%
25	Y0	85	75% 20% ••
26	R1	98	85% 9% ••
26	Y1	98	77% 22% •
27	R2	72	68% 26% ••
27	Y2	72	85% 11% •

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Mol	Chain	Length	Quality of chain
28	R3	60	 82% 17%
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%





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Mol	Chain	Length	Quality of chain
40	YG	182	80% 18% ...
41	RH	180	78% 17% ..
41	YH	180	84% 12% ..
42	RI	148	76% 16% . . .
42	YI	148	86% 9% ...
43	RN	140	79% 17% ...
43	YN	140	83% 14% ..
44	RO	122	78% 22%
44	YO	122	80% 20%
45	RP	150	75% 23% .
45	YP	150	81% 19% .
46	RQ	141	73% 24% ..
46	YQ	141	82% 18%
47	RR	118	81% 16% ..
47	YR	118	81% 16% ...
48	RS	112	78% 21% .
48	YS	112	79% 20% ..
49	RT	146	69% 23% . 6%
49	YT	146	77% 16% . 6%
50	RU	118	82% 15% ...
50	YU	118	84% 14% ..
51	RV	101	74% 21% ..
51	YV	101	74% 21% 5%
52	RW	113	88% 11% .
52	YW	113	79% 21%

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Mol	Chain	Length	Quality of chain
53	RX	96	 81% 15% .
53	YX	96	 81% 14% . .
54	RY	110	 79% 17% . .
54	YY	110	 89% 8% .
55	RZ	206	 76% 12% . 11%
55	YZ	206	 66% 23% 11%
56	ZA	3	 33% 33% 33%
56	ZB	3	 67% 33%

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
			Total	C	N	O	P			
1	QA	1510	Total 32452	C 14444	N 6009	O 10489	P 1510	0	0	0
1	XA	1507	Total 32389	C 14416	N 5999	O 10467	P 1507	0	0	0

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

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

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

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

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

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

- 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
			Total	C	N	O	S			
10	XJ	96	777	487	153	136	1	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S			
26	R1	94	Total 737	C 463	N 146	O 127	S 1	0	0	0
26	Y1	97	Total 763	C 481	N 150	O 131	S 1	0	0	0

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

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

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

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

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

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

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

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

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

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

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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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O			
47	YR	117	960	599	202	159	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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	QD	1	Total	Mg	0	0
			1	1		
57	QE	1	Total	Mg	0	0
			1	1		
57	QV	3	Total	Mg	0	0
			3	3		

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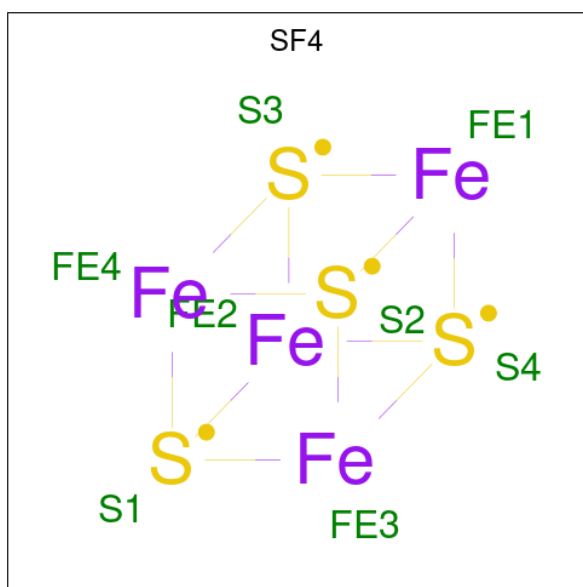
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QY	1	Total 1	Mg 1	0	0
57	R0	2	Total 2	Mg 2	0	0
57	R3	1	Total 1	Mg 1	0	0
57	RA	302	Total 302	Mg 302	0	0
57	RB	3	Total 3	Mg 3	0	0
57	RD	2	Total 2	Mg 2	0	0
57	RE	1	Total 1	Mg 1	0	0
57	RN	1	Total 1	Mg 1	0	0
57	RO	1	Total 1	Mg 1	0	0
57	RP	1	Total 1	Mg 1	0	0
57	RQ	4	Total 4	Mg 4	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RY	1	Total 1	Mg 1	0	0
57	XA	99	Total 99	Mg 99	0	0
57	XE	1	Total 1	Mg 1	0	0
57	XF	1	Total 1	Mg 1	0	0
57	XL	1	Total 1	Mg 1	0	0
57	XM	1	Total 1	Mg 1	0	0
57	XV	4	Total 4	Mg 4	0	0
57	Y0	2	Total 2	Mg 2	0	0
57	Y1	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y3	1	Total 1	Mg 1	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	Y9	1	Total 1	Mg 1	0	0
57	YA	335	Total 335	Mg 335	0	0
57	YB	3	Total 3	Mg 3	0	0
57	YD	4	Total 4	Mg 4	0	0
57	YE	5	Total 5	Mg 5	0	0
57	YF	1	Total 1	Mg 1	0	0
57	YG	1	Total 1	Mg 1	0	0
57	YO	1	Total 1	Mg 1	0	0
57	YP	1	Total 1	Mg 1	0	0
57	YQ	5	Total 5	Mg 5	0	0
57	YR	1	Total 1	Mg 1	0	0
57	YV	1	Total 1	Mg 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

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

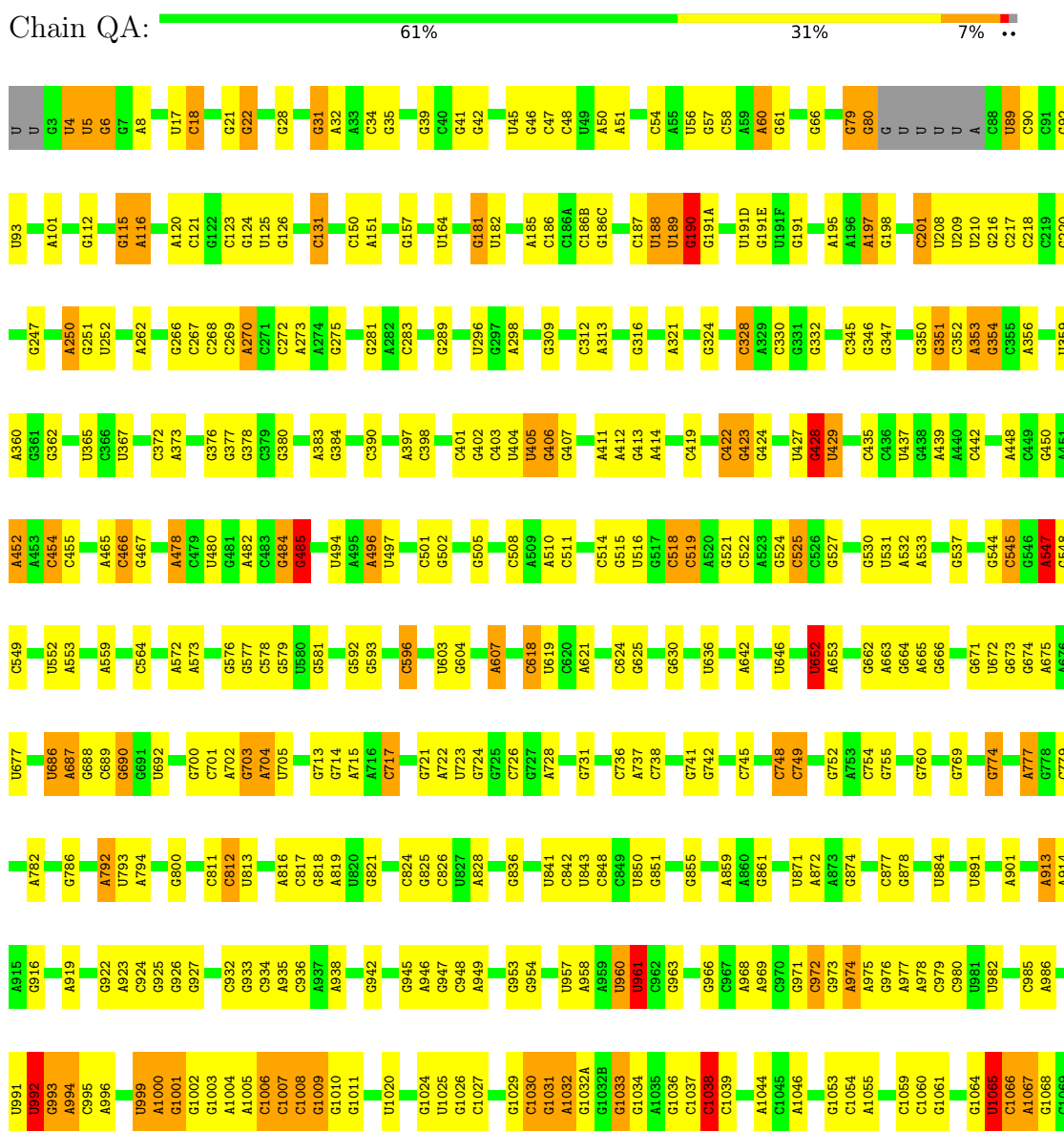
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	QN	1	Total	Zn	0	0
			1	1		
59	R4	1	Total	Zn	0	0
			1	1		
59	R5	1	Total	Zn	0	0
			1	1		
59	R6	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		
59	Y4	1	Total	Zn	0	0
			1	1		
59	Y6	1	Total	Zn	0	0
			1	1		

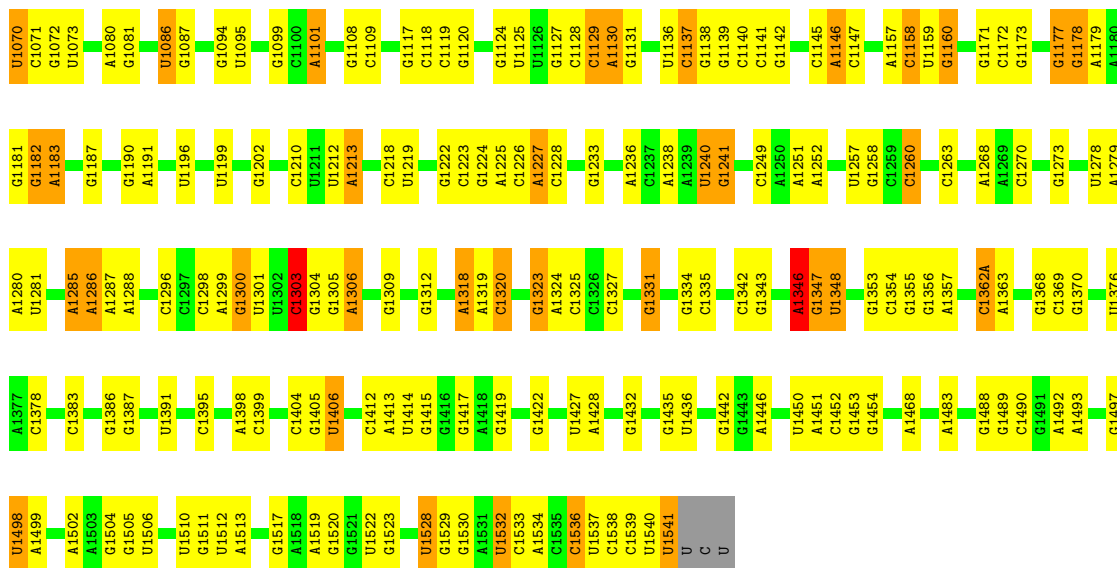
3 Residue-property plots [i](#)

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

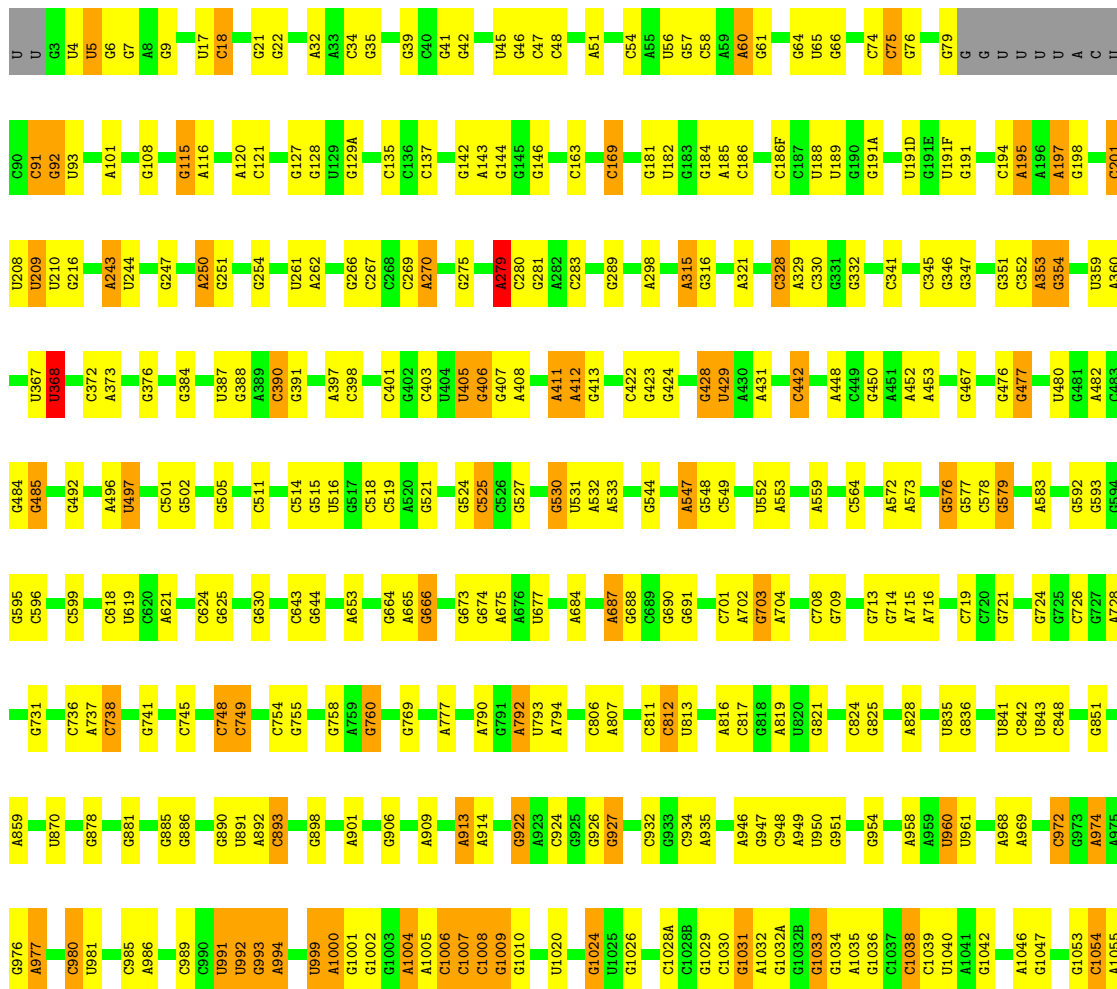
Note EDS failed to run properly.

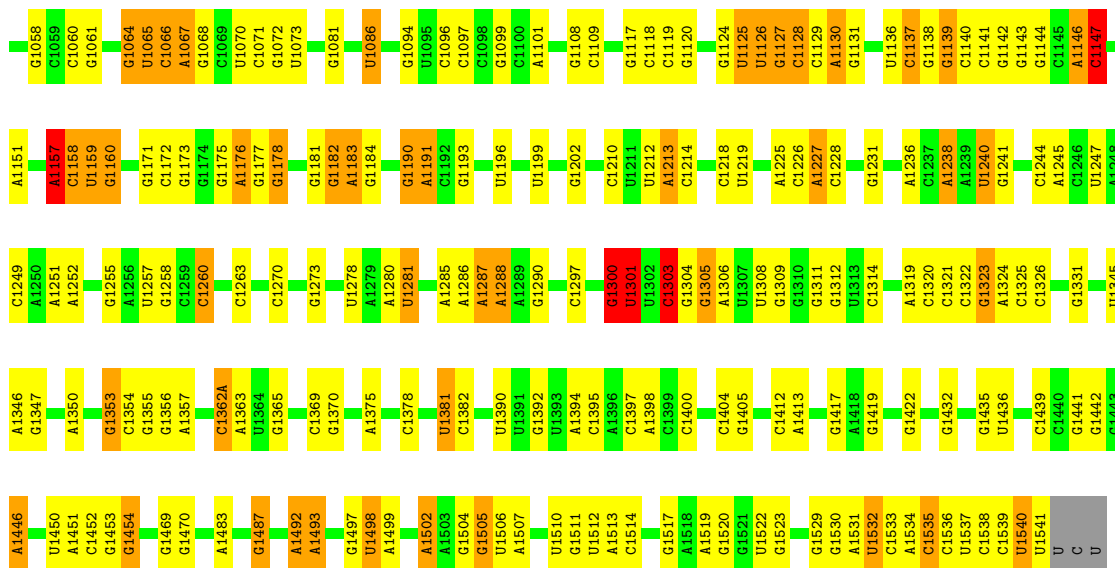
- Molecule 1: 16S rRNA





• Molecule 1: 16S rRNA

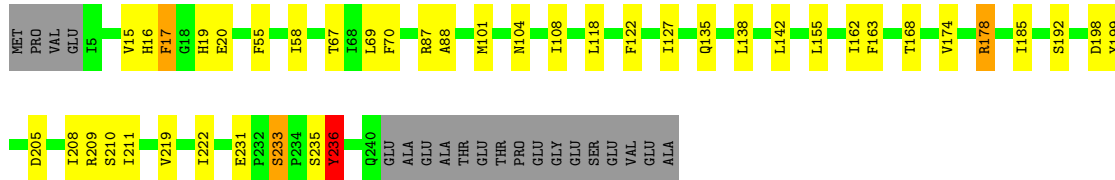
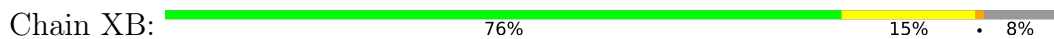




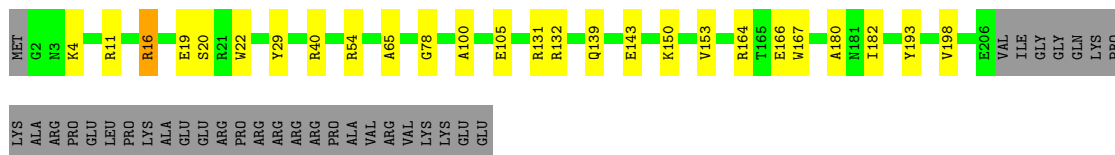
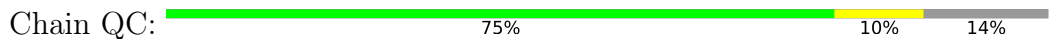
• Molecule 2: 30S ribosomal protein S2



• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3





- 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%



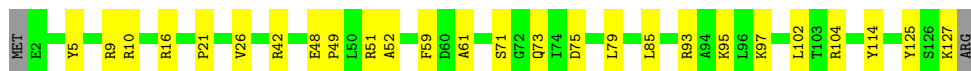
- Molecule 9: 30S ribosomal protein S9

Chain QI: 79% 19%

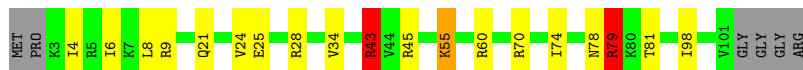
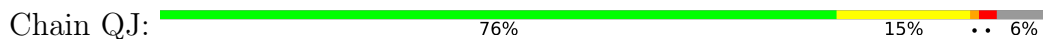


- Molecule 9: 30S ribosomal protein S9

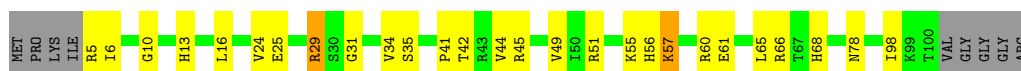
Chain XI: 78% 20%



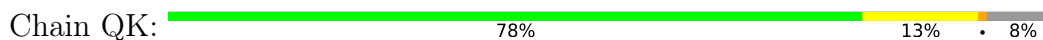
- Molecule 10: 30S ribosomal protein S10



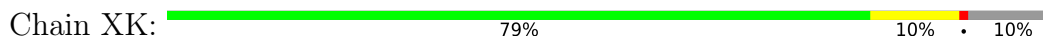
- Molecule 10: 30S ribosomal protein S10



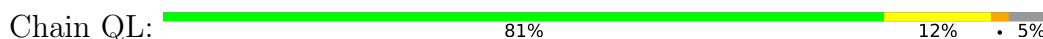
- Molecule 11: 30S ribosomal protein S11



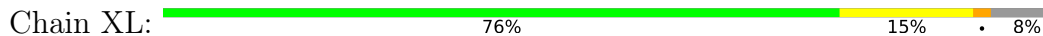
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

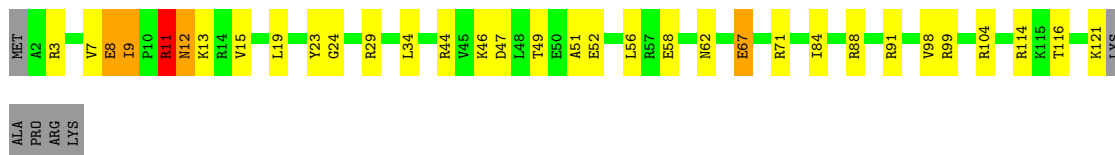


- Molecule 12: 30S ribosomal protein S12



- 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%



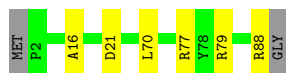
- Molecule 15: 30S ribosomal protein S15

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%



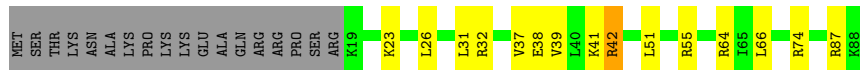
- Molecule 18: 30S ribosomal protein S18

Chain QR:  59% 19% • 20%



- Molecule 18: 30S ribosomal protein S18

Chain XR:  63% 16% • 20%



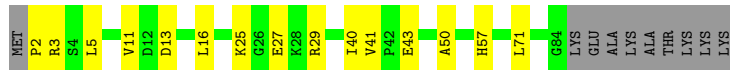
- Molecule 19: 30S ribosomal protein S19

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%




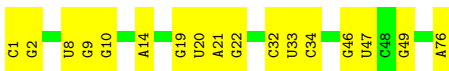
- Molecule 21: 30S ribosomal protein Thx

Chain XU:  70% 22% 7%




- Molecule 22: P-site tRNA-fMet

Chain QV:  78% 22%

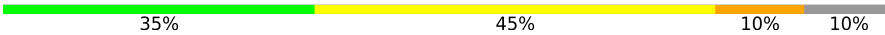


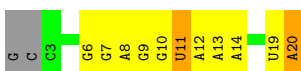
- Molecule 22: P-site tRNA-fMet

Chain XV:  81% 17% 2%

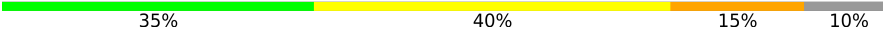


- Molecule 23: mRNA

Chain QX:  35% 45% 10% 10%




- Molecule 23: mRNA

Chain XX:  35% 40% 15% 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%




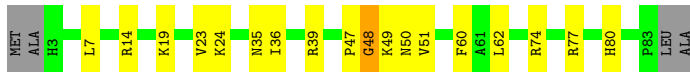
- Molecule 24: Addiction module toxin, Txe/YoeB family

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%



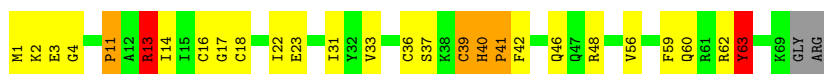
- Molecule 28: 50S ribosomal protein L30

Chain Y3:  83% 15%




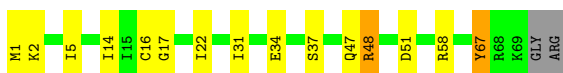
- Molecule 29: 50S ribosomal protein L31

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%




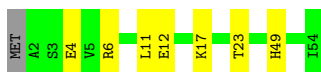
• Molecule 31: 50S ribosomal protein L33

Chain R6:  72% 22%




• Molecule 31: 50S ribosomal protein L33

Chain Y6:  85% 13%




• Molecule 32: 50S ribosomal protein L34

Chain R7:  88% 8%

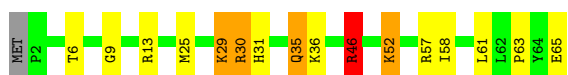


• Molecule 32: 50S ribosomal protein L34

Chain Y7:  84% 14%



• Molecule 33: 50S ribosomal protein L35



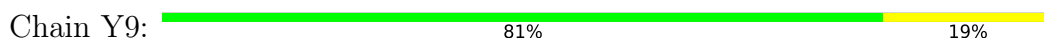
- Molecule 33: 50S ribosomal protein L35



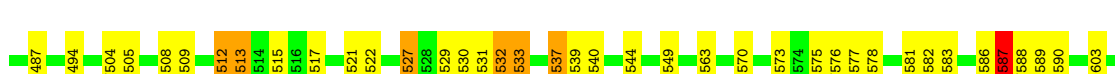
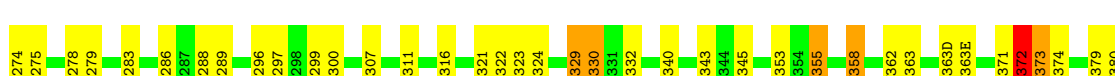
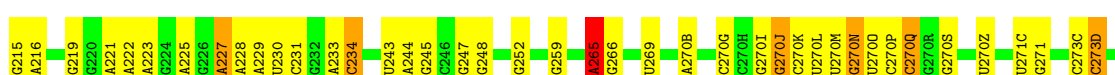
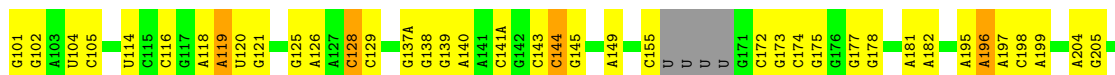
- Molecule 34: 50S ribosomal protein L36



- Molecule 34: 50S ribosomal protein L36



- Molecule 35: 23S rRNA



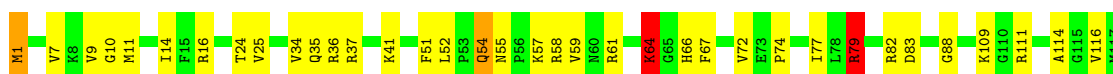
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A2020	C2021	U2022	G2023	G2024	C2025	C2026	G2027	U2028	A2029	C2030	A2031	G2032	A2033	A2034	G2035	G2036	G2037	G2038	U2041	A2042	C2043	G2052	C2055	G2056	A2059	A2060	G2061	A2062	C2063	C2064	C2065	G2069	C2073	U2074	U2075	U2086	G2093	U2096	U2099	C2103	C2111	G2112	U2113	A2114	G2115	G2116			
A1901	C1902	G1903	G1906	C1909	G1910	U1911	A1912	A1913	C1914	U1915	C1920	G1959	A1954	A1955	G1956	G1957	G1958	G1959	A1960	A1961	A1962	G1963	G1964	G1965	A1966	C1967	A1970	A1971	A1972	C1979	G1980	A1981	C1982	G1988	U1979	G1989	G1992	U1993	C1996	A2001	G2002	C2111	G2112	U2113	A2114	G2115	G2116		
G1763	G1764	G1769	A1773	C1774	U1779	A1780	C1781	A1782	A1783	A1784	C1788	A1791	G1792	U1798	G1799	C1800	G1801	A1802	A1809	G1816	A1819	U1820	G1824	C1827	G1828	A1829	C1830	G1831	G1835	A1847	G1858	A1859	A1872	G1878	C1881	C1882	G1883	G1888	A1889	G1899	A1900								
A1632	G1633	A1634	G1635	C1636	A1637	C1640	C1644	C1648	A1652	G1653	A1654	A1655	C1656	C1657	C1658	G1667	A1668	A1669	G1674	C1675	U1679	G1680	G1681	A1689	G1696	A1698	G1699	A1700	G1703	G1725	G1728	A1729	G1731	G1735	C1741	G1742	G1743	G1744	G1753	C1754	A1755	G1756	A1762						
U1516	G1522	U1523	G1524	G1525	A1528	U1535	A1536	C1537	G1538	G1539	G1540	A1543	C1544	A1545	C1547	A1554	A1558	G1559	G1560	A1566	G1567	A1568	A1569	A1570	A1571	A1572	U1578	A1579	A1580	C1585	A1586	A1587	C1588	C1598	U1602	C1607	A1608	G1613	A1614	A1618	G1622								
G1418	A1419	U1420	G1421	G1422	G1423	G1424	A1427	C1428	G1429	C1430	U1431	C1432	U1433	A1434	C1437	A1444	C1445	A1449	G1449A	G1455	G1459	A1460	G1461	C1462	C1463	C1464	C1467	A1471	C1474	G1475	G1480	U1482	G1483	G1488	U1489	A1490	C1493	C1499	G1500	G1505	C1509	A1510	G1512						
A1301	A1308	G1309	G1310	G1311	U1312	U1313	C1314	C1315	A1317	U1329	C1330	A1342	U1352	A1353	A1354	A1359	A1360	C1363	G1368	G1369	C1370	A1378	A1379	G1380	A1384	G1385	G1388	U1391	U1394	A1395	U1396	G1400	G1401	C1402	C1403	U1406	C1407	C1408	C1411	A1412	G1416	C1417							
G1187	U1188	G1191	G1195	C1196	A1204	U1205	A1210	U1211	G1212	A1213	A1214	A1220	C1225	G1226	A1227	G1228	C1233	G1236	A1237	G1243	A1247	G1248	G1252	A1253	A1254	U1255	G1266	C1267	U1267	A1265	U1266	U1267	A1272	A1278	G1279	G1280	G1281	U1294	U1300										
A1088	G1089	G1093	U1094	A1095	A1096	G1099	C11005	A1102	A1103	G1106	G1110	U1113	G1114	G1122	A1126	A1127	A1128	A1129	U1130	G1131	C1135	G1136	G1139	U1141	U1142	A1142A	A1143	U1148	C1152	U1152	A1156	U1165	G1170	G1171	G1173	A1174	U1175	A1177	C1178	U1179	A1180	G1184							
C992	G993	C994	C995	U996	G997	C998	U999	A1000	C1005	A1009	A1010	U1012	C1013	G1017	A1020	A1021	C1022	G1024	G1025	U1026	A1027	A1028	U1033	G1044	A1045	A1046	G1047	A1048	C1053	G1056	U1060	U1061	C1064	U1065	A1066	G1074	C1075	A980	A983	U1083	A1084	A1085	A1086	G1087					
A896	C897	C904	U905	G906	U907	A910	C915	G916	A917	A918	G919	G928	G929	U930	G931	G932	A933	G938	A941	A945	G946	A953	G956	A957	U958	A959	A960	C961	C964	C965	U968	U969	C970	C971	G972	G974	G975	A980	A983	U983	A984	A985	A990	C991					
C812	U813	C814	C817	U818	A819	A820	U822	G823	U827	U828	C831	G832	U833	C834	A835	G836	C837	C838	U839	G845	G848	A849	C850	U851	G852	C856	C857	U858	G859	U860	A861	C867	U868	G874	G875	G882	G883	A884	C885	C886	A887	C888	C889	A890	G892	C893	A894	U895	
G669	A670	G674	A675	A676	C679	G680	G681	G686	C692	C698	A699	G700	C708	U714	G717	A722	A727	C730	A734	A752	C753	A764	G768	G776	A782	U783	A784	G785	C786	U787	A788	A789	G792	A793	C797	G805	C806	U807	G866	U867	G868								
U614	G615	A616	G617	A621	G622	G623	C624	A627	G628	G629	G630	A633	C634	A637	G638	C640	C641	G642	C645	A646	C652	A653	A	C	G	G	G	C	C	C	C	C	C	C	C	C	C	A	A654V	C659	G660	G666	U667	G668					



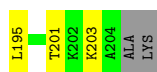
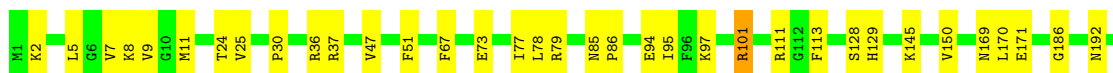
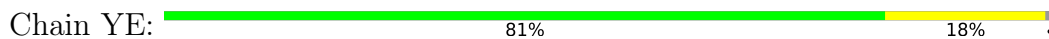
- Molecule 37: 50S ribosomal protein L2



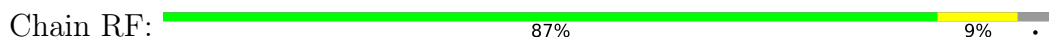
- Molecule 38: 50S ribosomal protein L3



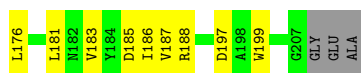
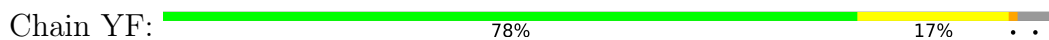
- Molecule 38: 50S ribosomal protein L3




- Molecule 39: 50S ribosomal protein L4

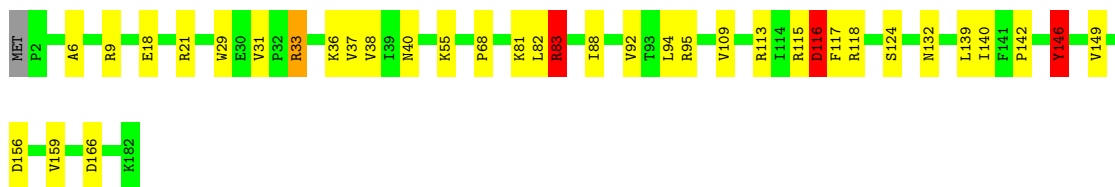


- Molecule 39: 50S ribosomal protein L4




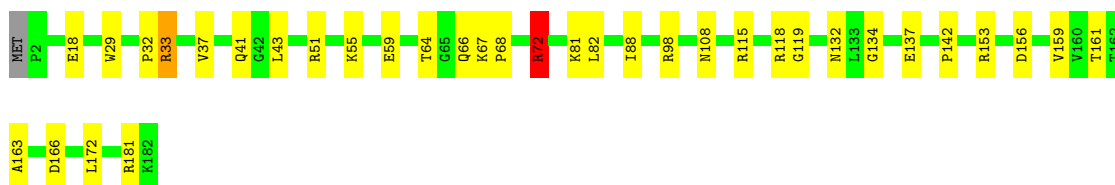
- Molecule 40: 50S ribosomal protein L5

Chain RG:  80% 18%




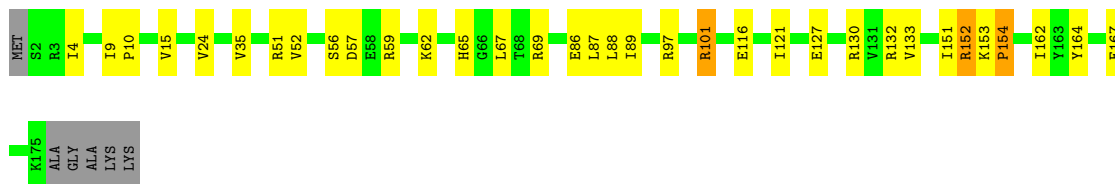
- Molecule 40: 50S ribosomal protein L5

Chain YG:  80% 18%




- Molecule 41: 50S ribosomal protein L6

Chain RH:  78% 17%




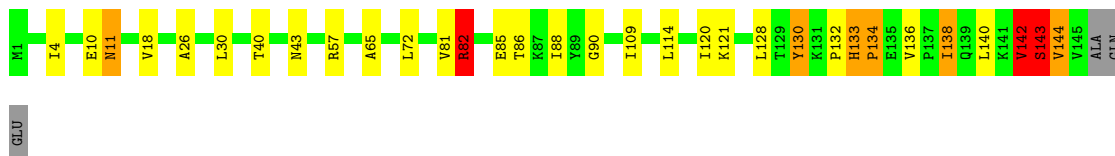
- Molecule 41: 50S ribosomal protein L6

Chain YH:  84% 12%




- Molecule 42: 50S ribosomal protein L9

Chain RI:  76% 16%

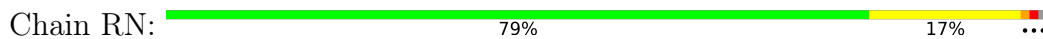


- Molecule 42: 50S ribosomal protein L9

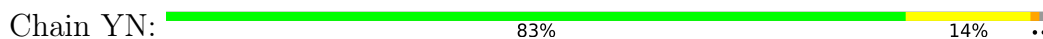
Chain YI:  86% 9%



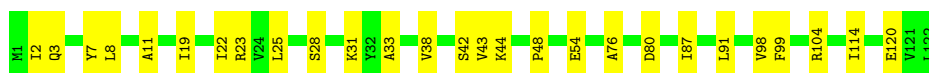
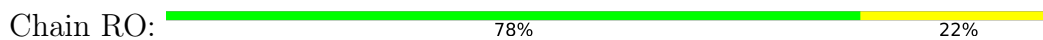
- Molecule 43: 50S ribosomal protein L13



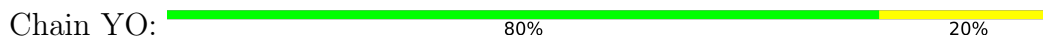
- Molecule 43: 50S ribosomal protein L13



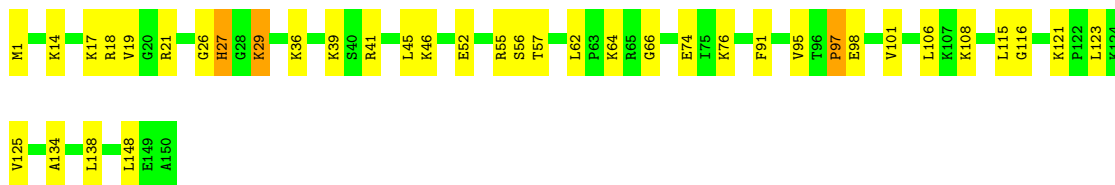
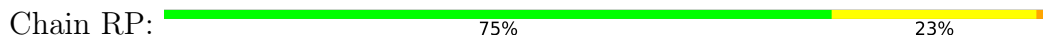
- Molecule 44: 50S ribosomal protein L14



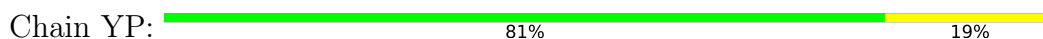
- Molecule 44: 50S ribosomal protein L14



- Molecule 45: 50S ribosomal protein L15

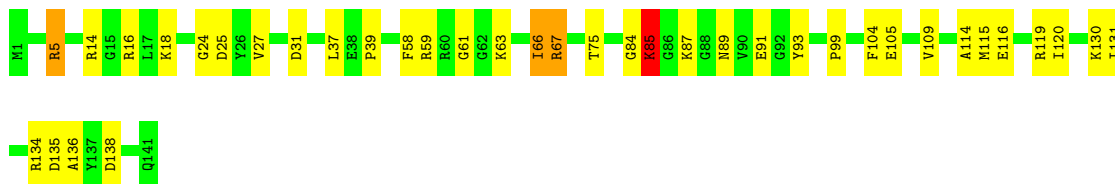


- Molecule 45: 50S ribosomal protein L15




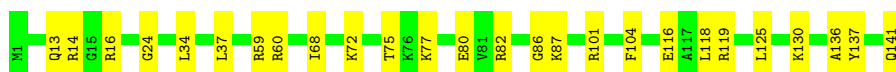
- Molecule 46: 50S ribosomal protein L16

Chain RQ:  73% 24% ..




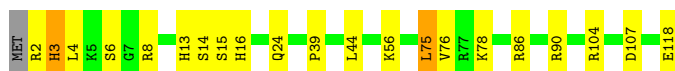
- Molecule 46: 50S ribosomal protein L16

Chain YQ:  82% 18%




- Molecule 47: 50S ribosomal protein L17

Chain RR:  81% 16% ..




- Molecule 47: 50S ribosomal protein L17

Chain YR:  81% 16% ...




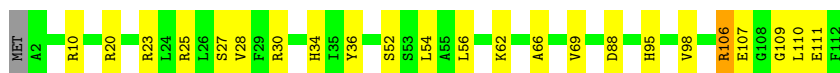
- Molecule 48: 50S ribosomal protein L18

Chain RS:  78% 21% .



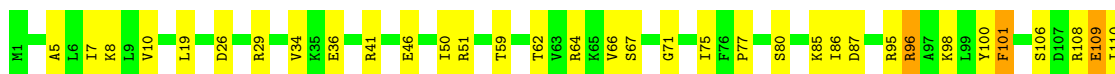
- Molecule 48: 50S ribosomal protein L18

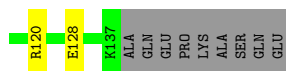
Chain YS:  79% 20% ..



- Molecule 49: 50S ribosomal protein L19

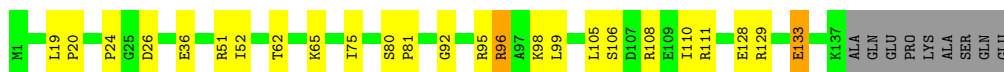
Chain RT:  69% 23% 6%





- Molecule 49: 50S ribosomal protein L19

Chain YT: 77% 16% 6%



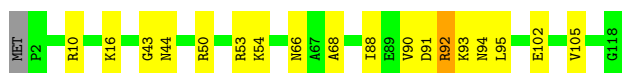
- Molecule 50: 50S ribosomal protein L20

Chain RU: 82% 15% ...



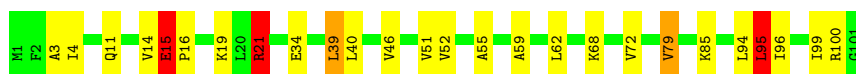
- Molecule 50: 50S ribosomal protein L20

Chain YU: 84% 14% ..



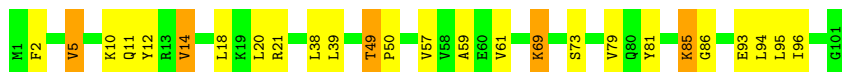
- Molecule 51: 50S ribosomal protein L21

Chain RV: 74% 21% ..



- Molecule 51: 50S ribosomal protein L21

Chain YV: 74% 21% 5%



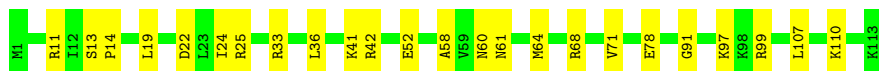
- Molecule 52: 50S ribosomal protein L22

Chain RW: 88% 11% .

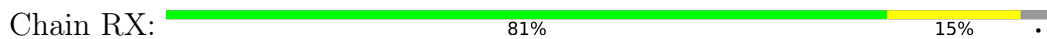


- Molecule 52: 50S ribosomal protein L22

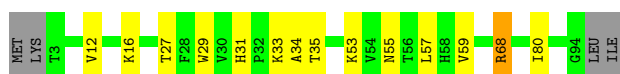
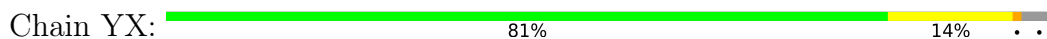
Chain YW: 79% 21%



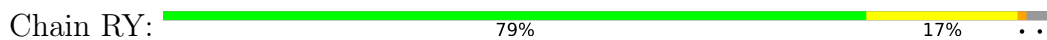
- Molecule 53: 50S ribosomal protein L23



- Molecule 53: 50S ribosomal protein L23



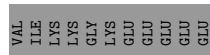
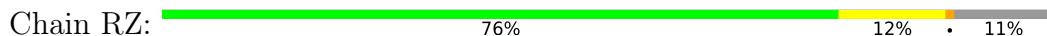
- Molecule 54: 50S ribosomal protein L24



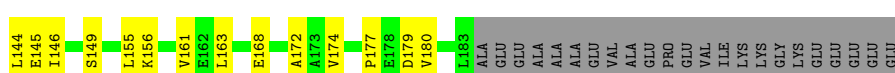
- Molecule 54: 50S ribosomal protein L24



- Molecule 55: 50S ribosomal protein L25



- Molecule 55: 50S ribosomal protein L25



- Molecule 56: CCPuro

Chain ZA:  33% 33% 33%

 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.49Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.216 , 0.246	Depositor
Wilson B-factor (Å ²)	89.9	Xtrriage
Anisotropy	0.032	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	295153	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PPU, MG, SF4, ZN, A3P

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 [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.

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:NZ	51:YV:85:LYS:CE	1.87	1.36
51:YV:85:LYS:CD	51:YV:85:LYS:CE	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 [i](#)

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
46	RQ	91	GLU
55	YZ	29	TYR
3	XC	111	LEU
53	YX	68	ARG
42	YI	10	GLU

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

Mol	Chain	Res	Type
55	RZ	151	HIS
13	XM	101	GLN
40	YG	132	ASN
9	QI	3	GLN
2	QB	16	HIS

5.3.3 RNA [i](#)

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	YA	119	A
36	YB	66	A
35	YA	752	A
35	YA	2144	U
35	RA	1022	G

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

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

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

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	ZA	3	PPU	N-CA-CB-CG
56	ZA	3	PPU	C-CA-CB-CG
56	ZA	3	PPU	C5-C6-N6-C9
56	ZB	3	PPU	N3'-C-CA-N

There are no ring outliers.

4 monomers are involved in 12 short contacts:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	QD	302	4	0,12,12	-	-	-		
58	SF4	XD	301	4	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	QD	302	4	-	-	0/6/5/5
58	SF4	XD	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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