



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 08:14 pm BST

PDB ID : 6BZ7
Title : Thermus thermophilus 70S containing 16S G299A point mutation and near-cognate ASL Leucine in A site.
Authors : Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.
Deposited on : 2017-12-22
Resolution : 3.68 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 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

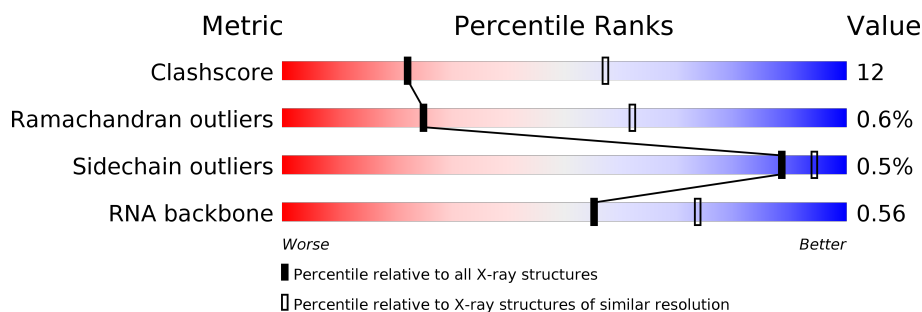
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.68 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	1070 (3.84-3.52)
Ramachandran outliers	138981	1036 (3.84-3.52)
Sidechain outliers	138945	1033 (3.84-3.52)
RNA backbone	3102	1024 (4.30-3.00)


























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 ≥ 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	1508	45% 44% 10% ..
1	XA	1508	44% 45% 10% .
2	QB	256	61% 30% . 8%
2	XB	256	63% 28% . 8%
3	QC	239	65% 21% 14%
3	XC	239	66% 20% 14%
4	QD	209	68% 31%

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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	QW	77	
22	XV	77	
22	XW	77	
23	QX	25	
23	XX	25	
24	QY	17	
24	XY	17	
25	RA	2915	
25	YA	2915	
26	RB	122	
26	YB	122	
27	RD	276	
27	YD	276	
28	RE	206	















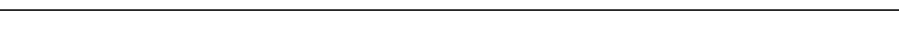




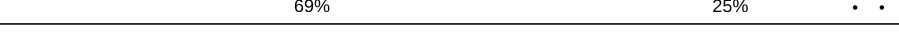





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Mol	Chain	Length	Quality of chain
28	YE	206	
29	RF	210	
29	YF	210	
30	RG	182	
30	YG	182	
31	RH	180	
31	YH	180	
32	RI	148	
32	YI	148	
33	RN	140	
33	YN	140	
34	RO	122	
34	YO	122	
35	RP	150	
35	YP	150	
36	RQ	141	
36	YQ	141	
37	RR	118	
37	YR	118	
38	RS	112	
38	YS	112	
39	RT	146	
39	YT	146	
40	RU	118	
40	YU	118	

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Mol	Chain	Length	Quality of chain
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	71	
51	R5	60	
51	Y5	60	
52	R6	54	
52	Y6	54	
53	R7	49	

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Mol	Chain	Length	Quality of chain
53	Y7	49	<div><div></div><div>71%</div><div>27%</div><div></div><div></div></div>
54	R8	65	<div><div></div><div>65%</div><div>31%</div><div></div><div></div></div>
54	Y8	65	<div><div></div><div>69%</div><div>26%</div><div></div><div></div></div>
55	R9	37	<div><div></div><div>38%</div><div>62%</div><div></div><div></div></div>
55	Y9	37	<div><div></div><div>24%</div><div>62%</div><div>14%</div><div></div></div>

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 295575 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1500	Total	C	N	O	P	0	0	0
			32246	14353	5981	10413	1499			
1	XA	1500	Total	C	N	O	P	0	0	0
			32248	14354	5984	10411	1499			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QA	299	A	G	engineered mutation	GB 55771382
XA	299	A	G	engineered mutation	GB 55771382

- 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			

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	QW	76	Total	C	N	O	P	0	0	0
			1618	722	292	529	75			
22	XV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	XW	76	Total	C	N	O	P	0	0	0
			1618	722	292	529	75			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total	C	N	O	P	0	0	0
			169	76	29	56	8			
23	XX	10	Total	C	N	O	P	0	0	0
			210	96	39	66	9			

- Molecule 24 is a RNA chain called ASL Leu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	17	Total	C	N	O	P	0	0	0
			358	162	64	116	16			
24	XY	17	Total	C	N	O	P	0	0	0
			358	162	64	116	16			

- Molecule 25 is a RNA chain called 23S rRNA.

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

- Molecule 26 is a RNA chain called 5S rRNA.

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
35	YP	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	Y0	75	Total	C	N	O	S	0	0	0
			599	370	127	101	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
47	Y1	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

- Molecule 52 is a protein called 50S ribosomal protein L33.

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

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

- Molecule 55 is a protein called 50S ribosomal protein L36.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	68	Total	Mg	0	0
			68	68		
56	RP	2	Total	Mg	0	0
			2	2		
56	YA	546	Total	Mg	0	0
			546	546		
56	RT	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	RN	1	Total 1	Mg 1	0	0
56	XE	1	Total 1	Mg 1	0	0
56	XS	1	Total 1	Mg 1	0	0
56	YD	2	Total 2	Mg 2	0	0
56	QV	6	Total 6	Mg 6	0	0
56	Y8	1	Total 1	Mg 1	0	0
56	YO	1	Total 1	Mg 1	0	0
56	XA	82	Total 82	Mg 82	0	0
56	YY	1	Total 1	Mg 1	0	0
56	RQ	2	Total 2	Mg 2	0	0
56	R0	4	Total 4	Mg 4	0	0
56	RU	1	Total 1	Mg 1	0	0
56	RO	2	Total 2	Mg 2	0	0
56	R4	1	Total 1	Mg 1	0	0
56	QH	1	Total 1	Mg 1	0	0
56	YQ	3	Total 3	Mg 3	0	0
56	RY	1	Total 1	Mg 1	0	0
56	QC	1	Total 1	Mg 1	0	0
56	R8	1	Total 1	Mg 1	0	0
56	YX	2	Total 2	Mg 2	0	0
56	RR	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	R1	2	Total 2	Mg 2	0	0
56	Y7	1	Total 1	Mg 1	0	0
56	QF	1	Total 1	Mg 1	0	0
56	Y9	1	Total 1	Mg 1	0	0
56	Y0	1	Total 1	Mg 1	0	0
56	XQ	1	Total 1	Mg 1	0	0
56	QQ	1	Total 1	Mg 1	0	0
56	RA	508	Total 508	Mg 508	0	0
56	YP	3	Total 3	Mg 3	0	0
56	R9	1	Total 1	Mg 1	0	0
56	RE	2	Total 2	Mg 2	0	0
56	XL	1	Total 1	Mg 1	0	0
56	YB	12	Total 12	Mg 12	0	0
56	QY	1	Total 1	Mg 1	0	0
56	XV	6	Total 6	Mg 6	0	0
56	RB	7	Total 7	Mg 7	0	0
56	QE	1	Total 1	Mg 1	0	0
56	RF	1	Total 1	Mg 1	0	0
56	XM	1	Total 1	Mg 1	0	0
56	YE	2	Total 2	Mg 2	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	Y9	1	Total	Zn	0	0
			1	1		
58	YY	1	Total	Zn	0	0
			1	1		
58	Y6	1	Total	Zn	0	0
			1	1		
58	QN	1	Total	Zn	0	0
			1	1		
58	XN	1	Total	Zn	0	0
			1	1		
58	RY	1	Total	Zn	0	0
			1	1		
58	Y4	1	Total	Zn	0	0
			1	1		
58	R6	1	Total	Zn	0	0
			1	1		
58	Y5	1	Total	Zn	0	0
			1	1		
58	R5	1	Total	Zn	0	0
			1	1		

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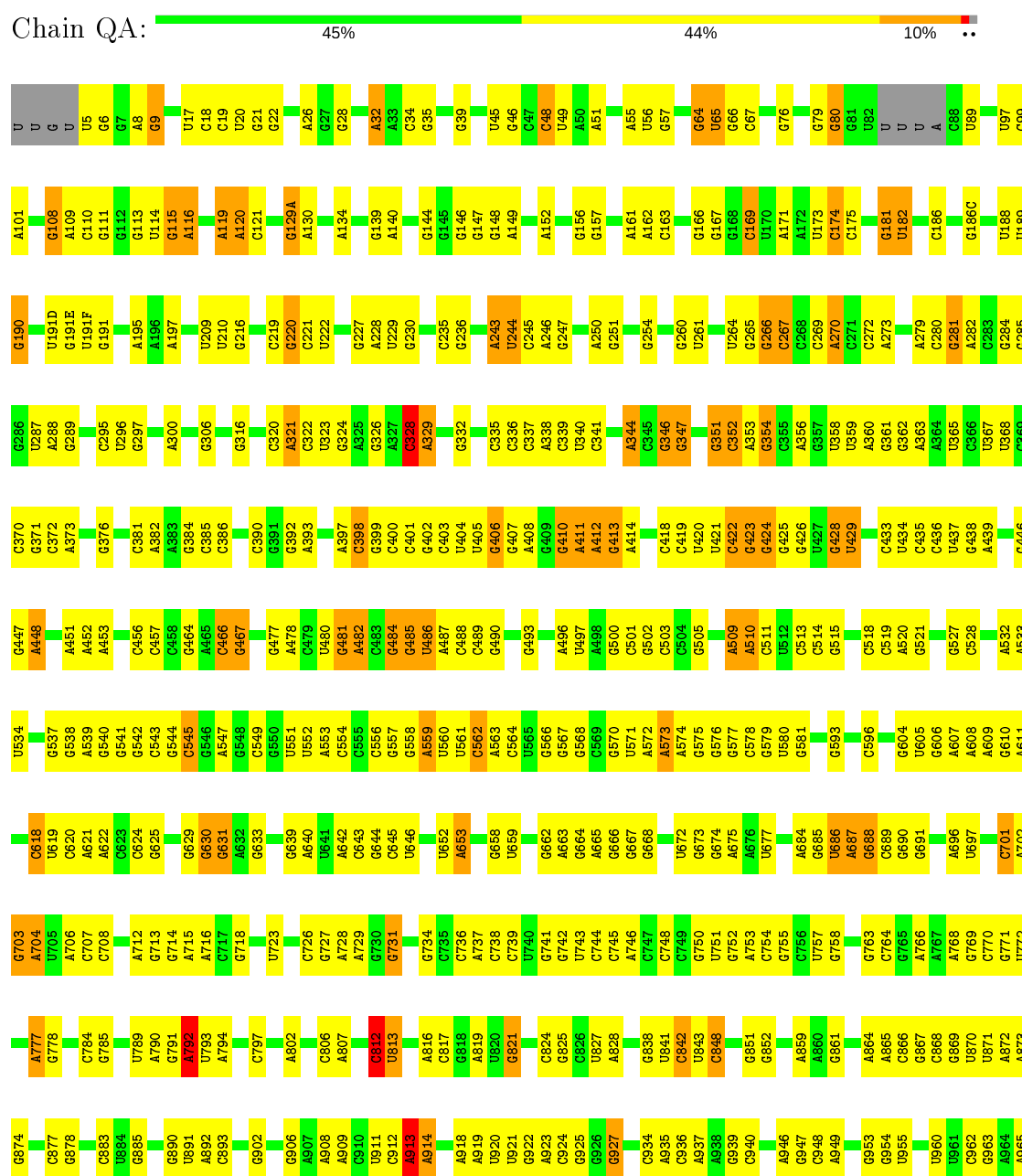
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	R4	1	Total 1	Zn 1	0	0
58	R9	1	Total 1	Zn 1	0	0

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.

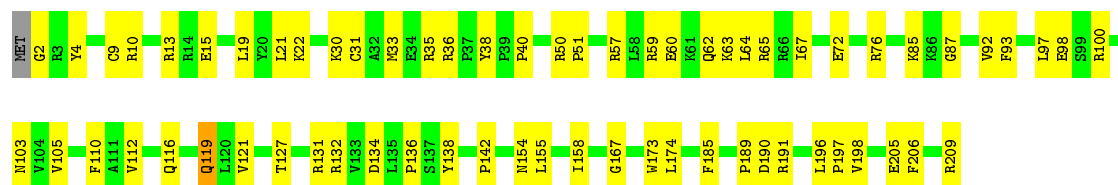
Note EDS failed to run properly.

• Molecule 1: 16S rRNA



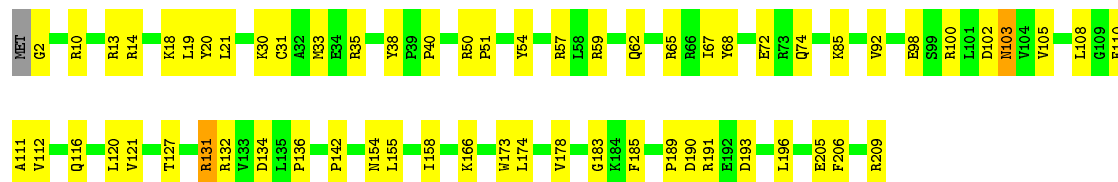






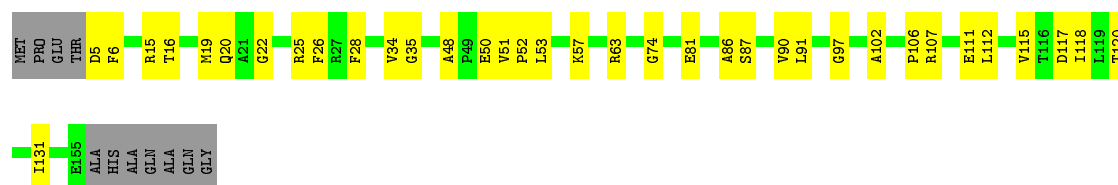
- Molecule 4: 30S ribosomal protein S4

Chain XD: 70% 29% .



- Molecule 5: 30S ribosomal protein S5

Chain QE: 71% 22% 7%



- Molecule 5: 30S ribosomal protein S5

Chain XE: 77% 17% 7%



- Molecule 6: 30S ribosomal protein S6

Chain QF: 74% 24% .




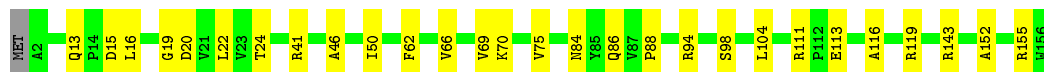
- Molecule 6: 30S ribosomal protein S6

Chain XF: 68% 32%




- Molecule 7: 30S ribosomal protein S7

Chain QG:  81% 18%




- Molecule 7: 30S ribosomal protein S7

Chain XG:  83% 16%




- Molecule 8: 30S ribosomal protein S8

Chain QH:  74% 25%



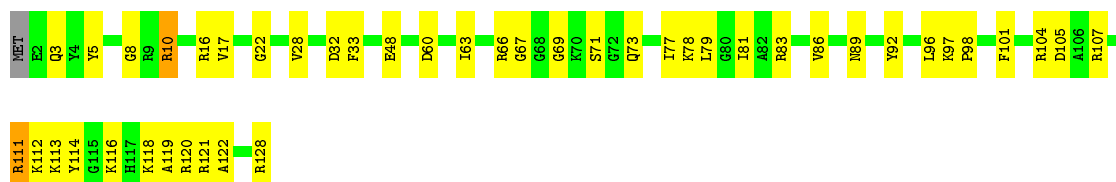
- Molecule 8: 30S ribosomal protein S8

Chain XH:  80% 20%



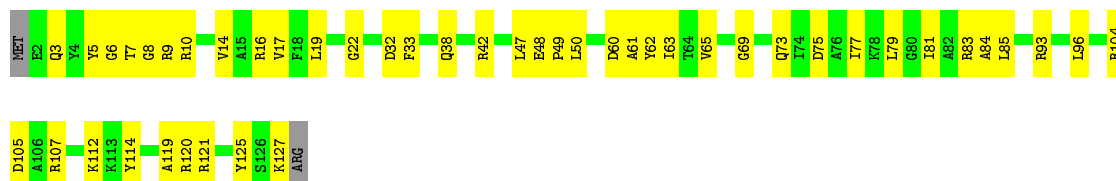
- Molecule 9: 30S ribosomal protein S9

Chain QI:  65% 33%

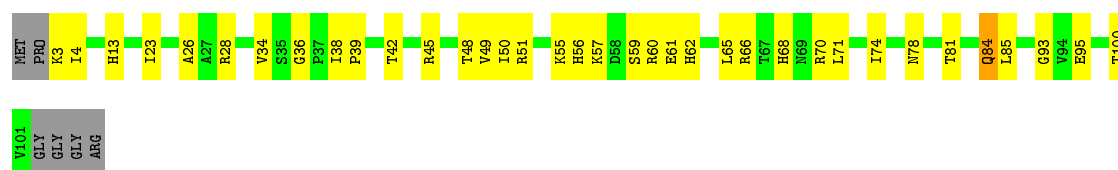


- Molecule 9: 30S ribosomal protein S9

Chain XI:  63% 36%



• Molecule 10: 30S ribosomal protein S10

Chain QJ: 

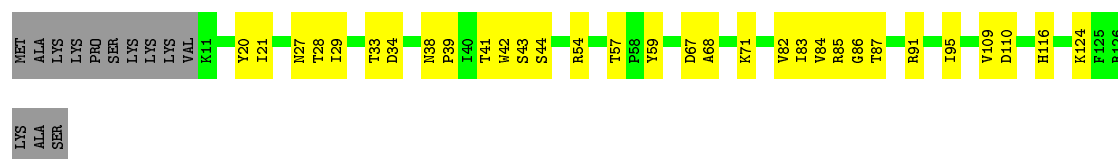
• Molecule 10: 30S ribosomal protein S10

Chain XJ: 

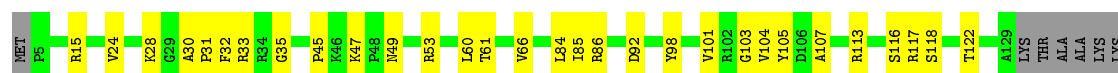
• Molecule 11: 30S ribosomal protein S11

Chain QK: 

• Molecule 11: 30S ribosomal protein S11

Chain XK: 

• Molecule 12: 30S ribosomal protein S12

Chain QL: 

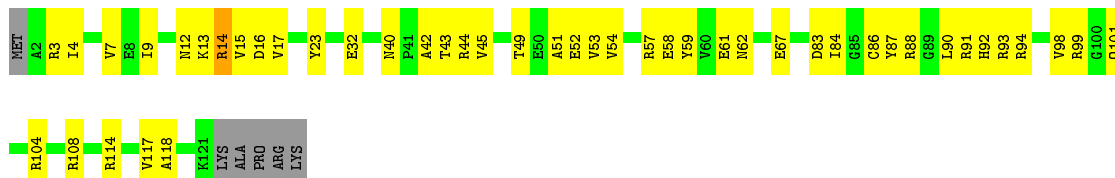
• Molecule 12: 30S ribosomal protein S12

Chain XL: 

LYS
LYS

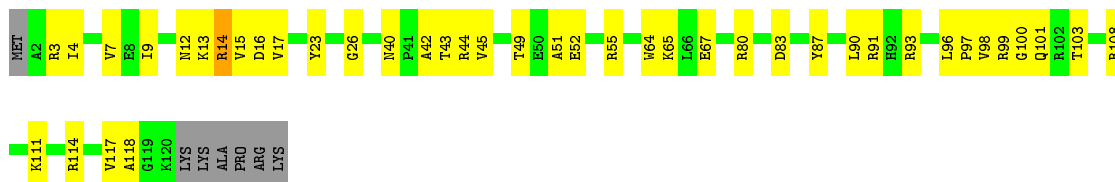
- Molecule 13: 30S ribosomal protein S13

Chain QM:  59% 36% • 5%



- Molecule 13: 30S ribosomal protein S13

Chain XM:  61% 33% • 6%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:  72% 25% • •




- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:  72% 25% • •



- Molecule 15: 30S ribosomal protein S15

Chain QO:  80% 19% •

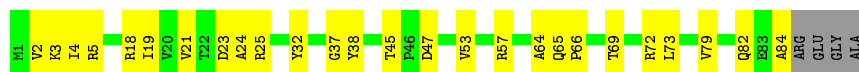


- Molecule 15: 30S ribosomal protein S15

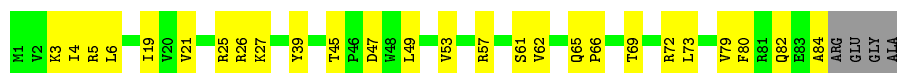
Chain XO:  72% 26% •



- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

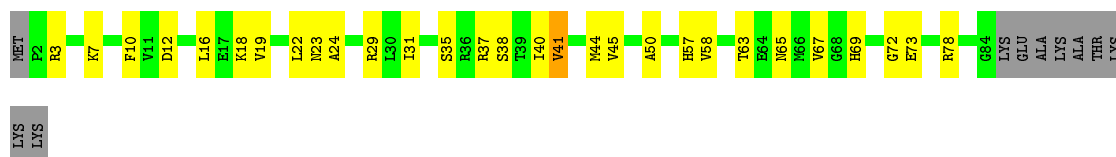


- Molecule 18: 30S ribosomal protein S18



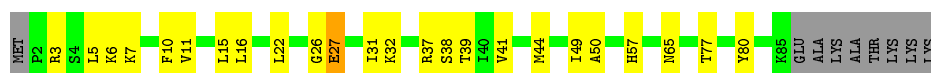
- Molecule 19: 30S ribosomal protein S19





- Molecule 19: 30S ribosomal protein S19

Chain XS: 65% 25% 10%



- Molecule 20: 30S ribosomal protein S20

Chain QT: 69% 25% 7%



- Molecule 20: 30S ribosomal protein S20

Chain XT: 72% 22% 7%



- Molecule 21: 30S ribosomal protein Thx

Chain QU: 67% 26% 7%



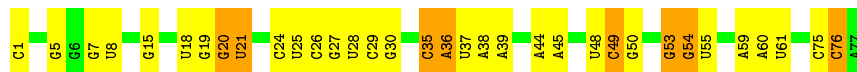
- Molecule 21: 30S ribosomal protein Thx

Chain XU: 52% 41% 7%

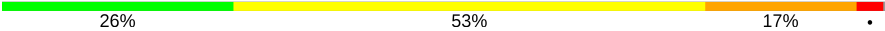


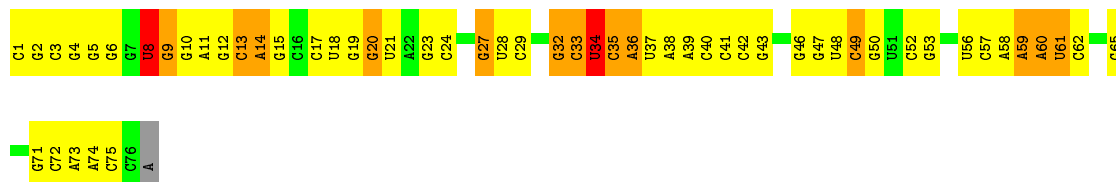
- Molecule 22: tRNA fMet

Chain QV: 56% 34% 10%



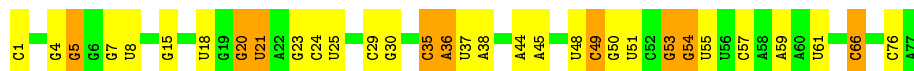
- Molecule 22: tRNA fMet

Chain QW:  26% 53% 17%



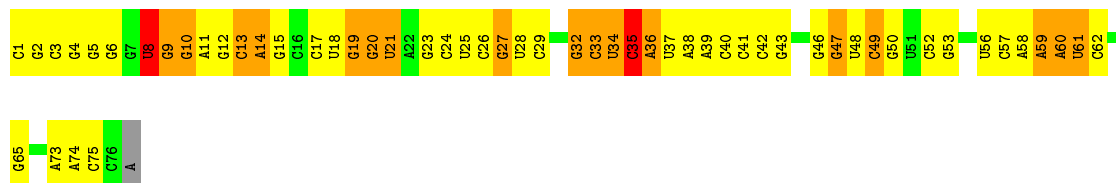
- Molecule 22: tRNA fMet

Chain XV:  58% 30% 12%



- Molecule 22: tRNA fMet

Chain XW:  26% 48% 22%



- Molecule 23: messenger RNA

Chain QX:  32% 68%



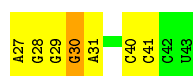
- Molecule 23: messenger RNA

Chain XX:  28% 8% 60%



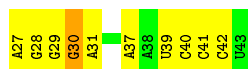
- Molecule 24: ASL Leu

Chain QY:  59% 35% 6%



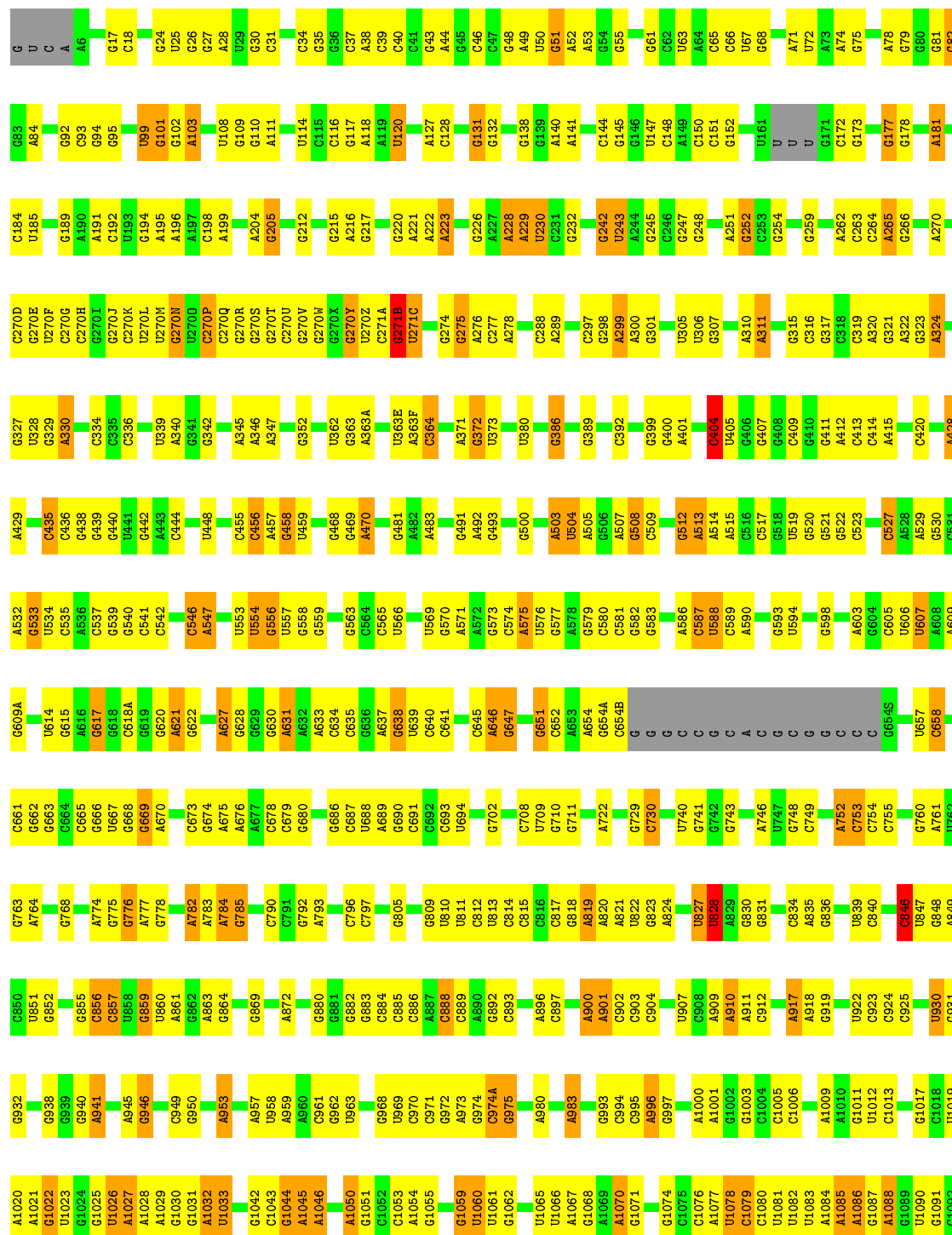
- Molecule 24: ASL Leu

Chain XY:  41% 53% 6%

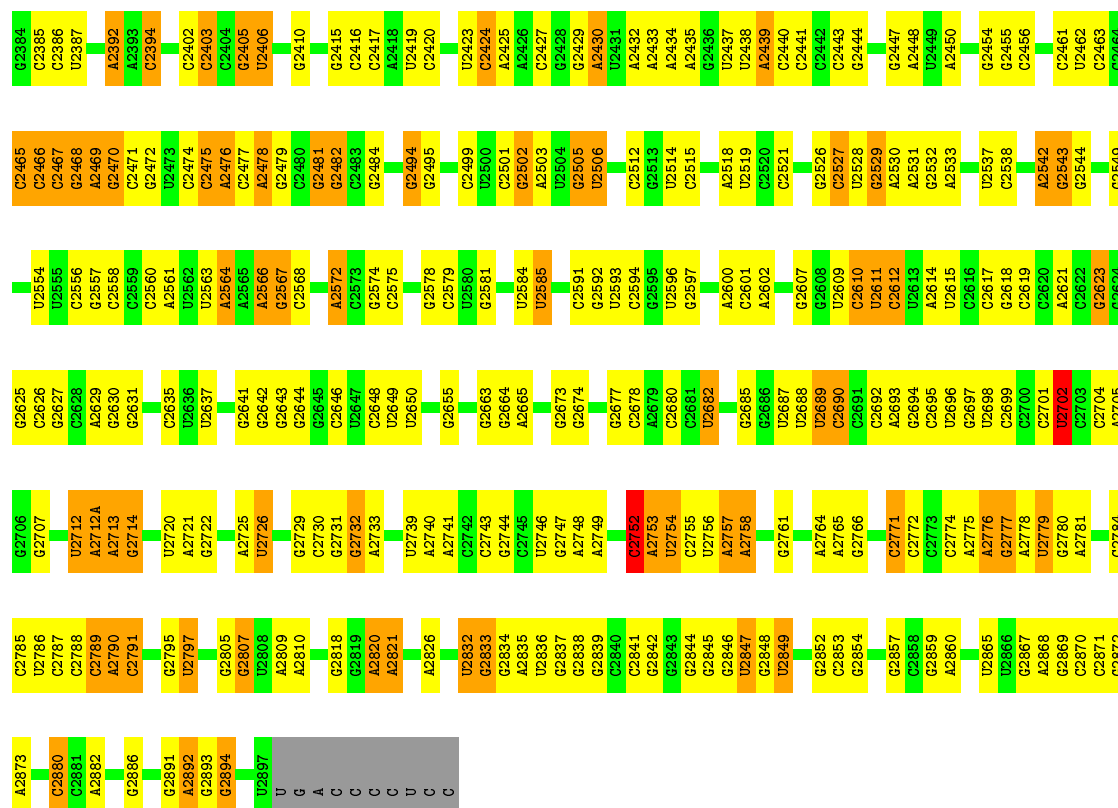


• Molecule 25: 23S rRNA

Chain RA: 48% 40% 10%

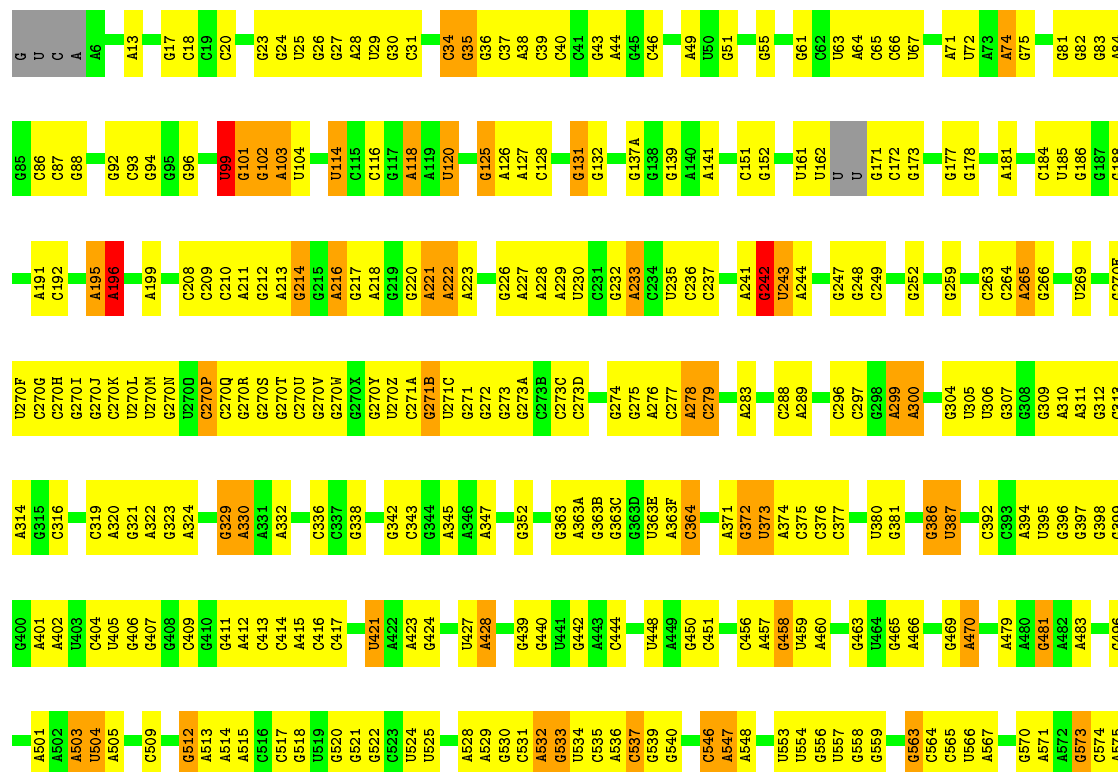






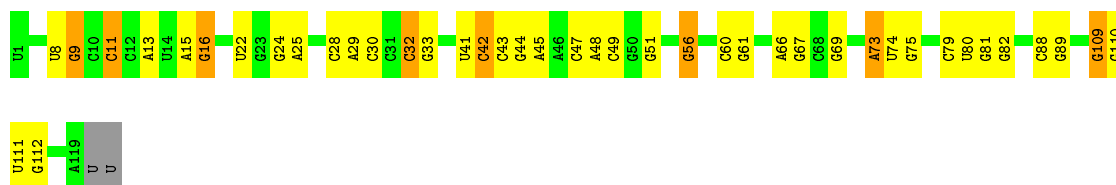
• Molecule 25: 23S rRNA

Chain YA: 46% 43% 9% ..



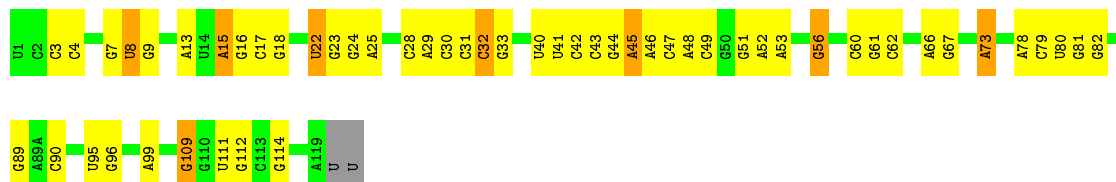
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G1591	C1592	G1595	A1596	G1597	C1598	C1599	C1600	A1603	C1604	C1605	G1606	C1607	A1608	A1609	A1610	G1613	A1616	C1617	G1622	G1628	G1629	G1636	G1637	G1638	A1639	C1640	G1641	G1642	C1643	G1644	G1645	G1646	G1647	G1648	G1649	G1650	G1651	A1652	G1653	G1654	G1655	G1656	C1657	C1658	U1659	C1660	G1661	C1662	C1663	A1668	A1669	C1670	
G1519	U1520	G1521	G1522	G1525	G1526	G1527	A1528	A1529	G1530	C1531	G1534	U1535	C1536	G1537	G1538	G1539	G1540	U1541	A1542	A1543	C1544	A1545	A1546	C1547	G1550	G1551	C1557	A1558	G1559	G1560	G1561	A1562	G1563	C1564	A1565	A1566	A1567	G1568	A1569	A1570	A1571	A1572	U1578	A1579	A1580	G1581	G1585	A1586	A1587	C1588	U1589	U1590	
A1439	G1440	G1441	G1442	A1444A	C1445	G1448	A1449	A1449A	A1453	U1454	G1455	C1458	G1459	A1460	G1461	C1464	C1467	G1470	A1471	G1474	G1475	G1476	A1477	G1478	G1479	G1480	U1482	G1483	A1490	C1493	A1496	U1497	C1498	C1499	G1500	G1505	C1506	A1507	A1508	C1509	A1510	A1511	A1512	A1513	U1514	C1518	A1569	C1570					
G1357	G1358	A1359	A1365	G1368	A1372	U1373	A1378	A1379	G1380	A1385	G1388	G1389	U1391	A1392	A1393	U1394	A1395	U1396	G1399	G1400	G1401	G1402	G1403	G1404	U1405	G1406	G1407	C1408	C1409	G1410	C1411	A1412	G1413	G1416	G1417	G1418	A1419	U1420	G1421	G1422	G1423	G1424	G1425	G1426	A1427	G1428	G1429	C1430	U1431	U1438			
G1264	A1265	G1266	G1270	G1271	A1272	U1273	A1278	G1290	C1291	U1292	C1293	G1296	C1297	G1298	G1299	U1300	A1301	G1302	G1303	A1308	G1309	G1310	U1313	G1314	G1315	U1316	G1317	G1318	G1319	G1320	A1321	A1322	U1329	C1330	G1331	G1332	C1333	G1334	G1338	G1344	C1345	G1346	G1347	G1348	A1349	U1352	A1353	A1354	G1438				
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U1083	A1084	A1085	A1086	G1087	A1088	G1093	U1094	A1095	A1096	U1097	A1103	C1104	U1108	C1109	G1110	A1111	G1112	U1113	G1114	G1115	G1116	G1117	A1129	U1130	G1135	G1136	G1137	G1138	G1139	C1140	U1141	U1142	A1142A	A1143	G1144	G1151	G1154	A1155	G1156	G1157	U1165	C1166	U1167	G1168	G1169	G1170	G1171	A1174	U1175	G1176			
C1008	A1009	A1010	G1011	U1012	A1013	G1014	G1015	G1016	G1017	A1021	C1022	U1023	G1024	G1025	U1026	A1027	A1028	A1029	U1033	G1042	C1043	G1044	A1045	A1046	G1047	A1048	C1049	A1050	G1059	U1060	U1061	G1062	G1063	C1064	U1065	U1066	A1067	G1068	A1069	U1070	G1071	C1072	A1073	G1074	C1075	G1076	A1077	U1078	C1079	C1080	U1081	C1082	
G934	C935	G938	G939	A941	G942	U943	A945	G946	G947	G948	G949	U953	U958	A959	C961	G962	U963	C964	C965	G968	G969	C970	C971	C972	C974A	A974	C975A	A976	G978	G979	A980	A983	A984	G993	C994	G995	A996	G997	C998	C999	A1000	A1001	C992	G848	A849	C850	U851	G852	C853	C854			
C856	C857	U858	G859	U860	A861	G862	A863	C865	A870	U871	A872	G873	G874	G875	G879	G880	G881	C884	C885	C886	A887	C888	C889	C890	C891	C892	U895	A896	C897	A898	A900	G906	U907	A910	A911	C914	C915	G916	C917	U918	U922	C923	C924	C925	G929	U930	G931	G932	A933				
A685	G686	A689	G690	C691	C692	C698	G704	C708	U709	G710	G711	G717	A718	C719	C720	C721	A722	G723	U724	G725	G726	A727	G728	C729	C730	A734	U740	G741	G742	G743	U747	G748	C749	A752	C753	C754	C755	C756	G760	A761	A764	U765	G766	U767	G768	U773	A774						
U576	G577	A578	G579	C580	C581	C582	G583	A586	C587	U588	C589	A590	C591	G592	G593	U594	C598	G600	A601	C603	G604	C605	U606	U607	A608	A609	G609A	C610	U614	G615	A616	G617	G618	G620	A621	G622	C623	C624	G625	U626	C627	G628	G629	G630	A631	A632	A633	C634	C635	G636	A637	G638	U639

A2892	G2794	G2635	C2540	G2454	A2361	C2283	G2182	C2107	G2038	A1960	G1858	G1772
G2893	G2795	C2638	A2541	G2455	G2362	A2287	C2183	C2108	C2039	A1963	A1859	A1773
G2894	G2796	G2639	A2542	C2456	C2363	A2288	C2184	U2109	U2040	U1964	G1860	U1779
U2897	G2797	G2640	G2543	G2457	G2364	G2289	G2185	G2110	G2041	G1965	A1780	C1781
G	A2798	G2641	G2544	U2462	G2365	G2290	G2186	G2111	C2042	A1966	G1862	C1782
G	C2803	G2642	G2545	C2463	A2369	U2291	G2190	U2113	G2043	C1967	G1863	C1783
C	C2804	C2646	U2546	A2469	A2370	C2292	G2191	G2114	G2044	U1968	U1864	A1784
C	G2805	U2647	G2547	G2470	G2379	C2293	G2192	G2115	U2046	G1969	G1869	A1785
C	G2806	C2648	G2548	C2471	G2380	C2294	G2193	G2116	G2045	A1970	C1870	A1786
C	U2807	U2649	G2549	G2472	G2381	C2295	G2194	A2117	G2046	A1971	A1871	A1787
U	A2808	U2650	U2554	U2473	G2382	A2298	G2195	U2118	C2047	A1972	A1872	C1788
U	A2809		U2555	C2474	C2383	A2299	G2196	A2119	A2051	U1973	G1873	A1789
C	A2810			C2475	C2384	A2300	G2197	G2120	G2052	U1974	C1874	C1789
C	C2811	A2660	C2558	C2476	A2392	G2303	A2199			U1975	C1875	C1790
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	G2839	U2692	U2516		A2434	G2331	U2247	A2158		A2018	A1829	A1829
	U2847	U2693	U2517		A2435	A2332	U2248	G2163	U2086	A2019	C1830	C1830
G2848	U2694	U2694	U2518		A2436	A2333	U2249	G2164	G2087	G2020	U1931	U1931
A2851	G2695	G2695	U2519		U2437	A2334	U2250	G2165	G2088	G2021	G1935	G1832
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			U2542		U2460	G2357	U2273	G2188		G2044	G1967	
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			U2554		U2472	G2369	U2285	G2200		G2056	G1979	
			U2555		U2473	A2370	U2286	G2201		G2057	G1980	
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			U2559		U2477	A2374	U2290	G2205		G2061	G1984	
			U2560		U2478	G2375	U2291	G2206		G2062	G1985	
			U2561		U2479	A2376	U2292	G2207		G2063	G1986	
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			U2586		U2504	G2401	U2317	G2232		G2088	G2011	
			U2587		U2505	A2402	U2318	G2233		G2089	G2012	
			U2588		U2506	G2403	U2319	G2234		G2090	G2013	
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			U2590		U25							



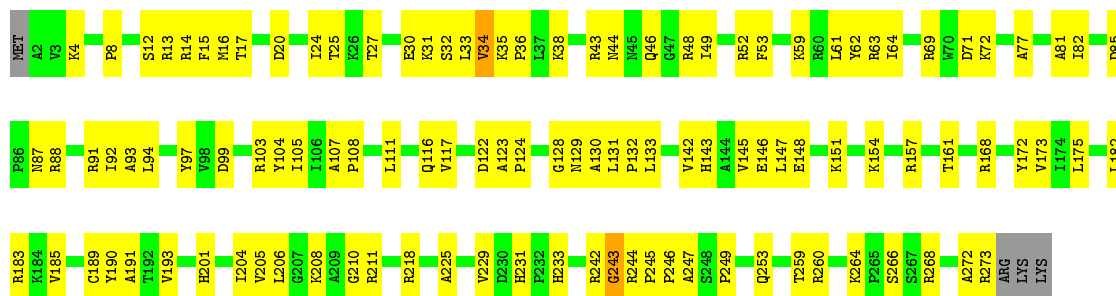
- Molecule 26: 5S rRNA

Chain YB:



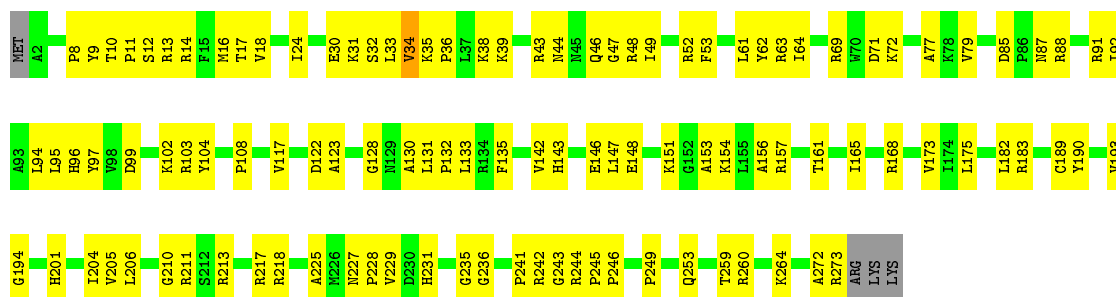
- Molecule 27: 50S ribosomal protein L2

Chain RD:



- Molecule 27: 50S ribosomal protein L2

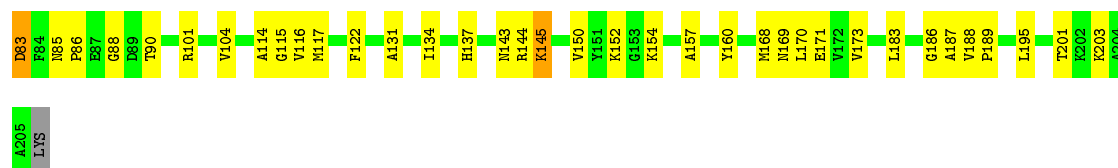
Chain YD:



- Molecule 28: 50S ribosomal protein L3

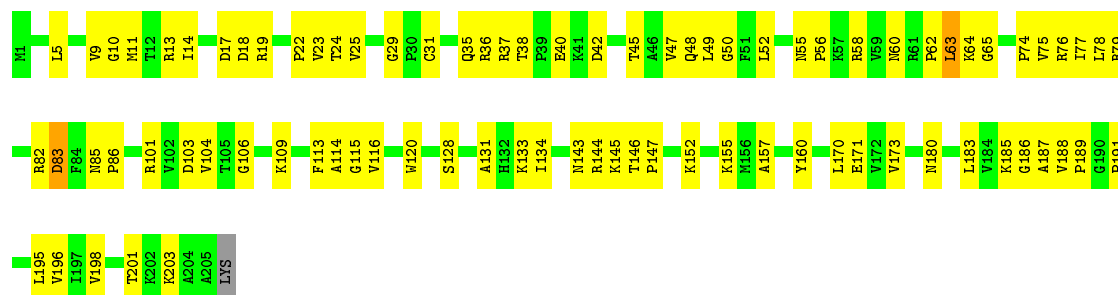
Chain RE:





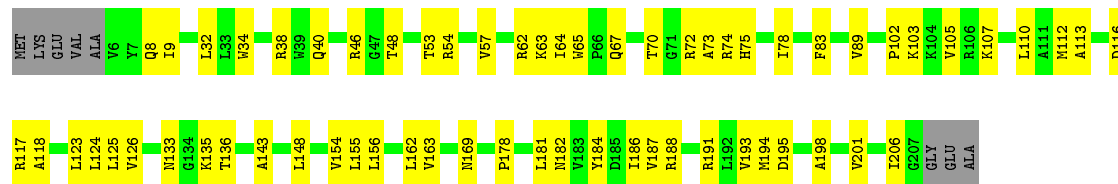
- Molecule 28: 50S ribosomal protein L3

Chain YE: 59% 40%



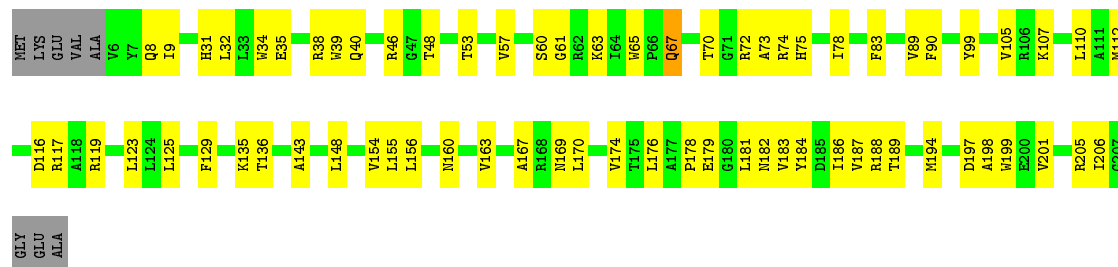
- Molecule 29: 50S ribosomal protein L4

Chain RF: 66% 30%



- Molecule 29: 50S ribosomal protein L4

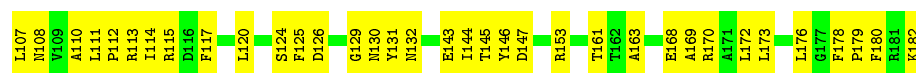
Chain YF: 63% 32%



- Molecule 30: 50S ribosomal protein L5

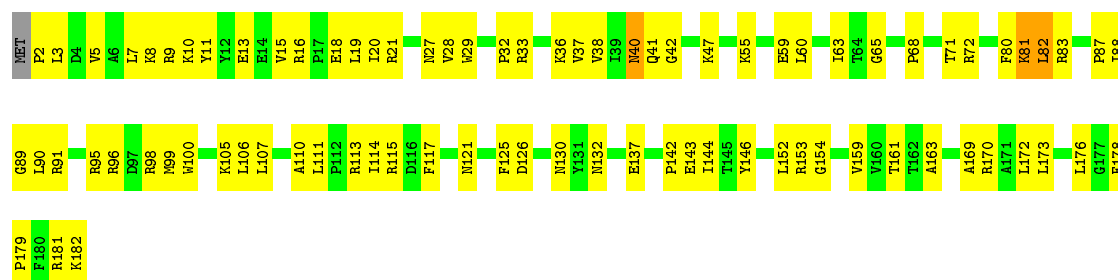
Chain RG: 59% 40%





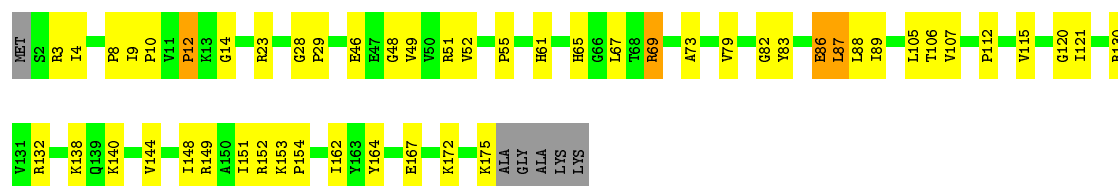
- Molecule 30: 50S ribosomal protein L5

Chain YG: 54% 44% ..



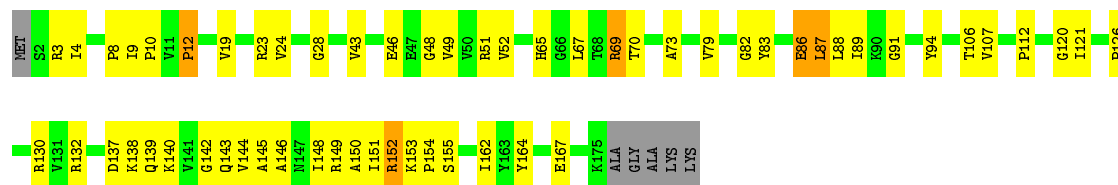
- Molecule 31: 50S ribosomal protein L6

Chain RH: 68% 26% ..



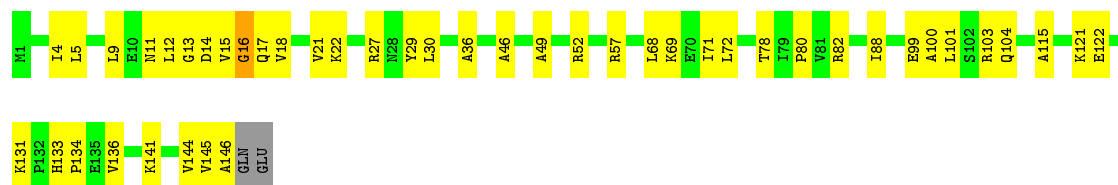
- Molecule 31: 50S ribosomal protein L6

Chain YH: 64% 29% ..



- Molecule 32: 50S ribosomal protein L9

Chain RI: 68% 30% ..



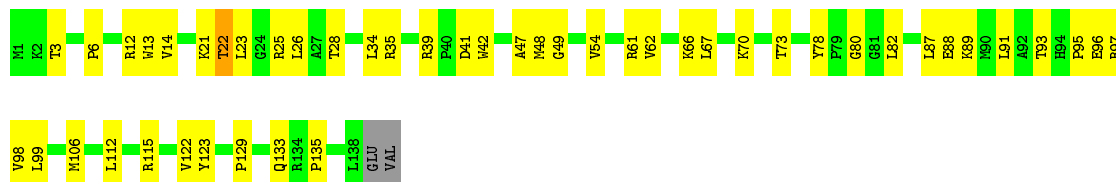
- Molecule 32: 50S ribosomal protein L9

Chain YI: 70% 27% ..



- Molecule 33: 50S ribosomal protein L13

Chain RN: 65% 33% ..



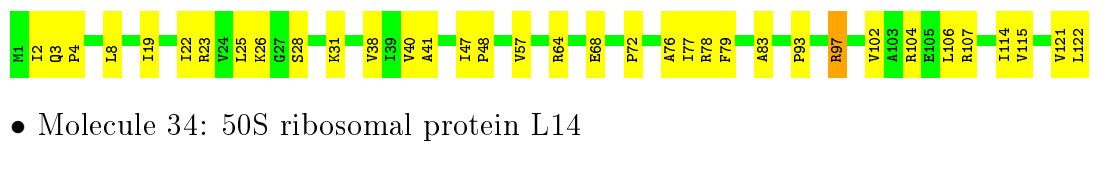
- Molecule 33: 50S ribosomal protein L13

Chain YN: 71% 26% ..



- Molecule 34: 50S ribosomal protein L14

Chain RO: 71% 28% .



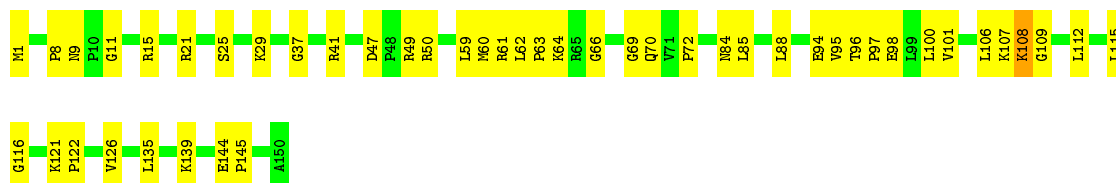
- Molecule 34: 50S ribosomal protein L14

Chain YO: 78% 21% .



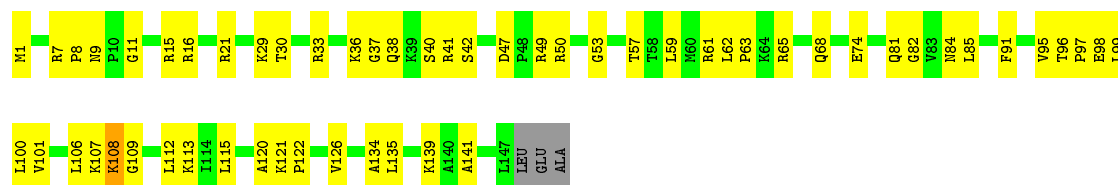
- Molecule 35: 50S ribosomal protein L15

Chain RP: 69% 31% .



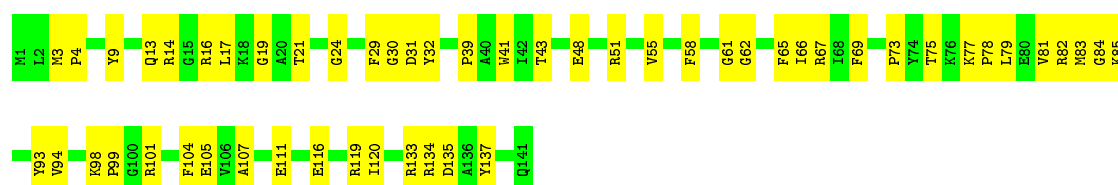
- Molecule 35: 50S ribosomal protein L15

Chain YP:  61% 37% ..



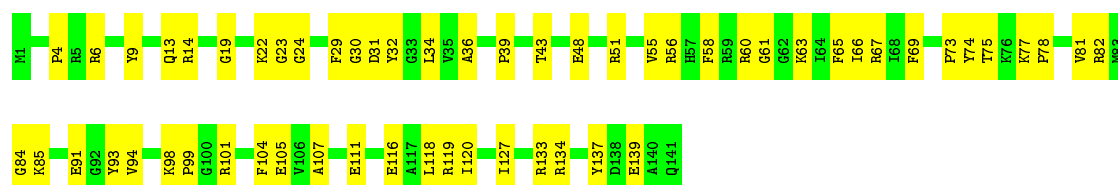
- Molecule 36: 50S ribosomal protein L16

Chain RQ:  62% 38%



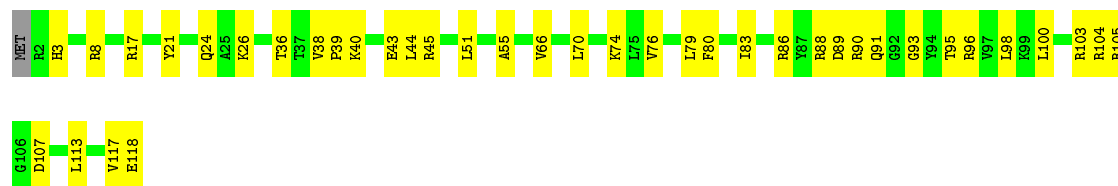
- Molecule 36: 50S ribosomal protein L16

Chain YQ:  60% 40%



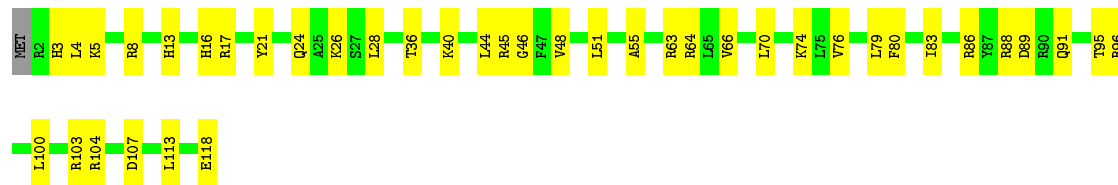
- Molecule 37: 50S ribosomal protein L17

Chain RR:  66% 33%



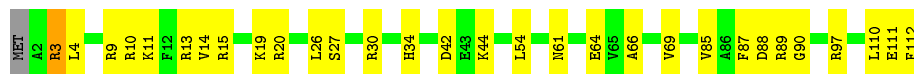
- Molecule 37: 50S ribosomal protein L17

Chain YR:  65% 34%



- Molecule 38: 50S ribosomal protein L18

Chain RS:  72% 26% ..



- Molecule 38: 50S ribosomal protein L18

Chain YS:  71% 28% ..



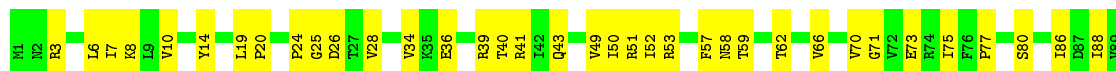
- Molecule 39: 50S ribosomal protein L19

Chain RT:  56% 37% 6% •



- Molecule 39: 50S ribosomal protein L19

Chain YT:  55% 38% 6% •



- Molecule 40: 50S ribosomal protein L20

Chain RU:  70% 27% ..

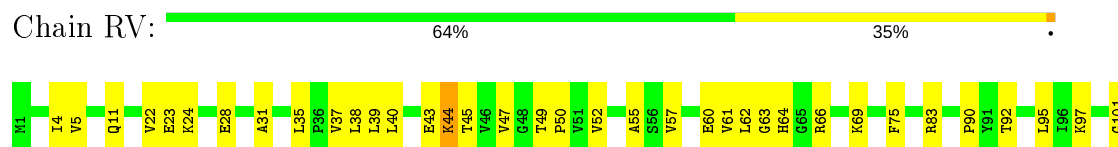


- Molecule 40: 50S ribosomal protein L20

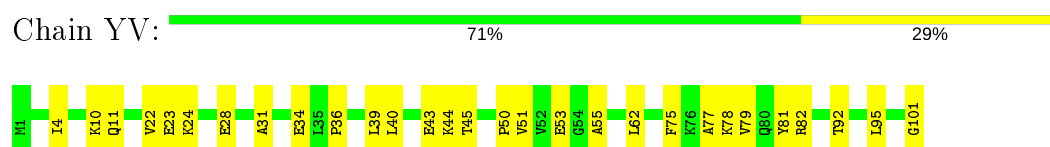
Chain YU:  70% 27% ..



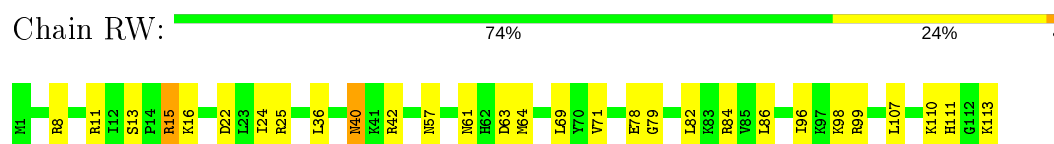
- Molecule 41: 50S ribosomal protein L21



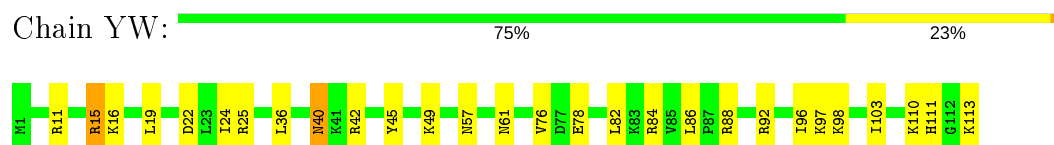
- Molecule 41: 50S ribosomal protein L21



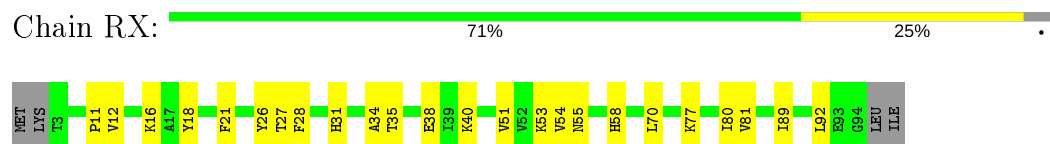
- Molecule 42: 50S ribosomal protein L22



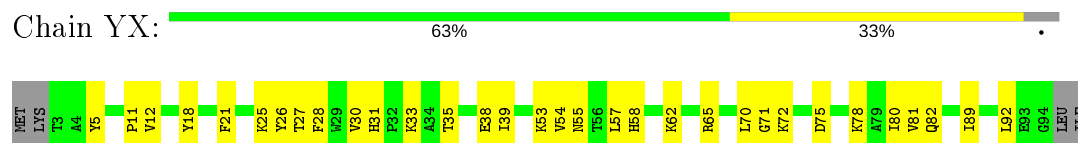
- Molecule 42: 50S ribosomal protein L22



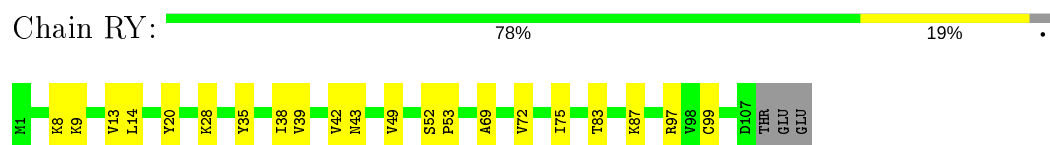
- Molecule 43: 50S ribosomal protein L23




- Molecule 43: 50S ribosomal protein L23



- Molecule 44: 50S ribosomal protein L24



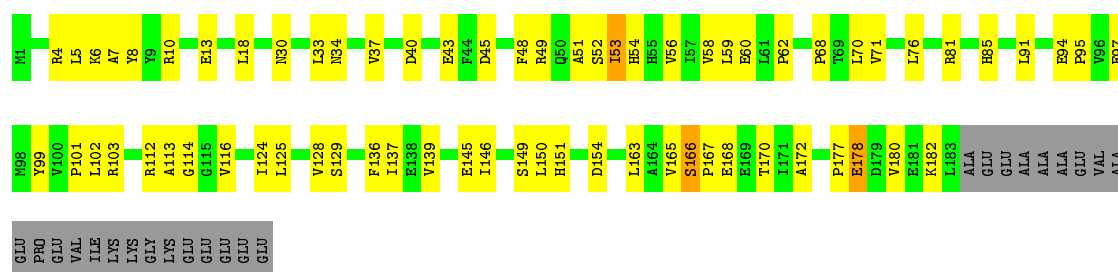
- Molecule 44: 50S ribosomal protein L24

Chain YY:  76% 21%



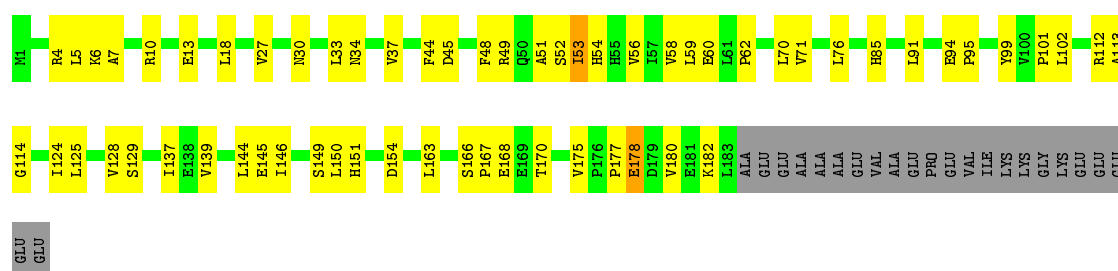
- Molecule 45: 50S ribosomal protein L25

Chain RZ:  56% 32% 11%



- Molecule 45: 50S ribosomal protein L25

Chain YZ:  59% 29% 11%



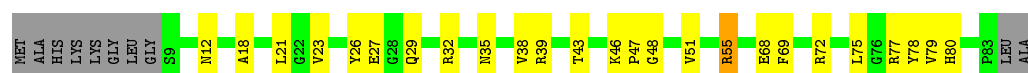
- Molecule 46: 50S ribosomal protein L27

Chain R0:  66% 29% 5%



- Molecule 46: 50S ribosomal protein L27

Chain Y0:  59% 28% 12%

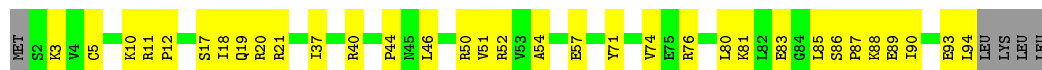


- Molecule 47: 50S ribosomal protein L28

Chain R1:  73% 26%



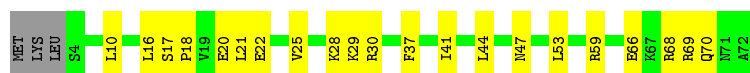
- Molecule 47: 50S ribosomal protein L28



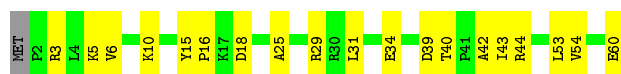
- Molecule 48: 50S ribosomal protein L29



- Molecule 49: 50S ribosomal protein L30



- Molecule 49: 50S ribosomal protein L30



- Molecule 49: 50S ribosomal protein L30



- Molecule 50: 50S ribosomal protein L31



- Molecule 50: 50S ribosomal protein L31





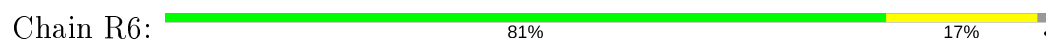
- Molecule 51: 50S ribosomal protein L32



- Molecule 51: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L34

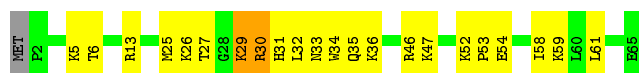


- Molecule 53: 50S ribosomal protein L34

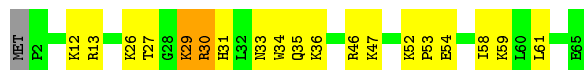


- Molecule 54: 50S ribosomal protein L35





- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



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	210.70Å 446.14Å 616.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.57 – 3.68	Depositor
% Data completeness (in resolution range)	99.3 (145.57-3.68)	Depositor
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.228 , 0.274	Depositor
Wilson B-factor (Å ²)	89.7	Xtriage
Anisotropy	0.196	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	295575	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, 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	0.22	0/36097	0.80	21/56339 (0.0%)
1	XA	0.22	0/36100	0.82	27/56344 (0.0%)
2	QB	0.26	0/1942	0.50	0/2619
2	XB	0.25	0/1950	0.49	0/2630
3	QC	0.25	0/1629	0.47	0/2195
3	XC	0.24	0/1629	0.46	0/2195
4	QD	0.35	1/1733 (0.1%)	0.49	1/2318 (0.0%)
4	XD	0.26	0/1733	0.47	0/2318
5	QE	0.24	0/1171	0.48	0/1576
5	XE	0.25	0/1171	0.49	0/1576
6	QF	0.24	0/856	0.49	0/1154
6	XF	0.24	0/856	0.48	0/1154
7	QG	0.24	0/1276	0.43	0/1709
7	XG	0.24	0/1276	0.42	0/1709
8	QH	0.24	0/1128	0.45	0/1517
8	XH	0.24	0/1128	0.46	0/1517
9	QI	0.26	0/1029	0.50	0/1379
9	XI	0.27	0/1017	0.52	0/1365
10	QJ	0.45	1/814 (0.1%)	0.63	3/1095 (0.3%)
10	XJ	0.24	0/790	0.49	0/1063
11	QK	0.25	0/900	0.46	0/1213
11	XK	0.24	0/879	0.47	0/1187
12	QL	0.26	0/991	0.59	0/1327
12	XL	0.26	0/972	0.63	1/1301 (0.1%)
13	QM	0.25	0/965	0.53	0/1292
13	XM	0.24	0/956	0.53	0/1281
14	QN	0.26	0/501	0.46	0/664
14	XN	0.25	0/501	0.46	0/664
15	QO	0.24	0/745	0.43	0/992
15	XO	0.23	0/740	0.40	0/987
16	QP	0.24	0/721	0.49	0/970
16	XP	0.24	0/721	0.49	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.24	0/847	0.46	0/1131
17	XQ	0.24	0/847	0.45	0/1131
18	QR	0.24	0/579	0.48	0/768
18	XR	0.24	0/579	0.49	0/768
19	QS	0.25	0/680	0.57	0/915
19	XS	0.26	0/689	0.57	0/926
20	QT	0.25	0/765	0.52	0/1007
20	XT	0.25	0/765	0.50	0/1007
21	QU	0.22	0/221	0.45	0/288
21	XU	0.23	0/221	0.46	0/288
22	QV	0.33	1/1836 (0.1%)	0.83	0/2859
22	QW	0.26	0/1807	0.92	2/2816 (0.1%)
22	XV	0.33	1/1836 (0.1%)	0.84	1/2859 (0.0%)
22	XW	0.26	0/1807	0.91	2/2816 (0.1%)
23	QX	0.19	0/188	0.73	0/290
23	XX	0.19	0/235	0.73	0/364
24	QY	0.19	0/400	0.80	0/621
24	XY	0.20	0/400	0.79	0/621
25	RA	0.24	0/69521	0.83	34/108529 (0.0%)
25	YA	0.27	6/69543 (0.0%)	0.85	91/108563 (0.1%)
26	RB	0.22	0/2878	0.81	1/4490 (0.0%)
26	YB	0.23	0/2878	0.82	0/4490
27	RD	0.28	0/2165	0.56	0/2919
27	YD	0.28	0/2165	0.56	0/2919
28	RE	0.26	0/1601	0.60	1/2160 (0.0%)
28	YE	0.26	0/1601	0.60	0/2160
29	RF	0.26	0/1620	0.50	0/2194
29	YF	0.27	0/1620	0.51	0/2194
30	RG	0.26	0/1499	0.55	0/2016
30	YG	0.26	0/1499	0.54	0/2016
31	RH	0.26	0/1362	0.57	1/1841 (0.1%)
31	YH	0.29	0/1362	0.62	1/1841 (0.1%)
32	RI	0.25	0/1151	0.56	0/1558
32	YI	0.25	0/1151	0.56	0/1558
33	RN	0.26	0/1131	0.58	0/1525
33	YN	0.26	0/1131	0.56	0/1525
34	RO	0.26	0/943	0.48	0/1269
34	YO	0.26	0/943	0.50	0/1269
35	RP	0.27	0/1162	0.61	0/1544
35	YP	0.27	0/1139	0.62	0/1514
36	RQ	0.26	0/1143	0.55	0/1527
36	YQ	0.26	0/1143	0.57	0/1527
37	RR	0.26	0/974	0.52	0/1302

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	YR	0.25	0/974	0.49	0/1302
38	RS	0.25	0/892	0.54	0/1187
38	YS	0.25	0/892	0.54	0/1187
39	RT	0.25	0/1155	0.53	0/1542
39	YT	0.25	0/1155	0.54	0/1542
40	RU	0.26	0/982	0.51	0/1306
40	YU	0.26	0/982	0.51	0/1306
41	RV	0.26	0/790	0.58	0/1057
41	YV	0.26	0/790	0.58	0/1057
42	RW	0.25	0/911	0.50	0/1220
42	YW	0.25	0/911	0.50	0/1220
43	RX	0.26	0/739	0.48	0/993
43	YX	0.26	0/739	0.48	0/993
44	RY	0.26	0/831	0.48	0/1108
44	YY	0.26	0/831	0.51	0/1108
45	RZ	0.25	0/1493	0.63	0/2026
45	YZ	0.26	0/1493	0.64	0/2026
46	R0	0.24	0/652	0.47	0/867
46	Y0	0.25	0/607	0.48	0/809
47	R1	0.27	0/770	0.55	0/1022
47	Y1	0.29	0/736	0.53	0/978
48	R2	0.24	0/583	0.49	0/771
48	Y2	0.24	0/583	0.51	0/771
49	R3	0.24	0/474	0.48	0/635
49	Y3	0.25	0/474	0.48	0/635
50	R4	0.25	0/578	0.53	0/776
50	Y4	0.27	0/578	0.54	0/776
51	R5	0.26	0/473	0.48	0/639
51	Y5	0.25	0/473	0.46	0/639
52	R6	0.22	0/460	0.47	0/613
52	Y6	0.22	0/460	0.47	0/613
53	R7	0.24	0/417	0.48	0/550
53	Y7	0.24	0/426	0.49	0/561
54	R8	0.33	0/525	0.67	0/691
54	Y8	0.33	0/525	0.67	0/691
55	R9	0.27	0/310	0.64	0/407
55	Y9	0.63	0/310	1.20	2/407 (0.5%)
All	All	0.25	10/319918 (0.0%)	0.76	189/478576 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
28	YE	0	2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	XV	1	C	OP3-P	-10.62	1.48	1.61
22	QV	1	C	OP3-P	-10.59	1.48	1.61
10	QJ	84	GLN	CD-NE2	9.70	1.57	1.32
4	QD	119	GLN	CB-CG	9.68	1.78	1.52
25	YA	2743	C	P-O5'	7.27	1.67	1.59

The worst 5 of 189 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	2743	C	O4'-C1'-N1	17.82	122.46	108.20
25	YA	2755	C	OP1-P-OP2	12.48	138.32	119.60
25	YA	2754	U	OP1-P-O3'	-11.78	79.29	105.20
25	YA	2525	G	O4'-C1'-N9	11.27	117.22	108.20
25	YA	2754	U	OP2-P-O3'	-11.23	80.50	105.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	YE	146	THR	Mainchain,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	32246	0	16278	644	0
1	XA	32248	0	16279	617	0
2	QB	1907	0	1958	51	0
2	XB	1915	0	1969	47	0
3	QC	1605	0	1668	37	0
3	XC	1605	0	1668	33	0
4	QD	1703	0	1766	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	XD	1703	0	1767	46	0
5	QE	1155	0	1213	23	0
5	XE	1155	0	1213	18	0
6	QF	843	0	857	18	0
6	XF	843	0	857	22	0
7	QG	1257	0	1296	20	0
7	XG	1257	0	1296	18	0
8	QH	1108	0	1165	23	0
8	XH	1108	0	1165	20	0
9	QI	1010	0	1037	35	0
9	XI	998	0	1024	39	0
10	QJ	801	0	849	39	0
10	XJ	777	0	816	24	0
11	QK	885	0	904	33	0
11	XK	864	0	881	25	0
12	QL	975	0	1062	26	0
12	XL	956	0	1046	28	0
13	QM	955	0	1021	46	0
13	XM	946	0	1007	36	0
14	QN	492	0	529	15	0
14	XN	492	0	529	12	0
15	QO	734	0	771	13	0
15	XO	729	0	768	17	0
16	QP	705	0	725	19	0
16	XP	705	0	725	22	0
17	QQ	834	0	904	14	0
17	XQ	834	0	904	21	0
18	QR	574	0	644	19	0
18	XR	574	0	644	22	0
19	QS	665	0	686	26	0
19	XS	674	0	699	21	0
20	QT	763	0	861	17	0
20	XT	763	0	861	19	0
21	QU	217	0	234	6	0
21	XU	217	0	234	10	0
22	QV	1644	0	836	21	0
22	QW	1618	0	826	45	0
22	XV	1644	0	836	19	0
22	XW	1618	0	826	44	0
23	QX	169	0	86	0	0
23	XX	210	0	109	3	0
24	QY	358	0	183	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	XY	358	0	184	5	0
25	RA	62071	0	31291	1006	0
25	YA	62091	0	31297	1166	0
26	RB	2573	0	1306	29	0
26	YB	2573	0	1306	42	0
27	RD	2115	0	2195	101	0
27	YD	2115	0	2195	102	0
28	RE	1568	0	1634	67	0
28	YE	1568	0	1634	64	0
29	RF	1585	0	1632	53	0
29	YF	1585	0	1632	55	0
30	RG	1474	0	1535	58	0
30	YG	1474	0	1535	69	0
31	RH	1336	0	1418	37	0
31	YH	1336	0	1418	72	0
32	RI	1136	0	1223	28	0
32	YI	1136	0	1223	27	0
33	RN	1104	0	1180	30	0
33	YN	1104	0	1180	25	0
34	RO	933	0	996	32	0
34	YO	933	0	996	26	0
35	RP	1145	0	1228	48	0
35	YP	1122	0	1206	50	0
36	RQ	1122	0	1179	49	0
36	YQ	1122	0	1179	47	0
37	RR	960	0	1021	30	0
37	YR	960	0	1021	27	0
38	RS	882	0	943	23	0
38	YS	882	0	943	27	0
39	RT	1141	0	1202	46	0
39	YT	1141	0	1202	49	0
40	RU	964	0	1022	47	0
40	YU	964	0	1022	45	0
41	RV	779	0	852	31	0
41	YV	779	0	852	24	0
42	RW	900	0	964	21	1
42	YW	900	0	964	21	0
43	RX	725	0	778	17	0
43	YX	725	0	778	25	0
44	RY	818	0	910	13	0
44	YY	818	0	912	14	1
45	RZ	1461	0	1493	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	YZ	1461	0	1493	46	0
46	R0	643	0	667	20	0
46	Y0	599	0	617	23	0
47	R1	763	0	848	18	0
47	Y1	729	0	802	22	0
48	R2	581	0	629	12	0
48	Y2	581	0	629	14	0
49	R3	469	0	518	14	0
49	Y3	469	0	518	16	0
50	R4	565	0	557	18	0
50	Y4	565	0	558	25	0
51	R5	459	0	477	5	0
51	Y5	459	0	480	10	0
52	R6	453	0	474	7	0
52	Y6	453	0	473	3	0
53	R7	409	0	454	12	0
53	Y7	418	0	467	9	0
54	R8	517	0	582	22	0
54	Y8	517	0	582	21	0
55	R9	307	0	338	22	0
55	Y9	307	0	338	141	0
56	QA	68	0	0	0	0
56	QC	1	0	0	0	0
56	QE	1	0	0	0	0
56	QF	1	0	0	0	0
56	QH	1	0	0	0	0
56	QQ	1	0	0	0	0
56	QV	6	0	0	0	0
56	QY	1	0	0	0	0
56	R0	4	0	0	0	0
56	R1	2	0	0	0	0
56	R4	1	0	0	0	0
56	R8	1	0	0	0	0
56	R9	1	0	0	0	0
56	RA	508	0	0	0	0
56	RB	7	0	0	0	0
56	RE	2	0	0	0	0
56	RF	1	0	0	0	0
56	RN	1	0	0	0	0
56	RO	2	0	0	0	0
56	RP	2	0	0	0	0
56	RQ	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	RR	1	0	0	0	0
56	RT	1	0	0	0	0
56	RU	1	0	0	0	0
56	RY	1	0	0	0	0
56	XA	82	0	0	0	0
56	XE	1	0	0	0	0
56	XL	1	0	0	0	0
56	XM	1	0	0	0	0
56	XQ	1	0	0	0	0
56	XS	1	0	0	0	0
56	XV	6	0	0	0	0
56	Y0	1	0	0	0	0
56	Y7	1	0	0	0	0
56	Y8	1	0	0	0	0
56	Y9	1	0	0	0	0
56	YA	546	0	0	0	0
56	YB	12	0	0	0	0
56	YD	2	0	0	0	0
56	YE	2	0	0	0	0
56	YO	1	0	0	0	0
56	YP	3	0	0	0	0
56	YQ	3	0	0	0	0
56	YX	2	0	0	0	0
56	YY	1	0	0	0	0
57	QD	8	0	0	1	0
57	XD	8	0	0	0	0
58	QN	1	0	0	0	0
58	R4	1	0	0	0	0
58	R5	1	0	0	0	0
58	R6	1	0	0	0	0
58	R9	1	0	0	0	0
58	RY	1	0	0	0	0
58	XN	1	0	0	0	0
58	Y4	1	0	0	0	0
58	Y5	1	0	0	0	0
58	Y6	1	0	0	0	0
58	Y9	1	0	0	0	0
58	YY	1	0	0	0	0
All	All	295575	0	199664	5705	1

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

The worst 5 of 5705 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)
4:QD:119:GLN:CB	4:QD:119:GLN:CG	1.78	1.55
25:YA:2755:C:H42	55:Y9:1:MET:HG2	1.08	1.16
25:RA:2747:G:N2	25:RA:2757:A:H62	1.43	1.15
25:YA:2742:C:H1'	55:Y9:26:ILE:HA	1.33	1.10
25:RA:2747:G:H21	25:RA:2757:A:N6	1.52	1.05

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:RW:63:ASP:OD1	44:YY:92:ASN:ND2[3_555]	2.18	0.02

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%)	29 (12%)	2 (1%)	17	54
2	XB	234/256 (91%)	202 (86%)	31 (13%)	1 (0%)	34	69
3	QC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
3	XC	203/239 (85%)	190 (94%)	13 (6%)	0	100	100
4	QD	206/209 (99%)	189 (92%)	17 (8%)	0	100	100
4	XD	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
5	QE	149/162 (92%)	141 (95%)	7 (5%)	1 (1%)	22	59
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	22	59
6	QF	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
7	QG	153/156 (98%)	147 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	XG	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
8	QH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
8	XH	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
9	QI	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
9	XI	124/128 (97%)	112 (90%)	12 (10%)	0	100	100
10	QJ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
10	XJ	94/105 (90%)	84 (89%)	10 (11%)	0	100	100
11	QK	117/129 (91%)	109 (93%)	8 (7%)	0	100	100
11	XK	114/129 (88%)	108 (95%)	6 (5%)	0	100	100
12	QL	123/132 (93%)	105 (85%)	18 (15%)	0	100	100
12	XL	120/132 (91%)	97 (81%)	22 (18%)	1 (1%)	19	56
13	QM	118/126 (94%)	96 (81%)	21 (18%)	1 (1%)	19	56
13	XM	117/126 (93%)	94 (80%)	22 (19%)	1 (1%)	17	54
14	QN	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	42
14	XN	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	42
15	QO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
15	XO	85/89 (96%)	84 (99%)	1 (1%)	0	100	100
16	QP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
17	XQ	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
18	QR	68/88 (77%)	64 (94%)	4 (6%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	81/93 (87%)	70 (86%)	11 (14%)	0	100	100
19	XS	82/93 (88%)	70 (85%)	11 (13%)	1 (1%)	13	49
20	QT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
20	XT	97/106 (92%)	87 (90%)	10 (10%)	0	100	100
21	QU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	XU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
27	RD	270/276 (98%)	235 (87%)	33 (12%)	2 (1%)	22	59
27	YD	270/276 (98%)	239 (88%)	29 (11%)	2 (1%)	22	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	RE	203/206 (98%)	163 (80%)	37 (18%)	3 (2%)	10	44
28	YE	203/206 (98%)	158 (78%)	42 (21%)	3 (2%)	10	44
29	RF	200/210 (95%)	183 (92%)	17 (8%)	0	100	100
29	YF	200/210 (95%)	185 (92%)	13 (6%)	2 (1%)	15	51
30	RG	179/182 (98%)	149 (83%)	29 (16%)	1 (1%)	25	62
30	YG	179/182 (98%)	148 (83%)	29 (16%)	2 (1%)	14	50
31	RH	172/180 (96%)	141 (82%)	28 (16%)	3 (2%)	9	42
31	YH	172/180 (96%)	137 (80%)	32 (19%)	3 (2%)	9	42
32	RI	144/148 (97%)	119 (83%)	22 (15%)	3 (2%)	7	38
32	YI	144/148 (97%)	117 (81%)	24 (17%)	3 (2%)	7	38
33	RN	136/140 (97%)	117 (86%)	17 (12%)	2 (2%)	10	44
33	YN	136/140 (97%)	117 (86%)	18 (13%)	1 (1%)	22	59
34	RO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
34	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
35	RP	148/150 (99%)	114 (77%)	33 (22%)	1 (1%)	22	59
35	YP	145/150 (97%)	112 (77%)	32 (22%)	1 (1%)	22	59
36	RQ	139/141 (99%)	114 (82%)	24 (17%)	1 (1%)	22	59
36	YQ	139/141 (99%)	116 (84%)	21 (15%)	2 (1%)	11	45
37	RR	115/118 (98%)	102 (89%)	13 (11%)	0	100	100
37	YR	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	17	54
38	RS	109/112 (97%)	86 (79%)	23 (21%)	0	100	100
38	YS	109/112 (97%)	87 (80%)	22 (20%)	0	100	100
39	RT	135/146 (92%)	115 (85%)	18 (13%)	2 (2%)	10	44
39	YT	135/146 (92%)	115 (85%)	18 (13%)	2 (2%)	10	44
40	RU	115/118 (98%)	109 (95%)	5 (4%)	1 (1%)	17	54
40	YU	115/118 (98%)	109 (95%)	5 (4%)	1 (1%)	17	54
41	RV	99/101 (98%)	86 (87%)	12 (12%)	1 (1%)	15	51
41	YV	99/101 (98%)	86 (87%)	13 (13%)	0	100	100
42	RW	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
42	YW	111/113 (98%)	98 (88%)	13 (12%)	0	100	100
43	RX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	YX	90/96 (94%)	88 (98%)	2 (2%)	0	100	100
44	RY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
44	YY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
45	RZ	181/206 (88%)	144 (80%)	33 (18%)	4 (2%)	6	37
45	YZ	181/206 (88%)	142 (78%)	36 (20%)	3 (2%)	9	42
46	R0	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
46	Y0	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
47	R1	95/98 (97%)	85 (90%)	9 (10%)	1 (1%)	14	50
47	Y1	91/98 (93%)	77 (85%)	13 (14%)	1 (1%)	14	50
48	R2	67/72 (93%)	62 (92%)	4 (6%)	1 (2%)	10	44
48	Y2	67/72 (93%)	61 (91%)	5 (8%)	1 (2%)	10	44
49	R3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
49	Y3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
50	R4	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	10	44
50	Y4	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	10	44
51	R5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
51	Y5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
52	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
52	Y6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
53	R7	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
53	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
54	R8	62/65 (95%)	46 (74%)	14 (23%)	2 (3%)	4	31
54	Y8	62/65 (95%)	47 (76%)	13 (21%)	2 (3%)	4	31
55	R9	35/37 (95%)	25 (71%)	10 (29%)	0	100	100
55	Y9	35/37 (95%)	18 (51%)	15 (43%)	2 (6%)	1	19
All	All	11452/12128 (94%)	10130 (88%)	1249 (11%)	73 (1%)	25	62

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	RE	18	ASP
31	RH	87	LEU
32	RI	15	VAL

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Mol	Chain	Res	Type
35	RP	108	LYS
39	RT	124	ASP

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%)	202 (100%)	1 (0%)	88	94
2	XB	204/220 (93%)	201 (98%)	3 (2%)	65	81
3	QC	159/188 (85%)	159 (100%)	0	100	100
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	180/181 (99%)	178 (99%)	2 (1%)	73	85
4	XD	180/181 (99%)	178 (99%)	2 (1%)	73	85
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	116 (100%)	0	100	100
6	QF	90/90 (100%)	88 (98%)	2 (2%)	52	72
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	118/119 (99%)	117 (99%)	1 (1%)	81	89
8	XH	118/119 (99%)	117 (99%)	1 (1%)	81	89
9	QI	98/99 (99%)	96 (98%)	2 (2%)	55	74
9	XI	97/99 (98%)	97 (100%)	0	100	100
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	104 (100%)	0	100	100
12	XL	103/109 (94%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	QM	96/101 (95%)	96 (100%)	0	100	100
13	XM	95/101 (94%)	95 (100%)	0	100	100
14	QN	49/50 (98%)	48 (98%)	1 (2%)	55	74
14	XN	49/50 (98%)	48 (98%)	1 (2%)	55	74
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	94 (99%)	1 (1%)	73	85
17	XQ	95/97 (98%)	94 (99%)	1 (1%)	73	85
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	71 (99%)	1 (1%)	67	82
19	XS	73/80 (91%)	73 (100%)	0	100	100
20	QT	76/82 (93%)	75 (99%)	1 (1%)	69	83
20	XT	76/82 (93%)	75 (99%)	1 (1%)	69	83
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
27	RD	214/218 (98%)	213 (100%)	1 (0%)	88	94
27	YD	214/218 (98%)	213 (100%)	1 (0%)	88	94
28	RE	165/166 (99%)	165 (100%)	0	100	100
28	YE	165/166 (99%)	165 (100%)	0	100	100
29	RF	161/166 (97%)	160 (99%)	1 (1%)	86	93
29	YF	161/166 (97%)	160 (99%)	1 (1%)	86	93
30	RG	155/156 (99%)	154 (99%)	1 (1%)	86	93
30	YG	155/156 (99%)	154 (99%)	1 (1%)	86	93
31	RH	145/148 (98%)	142 (98%)	3 (2%)	53	73
31	YH	145/148 (98%)	142 (98%)	3 (2%)	53	73
32	RI	122/124 (98%)	122 (100%)	0	100	100
32	YI	122/124 (98%)	122 (100%)	0	100	100
33	RN	117/119 (98%)	116 (99%)	1 (1%)	78	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	YN	117/119 (98%)	116 (99%)	1 (1%)	78	88
34	RO	100/100 (100%)	99 (99%)	1 (1%)	76	86
34	YO	100/100 (100%)	99 (99%)	1 (1%)	76	86
35	RP	116/116 (100%)	116 (100%)	0	100	100
35	YP	114/116 (98%)	114 (100%)	0	100	100
36	RQ	111/111 (100%)	111 (100%)	0	100	100
36	YQ	111/111 (100%)	111 (100%)	0	100	100
37	RR	100/101 (99%)	100 (100%)	0	100	100
37	YR	100/101 (99%)	100 (100%)	0	100	100
38	RS	87/88 (99%)	86 (99%)	1 (1%)	73	85
38	YS	87/88 (99%)	86 (99%)	1 (1%)	73	85
39	RT	120/127 (94%)	120 (100%)	0	100	100
39	YT	120/127 (94%)	120 (100%)	0	100	100
40	RU	93/94 (99%)	92 (99%)	1 (1%)	73	85
40	YU	93/94 (99%)	92 (99%)	1 (1%)	73	85
41	RV	82/82 (100%)	82 (100%)	0	100	100
41	YV	82/82 (100%)	82 (100%)	0	100	100
42	RW	92/92 (100%)	90 (98%)	2 (2%)	52	72
42	YW	92/92 (100%)	90 (98%)	2 (2%)	52	72
43	RX	74/78 (95%)	74 (100%)	0	100	100
43	YX	74/78 (95%)	74 (100%)	0	100	100
44	RY	88/91 (97%)	88 (100%)	0	100	100
44	YY	88/91 (97%)	88 (100%)	0	100	100
45	RZ	162/179 (90%)	161 (99%)	1 (1%)	86	93
45	YZ	162/179 (90%)	161 (99%)	1 (1%)	86	93
46	R0	65/67 (97%)	65 (100%)	0	100	100
46	Y0	61/67 (91%)	60 (98%)	1 (2%)	62	79
47	R1	82/83 (99%)	82 (100%)	0	100	100
47	Y1	78/83 (94%)	78 (100%)	0	100	100
48	R2	64/67 (96%)	64 (100%)	0	100	100
48	Y2	64/67 (96%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	R3	51/52 (98%)	51 (100%)	0	100	100
49	Y3	51/52 (98%)	51 (100%)	0	100	100
50	R4	62/63 (98%)	61 (98%)	1 (2%)	62	79
50	Y4	62/63 (98%)	60 (97%)	2 (3%)	39	64
51	R5	51/52 (98%)	51 (100%)	0	100	100
51	Y5	51/52 (98%)	51 (100%)	0	100	100
52	R6	51/52 (98%)	51 (100%)	0	100	100
52	Y6	51/52 (98%)	51 (100%)	0	100	100
53	R7	40/42 (95%)	40 (100%)	0	100	100
53	Y7	41/42 (98%)	41 (100%)	0	100	100
54	R8	54/55 (98%)	54 (100%)	0	100	100
54	Y8	54/55 (98%)	54 (100%)	0	100	100
55	R9	34/34 (100%)	34 (100%)	0	100	100
55	Y9	34/34 (100%)	33 (97%)	1 (3%)	42	66
All	All	9687/10066 (96%)	9635 (100%)	52 (0%)	88	94

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	RW	40	ASN
4	XD	103	ASN
46	Y0	55	ARG
45	RZ	34	ASN
2	XB	30	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
37	RR	71	GLN
39	RT	58	ASN
29	YF	40	GLN
30	RG	40	ASN
31	YH	74	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1508 (99%)	252 (16%)	34 (2%)
1	XA	1499/1508 (99%)	272 (18%)	37 (2%)
22	QV	76/77 (98%)	17 (22%)	3 (3%)
22	QW	75/77 (97%)	31 (41%)	2 (2%)
22	XV	76/77 (98%)	18 (23%)	3 (3%)
22	XW	75/77 (97%)	32 (42%)	2 (2%)
23	QX	7/25 (28%)	0	0
23	XX	9/25 (36%)	3 (33%)	0
24	QY	16/17 (94%)	2 (12%)	0
24	XY	16/17 (94%)	2 (12%)	0
25	RA	2879/2915 (98%)	599 (20%)	47 (1%)
25	YA	2880/2915 (98%)	570 (19%)	48 (1%)
26	RB	119/122 (97%)	17 (14%)	1 (0%)
26	YB	119/122 (97%)	19 (15%)	1 (0%)
All	All	9344/9482 (98%)	1834 (19%)	178 (1%)

5 of 1834 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	32	A
1	QA	39	G
1	QA	48	C

5 of 178 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2566	A
1	XA	352	C
25	YA	1819	A
25	RA	2689	U
1	XA	78	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1301 ligands modelled in this entry, 1299 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	$\# Z > 2$
57	SF4	XD	301	4	0,12,12	0.00	-	-		
57	SF4	QD	301	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
57	SF4	XD	301	4	-	-	0/6/5/5
57	SF4	QD	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	QD	301	SF4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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