



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 07:54 AM EDT

PDB ID : 6NSH
Title : Modified ASL proline bound to Thermus thermophilus 70S (near-cognate)
Authors : Hoffer, E.D.; Maehigashi, T.; Subaramanian, S.; Hong, S.; Dunham, C.M.
Deposited on : 2019-01-24
Resolution : 3.40 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)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

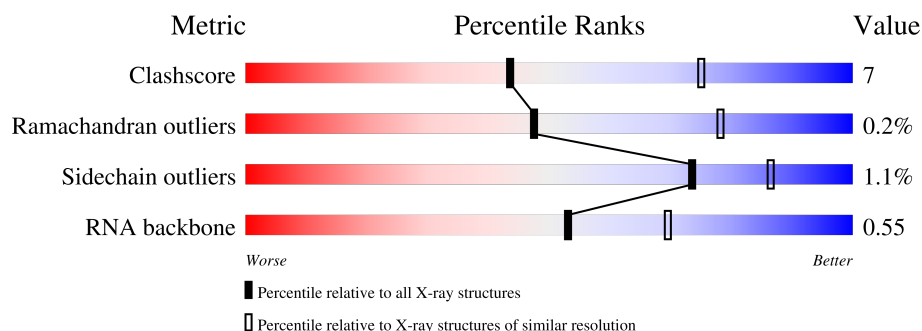
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RNA backbone	3102	1006 (3.84-2.96)


























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	RA	2915	
1	YA	2915	
2	RB	122	
2	YB	122	
3	RD	276	
3	YD	276	


























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Mol	Chain	Length	Quality of chain
4	RE	206	 78% 20% ..
4	YE	206	 76% 23% .
5	RF	210	 76% 20% .
5	YF	210	 72% 23% .
6	RG	182	 65% 30% ..
6	YG	182	 70% 27% ..
7	RH	180	 69% 24% . .
7	YH	180	 82% 13% . .
8	RI	148	 65% 28% 5% ..
8	YI	148	 66% 30% ..
9	RN	140	 76% 21% ..
9	YN	140	 78% 20% .
10	RO	122	 76% 23% .
10	YO	122	 83% 16% .
11	RP	150	 62% 34% ..
11	YP	150	 71% 25% . .
12	RQ	141	 65% 32% .
12	YQ	141	 82% 16% ..
13	RR	118	 83% 14% ..
13	YR	118	 82% 16% ..
14	RS	112	 75% 21% . .
14	YS	112	 87% 12% .
15	RT	146	 75% 18% . 6%
15	YT	146	 82% 12% 6%
16	RU	118	 79% 18% . .


























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Mol	Chain	Length	Quality of chain
16	YU	118	 82% 15% ..
17	RV	101	 77% 23%
17	YV	101	 83% 16% .
18	RW	113	 80% 18% .
18	YW	113	 82% 16% .
19	RX	96	 77% 19% .
19	YX	96	 76% 22% .
20	RY	110	 82% 15% ..
20	YY	110	 81% 15% ..
21	RZ	206	 67% 29% ..
21	YZ	206	 82% 15% .
22	R0	85	 75% 14% 11%
22	Y0	85	 69% 18% . 12%
23	R1	98	 81% 16% ..
23	Y1	98	 77% 18% 5%
24	R2	72	 74% 18% . .
24	Y2	72	 88% 12%
25	R3	60	 72% 25% ..
25	Y3	60	 72% 25% ..
26	R4	71	 61% 34% . .
26	Y4	71	 58% 34% 6% .
27	R5	60	 80% 18% .
27	Y5	60	 78% 20% .
28	R6	54	 93% 6% .
28	Y6	54	 85% 13% .

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


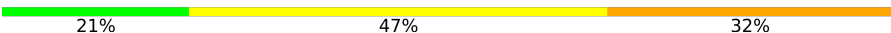
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Mol	Chain	Length	Quality of chain
41	XJ	105	
42	QK	129	
42	XK	129	
43	QL	132	
43	XL	132	
44	QM	126	
44	XM	126	
45	QN	61	
45	XN	61	
46	QO	89	
46	XO	89	
47	QP	88	
47	XP	88	
48	QQ	105	
48	XQ	105	
49	QR	88	
49	XR	88	
50	QS	93	
50	XS	93	
51	QT	106	
51	XT	106	
52	QU	27	
52	XU	27	
53	QV	17	
53	XV	17	

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Mol	Chain	Length	Quality of chain
54	QX	19	
54	XX	19	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	SF4	XD	301	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 290035 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	RA	2881	Total	C	N	O	P	0	0	0
			62051	27618	11609	19944	2880			
1	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
3	YD	273	Total	C	N	O	S	0	0	0
			2126	1341	424	358	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	RE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
4	YE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	RN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
9	YN	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	RP	148	Total	C	N	O	S	0	0	0
			1130	704	230	193	3			
11	YP	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	RR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	YR	117	Total	C	N	O		0	0	0
			960	599	202	159				

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	RS	111	Total	C	N	O	0	0	0
			882	556	176	150			
14	YS	110	Total	C	N	O	0	0	0
			877	553	175	149			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	RX	92	Total	C	N	O	S	0	0	0
			725	471	131	123				
19	YX	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	RZ	203	Total	C	N	O	S	0	0	0
			1601	1020	283	295	3			
21	YZ	201	Total	C	N	O	S	0	0	0
			1587	1012	281	291	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	R0	76	Total	C	N	O	S	0	0	0
			603	372	128	102	1			
22	Y0	75	Total	C	N	O	S	0	0	0
			599	370	127	101	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
24	Y2	72	Total	C	N	O	S	0	0	0
			606	375	122	107	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	R9	36	Total	C	N	O	S	0	0	0
			302	186	67	45	4			
31	Y9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	QA	1511	Total	C	N	O	P	0	0	0
			32469	14453	6011	10495	1510			
32	XA	1511	Total	C	N	O	P	0	0	0
			32471	14454	6014	10493	1510			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	QJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			
41	XJ	96	Total	C	N	O	S	0	0	0
			777	487	153	136	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	QK	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	XK	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
50	XS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

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

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

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

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

- Molecule 53 is a RNA chain called P-site ASLPro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	QV	17	Total	C	N	O	P	0	0	0
			365	163	65	120	17			
53	XV	15	Total	C	N	O	P	0	0	0
			322	144	57	106	15			

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	QX	18	Total	C	N	O	P	0	0	0
			389	174	76	121	18			
54	XX	19	Total	C	N	O	P	0	0	0
			412	184	81	128	19			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	RA	485	Total	Mg	0	0
			485	485		
55	RB	8	Total	Mg	0	0
			8	8		
55	RE	2	Total	Mg	0	0
			2	2		
55	RF	1	Total	Mg	0	0
			1	1		
55	RN	1	Total	Mg	0	0
			1	1		
55	RO	1	Total	Mg	0	0
			1	1		
55	RP	2	Total	Mg	0	0
			2	2		
55	RQ	2	Total	Mg	0	0
			2	2		
55	RT	1	Total	Mg	0	0
			1	1		
55	RX	1	Total	Mg	0	0
			1	1		
55	R0	1	Total	Mg	0	0
			1	1		
55	R1	1	Total	Mg	0	0
			1	1		
55	R5	1	Total	Mg	0	0
			1	1		
55	R8	1	Total	Mg	0	0
			1	1		

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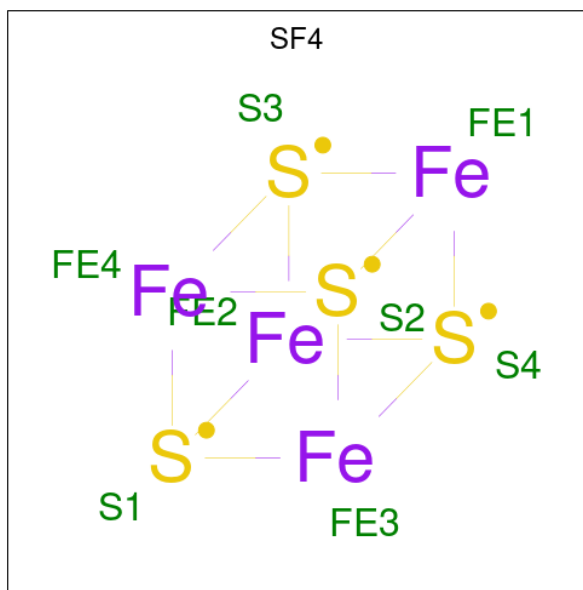
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	66	Total 66	Mg 66	0	0
55	QF	1	Total 1	Mg 1	0	0
55	YA	510	Total 510	Mg 510	0	0
55	YB	7	Total 7	Mg 7	0	0
55	YD	1	Total 1	Mg 1	0	0
55	YE	4	Total 4	Mg 4	0	0
55	YO	1	Total 1	Mg 1	0	0
55	YP	2	Total 2	Mg 2	0	0
55	YQ	1	Total 1	Mg 1	0	0
55	YR	1	Total 1	Mg 1	0	0
55	Y0	2	Total 2	Mg 2	0	0
55	Y1	1	Total 1	Mg 1	0	0
55	Y5	1	Total 1	Mg 1	0	0
55	Y7	1	Total 1	Mg 1	0	0
55	Y8	1	Total 1	Mg 1	0	0
55	XA	87	Total 87	Mg 87	0	0
55	XE	1	Total 1	Mg 1	0	0
55	XL	1	Total 1	Mg 1	0	0
55	XQ	1	Total 1	Mg 1	0	0
55	XS	1	Total 1	Mg 1	0	0

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

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

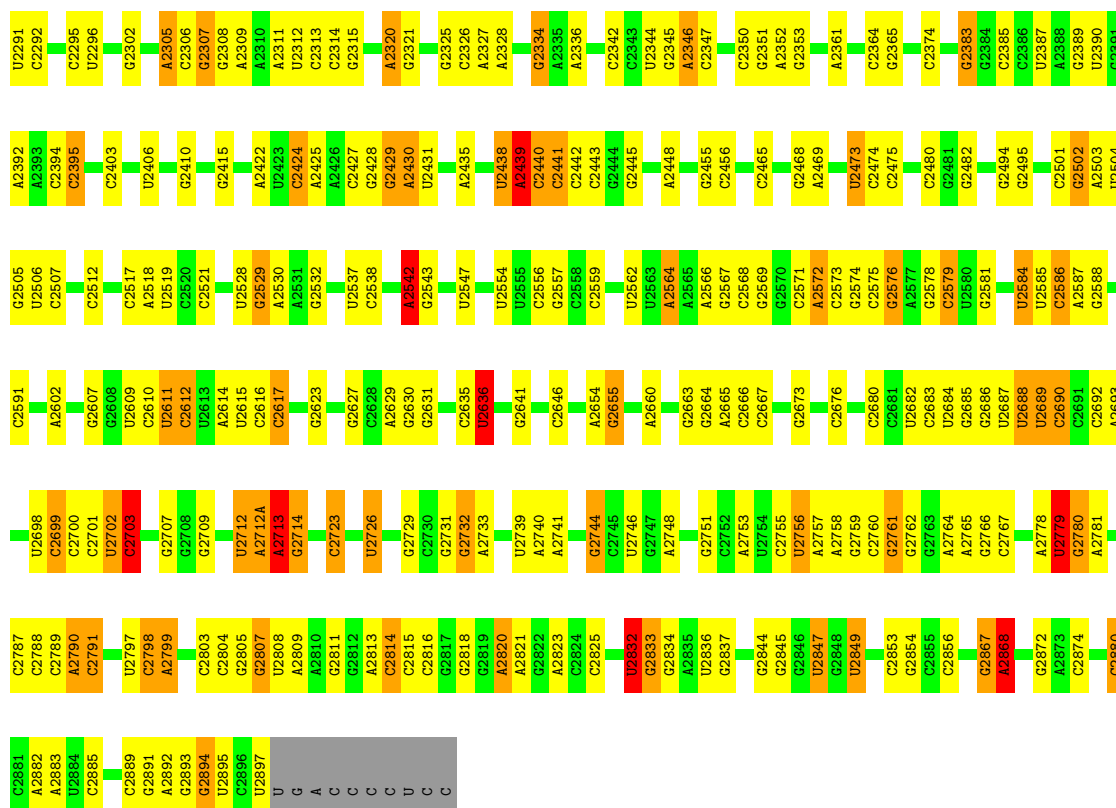
- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

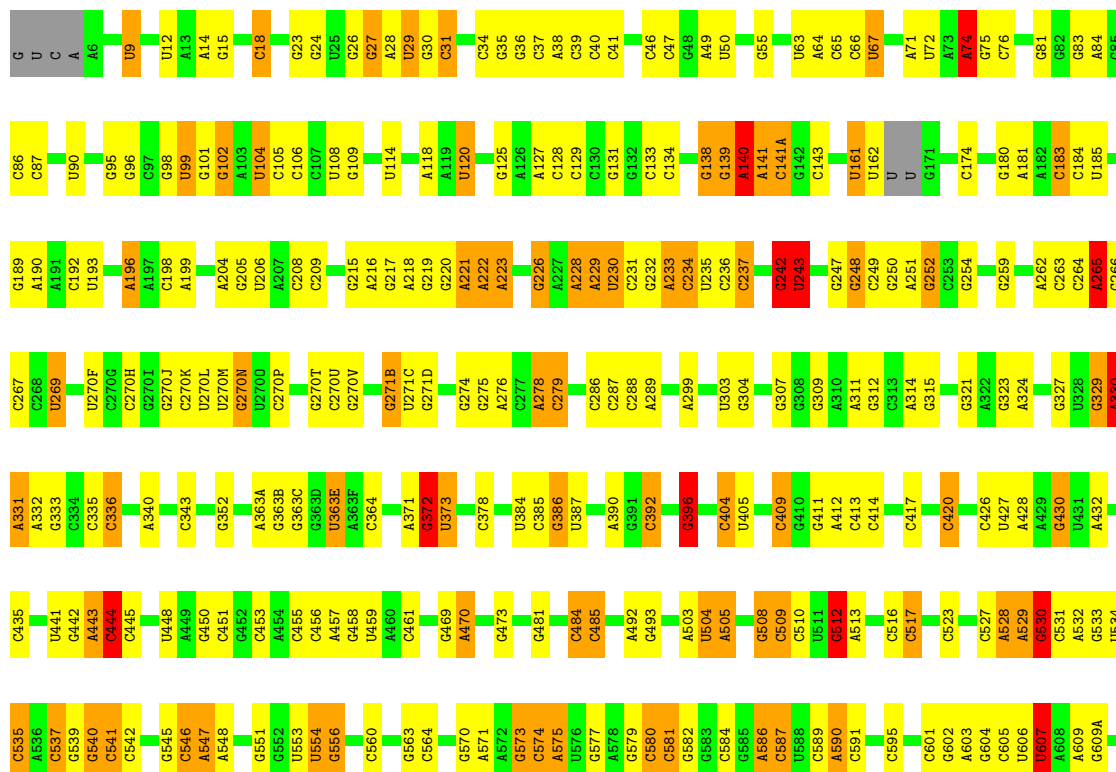


G2191	A2117	A1815	A1918	A1608	G1524	G1441	A1349	U1249	G1157	G1074	A1000	A910
G2192	U2118	G1816	A1919	A1609	G1525	G1442	U1352	G1250	C1158	C1075	A1001	A911
G2193		G1817	C1920	A1610	G1526		A1352	C1251	U1159	A1076	G1002	C912
U2197	G2123	U1818	A2031	C1611	G1527	A1444A	A1353	G1252		A1077	G1003	U913
A2198	G2124	A1819	G1929		A1528	C1445	A1354	A1253	U1165	U1078	C1004	C914
A2199	G2125	U1820	G1930	A1616	A1529			A1254	U1166	C1079	C1005	C915
C2205	A2126	G1823	U1931	C1617	C1533	G1448	A1359	U1255	G1171		C1006	G916
	G2127	G1824	C1934	A1618	C1534	A1449		G1256	U1082	U1082	G1007	A917
U2208	G2128	G1825	G1935	A1619	G1534	A1449A	A1365	C1257	U1083	U1083	C1008	A918
C2209	U2130	C1827	G1936	A1622	U1535			U1257	A1084	A1084	A1009	G919
G2210	G2131	G1828	A1937	A1624	A1536	G1455	G1368	A1262	U1085	A1085	A1010	
G2211	U2132	A1829	A1938	A1634	C1537	A1460	G1369	U1263	A1086	A1086	G1011	U922
A2212	G2133	C1830	U1939	G1635	C1538	G1461	C1370	G1264	C1178	C1178	U1012	C923
	A2134	C1831		C1636	C1539	G1462	G1371	A1265	G1087	A1087	C1013	C924
U2213	A2135	U1833	C1947	A1637	U1540	C1463	U1372	U1267	U1088	A1088		
G2215	C2136	U1834		U1638	G1542	C1464	C1375	C1267	U1089	U1089	U1019	
	C2137	G1835	G1950	U1639	A1543			A1272	U1090	U1090	A1020	
A2224	U2138	C1836	U1951	C1640	C1544	C1468	A1379	U1273	C1092	C1092	A1021	A941
A2225	G2139	C1844	A1952	C1644	A1545	A1471	A1384	A1274	G1183	G1183	U1023	
C2226	C2140	A1847	U1955	C1648	C1547	C1474	G1385	A1275	U1188	A1096	G1024	G944
	G2141	A1848	U1956		C1549		C1387	G1281	U1189	U1097	G1025	G946
U2233	C2145	A1883	C1961	G1653	C1550	G1478	U1390	U1282	G1190		A1027	A953
	G2146		G1962	A1654		G1479	U1391	G1283	G1100	C1100		G954
G2236	G2147	G1858	U1963	C1656	C1557	U1482		A1286	U1101	U1101	G1031	C955
G2237	G2148	A1859	C1967	C1657	A1558	U1483	U1394	U1288	C1102	C1102	A1032	G956
G2239	G2151	G1968	C1968	C1658	G1559	G1484	A1395	G1294	A1103		U1033	U958
U2243	G2152	U1864	A1969	U1659	G1560	G1485	U1396	U1296	C1203	C1109	C1041	A959
U2244	G2153	C1870	A1970	C1660	A1566	A1486	U1397	G1296	G1110	G1110	G1042	A960
U2245	G2154	A1871	A1971			G1487		C1296	A1111			C961
G2246	G2155	A1872	A1972	G1667	A1569	C1493	C1403	U1300	G1112		A1045	
A2247	G2156	G1878	A1973	A1668	C1577	A1494	C1404	A1301	U1113	U1113	A1046	C965
C2248	G2157	C1881	C1982	C1670	A1578	A1495	U1405	G1304	G1114	G1114	G1047	U969
U2249	G2158	G1882	C1983	G1674	A1579	A1496	C1407	C1306	G1115		A1048	
G2250	G2159	C1883	C1988	C1675	A1580	C1498	C1408	U1306	G1122		C1049	C970
	G2160	G1888	C1989	C1678	A1583	C1502	C1411	C1306	C1123		C1052	A973
C2254	G2161	A1889	U1991	A1679	C1585	U1503	G1416	G1310	C1124		C1053	G974
	C2163	C1892	G1992	U1680	A1586	C1504	C1417	U1312	A1129		A1054	C974A
C2260	G2164	C1899	C1993	G1681	A1587	C1505	G1418	U1313	U1130		G1055	G975
A2266	G2165	G1900	U1993	G1682	U1590	C1506	A1419	C1314	C1135		G1056	C976
A2269	U2167	A1900	C1996	C1683	G1592	A1507	U1420	G1224	C1136		A1057	A980
	A2169	G1903	G2002	C1686	C1593	C1509	G1421	A1321	G1137		G1058	
C2275	A2170	G1906	G2006	A1689	G1594	A1510		U1323	U1142		U1060	A983
A2278	G2173	G1907	C2006	A1690	G1595	G1511	G1427	G1329	U1143		U	A984
G2279	G2181	G1908	G2010	C1691	C1598	G1512	G1428	C1330	A142A		A1066	C992
	C2182	C1909	U2011	U1692	C1599	U1514	G1429	A1331	U1234		A1067	C993
C2283	G2183	C1913	G2012	C1694	C1603	C1515	U1431	G1332	G1149		G1068	G994
C2284	G2184	C1914	C2012	G1695	C1604	G1519	C1432	C1333	C1150		A1069	C995
A2286	G2187	U1915	A2019	G1696	C1605	G1522	U1433	U1341	C1154		A1070	C996
A2287	C2188	A1916	A2020	G1697	C1606	G1523	C1437	G1348	G1154		G1071	A996
A2288	U2189	C2021	U2022	A1698	C1607						C1072	C997
	G2190										A1073	

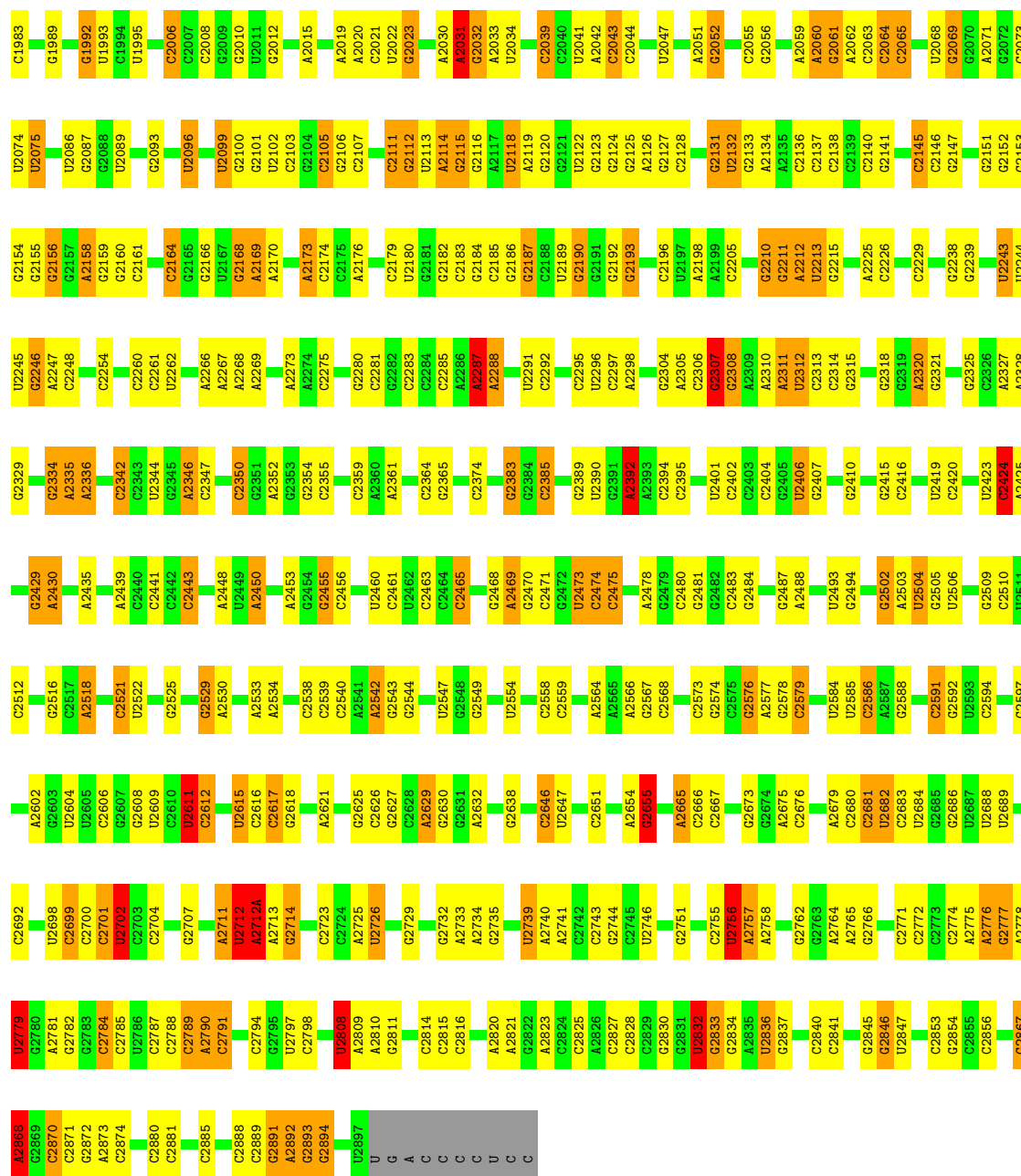


• Molecule 1: 23S rRNA

Chain YA: 54% 33% 11% ..

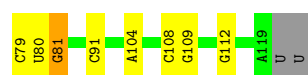
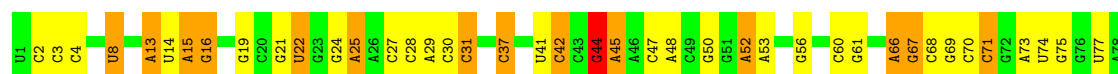






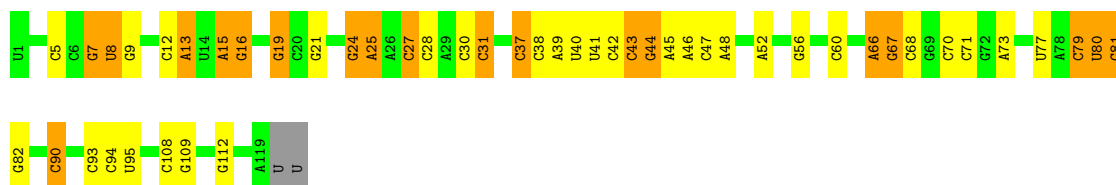
- Molecule 2: 5S rRNA

Chain RB: 58% 27% 12% ..



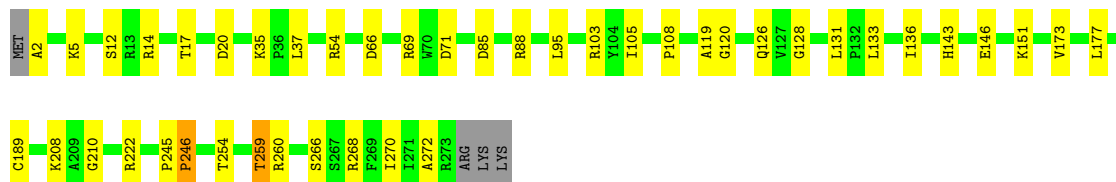
- Molecule 2: 5S rRNA

Chain YB: 58% 25% 16% .



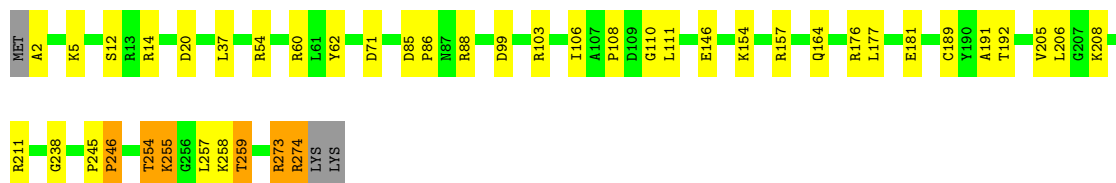
- Molecule 3: 50S ribosomal protein L2

Chain RD: 83% 15% ..



- Molecule 3: 50S ribosomal protein L2

Chain YD: 83% 13% ..



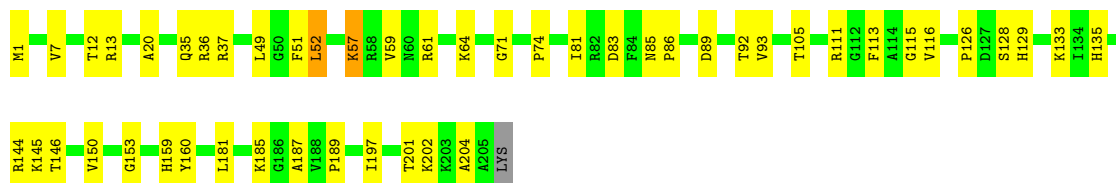
- Molecule 4: 50S ribosomal protein L3

Chain RE: 78% 20% ..



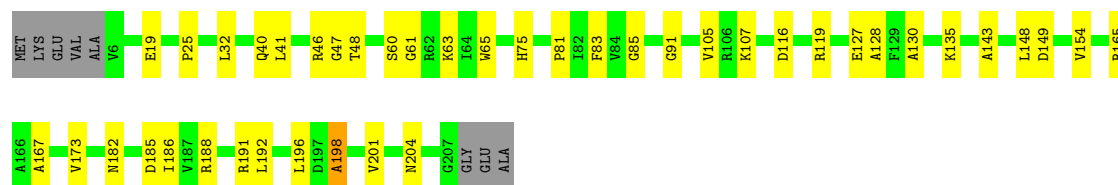
- Molecule 4: 50S ribosomal protein L3

Chain YE: 76% 23% .



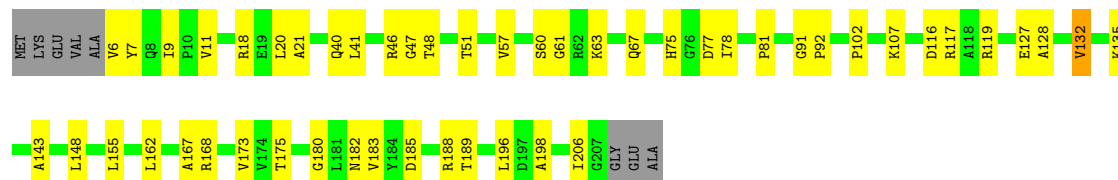
- Molecule 5: 50S ribosomal protein L4

Chain RF: 76% 20% .



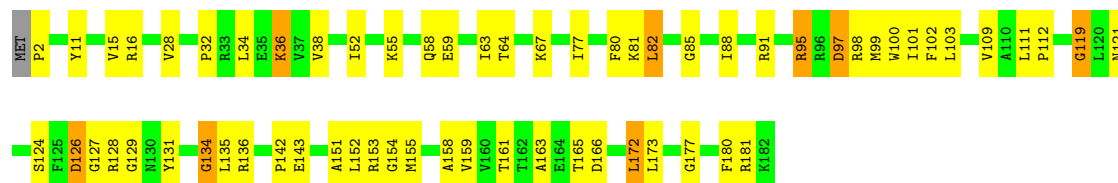
- Molecule 5: 50S ribosomal protein L4

Chain YF: 72% 23% .



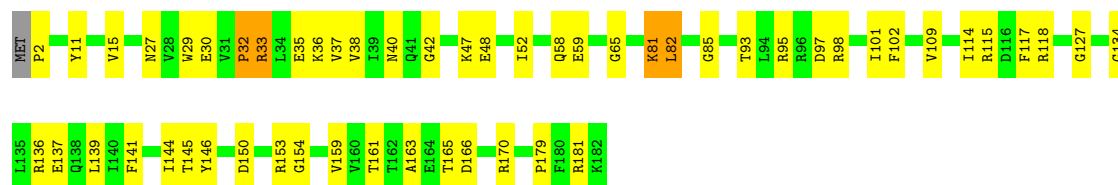
- Molecule 6: 50S ribosomal protein L5

Chain RG: 65% 30% . .



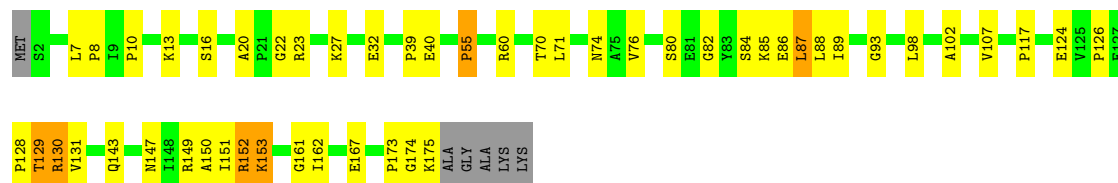
- Molecule 6: 50S ribosomal protein L5

Chain YG: 70% 27% . .



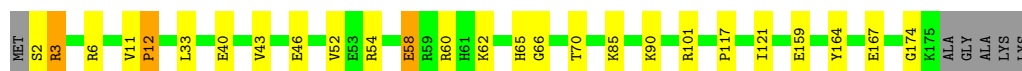
- Molecule 7: 50S ribosomal protein L6

Chain RH: 69% 24% . .



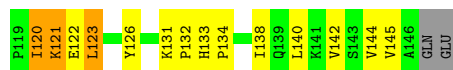
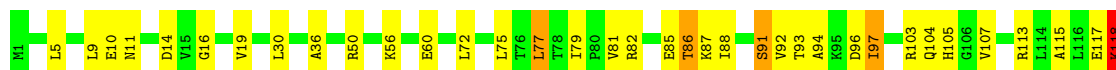
- Molecule 7: 50S ribosomal protein L6

Chain YH: 82% 13% . .



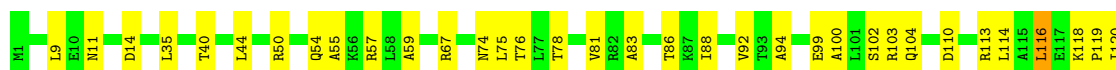
• Molecule 8: 50S ribosomal protein L9

Chain RI: 65% 28% 5% ..



• Molecule 8: 50S ribosomal protein L9

Chain YI: 66% 30% ..



• Molecule 9: 50S ribosomal protein L13

Chain RN: 76% 21% ..



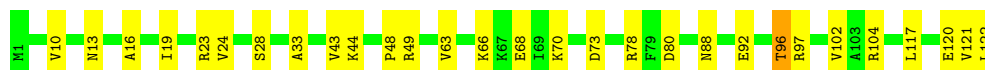
• Molecule 9: 50S ribosomal protein L13

Chain YN: 78% 20% .



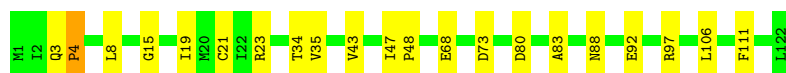
• Molecule 10: 50S ribosomal protein L14

Chain RO: 76% 23% .



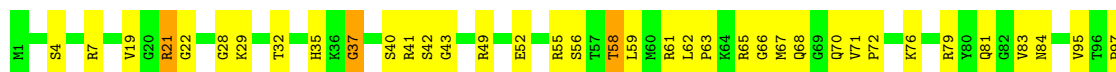
• Molecule 10: 50S ribosomal protein L14

Chain YO: 83% 16% .



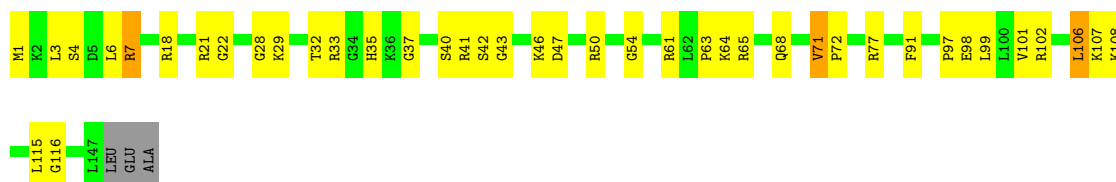
- Molecule 11: 50S ribosomal protein L15

Chain RP: 62% 34% ..



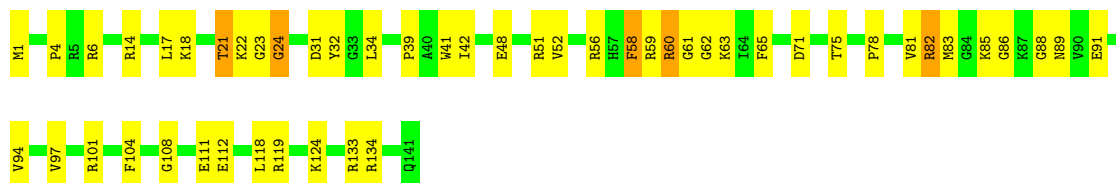
- Molecule 11: 50S ribosomal protein L15

Chain YP: 71% 25% ..



- Molecule 12: 50S ribosomal protein L16

Chain RQ: 65% 32% .



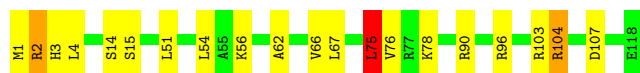
- Molecule 12: 50S ribosomal protein L16

Chain YQ: 82% 16% ..




- Molecule 13: 50S ribosomal protein L17

Chain RR: 83% 14% ..




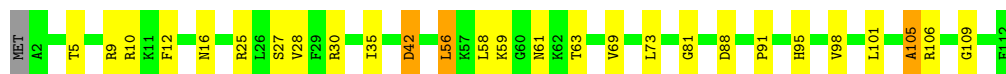
- Molecule 13: 50S ribosomal protein L17

Chain YR:  82% 16% ..




- Molecule 14: 50S ribosomal protein L18

Chain RS:  75% 21% ..




- Molecule 14: 50S ribosomal protein L18

Chain YS:  87% 12% .




- Molecule 15: 50S ribosomal protein L19

Chain RT:  75% 18% . 6%




- Molecule 15: 50S ribosomal protein L19

Chain YT:  82% 12% 6%




- Molecule 16: 50S ribosomal protein L20

Chain RU:  79% 18% ..




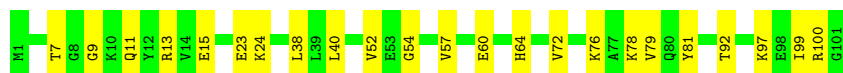
- Molecule 16: 50S ribosomal protein L20

Chain YU:  82% 15% ..




- Molecule 17: 50S ribosomal protein L21

Chain RV:  77% 23%




- Molecule 17: 50S ribosomal protein L21

Chain YV:  83% 16%




- Molecule 18: 50S ribosomal protein L22

Chain RW:  80% 18%




- Molecule 18: 50S ribosomal protein L22

Chain YW:  82% 16%




- Molecule 19: 50S ribosomal protein L23

Chain RX:  77% 19%




- Molecule 19: 50S ribosomal protein L23

Chain YX:  76% 22%




- Molecule 20: 50S ribosomal protein L24

Chain RY:  82% 15%



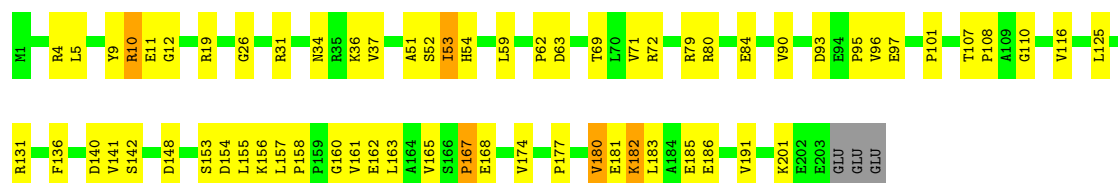
- Molecule 20: 50S ribosomal protein L24

Chain YY:  81% 15% ..




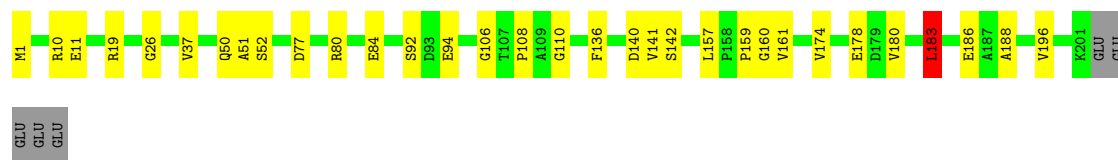
- Molecule 21: 50S ribosomal protein L25

Chain RZ:  67% 29% ..




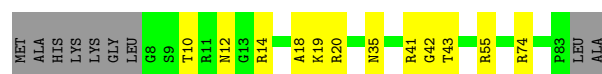
- Molecule 21: 50S ribosomal protein L25

Chain YZ:  82% 15% .



- Molecule 22: 50S ribosomal protein L27

Chain R0:  75% 14% 11%




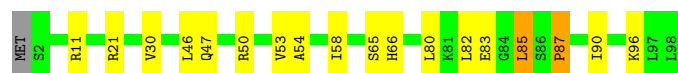
- Molecule 22: 50S ribosomal protein L27

Chain Y0:  69% 18% 12%




- Molecule 23: 50S ribosomal protein L28

Chain R1:  81% 16% ..



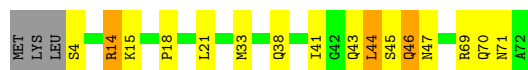
- Molecule 23: 50S ribosomal protein L28

Chain Y1:  77% 18% 5%



- Molecule 24: 50S ribosomal protein L29

Chain R2: 74% 18%



- Molecule 24: 50S ribosomal protein L29

Chain Y2: 88% 12%



- Molecule 25: 50S ribosomal protein L30

Chain R3: 72% 25%



- Molecule 25: 50S ribosomal protein L30

Chain Y3: 72% 25%



- Molecule 26: 50S ribosomal protein L31

Chain R4: 61% 34%



- Molecule 26: 50S ribosomal protein L31

Chain Y4: 58% 34% 6%



- Molecule 27: 50S ribosomal protein L32

Chain R5: 80% 18%



- Molecule 27: 50S ribosomal protein L32

Chain Y5: 78% 20% .



- Molecule 28: 50S ribosomal protein L33

Chain R6: 93% 6% .



- Molecule 28: 50S ribosomal protein L33

Chain Y6: 85% 13% .



- Molecule 29: 50S ribosomal protein L34

Chain R7: 80% 14% . .



- Molecule 29: 50S ribosomal protein L34

Chain Y7: 82% 16% .



- Molecule 30: 50S ribosomal protein L35

Chain R8: 74% 18% 6% .

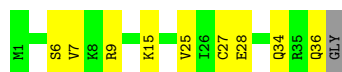


- Molecule 30: 50S ribosomal protein L35

Chain Y8: 69% 25% 5% .



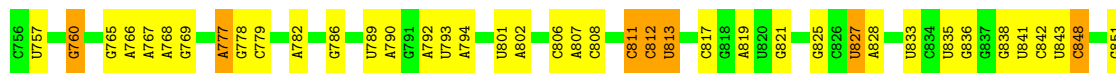
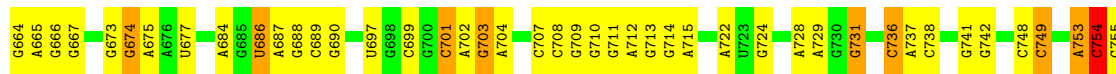
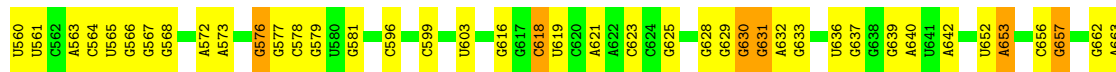
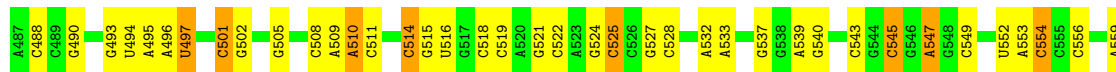
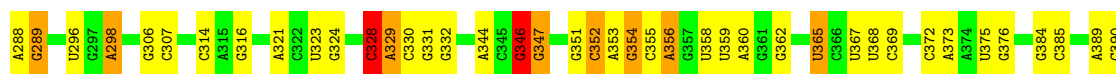
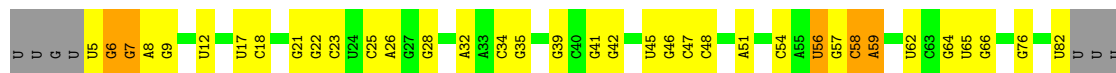
- Molecule 31: 50S ribosomal protein L36

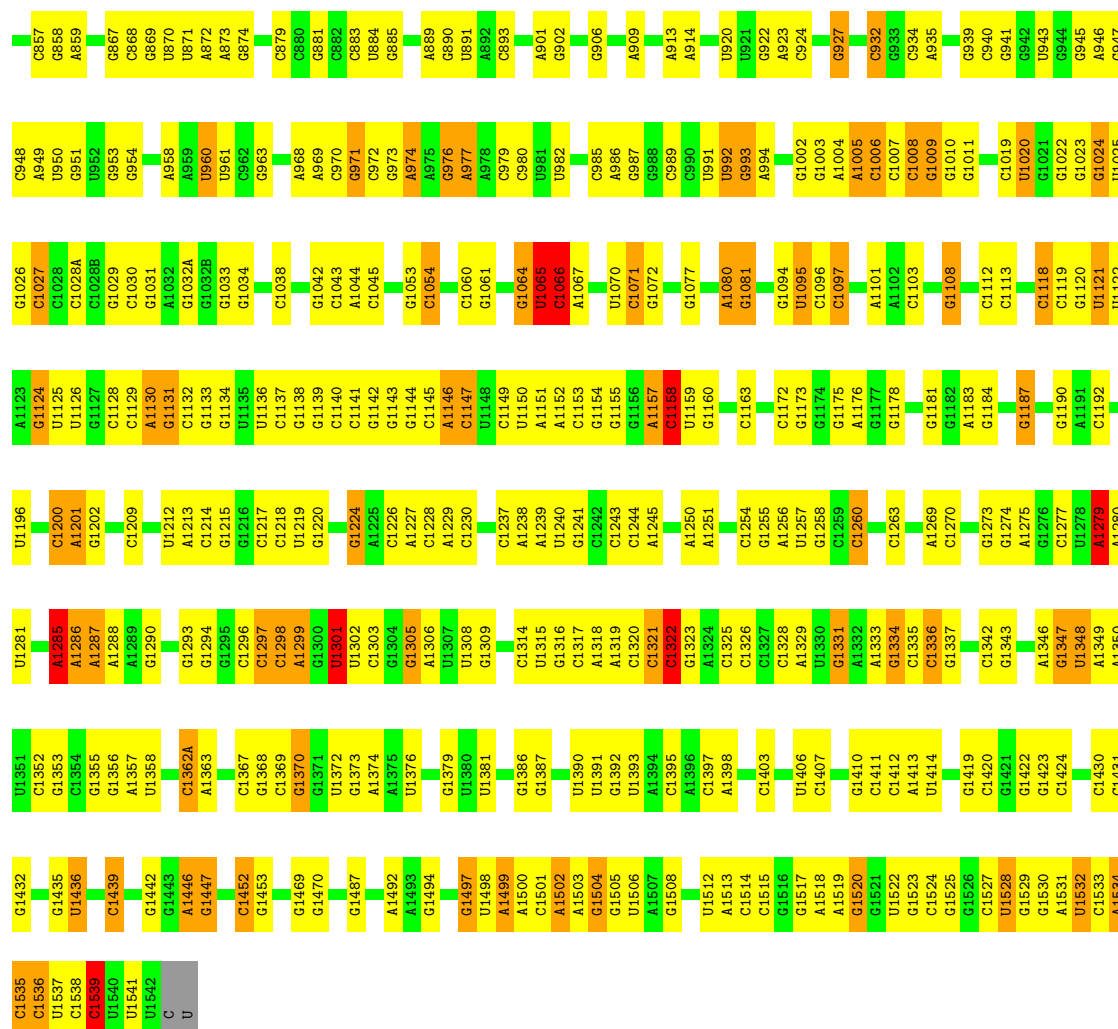


- Molecule 31: 50S ribosomal protein L36

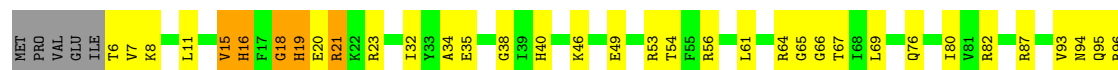


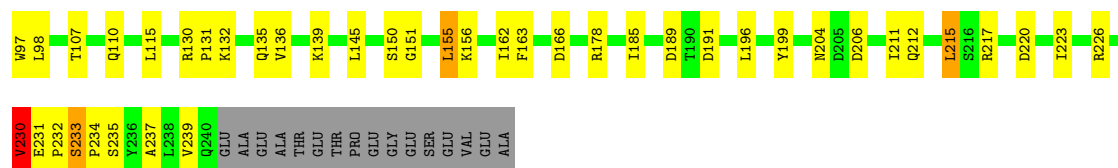
- Molecule 32: 16S rRNA





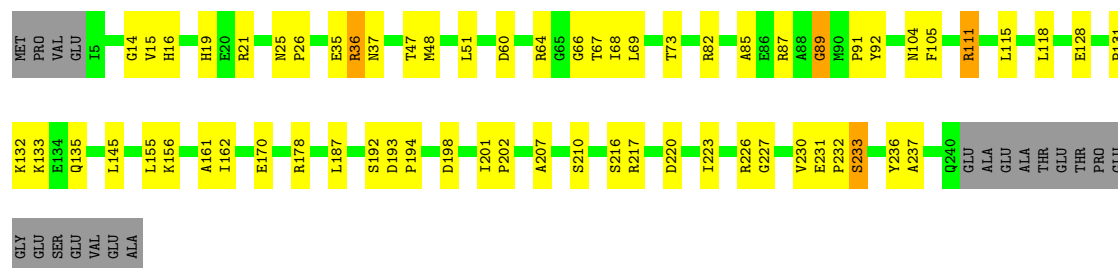
- Molecule 33: 30S ribosomal protein S2





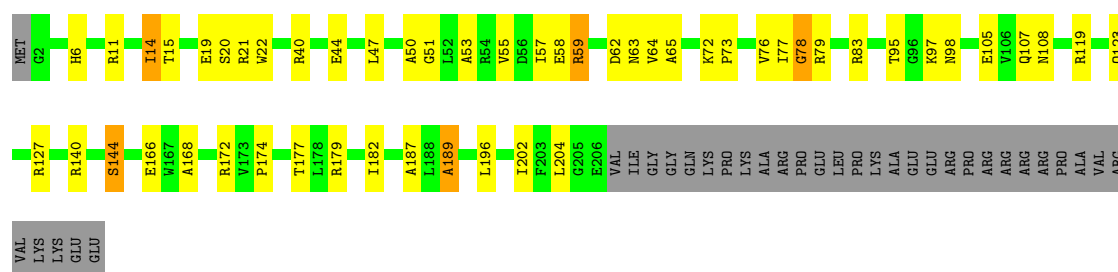
- Molecule 33: 30S ribosomal protein S2

Chain XB: 67% 23% 8%



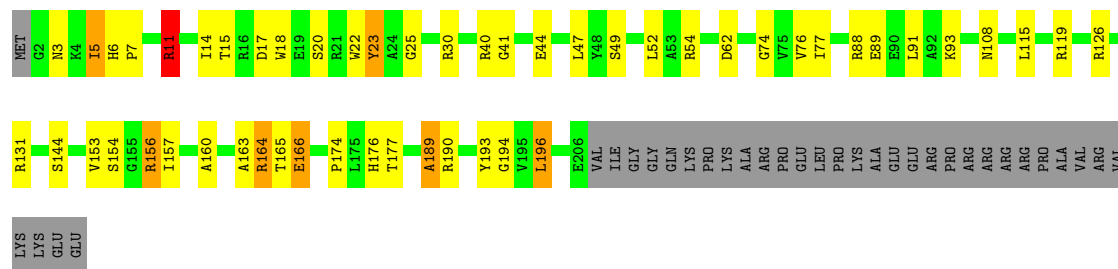
- Molecule 34: 30S ribosomal protein S3

Chain QC: 64% 20% 14%



- Molecule 34: 30S ribosomal protein S3

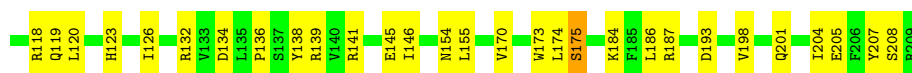
Chain XC: 64% 18% 14%



- Molecule 35: 30S ribosomal protein S4

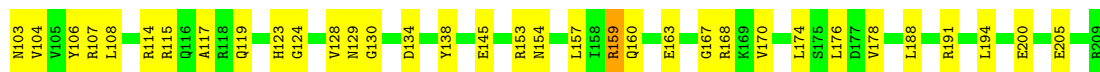
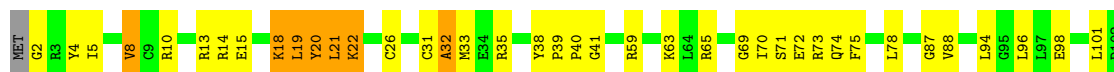
Chain QD: 68% 28% 0%





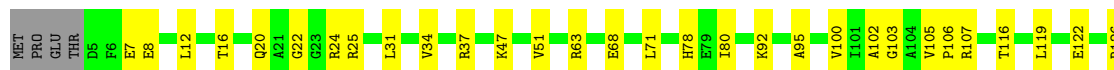
- Molecule 35: 30S ribosomal protein S4

Chain XD: 65% 31% .



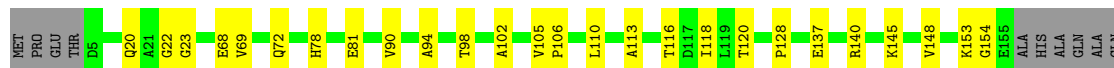
- Molecule 36: 30S ribosomal protein S5

Chain QE: 73% 20% 7%



- Molecule 36: 30S ribosomal protein S5

Chain XE: 77% 16% 7%



GLY

- Molecule 37: 30S ribosomal protein S6

Chain QF: 75% 25%




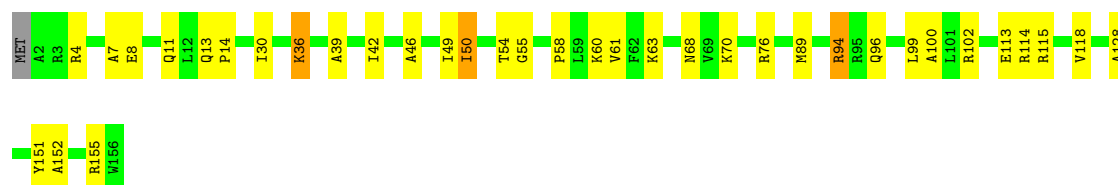
- Molecule 37: 30S ribosomal protein S6

Chain XF: 89% 11%



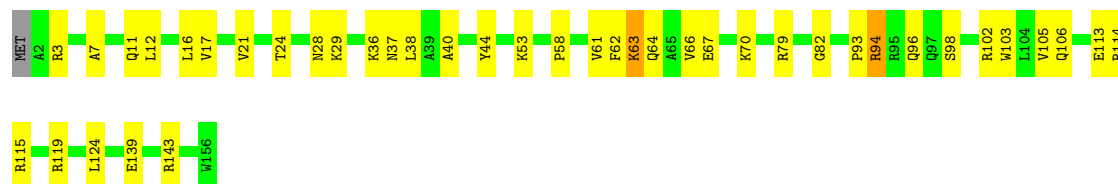
- Molecule 38: 30S ribosomal protein S7

Chain QG:  76% 21% ..




- Molecule 38: 30S ribosomal protein S7

Chain XG:  73% 25% ..




- Molecule 39: 30S ribosomal protein S8

Chain QH:  75% 24% .



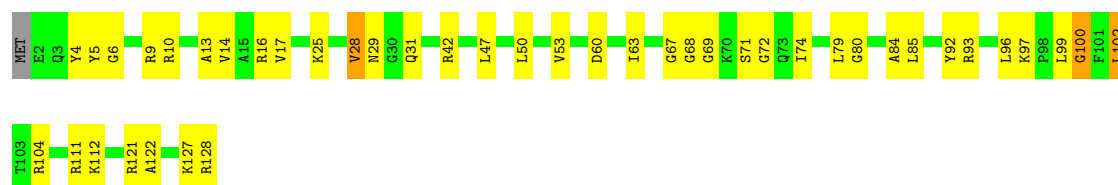
- Molecule 39: 30S ribosomal protein S8

Chain XH:  83% 17% .



- Molecule 40: 30S ribosomal protein S9

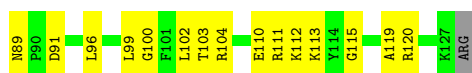
Chain QI:  66% 31% ..



- Molecule 40: 30S ribosomal protein S9

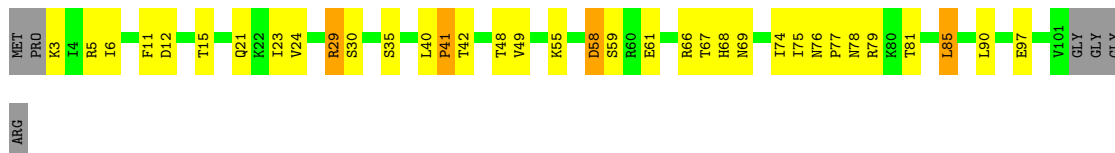
Chain XI:  59% 34% 6% .





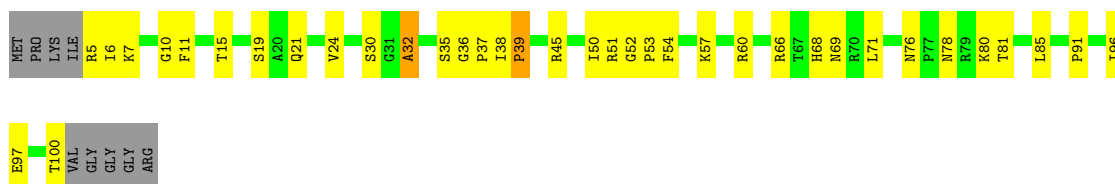
- Molecule 41: 30S ribosomal protein S10

Chain QJ: 61% 30% 6%



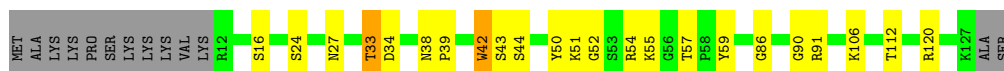
- Molecule 41: 30S ribosomal protein S10

Chain XJ: 56% 33% 9%



- Molecule 42: 30S ribosomal protein S11

Chain QK: 72% 16% 10%



- Molecule 42: 30S ribosomal protein S11

Chain XK: 73% 17% 10%



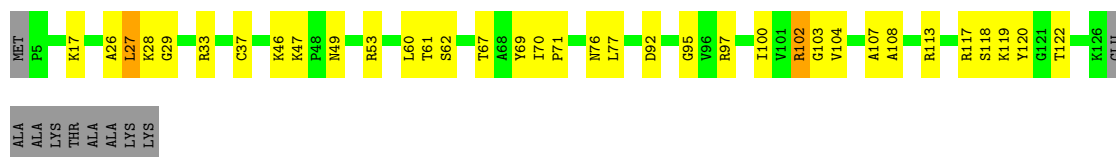
- Molecule 43: 30S ribosomal protein S12

Chain QL: 70% 24% 5%

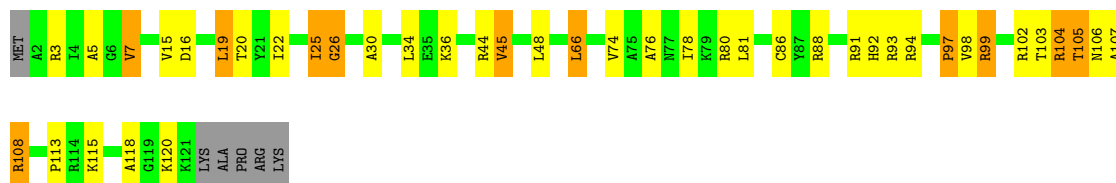


- Molecule 43: 30S ribosomal protein S12

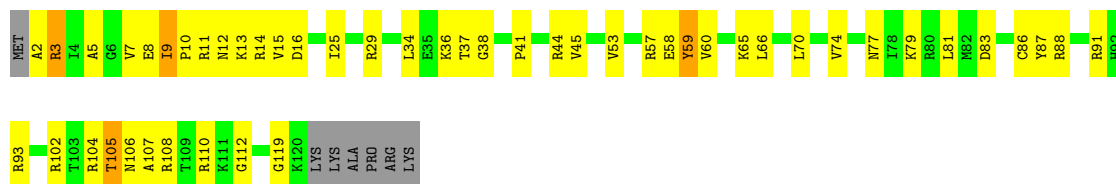
Chain XL: 66% 25% 8%



- Molecule 44: 30S ribosomal protein S13



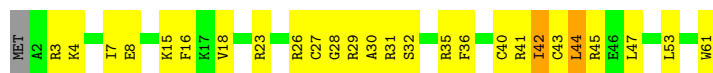
- Molecule 44: 30S ribosomal protein S13



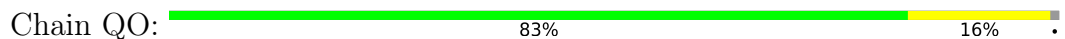
- Molecule 45: 30S ribosomal protein S14 type Z




- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15

Chain XO:  73% 24% ..



- Molecule 47: 30S ribosomal protein S16

Chain QP:  70% 24% • 5%




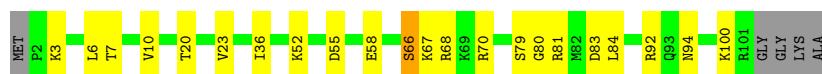
- Molecule 47: 30S ribosomal protein S16

Chain XP:  70% 23% • 5%



- Molecule 48: 30S ribosomal protein S17

Chain QQ:  74% 20% • 5%



- Molecule 48: 30S ribosomal protein S17

Chain XQ:  71% 23% • 5%



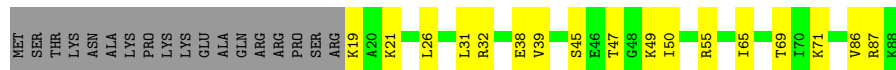
- Molecule 49: 30S ribosomal protein S18

Chain QR:  61% 18% 20%



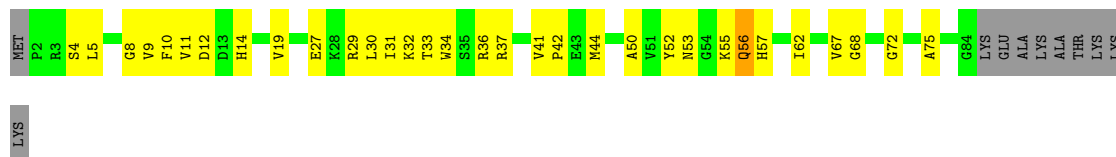
- Molecule 49: 30S ribosomal protein S18

Chain XR:  60% 19% 20%



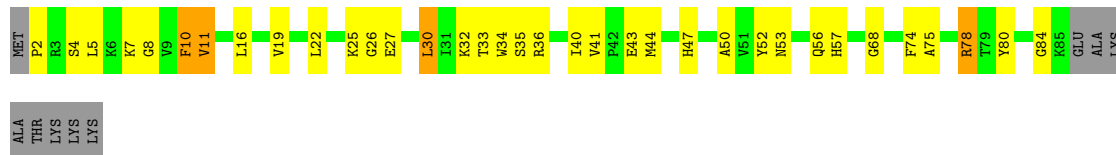
- Molecule 50: 30S ribosomal protein S19

Chain QS:  55% 33% 11%



- Molecule 50: 30S ribosomal protein S19

Chain XS:  53% 33% 10%



- Molecule 51: 30S ribosomal protein S20

Chain QT:  68% 23% 7%



- Molecule 51: 30S ribosomal protein S20

Chain XT:  62% 28% 7%



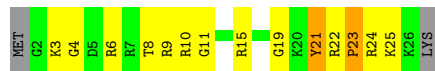
- Molecule 52: 30S ribosomal protein Thx

Chain QU:  56% 22% 11% 7%



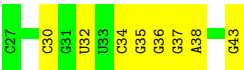
- Molecule 52: 30S ribosomal protein Thx

Chain XU:  41% 44% 7% 7%



- Molecule 53: P-site ASLPro

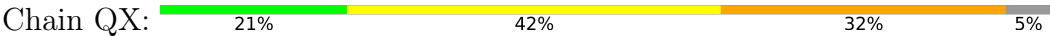
Chain QV:  53% 47%



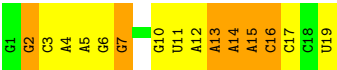
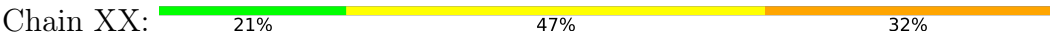
● Molecule 53: P-site ASLPro



● Molecule 54: mRNA



● Molecule 54: mRNA



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	210.12Å 451.80Å 622.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	188.68 – 3.40	Depositor
% Data completeness (in resolution range)	98.8 (188.68-3.40)	Depositor
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.198 , 0.237	Depositor
Wilson B-factor (Å ²)	79.0	Xtriage
Anisotropy	0.210	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	290035	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% 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: 1MG, MG, SF4, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	RA	1.16	19/69498 (0.0%)	1.25	634/108491 (0.6%)
1	YA	1.43	115/69543 (0.2%)	1.33	828/108563 (0.8%)
2	RB	0.85	0/2878	1.24	33/4490 (0.7%)
2	YB	1.23	0/2878	1.34	43/4490 (1.0%)
3	RD	0.68	0/2165	0.60	0/2919
3	YD	0.80	0/2176	0.63	0/2933
4	RE	0.66	0/1596	0.60	0/2153
4	YE	0.77	0/1601	0.68	0/2160
5	RF	0.64	0/1620	0.59	0/2194
5	YF	0.79	1/1620 (0.1%)	0.63	0/2194
6	RG	0.36	0/1499	0.64	1/2016 (0.0%)
6	YG	0.45	0/1499	0.60	0/2016
7	RH	0.44	0/1362	0.59	0/1841
7	YH	0.63	0/1362	0.56	0/1841
8	RI	0.48	0/1151	0.68	0/1558
8	YI	0.47	0/1151	0.66	0/1558
9	RN	0.59	0/1131	0.58	0/1525
9	YN	0.73	1/1148 (0.1%)	0.61	0/1547
10	RO	0.67	0/943	0.60	0/1269
10	YO	0.77	0/943	0.63	0/1269
11	RP	0.56	0/1147	0.68	1/1525 (0.1%)
11	YP	0.70	0/1139	0.70	1/1514 (0.1%)
12	RQ	0.59	1/1143 (0.1%)	0.65	0/1527
12	YQ	0.75	0/1143	0.60	0/1527
13	RR	0.58	0/982	0.65	1/1312 (0.1%)
13	YR	0.70	0/974	0.69	0/1302
14	RS	0.43	0/892	0.68	1/1187 (0.1%)
14	YS	0.61	0/887	0.57	0/1180
15	RT	0.58	0/1155	0.64	2/1542 (0.1%)
15	YT	0.65	0/1155	0.55	0/1542
16	RU	0.61	0/982	0.57	0/1306
16	YU	0.83	0/982	0.63	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	RV	0.54	0/790	0.58	0/1057
17	YV	0.77	0/790	0.66	0/1057
18	RW	0.66	0/911	0.56	0/1220
18	YW	0.80	0/911	0.60	0/1220
19	RX	0.60	0/739	0.60	0/993
19	YX	0.76	0/756	0.64	0/1014
20	RY	0.55	0/831	0.52	0/1108
20	YY	0.72	1/831 (0.1%)	0.56	0/1108
21	RZ	0.45	0/1634	0.65	1/2216 (0.0%)
21	YZ	0.57	0/1620	0.55	0/2197
22	R0	0.56	0/611	0.58	0/814
22	Y0	0.76	0/607	0.60	0/809
23	R1	0.58	0/770	0.61	0/1022
23	Y1	0.70	0/736	0.57	0/978
24	R2	0.41	0/583	0.49	0/771
24	Y2	0.57	0/608	0.52	0/803
25	R3	0.52	0/474	0.54	0/635
25	Y3	0.66	0/474	0.62	0/635
26	R4	0.35	0/578	0.59	0/776
26	Y4	0.38	0/578	0.67	0/776
27	R5	0.70	0/473	0.57	0/639
27	Y5	0.80	0/473	0.62	1/639 (0.2%)
28	R6	0.57	0/460	0.56	0/613
28	Y6	0.71	0/460	0.63	0/613
29	R7	0.69	0/417	0.52	0/550
29	Y7	0.85	1/426 (0.2%)	0.58	0/561
30	R8	0.57	0/525	0.62	0/691
30	Y8	0.71	0/525	0.65	0/691
31	R9	0.54	0/305	0.48	0/402
31	Y9	0.71	0/310	0.52	0/407
32	QA	0.87	1/36343 (0.0%)	1.17	200/56720 (0.4%)
32	XA	0.88	0/36346	1.17	213/56725 (0.4%)
33	QB	0.39	0/1942	0.62	1/2619 (0.0%)
33	XB	0.39	0/1950	0.58	0/2630
34	QC	0.35	0/1629	0.62	0/2195
34	XC	0.35	0/1629	0.57	0/2195
35	QD	0.51	0/1733	0.55	0/2318
35	XD	0.47	0/1733	0.56	0/2318
36	QE	0.45	0/1171	0.58	0/1576
36	XE	0.46	0/1171	0.54	0/1576
37	QF	0.48	0/856	0.56	0/1154
37	XF	0.46	0/856	0.52	0/1154
38	QG	0.33	0/1276	0.56	0/1709

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	XG	0.34	0/1276	0.53	0/1709
39	QH	0.51	0/1128	0.56	0/1517
39	XH	0.48	0/1128	0.57	0/1517
40	QI	0.32	0/1029	0.63	2/1379 (0.1%)
40	XI	0.34	0/1017	0.63	1/1365 (0.1%)
41	QJ	0.35	0/814	0.61	0/1095
41	XJ	0.32	0/790	0.53	0/1063
42	QK	0.44	0/879	0.54	0/1187
42	XK	0.44	0/879	0.53	0/1187
43	QL	0.56	0/991	0.59	0/1327
43	XL	0.51	0/972	0.62	0/1301
44	QM	0.36	0/965	0.64	1/1292 (0.1%)
44	XM	0.37	0/956	0.67	0/1281
45	QN	0.41	0/501	0.68	1/664 (0.2%)
45	XN	0.40	0/501	0.61	1/664 (0.2%)
46	QO	0.42	0/745	0.55	0/992
46	XO	0.44	0/740	0.47	0/987
47	QP	0.49	0/721	0.56	0/970
47	XP	0.44	0/721	0.57	0/970
48	QQ	0.51	0/847	0.55	0/1131
48	XQ	0.49	0/847	0.58	0/1131
49	QR	0.45	0/579	0.62	0/768
49	XR	0.44	0/579	0.60	0/768
50	QS	0.30	0/680	0.56	0/915
50	XS	0.31	0/689	0.65	2/926 (0.2%)
51	QT	0.39	0/765	0.52	0/1007
51	XT	0.35	0/765	0.52	0/1007
52	QU	0.34	0/221	0.66	0/288
52	XU	0.36	0/221	0.62	0/288
53	QV	0.55	0/380	1.09	2/590 (0.3%)
53	XV	0.56	0/332	1.15	5/515 (1.0%)
54	QX	0.61	0/436	1.06	1/678 (0.1%)
54	XX	0.52	0/462	1.17	5/719 (0.7%)
All	All	1.02	140/313742 (0.0%)	1.11	1982/468899 (0.4%)

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
3	RD	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	YD	0	10
4	RE	0	10
4	YE	0	13
5	RF	0	13
5	YF	0	9
6	RG	0	17
6	YG	0	18
7	RH	0	24
7	YH	0	5
8	RI	0	13
8	YI	0	18
9	RN	0	10
9	YN	0	6
10	RO	0	2
10	YO	0	2
11	RP	0	19
11	YP	0	18
12	RQ	0	11
12	YQ	0	8
13	RR	0	6
13	YR	0	5
14	RS	0	8
14	YS	0	2
15	RT	0	6
15	YT	0	4
16	RU	0	3
16	YU	0	5
17	RV	0	8
17	YV	0	4
18	RW	0	5
18	YW	0	5
19	RX	0	5
19	YX	0	4
20	RY	0	5
20	YY	0	2
21	RZ	0	22
21	YZ	0	9
22	R0	0	2
22	Y0	0	3
23	R1	0	6
23	Y1	0	2
24	R2	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	R3	0	3
25	Y3	0	1
26	R4	0	10
26	Y4	0	12
27	R5	0	1
27	Y5	0	2
29	R7	0	2
30	R8	0	7
30	Y8	0	4
31	Y9	0	1
33	QB	0	21
33	XB	0	18
34	QC	0	14
34	XC	0	17
35	QD	0	13
35	XD	0	13
36	QE	0	5
36	XE	0	5
37	QF	0	2
37	XF	0	1
38	QG	0	9
38	XG	0	6
39	QH	0	4
39	XH	0	8
40	QI	0	11
40	XI	0	19
41	QJ	0	6
41	XJ	0	9
42	QK	0	4
42	XK	0	5
43	QL	0	8
43	XL	0	12
44	QM	0	17
44	XM	0	14
45	QN	0	6
45	XN	0	5
46	QO	0	2
46	XO	0	3
47	QP	0	6
47	XP	0	7
48	QQ	0	2
48	XQ	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
49	QR	0	4
49	XR	0	4
50	QS	0	11
50	XS	0	14
51	QT	0	13
51	XT	0	13
52	QU	0	3
52	XU	0	5
All	All	0	749

The worst 5 of 140 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	YA	528	A	N9-C4	-9.09	1.32	1.37
1	YA	1021	A	N9-C4	-8.37	1.32	1.37
1	YA	1142(A)	A	N9-C4	-8.06	1.33	1.37
1	YA	676	A	N9-C4	-7.65	1.33	1.37
1	YA	1783	A	N9-C4	-6.76	1.33	1.37

The worst 5 of 1982 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	856	C	C6-N1-C2	-13.93	114.73	120.30
1	YA	856	C	C5-C6-N1	13.46	127.73	121.00
1	YA	1535	U	N1-C2-O2	13.33	132.13	122.80
1	RA	856	C	C6-N1-C2	-13.11	115.06	120.30
1	YA	2868	A	N7-C8-N9	12.59	120.10	113.80

There are no chirality outliers.

5 of 749 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	RD	119	ALA	Peptide
3	RD	120	GLY	Peptide
3	RD	126	GLN	Peptide
3	RD	2	ALA	Peptide
3	RD	246	PRO	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	RA	62051	0	31279	531	1
1	YA	62091	0	31300	497	0
2	RB	2573	0	1306	25	0
2	YB	2573	0	1306	16	0
3	RD	2115	0	2195	31	0
3	YD	2126	0	2208	39	0
4	RE	1563	0	1629	28	0
4	YE	1568	0	1633	30	0
5	RF	1585	0	1632	21	0
5	YF	1585	0	1632	28	0
6	RG	1474	0	1535	38	0
6	YG	1474	0	1535	26	0
7	RH	1336	0	1418	21	0
7	YH	1336	0	1418	23	1
8	RI	1136	0	1223	35	2
8	YI	1136	0	1223	21	0
9	RN	1104	0	1179	14	0
9	YN	1121	0	1194	16	0
10	RO	933	0	996	22	0
10	YO	933	0	995	14	0
11	RP	1130	0	1217	26	0
11	YP	1122	0	1206	23	0
12	RQ	1122	0	1178	48	0
12	YQ	1122	0	1179	16	0
13	RR	968	0	1033	10	0
13	YR	960	0	1021	10	0
14	RS	882	0	943	13	0
14	YS	877	0	938	9	0
15	RT	1141	0	1202	15	0
15	YT	1141	0	1202	11	0
16	RU	964	0	1022	21	0
16	YU	964	0	1022	19	0
17	RV	779	0	852	12	0
17	YV	779	0	852	17	0
18	RW	900	0	964	16	1
18	YW	900	0	964	12	0
19	RX	725	0	778	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	YX	742	0	803	9	0
20	RY	818	0	909	11	0
20	YY	818	0	909	9	2
21	RZ	1601	0	1630	43	0
21	YZ	1587	0	1622	16	0
22	R0	603	0	619	7	0
22	Y0	599	0	617	9	0
23	R1	763	0	848	10	0
23	Y1	729	0	802	12	0
24	R2	581	0	629	9	0
24	Y2	606	0	665	5	1
25	R3	469	0	518	7	0
25	Y3	469	0	518	12	0
26	R4	565	0	557	11	0
26	Y4	565	0	557	16	0
27	R5	459	0	476	10	0
27	Y5	459	0	476	9	0
28	R6	453	0	473	3	0
28	Y6	453	0	473	3	0
29	R7	409	0	454	6	0
29	Y7	418	0	466	4	0
30	R8	517	0	582	12	0
30	Y8	517	0	582	15	0
31	R9	302	0	332	7	0
31	Y9	307	0	335	9	0
32	QA	32469	0	16393	418	0
32	XA	32471	0	16393	441	2
33	QB	1907	0	1958	36	0
33	XB	1915	0	1969	28	0
34	QC	1605	0	1668	27	0
34	XC	1605	0	1668	28	0
35	QD	1703	0	1763	63	0
35	XD	1703	0	1764	50	0
36	QE	1155	0	1213	18	0
36	XE	1155	0	1213	11	0
37	QF	843	0	857	16	0
37	XF	843	0	857	13	0
38	QG	1257	0	1296	20	0
38	XG	1257	0	1296	24	0
39	QH	1108	0	1165	17	0
39	XH	1108	0	1165	11	0
40	QI	1010	0	1037	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	XI	998	0	1024	28	0
41	QJ	801	0	849	21	0
41	XJ	777	0	816	24	0
42	QK	864	0	881	15	0
42	XK	864	0	881	12	0
43	QL	975	0	1062	18	0
43	XL	956	0	1046	18	0
44	QM	955	0	1021	25	0
44	XM	946	0	1008	32	0
45	QN	492	0	529	10	0
45	XN	492	0	529	17	0
46	QO	734	0	771	11	0
46	XO	729	0	768	14	0
47	QP	705	0	725	12	0
47	XP	705	0	725	11	0
48	QQ	834	0	904	16	0
48	XQ	834	0	904	15	0
49	QR	574	0	644	9	0
49	XR	574	0	644	9	0
50	QS	665	0	686	16	0
50	XS	674	0	699	16	0
51	QT	763	0	861	12	0
51	XT	763	0	861	16	0
52	QU	217	0	234	9	0
52	XU	217	0	234	10	0
53	QV	365	0	186	5	0
53	XV	322	0	164	6	0
54	QX	389	0	197	27	0
54	XX	412	0	208	12	0
55	QA	66	0	0	0	0
55	QF	1	0	0	0	0
55	R0	1	0	0	0	0
55	R1	1	0	0	0	0
55	R5	1	0	0	0	0
55	R8	1	0	0	0	0
55	RA	485	0	0	0	0
55	RB	8	0	0	0	0
55	RE	2	0	0	0	0
55	RF	1	0	0	0	0
55	RN	1	0	0	0	0
55	RO	1	0	0	0	0
55	RP	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	RQ	2	0	0	0	0
55	RT	1	0	0	0	0
55	RX	1	0	0	0	0
55	XA	87	0	0	0	0
55	XE	1	0	0	0	0
55	XL	1	0	0	0	0
55	XQ	1	0	0	0	0
55	XS	1	0	0	0	0
55	Y0	2	0	0	0	0
55	Y1	1	0	0	0	0
55	Y5	1	0	0	0	0
55	Y7	1	0	0	0	0
55	Y8	1	0	0	0	0
55	YA	510	0	0	0	0
55	YB	7	0	0	0	0
55	YD	1	0	0	0	0
55	YE	4	0	0	0	0
55	YO	1	0	0	0	0
55	YP	2	0	0	0	0
55	YQ	1	0	0	0	0
55	YR	1	0	0	0	0
56	QN	1	0	0	0	0
56	R4	1	0	0	0	0
56	R5	1	0	0	0	0
56	R6	1	0	0	0	0
56	R9	1	0	0	0	0
56	RY	1	0	0	0	0
56	XN	1	0	0	0	0
56	Y4	1	0	0	0	0
56	Y5	1	0	0	0	0
56	Y6	1	0	0	0	0
56	Y9	1	0	0	0	0
56	YY	1	0	0	0	0
57	QD	8	0	0	1	0
57	XD	8	0	0	3	0
All	All	290035	0	196997	3129	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 3129 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)
32:QA:1535:C:N4	54:QX:9:G:C2	1.91	1.37
32:QA:1535:C:N4	54:QX:9:G:N2	1.78	1.30
17:YV:49:THR:OG1	17:YV:50:PRO:HD2	1.30	1.25
21:RZ:182:LYS:O	21:RZ:186:GLU:HG2	1.39	1.22
32:QA:1535:C:C4	54:QX:9:G:N2	2.07	1.22

All (5) 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)
1:RA:307:G:O6	24:Y2:71:ASN:O[3_555]	1.47	0.73
7:YH:46:GLU:CB	20:YY:22:GLY:O[4_445]	1.82	0.38
8:RI:82:ARG:NH1	32:XA:56:U:O2'[4_555]	2.05	0.15
8:RI:91:SER:OG	32:XA:368:U:OP1[4_555]	2.07	0.13
18:RW:63:ASP:OD1	20:YY:92:ASN:ND2[3_555]	2.08	0.12

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	RD	270/276 (98%)	257 (95%)	13 (5%)	0	100	100
3	YD	271/276 (98%)	261 (96%)	10 (4%)	0	100	100
4	RE	202/206 (98%)	190 (94%)	12 (6%)	0	100	100
4	YE	203/206 (98%)	170 (84%)	32 (16%)	1 (0%)	29	61
5	RF	200/210 (95%)	191 (96%)	9 (4%)	0	100	100
5	YF	200/210 (95%)	182 (91%)	18 (9%)	0	100	100
6	RG	179/182 (98%)	153 (86%)	25 (14%)	1 (1%)	25	57
6	YG	179/182 (98%)	151 (84%)	27 (15%)	1 (1%)	25	57
7	RH	172/180 (96%)	149 (87%)	21 (12%)	2 (1%)	13	41
7	YH	172/180 (96%)	164 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	RI	144/148 (97%)	119 (83%)	24 (17%)	1 (1%)	22	55
8	YI	144/148 (97%)	122 (85%)	22 (15%)	0	100	100
9	RN	136/140 (97%)	121 (89%)	15 (11%)	0	100	100
9	YN	138/140 (99%)	125 (91%)	12 (9%)	1 (1%)	22	55
10	RO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	RP	146/150 (97%)	122 (84%)	24 (16%)	0	100	100
11	YP	145/150 (97%)	129 (89%)	15 (10%)	1 (1%)	22	55
12	RQ	139/141 (99%)	120 (86%)	18 (13%)	1 (1%)	22	55
12	YQ	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
13	RR	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
13	YR	115/118 (98%)	106 (92%)	9 (8%)	0	100	100
14	RS	109/112 (97%)	91 (84%)	18 (16%)	0	100	100
14	YS	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
15	RT	135/146 (92%)	121 (90%)	14 (10%)	0	100	100
15	YT	135/146 (92%)	127 (94%)	8 (6%)	0	100	100
16	RU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	49
16	YU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	49
17	RV	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
17	YV	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	15	46
18	RW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
18	YW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
19	RX	90/96 (94%)	85 (94%)	5 (6%)	0	100	100
19	YX	92/96 (96%)	84 (91%)	8 (9%)	0	100	100
20	RY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
20	YY	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
21	RZ	201/206 (98%)	180 (90%)	20 (10%)	1 (0%)	29	61
21	YZ	199/206 (97%)	188 (94%)	9 (4%)	2 (1%)	15	46
22	R0	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
22	Y0	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
23	R1	95/98 (97%)	83 (87%)	12 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	Y1	91/98 (93%)	91 (100%)	0	0	100	100
24	R2	67/72 (93%)	64 (96%)	3 (4%)	0	100	100
24	Y2	70/72 (97%)	69 (99%)	1 (1%)	0	100	100
25	R3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
25	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	R4	67/71 (94%)	56 (84%)	11 (16%)	0	100	100
26	Y4	67/71 (94%)	58 (87%)	9 (13%)	0	100	100
27	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	Y5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	R7	45/49 (92%)	45 (100%)	0	0	100	100
29	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	R8	62/65 (95%)	54 (87%)	8 (13%)	0	100	100
30	Y8	62/65 (95%)	56 (90%)	6 (10%)	0	100	100
31	R9	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
31	Y9	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
33	QB	233/256 (91%)	201 (86%)	32 (14%)	0	100	100
33	XB	234/256 (91%)	205 (88%)	29 (12%)	0	100	100
34	QC	203/239 (85%)	187 (92%)	16 (8%)	0	100	100
34	XC	203/239 (85%)	186 (92%)	17 (8%)	0	100	100
35	QD	206/209 (99%)	191 (93%)	13 (6%)	2 (1%)	15	46
35	XD	206/209 (99%)	191 (93%)	13 (6%)	2 (1%)	15	46
36	QE	149/162 (92%)	139 (93%)	10 (7%)	0	100	100
36	XE	149/162 (92%)	135 (91%)	14 (9%)	0	100	100
37	QF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
37	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
38	QG	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
38	XG	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
39	QH	135/138 (98%)	123 (91%)	12 (9%)	0	100	100
39	XH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	QI	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
40	XI	124/128 (97%)	110 (89%)	14 (11%)	0	100	100
41	QJ	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
41	XJ	94/105 (90%)	84 (89%)	10 (11%)	0	100	100
42	QK	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
42	XK	114/129 (88%)	108 (95%)	6 (5%)	0	100	100
43	QL	123/132 (93%)	108 (88%)	15 (12%)	0	100	100
43	XL	120/132 (91%)	106 (88%)	14 (12%)	0	100	100
44	QM	118/126 (94%)	104 (88%)	13 (11%)	1 (1%)	19	51
44	XM	117/126 (93%)	105 (90%)	10 (8%)	2 (2%)	9	34
45	QN	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
45	XN	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
46	QO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	XO	85/89 (96%)	82 (96%)	3 (4%)	0	100	100
47	QP	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
47	XP	82/88 (93%)	75 (92%)	7 (8%)	0	100	100
48	QQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
48	XQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
49	QR	68/88 (77%)	62 (91%)	6 (9%)	0	100	100
49	XR	68/88 (77%)	64 (94%)	4 (6%)	0	100	100
50	QS	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
50	XS	82/93 (88%)	68 (83%)	13 (16%)	1 (1%)	13	41
51	QT	97/106 (92%)	89 (92%)	8 (8%)	0	100	100
51	XT	97/106 (92%)	86 (89%)	11 (11%)	0	100	100
52	QU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
52	XU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	11486/12128 (95%)	10518 (92%)	945 (8%)	23 (0%)	47	78

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	YV	49	THR
35	XD	32	ALA

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Mol	Chain	Res	Type
21	YZ	52	SER
16	RU	93	LYS
35	QD	32	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	RD	214/218 (98%)	214 (100%)	0	100	100
3	YD	215/218 (99%)	213 (99%)	2 (1%)	78	90
4	RE	165/166 (99%)	163 (99%)	2 (1%)	71	85
4	YE	165/166 (99%)	164 (99%)	1 (1%)	86	94
5	RF	161/166 (97%)	160 (99%)	1 (1%)	86	94
5	YF	161/166 (97%)	159 (99%)	2 (1%)	71	85
6	RG	155/156 (99%)	154 (99%)	1 (1%)	86	94
6	YG	155/156 (99%)	153 (99%)	2 (1%)	69	84
7	RH	145/148 (98%)	145 (100%)	0	100	100
7	YH	145/148 (98%)	143 (99%)	2 (1%)	67	83
8	RI	122/124 (98%)	109 (89%)	13 (11%)	6	24
8	YI	122/124 (98%)	121 (99%)	1 (1%)	81	91
9	RN	117/119 (98%)	116 (99%)	1 (1%)	78	90
9	YN	119/119 (100%)	118 (99%)	1 (1%)	81	91
10	RO	100/100 (100%)	100 (100%)	0	100	100
10	YO	100/100 (100%)	100 (100%)	0	100	100
11	RP	115/116 (99%)	113 (98%)	2 (2%)	60	80
11	YP	114/116 (98%)	113 (99%)	1 (1%)	78	90
12	RQ	111/111 (100%)	107 (96%)	4 (4%)	35	63
12	YQ	111/111 (100%)	109 (98%)	2 (2%)	59	79
13	RR	101/101 (100%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	YR	100/101 (99%)	100 (100%)	0	100	100
14	RS	87/88 (99%)	87 (100%)	0	100	100
14	YS	87/88 (99%)	87 (100%)	0	100	100
15	RT	120/127 (94%)	119 (99%)	1 (1%)	81	91
15	YT	120/127 (94%)	120 (100%)	0	100	100
16	RU	93/94 (99%)	93 (100%)	0	100	100
16	YU	93/94 (99%)	92 (99%)	1 (1%)	73	86
17	RV	82/82 (100%)	81 (99%)	1 (1%)	71	85
17	YV	82/82 (100%)	82 (100%)	0	100	100
18	RW	92/92 (100%)	92 (100%)	0	100	100
18	YW	92/92 (100%)	92 (100%)	0	100	100
19	RX	74/78 (95%)	73 (99%)	1 (1%)	67	83
19	YX	76/78 (97%)	73 (96%)	3 (4%)	32	61
20	RY	88/91 (97%)	88 (100%)	0	100	100
20	YY	88/91 (97%)	87 (99%)	1 (1%)	73	86
21	RZ	174/179 (97%)	169 (97%)	5 (3%)	42	69
21	YZ	173/179 (97%)	171 (99%)	2 (1%)	71	85
22	R0	61/67 (91%)	60 (98%)	1 (2%)	62	81
22	Y0	61/67 (91%)	60 (98%)	1 (2%)	62	81
23	R1	82/83 (99%)	82 (100%)	0	100	100
23	Y1	78/83 (94%)	78 (100%)	0	100	100
24	R2	64/67 (96%)	64 (100%)	0	100	100
24	Y2	67/67 (100%)	67 (100%)	0	100	100
25	R3	51/52 (98%)	49 (96%)	2 (4%)	32	61
25	Y3	51/52 (98%)	50 (98%)	1 (2%)	55	77
26	R4	62/63 (98%)	60 (97%)	2 (3%)	39	67
26	Y4	62/63 (98%)	62 (100%)	0	100	100
27	R5	51/52 (98%)	51 (100%)	0	100	100
27	Y5	51/52 (98%)	51 (100%)	0	100	100
28	R6	51/52 (98%)	51 (100%)	0	100	100
28	Y6	51/52 (98%)	49 (96%)	2 (4%)	32	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	R7	40/42 (95%)	40 (100%)	0	100	100
29	Y7	41/42 (98%)	41 (100%)	0	100	100
30	R8	54/55 (98%)	53 (98%)	1 (2%)	57	78
30	Y8	54/55 (98%)	54 (100%)	0	100	100
31	R9	34/34 (100%)	34 (100%)	0	100	100
31	Y9	34/34 (100%)	34 (100%)	0	100	100
33	QB	203/220 (92%)	201 (99%)	2 (1%)	76	88
33	XB	204/220 (93%)	204 (100%)	0	100	100
34	QC	159/188 (85%)	159 (100%)	0	100	100
34	XC	159/188 (85%)	157 (99%)	2 (1%)	69	84
35	QD	180/181 (99%)	178 (99%)	2 (1%)	73	86
35	XD	180/181 (99%)	173 (96%)	7 (4%)	32	61
36	QE	116/123 (94%)	113 (97%)	3 (3%)	46	72
36	XE	116/123 (94%)	115 (99%)	1 (1%)	78	90
37	QF	90/90 (100%)	90 (100%)	0	100	100
37	XF	90/90 (100%)	90 (100%)	0	100	100
38	QG	126/127 (99%)	124 (98%)	2 (2%)	62	81
38	XG	126/127 (99%)	124 (98%)	2 (2%)	62	81
39	QH	118/119 (99%)	118 (100%)	0	100	100
39	XH	118/119 (99%)	118 (100%)	0	100	100
40	QI	98/99 (99%)	97 (99%)	1 (1%)	76	88
40	XI	97/99 (98%)	97 (100%)	0	100	100
41	QJ	89/92 (97%)	86 (97%)	3 (3%)	37	65
41	XJ	86/92 (94%)	85 (99%)	1 (1%)	71	85
42	QK	88/99 (89%)	87 (99%)	1 (1%)	73	86
42	XK	88/99 (89%)	88 (100%)	0	100	100
43	QL	104/109 (95%)	104 (100%)	0	100	100
43	XL	103/109 (94%)	103 (100%)	0	100	100
44	QM	96/101 (95%)	93 (97%)	3 (3%)	40	68
44	XM	95/101 (94%)	92 (97%)	3 (3%)	39	67
45	QN	49/50 (98%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	XN	49/50 (98%)	49 (100%)	0	100	100
46	QO	79/80 (99%)	78 (99%)	1 (1%)	69	84
46	XO	79/80 (99%)	79 (100%)	0	100	100
47	QP	72/74 (97%)	70 (97%)	2 (3%)	43	70
47	XP	72/74 (97%)	70 (97%)	2 (3%)	43	70
48	QQ	95/97 (98%)	95 (100%)	0	100	100
48	XQ	95/97 (98%)	95 (100%)	0	100	100
49	QR	61/77 (79%)	61 (100%)	0	100	100
49	XR	61/77 (79%)	61 (100%)	0	100	100
50	QS	72/80 (90%)	72 (100%)	0	100	100
50	XS	73/80 (91%)	71 (97%)	2 (3%)	44	70
51	QT	76/82 (93%)	76 (100%)	0	100	100
51	XT	76/82 (93%)	76 (100%)	0	100	100
52	QU	20/22 (91%)	18 (90%)	2 (10%)	7	27
52	XU	20/22 (91%)	20 (100%)	0	100	100
All	All	9712/10066 (96%)	9607 (99%)	105 (1%)	73	86

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	QP	67	THR
11	YP	71	VAL
44	XM	7	VAL
52	QU	24	ARG
6	YG	33	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
41	QJ	69	ASN
6	YG	40	ASN
50	XS	83	HIS
39	XH	78	GLN
50	XS	53	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	RA	2877/2915 (98%)	581 (20%)	41 (1%)
1	YA	2880/2915 (98%)	558 (19%)	40 (1%)
2	RB	119/122 (97%)	19 (15%)	1 (0%)
2	YB	119/122 (97%)	23 (19%)	2 (1%)
32	QA	1510/1521 (99%)	292 (19%)	37 (2%)
32	XA	1509/1521 (99%)	277 (18%)	29 (1%)
53	QV	16/17 (94%)	1 (6%)	0
53	XV	14/17 (82%)	0	0
54	QX	17/19 (89%)	5 (29%)	1 (5%)
54	XX	18/19 (94%)	9 (50%)	1 (5%)
All	All	9079/9188 (98%)	1765 (19%)	152 (1%)

5 of 1765 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	RA	9	U
1	RA	15	G
1	RA	34	C
1	RA	35	G
1	RA	46	C

5 of 152 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	YA	2712	U
32	XA	992	U
1	YA	2867	G
32	XA	388	G
32	XA	1537	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	1MG	XV	37	53	18,26,27	0.66	0	19,39,42	1.00	2 (10%)
53	1MG	QV	37	53	18,26,27	0.67	0	19,39,42	1.09	3 (15%)

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
53	1MG	XV	37	53	-	0/3/25/26	0/3/3/3
53	1MG	QV	37	53	-	0/3/25/26	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
53	QV	37	1MG	C8-N7-C5	2.46	107.67	102.99
53	XV	37	1MG	C8-N7-C5	2.37	107.51	102.99
53	XV	37	1MG	C5-C6-N1	2.28	117.33	113.90
53	QV	37	1MG	C5-C6-N1	2.06	117.00	113.90
53	QV	37	1MG	CM1-N1-C6	2.04	120.35	117.55

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
53	XV	37	1MG	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1213 ligands modelled in this entry, 1211 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	35	0,12,12	-	-	-		
57	SF4	QD	301	35	0,12,12	-	-	-		

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	XD	301	SF4	3	0
57	QD	301	SF4	1	0

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.