



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 6, 2020 – 03:12 AM EDT

PDB ID : 6NTA
Title : Modified ASL proline bound to Thermus thermophilus 70S (cognate)
Authors : Hoffer, E.D.; Maehigashi, T.; Subaramanian, S.; Hong, S.; Dunham, C.M.
Deposited on : 2019-01-28
Resolution : 3.10 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) : 2.14.6

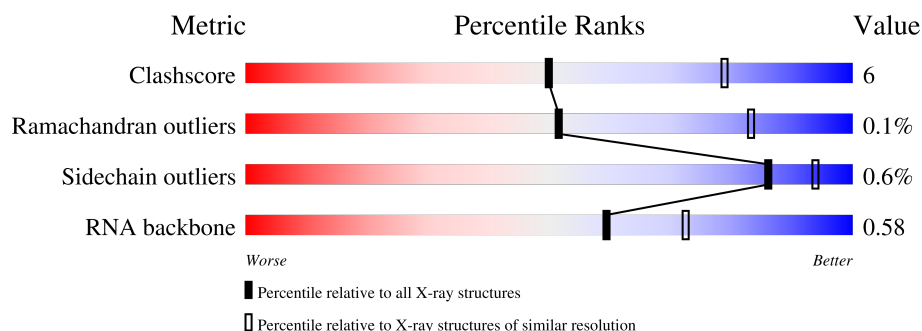
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)


























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	1521	56% 34% 8% ..
1	XA	1521	55% 35% 8% ..
2	QB	256	72% 18% • 8%
2	XB	256	69% 22% • 8%
3	QC	239	65% 20% • 14%
3	XC	239	60% 23% • 14%













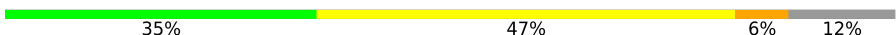
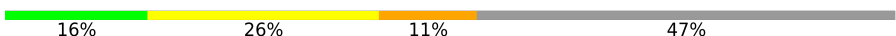











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Mol	Chain	Length	Quality of chain
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN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


























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Mol	Chain	Length	Quality of chain
16	XP	88	
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	17	
22	XV	17	
23	QX	19	
23	XX	19	
24	RA	2915	
24	YA	2915	
25	RB	122	
25	YB	122	
26	RD	276	
26	YD	276	
27	RE	206	
27	YE	206	
28	RF	210	
28	YF	210	

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Mol	Chain	Length	Quality of chain
29	RG	182	 66%31%..
29	YG	182	 77%20%...
30	RH	180	 75%19%..
30	YH	180	 85%11%..
31	RI	148	 78%19%..
31	YI	148	 79%15%5%.
32	RN	140	 76%22%.
32	YN	140	 78%19%..
33	RO	122	 72%27%.
33	YO	122	 82%18%
34	RP	150	 73%26%.
34	YP	150	 80%18%.
35	RQ	141	 67%30%.
35	YQ	141	 77%23%.
36	RR	118	 81%17%..
36	YR	118	 78%18%..
37	RS	112	 70%28%..
37	YS	112	 79%18%..
38	RT	146	 71%20%..6%
38	YT	146	 70%23%..6%
39	RU	118	 81%15%..
39	YU	118	 88%11%.
40	RV	101	 84%16%
40	YV	101	 89%11%
41	RW	113	 84%16%



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Mol	Chain	Length	Quality of chain
41	YW	113	
42	RX	96	
42	YX	96	
43	RY	110	
43	YY	110	
44	RZ	206	
44	YZ	206	
45	R0	85	
45	Y0	85	
46	R1	98	
46	Y1	98	
47	R2	72	
47	Y2	72	
48	R3	60	
48	Y3	60	
49	R4	71	
49	Y4	71	
50	R5	60	
50	Y5	60	
51	R6	54	
51	Y6	54	
52	R7	49	
52	Y7	49	
53	R8	65	
53	Y8	65	

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Mol	Chain	Length	Quality of chain	
54	R9	37		
54	Y9	37		

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 289311 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
			32247	14353	5981	10414	1499			
1	XA	1500	Total	C	N	O	P	0	0	0
			32249	14354	5984	10412	1499			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	XS	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			
20	XT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

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

- Molecule 22 is a RNA chain called P-site ASLPro.

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

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	10	Total	C	N	O	P	0	0	0
			217	97	43	67	10			
23	XX	12	Total	C	N	O	P	0	0	0
			262	117	53	80	12			

- Molecule 24 is a RNA chain called 23S rRNA.

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

- Molecule 25 is a RNA chain called 5S rRNA.

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

- Molecule 26 is a protein called 50S ribosomal protein L2.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L3.

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

- Molecule 28 is a protein called 50S ribosomal protein L4.

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

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

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
30	YH	173	Total	C	N	O	S	0	0	0
			1330	845	250	234	1			

- Molecule 31 is a protein called 50S ribosomal protein L9.

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

- Molecule 32 is a protein called 50S ribosomal protein L13.

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

- Molecule 33 is a protein called 50S ribosomal protein L14.

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

- Molecule 34 is a protein called 50S ribosomal protein L15.

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

- Molecule 35 is a protein called 50S ribosomal protein L16.

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

- Molecule 36 is a protein called 50S ribosomal protein L17.

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

- Molecule 37 is a protein called 50S ribosomal protein L18.

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

- Molecule 38 is a protein called 50S ribosomal protein L19.

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

- Molecule 39 is a protein called 50S ribosomal protein L20.

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

- Molecule 40 is a protein called 50S ribosomal protein L21.

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

- Molecule 41 is a protein called 50S ribosomal protein L22.

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

- Molecule 42 is a protein called 50S ribosomal protein L23.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L24.

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

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RZ	203	Total 1601	C 1020	N 283	O 295	S 3	0	0	0
44	YZ	203	Total 1601	C 1020	N 283	O 295	S 3	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L27.

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

- Molecule 46 is a protein called 50S ribosomal protein L28.

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

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
47	Y2	68	Total	C	N	O	S	0	0	0
			575	355	117	102	1			

- Molecule 48 is a protein called 50S ribosomal protein L30.

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

- Molecule 49 is a protein called 50S ribosomal protein L31.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

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

- Molecule 52 is a protein called 50S ribosomal protein L34.

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

- Molecule 53 is a protein called 50S ribosomal protein L35.

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

- Molecule 54 is a protein called 50S ribosomal protein L36.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	74	Total	Mg	0	0
			74	74		
55	RP	1	Total	Mg	0	0
			1	1		
55	YA	542	Total	Mg	0	0
			542	542		
55	QM	1	Total	Mg	0	0
			1	1		
55	YR	2	Total	Mg	0	0
			2	2		
55	RT	1	Total	Mg	0	0
			1	1		
55	RN	1	Total	Mg	0	0
			1	1		
55	XE	1	Total	Mg	0	0
			1	1		
55	XS	1	Total	Mg	0	0
			1	1		
55	Y1	1	Total	Mg	0	0
			1	1		
55	YD	3	Total	Mg	0	0
			3	3		
55	RX	1	Total	Mg	0	0
			1	1		
55	Y8	2	Total	Mg	0	0
			2	2		
55	YO	1	Total	Mg	0	0
			1	1		

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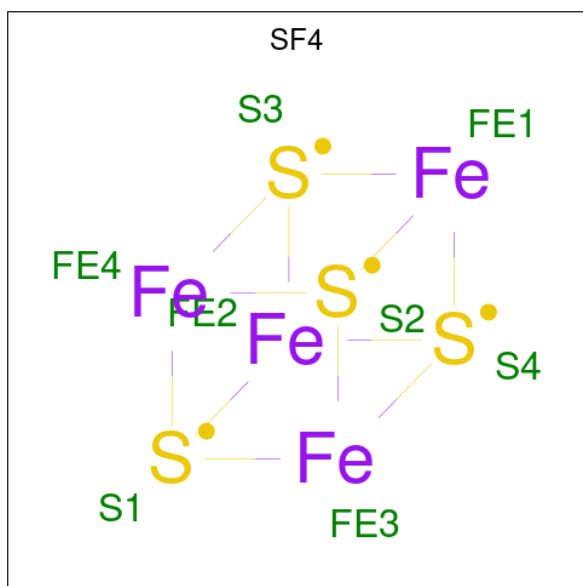
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	XA	92	Total 92	Mg 92	0	0
55	RQ	2	Total 2	Mg 2	0	0
55	R0	1	Total 1	Mg 1	0	0
55	RO	1	Total 1	Mg 1	0	0
55	QH	1	Total 1	Mg 1	0	0
55	YQ	3	Total 3	Mg 3	0	0
55	RY	1	Total 1	Mg 1	0	0
55	QC	1	Total 1	Mg 1	0	0
55	R8	1	Total 1	Mg 1	0	0
55	YX	2	Total 2	Mg 2	0	0
55	RR	2	Total 2	Mg 2	0	0
55	R1	2	Total 2	Mg 2	0	0
55	Y7	1	Total 1	Mg 1	0	0
55	QF	1	Total 1	Mg 1	0	0
55	XK	1	Total 1	Mg 1	0	0
55	Y0	2	Total 2	Mg 2	0	0
55	XQ	1	Total 1	Mg 1	0	0
55	RA	487	Total 487	Mg 487	0	0
55	Y5	1	Total 1	Mg 1	0	0
55	RE	4	Total 4	Mg 4	0	0
55	XL	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	YB	15	Total	Mg	0	0
			15	15		
55	XN	1	Total	Mg	0	0
			1	1		
55	RI	1	Total	Mg	0	0
			1	1		
55	RB	6	Total	Mg	0	0
			6	6		
55	RF	2	Total	Mg	0	0
			2	2		
55	XM	2	Total	Mg	0	0
			2	2		
55	YE	3	Total	Mg	0	0
			3	3		

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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

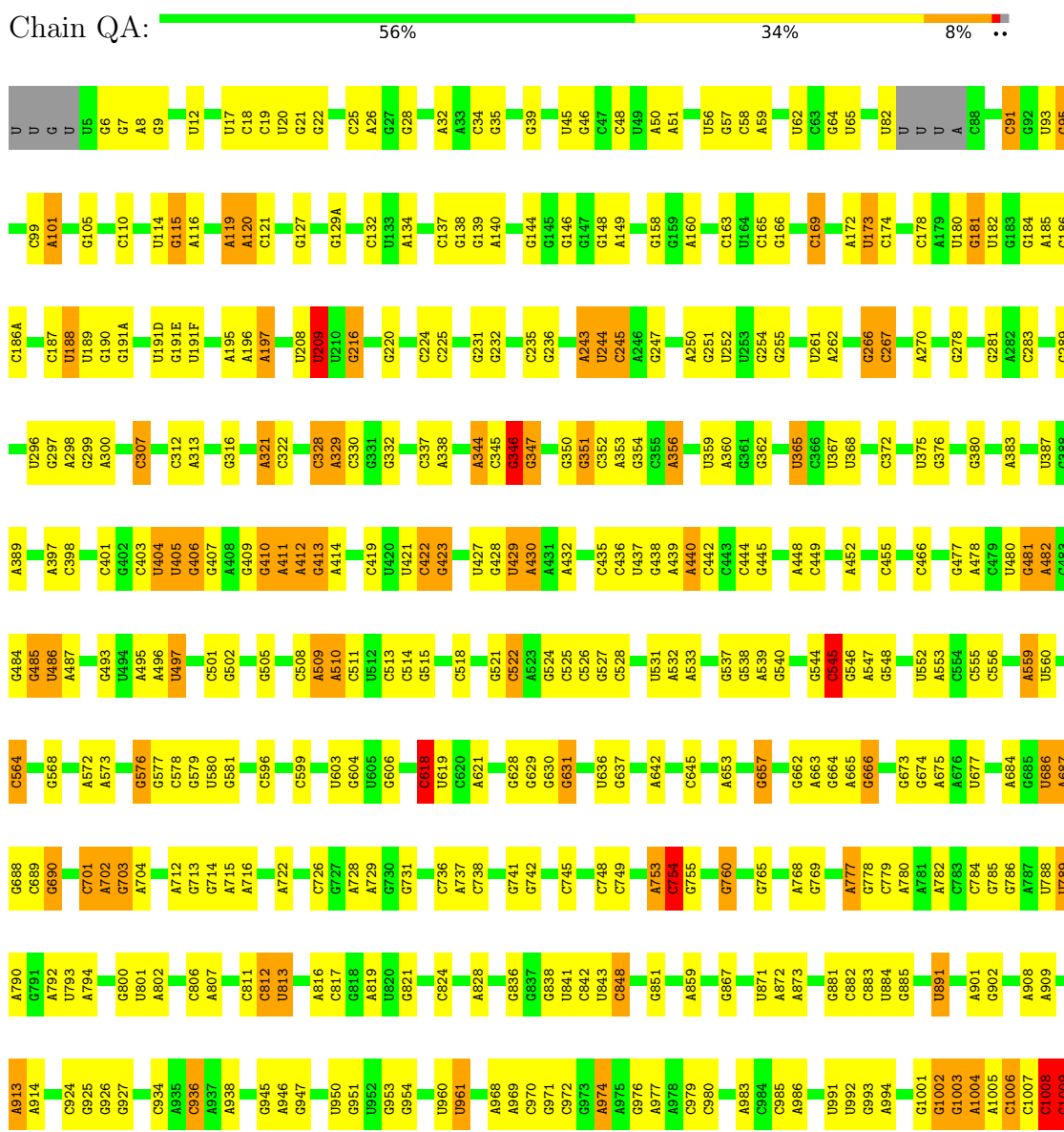
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y9	1	Total 1	Zn 1	0	0
57	YY	1	Total 1	Zn 1	0	0
57	Y6	1	Total 1	Zn 1	0	0
57	QN	1	Total 1	Zn 1	0	0
57	XN	1	Total 1	Zn 1	0	0
57	RY	1	Total 1	Zn 1	0	0
57	Y4	1	Total 1	Zn 1	0	0
57	R6	1	Total 1	Zn 1	0	0
57	Y5	1	Total 1	Zn 1	0	0
57	R5	1	Total 1	Zn 1	0	0
57	R4	1	Total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

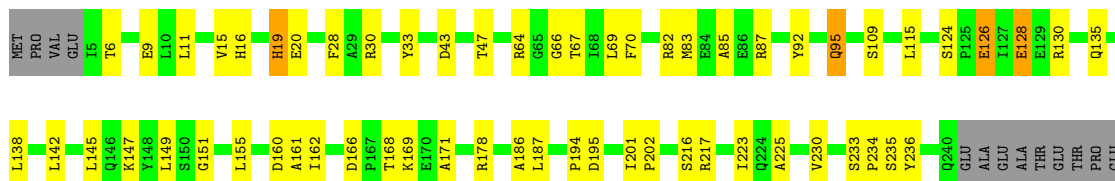
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

• Molecule 1: 16S rRNA

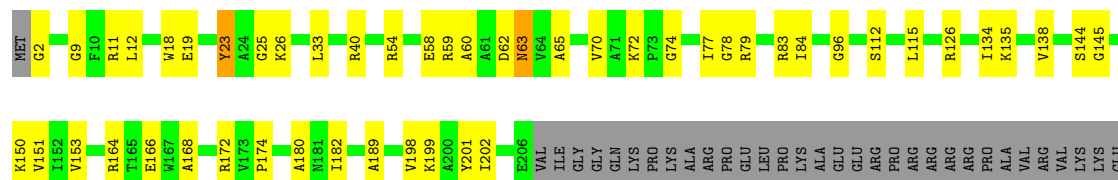




GLY
GLU
SER
GLU
VAL
GLU
ALA

- Molecule 3: 30S ribosomal protein S3

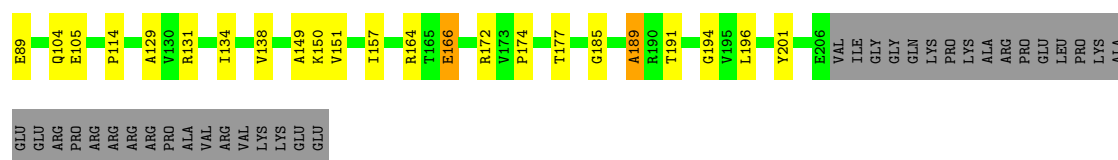
Chain QC:  65% 20% 14%




GLU

- Molecule 3: 30S ribosomal protein S3

Chain XC:  60% 23% 14%




- Molecule 4: 30S ribosomal protein S4

Chain QD:  72% 27% 1%




- Molecule 4: 30S ribosomal protein S4

Chain XD:  75% 23% 1%




- Molecule 5: 30S ribosomal protein S5

Chain QE:  77% 16% 7%




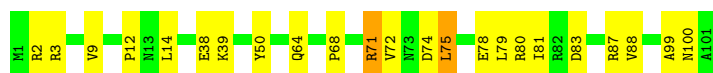
- Molecule 5: 30S ribosomal protein S5

Chain XE:  81% 12% 7%




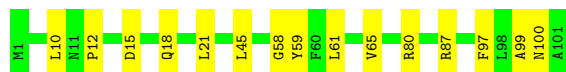
- Molecule 6: 30S ribosomal protein S6

Chain QF:  77% 21% 2%




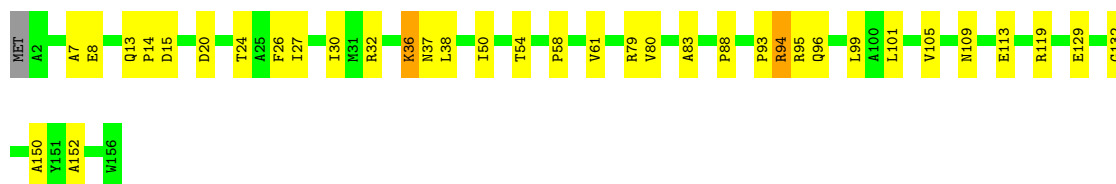
- Molecule 6: 30S ribosomal protein S6

Chain XF:  85% 15%




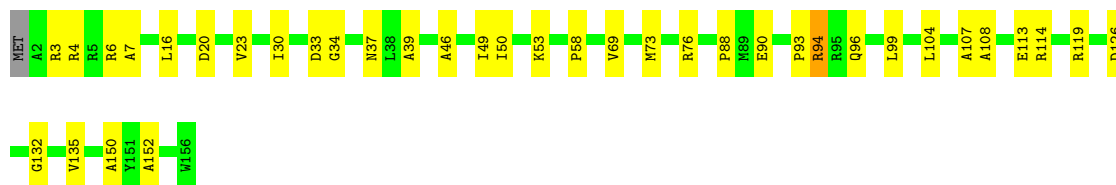
- Molecule 7: 30S ribosomal protein S7

Chain QG:  76% 22% 2%




- Molecule 7: 30S ribosomal protein S7

Chain XG:  76% 23% 1%



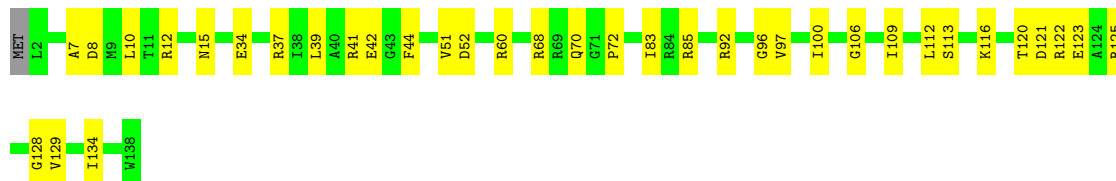
- Molecule 8: 30S ribosomal protein S8

Chain QH:  80% 20%



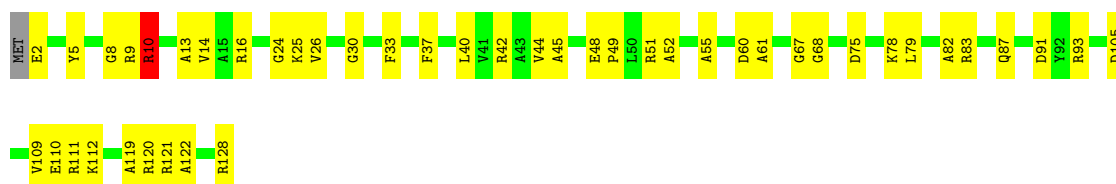
- Molecule 8: 30S ribosomal protein S8

Chain XH:  73% 26%



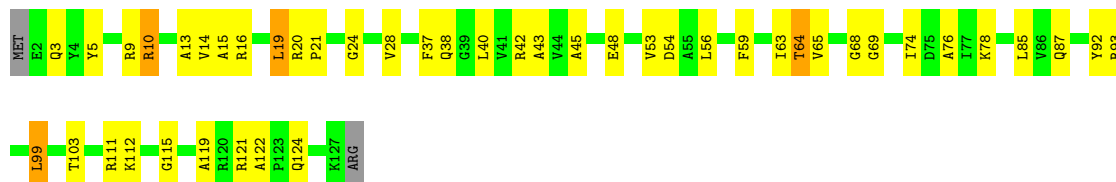
- Molecule 9: 30S ribosomal protein S9

Chain QI:  64% 34%



- Molecule 9: 30S ribosomal protein S9

Chain XI:  63% 32%



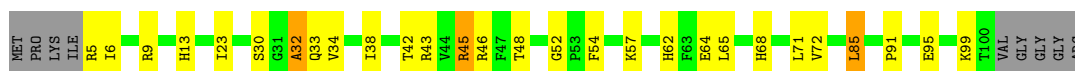
- Molecule 10: 30S ribosomal protein S10

Chain QJ:  66% 26% 6%

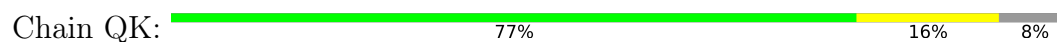


- Molecule 10: 30S ribosomal protein S10

Chain XJ:  65% 24% 9%



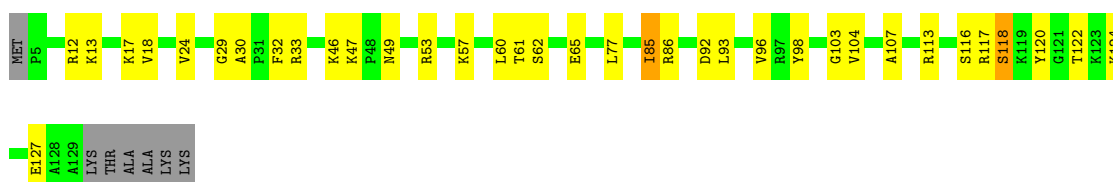
- Molecule 11: 30S ribosomal protein S11



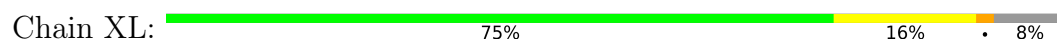
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12

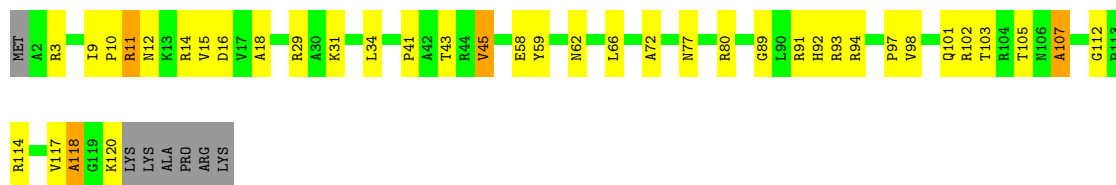


- Molecule 13: 30S ribosomal protein S13




- Molecule 13: 30S ribosomal protein S13

Chain XM:  63% 28% 6%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:  79% 18% ..




- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:  59% 36% ...



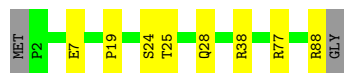
- Molecule 15: 30S ribosomal protein S15

Chain QO:  85% 13% .



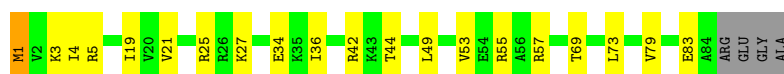
- Molecule 15: 30S ribosomal protein S15

Chain XO:  89% 9% .




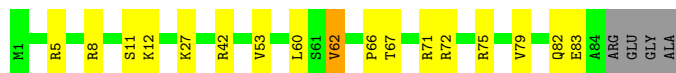
- Molecule 16: 30S ribosomal protein S16

Chain QP:  73% 22% . 5%




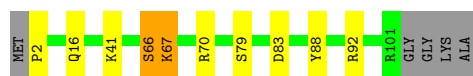
- Molecule 16: 30S ribosomal protein S16

Chain XP:  76% 18% . 5%



- Molecule 17: 30S ribosomal protein S17

Chain QQ:  86% 8% • 5%



- Molecule 17: 30S ribosomal protein S17

Chain XQ:  70% 23% • 5%



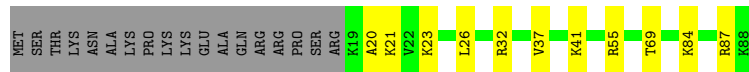
- Molecule 18: 30S ribosomal protein S18

Chain QR:  59% 19% • 20%



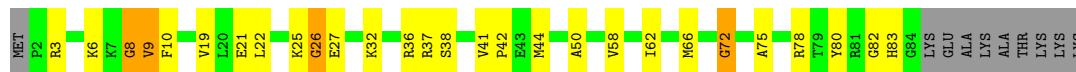
- Molecule 18: 30S ribosomal protein S18

Chain XR:  67% 13% 20%



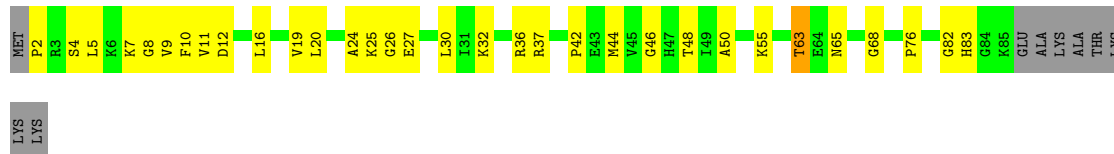
- Molecule 19: 30S ribosomal protein S19

Chain QS:  59% 26% • 11%



- Molecule 19: 30S ribosomal protein S19

Chain XS:  56% 33% • 10%



- Molecule 20: 30S ribosomal protein S20

Chain QT:  64% 25% • 7%



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx



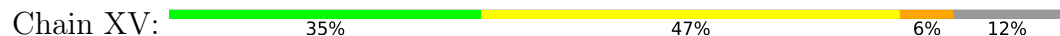
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: P-site ASLPro



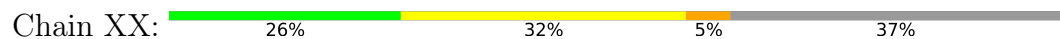
- Molecule 22: P-site ASLPro



- Molecule 23: mRNA



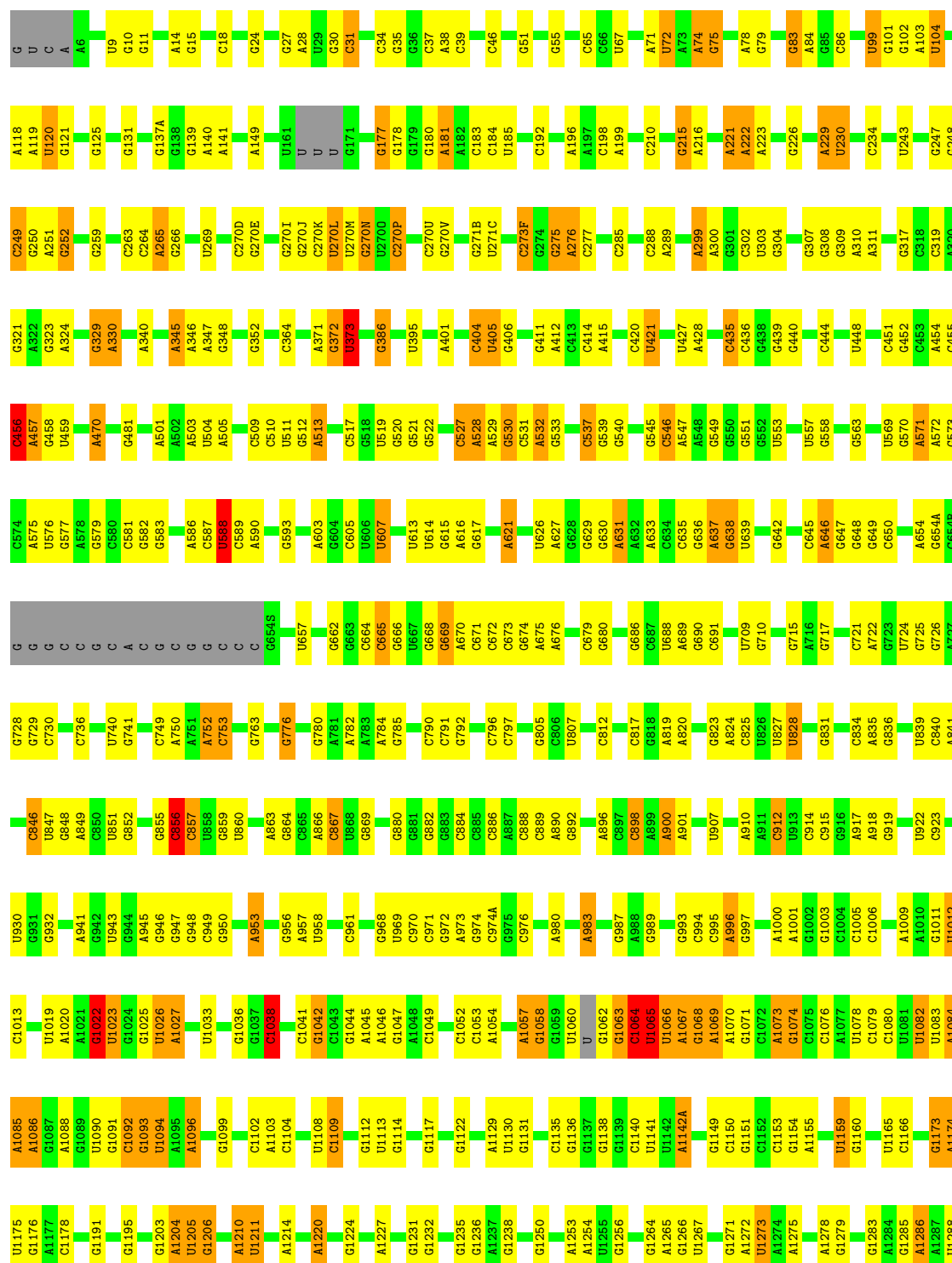
- Molecule 23: mRNA





Molecule 24: 23S rRNA

Chain RA: 61% 31% 7%

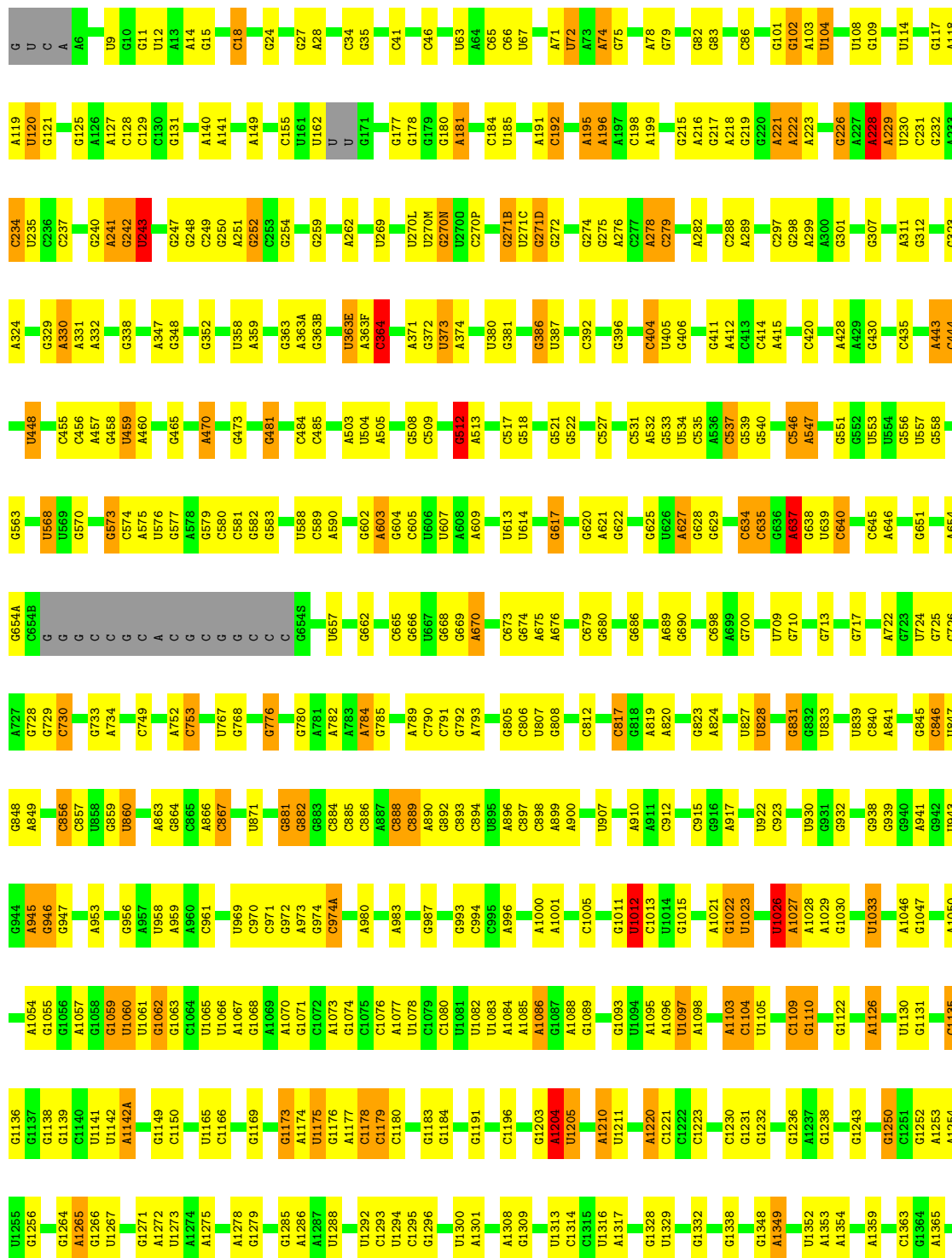






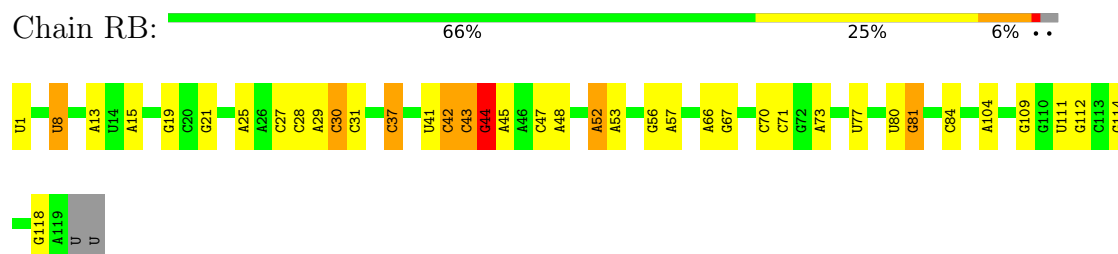
- Molecule 24: 23S rRNA

Chain YA:  62% 29% 7% 2%

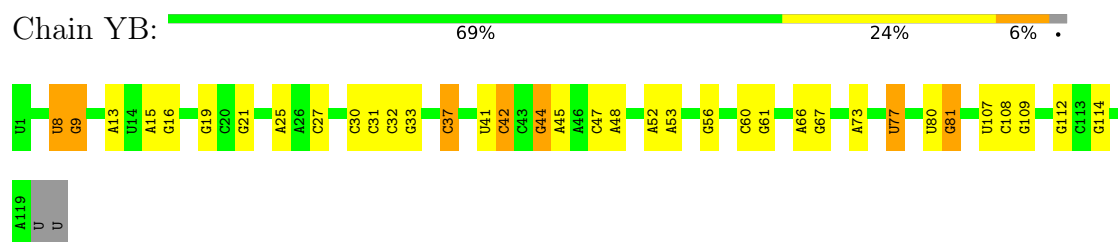


A2851	A2748	C2616	C2498	A2388	A2287	U2180	U2102	C1996	A1871	G1782	G1649	A1543	G1455	G1368
G2852	A2753	C2617	C2499	G2389	A2288	G2181	C2103	A2001	A1872	A1783	G1650	C1544	G1456	G1369
G2853				A2392	U2291	G2182	C2107	G2002	G1878	A1784	A1652	A1545	A1457	G1370
G2854	A2758	C2626	C2501	A2393	C2292	G2183			C1882	A1785	G1653	A1557	C1458	U1372
G2867		C2627	A2503	C2394		G2184	C2111	C2006	C1883	A1786	A1654	A1558	A1460	A1378
A2868	G2761	A2629	U2504		A2298	G2185	G2112	C2007	A1884	C1787		G1559	A1461	A1379
		G2630	G2505	C2402	G2304	G2186	U2113	C2008	G1888	A1789	C1657	G1560	C1462	
G2872	A2764	G2631	U2506	C2403	A2305	G2187	A2114	G2009	A1889	C1790	C1658	A1566	C1463	A1384
A2873	A2765		U2511	C2404	A2306	G2188	G2115	G2010	A1890	A1791	A1664	A1567	C1464	A1385
C2874	G2766	C2646		G2405	G2307	U2189	G2116		G1891	C1792		A1568	C1467	U1390
G2875		U2647	C2515	U2406	G2308	G2191	U2117	A2020	G1903	A1793	G1674	A1569	C1470	U1391
G2876	G2769	U2648	G2516	G2410	A2309	G2192	U2118	C2021	G1904	C1794		A1570	A1471	A1392
		U2649	C2517		A2310	G2193	A2119	U2022	G1905	C1795	G1678	A1571		
C2880	C2774		C2416		A2311	A2198	G2120	G2023	G1906	C1797	U1679	A1572		
G2889	A2775	A2654	C2417	A2422	U2312	A2199	G2125	A2030	A1912	U1798	C1683	C1577	C1474	A1395
G2891	A2776	G2655	C2521	U2423	C2313	A2200	A2126	A2031	A1913	C1799	U1689	U1578	C1475	U1396
A2892	A2778			G2424	C2314	G2210	G2127	G2032	C1914	C1800	C1686			U1397
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U	G	C2681	U2554	G2427	G2319	G2215	G2133		G1929	G1804	C1694	G1594	G1483	C1407
G		U2682		G2428	A2320	A2225	A2134	C2043	G1930	A1809	G1695	C1598	G1484	C1408
A	A2790			G2429	G2321	C2226	C2136		G1936	A1812		C1599	G1487	C1410
C	C2791	U2688	C2568	A2430			C2137	G2046	A1937	G1813	A1698		C1493	C1411
C		U2689	C2569	A2435	G2326	G2230	C2140	G2052	A1938	G1816	G1725	C1604		C1412
C	C2794	C2690	C2560	U2438	A2327	U2233	G2141		U1939	G1817	U1728	C1605	A1496	G1416
U	U2797	C2691		A2439	A2328		C2145	C2055	U1940	U1818	G1728	C1606	U1497	C1417
C		C2692	A2564	C2440	G2329	G2238	C2146	G2056	U1952	U1820	A1729	C1607	U1503	G1418
C	U2808	A2693	A2565	C2441	G2334	G2239	G2147	A2059	C1955	G1824	U1730	C1608	U1504	A1419
	A2809	G2694	A2566	C2442	A2335	A2241	U2150	A2060	U1956	A1825	A1732	A1610	C1506	U1420
	A2810	U2698	C2567	G2443	A2336	G2242	G2151	A2061	U1956	G1826	G1733	C1611	C1507	G1421
			C2568	G2444		U2243	G2152	A2062	C1961	C1827		C1612	A1507	
	C2814	U2702	C2573	G2445	U2344	U2244	G2153	A2063	C1962	G1828	G1743	C1617	A1508	G1426
	G2818	G2707	G2574		G2345	U2245	G2154	C2064	U1963	A1829	C1754	C1619	C1509	A1427
	A2820		U2580	A2448	A2346	G2246	G2155	C2065	C1964	C1830	A1756	G1622	A1510	C1428
	A2821	A2711	U2584	A2450	C2347	A2247	G2156	G2069	C1965	G1831	U1757	G1623	A1511	G1429
	G2822	U2712	U2585	C2456		C2258	G2157	G2070	G1967	G1832	U1629	G1628	G1512	C1430
A2823	A2712A		C2586	C2455	A2352	U2262	A2158	A2071	A1969	U1833	G1758	U1629	C1513	U1431
G2824	A2713	G2714							A1970	U1834		G1630	U1514	
C2825			A2590	C2465			C2161	U2074	A1971	G1835	A1762		G1522	A1434
	U2832	C2723	C2591	G2468	C2355	A2266	G2162	U2075	A1972	U1841	G1763	A1632		U1438
	G2833		G2592	A2469		A2267	C2163	U2086	G1973	G1842	G1764	A1633	A1528	A1439
A2835	U2726			G2470	G2358		G2164	G2087					A1529	
U2836	G2732		A2602	U2473	C2364	A2273	G2165	G2088	G1980	A1847	G1769	A1637	G1530	A1444A
G2837	A2733		G2603		G2365	A2274	G2166	U2089	A1981	C1638		C1638	G1534	C1445
G2838	G2734		U2604	A2478		C2275	G2167		C1982	U1773		U1639	U1535	G1448
G2839	G2735		G2608	G2479	C2374	A2278	A2169	G2093	C1989	C1774	A1775	C1640	A1536	A1449
	G2736		U2609	G2480	C2374	A2278	A2170		G1990	A1859	G1776	C1644	A1537	G1449A
			C2610	G2481	G2383	G2282	A2171	U2096	C1991	G1868		G1645	G1538	C1450
	U2739		U2611	G2384	G2384	C2283	U2172		U1991	A1859		G1646	G1539	C1451
			C2612	G2385	C2385	C2284	A2173	U2099	U1992	U1864	U1779	G1647	G1540	A1453
	G2744			C2386		G2285	G2100		U1993	G1869	A1780	A1453		A1454
			U2615	U2387		A2286	C2179	G2101		C1870				

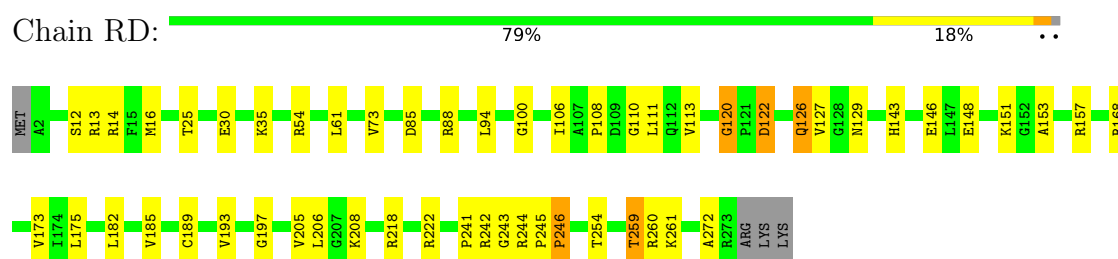
- Molecule 25: 5S rRNA



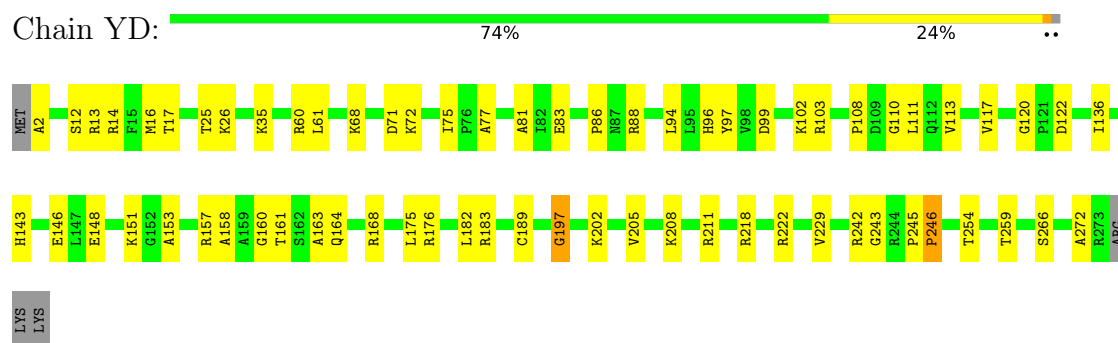
- Molecule 25: 5S rRNA



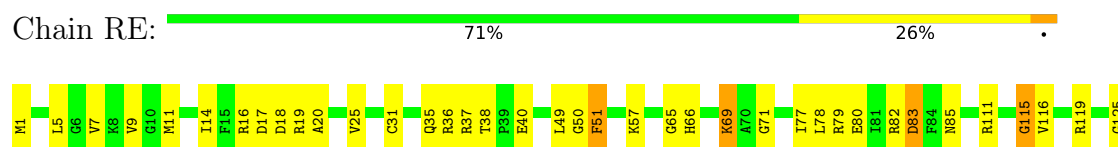
- Molecule 26: 50S ribosomal protein L2



- Molecule 26: 50S ribosomal protein L2



- Molecule 27: 50S ribosomal protein L3





- Molecule 27: 50S ribosomal protein L3

Chain YE: 83% 15%



- Molecule 28: 50S ribosomal protein L4

Chain RF: 78% 18%



- Molecule 28: 50S ribosomal protein L4

Chain YF: 76% 19%



- Molecule 29: 50S ribosomal protein L5

Chain RG: 66% 31%

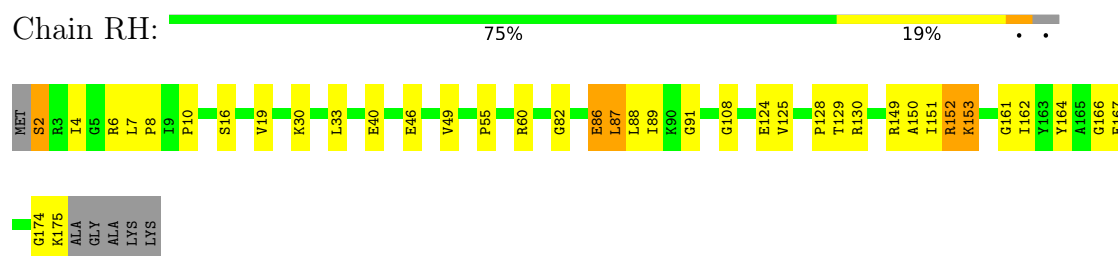


- Molecule 29: 50S ribosomal protein L5

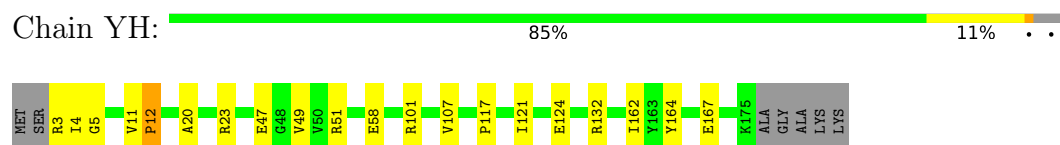
Chain YG: 77% 20%



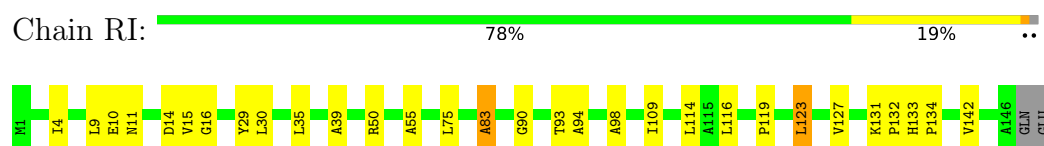
- Molecule 30: 50S ribosomal protein L6



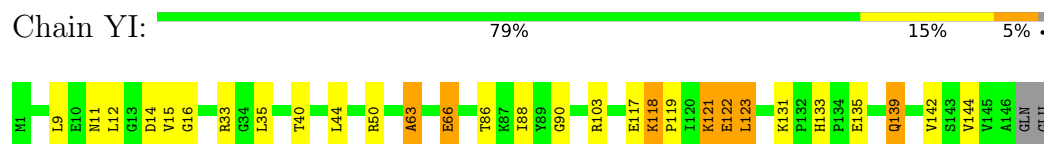
- Molecule 30: 50S ribosomal protein L6



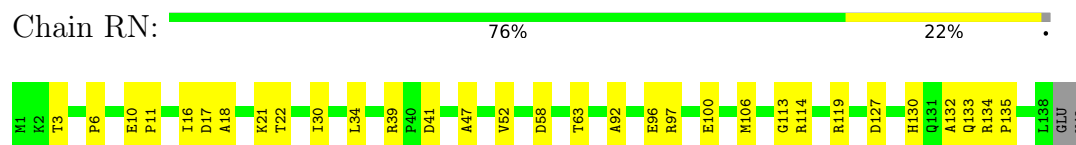
- Molecule 31: 50S ribosomal protein L9



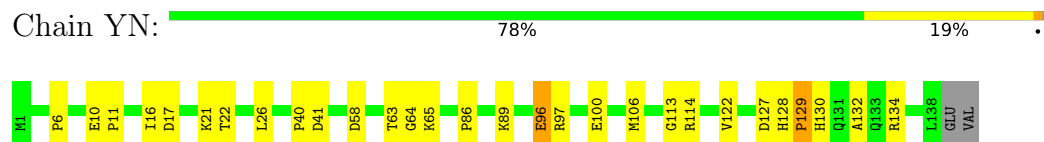
- Molecule 31: 50S ribosomal protein L9



- Molecule 32: 50S ribosomal protein L13

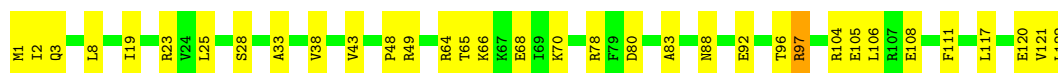


- Molecule 32: 50S ribosomal protein L13

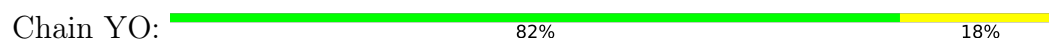


- Molecule 33: 50S ribosomal protein L14

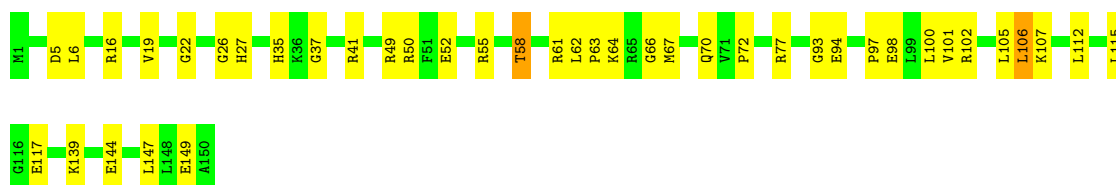
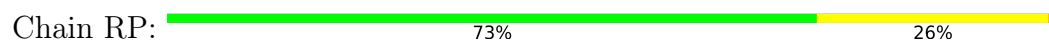




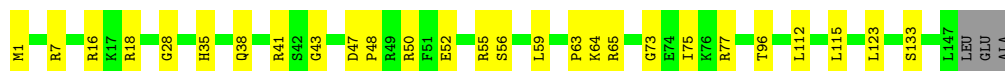
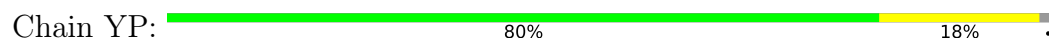
- Molecule 33: 50S ribosomal protein L14



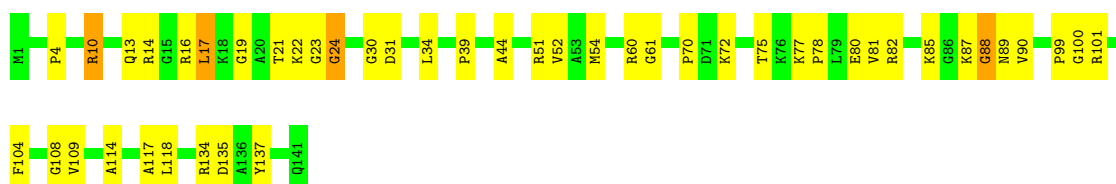
- Molecule 34: 50S ribosomal protein L15



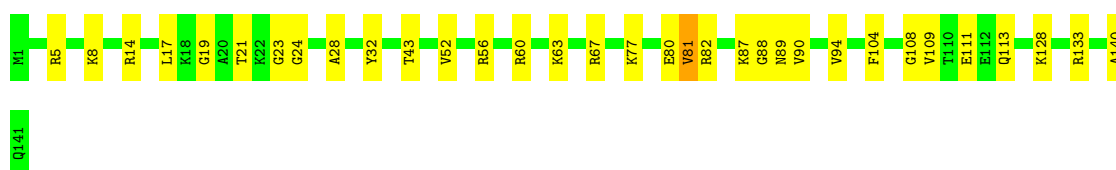
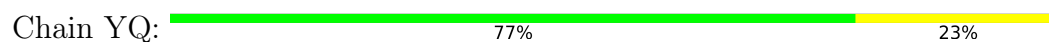
- Molecule 34: 50S ribosomal protein L15




- Molecule 35: 50S ribosomal protein L16



- Molecule 35: 50S ribosomal protein L16




- Molecule 36: 50S ribosomal protein L17

Chain RR:  81% 17% ..



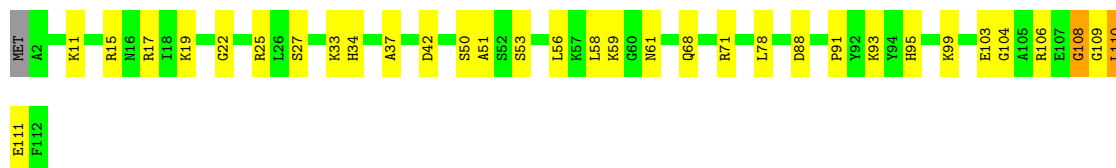
- Molecule 36: 50S ribosomal protein L17

Chain YR:  78% 18% ..




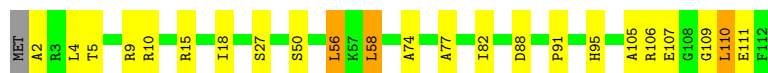
- Molecule 37: 50S ribosomal protein L18

Chain RS:  70% 28% ..



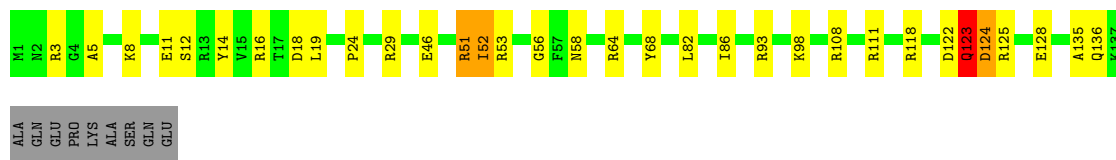
- Molecule 37: 50S ribosomal protein L18

Chain YS:  79% 18% ..



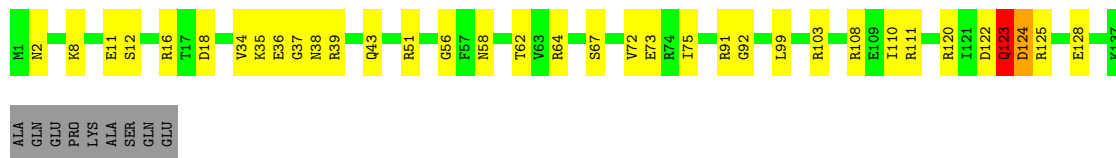
- Molecule 38: 50S ribosomal protein L19

Chain RT:  71% 20% .. 6%




- Molecule 38: 50S ribosomal protein L19

Chain YT:  70% 23% .. 6%



- Molecule 39: 50S ribosomal protein L20

Chain RU:  81% 15% ..




- Molecule 39: 50S ribosomal protein L20

Chain YU:  88% 11% .



- Molecule 40: 50S ribosomal protein L21

Chain RV:  84% 16%




- Molecule 40: 50S ribosomal protein L21

Chain YV:  89% 11%



- Molecule 41: 50S ribosomal protein L22

Chain RW:  84% 16%




- Molecule 41: 50S ribosomal protein L22

Chain YW:  90% 10%




- Molecule 42: 50S ribosomal protein L23

Chain RX:  83% 11% ..




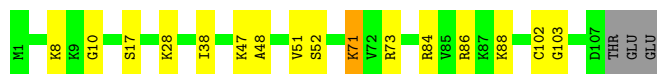
- Molecule 42: 50S ribosomal protein L23

Chain YX:  84% 11% .




- Molecule 43: 50S ribosomal protein L24

Chain RY:  83% 14% ..




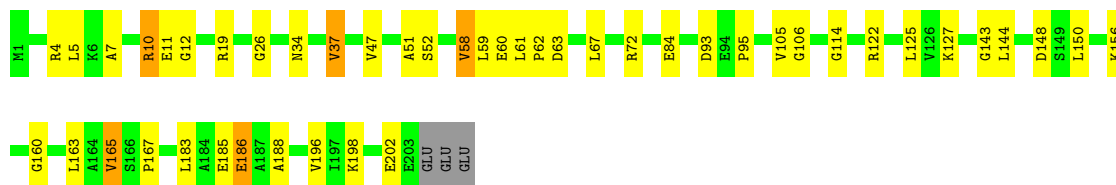
- Molecule 43: 50S ribosomal protein L24

Chain YY:  82% 15% .




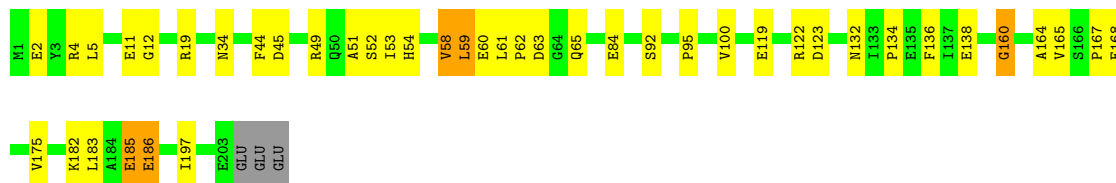
- Molecule 44: 50S ribosomal protein L25

Chain RZ:  76% 20% ..




- Molecule 44: 50S ribosomal protein L25

Chain YZ:  78% 18% ..




- Molecule 45: 50S ribosomal protein L27

Chain R0:  74% 15% 11%



- Molecule 45: 50S ribosomal protein L27

Chain Y0:  76% 12% 12%



- Molecule 46: 50S ribosomal protein L28

Chain R1: 81% 15% ..



- Molecule 46: 50S ribosomal protein L28

Chain Y1: 77% 15% • 5%



- Molecule 47: 50S ribosomal protein L29

Chain R2: 69% 25% ..



- Molecule 47: 50S ribosomal protein L29

Chain Y2: 72% 19% • 6%



- Molecule 48: 50S ribosomal protein L30

Chain R3: 70% 27% ..



- Molecule 48: 50S ribosomal protein L30

Chain Y3: 82% 17% •

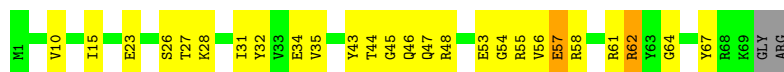


- Molecule 49: 50S ribosomal protein L31

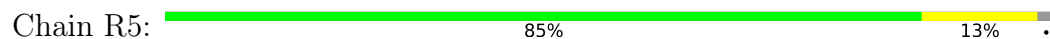
Chain R4: 70% 24% ..



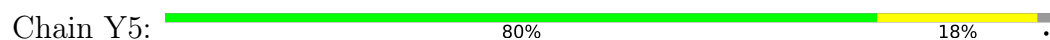
- Molecule 49: 50S ribosomal protein L31



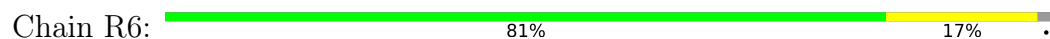
- Molecule 50: 50S ribosomal protein L32



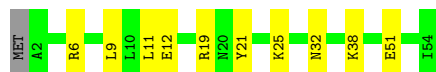
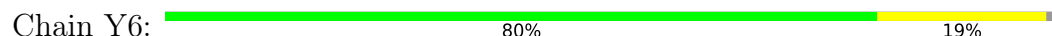
- Molecule 50: 50S ribosomal protein L32



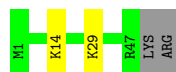
- Molecule 51: 50S ribosomal protein L33



- Molecule 51: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L34



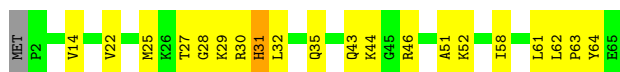
- Molecule 52: 50S ribosomal protein L34





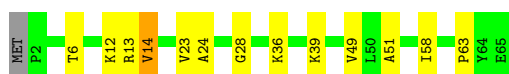
- Molecule 53: 50S ribosomal protein L35

Chain R8: 68% 29% ..



- Molecule 53: 50S ribosomal protein L35

Chain Y8: 78% 18% ..



- Molecule 54: 50S ribosomal protein L36

Chain R9: 78% 22%



- Molecule 54: 50S ribosomal protein L36

Chain Y9: 78% 22%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.79Å 451.91Å 621.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.71 – 3.10	Depositor
% Data completeness (in resolution range)	98.0 (152.71-3.10)	Depositor
R_{merge}	0.36	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.244 , 0.274	Depositor
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.231	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	289311	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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, 1MG, 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	0.36	0/36098	1.03	113/56341 (0.2%)
1	XA	0.37	2/36101 (0.0%)	1.04	128/56346 (0.2%)
2	QB	0.27	0/1942	0.54	0/2619
2	XB	0.27	0/1950	0.51	0/2630
3	QC	0.27	0/1629	0.53	0/2195
3	XC	0.26	0/1629	0.57	1/2195 (0.0%)
4	QD	0.44	0/1733	0.77	2/2318 (0.1%)
4	XD	0.35	0/1733	0.78	3/2318 (0.1%)
5	QE	0.27	0/1171	0.51	0/1576
5	XE	0.28	0/1171	0.51	0/1576
6	QF	0.26	0/856	0.46	0/1154
6	XF	0.25	0/856	0.47	0/1154
7	QG	0.27	0/1276	0.51	0/1709
7	XG	0.25	0/1276	0.48	0/1709
8	QH	0.27	0/1128	0.49	0/1517
8	XH	0.27	0/1128	0.49	0/1517
9	QI	0.27	0/1029	0.58	1/1379 (0.1%)
9	XI	0.28	0/1017	0.66	2/1365 (0.1%)
10	QJ	0.27	0/814	0.56	0/1095
10	XJ	0.27	0/790	0.51	0/1063
11	QK	0.27	0/900	0.51	0/1213
11	XK	0.26	0/879	0.49	0/1187
12	QL	0.29	0/991	0.52	0/1327
12	XL	0.28	0/972	0.52	0/1301
13	QM	0.27	0/965	0.57	0/1292
13	XM	0.26	0/956	0.55	0/1281
14	QN	0.30	0/501	0.58	1/664 (0.2%)
14	XN	0.29	0/501	0.55	1/664 (0.2%)
15	QO	0.26	0/745	0.48	0/992
15	XO	0.23	0/740	0.42	0/987
16	QP	0.27	0/721	0.50	0/970
16	XP	0.26	0/721	0.46	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.26	0/847	0.49	0/1131
17	XQ	0.27	0/847	0.47	0/1131
18	QR	0.27	0/579	0.56	0/768
18	XR	0.25	0/579	0.51	0/768
19	QS	0.27	0/680	0.60	0/915
19	XS	0.25	0/689	0.54	0/926
20	QT	0.28	0/765	0.52	0/1007
20	XT	0.24	0/765	0.54	1/1007 (0.1%)
21	QU	0.26	0/221	0.52	0/288
21	XU	0.25	0/221	0.53	0/288
22	QV	0.31	0/380	1.06	2/590 (0.3%)
22	XV	0.29	0/332	1.00	0/515
23	QX	0.53	0/243	1.05	0/377
23	XX	0.58	0/294	1.15	1/457 (0.2%)
24	RA	0.43	0/69498	1.05	263/108491 (0.2%)
24	YA	0.49	0/69543	1.05	237/108563 (0.2%)
25	RB	0.37	0/2878	1.11	19/4490 (0.4%)
25	YB	0.44	0/2878	1.10	17/4490 (0.4%)
26	RD	0.31	0/2165	0.49	0/2919
26	YD	0.33	0/2165	0.50	0/2919
27	RE	0.31	0/1601	0.58	0/2160
27	YE	0.32	0/1596	0.53	0/2153
28	RF	0.30	0/1620	0.50	0/2194
28	YF	0.32	0/1620	0.48	0/2194
29	RG	0.27	0/1499	0.57	0/2016
29	YG	0.27	0/1499	0.59	2/2016 (0.1%)
30	RH	0.28	0/1362	0.56	0/1841
30	YH	0.31	0/1356	0.52	0/1833
31	RI	0.27	0/1151	0.62	0/1558
31	YI	0.27	0/1151	0.57	0/1558
32	RN	0.28	0/1131	0.50	0/1525
32	YN	0.32	0/1131	0.51	0/1525
33	RO	0.31	0/943	0.50	0/1269
33	YO	0.32	0/943	0.52	0/1269
34	RP	0.30	0/1162	0.62	0/1544
34	YP	0.31	0/1139	0.54	0/1514
35	RQ	0.29	0/1143	0.56	0/1527
35	YQ	0.32	0/1143	0.57	0/1527
36	RR	0.28	0/974	0.53	0/1302
36	YR	0.30	0/974	0.55	1/1302 (0.1%)
37	RS	0.27	0/892	0.61	1/1187 (0.1%)
37	YS	0.29	0/892	0.61	1/1187 (0.1%)
38	RT	0.27	0/1155	0.56	0/1542

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YT	0.30	0/1155	0.55	1/1542 (0.1%)
39	RU	0.28	0/982	0.49	0/1306
39	YU	0.31	0/982	0.44	0/1306
40	RV	0.29	0/790	0.54	0/1057
40	YV	0.33	0/790	0.54	0/1057
41	RW	0.28	0/911	0.48	0/1220
41	YW	0.31	0/911	0.50	0/1220
42	RX	0.29	0/739	0.50	0/993
42	YX	0.31	0/739	0.52	0/993
43	RY	0.28	0/831	0.48	0/1108
43	YY	0.30	0/831	0.47	0/1108
44	RZ	0.32	0/1634	0.61	1/2216 (0.0%)
44	YZ	0.31	0/1634	0.56	0/2216
45	R0	0.29	0/611	0.49	0/814
45	Y0	0.32	0/607	0.50	0/809
46	R1	0.30	0/770	0.54	0/1022
46	Y1	0.31	0/736	0.54	0/978
47	R2	0.24	0/583	0.42	0/771
47	Y2	0.30	0/577	0.45	0/764
48	R3	0.26	0/474	0.51	0/635
48	Y3	0.27	0/474	0.52	0/635
49	R4	0.29	0/578	0.59	0/776
49	Y4	0.28	0/578	0.56	0/776
50	R5	0.30	0/473	0.48	0/639
50	Y5	0.32	0/473	0.49	0/639
51	R6	0.28	0/460	0.47	0/613
51	Y6	0.31	0/460	0.47	0/613
52	R7	0.27	0/417	0.42	0/550
52	Y7	0.30	0/426	0.45	0/561
53	R8	0.31	0/525	0.54	0/691
53	Y8	0.33	0/525	0.50	0/691
54	R9	0.27	0/310	0.44	0/407
54	Y9	0.31	0/310	0.45	0/407
All	All	0.39	2/312861 (0.0%)	0.94	799/467540 (0.2%)

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
1	XA	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	QB	0	17
2	XB	0	22
3	QC	0	16
3	XC	0	19
5	QE	0	5
5	XE	0	8
6	QF	0	5
7	QG	0	8
7	XG	0	8
8	QH	0	4
8	XH	0	5
9	QI	0	12
9	XI	0	11
10	QJ	0	12
10	XJ	0	9
11	QK	0	1
11	XK	0	4
12	QL	0	10
12	XL	0	10
13	QM	0	19
13	XM	0	15
14	QN	0	1
14	XN	0	7
15	QO	0	2
15	XO	0	2
16	QP	0	3
16	XP	0	4
17	QQ	0	3
17	XQ	0	4
18	QR	0	5
18	XR	0	3
19	QS	0	12
19	XS	0	21
20	QT	0	16
20	XT	0	12
21	QU	0	2
21	XU	0	2
26	RD	0	11
26	YD	0	8
27	RE	0	20
27	YE	0	7
28	RF	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
28	YF	0	14
29	RG	0	16
29	YG	0	13
30	RH	0	24
30	YH	0	2
31	RI	0	21
31	YI	0	22
32	RN	0	12
32	YN	0	10
33	RO	0	1
33	YO	0	1
34	RP	0	25
34	YP	0	8
35	RQ	0	14
35	YQ	0	13
36	RR	0	3
36	YR	0	5
37	RS	0	13
37	YS	0	9
38	RT	0	13
38	YT	0	11
39	RU	0	7
39	YU	0	2
40	RV	0	6
40	YV	0	6
41	RW	0	4
41	YW	0	3
42	RX	0	4
42	YX	0	2
43	RY	0	4
43	YY	0	4
44	RZ	0	20
44	YZ	0	16
45	R0	0	2
45	Y0	0	2
46	R1	0	7
46	Y1	0	8
47	R2	0	8
47	Y2	0	3
48	R3	0	1
48	Y3	0	2
49	R4	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
49	Y4	0	12
50	Y5	0	1
53	R8	0	12
53	Y8	0	1
54	R9	0	1
All	All	0	775

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	XA	358	U	O4'-C1'	-6.29	1.33	1.41
1	XA	358	U	C5'-C4'	5.05	1.57	1.51

The worst 5 of 799 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	359	U	C2-N1-C1'	-18.46	95.55	117.70
1	XA	359	U	O5'-P-OP1	-17.99	89.11	110.70
1	XA	359	U	C6-N1-C1'	16.75	144.64	121.20
1	XA	328	C	N1-C2-O2	13.70	127.12	118.90
24	RA	1092	C	N1-C2-O2	13.63	127.08	118.90

There are no chirality outliers.

5 of 775 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	15	VAL	Peptide
2	QB	19	HIS	Peptide
2	QB	21	ARG	Peptide
2	QB	22	LYS	Peptide
2	QB	34	ALA	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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16277	362	0
1	XA	32249	0	16278	389	0
2	QB	1907	0	1958	22	0
2	XB	1915	0	1969	24	0
3	QC	1605	0	1668	22	0
3	XC	1605	0	1668	28	0
4	QD	1703	0	1763	47	0
4	XD	1703	0	1763	36	0
5	QE	1155	0	1213	13	0
5	XE	1155	0	1213	8	0
6	QF	843	0	857	13	0
6	XF	843	0	857	9	0
7	QG	1257	0	1296	18	0
7	XG	1257	0	1296	20	0
8	QH	1108	0	1165	15	0
8	XH	1108	0	1165	20	0
9	QI	1010	0	1037	26	0
9	XI	998	0	1024	23	0
10	QJ	801	0	849	16	0
10	XJ	777	0	816	16	0
11	QK	885	0	904	14	0
11	XK	864	0	881	20	0
12	QL	975	0	1062	21	0
12	XL	956	0	1046	11	0
13	QM	955	0	1021	18	0
13	XM	946	0	1008	22	0
14	QN	492	0	529	10	0
14	XN	492	0	529	14	0
15	QO	734	0	771	7	0
15	XO	729	0	768	5	0
16	QP	705	0	725	13	0
16	XP	705	0	725	9	0
17	QQ	834	0	904	8	0
17	XQ	834	0	904	16	0
18	QR	574	0	644	8	0
18	XR	574	0	644	7	0
19	QS	665	0	686	15	0
19	XS	674	0	699	9	0
20	QT	763	0	861	16	0
20	XT	763	0	861	10	0
21	QU	217	0	234	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	XU	217	0	234	3	0
22	QV	365	0	186	4	0
22	XV	322	0	164	6	0
23	QX	217	0	110	5	0
23	XX	262	0	132	3	0
24	RA	62051	0	31280	482	0
24	YA	62091	0	31294	478	0
25	RB	2573	0	1306	20	0
25	YB	2573	0	1306	15	0
26	RD	2115	0	2195	37	0
26	YD	2115	0	2195	42	0
27	RE	1568	0	1634	32	0
27	YE	1563	0	1629	19	0
28	RF	1585	0	1632	19	0
28	YF	1585	0	1632	20	0
29	RG	1474	0	1535	31	0
29	YG	1474	0	1535	21	0
30	RH	1336	0	1418	12	0
30	YH	1330	0	1413	11	0
31	RI	1136	0	1223	6	0
31	YI	1136	0	1223	8	0
32	RN	1104	0	1180	13	0
32	YN	1104	0	1180	12	0
33	RO	933	0	996	22	0
33	YO	933	0	996	15	0
34	RP	1145	0	1227	14	0
34	YP	1122	0	1205	17	0
35	RQ	1122	0	1178	24	0
35	YQ	1122	0	1179	20	0
36	RR	960	0	1021	11	0
36	YR	960	0	1021	17	0
37	RS	882	0	943	17	0
37	YS	882	0	943	11	0
38	RT	1141	0	1202	19	0
38	YT	1141	0	1202	18	0
39	RU	964	0	1021	14	0
39	YU	964	0	1021	10	0
40	RV	779	0	852	6	0
40	YV	779	0	852	3	0
41	RW	900	0	964	9	0
41	YW	900	0	964	6	0
42	RX	725	0	778	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	YX	725	0	778	6	0
43	RY	818	0	909	11	0
43	YY	818	0	909	8	0
44	RZ	1601	0	1630	22	0
44	YZ	1601	0	1630	24	0
45	R0	603	0	620	7	0
45	Y0	599	0	617	5	0
46	R1	763	0	848	9	0
46	Y1	729	0	802	7	0
47	R2	581	0	629	7	0
47	Y2	575	0	624	9	0
48	R3	469	0	518	10	0
48	Y3	469	0	518	5	0
49	R4	565	0	557	9	0
49	Y4	565	0	557	12	0
50	R5	459	0	476	7	0
50	Y5	459	0	476	8	0
51	R6	453	0	473	6	0
51	Y6	453	0	473	7	0
52	R7	409	0	454	2	0
52	Y7	418	0	467	4	0
53	R8	517	0	582	10	0
53	Y8	517	0	582	8	0
54	R9	307	0	335	4	0
54	Y9	307	0	335	6	0
55	QA	74	0	0	0	0
55	QC	1	0	0	0	0
55	QF	1	0	0	0	0
55	QH	1	0	0	0	0
55	QM	1	0	0	0	0
55	R0	1	0	0	0	0
55	R1	2	0	0	0	0
55	R8	1	0	0	0	0
55	RA	487	0	0	0	0
55	RB	6	0	0	0	0
55	RE	4	0	0	0	0
55	RF	2	0	0	0	0
55	RI	1	0	0	0	0
55	RN	1	0	0	0	0
55	RO	1	0	0	0	0
55	RP	1	0	0	0	0
55	RQ	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	RR	2	0	0	0	0
55	RT	1	0	0	0	0
55	RX	1	0	0	0	0
55	RY	1	0	0	0	0
55	XA	92	0	0	0	0
55	XE	1	0	0	0	0
55	XK	1	0	0	0	0
55	XL	2	0	0	0	0
55	XM	2	0	0	0	0
55	XN	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	2	0	0	0	0
55	YA	542	0	0	0	0
55	YB	15	0	0	0	0
55	YD	3	0	0	0	0
55	YE	3	0	0	0	0
55	YO	1	0	0	0	0
55	YQ	3	0	0	0	0
55	YR	2	0	0	0	0
55	YX	2	0	0	0	0
56	QD	8	0	0	0	0
56	XD	8	0	0	0	0
57	QN	1	0	0	0	0
57	R4	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R9	1	0	0	0	0
57	RY	1	0	0	0	0
57	XN	1	0	0	0	0
57	Y4	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YY	1	0	0	0	0
All	All	289311	0	196538	2694	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 2694 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)
35:RQ:51:ARG:NH2	44:RZ:186:GLU:OE1	1.59	1.34
24:RA:2135:A:N6	24:RA:2156:G:H21	1.54	1.05
47:Y2:65:ASN:O	47:Y2:69:ARG:HG3	1.55	1.05
35:YQ:52:VAL:HG13	44:YZ:183:LEU:CD1	1.88	1.03
24:RA:2135:A:H62	24:RA:2156:G:N2	1.57	1.02

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	211 (91%)	22 (9%)	0	100	100
2	XB	234/256 (91%)	213 (91%)	21 (9%)	0	100	100
3	QC	203/239 (85%)	185 (91%)	18 (9%)	0	100	100
3	XC	203/239 (85%)	191 (94%)	12 (6%)	0	100	100
4	QD	206/209 (99%)	185 (90%)	18 (9%)	3 (2%)	10	39
4	XD	206/209 (99%)	189 (92%)	15 (7%)	2 (1%)	15	49
5	QE	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
5	XE	149/162 (92%)	139 (93%)	10 (7%)	0	100	100
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%)	148 (97%)	5 (3%)	0	100	100
7	XG	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
8	QH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
8	XH	135/138 (98%)	130 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	QI	125/128 (98%)	117 (94%)	8 (6%)	0	100	100
9	XI	124/128 (97%)	112 (90%)	12 (10%)	0	100	100
10	QJ	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
10	XJ	94/105 (90%)	90 (96%)	4 (4%)	0	100	100
11	QK	117/129 (91%)	110 (94%)	7 (6%)	0	100	100
11	XK	114/129 (88%)	109 (96%)	5 (4%)	0	100	100
12	QL	123/132 (93%)	113 (92%)	10 (8%)	0	100	100
12	XL	120/132 (91%)	107 (89%)	13 (11%)	0	100	100
13	QM	118/126 (94%)	105 (89%)	12 (10%)	1 (1%)	19	54
13	XM	117/126 (93%)	103 (88%)	14 (12%)	0	100	100
14	QN	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
14	XN	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
15	QO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	XO	85/89 (96%)	85 (100%)	0	0	100	100
16	QP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
17	XQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
18	QR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
19	XS	82/93 (88%)	71 (87%)	11 (13%)	0	100	100
20	QT	97/106 (92%)	92 (95%)	5 (5%)	0	100	100
20	XT	97/106 (92%)	89 (92%)	8 (8%)	0	100	100
21	QU	23/27 (85%)	23 (100%)	0	0	100	100
21	XU	23/27 (85%)	23 (100%)	0	0	100	100
26	RD	270/276 (98%)	258 (96%)	12 (4%)	0	100	100
26	YD	270/276 (98%)	257 (95%)	13 (5%)	0	100	100
27	RE	203/206 (98%)	171 (84%)	32 (16%)	0	100	100
27	YE	202/206 (98%)	193 (96%)	9 (4%)	0	100	100
28	RF	200/210 (95%)	189 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	YF	200/210 (95%)	189 (94%)	11 (6%)	0	100	100
29	RG	179/182 (98%)	158 (88%)	21 (12%)	0	100	100
29	YG	179/182 (98%)	161 (90%)	17 (10%)	1 (1%)	25	59
30	RH	172/180 (96%)	153 (89%)	18 (10%)	1 (1%)	25	59
30	YH	171/180 (95%)	163 (95%)	8 (5%)	0	100	100
31	RI	144/148 (97%)	125 (87%)	19 (13%)	0	100	100
31	YI	144/148 (97%)	129 (90%)	15 (10%)	0	100	100
32	RN	136/140 (97%)	124 (91%)	12 (9%)	0	100	100
32	YN	136/140 (97%)	125 (92%)	11 (8%)	0	100	100
33	RO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
33	YO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
34	RP	148/150 (99%)	133 (90%)	15 (10%)	0	100	100
34	YP	145/150 (97%)	137 (94%)	7 (5%)	1 (1%)	22	57
35	RQ	139/141 (99%)	122 (88%)	16 (12%)	1 (1%)	22	57
35	YQ	139/141 (99%)	120 (86%)	19 (14%)	0	100	100
36	RR	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
36	YR	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
37	RS	109/112 (97%)	95 (87%)	14 (13%)	0	100	100
37	YS	109/112 (97%)	95 (87%)	14 (13%)	0	100	100
38	RT	135/146 (92%)	123 (91%)	10 (7%)	2 (2%)	10	39
38	YT	135/146 (92%)	118 (87%)	15 (11%)	2 (2%)	10	39
39	RU	115/118 (98%)	108 (94%)	6 (5%)	1 (1%)	17	52
39	YU	115/118 (98%)	112 (97%)	3 (3%)	0	100	100
40	RV	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
40	YV	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
41	RW	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
41	YW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
42	RX	90/96 (94%)	88 (98%)	2 (2%)	0	100	100
42	YX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
43	RY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
43	YY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	RZ	201/206 (98%)	182 (90%)	19 (10%)	0	100	100
44	YZ	201/206 (98%)	181 (90%)	20 (10%)	0	100	100
45	R0	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
45	Y0	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
46	R1	95/98 (97%)	84 (88%)	11 (12%)	0	100	100
46	Y1	91/98 (93%)	83 (91%)	8 (9%)	0	100	100
47	R2	67/72 (93%)	66 (98%)	1 (2%)	0	100	100
47	Y2	66/72 (92%)	63 (96%)	2 (3%)	1 (2%)	10	39
48	R3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
48	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
49	R4	67/71 (94%)	57 (85%)	10 (15%)	0	100	100
49	Y4	67/71 (94%)	54 (81%)	13 (19%)	0	100	100
50	R5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
50	Y5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
51	R6	51/54 (94%)	51 (100%)	0	0	100	100
51	Y6	51/54 (94%)	51 (100%)	0	0	100	100
52	R7	45/49 (92%)	45 (100%)	0	0	100	100
52	Y7	46/49 (94%)	46 (100%)	0	0	100	100
53	R8	62/65 (95%)	49 (79%)	13 (21%)	0	100	100
53	Y8	62/65 (95%)	62 (100%)	0	0	100	100
54	R9	35/37 (95%)	35 (100%)	0	0	100	100
54	Y9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11484/12128 (95%)	10666 (93%)	802 (7%)	16 (0%)	51	83

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	QD	155	LEU
38	RT	124	ASP
4	XD	155	LEU
4	XD	171	GLY
34	YP	63	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	203/220 (92%)	203 (100%)	0	100	100
2	XB	204/220 (93%)	204 (100%)	0	100	100
3	QC	159/188 (85%)	158 (99%)	1 (1%)	86	94
3	XC	159/188 (85%)	157 (99%)	2 (1%)	69	87
4	QD	180/181 (99%)	174 (97%)	6 (3%)	38	69
4	XD	180/181 (99%)	178 (99%)	2 (1%)	73	89
5	QE	116/123 (94%)	113 (97%)	3 (3%)	46	74
5	XE	116/123 (94%)	116 (100%)	0	100	100
6	QF	90/90 (100%)	88 (98%)	2 (2%)	52	78
6	XF	90/90 (100%)	88 (98%)	2 (2%)	52	78
7	QG	126/127 (99%)	124 (98%)	2 (2%)	62	84
7	XG	126/127 (99%)	125 (99%)	1 (1%)	81	92
8	QH	118/119 (99%)	118 (100%)	0	100	100
8	XH	118/119 (99%)	118 (100%)	0	100	100
9	QI	98/99 (99%)	97 (99%)	1 (1%)	76	90
9	XI	97/99 (98%)	95 (98%)	2 (2%)	53	79
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%)	102 (99%)	1 (1%)	76	90
13	QM	96/101 (95%)	95 (99%)	1 (1%)	76	90
13	XM	95/101 (94%)	95 (100%)	0	100	100
14	QN	49/50 (98%)	49 (100%)	0	100	100
14	XN	49/50 (98%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	71 (99%)	1 (1%)	67	86
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	95 (100%)	0	100	100
17	XQ	95/97 (98%)	93 (98%)	2 (2%)	53	79
18	QR	61/77 (79%)	60 (98%)	1 (2%)	62	84
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	72 (100%)	0	100	100
19	XS	73/80 (91%)	72 (99%)	1 (1%)	67	86
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
26	RD	214/218 (98%)	213 (100%)	1 (0%)	88	94
26	YD	214/218 (98%)	214 (100%)	0	100	100
27	RE	165/166 (99%)	165 (100%)	0	100	100
27	YE	165/166 (99%)	164 (99%)	1 (1%)	86	94
28	RF	161/166 (97%)	161 (100%)	0	100	100
28	YF	161/166 (97%)	161 (100%)	0	100	100
29	RG	155/156 (99%)	155 (100%)	0	100	100
29	YG	155/156 (99%)	154 (99%)	1 (1%)	86	94
30	RH	145/148 (98%)	144 (99%)	1 (1%)	84	93
30	YH	144/148 (97%)	143 (99%)	1 (1%)	84	93
31	RI	122/124 (98%)	121 (99%)	1 (1%)	81	92
31	YI	122/124 (98%)	121 (99%)	1 (1%)	81	92
32	RN	117/119 (98%)	117 (100%)	0	100	100
32	YN	117/119 (98%)	116 (99%)	1 (1%)	78	91
33	RO	100/100 (100%)	99 (99%)	1 (1%)	76	90
33	YO	100/100 (100%)	100 (100%)	0	100	100
34	RP	116/116 (100%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	YP	114/116 (98%)	114 (100%)	0	100	100
35	RQ	111/111 (100%)	110 (99%)	1 (1%)	78	91
35	YQ	111/111 (100%)	110 (99%)	1 (1%)	78	91
36	RR	100/101 (99%)	99 (99%)	1 (1%)	76	90
36	YR	100/101 (99%)	100 (100%)	0	100	100
37	RS	87/88 (99%)	87 (100%)	0	100	100
37	YS	87/88 (99%)	87 (100%)	0	100	100
38	RT	120/127 (94%)	120 (100%)	0	100	100
38	YT	120/127 (94%)	120 (100%)	0	100	100
39	RU	93/94 (99%)	92 (99%)	1 (1%)	73	89
39	YU	93/94 (99%)	93 (100%)	0	100	100
40	RV	82/82 (100%)	82 (100%)	0	100	100
40	YV	82/82 (100%)	82 (100%)	0	100	100
41	RW	92/92 (100%)	92 (100%)	0	100	100
41	YW	92/92 (100%)	92 (100%)	0	100	100
42	RX	74/78 (95%)	74 (100%)	0	100	100
42	YX	74/78 (95%)	73 (99%)	1 (1%)	67	86
43	RY	88/91 (97%)	88 (100%)	0	100	100
43	YY	88/91 (97%)	88 (100%)	0	100	100
44	RZ	174/179 (97%)	172 (99%)	2 (1%)	73	89
44	YZ	174/179 (97%)	171 (98%)	3 (2%)	60	83
45	R0	61/67 (91%)	60 (98%)	1 (2%)	62	84
45	Y0	61/67 (91%)	60 (98%)	1 (2%)	62	84
46	R1	82/83 (99%)	82 (100%)	0	100	100
46	Y1	78/83 (94%)	78 (100%)	0	100	100
47	R2	64/67 (96%)	64 (100%)	0	100	100
47	Y2	64/67 (96%)	62 (97%)	2 (3%)	40	70
48	R3	51/52 (98%)	51 (100%)	0	100	100
48	Y3	51/52 (98%)	50 (98%)	1 (2%)	55	80
49	R4	62/63 (98%)	61 (98%)	1 (2%)	62	84
49	Y4	62/63 (98%)	62 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	R5	51/52 (98%)	51 (100%)	0	100	100
50	Y5	51/52 (98%)	51 (100%)	0	100	100
51	R6	51/52 (98%)	51 (100%)	0	100	100
51	Y6	51/52 (98%)	51 (100%)	0	100	100
52	R7	40/42 (95%)	40 (100%)	0	100	100
52	Y7	41/42 (98%)	41 (100%)	0	100	100
53	R8	54/55 (98%)	54 (100%)	0	100	100
53	Y8	54/55 (98%)	53 (98%)	1 (2%)	57	81
54	R9	34/34 (100%)	34 (100%)	0	100	100
54	Y9	34/34 (100%)	34 (100%)	0	100	100
All	All	9706/10066 (96%)	9649 (99%)	57 (1%)	86	94

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	RZ	34	ASN
4	XD	19	LEU
45	Y0	14	ARG
44	RZ	156	LYS
49	R4	61	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
35	RQ	123	HIS
16	XP	14	ASN
53	R8	31	HIS
10	QJ	84	GLN
39	RU	94	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1521 (98%)	276 (18%)	34 (2%)
1	XA	1499/1521 (98%)	278 (18%)	35 (2%)
22	QV	16/17 (94%)	1 (6%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	XV	14/17 (82%)	2 (14%)	0
23	QX	9/19 (47%)	4 (44%)	1 (11%)
23	XX	11/19 (57%)	5 (45%)	0
24	RA	2877/2915 (98%)	547 (19%)	37 (1%)
24	YA	2880/2915 (98%)	529 (18%)	41 (1%)
25	RB	119/122 (97%)	17 (14%)	1 (0%)
25	YB	119/122 (97%)	16 (13%)	1 (0%)
All	All	9042/9188 (98%)	1675 (18%)	150 (1%)

5 of 1675 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 150 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	RA	2439	A
1	XA	358	U
24	YA	1913	A
24	RA	2610	C
1	XA	115	G

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

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	$\# Z > 2$
22	1MG	QV	37	22	18,26,27	1.33	2 (11%)	19,39,42	1.58	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	1MG	XV	37	22	18,26,27	1.38	2 (11%)	19,39,42	1.63	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
22	1MG	QV	37	22	-	0/3/25/26	0/3/3/3
22	1MG	XV	37	22	-	0/3/25/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	XV	37	1MG	C6-C5	4.52	1.48	1.41
22	QV	37	1MG	C6-C5	4.31	1.48	1.41
22	XV	37	1MG	C5-C4	2.57	1.47	1.40
22	QV	37	1MG	C5-C4	2.57	1.47	1.40

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	XV	37	1MG	C2-N3-C4	5.77	121.94	115.36
22	QV	37	1MG	C2-N3-C4	5.56	121.70	115.36
22	XV	37	1MG	C4-C5-N7	-2.65	106.64	109.40
22	XV	37	1MG	C6-C5-C4	-2.50	118.36	119.96
22	QV	37	1MG	C4-C5-N7	-2.44	106.85	109.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1285 ligands modelled in this entry, 1283 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	$\# Z > 2$
56	SF4	XD	301	4	0,12,12	0.00	-	-		
56	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
56	SF4	XD	301	4	-	-	0/6/5/5
56	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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