



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 08:18 pm BST

PDB ID : 6BZ6  
Title : Thermus thermophilus 70S complex containing 16S G347U ram mutation and empty A site  
Authors : Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.  
Deposited on : 2017-12-22  
Resolution : 3.18 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	<b>FAILED</b>
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

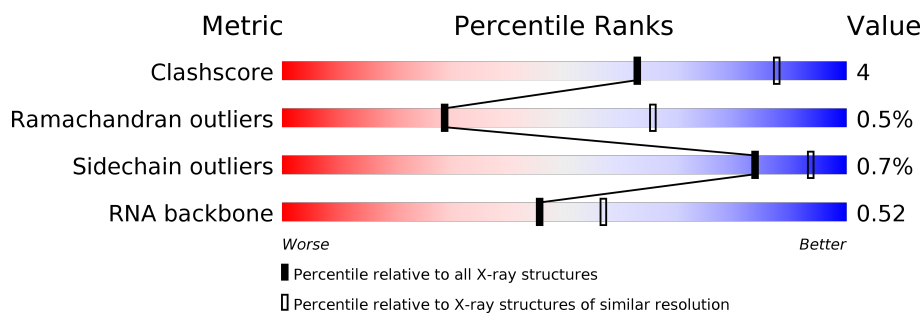
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.18 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	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RNA backbone	3102	1054 (3.50-2.86)


























The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	QA	1508	64% 29% 6% ..
1	XA	1508	66% 27% 6% ..
2	QB	256	77% 14% 8%
2	XB	256	79% 13% 8%
3	QC	239	72% 13% 14%
3	XC	239	72% 13% 14%
4	QD	209	87% 12%

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


























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Mol	Chain	Length	Quality of chain
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	25	
23	XX	25	
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	
29	RG	182	


























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Mol	Chain	Length	Quality of chain
29	YG	182	 81% 17% ..
30	RH	180	 79% 15% ...
30	YH	180	 78% 16% ...
31	RI	148	 79% 20% .
31	YI	148	 78% 21% .
32	RN	140	 88% 10% ..
32	YN	140	 91% 7% ..
33	RO	122	 89% 11% .
33	YO	122	 91% 8% .
34	RP	150	 79% 21%
34	YP	150	 78% 19% ..
35	RQ	141	 76% 24%
35	YQ	141	 79% 21%
36	RR	118	 86% 13% ..
36	YR	118	 81% 18% .
37	RS	112	 83% 15% ..
37	YS	112	 81% 17% ..
38	RT	146	 71% 22% . 6%
38	YT	146	 68% 25% . 6%
39	RU	118	 84% 14% ..
39	YU	118	 86% 11% ..
40	RV	101	 84% 15% .
40	YV	101	 84% 14% ..
41	RW	113	 88% 12% .
41	YW	113	 89% 11%


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Mol	Chain	Length	Quality of chain
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	
54	R9	37	

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Mol	Chain	Length	Quality of chain
54	Y9	37	 81% 19%

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 291753 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	1498	Total	C	N	O	P	0	0	0
			32202	14333	5970	10402	1497			
1	XA	1500	Total	C	N	O	P	0	0	0
			32246	14353	5981	10413	1499			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QA	347	U	G	engineered mutation	GB 55771382
XA	347	U	G	engineered mutation	GB 55771382

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	XV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	12	Total	C	N	O	P	0	0	0
			259	116	48	83	12			
23	XX	11	Total	C	N	O	P	0	0	0
			239	107	46	75	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	RA	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			
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			
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	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	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	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	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			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	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	69	Total	C	N	O	S	0	0	0
			581	358	118	104	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	S	0	0	0
			469	298	90	81				
48	Y3	59	Total	C	N	O	S	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	80	Total	Mg	0	0
			80	80		
55	RP	3	Total	Mg	0	0
			3	3		
55	YA	551	Total	Mg	0	0
			551	551		
55	Y5	1	Total	Mg	0	0
			1	1		
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		

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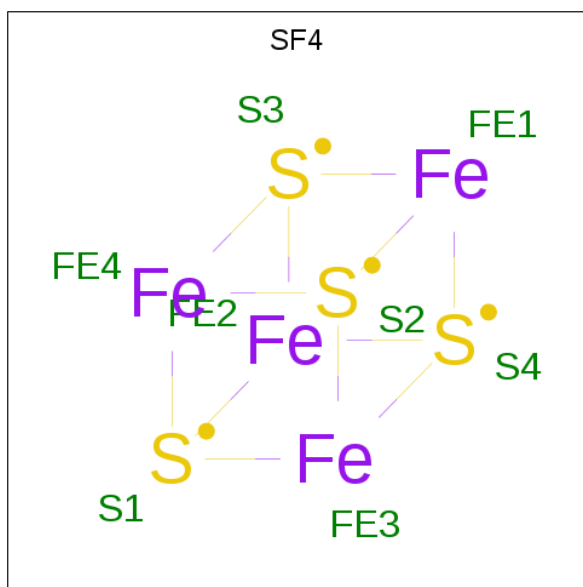
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	XX	1	Total 1	Mg 1	0	0
55	QV	6	Total 6	Mg 6	0	0
55	Y8	2	Total 2	Mg 2	0	0
55	YO	1	Total 1	Mg 1	0	0
55	XA	98	Total 98	Mg 98	0	0
55	YY	1	Total 1	Mg 1	0	0
55	RQ	3	Total 3	Mg 3	0	0
55	R0	2	Total 2	Mg 2	0	0
55	YU	1	Total 1	Mg 1	0	0
55	RO	1	Total 1	Mg 1	0	0
55	QH	1	Total 1	Mg 1	0	0
55	YQ	4	Total 4	Mg 4	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	RD	1	Total 1	Mg 1	0	0
55	Y7	1	Total 1	Mg 1	0	0
55	QF	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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	RA	521	Total 521	Mg 521	0	0
55	YF	1	Total 1	Mg 1	0	0
55	YP	2	Total 2	Mg 2	0	0
55	RE	4	Total 4	Mg 4	0	0
55	XL	2	Total 2	Mg 2	0	0
55	YB	12	Total 12	Mg 12	0	0
55	QT	1	Total 1	Mg 1	0	0
55	XV	8	Total 8	Mg 8	0	0
55	RB	11	Total 11	Mg 11	0	0
55	XM	2	Total 2	Mg 2	0	0
55	YE	4	Total 4	Mg 4	0	0

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



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).

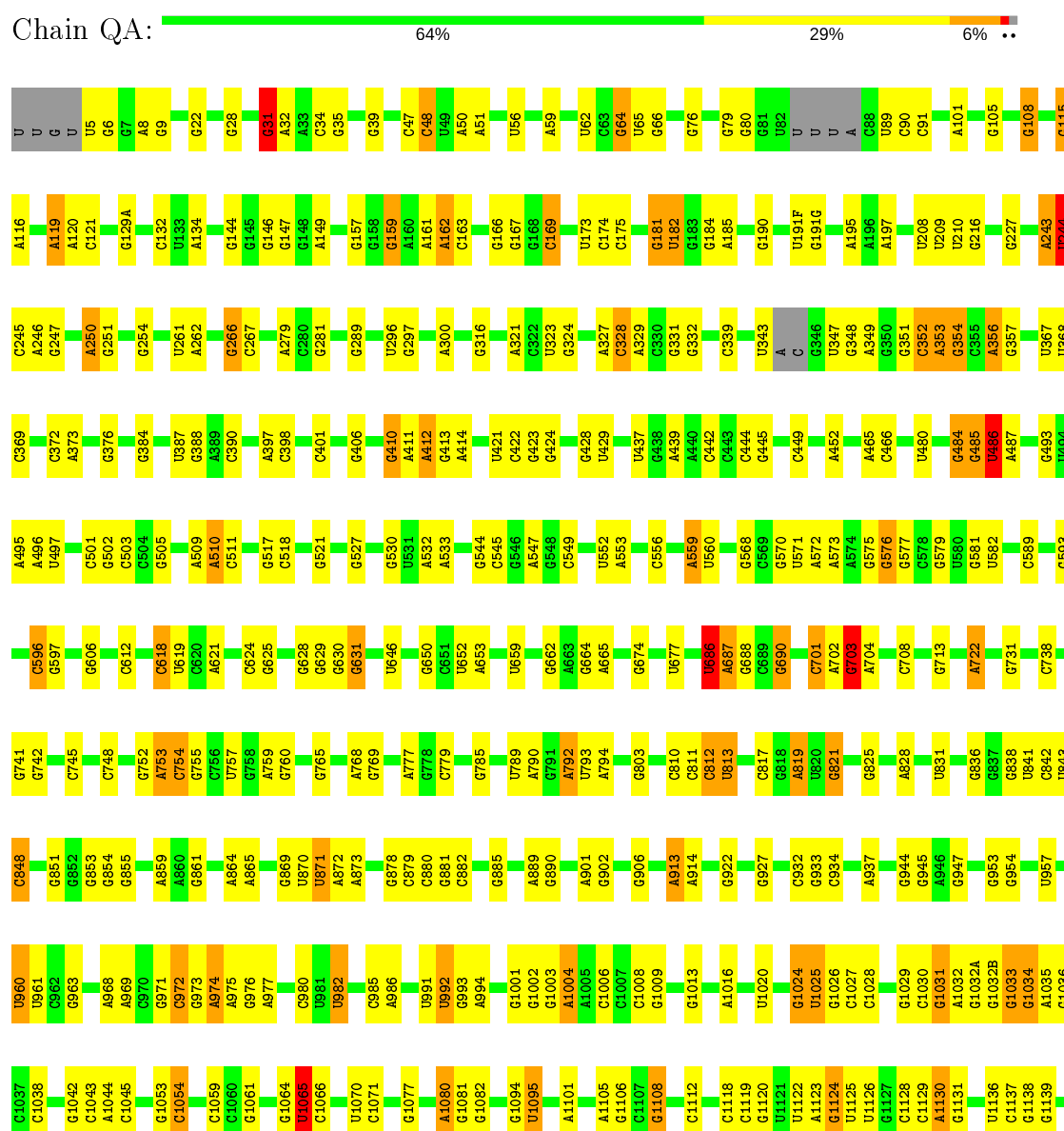
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y9	1	Total	Zn	0	0
			1	1		
57	YY	1	Total	Zn	0	0
			1	1		
57	Y6	1	Total	Zn	0	0
			1	1		
57	QN	1	Total	Zn	0	0
			1	1		
57	XN	1	Total	Zn	0	0
			1	1		
57	RY	1	Total	Zn	0	0
			1	1		
57	Y4	1	Total	Zn	0	0
			1	1		
57	R6	1	Total	Zn	0	0
			1	1		
57	Y5	1	Total	Zn	0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

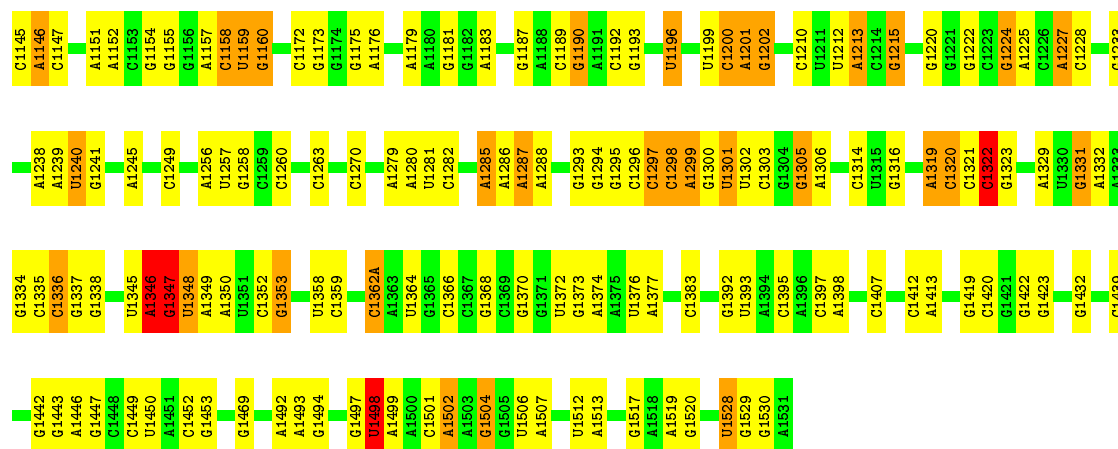
### 3 Residue-property plots

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

Note EDS failed to run properly.

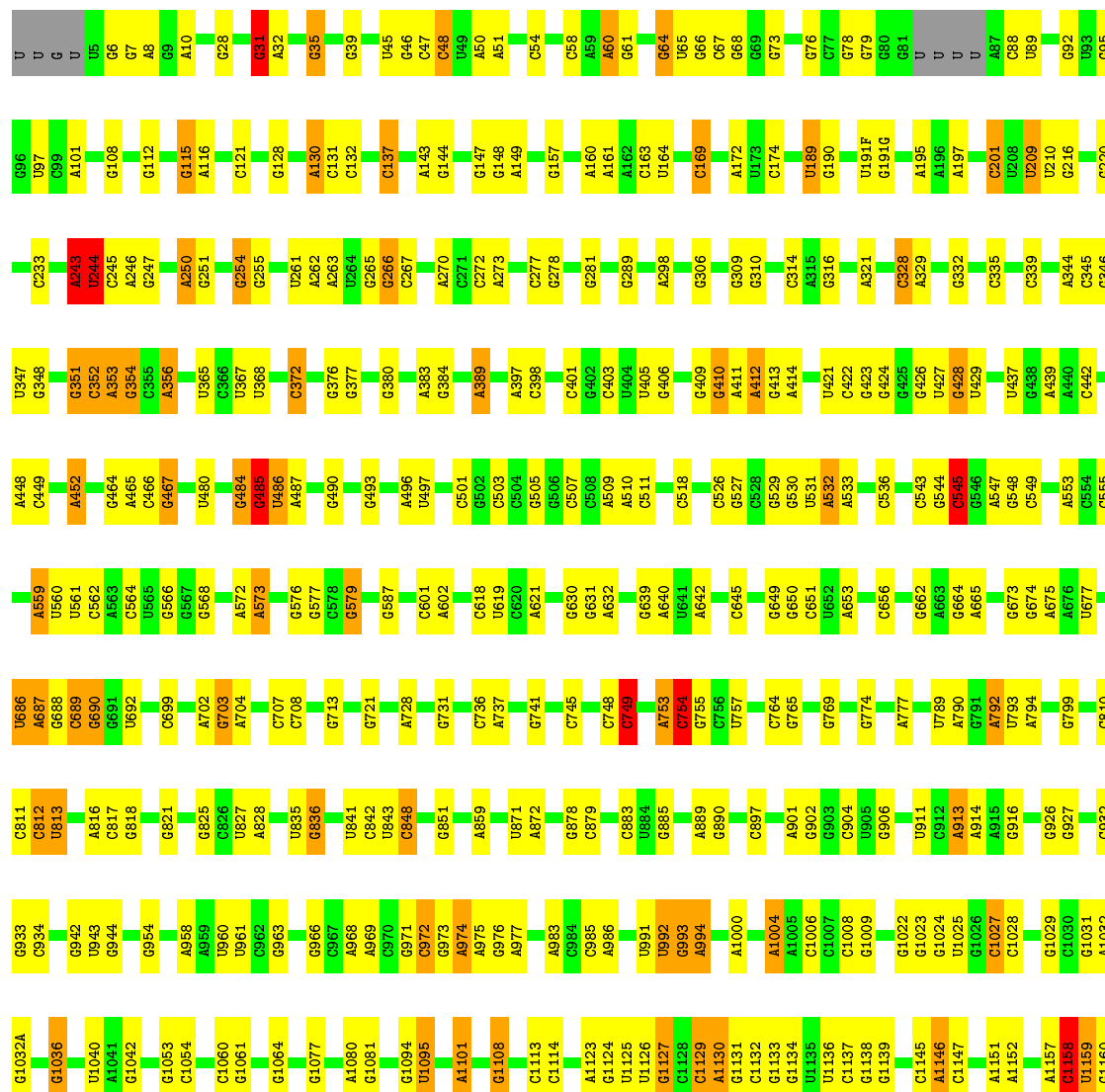
#### • Molecule 1: 16S rRNA

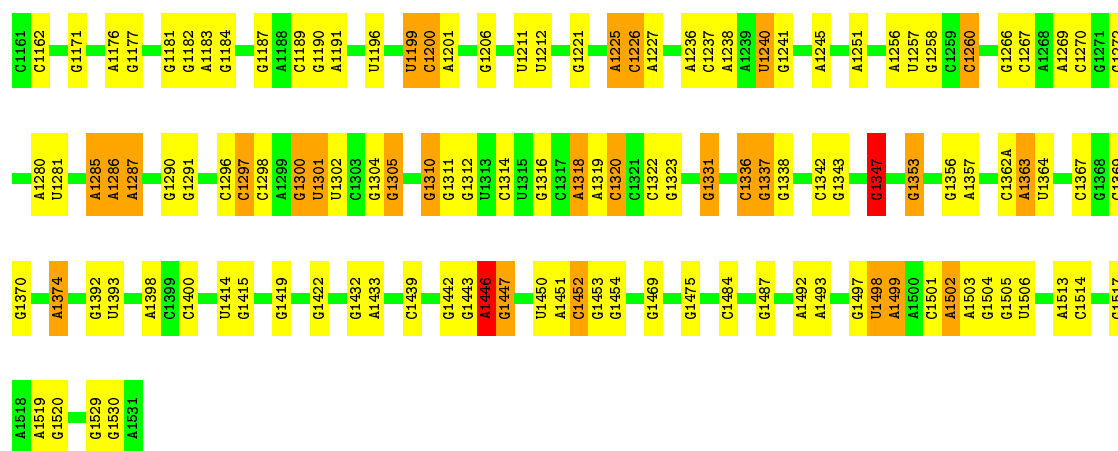




● Molecule 1: 16S rRNA

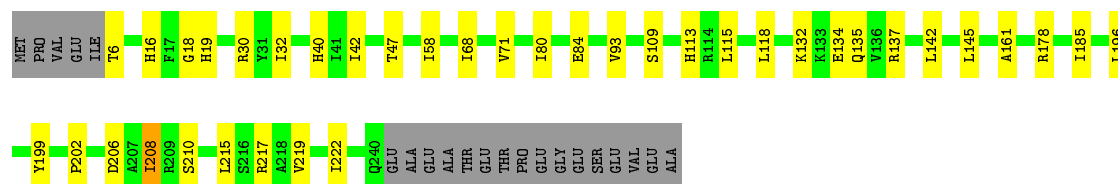
Chain XA:





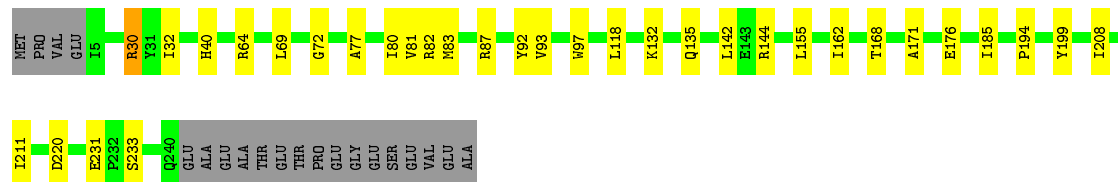
- Molecule 2: 30S ribosomal protein S2

Chain QB: 77% 14% 8%



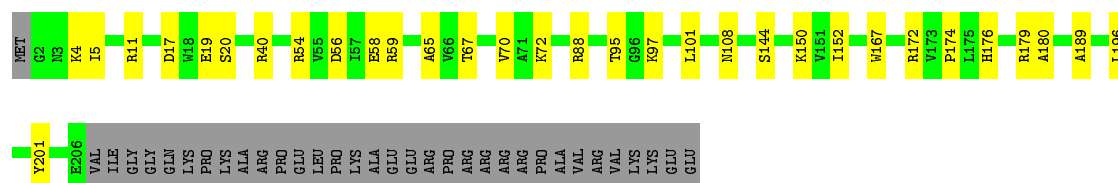
- Molecule 2: 30S ribosomal protein S2

Chain XB: 79% 13% 8%



- Molecule 3: 30S ribosomal protein S3

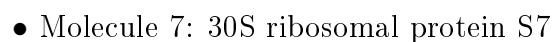
Chain QC: 72% 13% 14%




- Molecule 3: 30S ribosomal protein S3

Chain XC: 72% 13% 14%





Chain QG:  88% 10% ..




- Molecule 7: 30S ribosomal protein S7

Chain XG:  89% 10% ..




- Molecule 8: 30S ribosomal protein S8

Chain QH:  82% 17% .




- Molecule 8: 30S ribosomal protein S8

Chain XH:  83% 16% .



- Molecule 9: 30S ribosomal protein S9

Chain QI:  75% 23% ..



- Molecule 9: 30S ribosomal protein S9

Chain XI:  80% 17% ..



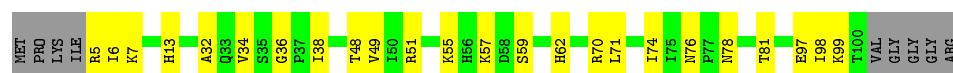
- Molecule 10: 30S ribosomal protein S10

Chain QJ:  70% 25% 6%



- Molecule 10: 30S ribosomal protein S10

Chain XJ: 




- Molecule 11: 30S ribosomal protein S11

Chain QK: 




- Molecule 11: 30S ribosomal protein S11

Chain XK: 



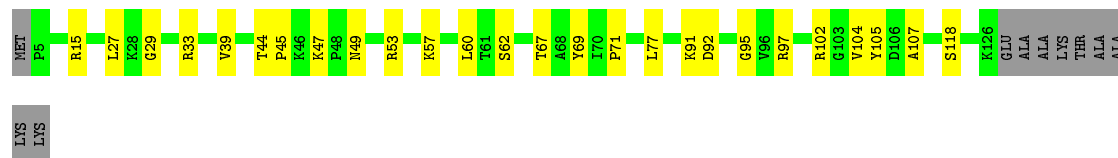
- Molecule 12: 30S ribosomal protein S12

Chain QL: 




- Molecule 12: 30S ribosomal protein S12

Chain XL: 




- Molecule 13: 30S ribosomal protein S13

Chain QM: 




- Molecule 13: 30S ribosomal protein S13

Chain XM: 




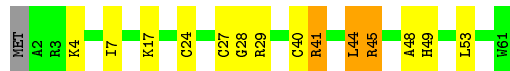
- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:  75% 20% ..



- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:  75% 18% 5% .



- Molecule 15: 30S ribosomal protein S15

Chain QO:  92% 7% .




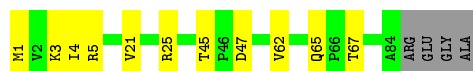
- Molecule 15: 30S ribosomal protein S15

Chain XO:  90% 8% .




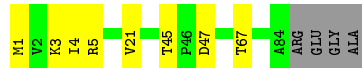
- Molecule 16: 30S ribosomal protein S16

Chain QP:  83% 13% 5%



- Molecule 16: 30S ribosomal protein S16

Chain XP:  86% 9% 5%




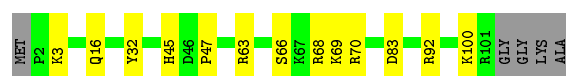
- Molecule 17: 30S ribosomal protein S17

Chain QQ:  89% 7% 5%



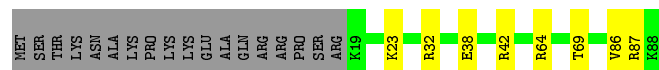
- Molecule 17: 30S ribosomal protein S17

Chain XQ:  83% 12% 5%



- Molecule 18: 30S ribosomal protein S18

Chain QR:  70% 9% 20%



- Molecule 18: 30S ribosomal protein S18

Chain XR:  69% 10% 20%




- Molecule 19: 30S ribosomal protein S19

Chain QS: 



- Molecule 19: 30S ribosomal protein S19

Chain XS:  78% 12% 10%



- Molecule 20: 30S ribosomal protein S20

Chain QT:  89% 5% 7%




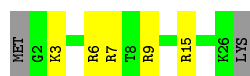
- Molecule 20: 30S ribosomal protein S20

Chain XT:  89% 5% 7%




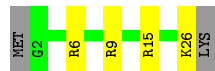
- Molecule 21: 30S ribosomal protein Thx

Chain QU:  74% 19% 7%




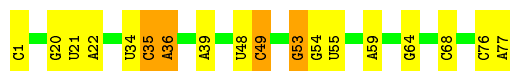
- Molecule 21: 30S ribosomal protein Thx

Chain XU:  78% 15% 7%




- Molecule 22: tRNA fMet

Chain QV:  77% 18% 5%



- Molecule 22: tRNA fMet

Chain XV:  74% 19% 5%




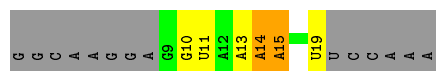
- Molecule 23: messenger RNA

Chain QX:  16% 28% 52%



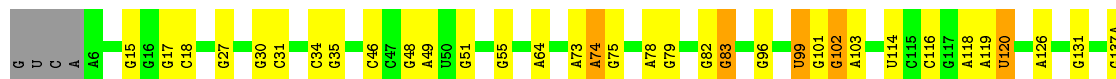
- Molecule 23: messenger RNA

Chain XX:  20% 16% 8% 56%

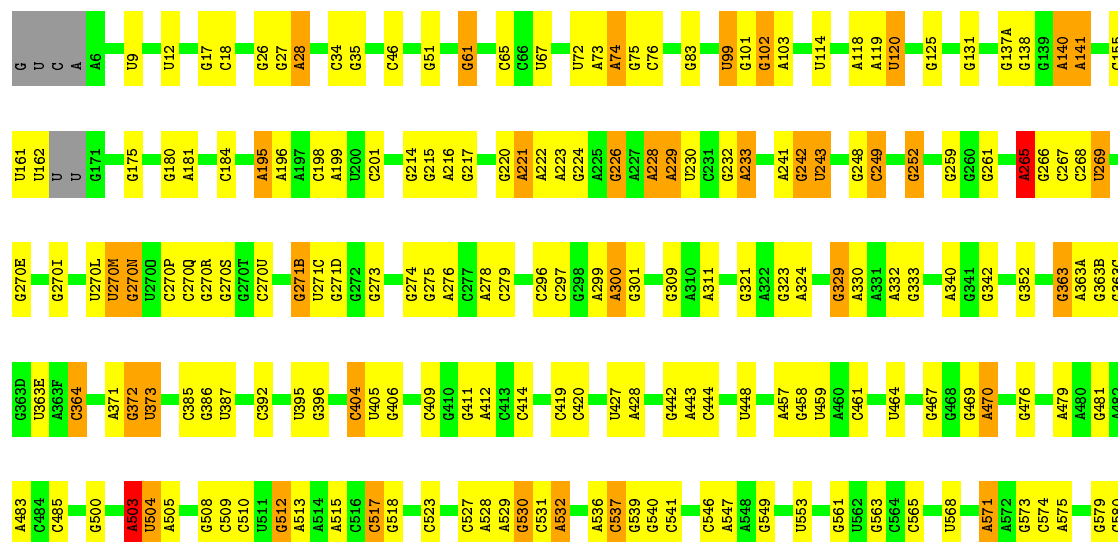


- Molecule 24: 23S rRNA

Chain RA:  67% 26% 6%

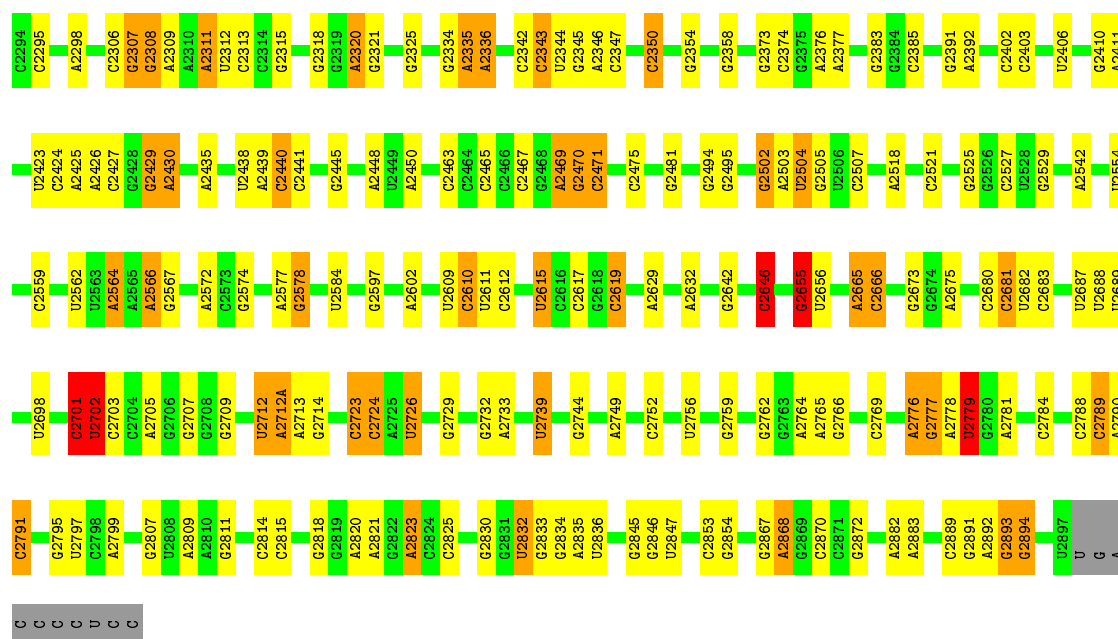


C1886	A1578	A1460	G1203	A1085	G1003	U907	C790	A654	U554	U448	U328	U269	G138
A1689	A1579	A1461	A1204	A1086	C1004	U907	C791	G654A	G556	A454	G329	A270	G139
C1694	A1580	A1471	G1206	A1088	C1005	A910	G792	G654B	G563	C455	A330	A140	A141
A1698	A1583	C1474	A1210	G1091	C1006	C914	A793	G	C565	C456	G333	G270H	U161
A1703	C1585	U1211	U1211	C1092	C1007	C915	A800	G	C565	A457	G336	G270J	U
G1725	A1586	A1214	A1214	G1093	C1008	C916	A800	C	G573	C458	C337	G270K	U
G1725	U1590	A1385	A1385	U1094	A1010	A917	G805	G	C574	A460	C337	U270L	U
G1728	G1591	U1482	U1482	A1095	G1011	A918	G806	G	A575	G461	U339	U270M	U
A1729	C1592	A1220	A1220	A1096	U1012	U922	U807	A	U576	C462	A340	G270N	G171
U1730	G1593	U1234	U1234	U1105	C1013	U922	G808	C	G577	G463	G341	G270P	G177
G1732	G1594	G1235	G1235	U1106	U1014	U930	G809	G	A578	U464	G342	G270Q	G177
G1733	G1595	G1236	G1236	G1110	G1015	U930	C812	C	G579	G465	G343	G270R	A181
C1742	C1598	A1237	A1237	A1111	G1016	U931	C817	G	G583	A466	G344	G270S	C184
G1743	G1607	G1238	G1238	G1112	G1017	G932	G818	C	G583	G467	G345	G270T	C184
G1750	C1608	U1379	U1379	G1122	U1018	G938	G819	C	A586	G468	A346	G270U	A196
C1754	A1609	G1252	G1252	G1123	U1019	U938	C817	C	C587	G469	G352	G270V	A197
A1755	A1610	C1257	C1257	G1124	A1020	A941	U827	G654S	U588	A470	G352	G270W	C198
G1756	C1617	G1258	G1258	G1125	A1021	A944	U828	G	G593	A480	C364	G270X	A199
A1762	G1622	A1264	A1264	G1126	U1022	G944	U828	U657	U594	C481	A371	G271B	U200
G1763	C1627	U1255	U1255	A1129	U1023	A945	U831	G662	C595	G489	G372	G271C	C201
G1764	U1639	C1267	C1267	U1130	G1024	G946	G834	G669	C601	A495	U373	G271D	G214
G1769	C1640	U1267	U1267	U1131	U1026	A953	C834	G	G602	G500	C385	G272	G215
A1773	C1644	G1271	G1271	G1132	A1027	G954	C838	C673	U613	G500	C385	G273F	A216
C1774	G1645	A1272	A1272	G1133	U1033	C955	C838	G674	G615	G500	C385	G273F	G217
H1775	C1646	U1273	U1273	U1134	G1042	A957	C846	A675	G615	A503	U387	G276	G220
G1776	C1648	U1288	U1288	U1142	G1043	U958	U847	A676	U607	U504	G388	G276	A221
U1779	A1652	C1407	C1407	A1142A	G1044	A959	G855	G686	U617	A505	C392	G277	A222
A1780	G1653	C1408	C1408	G1139	A1045	A960	C856	G	U613	C509	U395	A223	A223
C1781	A1654	A1411	A1411	U1140	A1046	C961	C857	G702	U614	G512	U284	A224	A225
C1782	A1655	A1412	A1412	U1141	A1050	C971	U858	G717	G615	A513	C288	A226	G226
A1783	C1656	G1413	G1413	U1142	A1054	A973	U860	G	G617	C517	A401	A228	A228
A1785	C1657	G1416	G1416	C1153	G1055	G974	A861	C721	C621	U405	C404	A229	A229
A1786	C1658	U1286	U1286	A1155	G1059	C974A	C869	A722	G622	C523	U405	U230	U230
A1791	G1662	U1300	U1300	G1171	U1059	A980	G882	G729	G625	C527	G408	C231	C231
G1799	A1663	A1301	A1301	A1173	U1061	A983	C883	C730	U626	A528	C409	G298	G298
C1800	G1666	U1304	U1304	A1174	G1062	A984	C884	C731	A627	A529	G410	A299	A299
G1801	A1667	G1309	G1309	U1175	U1065	C985	C885	A746	G630	C531	G411	A300	A300
C1804	A1668	U1312	U1312	G1176	A1066	C986	C886	C752	G630	A532	C413	G304	G304
G1816	C1669	A1314	A1314	U1177	A1067	C987	C887	A753	A633	G533	C414	G309	G309
G1817	A1670	C1314	C1314	G1178	G1068	A988	C888	C753	C634	G537	C419	A310	A310
U1818	G1674	U1331	U1331	C1179	A1069	G989	C889	G765	A637	G539	C420	A311	C253
A1819	C1675	G1332	G1332	C1180	A1070	C992	C893	G768	G638	G540	U427	G317	G254
		U1341	U1341	C1181	G1071	C993	C893	G776	G645	C546	A428	G321	G259
				G1184	A1077	C994	A896	G	A646	A547	A428	A322	A268
				G1187	U1078	C995	C897	G	A651	A547	A428	G323	G266
				U1188	C1079	G996	A900	A782	G651	A547	A428	A324	C267
				G1195	U1082	C998	A901	A783	G651	A547	A428	A324	C268
					U1083	C999	A901	A784	G651	A547	A428	A324	C268
					A1084	A1000	C904	G785	A653	U553	C444	G327	C268



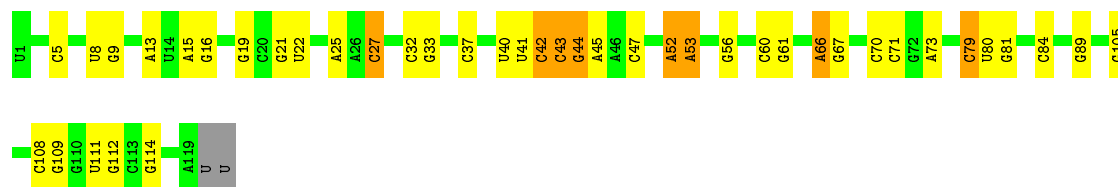


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G2181	G2100	A1970	G1859	A1729	G1595	G1491	C1375	C1223	U1105	A1020	U907	A783	g	C587
G2182	G2100	A1971	G1860	U1730	G1595	G1491	C1375	G1228	G1106	A1021	A910	A784	C	C
G2183	C2105	A1972	G1861	G1731	C1598	G1492	A1378	G1231	C1109	G1023	C915	G786	C	C
G2184	G2106	C1979	U1864	A1743	A1603	C1493	A1379	G1232	G1110	G1024	G916	U787	C	C591
G2185	C2107	G1980	G1869	G1750	C1607	A1496	A1384	G1236	A1111	G1025	A917	A788	A	A592
G2186	C2108	C1982	G1870	G1756	A1608	U1497	C1386	A1237	G1112	U1026	A918	G789	C	G593
U2189	C2111	U1991	A1872	C1754	G1612	G1500	U1391	G1238	G1114	A1027	U930	C791	C	C595
G2190	G2112	G1992	G1878	A1755	G1613	C1504	U1394	G1243	G1120	U1033	G931	G792	C	G598
G2191	U2113	U1993	G1879	G1756	G1613	C1505	U1395	G1252	G1121	U1035	G932	G794	C	C
G2192	A2114	C1996	C1880	G1762	C1617	G1506	U1396	G1253	G1122	G1036	A941	C795	C	C601
A2198	G2115	G1997	C1881	A1763	C1618	A1507	A1395	G1256	C1123	A1046	G942	A800	C	G602
A2199	G2116	G1997	C1882	G1763	C1617	A1508	U1396	A1257	C1124	G1047	U943	A800	C	A603
C2205	A2117	G1998	G1883	G1764	G1622	A1509	C1399	G1256	G1125	G1047	G944	G805	U	G604
U2218	U2118	C1999	G1888	G1769	G1625	A1510	C1402	C1257	A1126	A1050	A945	G805	U	G605
A2219	A2119	C2006	A1889	A1773	C1625	A1511	G1402	U1263	U1130	A1050	G946	C812	U	U607
G2212	G2121	G2007	G1899	U1773	C1638	G1512	C1407	U1263	G1131	A1054	A953	A819	U	G609A
U2213	U2122	C2008	G1900	U1774	C1638	A1528	C1407	G1264	G1135	G1055	U957	A820	U	C611
G2215	G2123	G2009	G1901	U1775	U1639	A1529	C1411	A1265	G1136	G1056	G956	C825	U	G612
G2216	G2124	G2010	G1902	G1776	C1640	G1530	C1411	G1266	U1142	G1057	U958	U826	U	G613
A2225	A2126	G2012	G1903	U1779	C1644	G1531	G1416	G1270	G1139	G1058	U959	U827	U	G614
G2238	G2127	C2013	G1904	A1780	G1645	G1532	G1417	G1271	U1143	G1059	A960	U828	U	G615
G2239	U2132	A2019	C1905	C1781	G1646	U1533	G1418	A1272	U1175	U1060	G961	A829	U	A616
G2240	G2133	C2020	G1906	U1781	C1646	A1534	A1419	G1272	A1142	U1061	U960	U829	U	G617
G2241	G2134	A2021	C1907	A1784	G1647	A1535	U1420	G1273	A1143	G1062	U961	A830	U	
A2242	A2135	U2022	G1908	U1785	C1648	G1536	G1421	G1274	G1176	G1063	A973	G831	U	
U2243	G2136	G2023	A1913	A1786	G1651	G1537	G1422	G1296	G1151	A1067	G974	C837	U	G620
U2244	C2136	A2030	C1914	A1787	A1652	G1540	G1423	U1300	G1173	G1068	C974A	C838	U	A621
U2245	C2140	A2031	A1919	A1791	G1653	U1542	G1424	A1301	G1174	A1069	G975	C838	U	G622
G2246	G2141	G2032	C1920	A1791	A1654	G1543	A1427	U1310	U1175	A1070	A980	C846	U	G625
A2247	C2145	A2033	G1929	C1795	C1656	A1544	C1428	G1311	G1176	G1071	C982	U847	U	G626
G2258	C2146	C2039	U1930	G1799	A1664	C1549	A1444A	U1312	C1178	C1076	A983	C856	U	G628
A2266	G2147	U1931	G1931	C1800	G1667	C1549	C1445	U1313	C1179	A1077	G987	U858	U	G629
A2267	C2148	C2043	A1936	G1801	A1668	A1558	A1449	C1314	C1180	U1078	G989	G859	U	G630
C2275	G2151	A2051	A1937	C1804	A1669	G1559	G1449A	U1329	G1184	U1082	C992	U860	U	A633
A2278	G2152	G2052	U1938	G1811	G1674	A1566	U1454	G1332	G1190	U1083	G993	A866	U	C634
G2279	G2153	C2053	U1939	U1815	C1686	A1567	G1455	G1338	G1195	A1084	C994	A752	U	C635
G2280	G2154	A2054	U1940	G1816	C1686	A1568	G1455	U1341	C1196	C995	C995	C753	U	A637
C2283	G2155	C2055	U1955	G1817	U1689	A1569	A1460	U1341	C1196	A1086	A996	C754	U	G638
G2284	G2156	G2056	U1956	U1818	A1689	C1575	G1461	A1349	U1204	G1087	A1000	C755	U	U639
A2287	A2157	C1957	C1957	U1819	U1689	C1575	G1467	U1349	A1205	A1088	C1005	C756	U	C645
A2288	U2167	C1958	C1958	A1819	C1693	U1578	C1467	A1349	G1206	G1089	C1005	C757	U	A646
G2289	G2168	U1963	G1959	G1826	C1694	A1579	A1471	U1352	A1210	U1093	U1011	A764	U	C650
G2290	A2169	U1963	U1963	G1827	G1695	G1581	C1474	A1359	U1211	A1094	G1012	C765	U	G651
U2291	G2170	G2068	G1964	U1828	A1698	G1581	C1474	A1359	C1217	A1095	U1012	C766	U	
C2292	A2171	G2069	U1965	A1829	G1703	C1585	G1479	A1365	A1220	A1096	G1017	A896	U	A654
G2293	U2172	A2071	A1966	G1835	G1725	A1586	G1480	G1368	G1221	U1097	G1017	C897	U	G654B
	A2173	U2089	G1968	A1847		A1587	G1483			A1103	C1018	A900	g	g



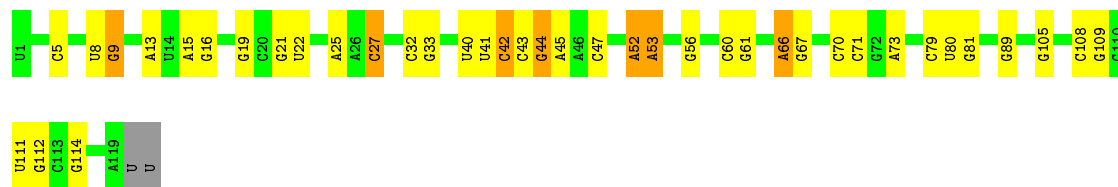
• Molecule 25: 5S rRNA

Chain RB: 




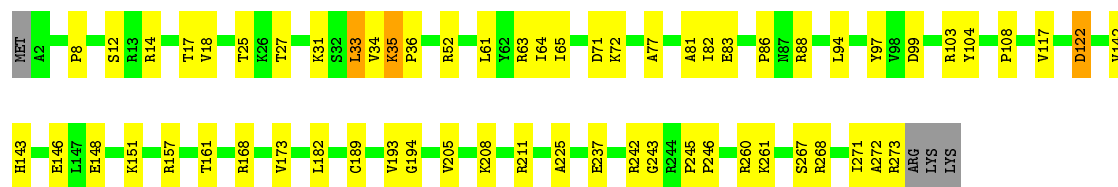
• Molecule 25: 5S rRNA

Chain YB: 




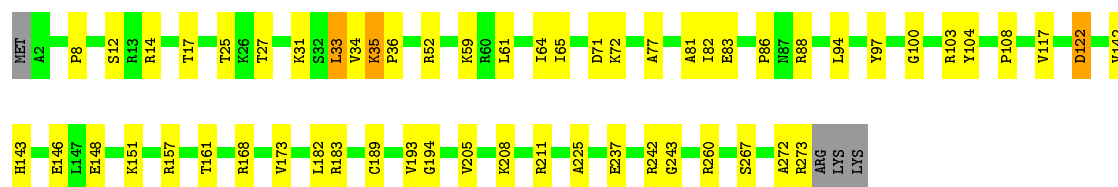
• Molecule 26: 50S ribosomal protein L2

Chain RD: 




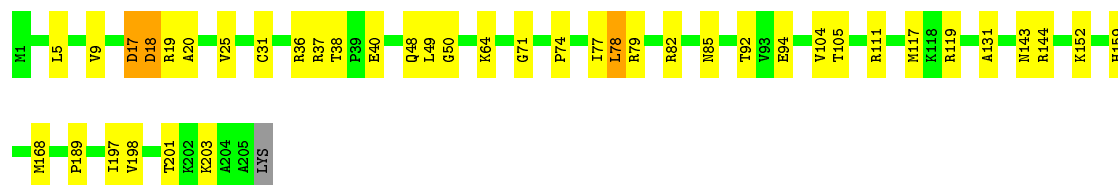
• Molecule 26: 50S ribosomal protein L2

Chain YD:  78% 20% ..




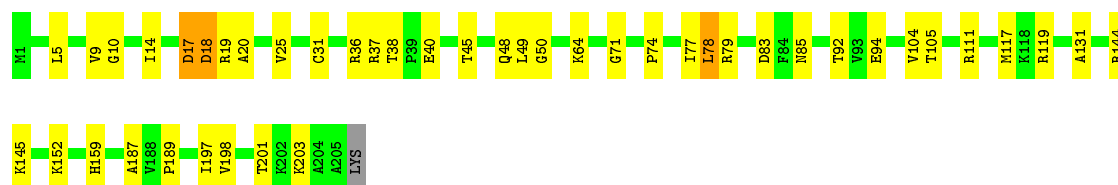
- Molecule 27: 50S ribosomal protein L3

Chain RE:  80% 18% .




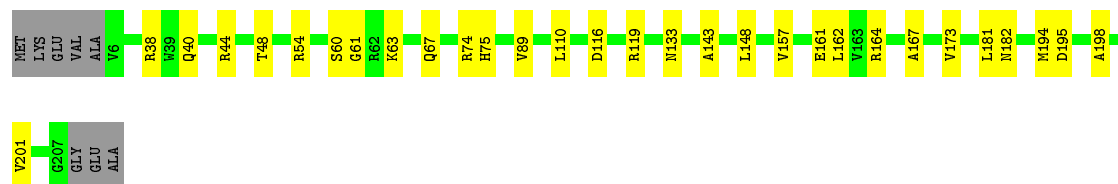
- Molecule 27: 50S ribosomal protein L3

Chain YE:  78% 20% .



- Molecule 28: 50S ribosomal protein L4

Chain RF:  82% 14% .




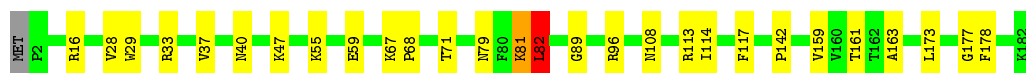
- Molecule 28: 50S ribosomal protein L4

Chain YF:  86% 10% .



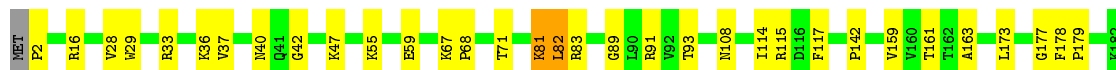
- Molecule 29: 50S ribosomal protein L5

Chain RG:  84% 14% ...



- Molecule 29: 50S ribosomal protein L5

Chain YG: 81% 17% ..



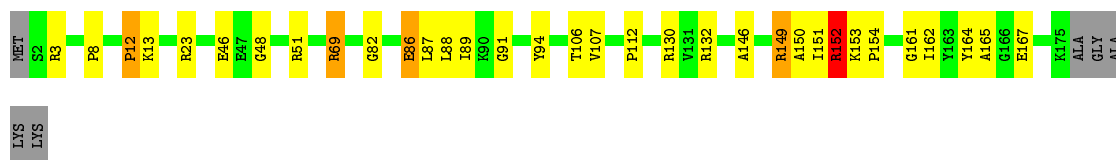
- Molecule 30: 50S ribosomal protein L6

Chain RH: 79% 15% ..



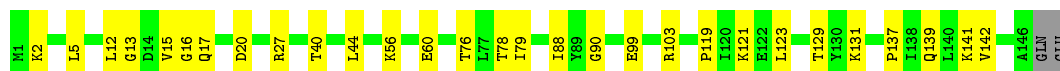
- Molecule 30: 50S ribosomal protein L6

Chain YH: 78% 16% ..



- Molecule 31: 50S ribosomal protein L9

Chain RI: 79% 20% .



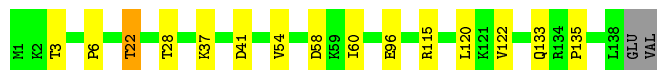
- Molecule 31: 50S ribosomal protein L9

Chain YI: 78% 21% .



- Molecule 32: 50S ribosomal protein L13

Chain RN: 88% 10% ..



- Molecule 32: 50S ribosomal protein L13

Chain YN:  91% 7% ..



- Molecule 33: 50S ribosomal protein L14

Chain RO:  89% 11% .




- Molecule 33: 50S ribosomal protein L14

Chain YO:  91% 8% .




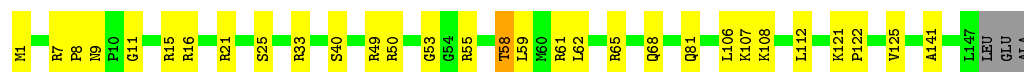
- Molecule 34: 50S ribosomal protein L15

Chain RP:  79% 21%



- Molecule 34: 50S ribosomal protein L15

Chain YP:  78% 19% ..




- Molecule 35: 50S ribosomal protein L16

Chain RQ:  76% 24%




- Molecule 35: 50S ribosomal protein L16

Chain YQ:  79% 21%




- Molecule 36: 50S ribosomal protein L17

Chain RR:  86% 13% ..




- Molecule 36: 50S ribosomal protein L17

Chain YR:  81% 18% .




- Molecule 37: 50S ribosomal protein L18

Chain RS:  83% 15% ..



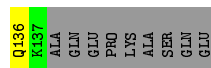
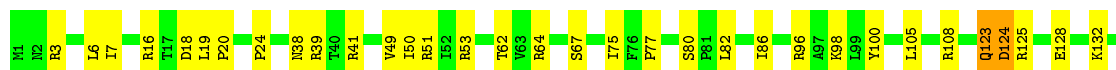
- Molecule 37: 50S ribosomal protein L18

Chain YS:  81% 17% ..



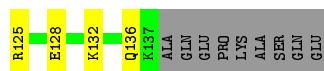
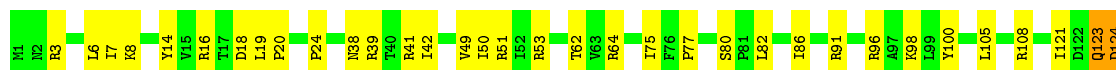
- Molecule 38: 50S ribosomal protein L19

Chain RT:  71% 22% • 6%



- Molecule 38: 50S ribosomal protein L19

Chain YT:  68% 25% • 6%



- Molecule 39: 50S ribosomal protein L20

MET
P2
R10
K19
W25
N44
R50
K51
R52
R53
K54
R55
D56
F57
R58
N75
Y76
I88
F89
V90
D91
R92
K93
N94
L95
G118

- |      |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |
|------|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
| ME-T | P2 | W25 | N44 | H49 | R50 | K51 | R52 | R53 | K54 | R55 | D56 | F57 | R58 | 188 | E89 | V90 | D91 | R92 | K93 | N94 | L95 | G118 |
|------|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|

- 
- | Category | Count |
|----------|-------|
| M1       | 1000  |
| I4       | 990   |
| Q11      | 980   |
| E23      | 970   |
| K24      | 960   |
| L39      | 950   |
| L40      | 940   |
| E43      | 930   |
| K44      | 920   |
| T49      | 910   |
| P50      | 900   |
| V51      | 890   |
| V52      | 880   |
| E53      | 870   |
| V61      | 860   |
| L62      | 850   |
| G63      | 840   |
| F75      | 830   |
| Q89      | 820   |
| T92      | 810   |
| G101     | 800   |


- |                   |
|-------------------|
| M1                |
| I4                |
| E23<br>K24        |
| L39<br>L40        |
| E43<br><b>K44</b> |
| T49               |
| P50<br>V51        |
| V52<br>E53        |
| V61               |
| L62<br>G63        |
| F75               |
| R88<br>Q89        |
| T92               |
| G101              |

- 
- | Item | Category |
|------|----------|
| M1   | Green    |
| R15  | Green    |
| R18  | Green    |
| N40  | Orange   |
| K41  | Green    |
| R42  | Yellow   |
| A58  | Green    |
| V59  | Green    |
| N60  | Green    |
| N61  | Green    |
| H62  | Green    |
| D63  | Green    |
| M64  | Green    |
| L65  | Green    |
| E66  | Green    |
| L86  | Green    |
| I96  | Green    |
| H11  | Green    |
| G12  | Green    |
| K13  | Green    |

- |      |
|------|
| M1   |
| R15  |
| I35  |
| T39  |
| N40  |
| K41  |
| R42  |
| A58  |
| M64  |
| L65  |
| E66  |
| L86  |
| I96  |
| H111 |
| G112 |
| K113 |


- |     |     |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | LYS | T3 | A4 | Y5 | K25 | Y26 | T35 | N41 | E44 | K53 | V54 | N55 | T56 | L57 | L66 | K78 | A79 | I80 | V81 | I89 | G94 | LEU | I1E |
|-----|-----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- WORLDWIDE  
 PDB  
PROTEIN DATA BANK

Chain YX:  77% 19% .




- Molecule 43: 50S ribosomal protein L24

Chain RY:  77% 20% .



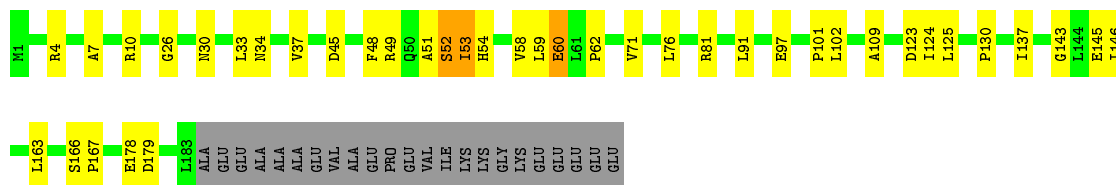
- Molecule 43: 50S ribosomal protein L24

Chain YY:  79% 18% .



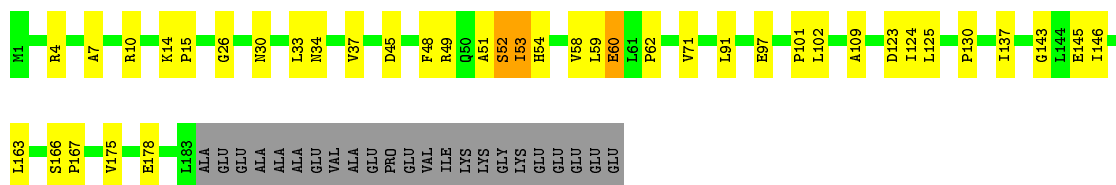
- Molecule 44: 50S ribosomal protein L25

Chain RZ:  69% 18% 11% .



- Molecule 44: 50S ribosomal protein L25

Chain YZ:  69% 18% 11% .



- Molecule 45: 50S ribosomal protein L27

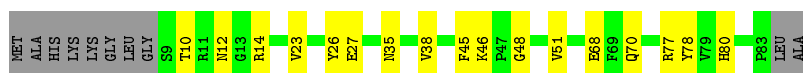
Chain R0:  75% 20% 5% .



- Molecule 45: 50S ribosomal protein L27

Chain Y0:  68% 20% 12% .

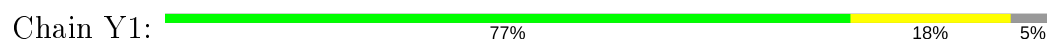




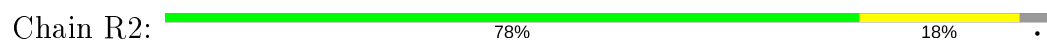
- Molecule 46: 50S ribosomal protein L28



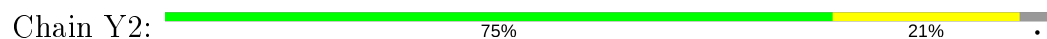
- Molecule 46: 50S ribosomal protein L28



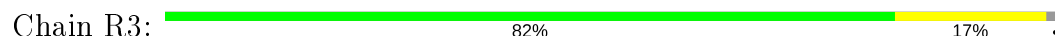
- Molecule 47: 50S ribosomal protein L29



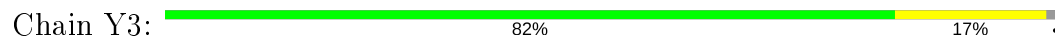
- Molecule 47: 50S ribosomal protein L29



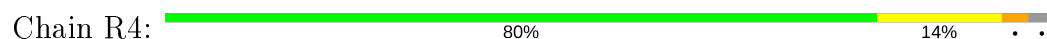
- Molecule 48: 50S ribosomal protein L30

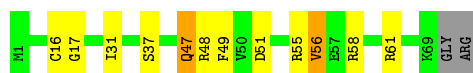


- Molecule 48: 50S ribosomal protein L30



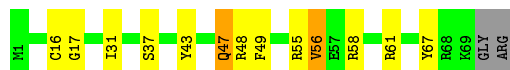
- Molecule 49: 50S ribosomal protein L31





- Molecule 49: 50S ribosomal protein L31

Chain Y4: 79% 15% . .



- Molecule 50: 50S ribosomal protein L32

Chain R5: 83% 15% .



- Molecule 50: 50S ribosomal protein L32

Chain Y5: 80% 18% .



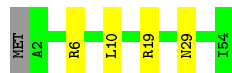
- Molecule 51: 50S ribosomal protein L33

Chain R6: 87% 11% .



- Molecule 51: 50S ribosomal protein L33

Chain Y6: 91% 7% .



- Molecule 52: 50S ribosomal protein L34

Chain R7: 88% 8% .



- Molecule 52: 50S ribosomal protein L34

Chain Y7: 86% 12% .



- Molecule 53: 50S ribosomal protein L35

Chain R8: 72% 20% 6%



- Molecule 53: 50S ribosomal protein L35

Chain Y8: 75% 17% 6%



- Molecule 54: 50S ribosomal protein L36

Chain R9: 81% 19%



- Molecule 54: 50S ribosomal protein L36

Chain Y9: 81% 19%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.65Å 447.95Å 618.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	124.48 – 3.18	Depositor
% Data completeness (in resolution range)	99.3 (124.48-3.18)	Depositor
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.12	Depositor
R, $R_{free}$	0.232 , 0.251	Depositor
Wilson B-factor (Å <sup>2</sup> )	76.7	Xtriage
Anisotropy	0.198	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	291753	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	QA	0.76	0/36046	1.03	110/56257 (0.2%)
1	XA	0.88	0/36097	1.04	113/56339 (0.2%)
2	QB	0.32	0/1942	0.58	0/2619
2	XB	0.37	0/1950	0.60	0/2630
3	QC	0.36	0/1629	0.53	0/2195
3	XC	0.36	0/1629	0.53	0/2195
4	QD	0.41	0/1733	0.55	0/2318
4	XD	0.41	0/1733	0.55	0/2318
5	QE	0.36	0/1171	0.55	0/1576
5	XE	0.36	0/1171	0.55	0/1576
6	QF	0.37	0/856	0.52	0/1154
6	XF	0.37	0/856	0.52	0/1154
7	QG	0.34	0/1276	0.47	0/1709
7	XG	0.33	0/1276	0.47	0/1709
8	QH	0.39	0/1128	0.54	0/1517
8	XH	0.39	0/1128	0.54	0/1517
9	QI	0.36	0/1029	0.60	0/1379
9	XI	0.43	1/1017 (0.1%)	0.62	0/1365
10	QJ	0.34	0/814	0.59	0/1095
10	XJ	0.39	0/790	0.60	0/1063
11	QK	0.38	0/900	0.55	0/1213
11	XK	0.43	0/879	0.56	0/1187
12	QL	0.45	0/991	0.64	0/1327
12	XL	0.54	0/972	0.66	0/1301
13	QM	0.36	0/965	0.61	0/1292
13	XM	0.37	0/956	0.63	0/1281
14	QN	0.43	0/501	0.64	1/664 (0.2%)
14	XN	0.43	0/501	0.64	1/664 (0.2%)
15	QO	0.32	0/745	0.51	0/992
15	XO	0.36	0/740	0.51	0/987
16	QP	0.43	0/721	0.56	0/970
16	XP	0.43	0/721	0.56	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	QQ	0.42	0/847	0.54	0/1131
17	XQ	0.42	0/847	0.54	0/1131
18	QR	0.36	0/579	0.56	0/768
18	XR	0.36	0/579	0.56	0/768
19	QS	0.33	0/680	0.67	0/915
19	XS	0.40	0/689	0.66	0/926
20	QT	0.32	0/765	0.57	0/1007
20	XT	0.32	0/765	0.56	0/1007
21	QU	0.40	0/221	0.69	0/288
21	XU	0.40	0/221	0.69	0/288
22	QV	0.85	1/1836 (0.1%)	1.01	6/2859 (0.2%)
22	XV	0.86	1/1836 (0.1%)	1.02	7/2859 (0.2%)
23	QX	0.59	0/290	1.08	2/450 (0.4%)
23	XX	0.65	0/268	0.84	0/416
24	RA	1.03	4/69521 (0.0%)	1.07	285/108529 (0.3%)
24	YA	1.16	8/69543 (0.0%)	1.11	344/108563 (0.3%)
25	RB	0.82	0/2878	1.01	6/4490 (0.1%)
25	YB	0.82	0/2878	1.01	5/4490 (0.1%)
26	RD	0.61	0/2165	0.71	1/2919 (0.0%)
26	YD	0.61	0/2165	0.71	1/2919 (0.0%)
27	RE	0.53	0/1601	0.71	2/2160 (0.1%)
27	YE	0.53	0/1601	0.71	2/2160 (0.1%)
28	RF	0.55	0/1620	0.59	0/2194
28	YF	0.55	0/1620	0.59	0/2194
29	RG	0.40	0/1499	0.65	2/2016 (0.1%)
29	YG	0.40	0/1499	0.65	2/2016 (0.1%)
30	RH	0.41	0/1362	0.65	0/1841
30	YH	0.41	0/1362	0.65	0/1841
31	RI	0.35	0/1151	0.66	0/1558
31	YI	0.35	0/1151	0.66	0/1558
32	RN	0.49	0/1131	0.65	1/1525 (0.1%)
32	YN	0.49	0/1131	0.65	1/1525 (0.1%)
33	RO	0.55	0/943	0.61	0/1269
33	YO	0.55	0/943	0.61	0/1269
34	RP	0.45	0/1162	0.76	1/1544 (0.1%)
34	YP	0.50	0/1139	0.79	1/1514 (0.1%)
35	RQ	0.50	0/1143	0.66	0/1527
35	YQ	0.50	0/1143	0.66	0/1527
36	RR	0.49	0/974	0.69	1/1302 (0.1%)
36	YR	0.51	0/974	0.67	1/1302 (0.1%)
37	RS	0.39	0/892	0.71	0/1187
37	YS	0.39	0/892	0.71	0/1187
38	RT	0.48	0/1155	0.66	1/1542 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	YT	0.47	0/1155	0.66	1/1542 (0.1%)
39	RU	0.52	0/982	0.61	0/1306
39	YU	0.52	0/982	0.61	0/1306
40	RV	0.46	0/790	0.67	0/1057
40	YV	0.46	0/790	0.67	0/1057
41	RW	0.54	0/911	0.61	0/1220
41	YW	0.54	0/911	0.61	0/1220
42	RX	0.53	0/739	0.58	0/993
42	YX	0.53	0/739	0.58	0/993
43	RY	0.50	0/831	0.55	0/1108
43	YY	0.50	0/831	0.55	0/1108
44	RZ	0.39	0/1493	0.71	0/2026
44	YZ	0.39	0/1493	0.70	0/2026
45	R0	0.47	0/652	0.56	0/867
45	Y0	0.56	0/607	0.60	0/809
46	R1	0.54	0/770	0.65	0/1022
46	Y1	0.54	0/736	0.65	0/978
47	R2	0.36	0/583	0.53	0/771
47	Y2	0.36	0/583	0.53	0/771
48	R3	0.44	0/474	0.61	0/635
48	Y3	0.43	0/474	0.61	0/635
49	R4	0.36	0/578	0.62	0/776
49	Y4	0.36	0/578	0.62	0/776
50	R5	0.49	0/473	0.56	0/639
50	Y5	0.49	0/473	0.56	0/639
51	R6	0.32	0/460	0.50	0/613
51	Y6	0.32	0/460	0.50	0/613
52	R7	0.52	0/417	0.56	0/550
52	Y7	0.62	0/426	0.59	0/561
53	R8	0.54	0/525	0.83	2/691 (0.3%)
53	Y8	0.54	0/525	0.82	2/691 (0.3%)
54	R9	0.41	0/310	0.49	0/407
54	Y9	0.41	0/310	0.49	0/407
All	All	0.88	15/315585 (0.0%)	0.97	902/471827 (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
4	QD	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	XD	0	2
12	QL	0	2
12	XL	0	2
19	QS	0	1
26	RD	0	4
26	YD	0	4
27	RE	0	4
27	YE	0	4
29	RG	0	1
29	YG	0	1
30	RH	0	2
30	YH	0	2
31	RI	0	2
31	YI	0	2
32	RN	0	1
32	YN	0	1
34	RP	0	1
34	YP	0	3
35	RQ	0	1
35	YQ	0	1
39	RU	0	1
39	YU	0	1
40	RV	0	2
40	YV	0	2
44	RZ	0	4
44	YZ	0	4
47	R2	0	1
47	Y2	0	1
49	R4	0	2
49	Y4	0	2
53	R8	0	4
53	Y8	0	4
All	All	0	71

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	1	C	OP3-P	-10.78	1.48	1.61
22	XV	1	C	OP3-P	-10.77	1.48	1.61
24	YA	1142(A)	A	N9-C4	-5.74	1.34	1.37
24	YA	528	A	N9-C4	-5.62	1.34	1.37
9	XI	121	ARG	C-N	-5.60	1.21	1.34



The worst 5 of 902 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	1301	U	N1-C2-O2	13.33	132.13	122.80
1	XA	1158	C	N1-C2-O2	12.35	126.31	118.90
1	QA	1301	U	N3-C2-O2	-11.96	113.83	122.20
1	QA	1158	C	C2-N1-C1'	11.77	131.75	118.80
1	QA	1301	U	C2-N1-C1'	11.74	131.79	117.70

There are no chirality outliers.

5 of 71 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	QD	19	LEU	Peptide
4	QD	33	MET	Peptide
12	QL	104	VAL	Peptide
12	QL	47	LYS	Peptide
19	QS	41	VAL	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32202	0	16255	204	0
1	XA	32246	0	16277	177	0
2	QB	1907	0	1958	20	0
2	XB	1915	0	1969	17	0
3	QC	1605	0	1668	21	0
3	XC	1605	0	1668	20	2
4	QD	1703	0	1766	17	0
4	XD	1703	0	1767	22	0
5	QE	1155	0	1213	11	0
5	XE	1155	0	1213	7	0
6	QF	843	0	857	10	0
6	XF	843	0	857	8	0
7	QG	1257	0	1296	11	0
7	XG	1257	0	1296	10	0
8	QH	1108	0	1164	16	0
8	XH	1108	0	1165	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	QI	1010	0	1037	26	0
9	XI	998	0	1023	16	0
10	QJ	801	0	849	18	0
10	XJ	777	0	816	19	0
11	QK	885	0	904	19	2
11	XK	864	0	881	15	0
12	QL	975	0	1062	12	0
12	XL	956	0	1046	16	0
13	QM	955	0	1021	14	0
13	XM	946	0	1008	17	0
14	QN	492	0	529	7	0
14	XN	492	0	529	8	0
15	QO	734	0	771	5	0
15	XO	729	0	768	4	0
16	QP	705	0	725	7	0
16	XP	705	0	725	4	0
17	QQ	834	0	904	6	0
17	XQ	834	0	904	13	0
18	QR	574	0	644	6	0
18	XR	574	0	644	7	0
19	QS	665	0	686	15	0
19	XS	674	0	699	8	0
20	QT	763	0	860	5	0
20	XT	763	0	861	5	0
21	QU	217	0	234	5	0
21	XU	217	0	234	4	0
22	QV	1644	0	836	3	0
22	XV	1644	0	836	4	0
23	QX	259	0	129	2	0
23	XX	239	0	119	1	0
24	RA	62071	0	31285	264	0
24	YA	62091	0	31293	267	0
25	RB	2573	0	1306	15	0
25	YB	2573	0	1306	13	0
26	RD	2115	0	2195	42	0
26	YD	2115	0	2195	40	0
27	RE	1568	0	1634	25	0
27	YE	1568	0	1634	26	0
28	RF	1585	0	1632	20	0
28	YF	1585	0	1632	15	0
29	RG	1474	0	1535	17	0
29	YG	1474	0	1535	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	RH	1336	0	1418	19	0
30	YH	1336	0	1418	20	1
31	RI	1136	0	1223	17	0
31	YI	1136	0	1223	19	0
32	RN	1104	0	1180	9	0
32	YN	1104	0	1180	5	0
33	RO	933	0	996	12	0
33	YO	933	0	996	10	0
34	RP	1145	0	1227	22	0
34	YP	1122	0	1206	22	0
35	RQ	1122	0	1179	25	0
35	YQ	1122	0	1179	21	0
36	RR	960	0	1021	9	0
36	YR	960	0	1021	13	0
37	RS	882	0	943	11	0
37	YS	882	0	943	14	0
38	RT	1141	0	1202	22	0
38	YT	1141	0	1202	23	0
39	RU	964	0	1022	19	0
39	YU	964	0	1021	18	0
40	RV	779	0	852	11	0
40	YV	779	0	852	10	3
41	RW	900	0	964	7	2
41	YW	900	0	964	5	0
42	RX	725	0	778	10	0
42	YX	725	0	778	13	0
43	RY	818	0	909	14	4
43	YY	818	0	909	12	3
44	RZ	1461	0	1493	22	0
44	YZ	1461	0	1493	21	0
45	R0	643	0	667	11	0
45	Y0	599	0	617	12	0
46	R1	763	0	848	16	0
46	Y1	729	0	802	9	0
47	R2	581	0	629	6	0
47	Y2	581	0	629	7	4
48	R3	469	0	518	8	0
48	Y3	469	0	518	6	0
49	R4	565	0	557	7	0
49	Y4	565	0	557	8	0
50	R5	459	0	476	8	0
50	Y5	459	0	479	8	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	R6	453	0	473	5	0
51	Y6	453	0	473	3	0
52	R7	409	0	454	2	0
52	Y7	418	0	467	5	0
53	R8	517	0	582	14	0
53	Y8	517	0	582	9	0
54	R9	307	0	335	4	0
54	Y9	307	0	335	4	0
55	QA	80	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	QT	1	0	0	0	0
55	QV	6	0	0	0	0
55	R0	2	0	0	0	0
55	R8	1	0	0	0	0
55	RA	521	0	0	0	0
55	RB	11	0	0	0	0
55	RD	1	0	0	0	0
55	RE	4	0	0	0	0
55	RN	1	0	0	0	0
55	RO	1	0	0	0	0
55	RP	3	0	0	0	0
55	RQ	3	0	0	0	0
55	RR	2	0	0	0	0
55	RT	1	0	0	0	0
55	XA	98	0	0	0	0
55	XE	1	0	0	0	0
55	XL	2	0	0	0	0
55	XM	2	0	0	0	0
55	XQ	1	0	0	0	0
55	XS	1	0	0	0	0
55	XV	8	0	0	0	0
55	XX	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	551	0	0	0	0
55	YB	12	0	0	0	0
55	YD	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	YE	4	0	0	0	0
55	YF	1	0	0	0	0
55	YO	1	0	0	0	0
55	YP	2	0	0	0	0
55	YQ	4	0	0	0	0
55	YU	1	0	0	0	0
55	YX	2	0	0	0	0
55	YY	1	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	291753	0	197645	1817	12

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 4.

The worst 5 of 1817 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)
24:RA:602:G:HO2'	24:RA:604:G:HO2'	1.26	0.80
46:Y1:91:LYS:HE2	46:Y1:92:LYS:HE2	1.69	0.74
1:QA:664:G:H22	1:QA:741:G:H1	1.36	0.74
1:XA:686:U:H1'	11:XK:42:TRP:HE1	1.54	0.73
24:RA:676:A:H8	24:RA:2069:G:H21	1.36	0.72

The worst 5 of 12 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)
43:RY:21:LYS:NZ	47:Y2:71:ASN:CB[3_555]	1.64	0.56
43:RY:19:LYS:O	47:Y2:71:ASN:ND2[3_555]	1.79	0.41
41:RW:63:ASP:OD1	43:YY:92:ASN:ND2[3_555]	1.88	0.32
40:YV:49:THR:O	50:Y5:59:GLU:OE2[4_445]	1.90	0.30
40:YV:49:THR:OG1	50:Y5:60:VAL:O[4_445]	1.91	0.29

## 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	
2	QB	233/256 (91%)	205 (88%)	27 (12%)	1 (0%)	34	69
2	XB	234/256 (91%)	210 (90%)	24 (10%)	0	100	100
3	QC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
3	XC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
4	QD	206/209 (99%)	193 (94%)	13 (6%)	0	100	100
4	XD	206/209 (99%)	193 (94%)	13 (6%)	0	100	100
5	QE	149/162 (92%)	142 (95%)	6 (4%)	1 (1%)	22	60
5	XE	149/162 (92%)	142 (95%)	6 (4%)	1 (1%)	22	60
6	QF	99/101 (98%)	99 (100%)	0	0	100	100
6	XF	99/101 (98%)	99 (100%)	0	0	100	100
7	QG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
7	XG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
8	QH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
8	XH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
9	QI	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
9	XI	124/128 (97%)	114 (92%)	10 (8%)	0	100	100
10	QJ	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
10	XJ	94/105 (90%)	83 (88%)	11 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	QK	117/129 (91%)	109 (93%)	8 (7%)	0	100	100
11	XK	114/129 (88%)	107 (94%)	7 (6%)	0	100	100
12	QL	123/132 (93%)	104 (85%)	19 (15%)	0	100	100
12	XL	120/132 (91%)	105 (88%)	14 (12%)	1 (1%)	19	56
13	QM	118/126 (94%)	101 (86%)	16 (14%)	1 (1%)	19	56
13	XM	117/126 (93%)	100 (86%)	17 (14%)	0	100	100
14	QN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9	40
14	XN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9	40
15	QO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	XO	85/89 (96%)	85 (100%)	0	0	100	100
16	QP	82/88 (93%)	81 (99%)	1 (1%)	0	100	100
16	XP	82/88 (93%)	81 (99%)	1 (1%)	0	100	100
17	QQ	98/105 (93%)	97 (99%)	1 (1%)	0	100	100
17	XQ	98/105 (93%)	97 (99%)	1 (1%)	0	100	100
18	QR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
18	XR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
19	QS	81/93 (87%)	71 (88%)	10 (12%)	0	100	100
19	XS	82/93 (88%)	66 (80%)	15 (18%)	1 (1%)	13	48
20	QT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
20	XT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
21	QU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	XU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
26	RD	270/276 (98%)	246 (91%)	23 (8%)	1 (0%)	34	69
26	YD	270/276 (98%)	246 (91%)	23 (8%)	1 (0%)	34	69
27	RE	203/206 (98%)	165 (81%)	37 (18%)	1 (0%)	29	66
27	YE	203/206 (98%)	165 (81%)	37 (18%)	1 (0%)	29	66
28	RF	200/210 (95%)	186 (93%)	14 (7%)	0	100	100
28	YF	200/210 (95%)	186 (93%)	14 (7%)	0	100	100
29	RG	179/182 (98%)	152 (85%)	26 (14%)	1 (1%)	25	63
29	YG	179/182 (98%)	152 (85%)	26 (14%)	1 (1%)	25	63
30	RH	172/180 (96%)	149 (87%)	19 (11%)	4 (2%)	6	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	YH	172/180 (96%)	149 (87%)	19 (11%)	4 (2%)	6	32
31	RI	144/148 (97%)	126 (88%)	16 (11%)	2 (1%)	11	44
31	YI	144/148 (97%)	126 (88%)	16 (11%)	2 (1%)	11	44
32	RN	136/140 (97%)	124 (91%)	11 (8%)	1 (1%)	22	60
32	YN	136/140 (97%)	124 (91%)	11 (8%)	1 (1%)	22	60
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%)	122 (82%)	25 (17%)	1 (1%)	22	60
34	YP	145/150 (97%)	115 (79%)	29 (20%)	1 (1%)	22	60
35	RQ	139/141 (99%)	117 (84%)	21 (15%)	1 (1%)	22	60
35	YQ	139/141 (99%)	117 (84%)	21 (15%)	1 (1%)	22	60
36	RR	115/118 (98%)	107 (93%)	8 (7%)	0	100	100
36	YR	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	54
37	RS	109/112 (97%)	91 (84%)	17 (16%)	1 (1%)	17	54
37	YS	109/112 (97%)	91 (84%)	17 (16%)	1 (1%)	17	54
38	RT	135/146 (92%)	120 (89%)	13 (10%)	2 (2%)	10	43
38	YT	135/146 (92%)	120 (89%)	13 (10%)	2 (2%)	10	43
39	RU	115/118 (98%)	107 (93%)	8 (7%)	0	100	100
39	YU	115/118 (98%)	107 (93%)	8 (7%)	0	100	100
40	RV	99/101 (98%)	84 (85%)	14 (14%)	1 (1%)	15	52
40	YV	99/101 (98%)	84 (85%)	14 (14%)	1 (1%)	15	52
41	RW	111/113 (98%)	105 (95%)	5 (4%)	1 (1%)	17	54
41	YW	111/113 (98%)	105 (95%)	5 (4%)	1 (1%)	17	54
42	RX	90/96 (94%)	87 (97%)	3 (3%)	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%)	98 (93%)	7 (7%)	0	100	100
44	RZ	181/206 (88%)	148 (82%)	30 (17%)	3 (2%)	9	40
44	YZ	181/206 (88%)	148 (82%)	30 (17%)	3 (2%)	9	40
45	R0	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
45	Y0	73/85 (86%)	69 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	R1	95/98 (97%)	84 (88%)	11 (12%)	0	100	100
46	Y1	91/98 (93%)	80 (88%)	11 (12%)	0	100	100
47	R2	67/72 (93%)	62 (92%)	4 (6%)	1 (2%)	10	43
47	Y2	67/72 (93%)	62 (92%)	4 (6%)	1 (2%)	10	43
48	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
48	Y3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
49	R4	67/71 (94%)	55 (82%)	11 (16%)	1 (2%)	10	43
49	Y4	67/71 (94%)	55 (82%)	11 (16%)	1 (2%)	10	43
50	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
50	Y5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
51	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
51	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
52	R7	45/49 (92%)	45 (100%)	0	0	100	100
52	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
53	R8	62/65 (95%)	49 (79%)	11 (18%)	2 (3%)	4	23
53	Y8	62/65 (95%)	49 (79%)	11 (18%)	2 (3%)	4	23
54	R9	35/37 (95%)	35 (100%)	0	0	100	100
54	Y9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11452/12128 (94%)	10380 (91%)	1015 (9%)	57 (0%)	29	66

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	RE	18	ASP
31	RI	15	VAL
38	RT	124	ASP
44	RZ	53	ILE
12	XL	105	TYR

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	203/220 (92%)	202 (100%)	1 (0%)	88	95
2	XB	204/220 (93%)	200 (98%)	4 (2%)	55	79
3	QC	159/188 (85%)	159 (100%)	0	100	100
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	180/181 (99%)	180 (100%)	0	100	100
4	XD	180/181 (99%)	180 (100%)	0	100	100
5	QE	116/123 (94%)	115 (99%)	1 (1%)	78	91
5	XE	116/123 (94%)	115 (99%)	1 (1%)	78	91
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	125 (99%)	1 (1%)	81	92
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%)	96 (98%)	2 (2%)	55	79
9	XI	97/99 (98%)	97 (100%)	0	100	100
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	104 (100%)	0	100	100
12	XL	103/109 (94%)	103 (100%)	0	100	100
13	QM	96/101 (95%)	96 (100%)	0	100	100
13	XM	95/101 (94%)	95 (100%)	0	100	100
14	QN	49/50 (98%)	46 (94%)	3 (6%)	18	51
14	XN	49/50 (98%)	46 (94%)	3 (6%)	18	51
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	85
16	XP	72/74 (97%)	71 (99%)	1 (1%)	67	85
17	QQ	95/97 (98%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	72 (100%)	0	100	100
19	XS	73/80 (91%)	73 (100%)	0	100	100
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
26	RD	214/218 (98%)	211 (99%)	3 (1%)	67	85
26	YD	214/218 (98%)	211 (99%)	3 (1%)	67	85
27	RE	165/166 (99%)	165 (100%)	0	100	100
27	YE	165/166 (99%)	165 (100%)	0	100	100
28	RF	161/166 (97%)	159 (99%)	2 (1%)	71	87
28	YF	161/166 (97%)	159 (99%)	2 (1%)	71	87
29	RG	155/156 (99%)	154 (99%)	1 (1%)	86	94
29	YG	155/156 (99%)	154 (99%)	1 (1%)	86	94
30	RH	145/148 (98%)	141 (97%)	4 (3%)	43	73
30	YH	145/148 (98%)	141 (97%)	4 (3%)	43	73
31	RI	122/124 (98%)	122 (100%)	0	100	100
31	YI	122/124 (98%)	122 (100%)	0	100	100
32	RN	117/119 (98%)	116 (99%)	1 (1%)	78	91
32	YN	117/119 (98%)	116 (99%)	1 (1%)	78	91
33	RO	100/100 (100%)	99 (99%)	1 (1%)	76	89
33	YO	100/100 (100%)	99 (99%)	1 (1%)	76	89
34	RP	116/116 (100%)	116 (100%)	0	100	100
34	YP	114/116 (98%)	112 (98%)	2 (2%)	59	81
35	RQ	111/111 (100%)	111 (100%)	0	100	100
35	YQ	111/111 (100%)	111 (100%)	0	100	100
36	RR	100/101 (99%)	99 (99%)	1 (1%)	76	89
36	YR	100/101 (99%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	RS	87/88 (99%)	86 (99%)	1 (1%)	73	88
37	YS	87/88 (99%)	86 (99%)	1 (1%)	73	88
38	RT	120/127 (94%)	119 (99%)	1 (1%)	81	92
38	YT	120/127 (94%)	119 (99%)	1 (1%)	81	92
39	RU	93/94 (99%)	92 (99%)	1 (1%)	73	88
39	YU	93/94 (99%)	92 (99%)	1 (1%)	73	88
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%)	90 (98%)	2 (2%)	52	78
41	YW	92/92 (100%)	90 (98%)	2 (2%)	52	78
42	RX	74/78 (95%)	73 (99%)	1 (1%)	67	85
42	YX	74/78 (95%)	73 (99%)	1 (1%)	67	85
43	RY	88/91 (97%)	88 (100%)	0	100	100
43	YY	88/91 (97%)	88 (100%)	0	100	100
44	RZ	162/179 (90%)	161 (99%)	1 (1%)	86	94
44	YZ	162/179 (90%)	161 (99%)	1 (1%)	86	94
45	R0	65/67 (97%)	64 (98%)	1 (2%)	65	85
45	Y0	61/67 (91%)	60 (98%)	1 (2%)	62	83
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%)	64 (100%)	0	100	100
48	R3	51/52 (98%)	50 (98%)	1 (2%)	55	79
48	Y3	51/52 (98%)	50 (98%)	1 (2%)	55	79
49	R4	62/63 (98%)	60 (97%)	2 (3%)	39	70
49	Y4	62/63 (98%)	60 (97%)	2 (3%)	39	70
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	54 (100%)	0	100	100
54	R9	34/34 (100%)	34 (100%)	0	100	100
54	Y9	34/34 (100%)	34 (100%)	0	100	100
All	All	9687/10066 (96%)	9619 (99%)	68 (1%)	84	93

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	R3	30	ARG
7	XG	94	ARG
42	YX	66	LEU
49	R4	56	VAL
2	XB	64	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
50	R5	23	HIS
6	XF	7	ASN
47	Y2	46	GLN
2	XB	40	HIS
4	XD	119	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1496/1508 (99%)	280 (18%)	35 (2%)
1	XA	1498/1508 (99%)	281 (18%)	31 (2%)
22	QV	76/77 (98%)	14 (18%)	2 (2%)
22	XV	76/77 (98%)	14 (18%)	2 (2%)
23	QX	11/25 (44%)	5 (45%)	1 (9%)
23	XX	10/25 (40%)	6 (60%)	0
24	RA	2879/2915 (98%)	577 (20%)	38 (1%)
24	YA	2880/2915 (98%)	573 (19%)	40 (1%)
25	RB	119/122 (97%)	22 (18%)	2 (1%)
25	YB	119/122 (97%)	22 (18%)	2 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9164/9294 (98%)	1794 (19%)	153 (1%)

5 of 1794 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	22	G
1	QA	32	A
1	QA	39	G

5 of 153 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	RA	2126	A
1	XA	250	A
24	YA	1930	G
24	RA	2566	A
25	RB	108	C

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1358 ligands modelled in this entry, 1356 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	QD	301	4	0,12,12	0.00	-	-		
56	SF4	XD	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	QD	301	4	-	-	0/6/5/5
56	SF4	XD	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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