



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 4, 2020 – 11:22 pm BST

PDB ID : 5J30
Title : Thermus thermophilus 70S termination complex containing E. coli RF1
Authors : Hoffer, E.D.; Dunham, C.M.
Deposited on : 2016-03-30
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

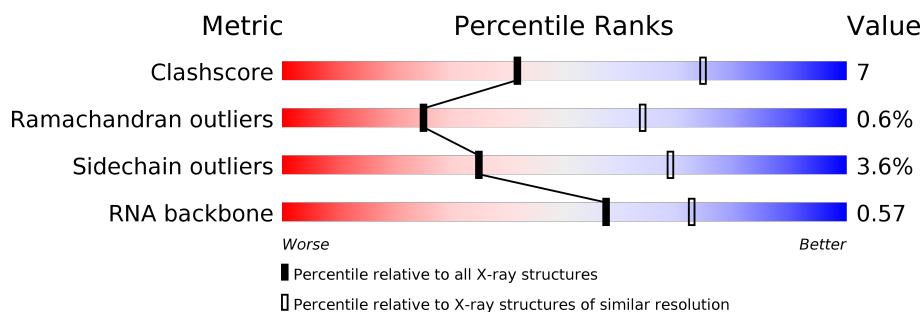
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)















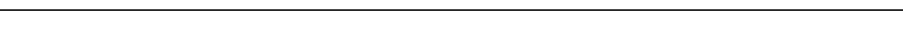




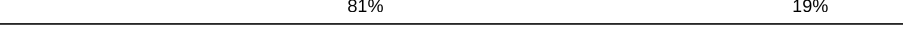





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	RA	2915	65% 27% 6% .
1	YA	2915	64% 27% 6% .
2	RB	122	82% 16% ..
2	YB	122	68% 26% . .
3	RD	276	82% 16% .
3	YD	276	84% 14% .
4	RE	206	81% 16% ..


























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Mol	Chain	Length	Quality of chain
4	YE	206	 78%19%..
5	RF	210	 75%20%..
5	YF	210	 71%20%5%.
6	RG	182	 74%23%..
6	YG	182	 63%32%..
7	RH	180	 79%17%..
7	YH	180	 66%26%..
8	RI	148	 78%20%..
8	YI	148	 78%17%..
9	RN	140	 81%16%.
9	YN	140	 81%17%.
10	RO	122	 89%11%
10	YO	122	 86%14%
11	RP	150	 79%19%..
11	YP	150	 77%21%..
12	RQ	141	 79%20%.
12	YQ	141	 79%18%.
13	RR	118	 81%17%.
13	YR	118	 81%19%
14	RS	112	 85%12%..
14	YS	112	 78%20%..
15	RT	146	 68%21%10%
15	YT	146	 75%14%10%
16	RU	118	 83%14%..
16	YU	118	 84%14%..















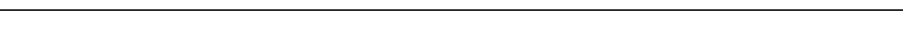




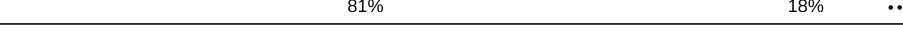





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Mol	Chain	Length	Quality of chain
17	RV	101	
17	YV	101	
18	RW	113	
18	YW	113	
19	RX	96	
19	YX	96	
20	RY	110	
20	YY	110	
21	RZ	206	
21	YZ	206	
22	R0	85	
22	Y0	85	
23	R1	98	
23	Y1	98	
24	R2	72	
24	Y2	72	
25	R3	60	
25	Y3	60	
26	R4	71	
26	Y4	71	
27	R5	60	
27	Y5	60	
28	R6	54	
28	Y6	54	
29	R7	49	


























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

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Mol	Chain	Length	Quality of chain
42	QK	129	
42	XK	129	
43	QL	132	
43	XL	132	
44	QM	126	
44	XM	126	
45	QN	61	
45	XN	61	
46	QO	89	
46	XO	89	
47	QP	88	
47	XP	88	
48	QQ	105	
48	XQ	105	
49	QR	88	
49	XR	88	
50	QS	93	
50	XS	93	
51	QT	106	
51	XT	106	
52	QU	27	
52	XU	27	
53	QV	77	
53	XV	77	
54	QX	25	

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Mol	Chain	Length	Quality of chain
54	XX	25	<div><div></div><div></div><div></div><div></div></div> <div>12%16%8%64%</div>
55	QY	360	<div><div></div><div></div><div></div><div></div></div> <div>46%23%•28%</div>
55	XY	360	<div><div></div><div></div><div></div><div></div></div> <div>45%24%•28%</div>

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 294739 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	RA	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			
1	YA	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	RB	120	Total	C	N	O	P	0	0	0
			2572	1145	476	832	119			
2	YB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	RD	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
3	YD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	RE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	YE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	RF	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	YF	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	RG	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
6	YG	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	RH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	YH	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	RI	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	YI	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	RN	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
9	YN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	RP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
11	YP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	RS	110	Total	C	N	O	0	0	0
			877	553	175	149			
14	YS	110	Total	C	N	O	0	0	0
			870	549	173	148			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	RT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
15	YT	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	RU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	YU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	RV	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
17	YV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	RW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
18	YW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	RX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	YX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	RY	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
20	YY	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	RZ	189	Total	C	N	O	S	0	0	0
			1485	946	265	272	2			
21	YZ	189	Total	C	N	O	S	0	0	0
			1469	938	259	270	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	R0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	Y0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	R1	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			
23	Y1	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	Y2	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	R3	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	Y3	59	Total	C	N	O	0	0	0
			464	296	90	78			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R4	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y4	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	Y5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	Y6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	QA	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	XA	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	QB	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
33	XB	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	QC	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
34	XC	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	QD	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
35	XD	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	QE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
36	XE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	QF	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
37	XF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	QG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
38	XG	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	QH	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
39	XH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	QI	127	Total	C	N	O	0	0	0
			986	625	193	168			
40	XI	126	Total	C	N	O	0	0	0
			966	613	186	167			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	QJ	97	Total	C	N	O	0	0	0
			719	446	142	131			
41	XJ	96	Total	C	N	O	0	0	0
			710	442	137	131			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	QK	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	XK	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	QL	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
43	XL	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	QM	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	XM	114	Total	C	N	O	S	0	0	0
			895	550	186	157	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	QO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
46	XO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	QP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
47	XP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	QQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	XQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	QR	68	Total	C	N	O		0	0	0
			555	355	108	92				
49	XR	68	Total	C	N	O		0	0	0
			555	355	108	92				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	QS	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
50	XS	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	QT	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
51	XT	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	QU	23	Total	C	N	O	0	0	0
			199	122	48	29			
52	XU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a RNA chain called P-site tRNA fMet.

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

- Molecule 54 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	QX	10	Total	C	N	O	P	0	0	0
			215	97	42	66	10			
54	XX	9	Total	C	N	O	P	0	0	0
			193	87	37	60	9			

- Molecule 55 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	QY	258	Total	C	N	O	S	0	0	0
			2014	1235	382	389	8			
55	XY	259	Total	C	N	O	S	0	0	0
			2023	1240	384	391	8			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	256	Total	Mg	0	0
			256	256		
56	YV	1	Total	Mg	0	0
			1	1		
56	RP	1	Total	Mg	0	0
			1	1		
56	R7	2	Total	Mg	0	0
			2	2		
56	YA	744	Total	Mg	0	0
			744	744		
56	QM	1	Total	Mg	0	0
			1	1		
56	YR	1	Total	Mg	0	0
			1	1		
56	RT	2	Total	Mg	0	0
			2	2		
56	QD	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	RN	2	Total 2	Mg 2	0	0
56	XE	1	Total 1	Mg 1	0	0
56	RG	4	Total 4	Mg 4	0	0
56	QI	1	Total 1	Mg 1	0	0
56	YD	9	Total 9	Mg 9	0	0
56	XX	1	Total 1	Mg 1	0	0
56	QV	6	Total 6	Mg 6	0	0
56	RX	1	Total 1	Mg 1	0	0
56	Y8	2	Total 2	Mg 2	0	0
56	YO	2	Total 2	Mg 2	0	0
56	XA	183	Total 183	Mg 183	0	0
56	Y1	1	Total 1	Mg 1	0	0
56	RQ	6	Total 6	Mg 6	0	0
56	R0	4	Total 4	Mg 4	0	0
56	XT	1	Total 1	Mg 1	0	0
56	QR	1	Total 1	Mg 1	0	0
56	QL	2	Total 2	Mg 2	0	0
56	RU	2	Total 2	Mg 2	0	0
56	QG	2	Total 2	Mg 2	0	0
56	RO	1	Total 1	Mg 1	0	0
56	XJ	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	Y7	2	Total 2	Mg 2	0	0
56	QH	1	Total 1	Mg 1	0	0
56	YG	2	Total 2	Mg 2	0	0
56	YQ	2	Total 2	Mg 2	0	0
56	RY	1	Total 1	Mg 1	0	0
56	YN	1	Total 1	Mg 1	0	0
56	R8	1	Total 1	Mg 1	0	0
56	YX	1	Total 1	Mg 1	0	0
56	RR	3	Total 3	Mg 3	0	0
56	RD	15	Total 15	Mg 15	0	0
56	R1	4	Total 4	Mg 4	0	0
56	XL	1	Total 1	Mg 1	0	0
56	QO	1	Total 1	Mg 1	0	0
56	YT	4	Total 4	Mg 4	0	0
56	RV	4	Total 4	Mg 4	0	0
56	QF	1	Total 1	Mg 1	0	0
56	RH	1	Total 1	Mg 1	0	0
56	R5	3	Total 3	Mg 3	0	0
56	Y0	1	Total 1	Mg 1	0	0
56	QQ	1	Total 1	Mg 1	0	0
56	RA	1039	Total 1039	Mg 1039	0	0

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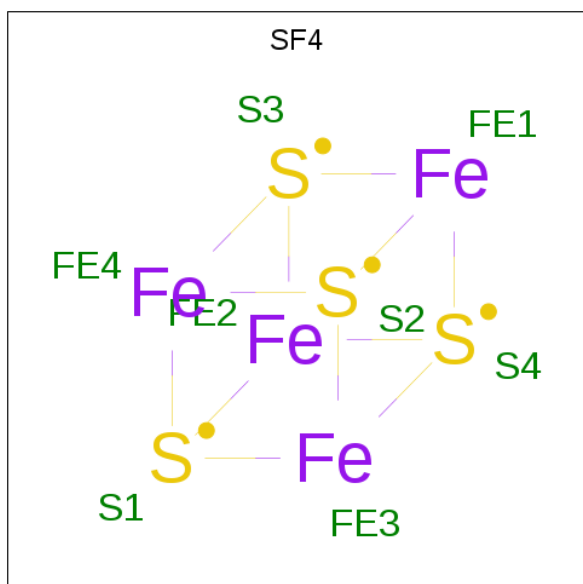
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	YF	3	Total 3	Mg 3	0	0
56	YP	1	Total 1	Mg 1	0	0
56	RZ	1	Total 1	Mg 1	0	0
56	QB	1	Total 1	Mg 1	0	0
56	Y5	1	Total 1	Mg 1	0	0
56	RE	8	Total 8	Mg 8	0	0
56	XK	1	Total 1	Mg 1	0	0
56	YB	18	Total 18	Mg 18	0	0
56	XR	1	Total 1	Mg 1	0	0
56	QT	2	Total 2	Mg 2	0	0
56	QN	2	Total 2	Mg 2	0	0
56	YW	2	Total 2	Mg 2	0	0
56	RW	2	Total 2	Mg 2	0	0
56	XV	4	Total 4	Mg 4	0	0
56	RB	27	Total 27	Mg 27	0	0
56	YI	1	Total 1	Mg 1	0	0
56	QE	2	Total 2	Mg 2	0	0
56	XF	2	Total 2	Mg 2	0	0
56	RF	12	Total 12	Mg 12	0	0
56	R3	2	Total 2	Mg 2	0	0
56	YE	5	Total 5	Mg 5	0	0

- 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		

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



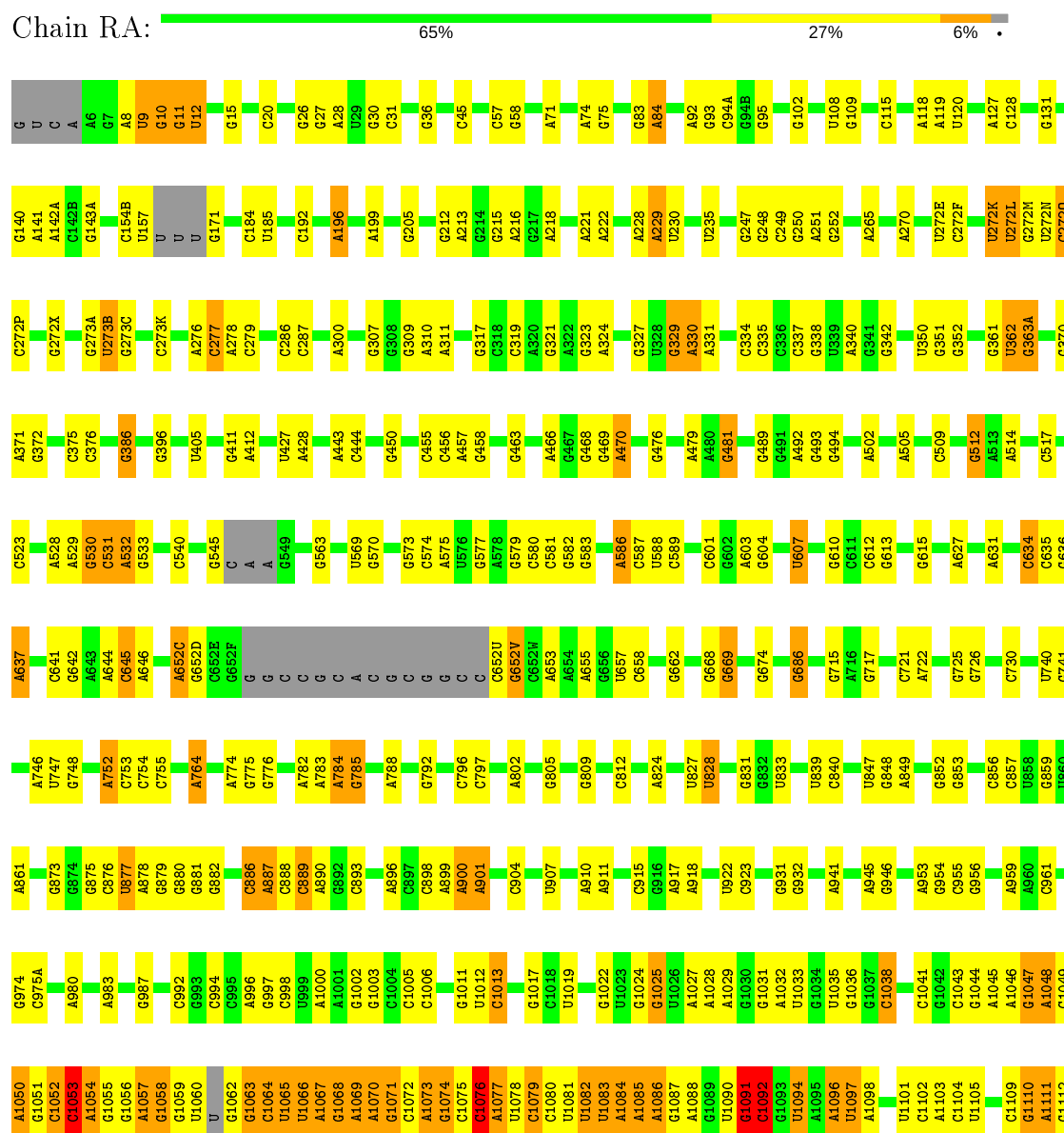
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	QD	1	Total 8	Fe 4	S 4	0	0
58	XD	1	Total 8	Fe 4	S 4	0	0

3 Residue-property plots [i](#)

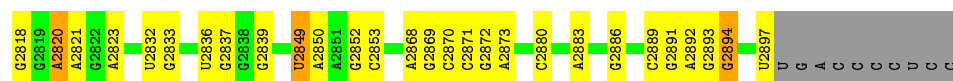
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: 23S rRNA

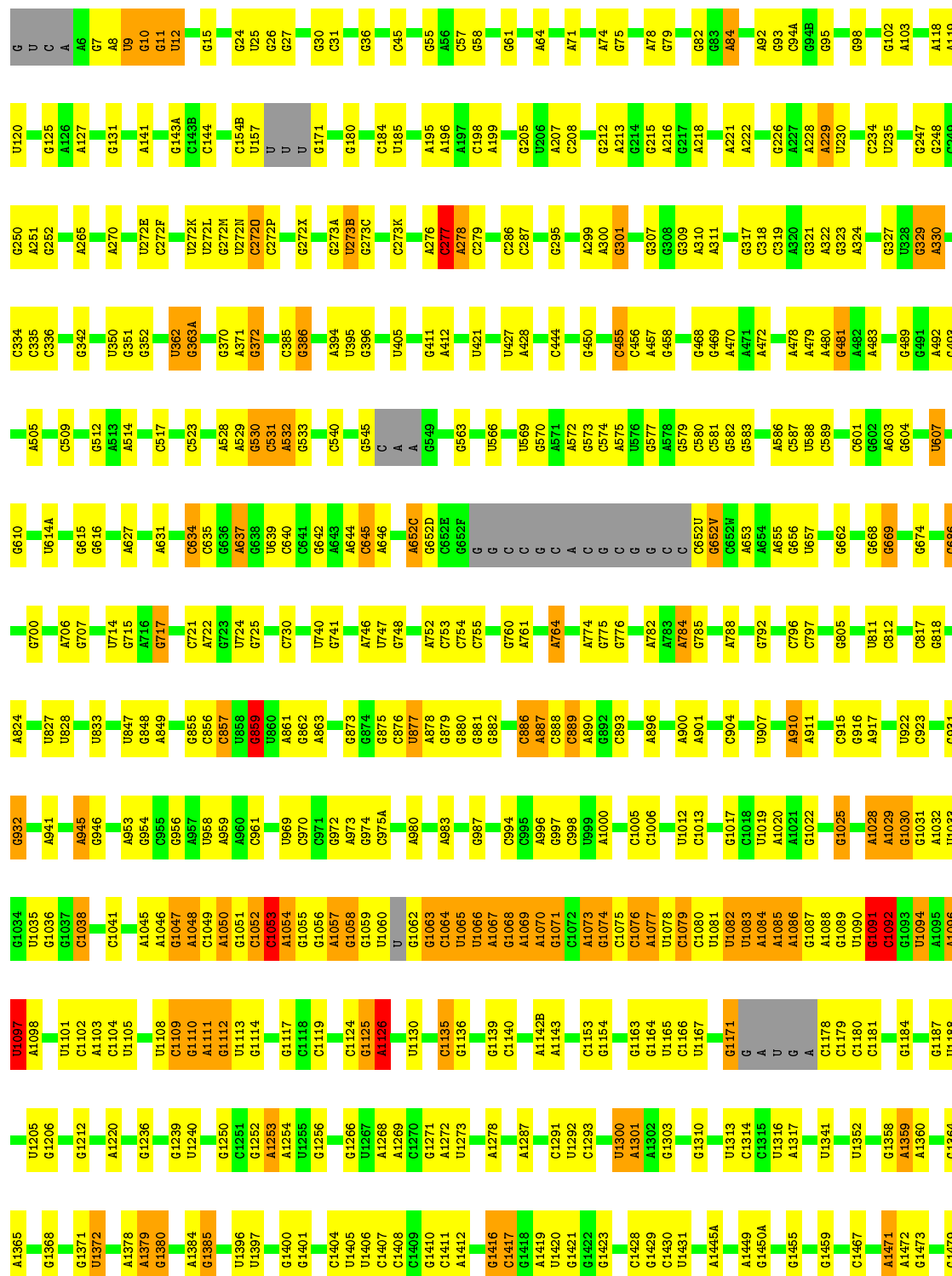


U2726	C2573	U2438	G2342	G2238	C2142	A2060	A1927	U1779	A1614	U1503	A1392	G1239	U1113
G2732	G2574	A2439	C2343	G2239	C2143	G2061	A1928	A1780	G1622	C1504	A1393	U1240	G1114
A2733	G2578	C2440	U2344	G2240	U2144	A2062	G1929	A1784	G1626	C1505	A1396	G1280	G1117
G2734	A2602	G2445	G2345	U2243	C2145	G2069	U1931	A1785	A1637	G1506	U1397	A1253	C1118
G2735	G2603	A2446	G2346	U2244	G2146	U2074	A1932	A1786	U1638	A1507	U1397	A1254	C1119
C2742	U2604	A2448	C2347	G2289	G2148	U2075	G1933	C1790	G1637	A1508	G1400	G1266	G1125
C2743	C2350	G2445	C2350	U2282	U2150	U2076	A1936	A1791	U1638	C1509A	G1401	U1270	A1126
G2744	G2354	G2455	G2354	U2262	G2152	U2086	A1937	U1794	U1639	C1509B	G1401	G1271	U1130
C2745	C2355	U2461	C2355	G2269	G2153	U2087	A1938	C1795	A1641	A1509C	C1404	G1272	G1135
U2746	U2462	U2462	C2358	A2274	G2154	U2092	U1939	C1796	G1642	C1511	U1405	G1273	G1136
U2747	C2463	C2463	C2359	G2275	G2155	G2093	U1940	C1797	G1648	U1514	U1406	C1270	C1135
A2748	C2464	C2464	A2360	G2276	G2156	G2094	C1941	C1798	G1653	G1515	C1407	G1271	G1136
A2749	C2465	C2465	C2361	G2277	A2158	U2096	U1955	U1799	G1657	C1530	G1410	G1272	G1139
G2750	C2466	C2466	C2362	G2278	G2157	U2097	U1962	C1801	C1658	C1531	U1273	A1274	U1140
G2751	C2364	C2364	C2365	A2278	G2159	U2098	U1963	A1802	G1667	G1532	U1420	U1291	U1141
A2629	G2365	C2372	G2372	G2282	G2160	U2099	C1967	C1803	A1669	U	C1291	C1293	G1153
G2630	C2372	G2372	G2373	G2283	G2161	U2102	U1970	A1810	G1674	G1536	G1422	G1293	G1154
G2643	C2373	G2373	C2374	G2284	C2162	C2103	A1971	G1811	C1686	A1542	C1428	C1297	U1165
G2644	C2374	G2374	G2375	G2285	C2164	U2109	U1975	G1813	G1687	C1543	C1428	U1300	C1166
G2645	G2375	G2375	A2286	G2286	G2165	G2104	U1991	A1815	U1688	C1547	G1429	U1301	U1167
U2647	A2376	C2376	A2287	G2287	G2166	C2105	G1992	G1816	A1689	C1431	U1431	G1309	G1171
C2498	A2377	G2377	A2288	G2288	U2167	G2106	U1993	G1824	U1693	C1557	C1432	G1309	G
G2502	G2378	G2378	G2289	G2289	G2168	C2107	G1997	G1827	C1694	A1588	C1432	G1310	A
A2503	G2379	G2379	U2291	U2291	A2171	C2108	A2001	C1827	G1695	G1559	A1445A	U1313	U
U2504	G2382	G2382	G2304	A2305	U2172	U2110	G2002	G1835	G1700	A1566	G1450A	C1314	G
U2505	G2383	G2383	A2306	A2306	A2173	C2111	G2010	A1847	A1701	A1569	U1453	G1327	C1178
U2506	G2384	G2384	G2307	G2307	A2176	U2112	G2012	A1848	G1704	A1570	U1453	U1340	C1179
C2507	C2385	C2385	G2308	G2308	G2178	U2113	G2011	G1877	G1721	A1571	G1459	U1341	C1180
C2512	G2389	G2389	U2390	U2390	U2180	G2115	G2010	G1878	A1722	U1578	C1467	U1352	G1201
G2513	G2391	G2391	G2391	G2391	G2181	G2116	G2011	G1878	A1739	A1580	G1468	U1358	U1205
A2518	C2394	C2394	C2311	U2312	G2182	U2118	G2012	G1878	G1740	C1582	A1471	A1360	G1206
G2526	G2394	G2394	C2313	C2313	G2185	A2119	G2011	G1889	A1741	U1583	G1470	A1369	U1205
C2527	U2528	U2528	C2314	C2314	C2186	G2120	G2012	A1890	G1750	C1584	A1472	A1365	U1211
G2529	C2401	C2401	G2315	G2315	G2187	G2121	G2013	G1899	G1756	A1586	G1473	A1365	G1212
A2530	C2402	C2402	C2316	C2316	U2189	U2122	G2015	A1900	U1757	C1587	G1479	G1368	A1220
C2530	U2406	U2406	G2317	G2317	G2190	G2123	U2016	G1906	G1758	C1588	G1482	U1372	G1223
U2537	G2410	G2410	G2319	G2319	G2192	A2126	U2022	G1913	A1762	G1593	G1492	A1379	G1223
C2538	G2420	G2420	G2320	G2320	G2193	G2127	G2023	C1914	G1763	G1594	C1493	A1379	G1223
G2543	G2421	G2421	G2321	G2321	A2198	U2130	A2031	U1915	G1764	C1607	C1493	G1380	G1225
G2544	A2422	A2422	G2325	G2325	G2206	U2132	G2032	U1916	A1773	A1608	A1494	A1226	A1226
U2552	U2423	U2423	G2336	G2336	G2207	G2133	A2033	U1917	U1778	A1610	A1496	A1384	G1236
G2553	C2424	C2424	A2327	A2327	A2208	A2134	G2043	G1914	A1778	G1594	G1482	U1372	A1220
U2554	A2425	A2425	A2328	A2328	U2218	A2135	C2043	C1914	A1762	G1594	G1482	U1372	A1220
U2555	G2429	G2429	G2330	G2330	U2218	A2136	C2043	U1915	A1762	G1594	G1482	U1372	A1220
A2566	A2430	A2430	G2331	G2331	A2225	C2137	A2051	U1916	A1762	G1594	G1482	U1372	A1220
G2567	A2434	A2434	G2331	G2331	A2225	C2137	A2051	U1916	A1762	G1594	G1482	U1372	A1220
C2568	A2435	A2435	G2334	G2334	G2228	C2139	C2055	U1923	A1773	A1609	A1496	A1384	G1236
A2572	G2435	G2435	A2336	A2336	G2234	G2141	G2056	U1923	U1778	A1610	A1496	A1384	G1236

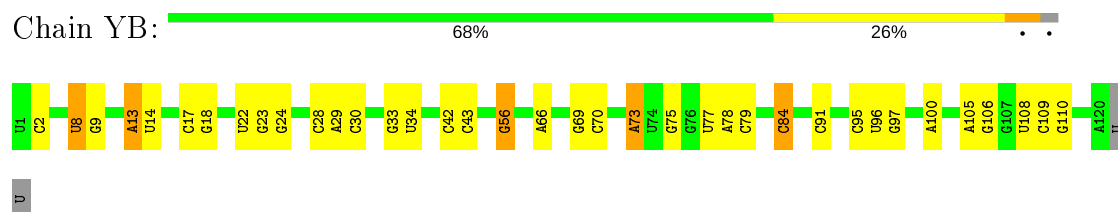


• Molecule 1: 23S rRNA

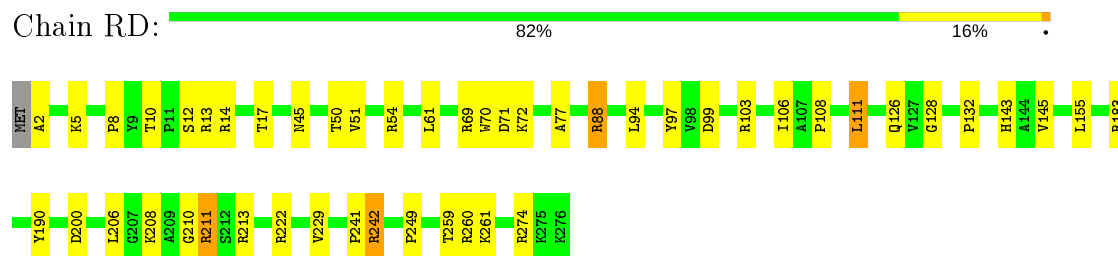
Chain YA: 64% 27% 6%



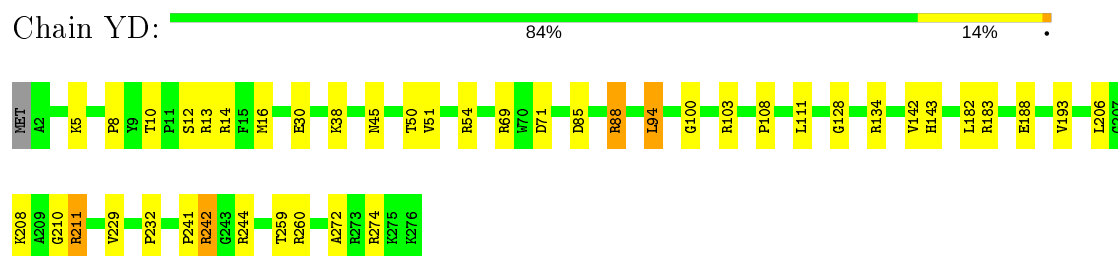
- Molecule 2: 5S rRNA



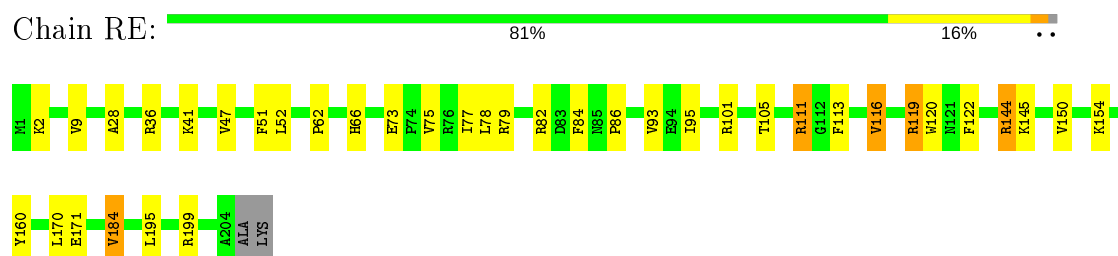
- Molecule 3: 50S ribosomal protein L2



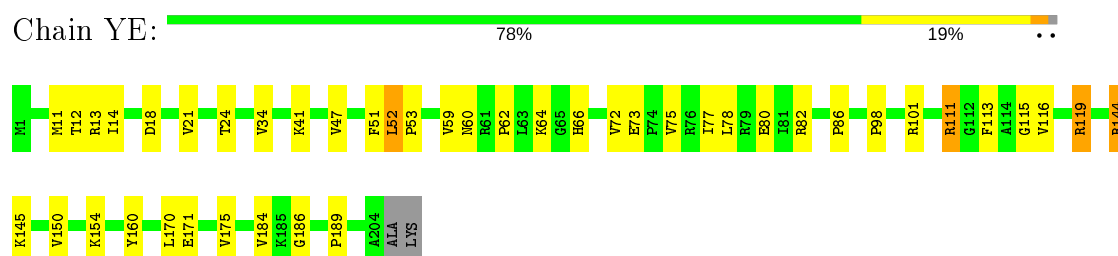
- Molecule 3: 50S ribosomal protein L2




- Molecule 4: 50S ribosomal protein L3

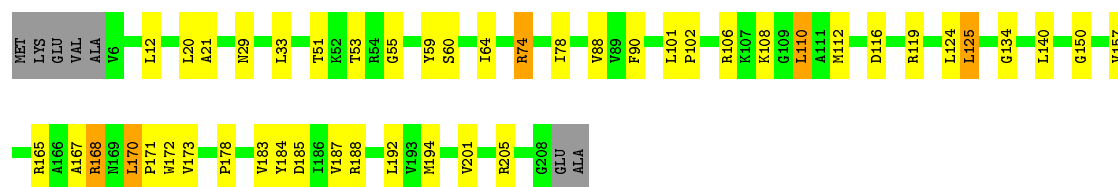


- Molecule 4: 50S ribosomal protein L3



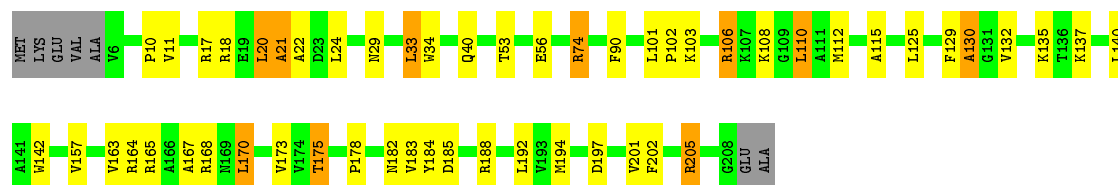
- Molecule 5: 50S ribosomal protein L4

Chain RF:  75% 20% ..



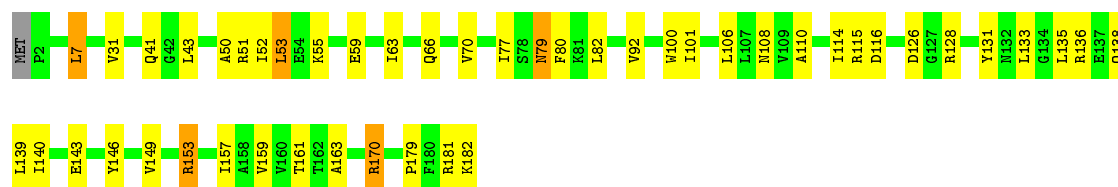
- Molecule 5: 50S ribosomal protein L4

Chain YF:  71% 20% 5% .



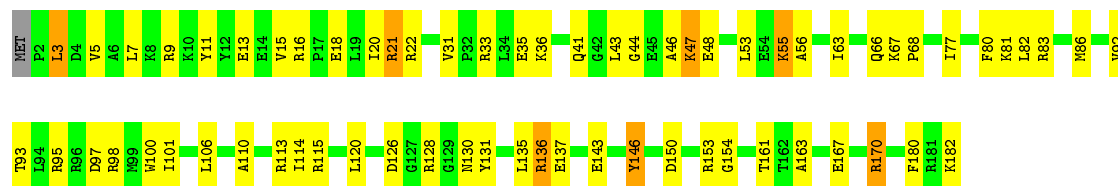
- Molecule 6: 50S ribosomal protein L5

Chain RG:  74% 23% ..




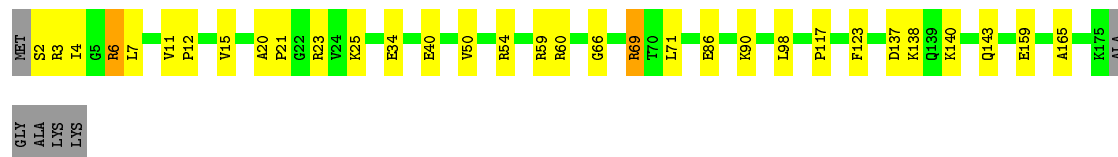
- Molecule 6: 50S ribosomal protein L5

Chain YG:  63% 32% ..



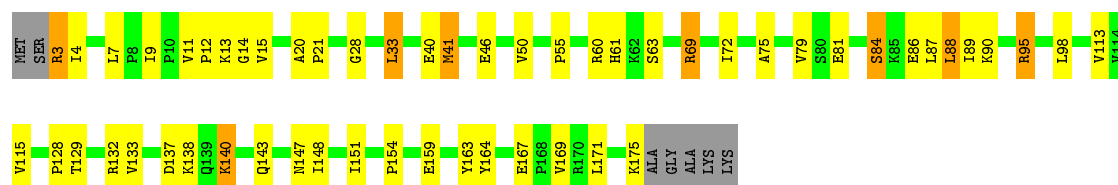
- Molecule 7: 50S ribosomal protein L6

Chain RH:  79% 17% ..




- Molecule 7: 50S ribosomal protein L6

Chain YH:  66% 26%




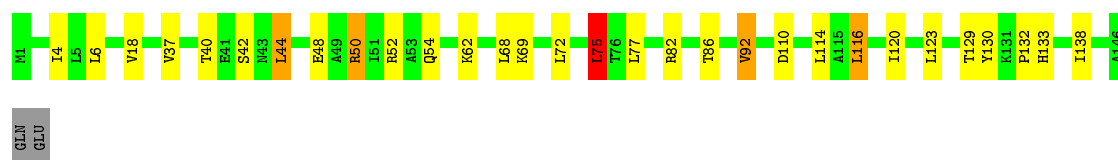
- Molecule 8: 50S ribosomal protein L9

Chain RI:  78% 20%




- Molecule 8: 50S ribosomal protein L9

Chain YI:  78% 17%




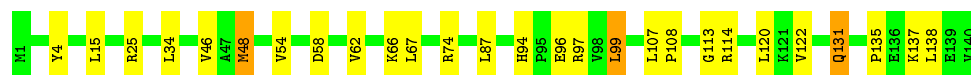
- Molecule 9: 50S ribosomal protein L13

Chain RN:  81% 16%



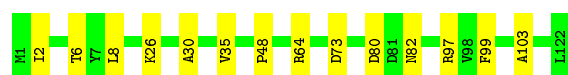
- Molecule 9: 50S ribosomal protein L13

Chain YN:  81% 17%



- Molecule 10: 50S ribosomal protein L14

Chain RO:  89% 11%

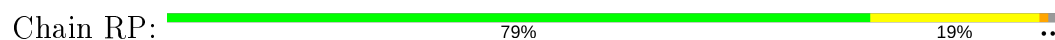


- Molecule 10: 50S ribosomal protein L14

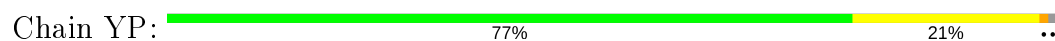
Chain YO:  86% 14%



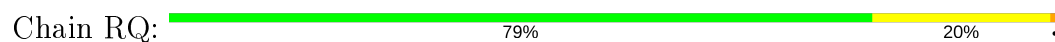
- Molecule 11: 50S ribosomal protein L15



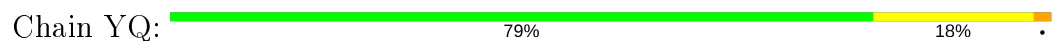
- Molecule 11: 50S ribosomal protein L15



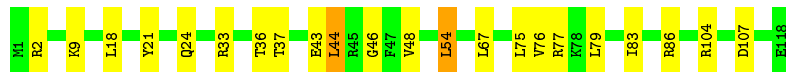
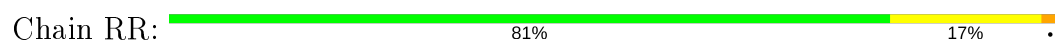
- Molecule 12: 50S ribosomal protein L16



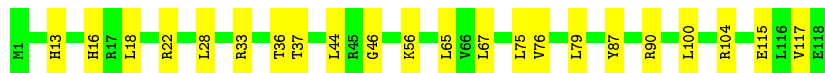
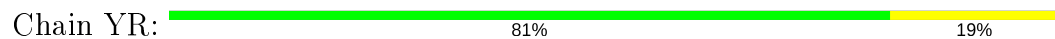
- Molecule 12: 50S ribosomal protein L16



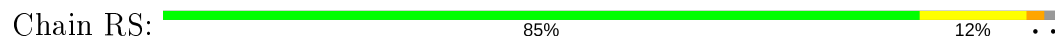
- Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18





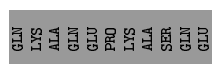
- Molecule 14: 50S ribosomal protein L18

Chain YS: 78% 20% ..



- Molecule 15: 50S ribosomal protein L19

Chain RT: 68% 21% • 10%



- Molecule 15: 50S ribosomal protein L19

Chain YT: 75% 14% • 10%



- Molecule 16: 50S ribosomal protein L20

Chain RU: 83% 14% ..



- Molecule 16: 50S ribosomal protein L20

Chain YU: 84% 14% ..




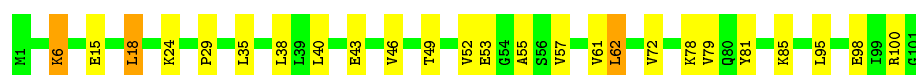
- Molecule 17: 50S ribosomal protein L21

Chain RV: 89% 10% •



- Molecule 17: 50S ribosomal protein L21

Chain YV:  75% 22% .



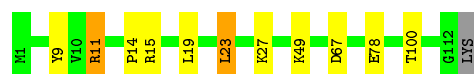
- Molecule 18: 50S ribosomal protein L22

Chain RW:  82% 13% . .




- Molecule 18: 50S ribosomal protein L22

Chain YW:  89% 8% . .




- Molecule 19: 50S ribosomal protein L23

Chain RX:  79% 20% .




- Molecule 19: 50S ribosomal protein L23

Chain YX:  78% 21% .



- Molecule 20: 50S ribosomal protein L24

Chain RY:  77% 18% . .




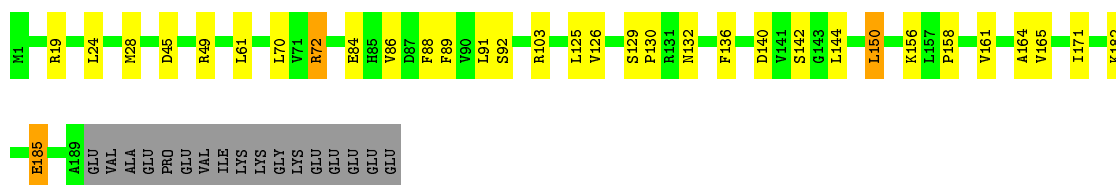
- Molecule 20: 50S ribosomal protein L24

Chain YY:  72% 24% . .



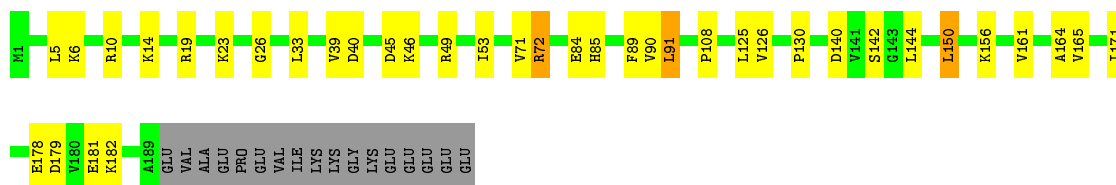
- Molecule 21: 50S ribosomal protein L25

Chain RZ:  76% 15% 8%




- Molecule 21: 50S ribosomal protein L25

Chain YZ:  73% 17% 8%



- Molecule 22: 50S ribosomal protein L27

Chain R0:  76% 12% 9%




- Molecule 22: 50S ribosomal protein L27

Chain Y0:  72% 19% 9%



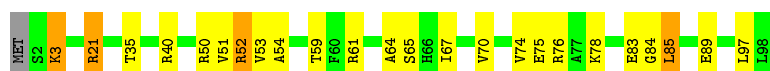
- Molecule 23: 50S ribosomal protein L28

Chain R1:  84% 13% ..




- Molecule 23: 50S ribosomal protein L28

Chain Y1:  74% 20% ..



- Molecule 24: 50S ribosomal protein L29

Chain R2:  88% 8% ..



- Molecule 24: 50S ribosomal protein L29

Chain Y2: 81% 15% ..



- Molecule 25: 50S ribosomal protein L30

Chain R3: 92% 7% .



- Molecule 25: 50S ribosomal protein L30

Chain Y3: 77% 18% ..



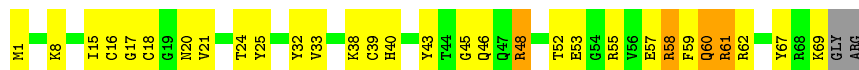
- Molecule 26: 50S ribosomal protein L31

Chain R4: 56% 37% . .



- Molecule 26: 50S ribosomal protein L31

Chain Y4: 55% 37% 6% .



- Molecule 27: 50S ribosomal protein L32

Chain R5: 75% 22% ..



- Molecule 27: 50S ribosomal protein L32

Chain Y5: 85% 12% ..



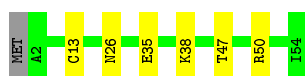
- Molecule 28: 50S ribosomal protein L33

Chain R6: 76% 20%



- Molecule 28: 50S ribosomal protein L33

Chain Y6: 87% 11%



- Molecule 29: 50S ribosomal protein L34

Chain R7: 76% 22%



- Molecule 29: 50S ribosomal protein L34

Chain Y7: 78% 20%



- Molecule 30: 50S ribosomal protein L35

Chain R8: 69% 28%



- Molecule 30: 50S ribosomal protein L35

Chain Y8: 78% 18%



- Molecule 31: 50S ribosomal protein L36

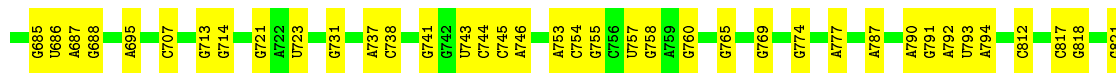
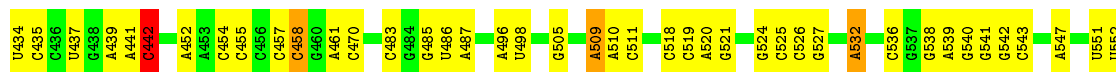
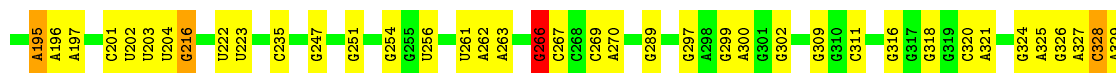
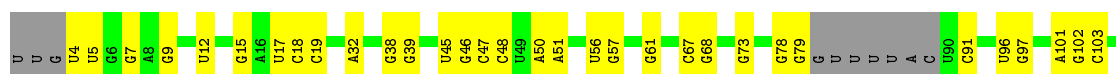
Chain R9: 81% 19%



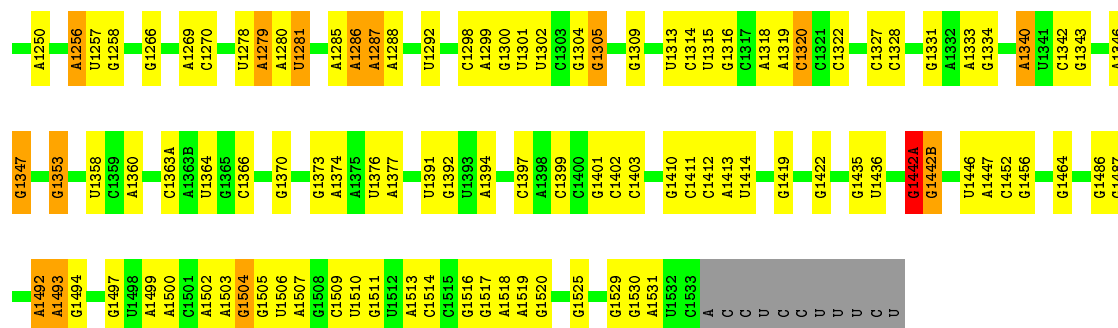
- Molecule 31: 50S ribosomal protein L36



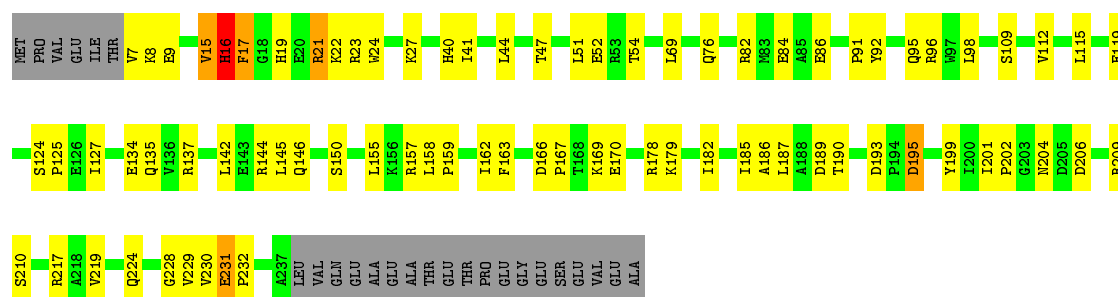
- Molecule 32: 16S rRNA



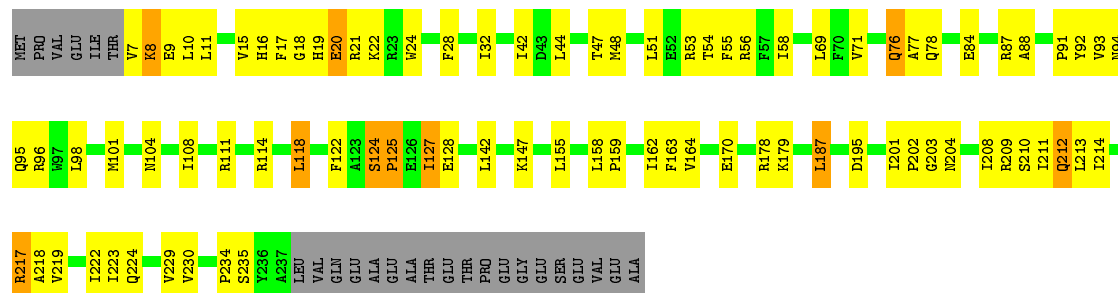




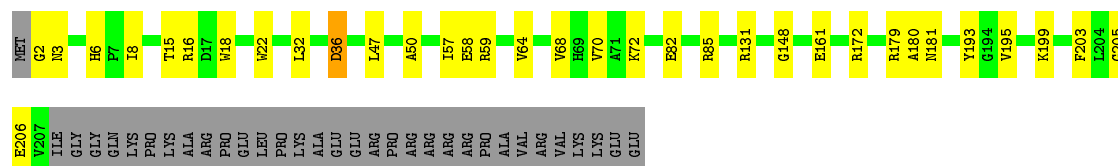
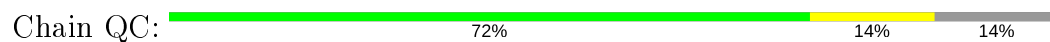
• Molecule 33: 30S ribosomal protein S2



• Molecule 33: 30S ribosomal protein S2

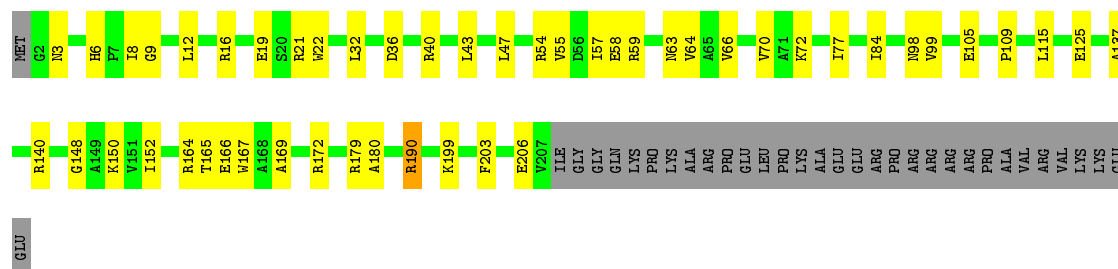


• Molecule 34: 30S ribosomal protein S3

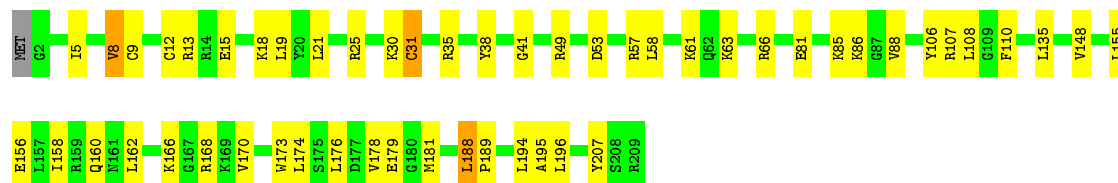
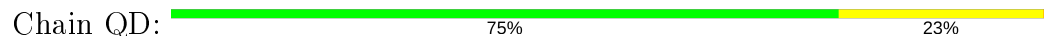


• Molecule 34: 30S ribosomal protein S3

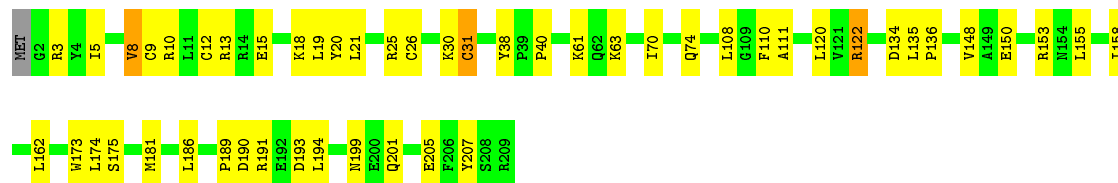
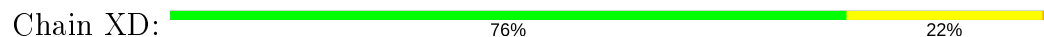




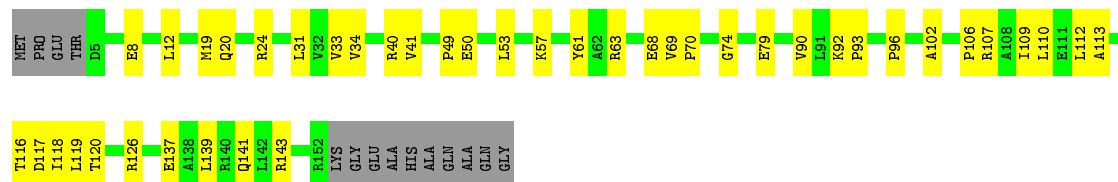
- Molecule 35: 30S ribosomal protein S4



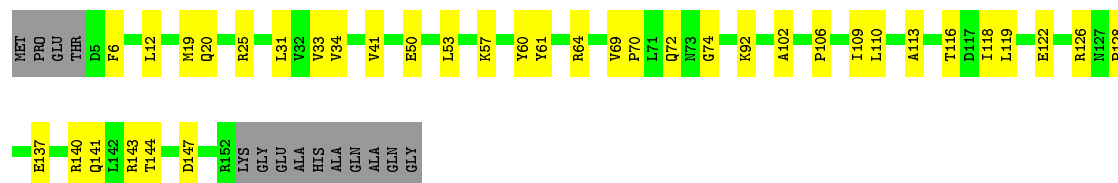
- Molecule 35: 30S ribosomal protein S4




- Molecule 36: 30S ribosomal protein S5

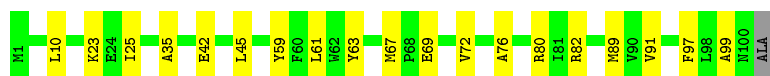


- Molecule 36: 30S ribosomal protein S5




- Molecule 37: 30S ribosomal protein S6

Chain QF:  80% 19%




- Molecule 37: 30S ribosomal protein S6

Chain XF:  83% 16%




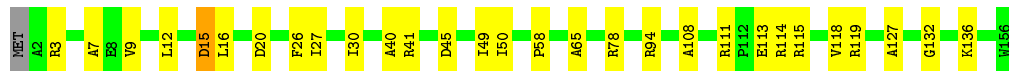
- Molecule 38: 30S ribosomal protein S7

Chain QG:  80% 19%




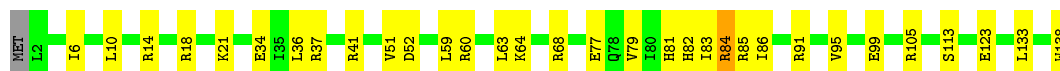
- Molecule 38: 30S ribosomal protein S7

Chain XG:  81% 18%




- Molecule 39: 30S ribosomal protein S8

Chain QH:  76% 22%



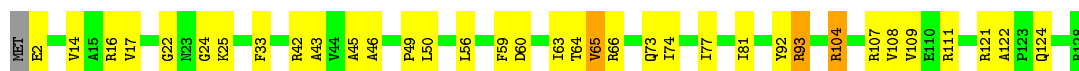
- Molecule 39: 30S ribosomal protein S8

Chain XH:  82% 16%

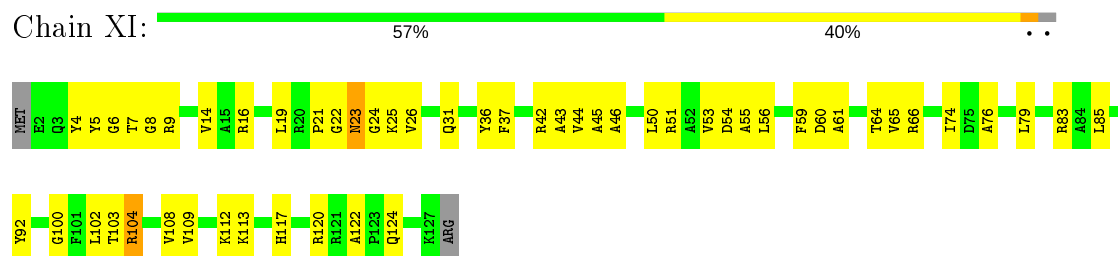


- Molecule 40: 30S ribosomal protein S9

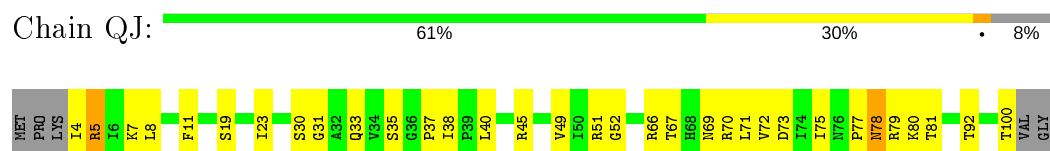
Chain QI:  72% 25%



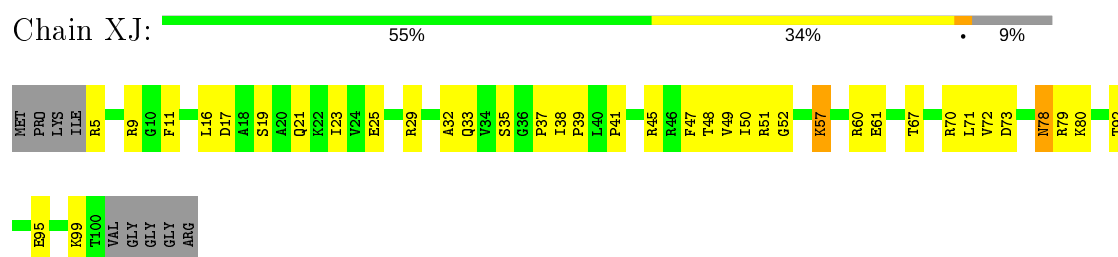
- Molecule 40: 30S ribosomal protein S9



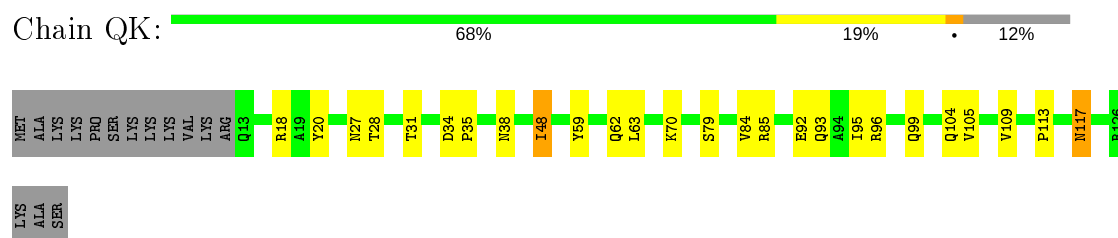
- Molecule 41: 30S ribosomal protein S10



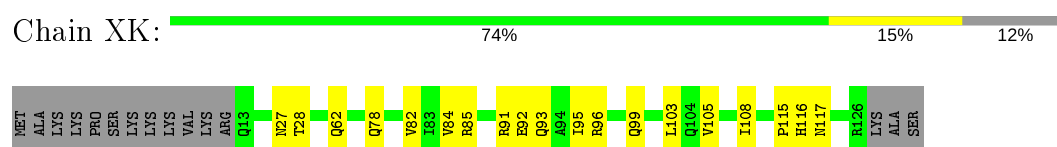
- Molecule 41: 30S ribosomal protein S10



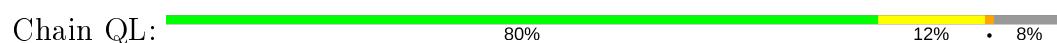
- Molecule 42: 30S ribosomal protein S11



- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12





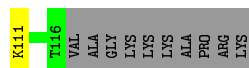
- Molecule 43: 30S ribosomal protein S12



- Molecule 44: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z

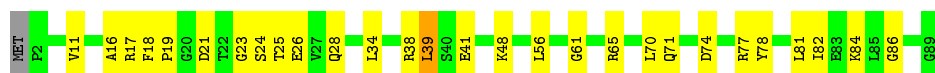


- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15





- Molecule 46: 30S ribosomal protein S15

Chain XO: 82% 15% ..



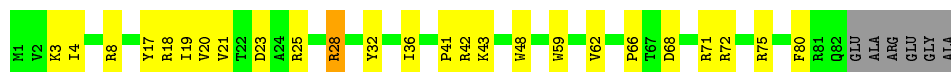
- Molecule 47: 30S ribosomal protein S16

Chain QP: 77% 15% 7%



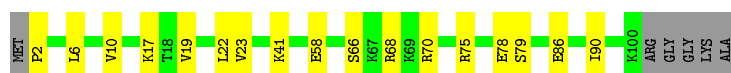
- Molecule 47: 30S ribosomal protein S16

Chain XP: 65% 27% 7%



- Molecule 48: 30S ribosomal protein S17

Chain QQ: 78% 16% 6%



- Molecule 48: 30S ribosomal protein S17

Chain XQ: 86% 9% 6%



- Molecule 49: 30S ribosomal protein S18

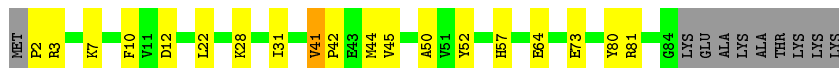
Chain QR: 64% 14% 23%



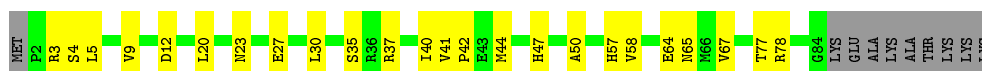
- Molecule 49: 30S ribosomal protein S18

Chain XR: 57% 19% 23%

- Molecule 50: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S19



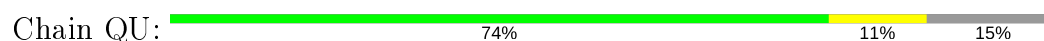
- Molecule 51: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



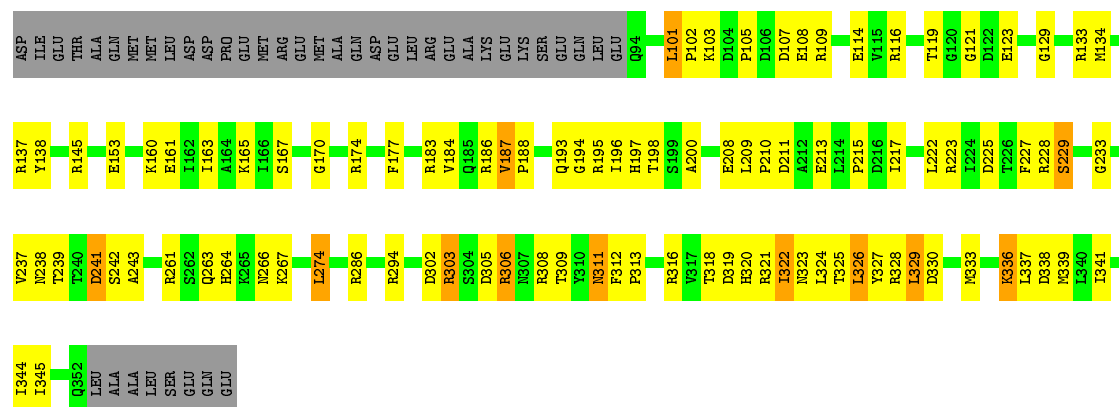
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: P-site tRNA fMet







4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.03Å 449.71Å 620.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 3.20	Depositor
% Data completeness (in resolution range)	99.9 (49.81-3.20)	Depositor
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.214 , 0.244	Depositor
Wilson B-factor (Å ²)	93.8	Xtriage
Anisotropy	0.251	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	294739	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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: 5MU, ZN, MEQ, OMG, MA6, SF4, 0TD, MG, 2MA, 2MU, 2MG, 5MC, UR3, 4OC, M2G, 7MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	RA	0.26	0/68901	0.85	52/107544 (0.0%)
1	YA	0.30	4/68901 (0.0%)	0.87	72/107544 (0.1%)
2	RB	0.25	0/2876	0.83	0/4486
2	YB	0.27	0/2878	0.84	0/4490
3	RD	0.30	0/2181	0.54	0/2940
3	YD	0.30	0/2186	0.56	0/2944
4	RE	0.29	0/1592	0.53	0/2149
4	YE	0.31	0/1592	0.57	1/2149 (0.0%)
5	RF	0.28	0/1619	0.52	0/2193
5	YF	0.30	0/1615	0.53	0/2188
6	RG	0.28	0/1451	0.53	0/1961
6	YG	0.29	0/1449	0.52	0/1957
7	RH	0.28	0/1356	0.50	0/1834
7	YH	0.29	0/1350	0.56	2/1826 (0.1%)
8	RI	0.27	0/1109	0.54	0/1512
8	YI	0.27	0/1091	0.55	1/1490 (0.1%)
9	RN	0.28	0/1148	0.51	0/1547
9	YN	0.28	0/1144	0.50	0/1543
10	RO	0.29	0/943	0.55	0/1269
10	YO	0.29	0/943	0.55	0/1269
11	RP	0.28	0/1152	0.56	0/1533
11	YP	0.28	0/1152	0.56	0/1533
12	RQ	0.30	0/1143	0.52	0/1527
12	YQ	0.29	0/1143	0.51	0/1527
13	RR	0.27	0/982	0.54	0/1312
13	YR	0.27	0/982	0.53	0/1312
14	RS	0.27	0/887	0.52	0/1180
14	YS	0.29	0/880	0.52	0/1172
15	RT	0.29	0/1105	0.58	0/1477
15	YT	0.28	0/1097	0.55	0/1468
16	RU	0.29	0/977	0.45	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	YU	0.30	0/977	0.46	0/1301
17	RV	0.28	0/786	0.52	0/1053
17	YV	0.32	0/782	0.57	0/1049
18	RW	0.27	0/897	0.48	0/1205
18	YW	0.28	0/897	0.50	0/1205
19	RX	0.30	0/764	0.53	0/1025
19	YX	0.30	0/764	0.53	0/1025
20	RY	0.29	0/823	0.55	0/1099
20	YY	0.33	0/823	0.55	0/1100
21	RZ	0.31	0/1517	0.53	0/2062
21	YZ	0.28	0/1501	0.52	0/2043
22	R0	0.28	0/616	0.53	0/821
22	Y0	0.27	0/616	0.55	0/821
23	R1	0.27	0/761	0.53	0/1013
23	Y1	0.28	0/766	0.56	0/1018
24	R2	0.29	0/590	0.51	0/781
24	Y2	0.26	0/594	0.46	0/785
25	R3	0.28	0/474	0.51	0/635
25	Y3	0.29	0/469	0.54	0/630
26	R4	0.32	0/559	0.66	0/754
26	Y4	0.37	0/549	0.63	0/741
27	R5	0.33	0/473	0.54	0/639
27	Y5	0.32	0/469	0.54	0/635
28	R6	0.28	0/460	0.53	0/613
28	Y6	0.23	0/456	0.46	0/608
29	R7	0.26	0/426	0.49	0/561
29	Y7	0.26	0/426	0.45	0/561
30	R8	0.29	0/525	0.52	0/691
30	Y8	0.28	0/525	0.51	0/691
31	R9	0.23	0/310	0.47	0/407
31	Y9	0.26	0/310	0.51	0/407
32	QA	0.26	0/35795	0.86	38/55864 (0.1%)
32	XA	0.26	0/35890	0.85	30/56012 (0.1%)
33	QB	0.28	0/1876	0.54	0/2533
33	XB	0.30	0/1860	0.57	0/2518
34	QC	0.27	0/1582	0.52	0/2137
34	XC	0.28	0/1566	0.52	0/2119
35	QD	0.28	0/1695	0.50	0/2274
35	XD	0.27	0/1698	0.47	0/2277
36	QE	0.30	0/1149	0.52	0/1548
36	XE	0.28	0/1149	0.51	0/1548
37	QF	0.26	0/827	0.51	0/1120
37	XF	0.26	0/829	0.52	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	QG	0.27	0/1254	0.43	0/1683
38	XG	0.27	0/1248	0.45	0/1676
39	QH	0.27	0/1118	0.50	0/1506
39	XH	0.28	0/1108	0.51	0/1494
40	QI	0.28	0/1005	0.53	0/1351
40	XI	0.28	0/985	0.52	0/1329
41	QJ	0.26	0/732	0.51	0/993
41	XJ	0.26	0/723	0.51	0/984
42	QK	0.26	0/849	0.48	0/1150
42	XK	0.26	0/848	0.53	0/1149
43	QL	0.28	0/937	0.54	0/1260
43	XL	0.29	0/937	0.59	0/1260
44	QM	0.26	0/924	0.52	0/1242
44	XM	0.26	0/905	0.50	0/1217
45	QN	0.28	0/501	0.44	0/664
45	XN	0.29	0/501	0.46	0/664
46	QO	0.26	0/739	0.48	0/985
46	XO	0.26	0/739	0.49	0/985
47	QP	0.28	0/697	0.51	0/939
47	XP	0.28	0/693	0.50	0/935
48	QQ	0.26	0/836	0.50	0/1117
48	XQ	0.26	0/836	0.50	0/1117
49	QR	0.26	0/560	0.51	0/746
49	XR	0.26	0/560	0.51	0/746
50	QS	0.27	0/663	0.57	0/895
50	XS	0.27	0/660	0.55	0/893
51	QT	0.27	0/734	0.48	0/969
51	XT	0.27	0/736	0.42	0/976
52	QU	0.25	0/203	0.52	0/266
52	XU	0.30	0/203	0.52	0/266
53	QV	0.33	1/1836 (0.1%)	0.82	0/2859
53	XV	0.34	1/1836 (0.1%)	0.82	0/2859
54	QX	0.33	0/241	0.95	0/373
54	XX	0.27	0/216	0.89	0/334
55	QY	0.31	0/2035	0.51	0/2742
55	XY	0.29	0/2044	0.51	0/2754
All	All	0.28	6/316288 (0.0%)	0.78	196/472607 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	RS	0	1
26	R4	0	1
33	QB	0	1
43	XL	0	1
All	All	0	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	XV	1	C	OP3-P	-10.46	1.48	1.61
53	QV	1	C	OP3-P	-10.44	1.48	1.61
1	YA	2751	G	N1-C2	-8.70	1.30	1.37
1	YA	2751	G	C2-N3	-6.96	1.27	1.32
1	YA	1029	A	N3-C4	-5.78	1.31	1.34

The worst 5 of 196 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	1029	A	N1-C2-N3	12.53	135.56	129.30
32	QA	576	G	OP1-P-O3'	-11.19	80.59	105.20
1	RA	2602	A	OP2-P-O3'	-11.18	80.60	105.20
32	QA	576	G	OP2-P-O3'	-10.40	82.31	105.20
1	RA	1050	A	N1-C2-N3	10.32	134.46	129.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	QB	231	GLU	Peptide
26	R4	67	TYR	Peptide
14	RS	58	LEU	Peptide
43	XL	86	ARG	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	RA	61758	0	31145	564	0
1	YA	61758	0	31148	595	1
2	RB	2572	0	1305	8	0
2	YB	2573	0	1306	23	0
3	RD	2131	0	2207	42	0
3	YD	2136	0	2218	37	0
4	RE	1559	0	1618	27	0
4	YE	1559	0	1618	30	0
5	RF	1584	0	1625	31	0
5	YF	1580	0	1619	42	0
6	RG	1426	0	1445	34	0
6	YG	1424	0	1441	45	0
7	RH	1330	0	1407	24	0
7	YH	1324	0	1402	36	0
8	RI	1094	0	1127	23	0
8	YI	1076	0	1094	21	0
9	RN	1121	0	1195	14	0
9	YN	1117	0	1184	21	0
10	RO	933	0	996	9	0
10	YO	933	0	996	10	0
11	RP	1135	0	1212	25	0
11	YP	1135	0	1212	32	0
12	RQ	1122	0	1179	22	0
12	YQ	1122	0	1179	20	0
13	RR	968	0	1033	15	0
13	YR	968	0	1033	11	0
14	RS	877	0	938	9	0
14	YS	870	0	923	14	0
15	RT	1091	0	1151	21	0
15	YT	1083	0	1136	19	0
16	RU	959	0	1019	12	0
16	YU	959	0	1019	13	0
17	RV	775	0	841	7	0
17	YV	771	0	830	15	0
18	RW	886	0	940	13	0
18	YW	886	0	940	8	0
19	RX	750	0	814	17	0
19	YX	750	0	814	12	0
20	RY	810	0	892	14	0
20	YY	810	0	888	18	0
21	RZ	1485	0	1493	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	YZ	1469	0	1467	26	0
22	R0	608	0	622	10	0
22	Y0	608	0	622	14	0
23	R1	754	0	823	10	0
23	Y1	759	0	837	20	0
24	R2	588	0	643	5	1
24	Y2	592	0	654	7	0
25	R3	469	0	518	4	0
25	Y3	464	0	514	7	0
26	R4	546	0	522	26	0
26	Y4	536	0	514	28	0
27	R5	459	0	476	11	0
27	Y5	455	0	465	7	0
28	R6	453	0	473	14	0
28	Y6	449	0	469	4	0
29	R7	418	0	467	13	0
29	Y7	418	0	467	8	0
30	R8	517	0	582	21	0
30	Y8	517	0	582	17	0
31	R9	307	0	335	9	0
31	Y9	307	0	335	15	0
32	QA	32246	0	16294	310	0
32	XA	32331	0	16338	344	0
33	QB	1842	0	1862	55	0
33	XB	1825	0	1828	57	0
34	QC	1558	0	1557	30	0
34	XC	1542	0	1517	38	0
35	QD	1665	0	1688	42	0
35	XD	1668	0	1704	39	0
36	QE	1133	0	1191	31	0
36	XE	1133	0	1191	24	0
37	QF	814	0	808	14	0
37	XF	816	0	808	11	0
38	QG	1235	0	1249	20	0
38	XG	1229	0	1238	16	0
39	QH	1098	0	1143	26	0
39	XH	1088	0	1126	14	0
40	QI	986	0	990	28	0
40	XI	966	0	953	37	0
41	QJ	719	0	672	22	0
41	XJ	710	0	661	30	0
42	QK	834	0	838	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	XK	833	0	836	12	0
43	QL	932	0	980	14	0
43	XL	932	0	981	20	0
44	QM	914	0	954	30	0
44	XM	895	0	920	24	0
45	QN	492	0	529	19	0
45	XN	492	0	529	19	0
46	QO	728	0	760	17	0
46	XO	728	0	760	9	0
47	QP	681	0	697	11	0
47	XP	677	0	686	19	0
48	QQ	823	0	891	12	0
48	XQ	823	0	891	7	0
49	QR	555	0	618	11	0
49	XR	555	0	618	14	0
50	QS	648	0	658	16	0
50	XS	645	0	635	27	0
51	QT	732	0	809	16	0
51	XT	733	0	795	15	0
52	QU	199	0	208	2	0
52	XU	199	0	208	7	0
53	QV	1644	0	835	23	0
53	XV	1644	0	836	15	0
54	QX	215	0	109	1	0
54	XX	193	0	97	5	0
55	QY	2014	0	1981	60	0
55	XY	2023	0	1988	78	0
56	QA	256	0	0	0	0
56	QB	1	0	0	0	0
56	QD	3	0	0	0	0
56	QE	2	0	0	0	0
56	QF	1	0	0	0	0
56	QG	2	0	0	0	0
56	QH	1	0	0	0	0
56	QI	1	0	0	0	0
56	QL	2	0	0	0	0
56	QM	1	0	0	0	0
56	QN	2	0	0	0	0
56	QO	1	0	0	0	0
56	QQ	1	0	0	0	0
56	QR	1	0	0	0	0
56	QT	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	QV	6	0	0	0	0
56	R0	4	0	0	0	0
56	R1	4	0	0	0	0
56	R3	2	0	0	0	0
56	R5	3	0	0	0	0
56	R7	2	0	0	0	0
56	R8	1	0	0	0	0
56	RA	1039	0	0	0	0
56	RB	27	0	0	0	0
56	RD	15	0	0	0	0
56	RE	8	0	0	0	0
56	RF	12	0	0	0	0
56	RG	4	0	0	0	0
56	RH	1	0	0	0	0
56	RN	2	0	0	0	0
56	RO	1	0	0	0	0
56	RP	1	0	0	0	0
56	RQ	6	0	0	0	0
56	RR	3	0	0	0	0
56	RT	2	0	0	0	0
56	RU	2	0	0	0	0
56	RV	4	0	0	0	0
56	RW	2	0	0	0	0
56	RX	1	0	0	0	0
56	RY	1	0	0	0	0
56	RZ	1	0	0	0	0
56	XA	183	0	0	0	0
56	XE	1	0	0	0	0
56	XF	2	0	0	0	0
56	XJ	1	0	0	0	0
56	XK	1	0	0	0	0
56	XL	1	0	0	0	0
56	XR	1	0	0	0	0
56	XT	1	0	0	0	0
56	XV	4	0	0	0	0
56	XX	1	0	0	0	0
56	Y0	1	0	0	0	0
56	Y1	1	0	0	0	0
56	Y5	1	0	0	0	0
56	Y7	2	0	0	0	0
56	Y8	2	0	0	0	0
56	YA	744	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	YB	18	0	0	0	0
56	YD	9	0	0	0	0
56	YE	5	0	0	0	0
56	YF	3	0	0	0	0
56	YG	2	0	0	0	0
56	YI	1	0	0	0	0
56	YN	1	0	0	0	0
56	YO	2	0	0	0	0
56	YP	1	0	0	0	0
56	YQ	2	0	0	0	0
56	YR	1	0	0	0	0
56	YT	4	0	0	0	0
56	YV	1	0	0	0	0
56	YW	2	0	0	0	0
56	YX	1	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
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
All	All	294739	0	198434	3343	1

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

The worst 5 of 3343 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)
1:YA:2552:2MU:C5	1:YA:2552:2MU:C4	1.80	1.59
1:RA:2552:2MU:C4	1:RA:2552:2MU:C5	1.80	1.58
32:XA:1003:G:H2'	32:XA:1004:A:H4'	1.32	1.08
1:YA:1029:A:N6	1:YA:1125:G:O2'	1.87	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y4:59:PHE:HA	26:Y4:61:ARG:N	1.76	1.00

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:R2:46:GLN:OE1	1:YA:277:C:O2'[3_555]	2.14	0.06

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	
3	RD	273/276 (99%)	261 (96%)	12 (4%)	0	100	100
3	YD	273/276 (99%)	262 (96%)	11 (4%)	0	100	100
4	RE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	67
4	YE	202/206 (98%)	195 (96%)	7 (4%)	0	100	100
5	RF	201/210 (96%)	197 (98%)	4 (2%)	0	100	100
5	YF	201/210 (96%)	196 (98%)	3 (2%)	2 (1%)	15	54
6	RG	179/182 (98%)	166 (93%)	12 (7%)	1 (1%)	25	64
6	YG	179/182 (98%)	170 (95%)	8 (4%)	1 (1%)	25	64
7	RH	172/180 (96%)	167 (97%)	5 (3%)	0	100	100
7	YH	171/180 (95%)	164 (96%)	7 (4%)	0	100	100
8	RI	145/148 (98%)	135 (93%)	10 (7%)	0	100	100
8	YI	144/148 (97%)	137 (95%)	7 (5%)	0	100	100
9	RN	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
9	YN	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
10	RO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	RP	147/150 (98%)	142 (97%)	4 (3%)	1 (1%)	22	61
11	YP	147/150 (98%)	142 (97%)	4 (3%)	1 (1%)	22	61
12	RQ	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
12	YQ	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
13	RR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
13	YR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
14	RS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	17	56
14	YS	108/112 (96%)	105 (97%)	3 (3%)	0	100	100
15	RT	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
15	YT	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
16	RU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	YU	114/118 (97%)	114 (100%)	0	0	100	100
17	RV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	54
17	YV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	54
18	RW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	YW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	RX	93/96 (97%)	92 (99%)	1 (1%)	0	100	100
19	YX	93/96 (97%)	92 (99%)	1 (1%)	0	100	100
20	RY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
20	YY	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
21	RZ	187/206 (91%)	182 (97%)	5 (3%)	0	100	100
21	YZ	187/206 (91%)	181 (97%)	6 (3%)	0	100	100
22	R0	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
22	Y0	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
23	R1	95/98 (97%)	94 (99%)	0	1 (1%)	14	51
23	Y1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	51
24	R2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	Y2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	R4	67/71 (94%)	56 (84%)	7 (10%)	4 (6%)	1	12
26	Y4	67/71 (94%)	55 (82%)	9 (13%)	3 (4%)	2	18
27	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	Y5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	R7	46/49 (94%)	46 (100%)	0	0	100	100
29	Y7	46/49 (94%)	46 (100%)	0	0	100	100
30	R8	62/65 (95%)	62 (100%)	0	0	100	100
30	Y8	62/65 (95%)	62 (100%)	0	0	100	100
31	R9	35/37 (95%)	35 (100%)	0	0	100	100
31	Y9	35/37 (95%)	35 (100%)	0	0	100	100
33	QB	229/256 (90%)	201 (88%)	24 (10%)	4 (2%)	9	42
33	XB	229/256 (90%)	205 (90%)	19 (8%)	5 (2%)	6	35
34	QC	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
34	XC	204/239 (85%)	189 (93%)	15 (7%)	0	100	100
35	QD	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
35	XD	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
36	QE	146/162 (90%)	144 (99%)	2 (1%)	0	100	100
36	XE	146/162 (90%)	144 (99%)	2 (1%)	0	100	100
37	QF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	XF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	QG	153/156 (98%)	151 (99%)	2 (1%)	0	100	100
38	XG	153/156 (98%)	149 (97%)	3 (2%)	1 (1%)	22	61
39	QH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
39	XH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
40	QI	125/128 (98%)	116 (93%)	9 (7%)	0	100	100
40	XI	124/128 (97%)	113 (91%)	9 (7%)	2 (2%)	9	43
41	QJ	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	3	20
41	XJ	94/105 (90%)	84 (89%)	8 (8%)	2 (2%)	7	37
42	QK	112/129 (87%)	105 (94%)	6 (5%)	1 (1%)	17	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	XK	112/129 (87%)	106 (95%)	6 (5%)	0	100	100
43	QL	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
43	XL	119/132 (90%)	116 (98%)	3 (2%)	0	100	100
44	QM	114/126 (90%)	105 (92%)	7 (6%)	2 (2%)	8	41
44	XM	112/126 (89%)	105 (94%)	6 (5%)	1 (1%)	17	56
45	QN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	XN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
46	QO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
46	XO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
47	QP	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
47	XP	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
48	QQ	97/105 (92%)	94 (97%)	2 (2%)	1 (1%)	15	54
48	XQ	97/105 (92%)	95 (98%)	2 (2%)	0	100	100
49	QR	66/88 (75%)	66 (100%)	0	0	100	100
49	XR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	QS	81/93 (87%)	78 (96%)	2 (2%)	1 (1%)	13	49
50	XS	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
51	QT	94/106 (89%)	88 (94%)	5 (5%)	1 (1%)	14	51
51	XT	96/106 (91%)	89 (93%)	5 (5%)	2 (2%)	7	37
52	QU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	XU	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	17
55	QY	255/360 (71%)	224 (88%)	17 (7%)	14 (6%)	2	14
55	XY	256/360 (71%)	222 (87%)	25 (10%)	9 (4%)	3	24
All	All	11925/12848 (93%)	11396 (96%)	459 (4%)	70 (1%)	25	64

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	R4	49	PHE
33	QB	16	HIS
33	QB	22	LYS
51	QT	95	ALA
55	QY	215	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	
3	RD	214/218 (98%)	206 (96%)	8 (4%)	34	68
3	YD	215/218 (99%)	210 (98%)	5 (2%)	50	78
4	RE	164/166 (99%)	157 (96%)	7 (4%)	29	64
4	YE	164/166 (99%)	156 (95%)	8 (5%)	25	61
5	RF	160/166 (96%)	151 (94%)	9 (6%)	21	57
5	YF	159/166 (96%)	149 (94%)	10 (6%)	18	52
6	RG	144/156 (92%)	136 (94%)	8 (6%)	21	57
6	YG	142/156 (91%)	131 (92%)	11 (8%)	13	44
7	RH	144/148 (97%)	141 (98%)	3 (2%)	53	79
7	YH	143/148 (97%)	133 (93%)	10 (7%)	15	48
8	RI	111/124 (90%)	102 (92%)	9 (8%)	11	42
8	YI	108/124 (87%)	101 (94%)	7 (6%)	17	51
9	RN	119/119 (100%)	111 (93%)	8 (7%)	16	50
9	YN	118/119 (99%)	114 (97%)	4 (3%)	37	70
10	RO	100/100 (100%)	100 (100%)	0	100	100
10	YO	100/100 (100%)	100 (100%)	0	100	100
11	RP	115/116 (99%)	113 (98%)	2 (2%)	60	83
11	YP	115/116 (99%)	113 (98%)	2 (2%)	60	83
12	RQ	111/111 (100%)	108 (97%)	3 (3%)	44	75
12	YQ	111/111 (100%)	105 (95%)	6 (5%)	22	58
13	RR	101/101 (100%)	95 (94%)	6 (6%)	19	54
13	YR	101/101 (100%)	95 (94%)	6 (6%)	19	54
14	RS	87/88 (99%)	85 (98%)	2 (2%)	50	78
14	YS	85/88 (97%)	83 (98%)	2 (2%)	49	77
15	RT	115/127 (91%)	111 (96%)	4 (4%)	36	69
15	YT	113/127 (89%)	110 (97%)	3 (3%)	44	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	RU	93/94 (99%)	89 (96%)	4 (4%)	29	64
16	YU	93/94 (99%)	90 (97%)	3 (3%)	39	71
17	RV	81/82 (99%)	77 (95%)	4 (5%)	25	61
17	YV	80/82 (98%)	76 (95%)	4 (5%)	24	60
18	RW	90/92 (98%)	84 (93%)	6 (7%)	16	50
18	YW	90/92 (98%)	87 (97%)	3 (3%)	38	71
19	RX	77/78 (99%)	76 (99%)	1 (1%)	69	87
19	YX	77/78 (99%)	77 (100%)	0	100	100
20	RY	86/91 (94%)	84 (98%)	2 (2%)	50	78
20	YY	86/91 (94%)	83 (96%)	3 (4%)	36	69
21	RZ	159/179 (89%)	153 (96%)	6 (4%)	33	67
21	YZ	156/179 (87%)	150 (96%)	6 (4%)	33	67
22	R0	61/67 (91%)	59 (97%)	2 (3%)	38	71
22	Y0	61/67 (91%)	60 (98%)	1 (2%)	62	84
23	R1	79/83 (95%)	77 (98%)	2 (2%)	47	77
23	Y1	81/83 (98%)	77 (95%)	4 (5%)	25	61
24	R2	65/67 (97%)	63 (97%)	2 (3%)	40	72
24	Y2	66/67 (98%)	64 (97%)	2 (3%)	41	73
25	R3	51/52 (98%)	51 (100%)	0	100	100
25	Y3	50/52 (96%)	44 (88%)	6 (12%)	5	22
26	R4	58/63 (92%)	56 (97%)	2 (3%)	37	70
26	Y4	54/63 (86%)	46 (85%)	8 (15%)	3	14
27	R5	51/52 (98%)	49 (96%)	2 (4%)	32	67
27	Y5	50/52 (96%)	48 (96%)	2 (4%)	31	66
28	R6	51/52 (98%)	49 (96%)	2 (4%)	32	67
28	Y6	50/52 (96%)	50 (100%)	0	100	100
29	R7	41/42 (98%)	41 (100%)	0	100	100
29	Y7	41/42 (98%)	41 (100%)	0	100	100
30	R8	54/55 (98%)	51 (94%)	3 (6%)	21	57
30	Y8	54/55 (98%)	52 (96%)	2 (4%)	34	68
31	R9	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	Y9	34/34 (100%)	34 (100%)	0	100	100
33	QB	191/220 (87%)	180 (94%)	11 (6%)	20	55
33	XB	187/220 (85%)	173 (92%)	14 (8%)	13	45
34	QC	144/188 (77%)	142 (99%)	2 (1%)	67	86
34	XC	140/188 (74%)	137 (98%)	3 (2%)	53	79
35	QD	171/181 (94%)	166 (97%)	5 (3%)	42	74
35	XD	172/181 (95%)	169 (98%)	3 (2%)	60	83
36	QE	114/123 (93%)	113 (99%)	1 (1%)	78	91
36	XE	114/123 (93%)	113 (99%)	1 (1%)	78	91
37	QF	85/90 (94%)	85 (100%)	0	100	100
37	XF	85/90 (94%)	84 (99%)	1 (1%)	71	88
38	QG	120/127 (94%)	114 (95%)	6 (5%)	24	60
38	XG	119/127 (94%)	115 (97%)	4 (3%)	37	70
39	QH	116/119 (98%)	113 (97%)	3 (3%)	46	76
39	XH	114/119 (96%)	110 (96%)	4 (4%)	36	69
40	QI	91/99 (92%)	83 (91%)	8 (9%)	10	36
40	XI	88/99 (89%)	83 (94%)	5 (6%)	20	56
41	QJ	68/92 (74%)	66 (97%)	2 (3%)	42	74
41	XJ	68/92 (74%)	67 (98%)	1 (2%)	65	85
42	QK	83/99 (84%)	81 (98%)	2 (2%)	49	77
42	XK	83/99 (84%)	83 (100%)	0	100	100
43	QL	96/108 (89%)	95 (99%)	1 (1%)	76	90
43	XL	96/108 (89%)	95 (99%)	1 (1%)	76	90
44	QM	90/101 (89%)	87 (97%)	3 (3%)	38	71
44	XM	87/101 (86%)	86 (99%)	1 (1%)	73	88
45	QN	49/50 (98%)	44 (90%)	5 (10%)	7	29
45	XN	49/50 (98%)	48 (98%)	1 (2%)	55	80
46	QO	78/80 (98%)	74 (95%)	4 (5%)	24	60
46	XO	78/80 (98%)	75 (96%)	3 (4%)	33	67
47	QP	69/74 (93%)	68 (99%)	1 (1%)	67	86
47	XP	68/74 (92%)	66 (97%)	2 (3%)	42	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	QQ	94/97 (97%)	94 (100%)	0	100	100
48	XQ	94/97 (97%)	94 (100%)	0	100	100
49	QR	59/77 (77%)	59 (100%)	0	100	100
49	XR	59/77 (77%)	58 (98%)	1 (2%)	60	83
50	QS	68/80 (85%)	66 (97%)	2 (3%)	42	74
50	XS	67/80 (84%)	67 (100%)	0	100	100
51	QT	71/82 (87%)	68 (96%)	3 (4%)	30	65
51	XT	70/82 (85%)	69 (99%)	1 (1%)	67	86
52	QU	18/22 (82%)	18 (100%)	0	100	100
52	XU	18/22 (82%)	17 (94%)	1 (6%)	21	57
55	QY	210/299 (70%)	200 (95%)	10 (5%)	25	61
55	XY	211/299 (71%)	198 (94%)	13 (6%)	18	53
All	All	9765/10662 (92%)	9411 (96%)	354 (4%)	35	69

5 of 354 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	QP	5	ARG
5	YF	205	ARG
40	XI	102	LEU
51	QT	65	LYS
3	YD	242	ARG

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

Mol	Chain	Res	Type
9	YN	131	GLN
50	XS	23	ASN
34	XC	6	HIS
31	R9	20	HIS
40	XI	124	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	RA	2855/2915 (97%)	442 (15%)	27 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	YA	2855/2915 (97%)	439 (15%)	25 (0%)
2	RB	119/122 (97%)	9 (7%)	0
2	YB	119/122 (97%)	10 (8%)	0
32	QA	1494/1521 (98%)	229 (15%)	16 (1%)
32	XA	1498/1521 (98%)	227 (15%)	19 (1%)
53	QV	76/77 (98%)	15 (19%)	0
53	XV	76/77 (98%)	15 (19%)	1 (1%)
54	QX	9/25 (36%)	2 (22%)	0
54	XX	8/25 (32%)	3 (37%)	0
All	All	9109/9320 (97%)	1391 (15%)	88 (0%)

5 of 1391 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	RA	10	G
1	RA	11	G
1	RA	12	U
1	RA	15	G
1	RA	45	C

5 of 88 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	QA	1256	A
1	YA	856	C
32	XA	1067	A
32	QA	1281	U
1	YA	196	A

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

50 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
32	5MC	XA	1400	32	15,22,23	3.23	5 (33%)	19,32,35	1.31	2 (10%)
1	PSU	YA	1917	1	17,21,22	3.72	8 (47%)	20,30,33	3.24	6 (30%)
43	0TD	QL	92	43	4,9,10	1.15	0	3,11,13	2.83	2 (66%)
32	UR3	QA	1498	32	14,22,23	3.49	3 (21%)	15,32,35	0.74	0
32	M2G	QA	966	32	20,27,28	4.15	6 (30%)	22,40,43	2.54	8 (36%)
32	2MG	QA	1207	32,56	19,26,27	4.42	6 (31%)	21,38,41	2.67	8 (38%)
32	5MC	QA	1400	32	15,22,23	3.22	5 (33%)	19,32,35	1.39	3 (15%)
1	5MU	RA	1915	1	15,22,23	2.86	3 (20%)	16,32,35	2.66	2 (12%)
32	2MG	XA	1207	32	19,26,27	4.38	6 (31%)	21,38,41	2.52	7 (33%)
1	2MA	YA	2503	1,56	17,25,26	4.23	6 (35%)	19,37,40	2.89	5 (26%)
1	5MC	YA	1962	1,56	15,22,23	3.25	5 (33%)	19,32,35	1.35	2 (10%)
55	MEQ	XY	235	55	8,9,10	0.90	0	5,10,12	0.80	0
1	2MU	YA	2552	1,56	14,22,24	8.48	9 (64%)	14,31,36	1.04	0
1	4OC	RA	1920	1	15,22,24	3.63	6 (40%)	17,31,35	1.67	3 (17%)
32	PSU	XA	516	32	17,21,22	3.73	9 (52%)	20,30,33	3.15	6 (30%)
1	5MC	RA	1942	1,56	15,22,23	3.28	5 (33%)	19,32,35	1.25	3 (15%)
55	MEQ	QY	235	55	8,9,10	0.93	0	5,10,12	1.08	1 (20%)
1	5MU	RA	1939	1	15,22,23	2.80	3 (20%)	16,32,35	2.99	2 (12%)
32	4OC	QA	1402	32	16,23,24	3.56	6 (37%)	17,32,35	1.75	1 (5%)
1	2MA	RA	2503	1,56	17,25,26	4.19	6 (35%)	19,37,40	2.87	5 (26%)
32	MA6	QA	1519	32	19,26,27	1.13	2 (10%)	18,38,41	3.55	2 (11%)
1	2MU	RA	2552	1,56	14,22,24	8.46	9 (64%)	14,31,36	1.03	0
1	5MC	RA	1962	1,56	15,22,23	3.24	5 (33%)	19,32,35	1.33	3 (15%)
32	PSU	QA	516	32,56	17,21,22	3.71	9 (52%)	20,30,33	3.11	6 (30%)
32	MA6	XA	1519	32	19,26,27	1.12	2 (10%)	18,38,41	3.54	2 (11%)
32	5MC	QA	1404	32	15,22,23	3.22	5 (33%)	19,32,35	1.47	4 (21%)
1	PSU	YA	2605	1	17,21,22	3.69	8 (47%)	20,30,33	3.07	6 (30%)
32	7MG	QA	527	32,56	22,26,27	4.67	10 (45%)	28,39,42	1.99	11 (39%)
1	PSU	RA	1911	1	17,21,22	3.74	9 (52%)	20,30,33	3.27	5 (25%)
1	4OC	YA	1920	1	15,22,24	3.61	6 (40%)	17,31,35	1.61	3 (17%)
32	UR3	XA	1498	32,56	14,22,23	3.52	3 (21%)	15,32,35	0.76	0
32	5MC	QA	967	32	15,22,23	3.28	5 (33%)	19,32,35	1.30	2 (10%)
1	OMG	RA	2251	1,56,53	18,26,27	3.57	7 (38%)	20,38,41	2.54	8 (40%)
32	MA6	QA	1518	32	19,26,27	1.14	2 (10%)	18,38,41	3.50	2 (11%)
1	5MU	YA	1939	1,56	15,22,23	2.79	3 (20%)	16,32,35	2.96	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	YA	1911	1	17,21,22	3.74	8 (47%)	20,30,33	3.25	6 (30%)
32	5MC	XA	1404	32	15,22,23	3.17	5 (33%)	19,32,35	1.42	3 (15%)
32	M2G	XA	966	32	20,27,28	4.08	6 (30%)	22,40,43	2.53	7 (31%)
1	PSU	RA	1917	1	17,21,22	3.75	8 (47%)	20,30,33	3.40	6 (30%)
32	5MC	QA	1407	32	15,22,23	3.21	5 (33%)	19,32,35	1.47	3 (15%)
1	5MC	YA	1942	1	15,22,23	3.27	5 (33%)	19,32,35	1.32	3 (15%)
1	PSU	RA	2605	1	17,21,22	3.70	8 (47%)	20,30,33	3.05	6 (30%)
1	OMG	YA	2251	1,56,53	18,26,27	3.54	7 (38%)	20,38,41	2.48	8 (40%)
32	4OC	XA	1402	32	16,23,24	3.38	6 (37%)	17,32,35	2.87	1 (5%)
32	7MG	XA	527	32,56	22,26,27	4.67	10 (45%)	28,39,42	1.92	11 (39%)
43	0TD	XL	92	43	4,9,10	1.14	0	3,11,13	2.75	2 (66%)
32	5MC	XA	1407	32	15,22,23	3.21	5 (33%)	19,32,35	1.30	2 (10%)
32	5MC	XA	967	32	15,22,23	3.23	5 (33%)	19,32,35	1.37	4 (21%)
1	5MU	YA	1915	1,56	15,22,23	2.87	3 (20%)	16,32,35	2.68	2 (12%)
32	MA6	XA	1518	32	19,26,27	1.06	2 (10%)	18,38,41	3.59	2 (11%)

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
32	5MC	XA	1400	32	-	4/5/25/26	0/2/2/2
1	PSU	YA	1917	1	-	0/7/25/26	0/2/2/2
43	0TD	QL	92	43	-	1/3/12/14	-
32	UR3	QA	1498	32	-	0/5/25/26	0/2/2/2
32	M2G	QA	966	32	-	0/7/29/30	0/3/3/3
32	2MG	QA	1207	32,56	-	0/5/27/28	0/3/3/3
32	5MC	QA	1400	32	-	2/5/25/26	0/2/2/2
1	5MU	RA	1915	1	-	2/5/25/26	0/2/2/2
32	2MG	XA	1207	32	-	0/5/27/28	0/3/3/3
1	2MA	YA	2503	1,56	-	1/3/25/26	0/3/3/3
1	5MC	YA	1962	1,56	-	2/5/25/26	0/2/2/2
55	MEQ	XY	235	55	-	4/8/9/11	-
1	2MU	YA	2552	1,56	-	0/7/27/28	0/2/2/2
1	4OC	RA	1920	1	-	0/7/27/30	0/2/2/2
32	PSU	XA	516	32	-	0/7/25/26	0/2/2/2
1	5MC	RA	1942	1,56	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	MEQ	QY	235	55	-	2/8/9/11	-
1	5MU	RA	1939	1	-	0/5/25/26	0/2/2/2
32	4OC	QA	1402	32	-	3/9/29/30	0/2/2/2
1	2MA	RA	2503	1,56	-	1/3/25/26	0/3/3/3
32	MA6	QA	1519	32	-	2/7/29/30	0/3/3/3
1	2MU	RA	2552	1,56	-	0/7/27/28	0/2/2/2
1	5MC	RA	1962	1,56	-	2/5/25/26	0/2/2/2
32	PSU	QA	516	32,56	-	0/7/25/26	0/2/2/2
32	MA6	XA	1519	32	-	2/7/29/30	0/3/3/3
32	5MC	QA	1404	32	-	0/5/25/26	0/2/2/2
1	PSU	YA	2605	1	-	0/7/25/26	0/2/2/2
32	7MG	QA	527	32,56	-	2/7/37/38	0/3/3/3
1	PSU	RA	1911	1	-	0/7/25/26	0/2/2/2
1	4OC	YA	1920	1	-	1/7/27/30	0/2/2/2
32	UR3	XA	1498	32,56	-	0/5/25/26	0/2/2/2
32	5MC	QA	967	32	-	0/5/25/26	0/2/2/2
1	OMG	RA	2251	1,56,53	-	0/5/27/28	0/3/3/3
32	MA6	QA	1518	32	-	0/7/29/30	0/3/3/3
1	5MU	YA	1939	1,56	-	0/5/25/26	0/2/2/2
1	PSU	YA	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	XA	1404	32	-	0/5/25/26	0/2/2/2
32	M2G	XA	966	32	-	0/7/29/30	0/3/3/3
1	PSU	RA	1917	1	-	0/7/25/26	0/2/2/2
32	5MC	QA	1407	32	-	0/5/25/26	0/2/2/2
1	5MC	YA	1942	1	-	0/5/25/26	0/2/2/2
1	PSU	RA	2605	1	-	0/7/25/26	0/2/2/2
1	OMG	YA	2251	1,56,53	-	0/5/27/28	0/3/3/3
32	4OC	XA	1402	32	-	2/9/29/30	0/2/2/2
32	7MG	XA	527	32,56	-	2/7/37/38	0/3/3/3
43	0TD	XL	92	43	-	2/3/12/14	-
32	5MC	XA	1407	32	-	0/5/25/26	0/2/2/2
32	5MC	XA	967	32	-	0/5/25/26	0/2/2/2
1	5MU	YA	1915	1,56	-	2/5/25/26	0/2/2/2
32	MA6	XA	1518	32	-	0/7/29/30	0/3/3/3

The worst 5 of 265 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	YA	2552	2MU	C6-N1	24.02	1.65	1.35
1	RA	2552	2MU	C6-N1	23.98	1.65	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	QA	1207	2MG	C2-N2	13.10	1.45	1.34
32	XA	1207	2MG	C2-N2	13.04	1.45	1.34
1	RA	2552	2MU	O4'-C1'	12.01	1.57	1.41

The worst 5 of 188 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	QA	1519	MA6	N1-C6-N6	-14.19	102.12	117.06
32	XA	1518	MA6	N1-C6-N6	-14.17	102.14	117.06
32	XA	1519	MA6	N1-C6-N6	-13.85	102.48	117.06
32	QA	1518	MA6	N1-C6-N6	-13.80	102.54	117.06
32	XA	1402	4OC	CM4-N4-C4	-11.49	113.10	122.97

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	XA	1400	5MC	O4'-C1'-N1-C6
32	XA	1400	5MC	C2'-C1'-N1-C6
43	QL	92	0TD	CG-CB-SB-CSB
1	RA	1915	5MU	O4'-C4'-C5'-O5'
1	YA	1962	5MC	O4'-C1'-N1-C6

There are no ring outliers.

21 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	YA	1917	PSU	1	0
32	QA	966	M2G	1	0
32	XA	1207	2MG	1	0
1	YA	2503	2MA	2	0
1	YA	1962	5MC	1	0
1	YA	2552	2MU	4	0
1	RA	1942	5MC	1	0
1	RA	1939	5MU	1	0
32	QA	1402	4OC	2	0
1	RA	2503	2MA	2	0
32	QA	1519	MA6	3	0
1	RA	2552	2MU	4	0
1	RA	1962	5MC	1	0
32	XA	1519	MA6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	QA	1518	MA6	1	0
1	YA	1939	5MU	1	0
1	RA	1917	PSU	1	0
1	YA	1942	5MC	1	0
32	XA	1402	4OC	3	0
43	XL	92	0TD	1	0
32	XA	1518	MA6	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2445 ligands modelled in this entry, 2443 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	SF4	QD	302	35	0,12,12	0.00	-	-		
58	SF4	XD	301	-	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
58	SF4	QD	302	35	-	-	0/6/5/5
58	SF4	XD	301	-	-	-	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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