



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 19, 2017 – 10:01 PM EST

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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : **FAILED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

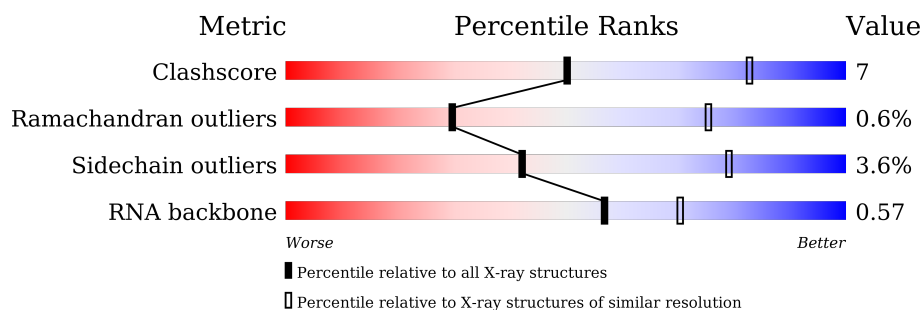
1 Overall quality at a glance

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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RNA backbone	2183	1079 (3.70-2.70)


























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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	RA	2915	
1	YA	2915	
2	RB	122	
2	YB	122	
3	RD	276	
3	YD	276	












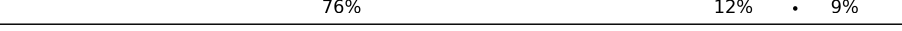







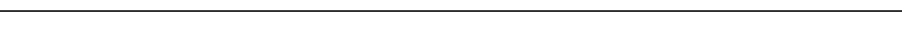

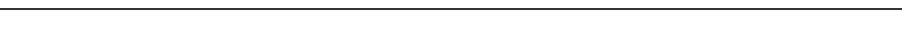
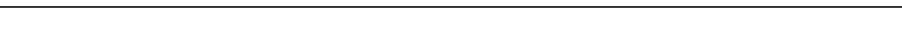


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Mol	Chain	Length	Quality of chain
4	RE	206	 81% 16% ..
4	YE	206	 78% 19% ..
5	RF	210	 75% 20% ..
5	YF	210	 71% 20% 5% .
6	RG	182	 74% 23% ..
6	YG	182	 63% 32% ..
7	RH	180	 79% 17% ..
7	YH	180	 66% 26% . .
8	RI	148	 78% 20% ..
8	YI	148	 78% 17% ..
9	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% ..


























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Mol	Chain	Length	Quality of chain
16	YU	118	 84% 14% ..
17	RV	101	 89% 10% .
17	YV	101	 75% 22% .
18	RW	113	 82% 13% ..
18	YW	113	 89% 8% ..
19	RX	96	 79% 20% .
19	YX	96	 78% 21% .
20	RY	110	 77% 18% ..
20	YY	110	 72% 24% ..
21	RZ	206	 76% 15% . 8%
21	YZ	206	 73% 17% . 8%
22	R0	85	 76% 12% . 9%
22	Y0	85	 72% 19% 9%
23	R1	98	 84% 13% ..
23	Y1	98	 74% 20% ..
24	R2	72	 88% 8% ..
24	Y2	72	 81% 15% ..
25	R3	60	 92% 7% .
25	Y3	60	 77% 18% ..
26	R4	71	 56% 37% ..
26	Y4	71	 55% 37% 6% .
27	R5	60	 75% 22% ..
27	Y5	60	 85% 12% ..
28	R6	54	 76% 20% ..
28	Y6	54	 87% 11% .


























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




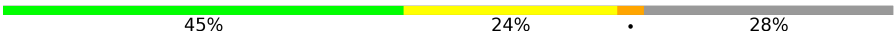
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Mol	Chain	Length	Quality of chain
41	XJ	105	
42	QK	129	
42	XK	129	
43	QL	132	
43	XL	132	
44	QM	126	
44	XM	126	
45	QN	61	
45	XN	61	
46	QO	89	
46	XO	89	
47	QP	88	
47	XP	88	
48	QQ	105	
48	XQ	105	
49	QR	88	
49	XR	88	
50	QS	93	
50	XS	93	
51	QT	106	
51	XT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

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Mol	Chain	Length	Quality of chain
54	QX	25	
54	XX	25	
55	QY	360	
55	XY	360	

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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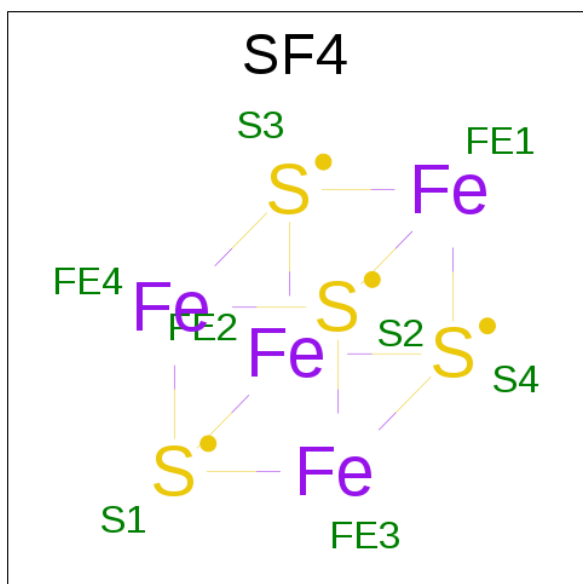
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	YF	3	Total 3	Mg 3	0	0
56	YP	1	Total 1	Mg 1	0	0
56	RZ	1	Total 1	Mg 1	0	0
56	QB	1	Total 1	Mg 1	0	0
56	Y5	1	Total 1	Mg 1	0	0
56	RE	8	Total 8	Mg 8	0	0
56	XK	1	Total 1	Mg 1	0	0
56	YB	18	Total 18	Mg 18	0	0
56	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).



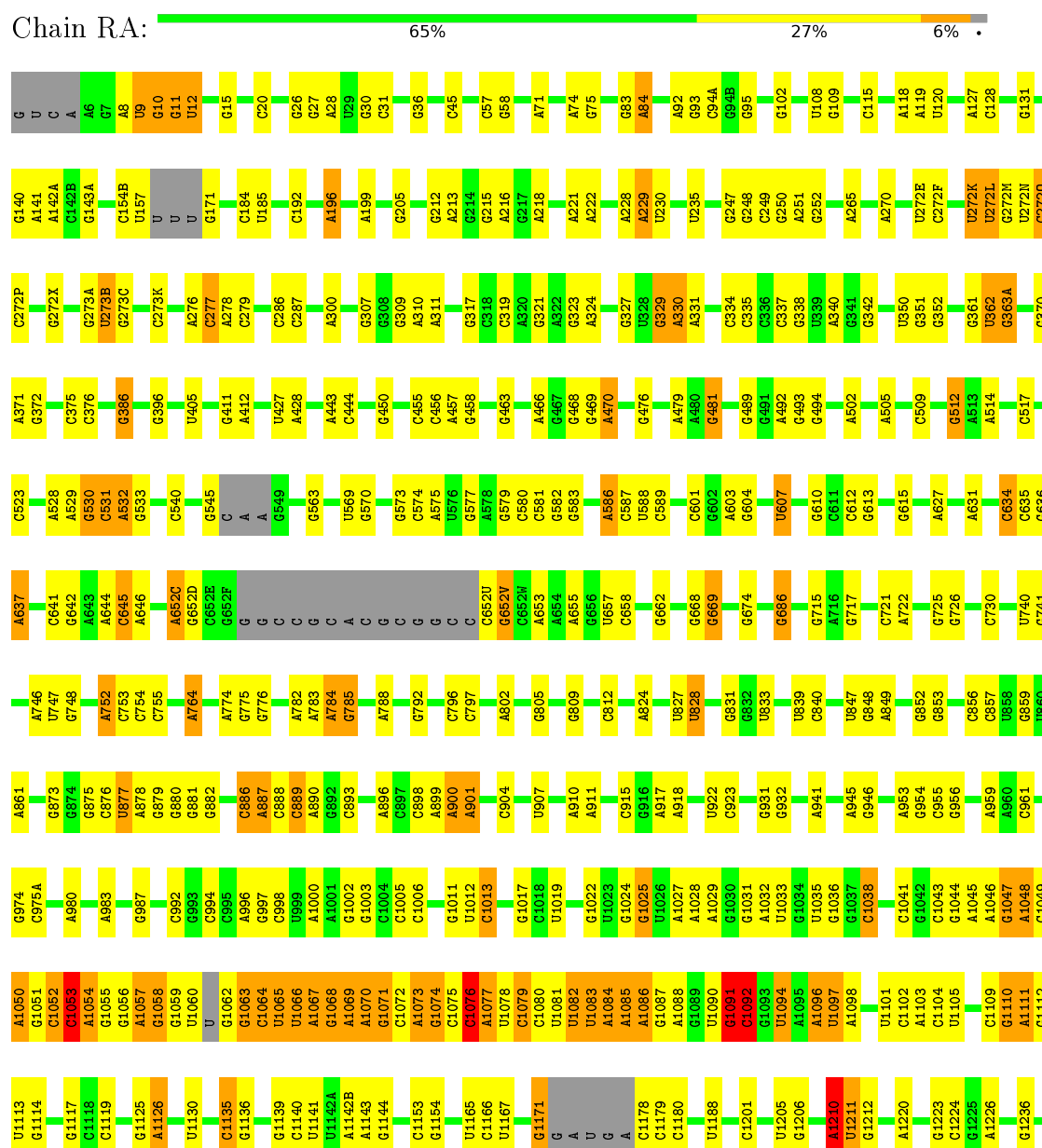
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	QD	1	Total 8	Fe 4	S 4	0	0
58	XD	1	Total 8	Fe 4	S 4	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

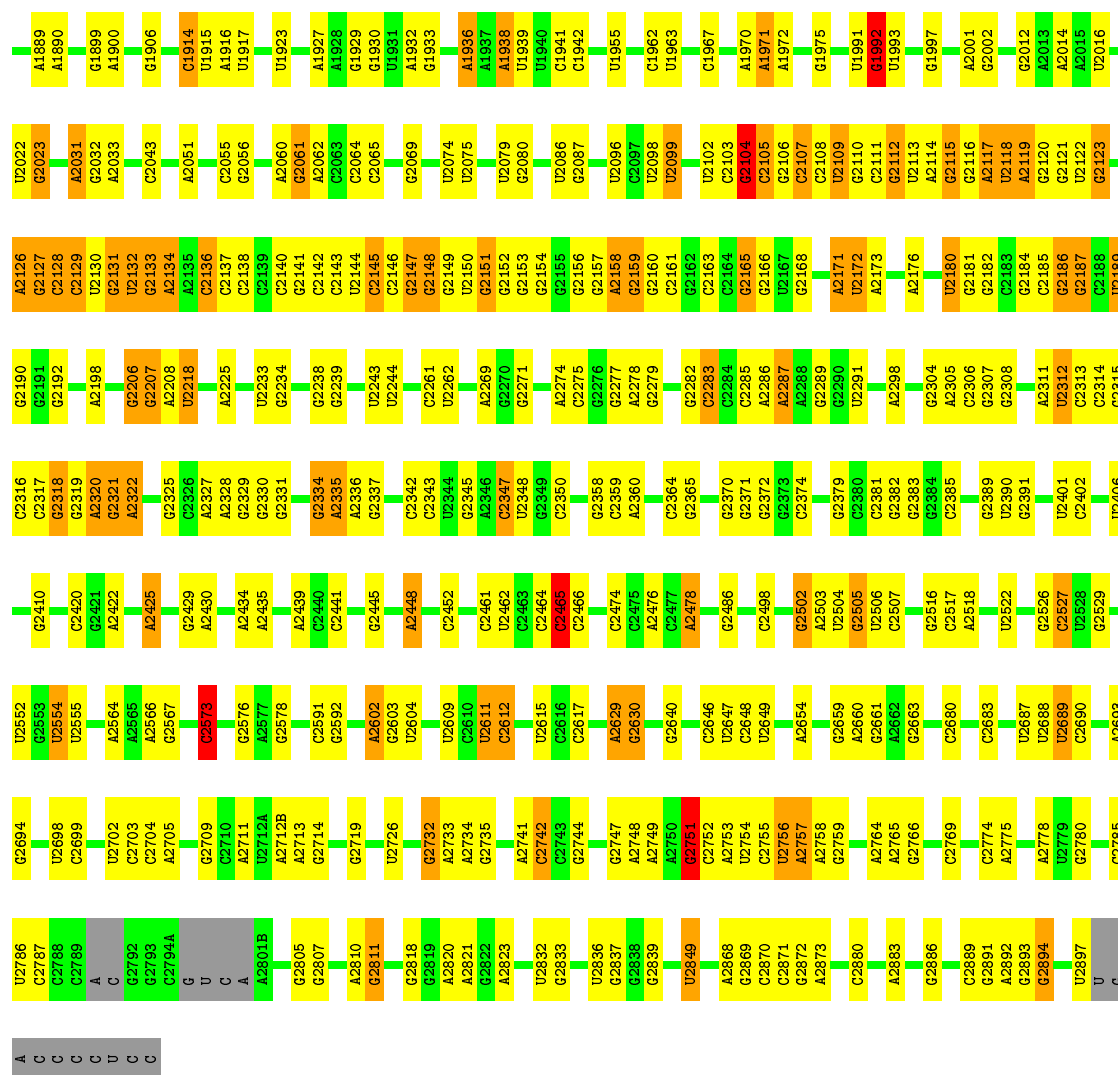
Note EDS failed to run properly.

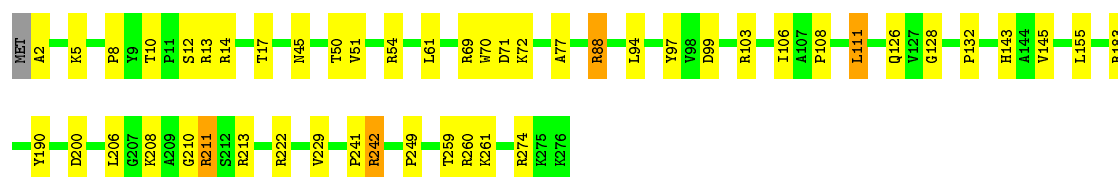
• Molecule 1: 23S rRNA



G1239	U1240	A1392	A1393	U1503	A1614	U1779	A1927	A2060	C2142	G2238	C2342	U2438	C2573	U2726	G2819
G1250	G1251	A1396	U1397	C1505	G1622	A1780	A1928	G2061	C2143	G2239	C2343	A2439	G2574	G2732	G2820
A1253	A1254	U1396	U1397	C1506	G1626	A1784	G1930	A2062	U2144	U2243	U2344	C2440	G2578	A2733	A2821
U1255	U1256	C1507	U1397	C1508	A1637	A1786	A1932	G2069	C2146	U2244	A2346	G2445	A2602	A2734	G2822
G1266	G1267	A1508	A1509A	C1509B	A1638	C1790	A1936	U2074	G2147	G2249	C2347	A2448	G2603	G2735	A2823
G1270	G1271	A1509C	A1510	C1511	A1640	A1791	A1937	U2075	G2148	U2262	C2350	G2455	U2604	C2742	U2832
G1272	G1273	U1404	U1405	U1406	A1641	U1794	A1938	U2086	G2151	U2269	G2354	C2461	C2605	C2743	G2833
A1274	A1275	U1406	U1407	U1514	G1642	U1796	A1939	U2087	G2152	A2274	C2355	U2462	U2611	U2746	U2836
A1278	U1288	C1410	C1411	G1515	G1648	U1797	U1940	U2088	G2153	C2276	G2356	C2463	C2612	G2747	G2838
C1291	U1292	G1416	G1417	C1530	G1653	U1798	C1941	G2093	G2156	C2277	C2359	C2464	U2615	A2748	G2839
C1293	U1300	U1419	U1420	C1531	G1657	U1799	C1942	G2094	G2157	C2278	A2360	C2465	C2616	A2749	U2849
U1301	U1302	G1421	G1422	C1532	A1668	C1800	C1943	U2096	A2158	C2279	C2364	C2466	C2617	C2751	A2850
U1309	G1310	G1423	G1428	C1533	G1667	A1801	U1955	C2097	G2159	A2278	C2365	C2474	A2629	C2752	G2852
U1313	C1314	U1431	C1432	C1536	A1669	A1802	C1962	U2098	G2160	C2282	G2372	C2475	G2630	A2753	C2853
C1327	U1340	U1453	U1455	U1559	G1674	A1810	C1967	U2102	C2161	C2283	G2373	A2476	G2643	U2756	A2868
U1341	U1352	G1467	G1468	G1559	A1700	A1811	A1970	G2103	G2162	C2284	G2374	A2477	G2644	A2757	G2869
G1358	A1359	A1469	A1470	A1471	A1701	A1812	A1971	G2104	C2163	C2285	C2375	A2478	G2645	A2758	C2870
A1360	A1365	A1472	G1473	C1582	A1701	A1813	A1972	G2105	C2164	C2286	G2376	C2479	G2646	G2759	C2871
G1368	U1372	G1479	G1482	A1587	A1701	A1814	A1972	G2106	U2165	A2287	A2377	G2502	U2647	A2764	G2872
A1378	A1379	G1492	C1493	A1588	A1701	A1815	A1972	G2107	U2166	C2288	A2378	G2503	U2648	A2765	A2873
G1380	A1384	A1494	A1495	C1588	A1701	A1816	A1972	G2108	U2167	C2289	A2379	G2504	U2649	C2766	C2880
A1385	U1497	A1608	A1609	A1589	A1701	A1817	A1972	G2109	U2168	C2290	A2380	G2505	U2650	C2769	A2883
		A1610	A1610	A1589	A1701	A1818	A1972	G2110	U2169	C2291	A2381	G2506	U2651	A2778	G2886
				A1570	A1701	A1819	A1972	G2111	U2170	C2292	A2382	G2507	U2652	G2779	C2889
				A1571	A1701	A1820	A1972	G2112	U2171	C2293	A2383	G2508	U2653	A2780	C2891
				A1572	A1701	A1821	A1972	G2113	U2172	C2294	A2384	G2509	U2654	G2781	A2892
				A1573	A1701	A1822	A1972	G2114	U2173	C2295	A2385	G2510	U2655	G2782	G2893
				A1574	A1701	A1823	A1972	G2115	U2174	C2296	A2386	G2511	U2656	C2785	G2894
				A1575	A1701	A1824	A1972	G2116	U2175	C2297	A2387	G2512	U2657	U2786	U2897
				A1576	A1701	A1825	A1972	G2117	U2176	C2298	A2388	G2513	U2658	A	G
				A1577	A1701	A1826	A1972	G2118	U2177	C2299	A2389	G2514	U2659	C	A
				A1578	A1701	A1827	A1972	U2119	U2178	C2300	A2390	G2515	U2660	C	C
				A1579	A1701	A1828	A1972	U2120	U2179	C2301	A2391	G2516	U2661	C	C
				A1580	A1701	A1829	A1972	U2121	U2180	C2302	A2392	G2517	U2662	C	C
				A1581	A1701	A1830	A1972	U2122	U2181	C2303	A2393	G2518	U2663	C	C
				A1582	A1701	A1831	A1972	U2123	U2182	C2304	A2394	G2519	U2664	C	C
				A1583	A1701	A1832	A1972	U2124	U2183	C2305	A2395	G2520	U2665	C	C
				A1584	A1701	A1833	A1972	U2125	U2184	C2306	A2396	G2521	U2666	C	C
				A1585	A1701	A1834	A1972	U2126	U2185	C2307	A2397	G2522	U2667	C	C
				A1586	A1701	A1835	A1972	U2127	U2186	C2308	A2398	G2523	U2668	C	C
				A1587	A1701	A1836	A1972	U2128	U2187	C2309	A2399	G2524	U2669	C	C
				A1588	A1701	A1837	A1972	U2129	U2188	C2310	A2400	G2525	U2670	C	C
				A1589	A1701	A1838	A1972	U2130	U2189	C2311	A2401	G2526	U2671	C	C
				A1590	A1701	A1839	A1972	U2131	U2190	C2312	A2402	G2527	U2672	C	C
				A1591	A1701	A1840	A1972	U2132	U2191	C2313	A2403	G2528	U2673	C	C
				A1592	A1701	A1841	A1972	U2133	U2192	C2314	A2404	G2529	U2674	C	C
				A1593	A1701	A1842	A1972	U2134	U2193	C2315	A2405	G2530	U2675	C	C
				A1594	A1701	A1843	A1972	U2135	U2194	C2316	A2406	G2531	U2676	C	C
				A1595	A1701	A1844	A1972	U2136	U2195	C2317	A2407	G2532	U2677	C	C
				A1596	A1701	A1845	A1972	U2137	U2196	C2318	A2408	G2533	U2678	C	C
				A1597	A1701	A1846	A1972	U2138	U2197	C2319	A2409	G2534	U2679	C	C
				A1598	A1701	A1847	A1972	U2139	U2198	C2320	A2410	G2535	U2680	C	C
				A1599	A1701	A1848	A1972	U2140	U2199	C2321	A2411	G2536	U2681	C	C
				A1600	A1701	A1849	A1972	U2141	U2200	C2322	A2412	G2537	U2682	C	C
				A1601	A1701	A1850	A1972	U2142	U2201	C2323	A2413	G2538	U2683	C	C
				A1602	A1701	A1851	A1972	U2143	U2202	C2324	A2414	G2539	U2684	C	C
				A1603	A1701	A1852	A1972	U2144	U2203	C2325	A2415	G2540	U2685	C	C
				A1604	A1701	A1853	A1972	U2145	U2204	C2326	A2416	G2541	U2686	C	C
				A1605	A1701	A1854	A1972	U2146	U2205	C2327	A2417	G2542	U2687	C	C
				A1606	A1701	A1855	A1972	U2147	U2206	C2328	A2418	G2543	U2688	C	C
				A1607	A1701	A1856	A1972	U2148	U2207	C2329	A2419	G2544	U2689	C	C
				A1608	A1701	A1857	A1972	U2149	U2208	C2330	A2420	G2545	U2690	C	C
				A1609	A1701	A1858	A1972	U2150	U2209	C2331	A2421	G2546	U2691	C	C
				A1610	A1701	A1859	A1972	U2151	U2210	C2332	A2422	G2547	U2692	C	C
				A1611	A1701	A1860	A1972	U2152	U2211	C2333	A2423	G2548	U2693	C	C
				A1612	A1701	A1861	A1972	U2153	U2212	C2334	A2424	G2549	U2694	C	C
				A1613	A1701	A1862	A1972	U2154	U2213	C2335	A2425	G2550	U2695	C	C
				A1614	A1701	A1863	A1972	U2155	U2214	C2336	A2426	G2551	U2696	C	C
				A1615	A1701	A1864	A1972	U2156	U2215	C2337	A2427	G2552	U2697	C	C
				A1616	A1701	A1865	A1972	U2157	U2216	C2338	A2428	G2553	U2698	C	C
				A1617	A1701	A1866	A1972	U2158	U2217	C2339	A2429	G2554	U2699	C	C
				A1618	A1701	A1867	A1972	U2159	U2218	C2340	A2430	G2555	U2700	C	C
				A1619	A1701	A1868	A1972	U2160	U2219	C2341	A2431	G2556	U2701	C	C
				A1620	A1701	A1869	A1972	U2161	U2220	C2342	A2432	G2557	U2702	C	C
				A1621	A1701	A1870	A1972	U2162	U2221	C2343	A2433	G2558	U2703	C	C
				A1622	A1701	A1871	A1972	U2163	U2222	C2344	A2434	G2559	U2704	C	C
				A1623	A1701	A1872	A1972	U2164	U2223	C2345	A2435	G2560	U2705	C	C
				A1624	A1701	A1873	A1972	U2165	U2224	C2346	A2436	G2561	U2706	C	C
				A1625	A1701	A1874	A1972	U2166	U2225	C2347	A2437	G2562	U2707	C	C
				A1626	A1701	A1875	A1972	U2167	U2226	C2348	A2438	G2563	U2708	C	C
				A1627	A1701	A1876	A1972	U2168	U2227	C2349	A2439	G2564	U2709	C	C
				A1628	A1701	A1877	A1972	U2169	U2228	C2350	A2440	G2565	U2710	C	C
				A1629	A1701	A1878	A1972	U2170	U2229	C2351	A2441	G2566	U2711	C	C
				A1630	A1701	A1879	A1972	U2171	U2230	C2352	A2442	G2567	U2712	C	C
				A1631	A1701	A1880	A1972	U2172	U2231	C2353	A2443	G2568	U2713	C	C
				A1632	A1701	A1881	A1972	U2173	U2232	C2354	A2444	G2569	U2714	C	C
				A1633	A1701	A1882	A1972	U2174	U2233	C2355	A2445	G2570	U2715	C	C
				A1634	A1701	A1883	A1972	U2175	U2234	C2356	A2446	G2571	U2716	C	C
				A1635	A1701	A1884	A1972	U2176	U2235	C2357	A2447	G2572	U2717	C	C
				A1636	A1701	A1885	A1972	U2177	U2236	C2358	A2448	G2573	U2718	C	C
				A1637	A1701	A1886	A1972	U2178	U2237	C2359	A2449	G2574	U2719	C	C
				A1638	A1701	A1887	A1972	U2179	U2238	C2360	A2450	G2575	U2720	C	C
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				A1640	A1701										

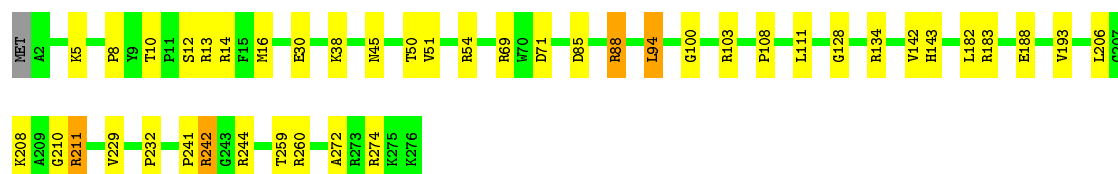






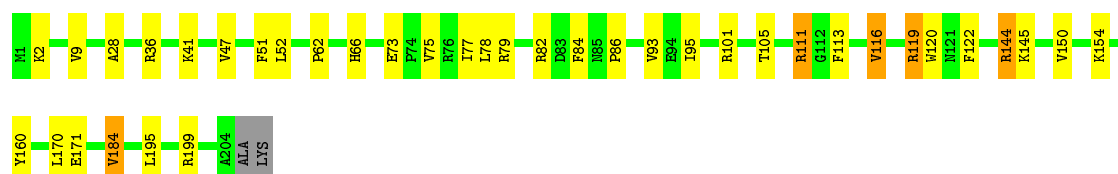
• Molecule 3: 50S ribosomal protein L2

Chain YD: 84% 14% .



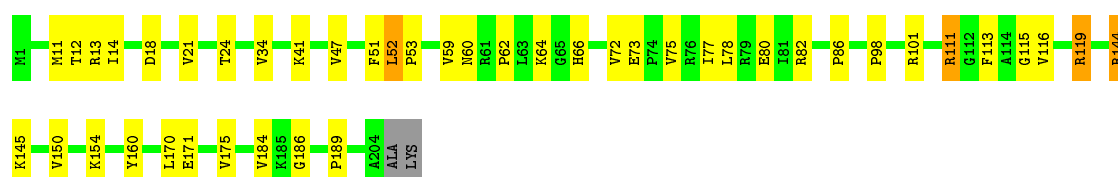
• Molecule 4: 50S ribosomal protein L3

Chain RE: 81% 16% ..



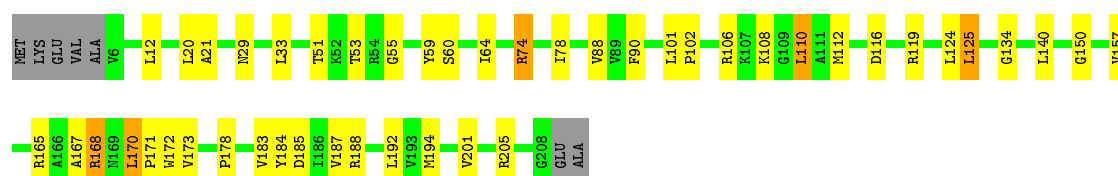
• Molecule 4: 50S ribosomal protein L3

Chain YE: 78% 19% ..



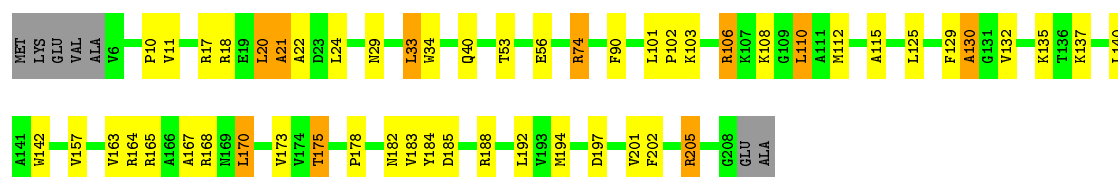
• Molecule 5: 50S ribosomal protein L4

Chain RF: 75% 20% ..



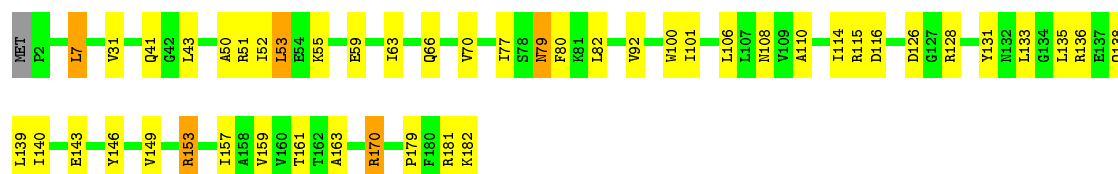
• Molecule 5: 50S ribosomal protein L4

Chain YF: 71% 20% 5% .



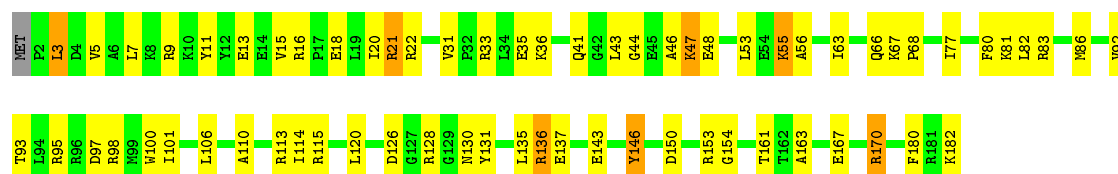
- Molecule 6: 50S ribosomal protein L5

Chain RG: 74% 23% ..



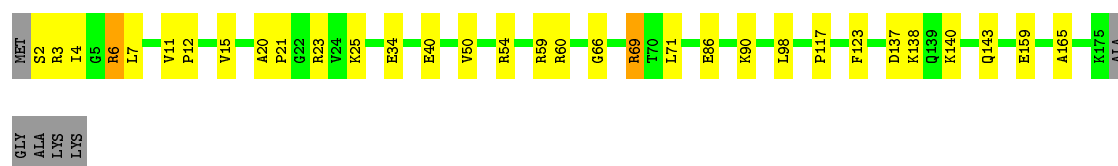
- Molecule 6: 50S ribosomal protein L5

Chain YG: 63% 32% ..



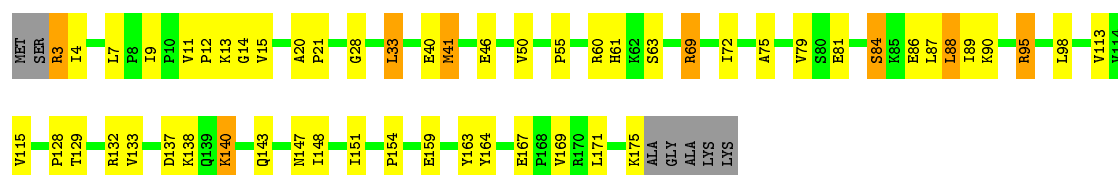
- Molecule 7: 50S ribosomal protein L6

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

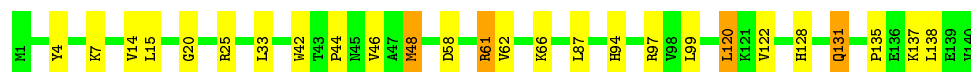
Chain YI: 78% 17% ..



GLU
GLU

- Molecule 9: 50S ribosomal protein L13

Chain RN: 81% 16% .



- Molecule 9: 50S ribosomal protein L13

Chain YN: 81% 17% .



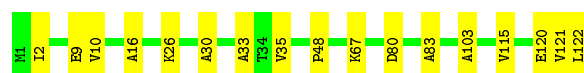
- Molecule 10: 50S ribosomal protein L14

Chain RO: 89% 11%



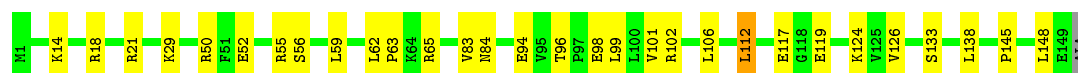
- Molecule 10: 50S ribosomal protein L14

Chain YO: 86% 14%



- Molecule 11: 50S ribosomal protein L15

Chain RP: 79% 19% ..



- Molecule 11: 50S ribosomal protein L15

Chain YP: 77% 21% ..



- Molecule 12: 50S ribosomal protein L16

Chain RQ: 79% 20% .



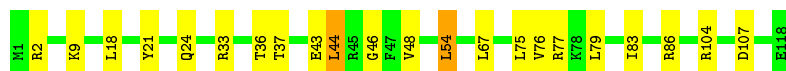
- Molecule 12: 50S ribosomal protein L16

Chain YQ: 79% 18% .



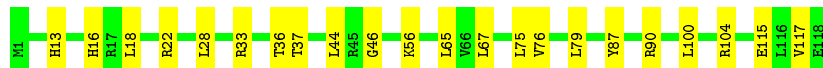
- Molecule 13: 50S ribosomal protein L17

Chain RR: 81% 17% .



- Molecule 13: 50S ribosomal protein L17

Chain YR: 81% 19% .



- Molecule 14: 50S ribosomal protein L18

Chain RS: 85% 12% . .



- Molecule 14: 50S ribosomal protein L18

Chain YS: 78% 20% . .




- Molecule 15: 50S ribosomal protein L19

Chain RT: 68% 21% 10% .




GLN
LYS
ALA
GLN
GLU
PRO
LYS
ALA
SER
GLN
GLU

- 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% ..




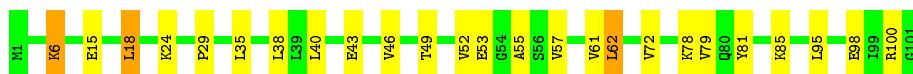
- Molecule 17: 50S ribosomal protein L21

Chain RV:  89% 10% .




- Molecule 17: 50S ribosomal protein L21

Chain YV:  75% 22% .



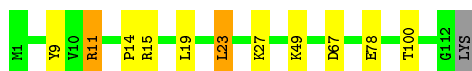
- Molecule 18: 50S ribosomal protein L22

Chain RW:  82% 13% ..




- Molecule 18: 50S ribosomal protein L22

Chain YW:  89% 8% ..




- Molecule 19: 50S ribosomal protein L23

Chain RX:  79% 20%




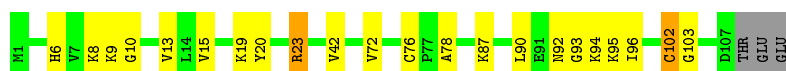
- Molecule 19: 50S ribosomal protein L23

Chain YX:  78% 21%



- Molecule 20: 50S ribosomal protein L24

Chain RY:  77% 18%




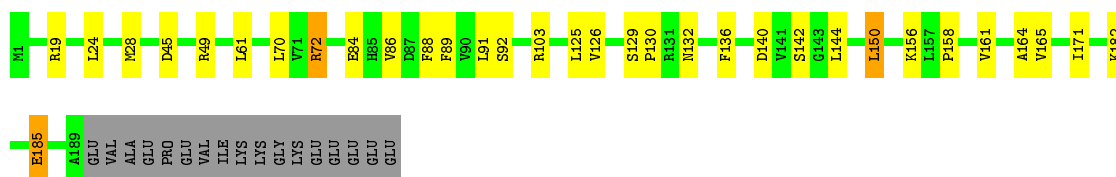
- Molecule 20: 50S ribosomal protein L24

Chain YY:  72% 24%




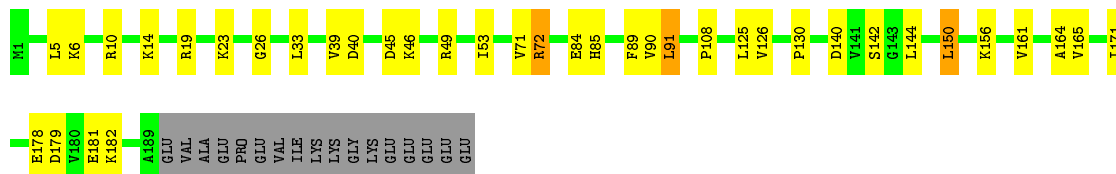
- Molecule 21: 50S ribosomal protein L25

Chain RZ:  76% 15% 8%




- Molecule 21: 50S ribosomal protein L25

Chain YZ:  73% 17% 8%



- Molecule 22: 50S ribosomal protein L27

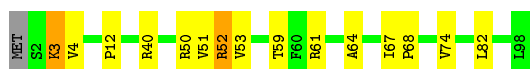
Chain R0:  76% 12% 9%



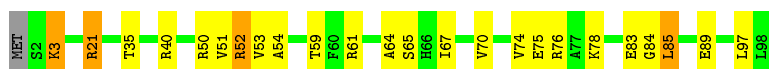
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



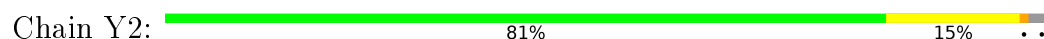
- Molecule 23: 50S ribosomal protein L28



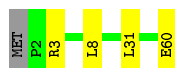
- Molecule 24: 50S ribosomal protein L29



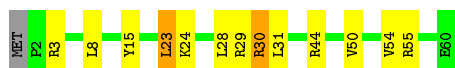
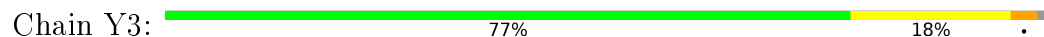
- Molecule 24: 50S ribosomal protein L29



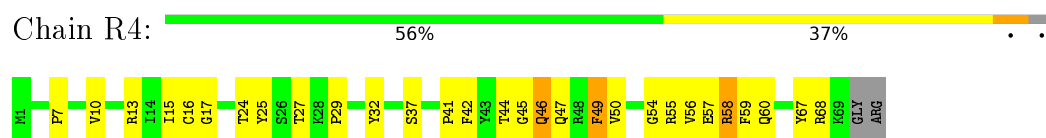
- Molecule 25: 50S ribosomal protein L30



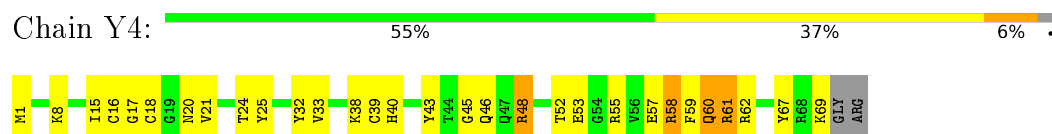
- Molecule 25: 50S ribosomal protein L30



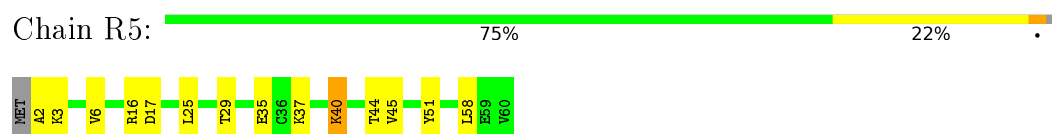
- Molecule 26: 50S ribosomal protein L31



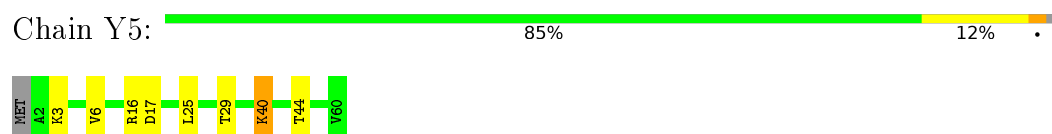
- Molecule 26: 50S ribosomal protein L31



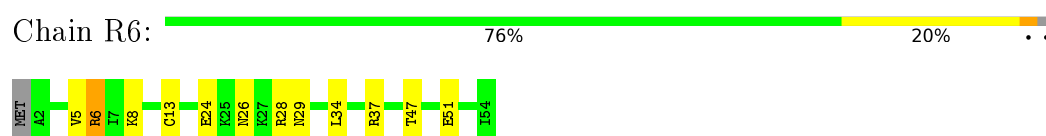
- Molecule 27: 50S ribosomal protein L32



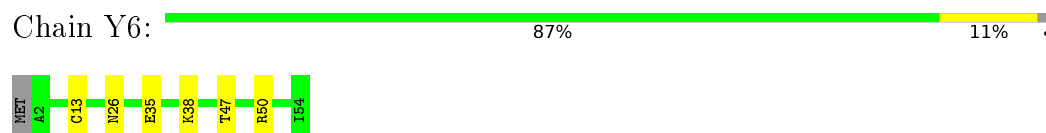
- Molecule 27: 50S ribosomal protein L32



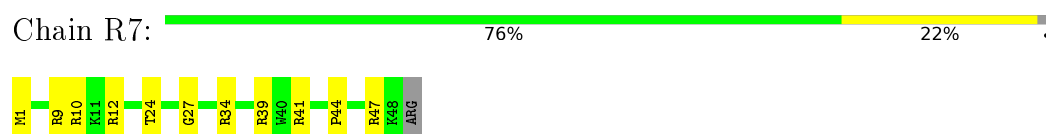
- Molecule 28: 50S ribosomal protein L33



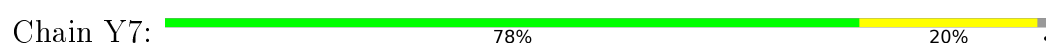
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34





- 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%



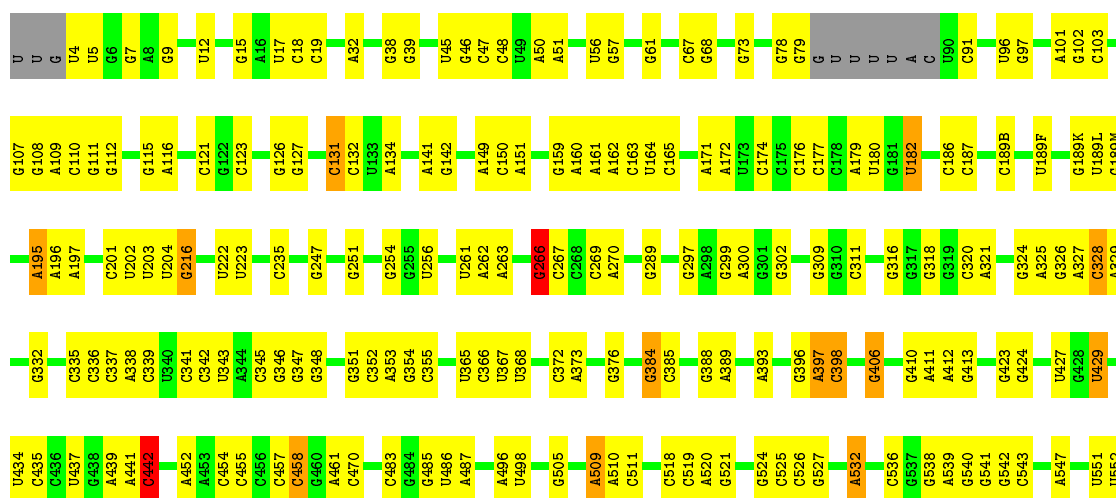
- Molecule 31: 50S ribosomal protein L36

Chain Y9: 70% 30%

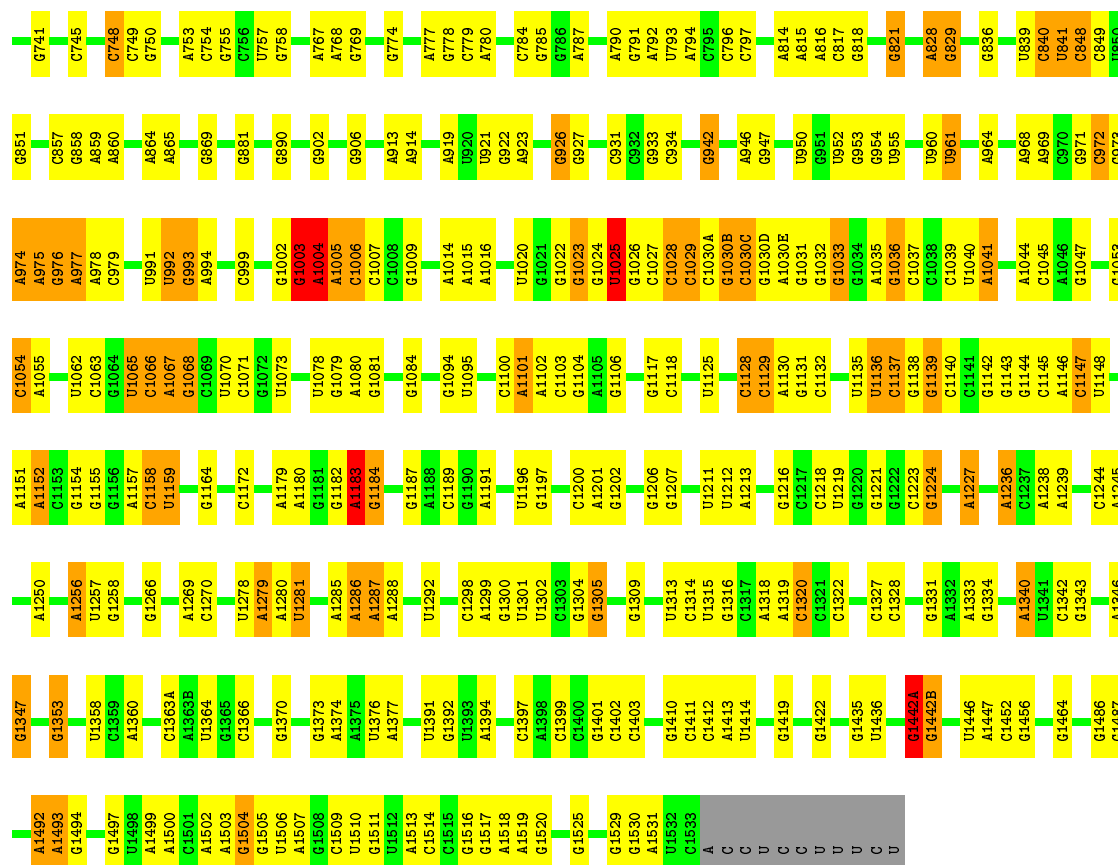


- Molecule 32: 16S rRNA

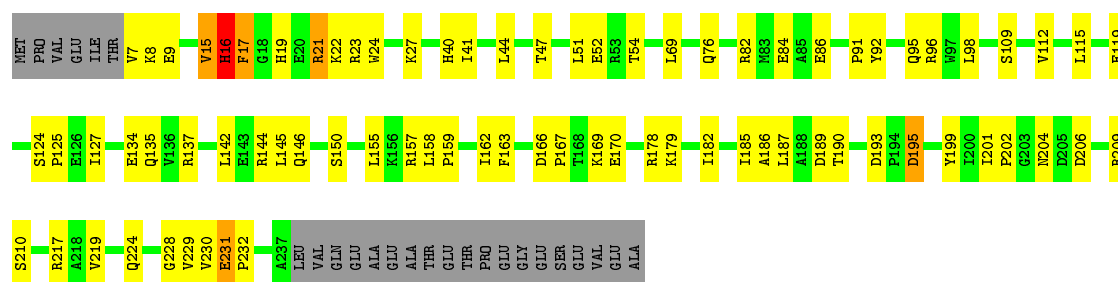
Chain QA: 63% 29% 5% ..



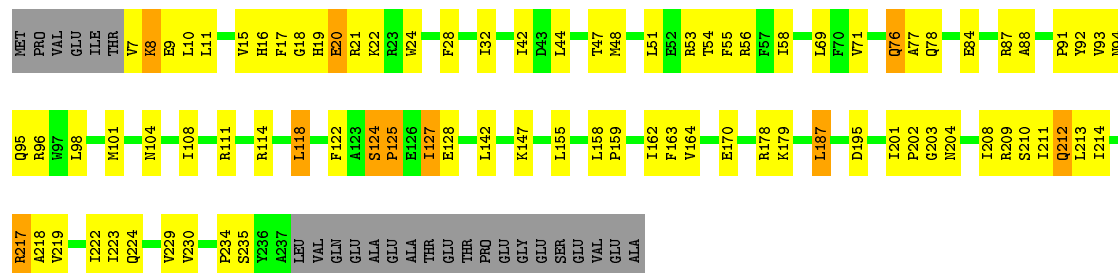




• Molecule 33: 30S ribosomal protein S2

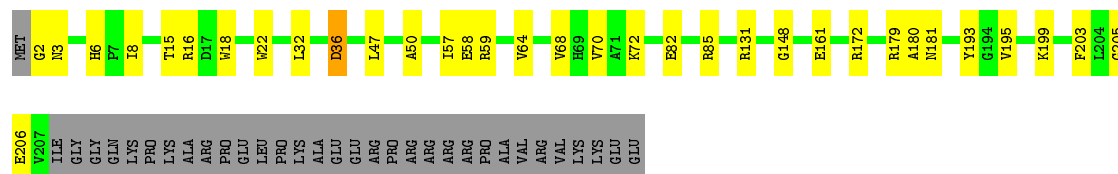


• Molecule 33: 30S ribosomal protein S2



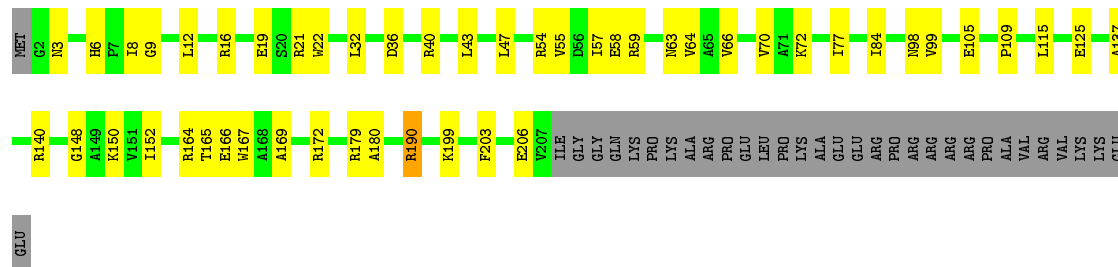
- Molecule 34: 30S ribosomal protein S3

Chain QC:  72% 14% 14%




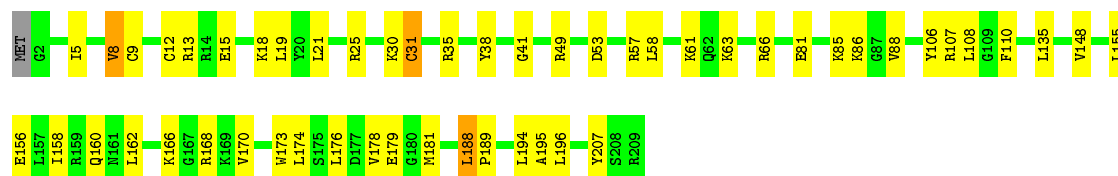
- Molecule 34: 30S ribosomal protein S3

Chain XC:  66% 20% 14%




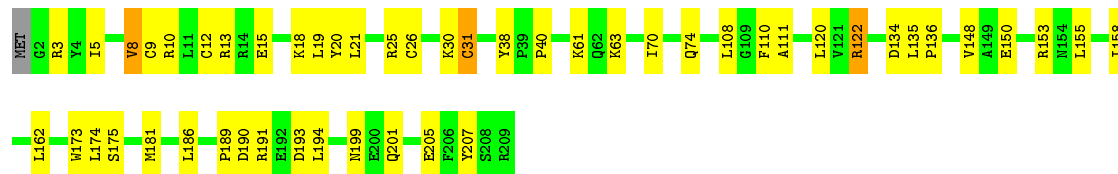
- Molecule 35: 30S ribosomal protein S4

Chain QD:  75% 23% .



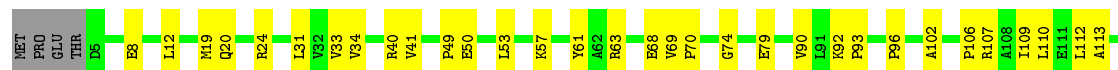
- Molecule 35: 30S ribosomal protein S4

Chain XD:  76% 22% .



- Molecule 36: 30S ribosomal protein S5

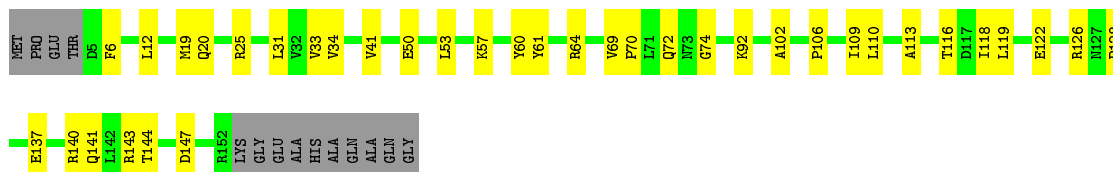
Chain QE:  65% 26% 9%





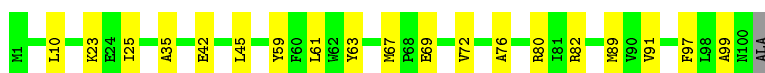
- Molecule 36: 30S ribosomal protein S5

Chain XE: 69% 23% 9%



- Molecule 37: 30S ribosomal protein S6

Chain QF: 80% 19%



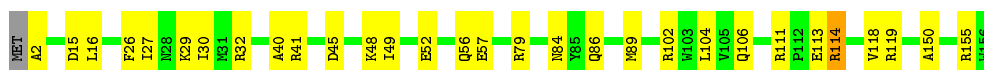
- Molecule 37: 30S ribosomal protein S6

Chain XF: 83% 16%



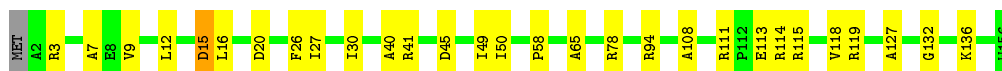
- Molecule 38: 30S ribosomal protein S7

Chain QG: 80% 19%



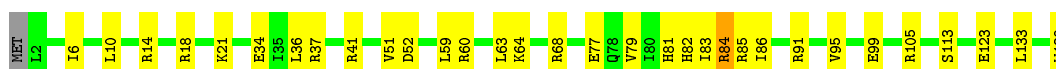
- Molecule 38: 30S ribosomal protein S7

Chain XG: 81% 18%




- Molecule 39: 30S ribosomal protein S8

Chain QH: 76% 22%



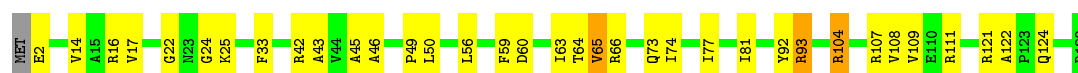
- Molecule 39: 30S ribosomal protein S8

Chain XH:  82% 16% ..



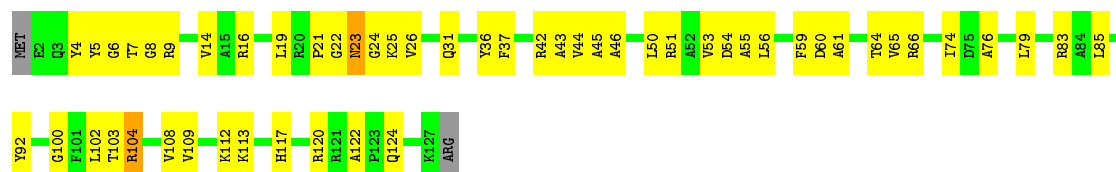
- Molecule 40: 30S ribosomal protein S9

Chain QI:  72% 25% ..



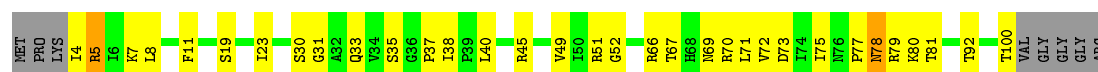
- Molecule 40: 30S ribosomal protein S9

Chain XI:  57% 40% ..



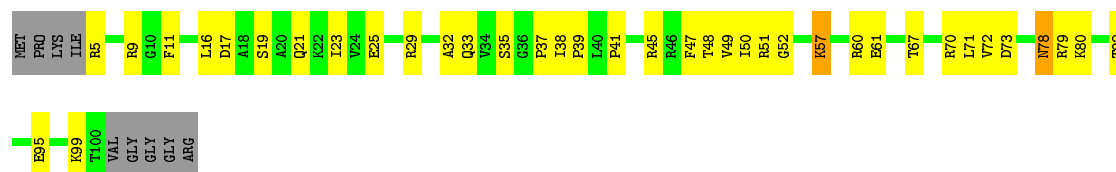
- Molecule 41: 30S ribosomal protein S10

Chain QJ:  61% 30% 8%



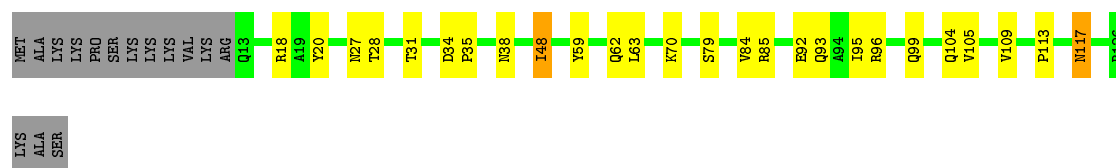
- Molecule 41: 30S ribosomal protein S10

Chain XJ:  55% 34% 9%




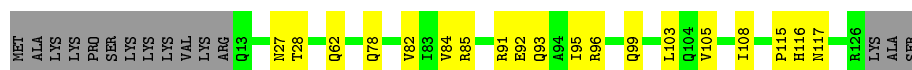
- Molecule 42: 30S ribosomal protein S11

Chain QK:  68% 19% 12%




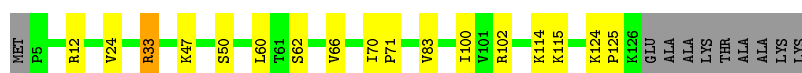
- Molecule 42: 30S ribosomal protein S11

Chain XK:  74% 15% 12%



- Molecule 43: 30S ribosomal protein S12

Chain QL:  80% 12% 8%



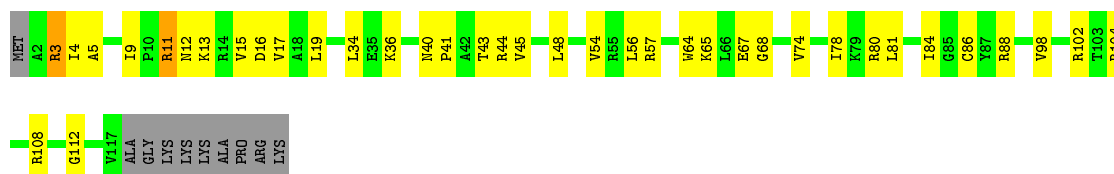
- Molecule 43: 30S ribosomal protein S12

Chain XL:  75% 17% 8%



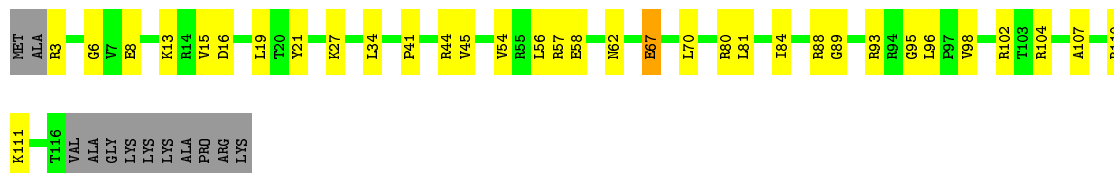
- Molecule 44: 30S ribosomal protein S13

Chain QM:  62% 29% 8%



- Molecule 44: 30S ribosomal protein S13

Chain XM:  63% 26% 10%



- Molecule 45: 30S ribosomal protein S14 type Z

Chain QN:  66% 26% 7%



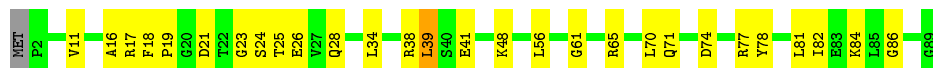
- Molecule 45: 30S ribosomal protein S14 type Z

Chain XN:  74% 23%



- Molecule 46: 30S ribosomal protein S15

Chain QO: 67% 30% ..



- Molecule 46: 30S ribosomal protein S15

Chain XO: 82% 15% ..



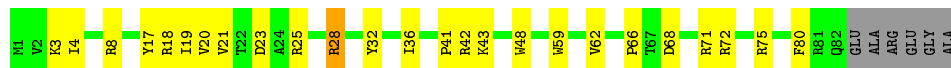
- Molecule 47: 30S ribosomal protein S16

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% ..



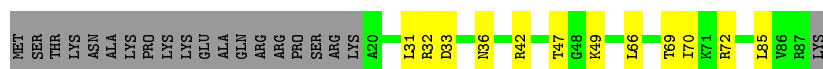
- Molecule 48: 30S ribosomal protein S17

Chain XQ: 86% 9% 6% ..

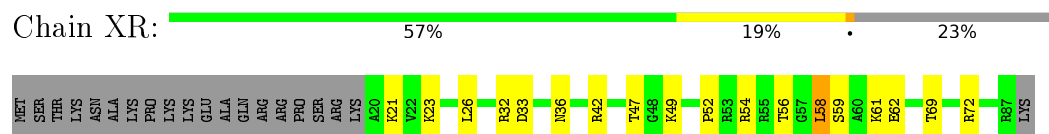


- Molecule 49: 30S ribosomal protein S18

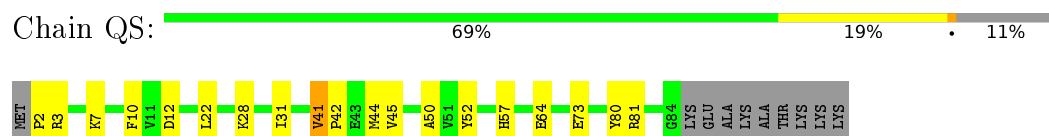
Chain QR: 64% 14% 23%



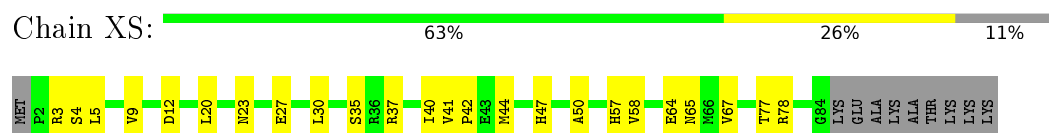
- Molecule 49: 30S ribosomal protein S18



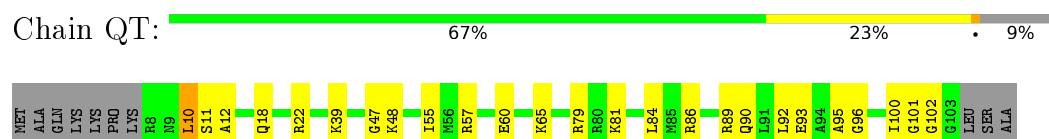
- Molecule 50: 30S ribosomal protein S19



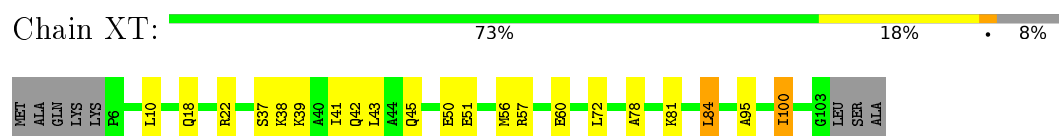
- Molecule 50: 30S ribosomal protein S19



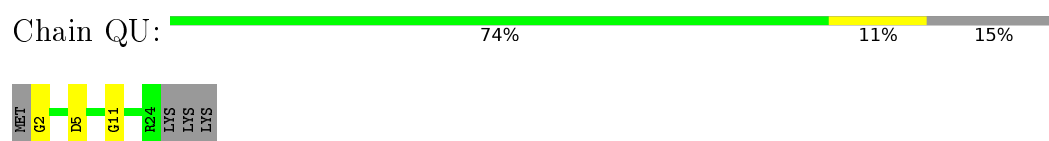
- Molecule 51: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: P-site tRNA fMet

C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	C12	C13	C14	C15	C16	C17	C18	C19	C20	C21	C22	C23	C24	C25	C26	C27	C28	C29	C30	C31	C32	C33	C34	C35	C36	C37	C38	C39	C40	C41	C42	C43	C44	C45	C46	C47	C48	C49	C50	C51	C52	C53	C54	C55	C56	C57	C58	C59	C60	C61	C62	C63	C64	C65	C66	C67	C68	C69	C70	C71	C72	C73	C74	C75	C76	C77	C78	C79	C80	C81	C82	C83	C84	C85	C86	C87	C88	C89	C90	C91	C92	C93	C94	C95	C96	C97	C98	C99	C100	C101	C102	C103	C104	C105	C106	C107	C108	C109	C110	C111	C112	C113	C114	C115	C116	C117	C118	C119	C120	C121	C122	C123	C124	C125	C126	C127	C128	C129	C130	C131	C132	C133	C134	C135	C136	C137	C138	C139	C140	C141	C142	C143	C144	C145	C146	C147	C148	C149	C150	C151	C152	C153	C154	C155	C156	C157	C158	C159	C160	C161	C162	C163	C164	C165	C166	C167	C168	C169	C170	C171	C172	C173	C174	C175	C176	C177	C178	C179	C180	C181	C182	C183	C184	C185	C186	C187	C188	C189	C190	C191	C192	C193	C194	C195	C196	C197	C198	C199	C200	C201	C202	C203	C204	C205	C206	C207	C208	C209	C210	C211	C212	C213	C214	C215	C216	C217	C218	C219	C220	C221	C222	C223	C224	C225	C226	C227	C228	C229	C230	C231	C232	C233	C234	C235	C236	C237	C238	C239	C240	C241	C242	C243	C244	C245	C246	C247	C248	C249	C250	C251	C252	C253	C254	C255	C256	C257	C258	C259	C260	C261	C262	C263	C264	C265	C266	C267	C268	C269	C270	C271	C272	C273	C274	C275	C276	C277	C278	C279	C280	C281	C282	C283	C284	C285	C286	C287	C288	C289	C290	C291	C292	C293	C294	C295	C296	C297	C298	C299	C300	C301	C302	C303	C304	C305	C306	C307	C308	C309	C310	C311	C312	C313	C314	C315	C316	C317	C318	C319	C320	C321	C322	C323	C324	C325	C326	C327	C328	C329	C330	C331	C332	C333	C334	C335	C336	C337	C338	C339	C340	C341	C342	C343	C344	C345	C346	C347	C348	C349	C350	C351	C352	C353	C354	C355	C356	C357	C358	C359	C360	C361	C362	C363	C364	C365	C366	C367	C368	C369	C370	C371	C372	C373	C374	C375	C376	C377	C378	C379	C380	C381	C382	C383	C384	C385	C386	C387	C388	C389	C390	C391	C392	C393	C394	C395	C396	C397	C398	C399	C400	C401	C402	C403	C404	C405	C406	C407	C408	C409	C410	C411	C412	C413	C414	C415	C416	C417	C418	C419	C420	C421	C422	C423	C424	C425	C426	C427	C428	C429	C430	C431	C432	C433	C434	C435	C436	C437	C438	C439	C440	C441	C442	C443	C444	C445	C446	C447	C448	C449	C450	C451	C452	C453	C454	C455	C456	C457	C458	C459	C460	C461	C462	C463	C464	C465	C466	C467	C468	C469	C470	C471	C472	C473	C474	C475	C476	C477	C478	C479	C480	C481	C482	C483	C484	C485	C486	C487	C488	C489	C490	C491	C492	C493	C494	C495	C496	C497	C498	C499	C500	C501	C502	C503	C504	C505	C506	C507	C508	C509	C510	C511	C512	C513	C514	C515	C516	C517	C518	C519	C520	C521	C522	C523	C524	C5
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| C1 | C2 | C3 | C4 | C5 | G9 | G10 | C16 | C17 | U17A | C18 | C19 | U20 | A21 | U24 | C25 | G26 | C31 | C32 | A43 | A44 | G45 | G46 | U47 | C48 | G49 | U50 | G51 | G52 | G53 | U54 | C61 | G64 | C75 | A76 | C77 |
|----|----|----|----|----|----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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| MET | LYS | PRO | SER | ILE | VAL | ALA | LYS | LEU | GLU | LEU | ALA | LEU | HIS | GLU | ARG | GLY | HIS | GLU | GLU | VAL | GLN | ALA | ALA | LEU | GLY | ASP | ASP | GLN | THR | THR | ILE | ALA | ALA | ASP | GLN | GLU | GLU | ARG | PHE | ARG | ALA | LEU | SER | SER | GLY | TYR | GLN | ALA | LEU | ASP | SER | VAL | SER | ARG | CYS | PHE | THR | ASP | TRP | GLN | GLN | VAL | GLN | GLN |
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[illegible]

I162	I163	Y172	F177	H182	R183	V184	Q185	R186	V187	P188	Q193	G194	R195	T198	A204	L209	L214	P215	T216	T217	M218	P219	A220	D221	L222	G233	G234	Q235	H236	V237	N238	T239	T240	D241	S242	R245	I246	T247	H248	L249	P250	V254	V255	E256	C257	S262
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Q263	Q264	R265	N266	K267	L274	R294	L298	G299	R303	R306	T309	T310	N311	F312	P313	Q314	G315	R316	V317	T318	R321	I322	N323	L324	T325	T326	V327	R328	L329	V332	R333	E334	G335	K336	L337	R338	M339	L340	T341	T345	D351	G51	LEU	ALA	ALA	LEU	SER	GLU	GLN
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| MET | LYS | PRO | SER | ILE | VAL | ALA | LYS | LEU | GLU | ALA | LEU | HIS | GLU | ARG | GLY | HIS | GLU | GLU | VAL | GLN | ALA | LEU | LEU | GLY | ASP | ALA | GLN | THR | ILE | ALA | ASP | GLN | GLU | ARG | PHE | ARG | ALA | LEU | SER | SER | CYS | PHE | THR | ASP | TRP | GLN | GLN | VAL | GLN | GLN |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

ASP	ASP	R137	V237	I344
ILE	ILE	Y138	N238	I345
GLU	GLU		T239	Q352
THR	THR	R145	T240	LEU
ALA	ALA	E153	D241	ALA
GLN	GLN		S242	ALA
MET	MET		A243	LEU
MET	MET	K160	R261	SER
LEU	LEU	E161	S262	GLU
ASP	ASP	I163	Q263	GLN
PRO	PRO	A164	H264	GLU
GLU	GLU	K165	K265	GLU
MET	MET	I166	N266	
ARG	ARG	S167	K267	
GLU	GLU		L274	
MET	MET	G170	R286	
ALA	ALA	R174	R294	
GLN	GLN		D302	
ASP	ASP	F177	R303	
LEU	LEU		V184	
ARG	ARG	R183	S304	
GLU	GLU	V184	D305	
ALA	ALA	Q185	R306	
LYS	LYS	R186	N307	
GLU	GLU	V187	R308	
LYS	LYS	P188	T309	
SER	SER		V310	
GLU	GLU	Q193	R311	
GLN	GLN	G194	F312	
LEU	LEU	R195	P313	
LEU	LEU	I196		
GLU	GLU	H197	R316	
		T198	V317	
		Q94	T318	
			D319	
		L101	R320	
		P102	R321	
		K103	I322	
		D104	N323	
		P105	L324	
		D106	T325	
		D107	L326	
		E108	Y327	
		R109	R328	
			L329	
		E114	D330	
		V115	N333	
		R116	K336	
			L337	
		T119	D338	
		G120	H339	
		G121	L340	
		D122	I341	
		E123		
		G129		
		R133		
		M134		
		G233		

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 (phenix.refine: 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%)	34	78
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%)	19	65
6	RG	179/182 (98%)	166 (93%)	12 (7%)	1 (1%)	30	75
6	YG	179/182 (98%)	170 (95%)	8 (4%)	1 (1%)	30	75
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%)	26	72
11	YP	147/150 (98%)	142 (97%)	4 (3%)	1 (1%)	26	72
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%)	21	67
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%)	19	65
17	YV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	19	65
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%)	17	62
23	Y1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	17	62
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%)	2	16
26	Y4	67/71 (94%)	55 (82%)	9 (13%)	3 (4%)	3	24
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%)	11	52
33	XB	229/256 (90%)	205 (90%)	19 (8%)	5 (2%)	8	45
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%)	26	72
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%)	12	54
41	QJ	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	3	26
41	XJ	94/105 (90%)	84 (89%)	8 (8%)	2 (2%)	9	46
42	QK	112/129 (87%)	105 (94%)	6 (5%)	1 (1%)	21	67

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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%)	11	51
44	XM	112/126 (89%)	105 (94%)	6 (5%)	1 (1%)	21	67
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%)	19	65
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%)	16	60
50	XS	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
51	QT	94/106 (89%)	88 (94%)	5 (5%)	1 (1%)	17	62
51	XT	96/106 (91%)	89 (93%)	5 (5%)	2 (2%)	9	46
52	QU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	XU	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	3	22
55	QY	255/360 (71%)	224 (88%)	17 (7%)	14 (6%)	2	18
55	XY	256/360 (71%)	222 (87%)	25 (10%)	9 (4%)	4	31
All	All	11925/12848 (93%)	11396 (96%)	459 (4%)	70 (1%)	30	75

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%)	41	79
3	YD	215/218 (99%)	210 (98%)	5 (2%)	58	87
4	RE	164/166 (99%)	157 (96%)	7 (4%)	35	75
4	YE	164/166 (99%)	156 (95%)	8 (5%)	31	72
5	RF	160/166 (96%)	151 (94%)	9 (6%)	26	68
5	YF	159/166 (96%)	149 (94%)	10 (6%)	22	63
6	RG	144/156 (92%)	136 (94%)	8 (6%)	26	68
6	YG	142/156 (91%)	131 (92%)	11 (8%)	16	54
7	RH	144/148 (97%)	141 (98%)	3 (2%)	61	88
7	YH	143/148 (97%)	133 (93%)	10 (7%)	19	58
8	RI	111/124 (90%)	102 (92%)	9 (8%)	15	51
8	YI	108/124 (87%)	101 (94%)	7 (6%)	21	61
9	RN	119/119 (100%)	111 (93%)	8 (7%)	20	60
9	YN	118/119 (99%)	114 (97%)	4 (3%)	44	80
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%)	68	90
11	YP	115/116 (99%)	113 (98%)	2 (2%)	68	90
12	RQ	111/111 (100%)	108 (97%)	3 (3%)	52	85
12	YQ	111/111 (100%)	105 (95%)	6 (5%)	27	68
13	RR	101/101 (100%)	95 (94%)	6 (6%)	24	65
13	YR	101/101 (100%)	95 (94%)	6 (6%)	24	65
14	RS	87/88 (99%)	85 (98%)	2 (2%)	58	87
14	YS	85/88 (97%)	83 (98%)	2 (2%)	57	86
15	RT	115/127 (91%)	111 (96%)	4 (4%)	43	80
15	YT	113/127 (89%)	110 (97%)	3 (3%)	52	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	RU	93/94 (99%)	89 (96%)	4 (4%)	35	75
16	YU	93/94 (99%)	90 (97%)	3 (3%)	46	81
17	RV	81/82 (99%)	77 (95%)	4 (5%)	31	72
17	YV	80/82 (98%)	76 (95%)	4 (5%)	30	71
18	RW	90/92 (98%)	84 (93%)	6 (7%)	20	60
18	YW	90/92 (98%)	87 (97%)	3 (3%)	45	81
19	RX	77/78 (99%)	76 (99%)	1 (1%)	76	92
19	YX	77/78 (99%)	77 (100%)	0	100	100
20	RY	86/91 (94%)	84 (98%)	2 (2%)	58	87
20	YY	86/91 (94%)	83 (96%)	3 (4%)	43	80
21	RZ	159/179 (89%)	153 (96%)	6 (4%)	40	78
21	YZ	156/179 (87%)	150 (96%)	6 (4%)	40	78
22	R0	61/67 (91%)	59 (97%)	2 (3%)	45	81
22	Y0	61/67 (91%)	60 (98%)	1 (2%)	70	91
23	R1	79/83 (95%)	77 (98%)	2 (2%)	55	86
23	Y1	81/83 (98%)	77 (95%)	4 (5%)	31	72
24	R2	65/67 (97%)	63 (97%)	2 (3%)	47	82
24	Y2	66/67 (98%)	64 (97%)	2 (3%)	48	82
25	R3	51/52 (98%)	51 (100%)	0	100	100
25	Y3	50/52 (96%)	44 (88%)	6 (12%)	6	28
26	R4	58/63 (92%)	56 (97%)	2 (3%)	44	80
26	Y4	54/63 (86%)	46 (85%)	8 (15%)	4	18
27	R5	51/52 (98%)	49 (96%)	2 (4%)	39	78
27	Y5	50/52 (96%)	48 (96%)	2 (4%)	38	77
28	R6	51/52 (98%)	49 (96%)	2 (4%)	39	78
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%)	26	68
30	Y8	54/55 (98%)	52 (96%)	2 (4%)	41	79
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%)	25	66
33	XB	187/220 (85%)	173 (92%)	14 (8%)	17	55
34	QC	144/188 (77%)	142 (99%)	2 (1%)	74	92
34	XC	140/188 (74%)	137 (98%)	3 (2%)	61	88
35	QD	171/181 (94%)	166 (97%)	5 (3%)	50	83
35	XD	172/181 (95%)	169 (98%)	3 (2%)	68	90
36	QE	114/123 (93%)	113 (99%)	1 (1%)	84	95
36	XE	114/123 (93%)	113 (99%)	1 (1%)	84	95
37	QF	85/90 (94%)	85 (100%)	0	100	100
37	XF	85/90 (94%)	84 (99%)	1 (1%)	78	93
38	QG	120/127 (94%)	114 (95%)	6 (5%)	30	71
38	XG	119/127 (94%)	115 (97%)	4 (3%)	44	80
39	QH	116/119 (98%)	113 (97%)	3 (3%)	54	85
39	XH	114/119 (96%)	110 (96%)	4 (4%)	43	80
40	QI	91/99 (92%)	83 (91%)	8 (9%)	12	45
40	XI	88/99 (89%)	83 (94%)	5 (6%)	25	67
41	QJ	68/92 (74%)	66 (97%)	2 (3%)	50	83
41	XJ	68/92 (74%)	67 (98%)	1 (2%)	72	91
42	QK	83/99 (84%)	81 (98%)	2 (2%)	57	86
42	XK	83/99 (84%)	83 (100%)	0	100	100
43	QL	96/108 (89%)	95 (99%)	1 (1%)	82	95
43	XL	96/108 (89%)	95 (99%)	1 (1%)	82	95
44	QM	90/101 (89%)	87 (97%)	3 (3%)	45	81
44	XM	87/101 (86%)	86 (99%)	1 (1%)	80	94
45	QN	49/50 (98%)	44 (90%)	5 (10%)	9	36
45	XN	49/50 (98%)	48 (98%)	1 (2%)	63	88
46	QO	78/80 (98%)	74 (95%)	4 (5%)	29	70
46	XO	78/80 (98%)	75 (96%)	3 (4%)	40	78
47	QP	69/74 (93%)	68 (99%)	1 (1%)	74	92
47	XP	68/74 (92%)	66 (97%)	2 (3%)	50	83

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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%)	68	90
50	QS	68/80 (85%)	66 (97%)	2 (3%)	50	83
50	XS	67/80 (84%)	67 (100%)	0	100	100
51	QT	71/82 (87%)	68 (96%)	3 (4%)	36	75
51	XT	70/82 (85%)	69 (99%)	1 (1%)	74	92
52	QU	18/22 (82%)	18 (100%)	0	100	100
52	XU	18/22 (82%)	17 (94%)	1 (6%)	26	68
55	QY	210/299 (70%)	200 (95%)	10 (5%)	31	72
55	XY	211/299 (71%)	198 (94%)	13 (6%)	23	64
All	All	9765/10662 (92%)	9411 (96%)	354 (4%)	42	79

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	2MG	QA	1207	32,56	18,26,27	3.81	6 (33%)	21,38,41	2.64	7 (33%)
32	5MC	QA	1400	32	14,22,23	3.22	5 (35%)	17,32,35	0.91	0
32	4OC	QA	1402	32	15,23,24	3.49	5 (33%)	21,32,35	2.02	3 (14%)
32	5MC	QA	1404	32	14,22,23	3.22	5 (35%)	17,32,35	0.98	2 (11%)
32	5MC	QA	1407	32	14,22,23	3.21	5 (35%)	17,32,35	1.01	1 (5%)
32	UR3	QA	1498	32	13,22,23	3.52	3 (23%)	18,32,35	0.73	0
32	MA6	QA	1518	32	18,26,27	1.10	2 (11%)	15,38,41	2.90	2 (13%)
32	MA6	QA	1519	32	18,26,27	1.10	2 (11%)	15,38,41	2.65	2 (13%)
32	PSU	QA	516	32,56	15,21,22	3.76	7 (46%)	16,30,33	1.84	3 (18%)
32	7MG	QA	527	32,56	20,26,27	4.64	8 (40%)	23,39,42	2.25	8 (34%)
32	M2G	QA	966	32	18,27,28	3.99	5 (27%)	22,40,43	3.38	7 (31%)
32	5MC	QA	967	32	14,22,23	3.28	5 (35%)	17,32,35	0.79	1 (5%)
43	0TD	QL	92	43	4,9,10	1.08	0	4,11,13	2.84	2 (50%)
55	MEQ	QY	235	55	7,9,10	0.79	0	8,10,12	1.02	1 (12%)
1	PSU	RA	1911	1	15,21,22	3.79	7 (46%)	16,30,33	1.91	3 (18%)
1	5MU	RA	1915	1	13,22,23	1.60	2 (15%)	16,32,35	1.65	2 (12%)
1	PSU	RA	1917	1	15,21,22	3.79	7 (46%)	16,30,33	2.04	4 (25%)
1	4OC	RA	1920	1	15,22,24	3.50	6 (40%)	20,31,35	1.57	2 (10%)
1	5MU	RA	1939	1	13,22,23	1.41	2 (15%)	16,32,35	1.67	2 (12%)
1	5MC	RA	1942	1,56	14,22,23	3.28	5 (35%)	17,32,35	0.85	1 (5%)
1	5MC	RA	1962	1,56	14,22,23	3.24	5 (35%)	17,32,35	0.82	1 (5%)
1	OMG	RA	2251	1,56,53	18,26,27	3.33	6 (33%)	21,38,41	2.56	6 (28%)
1	2MA	RA	2503	1,56	17,25,26	3.99	5 (29%)	18,37,40	4.48	4 (22%)
1	2MU	RA	2552	1,56	14,22,24	8.18	9 (64%)	19,31,36	1.37	2 (10%)
1	PSU	RA	2605	1	15,21,22	3.77	7 (46%)	16,30,33	1.91	4 (25%)
32	2MG	XA	1207	32	18,26,27	3.77	6 (33%)	21,38,41	2.46	6 (28%)
32	5MC	XA	1400	32	14,22,23	3.23	5 (35%)	17,32,35	0.84	1 (5%)
32	4OC	XA	1402	32	15,23,24	3.34	5 (33%)	21,32,35	2.84	3 (14%)
32	5MC	XA	1404	32	14,22,23	3.17	5 (35%)	17,32,35	0.90	1 (5%)
32	5MC	XA	1407	32	14,22,23	3.22	5 (35%)	17,32,35	0.91	1 (5%)
32	UR3	XA	1498	32,56	13,22,23	3.55	3 (23%)	18,32,35	0.73	0
32	MA6	XA	1518	32	18,26,27	1.04	2 (11%)	15,38,41	2.84	2 (13%)
32	MA6	XA	1519	32	18,26,27	1.06	2 (11%)	15,38,41	3.03	3 (20%)
32	PSU	XA	516	32	15,21,22	3.78	7 (46%)	16,30,33	1.95	3 (18%)
32	7MG	XA	527	32,56	20,26,27	4.65	9 (45%)	23,39,42	2.23	8 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	M2G	XA	966	32	18,27,28	3.93	5 (27%)	22,40,43	3.21	6 (27%)
32	5MC	XA	967	32	14,22,23	3.23	5 (35%)	17,32,35	0.90	1 (5%)
43	0TD	XL	92	43	4,9,10	1.08	0	4,11,13	2.76	2 (50%)
55	MEQ	XY	235	55	7,9,10	0.81	0	8,10,12	0.81	0
1	PSU	YA	1911	1	15,21,22	3.78	7 (46%)	16,30,33	1.98	4 (25%)
1	5MU	YA	1915	1,56	13,22,23	1.56	2 (15%)	16,32,35	1.69	3 (18%)
1	PSU	YA	1917	1	15,21,22	3.76	7 (46%)	16,30,33	1.97	4 (25%)
1	4OC	YA	1920	1	15,22,24	3.47	6 (40%)	20,31,35	1.63	2 (10%)
1	5MU	YA	1939	1,56	13,22,23	1.38	2 (15%)	16,32,35	1.81	3 (18%)
1	5MC	YA	1942	1	14,22,23	3.27	5 (35%)	17,32,35	0.90	1 (5%)
1	5MC	YA	1962	1,56	14,22,23	3.25	5 (35%)	17,32,35	0.83	1 (5%)
1	OMG	YA	2251	1,56,53	18,26,27	3.30	6 (33%)	21,38,41	2.51	6 (28%)
1	2MA	YA	2503	1,56	17,25,26	4.04	5 (29%)	18,37,40	4.44	4 (22%)
1	2MU	YA	2552	1,56	14,22,24	8.21	9 (64%)	19,31,36	1.42	2 (10%)
1	PSU	YA	2605	1	15,21,22	3.74	7 (46%)	16,30,33	1.84	4 (25%)

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	2MG	QA	1207	32,56	-	0/5/27/28	0/3/3/3
32	5MC	QA	1400	32	-	0/3/25/26	0/2/2/2
32	4OC	QA	1402	32	-	0/7/29/30	0/2/2/2
32	5MC	QA	1404	32	-	0/3/25/26	0/2/2/2
32	5MC	QA	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	QA	1498	32	-	0/3/25/26	0/2/2/2
32	MA6	QA	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	QA	1519	32	-	0/7/29/30	0/3/3/3
32	PSU	QA	516	32,56	-	0/7/25/26	0/2/2/2
32	7MG	QA	527	32,56	-	0/7/37/38	0/3/3/3
32	M2G	QA	966	32	-	0/7/29/30	0/3/3/3
32	5MC	QA	967	32	-	0/3/25/26	0/2/2/2
43	0TD	QL	92	43	-	0/2/12/14	0/0/0/0
55	MEQ	QY	235	55	-	0/7/9/11	0/0/0/0
1	PSU	RA	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	RA	1915	1	-	0/3/25/26	0/2/2/2
1	PSU	RA	1917	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4OC	RA	1920	1	-	0/5/27/30	0/2/2/2
1	5MU	RA	1939	1	-	0/3/25/26	0/2/2/2
1	5MC	RA	1942	1,56	-	0/3/25/26	0/2/2/2
1	5MC	RA	1962	1,56	-	0/3/25/26	0/2/2/2
1	OMG	RA	2251	1,56,53	-	0/5/27/28	0/3/3/3
1	2MA	RA	2503	1,56	-	0/3/25/26	0/3/3/3
1	2MU	RA	2552	1,56	-	0/5/27/28	0/2/2/2
1	PSU	RA	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	XA	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	XA	1400	32	-	0/3/25/26	0/2/2/2
32	4OC	XA	1402	32	-	0/7/29/30	0/2/2/2
32	5MC	XA	1404	32	-	0/3/25/26	0/2/2/2
32	5MC	XA	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	XA	1498	32,56	-	0/3/25/26	0/2/2/2
32	MA6	XA	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	XA	1519	32	-	0/7/29/30	0/3/3/3
32	PSU	XA	516	32	-	0/7/25/26	0/2/2/2
32	7MG	XA	527	32,56	-	0/7/37/38	0/3/3/3
32	M2G	XA	966	32	-	0/7/29/30	0/3/3/3
32	5MC	XA	967	32	-	0/3/25/26	0/2/2/2
43	0TD	XL	92	43	-	0/2/12/14	0/0/0/0
55	MEQ	XY	235	55	-	0/7/9/11	0/0/0/0
1	PSU	YA	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	YA	1915	1,56	-	0/3/25/26	0/2/2/2
1	PSU	YA	1917	1	-	0/7/25/26	0/2/2/2
1	4OC	YA	1920	1	-	0/5/27/30	0/2/2/2
1	5MU	YA	1939	1,56	-	0/3/25/26	0/2/2/2
1	5MC	YA	1942	1	-	0/3/25/26	0/2/2/2
1	5MC	YA	1962	1,56	-	0/3/25/26	0/2/2/2
1	OMG	YA	2251	1,56,53	-	0/5/27/28	0/3/3/3
1	2MA	YA	2503	1,56	-	0/3/25/26	0/3/3/3
1	2MU	YA	2552	1,56	-	0/5/27/28	0/2/2/2
1	PSU	YA	2605	1	-	0/7/25/26	0/2/2/2

The worst 5 of 239 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	YA	2552	2MU	C6-C5	-9.51	1.17	1.38
1	RA	2552	2MU	C6-C5	-9.50	1.17	1.38
1	YA	2552	2MU	C3'-C2'	-8.51	1.33	1.53
1	RA	2552	2MU	C3'-C2'	-8.26	1.34	1.53
1	RA	2552	2MU	C4-N3	-6.87	1.20	1.33

The worst 5 of 141 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	QA	966	M2G	C1'-N9-C4	-12.99	112.31	126.81
1	RA	2503	2MA	C1'-N9-C4	-11.96	113.46	126.81
1	YA	2503	2MA	C1'-N9-C4	-11.95	113.47	126.81
32	XA	966	M2G	C1'-N9-C4	-11.61	113.85	126.81
32	XA	1402	4OC	CM4-N4-C4	-11.59	113.10	122.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	QA	1402	4OC	2	0
32	QA	1518	MA6	1	0
32	QA	1519	MA6	3	0
32	QA	966	M2G	1	0
1	RA	1917	PSU	1	0
1	RA	1939	5MU	1	0
1	RA	1942	5MC	1	0
1	RA	1962	5MC	1	0
1	RA	2503	2MA	2	0
1	RA	2552	2MU	4	0
32	XA	1207	2MG	1	0
32	XA	1402	4OC	3	0
32	XA	1518	MA6	2	0
32	XA	1519	MA6	1	0
43	XL	92	0TD	1	0
1	YA	1917	PSU	1	0
1	YA	1939	5MU	1	0
1	YA	1942	5MC	1	0
1	YA	1962	5MC	1	0
1	YA	2503	2MA	2	0
1	YA	2552	2MU	4	0

5.5 Carbohydrates

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	-	0,24,24	0.00	-
58	SF4	XD	301	-	0,12,12	0.00	-	0,24,24	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	-	0/0/48/48	0/6/5/5
58	SF4	XD	301	-	-	0/0/48/48	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.