



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2017 – 02:50 PM EDT

PDB ID : 5J30
Title : Thermus thermophilus 70S termination complex containing E. coli RF1
Authors : Hoffer, E.D.; Dunham, C.M.
Deposited on : unknown
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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : **FAILED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

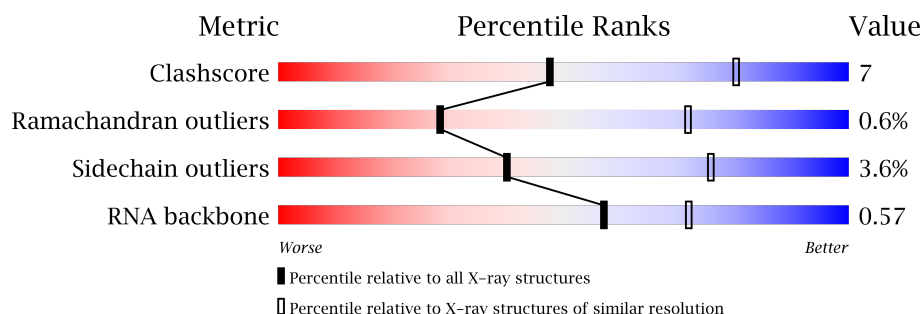
1 Overall quality at a glance

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	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RNA backbone	2435	1045 (3.60-2.80)


























The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	












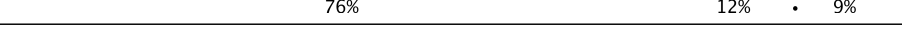







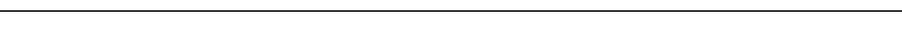

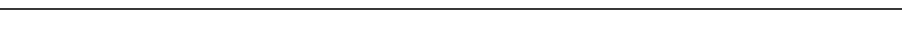
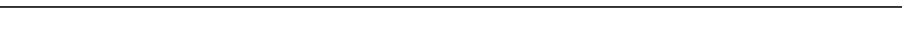


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Mol	Chain	Length	Quality of chain
4	RE	206	 81% 16% ..
4	YE	206	 78% 19% ..
5	RF	210	 75% 20% ..
5	YF	210	 71% 20% 5% .
6	RG	182	 74% 23% ..
6	YG	182	 63% 32% ..
7	RH	180	 79% 17% ..
7	YH	180	 66% 26% . .
8	RI	148	 78% 20% ..
8	YI	148	 78% 17% ..
9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









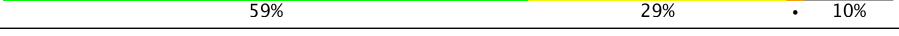

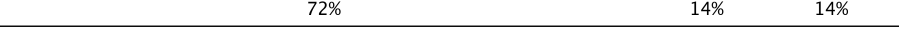
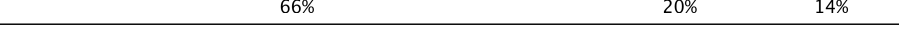

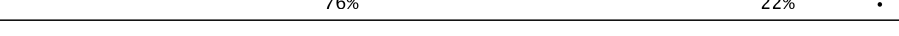


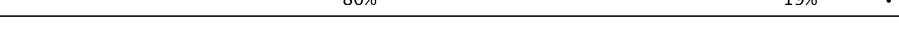

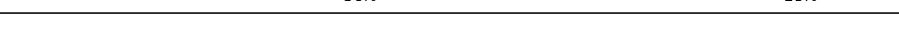






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Mol	Chain	Length	Quality of chain
16	YU	118	 84% 14% ..
17	RV	101	 89% 10% .
17	YV	101	 75% 22% .
18	RW	113	 82% 13% ..
18	YW	113	 89% 8% ..
19	RX	96	 79% 20% .
19	YX	96	 78% 21% .
20	RY	110	 77% 18% ..
20	YY	110	 72% 24% ..
21	RZ	206	 76% 15% . 8%
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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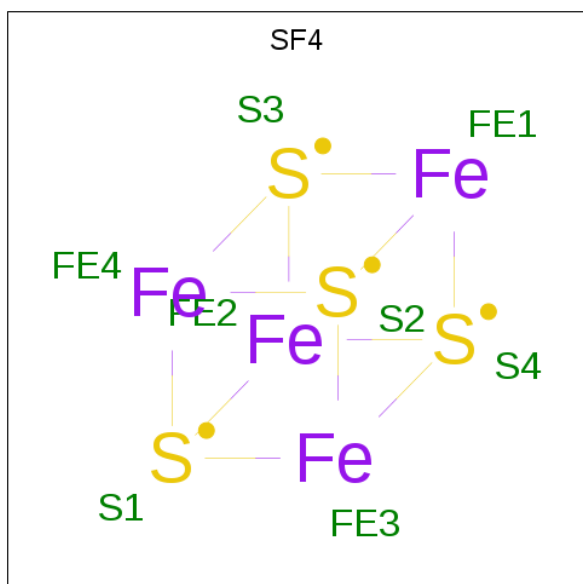
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	YF	3	Total 3	Mg 3	0	0
56	YP	1	Total 1	Mg 1	0	0
56	RZ	1	Total 1	Mg 1	0	0
56	QB	1	Total 1	Mg 1	0	0
56	Y5	1	Total 1	Mg 1	0	0
56	RE	8	Total 8	Mg 8	0	0
56	XK	1	Total 1	Mg 1	0	0
56	YB	18	Total 18	Mg 18	0	0
56	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		

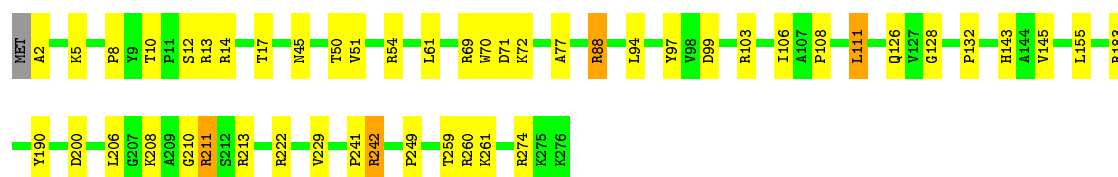
- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

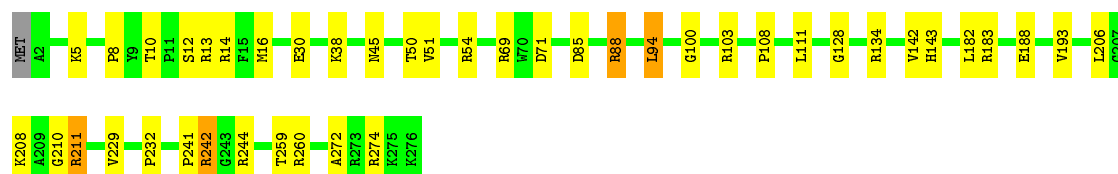
G1239	U1240	A1392	A1393	U1503	A1614	U1779	A1927	A2060	C2142	G2238	C2342	U2438	C2573	U2726	G2819
G1250	G1251	A1396	U1397	C1505	G1622	A1780	A1928	G2061	C2143	G2239	C2343	A2439	G2574	G2732	G2820
A1253	A1254	U1396	U1397	C1506	G1626	A1784	G1930	A2062	U2144	U2243	U2344	C2440	G2578	A2733	A2821
U1255	U1256	C1507	U1397	C1508	A1637	A1786	A1932	G2069	C2146	U2244	A2345	G2445	A2602	A2734	G2822
G1266	G1267	A1508	U1397	C1509A	A1638	C1790	A1936	U2074	G2147	G2249	C2347	A2448	G2603	G2735	A2823
G1270	G1271	A1509B	U1397	C1509C	A1640	A1791	A1937	U2075	G2148	U2250	C2350	G2455	U2604	C2742	U2832
G1272	U1273	A1509C	U1397	C1510	A1641	U1794	A1938	U2086	G2151	U2262	G2354	G2461	C2610	C2743	G2833
A1274	A1275	C1511	U1397	C1511	A1642	U1795	A1939	U2087	G2152	A2269	C2355	U2462	C2611	C2744	U2836
A1278	U1288	U1514	U1397	C1512	G1648	U1796	U1940	U2088	G2153	A2274	G2356	C2463	C2612	U2746	G2838
C1291	U1292	U1515	U1397	C1513	G1653	U1797	C1941	U2089	G2156	C2275	C2359	C2464	U2615	A2748	G2839
C1293	U1297	U1516	U1397	C1514	G1657	U1798	C1942	U2090	G2157	C2276	A2360	C2465	C2616	A2749	U2849
U1300	U1301	U1517	U1397	C1515	G1667	U1799	U1955	U2091	A2158	C2277	C2364	C2466	C2617	C2751	A2850
U1309	G1310	U1518	U1397	C1516	G1668	U1801	U1962	U2092	G2159	A2278	C2365	C2474	A2629	C2752	G2852
U1313	C1314	U1519	U1397	C1517	G1674	U1802	U1963	U2093	G2160	C2282	G2372	C2475	G2630	A2753	C2853
C1327	U1340	U1520	U1397	C1518	G1686	U1803	C1967	U2102	C2161	C2283	G2373	C2476	G2643	U2756	A2868
U1352	G1358	U1521	U1397	C1519	G1687	U1804	U1970	G2103	C2162	C2284	G2374	A2477	G2644	A2757	G2869
G1359	A1359	U1522	U1397	C1520	G1688	U1805	A1971	G2104	C2163	C2285	C2375	A2478	G2645	A2758	C2870
A1360	A1365	U1523	U1397	C1521	G1689	U1806	A1972	G2105	G2165	A2286	A2376	C2498	G2646	G2759	C2871
A1368	U1372	U1524	U1397	C1522	G1696	U1807	A1973	G2106	U2167	A2288	A2377	G2502	U2647	A2764	G2872
A1378	G1380	U1525	U1397	C1523	G1697	U1808	U1974	G2107	C2168	C2289	A2378	G2503	U2648	A2765	A2873
A1384	G1385	U1526	U1397	C1524	G1698	U1809	U1975	G2108	A2171	U2291	G2382	G2504	U2649	C2769	C2880
		U1527	U1397	C1525	G1699	U1810	U1976	G2109	A2172	G2390	G2383	G2505		A2778	A2883
		U1528	U1397	C1526	G1700	U1811	U1977	G2110	C2169	G2391	G2384	G2506		U2779	G2886
		U1529	U1397	C1527	A1701	U1812	U1978	G2111	U2170	G2392	G2385	G2507		A2780	C2889
		U1530	U1397	C1528	A1702	U1813	U1979	G2112	A2171	G2393	G2390	G2508		G2782	A2892
		U1531	U1397	C1529	A1703	U1814	U1980	G2113	C2170	U2311	G2394	G2509		C2785	G2893
		U1532	U1397	C1530	A1704	U1815	U1981	G2114	C2171	U2312	U2401	G2510		U2786	G2894
		U1533	U1397	C1531	A1705	U1816	U1982	G2115	C2172	U2313	U2402	G2511		C2789	U2897
		U1534	U1397	C1532	A1706	U1817	U1983	G2116	C2173	U2314	C2403	G2512		A	G
		U1535	U1397	C1533	A1707	U1818	U1984	G2117	C2174	U2315	U2404	G2513		C	A
		U1536	U1397	C1534	A1708	U1819	U1985	G2118	C2175	U2316	U2405	G2514		C	C
		U1537	U1397	C1535	A1709	U1820	U1986	G2119	C2176	U2317	U2406	G2515		C	C
		U1538	U1397	C1536	A1710	U1821	U1987	G2120	C2177	U2318	U2407	G2516		C	C
		U1539	U1397	C1537	A1711	U1822	U1988	G2121	C2178	U2319	U2408	G2517		C	C
		U1540	U1397	C1538	A1712	U1823	U1989	G2122	C2179	U2320	U2409	G2518		C	C
		U1541	U1397	C1539	A1713	U1824	U1990	G2123	C2180	U2321	U2410	G2519		C	C
		U1542	U1397	C1540	A1714	U1825	U1991	G2124	C2181	U2322	U2411	G2520		C	C
		U1543	U1397	C1541	A1715	U1826	U1992	G2125	C2182	U2323	U2412	G2521		C	C
		U1544	U1397	C1542	A1716	U1827	U1993	G2126	C2183	U2324	U2413	G2522		C	C
		U1545	U1397	C1543	A1717	U1828	U1994	G2127	C2184	U2325	U2414	G2523		C	C
		U1546	U1397	C1544	A1718	U1829	U1995	G2128	C2185	U2326	U2415	G2524		C	C
		U1547	U1397	C1545	A1719	U1830	U1996	G2129	C2186	U2327	U2416	G2525		C	C
		U1548	U1397	C1546	A1720	U1831	U1997	G2130	C2187	U2328	U2417	G2526		C	C
		U1549	U1397	C1547	A1721	U1832	U1998	G2131	C2188	U2329	U2418	G2527		C	C
		U1550	U1397	C1548	A1722	U1833	U1999	G2132	C2189	U2330	U2419	G2528		C	C
		U1551	U1397	C1549	A1723	U1834	U2000	G2133	C2190	U2331	U2420	G2529		C	C
		U1552	U1397	C1550	A1724	U1835	U2001	G2134	C2191	U2332	U2421	G2530		C	C
		U1553	U1397	C1551	A1725	U1836	U2002	G2135	C2192	U2333	U2422	G2531		C	C
		U1554	U1397	C1552	A1726	U1837	U2003	G2136	C2193	U2334	U2423	G2532		C	C
		U1555	U1397	C1553	A1727	U1838	U2004	G2137	C2194	U2335	U2424	G2533		C	C
		U1556	U1397	C1554	A1728	U1839	U2005	G2138	C2195	U2336	U2425	G2534		C	C
		U1557	U1397	C1555	A1729	U1840	U2006	G2139	C2196	U2337	U2426	G2535		C	C
		U1558	U1397	C1556	A1730	U1841	U2007	G2140	C2197	U2338	U2427	G2536		C	C
		U1559	U1397	C1557	A1731	U1842	U2008	G2141	C2198	U2339	U2428	G2537		C	C
		U1560	U1397	C1558	A1732	U1843	U2009	G2142	C2199	U2340	U2429	G2538		C	C
		U1561	U1397	C1559	A1733	U1844	U2010	G2143	C2200	U2341	U2430	G2539		C	C
		U1562	U1397	C1560	A1734	U1845	U2011	G2144	C2201	U2342	U2431	G2540		C	C
		U1563	U1397	C1561	A1735	U1846	U2012	G2145	C2202	U2343	U2432	G2541		C	C
		U1564	U1397	C1562	A1736	U1847	U2013	G2146	C2203	U2344	U2433	G2542		C	C
		U1565	U1397	C1563	A1737	U1848	U2014	G2147	C2204	U2345	U2434	G2543		C	C
		U1566	U1397	C1564	A1738	U1849	U2015	G2148	C2205	U2346	U2435	G2544		C	C
		U1567	U1397	C1565	A1739	U1850	U2016	G2149	C2206	U2347	U2436	G2545		C	C
		U1568	U1397	C1566	A1740	U1851	U2017	G2150	C2207	U2348	U2437	G2546		C	C
		U1569	U1397	C1567	A1741	U1852	U2018	G2151	C2208	U2349	U2438	G2547		C	C
		U1570	U1397	C1568	A1742	U1853	U2019	G2152	C2209	U2350	U2439	G2548		C	C
		U1571	U1397	C1569	A1743	U1854	U2020	G2153	C2210	U2351	U2440	G2549		C	C
		U1572	U1397	C1570	A1744	U1855	U2021	G2154	C2211	U2352	U2441	G2550		C	C
		U1573	U1397	C1571	A1745	U1856	U2022	G2155	C2212	U2353	U2442	G2551		C	C
		U1574	U1397	C1572	A1746	U1857	U2023	G2156	C2213	U2354	U2443	G2552		C	C
		U1575	U1397	C1573	A1747	U1858	U2024	G2157	C2214	U2355	U2444	G2553		C	C
		U1576	U1397	C1574	A1748	U1859	U2025	G2158	C2215	U2356	U2445	G2554		C	C
		U1577	U1397	C1575	A1749	U1860	U2026	G2159	C2216	U2357	U2446	G2555		C	C
		U1578	U1397	C1576	A1750	U1861	U2027	G2160	C2217	U2358	U2447	G2556		C	C
		U1579	U1397	C1577	A1751	U1862	U2028	G2161	C2218	U2359	U2448	G2557		C	C
		U1580	U1397	C1578	A1752	U1863	U2029	G2162	C2219	U2360	U2449	G2558		C	C
		U1581	U1397	C1579	A1753	U1864	U2030	G2163	C2220	U2361	U2450	G2559		C	C
		U1582	U1397	C1580	A1754	U1865	U2031	G2164	C2221	U2362	U2451	G2560		C	C
		U1583	U1397	C1581	A1755	U1866	U2032	G2165	C2222	U2363	U2452	G2561		C	C
		U1584	U1397	C1582	A1756	U1867	U2033	G2166	C2223	U2364	U2453	G2562		C	C
		U1585	U1397	C1583	A1757	U1868	U2034	G2167	C2224	U2365	U2454	G2563		C	C
		U1586	U1397	C1584	A1758	U1869	U2035	G2168	C2225	U2366	U2455	G2564		C	C
		U1587	U1397	C1585	A1759	U1870	U2036	G2169	C2226	U2367	U2456	G2565		C	C
		U1588	U1397	C1586	A1760	U1871	U2037	G2170	C2227	U2368	U2457	G2566		C	C
		U1589	U1397	C1587	A1761	U1872	U2038	G2171	C2228	U2369	U2458	G2567		C	C
		U1590	U1397	C1588	A1762	U1873	U2039	G2172	C2229	U2370	U2459	G2568		C	C
		U1591	U1397	C1589	A1763	U1874	U2040	G2173	C2230	U2371	U2460	G2569		C	C
		U1592	U1397	C1590	A1764	U1875	U2041	G2174	C2231	U2372	U2461	G2570		C	C
		U1593	U1397	C1591	A1765	U1876	U2042	G2175	C2232	U2373	U2462	G2571		C	C
		U1594	U1397	C1592	A1766	U1877	U2043	G2176	C2233	U2374	U2463	G2572			

A1741	A1579	A1365	U1205	U1097	G1034	G982	A824	G700	G610	A505	C334	G250	U120	G
G1750	A1580	G1368	G1206	A1098	U1035	A941	U827	A706	U614A	C509	C336	A251	G125	U
G1753	C1584	G1492	G1212	U1101	G1036	A945	U828	A707	G615	C509	C336	G252	A126	C
G1756	C1587	G1371	G1212	A1103	G1038	A946	U833	G707	G616	G512	G342	A265	A127	A
U1757	C1588	A1378	A1220	C1104	C1041	A953	U847	U714	A827	A513	U850	A270	G131	G7
G1758	C1592	A1379	G1236	U1105	A1045	G954	G848	G715	A827	A514	G351	U272E	G131	A8
A1759	G1593	G1380	U1236	U1108	A1046	C955	A849	G717	A831	C517	G352	C272F	A141	U9
G1594	G1590	A1384	G1239	C1109	G1047	G956	U855	U714	A831	C523	U362	C272F	G143A	G11
G1595	C1504	A1385	U1240	G1110	A1048	A957	C856	G721	C634	C523	G363A	U272K	C143B	U12
C1607	C1505	U1396	G1250	G1111	A1049	U958	C857	A722	C635	A528	G370	U272L	C144	G15
A1608	C1506	G1251	G1251	U1112	A1050	A959	C857	G723	G636	A529	A371	U272M	C145B	G24
A1609	A1507	U1397	G1252	U1113	G1051	A960	U858	U724	A637	A530	G372	U272N	U157	U25
A1610	A1508	U1397	G1252	U1114	C1052	C961	U859	G725	U639	C531	G372	U272P	U	G26
G1622	A1509A	G1400	A1254	G1117	C1053	U969	U860	C730	C641	A532	C385	U272X	U	G27
A1632	A1509B	G1401	U1255	C1118	A1054	C970	G862	U740	C642	G533	G386	U272X	G171	G30
C1638	A1509C	C1404	G1266	G1119	A1057	C971	A863	G741	G643	C540	A394	U273A	G171	C31
A1639	C1511	U1405	U1267	C1124	G1058	A973	G873	G741	A644	G545	A394	U273B	G180	G36
U1639	U1514	U1406	U1267	G1125	G1059	G974	G874	A746	A645	C	G396	U273C	C184	G36
C1640	G1515	C1407	A1268	A1126	U1060	C975A	C876	U747	A646	A	U405	C273K	U185	C45
A1641	C1408	C1408	A1269	U1130	U	A880	C876	G748	A652C	A	U405	C273K	U185	C45
G1642	C1409	C1410	G1270	U1130	G1062	A880	U877	A752	G652D	G549	G411	A276	A195	G55
C1648	G1410	C1411	G1271	C1135	G1063	A886	A878	C753	C652E	A56	A412	C277	A195	A56
C1657	A1411	A1412	U1272	G1136	A983	C887	G879	C754	G652F	G563	A421	A278	A197	C57
C1658	G1416	G1417	U1273	G1139	U1065	G887	G881	C755	G	U566	U421	C279	C198	G58
A1665	C1417	C1417	A1278	G1140	A1067	C994	G882	G760	C	U566	U427	C286	A199	G61
C1665	C1418	C1418	A1287	C1140	G1068	C995	C886	A761	C	U569	A428	C287	G205	A64
A1668	A1419	A1420	C1291	A1142B	A1069	A996	C887	A764	C	A571	C444	G295	U206	A71
A1669	G1421	G1421	U1292	A1143	A1070	G997	C888	A764	C	A572	C444	G295	C208	A71
G1674	G1422	G1423	C1293	C1153	C1072	C998	C889	A774	C	G573	G450	A299	G212	A74
C1804	U	U	U1300	G1154	G1073	U999	A890	G775	C	A575	G450	A300	G212	A74
U1805	A	A	A1301	G1163	G1074	A1000	C893	G776	C	A576	C455	G301	A213	G75
C1683	C1536	C1428	A1302	G1164	C1075	C994	C896	A782	C	U576	C456	A300	A213	G75
C1684	G1539	G1429	G1303	U1165	A1077	C995	C897	A783	C	A577	C457	G307	G215	A78
U1688	A1542	U1431	G1340	C1166	U1078	C998	C898	A784	C	A578	G458	G308	G217	G79
U1693	C1543	A1445A	G1340	U1167	C1079	U1012	A900	G785	C	G579	G468	A310	A218	G82
C1694	C1547	A1449	C1314	G1171	U1081	C1013	A901	G785	C	C580	G469	A311	G218	G83
G1695	C1557	G1450A	G1315	G	U1082	C1017	C904	A788	C	C581	G469	A311	G218	G83
G1696	A1558	G1455	U1316	U	U1083	G1018	C904	A788	C	C582	G469	A311	G218	G83
A1700	A1559	G1459	A1317	G	A1084	U1019	C907	G792	C	C583	G469	A311	G218	G83
A1701	G1560	G1459	U1341	A	A1085	A1020	A910	G796	C	A586	G469	A311	G218	G83
U1709	A1566	C1467	U1352	C1178	A1086	A1021	A911	C797	C	C587	G469	A311	G218	G83
C1710	A1569	A1471	G1358	C1179	G1087	G1022	C915	G805	C	C588	G469	A311	G218	G83
G1721	A1570	A1472	A1359	C1180	A1088	G1025	C915	G805	C	C589	G469	A311	G218	G83
A1722	A1571	G1473	A1360	C1181	A1089	G1025	C915	G805	C	C590	G469	A311	G218	G83
U1739	U1578	U1479	G1364	G1184	U1090	G1025	C915	G805	C	C591	G469	A311	G218	G83
A1777	U1578	U1479	G1364	G1184	U1090	G1025	C915	G805	C	C592	G469	A311	G218	G83
G1878	U1578	U1479	G1364	G1184	U1090	G1025	C915	G805	C	C593	G469	A311	G218	G83



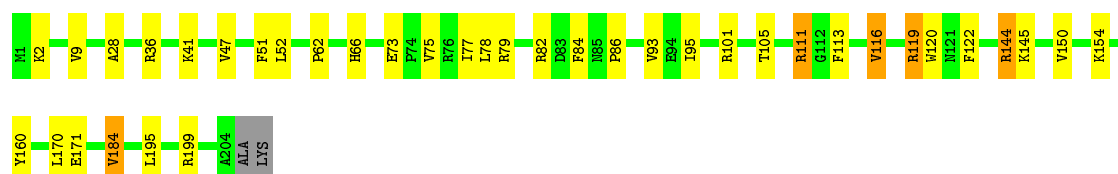
• Molecule 3: 50S ribosomal protein L2

Chain YD: 84% 14% .



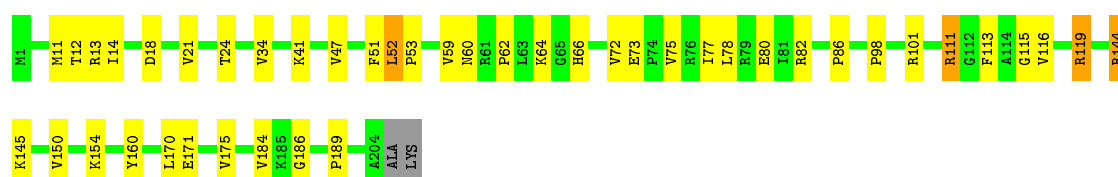
• Molecule 4: 50S ribosomal protein L3

Chain RE: 81% 16% ..



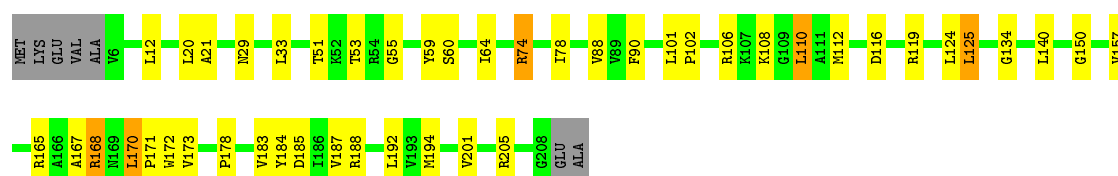
• Molecule 4: 50S ribosomal protein L3

Chain YE: 78% 19% ..



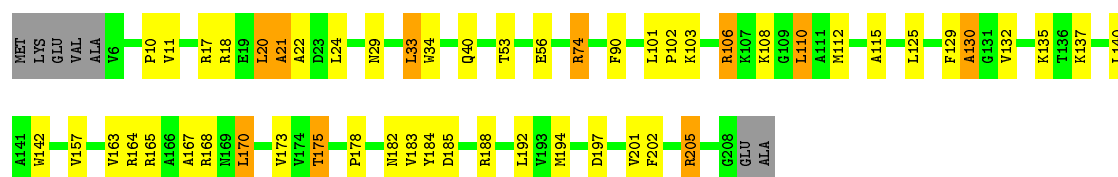
• Molecule 5: 50S ribosomal protein L4

Chain RF: 75% 20% ..



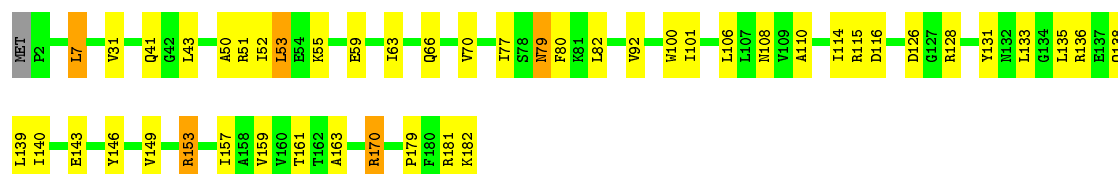
• Molecule 5: 50S ribosomal protein L4

Chain YF: 71% 20% 5% .



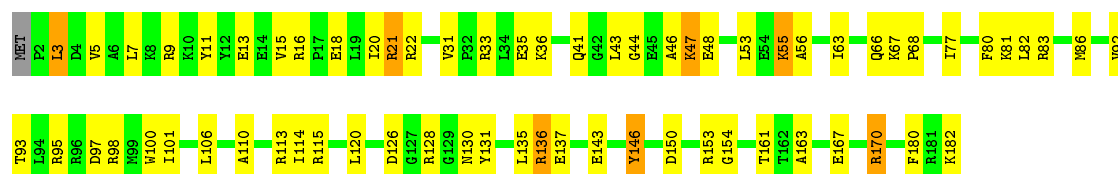
- Molecule 6: 50S ribosomal protein L5

Chain RG: 74% 23% ..



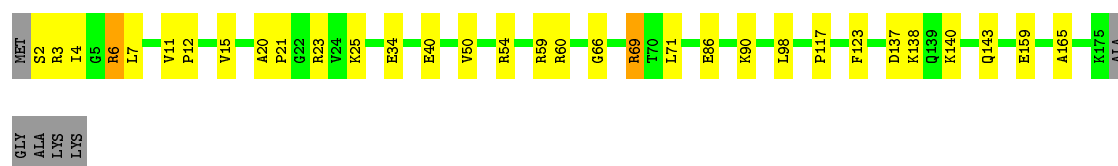
- Molecule 6: 50S ribosomal protein L5

Chain YG: 63% 32% ..



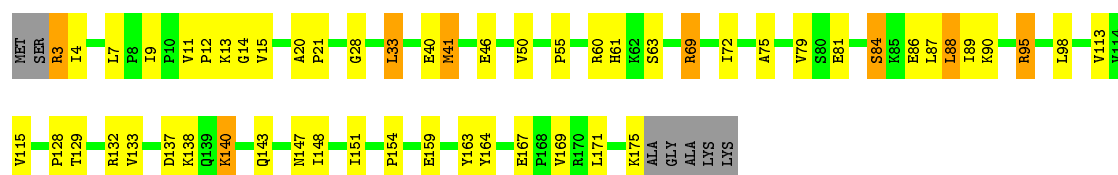
- Molecule 7: 50S ribosomal protein L6

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

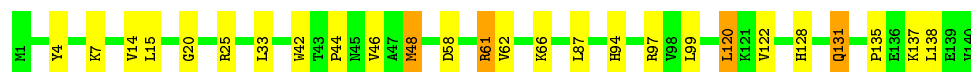
Chain YI: 78% 17%



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%



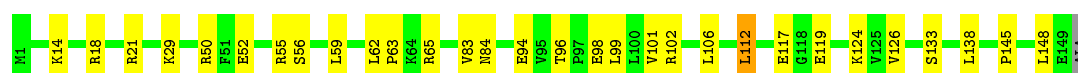
- Molecule 10: 50S ribosomal protein L14

Chain YO: 86% 14%



- Molecule 11: 50S ribosomal protein L15

Chain RP: 79% 19%



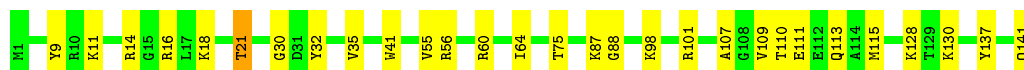
- Molecule 11: 50S ribosomal protein L15

Chain YP: 77% 21%



- Molecule 12: 50S ribosomal protein L16

Chain RQ: 79% 20% .



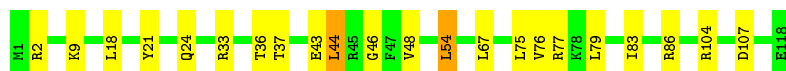
- Molecule 12: 50S ribosomal protein L16

Chain YQ: 79% 18% .



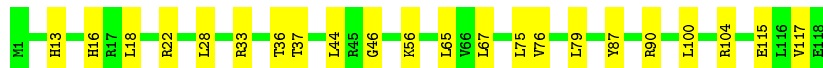
- Molecule 13: 50S ribosomal protein L17

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% .



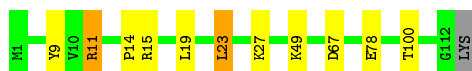
- Molecule 18: 50S ribosomal protein L22

Chain RW:  82% 13% ..




- Molecule 18: 50S ribosomal protein L22

Chain YW:  89% 8% ..




- Molecule 19: 50S ribosomal protein L23

Chain RX:  79% 20%




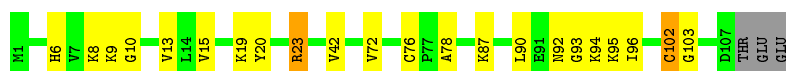
- Molecule 19: 50S ribosomal protein L23

Chain YX:  78% 21%



- Molecule 20: 50S ribosomal protein L24

Chain RY:  77% 18%




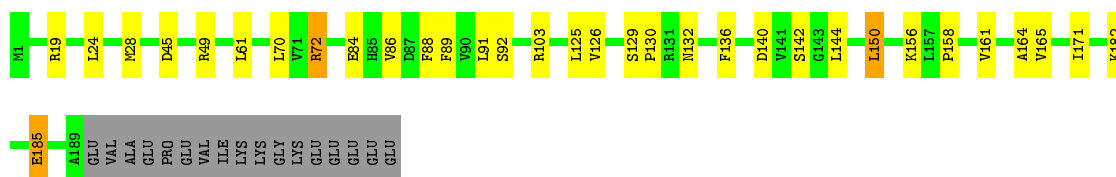
- Molecule 20: 50S ribosomal protein L24

Chain YY:  72% 24%



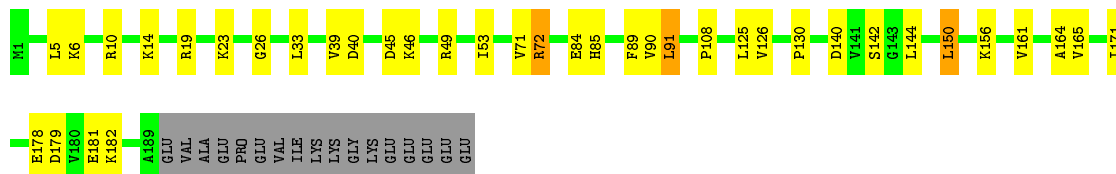
- Molecule 21: 50S ribosomal protein L25

Chain RZ:  76% 15% 8%




- Molecule 21: 50S ribosomal protein L25

Chain YZ:  73% 17% 8%



- Molecule 22: 50S ribosomal protein L27

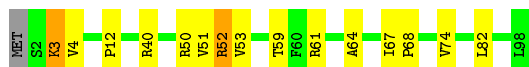
Chain R0:  76% 12% 9%



- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



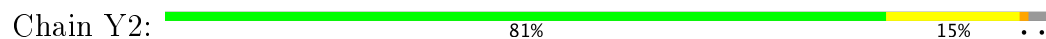
- Molecule 23: 50S ribosomal protein L28



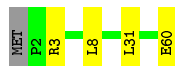
- Molecule 24: 50S ribosomal protein L29



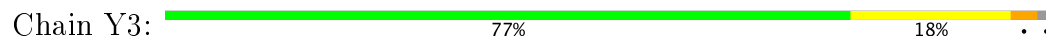
- Molecule 24: 50S ribosomal protein L29



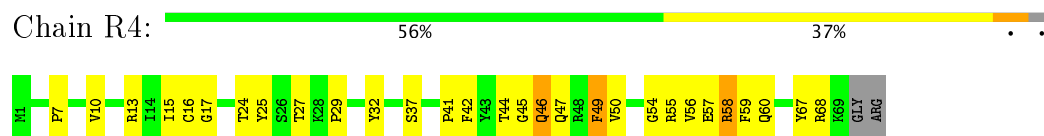
- Molecule 25: 50S ribosomal protein L30



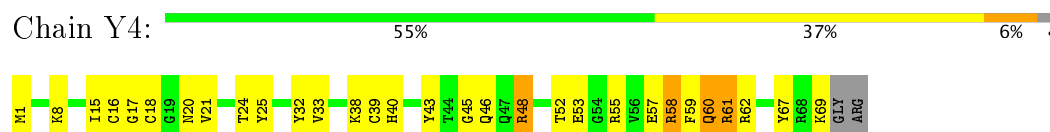
- Molecule 25: 50S ribosomal protein L30



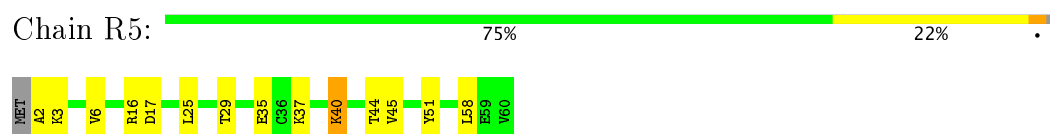
- Molecule 26: 50S ribosomal protein L31



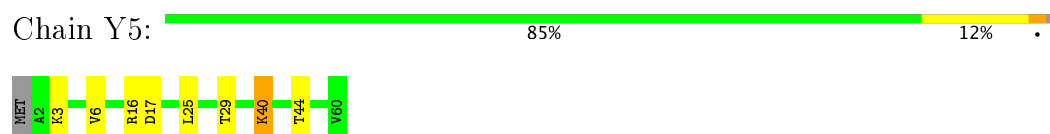
- Molecule 26: 50S ribosomal protein L31



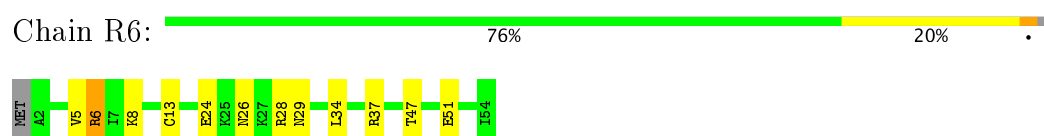
- Molecule 27: 50S ribosomal protein L32



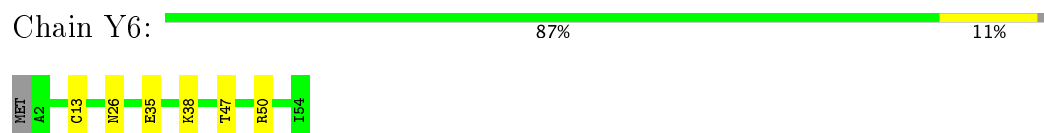
- Molecule 27: 50S ribosomal protein L32



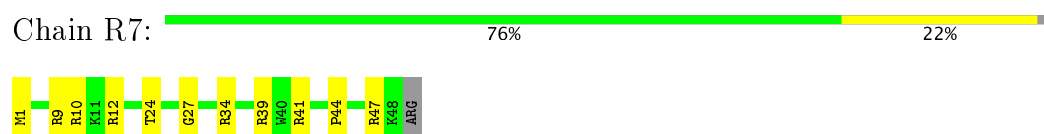
- Molecule 28: 50S ribosomal protein L33



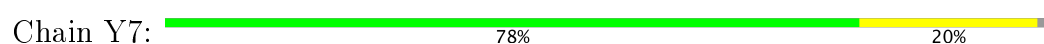
- Molecule 28: 50S ribosomal protein L33



- 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%



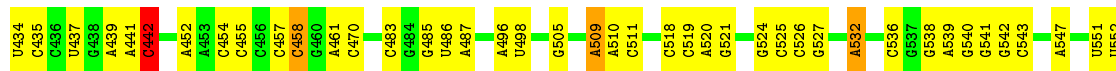
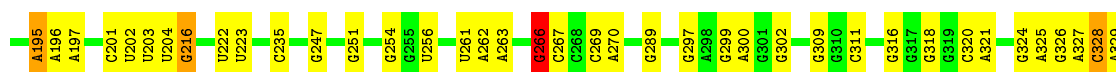
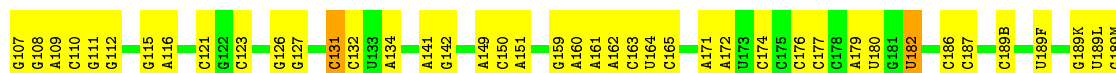
- Molecule 31: 50S ribosomal protein L36

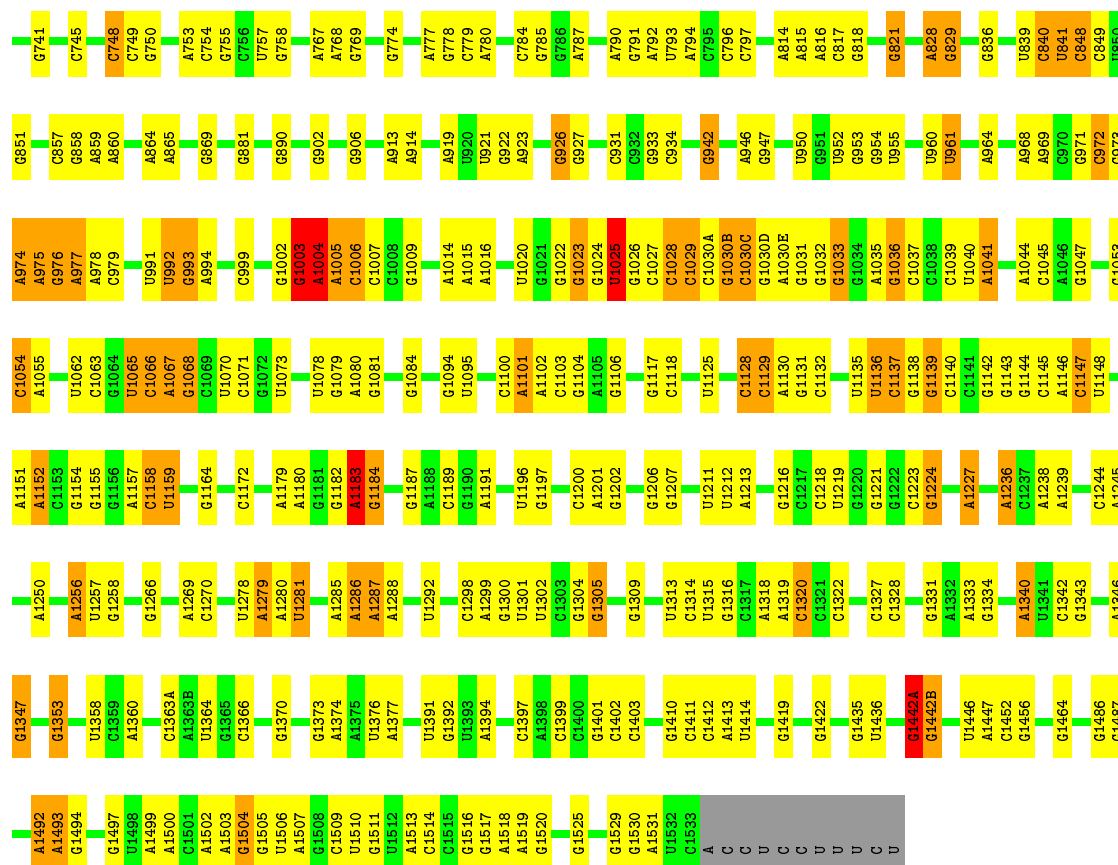
Chain Y9: 70% 30%



- Molecule 32: 16S rRNA

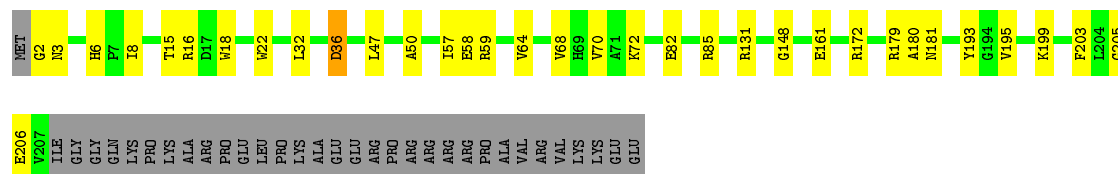
Chain QA: 63% 29% 5% ..





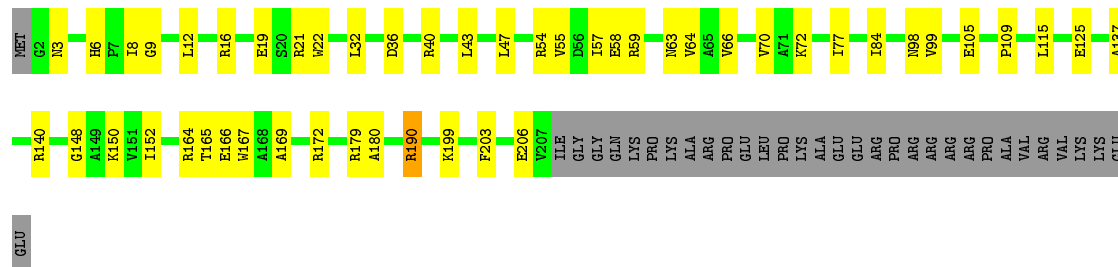
- Molecule 34: 30S ribosomal protein S3

Chain QC:  72% 14% 14%




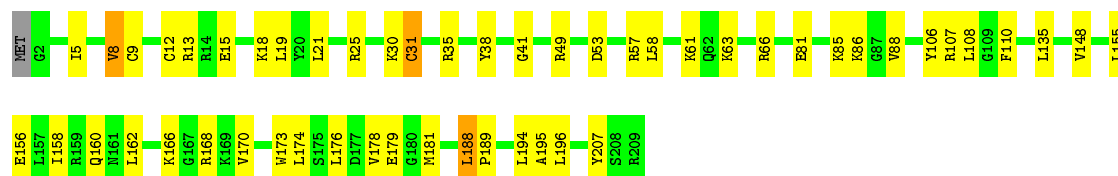
- Molecule 34: 30S ribosomal protein S3

Chain XC:  66% 20% 14%




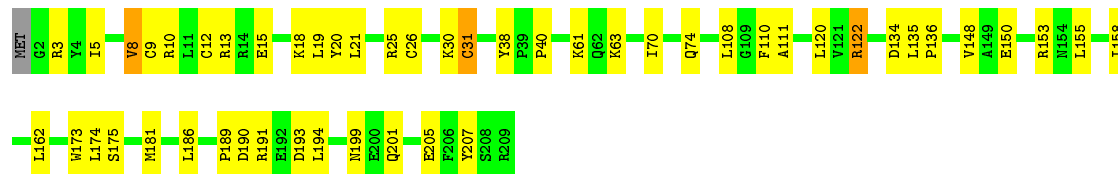
- Molecule 35: 30S ribosomal protein S4

Chain QD:  75% 23% .



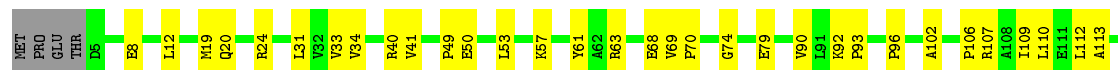
- Molecule 35: 30S ribosomal protein S4

Chain XD:  76% 22% .



- Molecule 36: 30S ribosomal protein S5

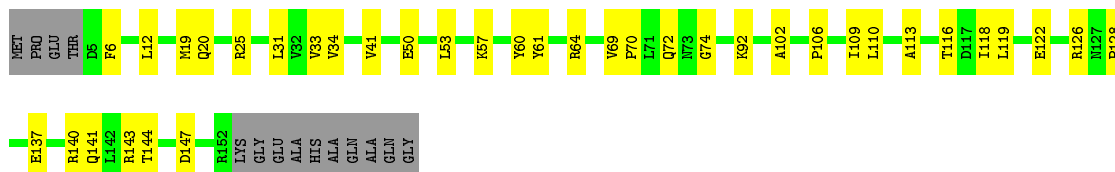
Chain QE:  65% 26% 9%





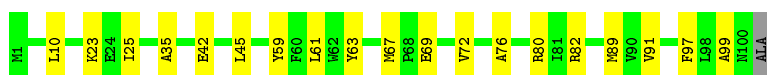
- Molecule 36: 30S ribosomal protein S5

Chain XE:



- Molecule 37: 30S ribosomal protein S6

Chain QF:



- Molecule 37: 30S ribosomal protein S6

Chain XF:



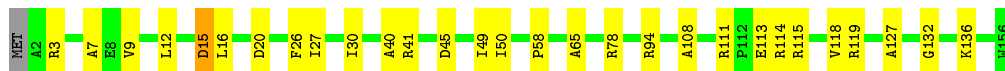
- Molecule 38: 30S ribosomal protein S7

Chain QG:



- Molecule 38: 30S ribosomal protein S7

Chain XG:




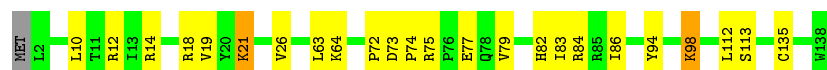
- Molecule 39: 30S ribosomal protein S8

Chain QH:



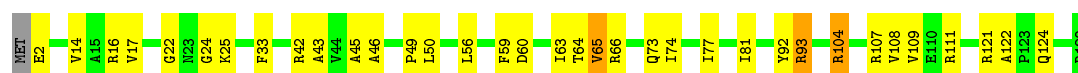
- Molecule 39: 30S ribosomal protein S8

Chain XH:  82% 16% ..



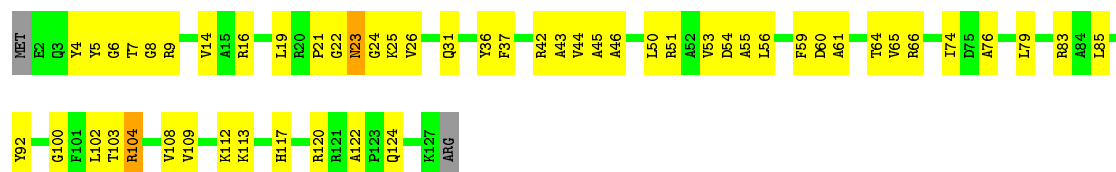
- Molecule 40: 30S ribosomal protein S9

Chain QI:  72% 25% ..



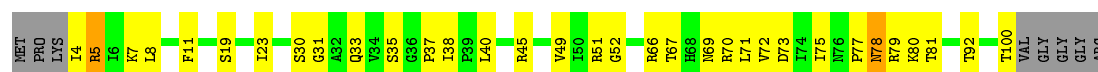
- Molecule 40: 30S ribosomal protein S9

Chain XI:  57% 40% ..



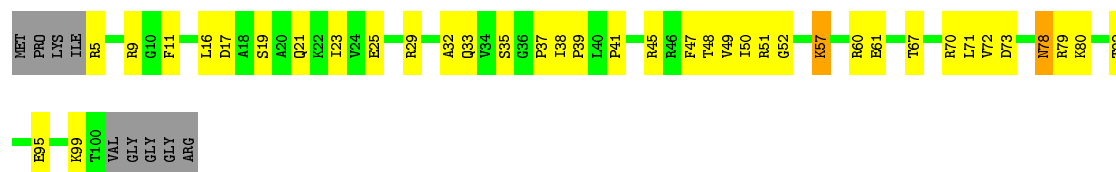
- Molecule 41: 30S ribosomal protein S10

Chain QJ:  61% 30% 8% .



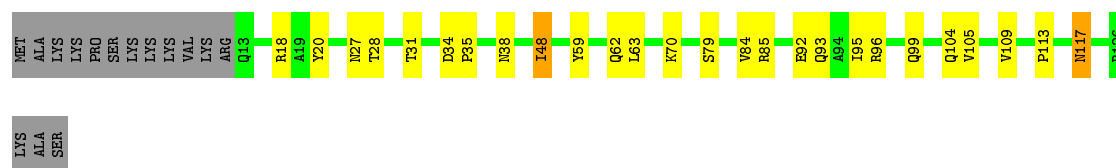
- Molecule 41: 30S ribosomal protein S10

Chain XJ:  55% 34% 9% .




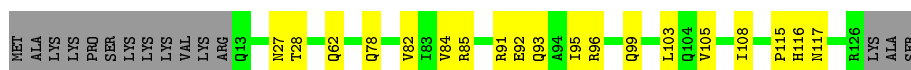
- Molecule 42: 30S ribosomal protein S11

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%



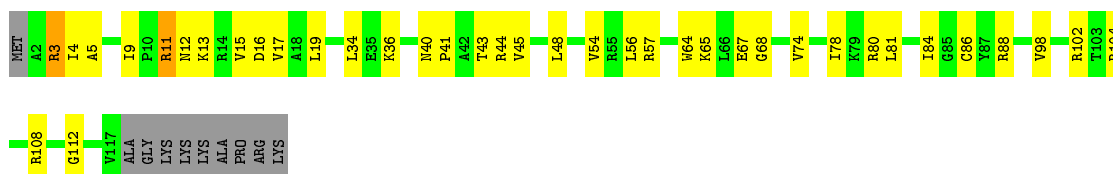
- Molecule 43: 30S ribosomal protein S12

Chain XL:  75% 17% 8%



- Molecule 44: 30S ribosomal protein S13

Chain QM:  62% 29% 8%



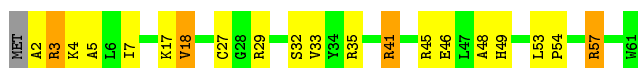
- Molecule 44: 30S ribosomal protein S13

Chain XM:  63% 26% 10%



- Molecule 45: 30S ribosomal protein S14 type Z

Chain QN:  66% 26% 7%

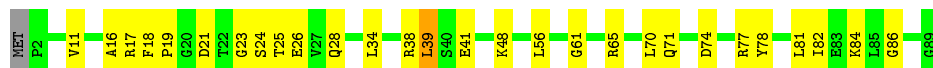


- Molecule 45: 30S ribosomal protein S14 type Z

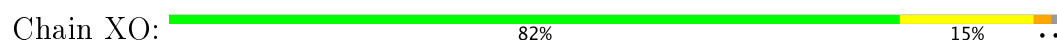
Chain XN:  74% 23% 3%



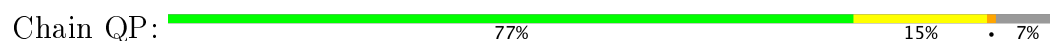
- Molecule 46: 30S ribosomal protein S15



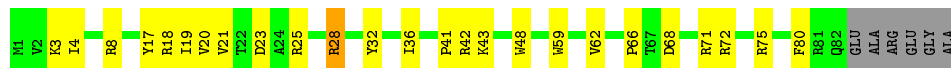
- Molecule 46: 30S ribosomal protein S15



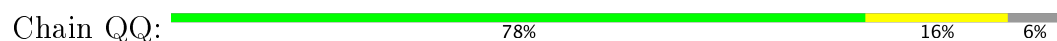
- Molecule 47: 30S ribosomal protein S16



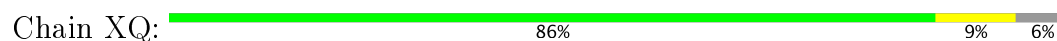
- Molecule 47: 30S ribosomal protein S16



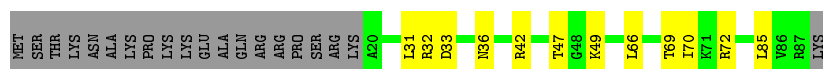
- Molecule 48: 30S ribosomal protein S17



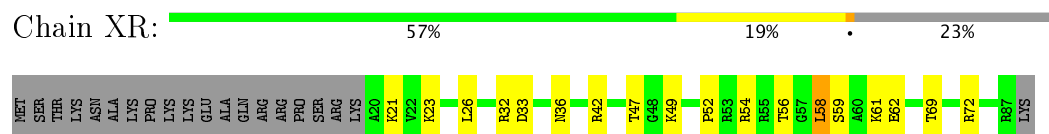
- Molecule 48: 30S ribosomal protein S17



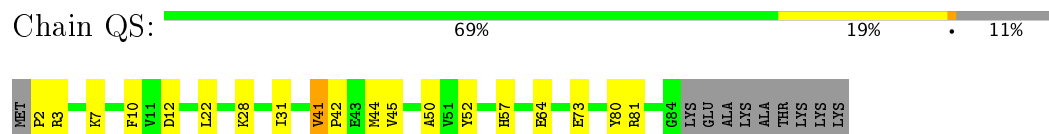
- Molecule 49: 30S ribosomal protein S18



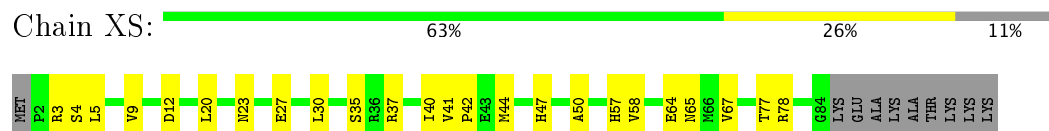
- Molecule 49: 30S ribosomal protein S18



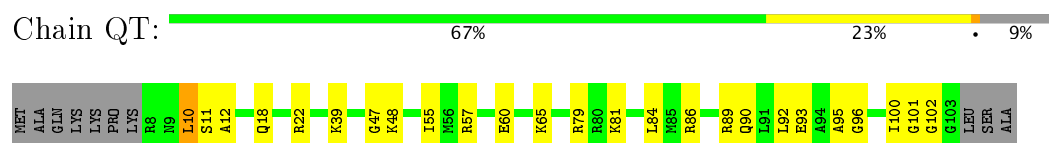
- Molecule 50: 30S ribosomal protein S19



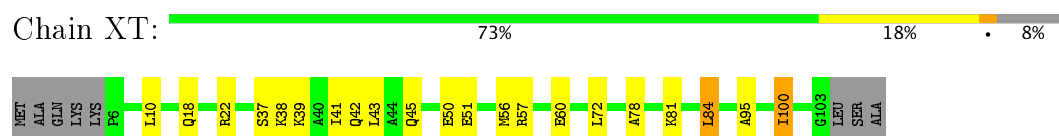
- Molecule 50: 30S ribosomal protein S19



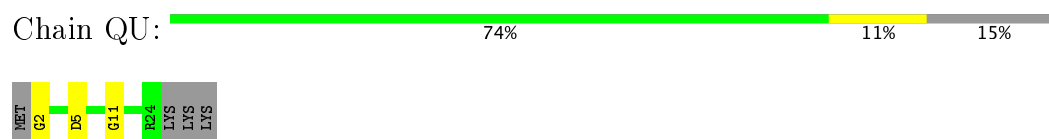
- Molecule 51: 30S ribosomal protein S20



- 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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| G1 | G2 | G3 | G4 | G5 | G9 | G10 | G16 | G17 | G18 | G19 | G20 | A21 | U24 | G25 | G26 | G31 | G32 | A43 | A44 | G45 | G46 | U47 | G48 | G49 | U50 | G51 | G52 | G53 | U54 | G61 | G64 | G75 | A76 | A77 |
|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- G G C A A G G A G G U A A A14 A20 A21 C22 A23 G A

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| G | G | C | A | A | G | G | A | G | G | G | U | A | A | A14 | A15 | A16 | U17 | G18 | U19 | A20 | A21 | C22 | A | G | A |
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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 | LEU | GLY | ASP | GLN | THR | ILE | ALA | ASP | GLN | GLU | ARG | PHE | ARG | ALA | LEU | SER | SER | CYS | PHE | THR | ASP | TRP | GLN | VAL | GLN |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

ASP	IIE	GIU	THR	ALA	GLN	MET	MET	LEU	ASP	ASP	PRO	GLU	MET	MET	ARG	GLU	MET	MET	ALA	GLN	ASP	ASP	GLU	LEU	ARG	GLU	ALA	LYS	GLU	LVS	SER	GLU	GLN	LEU	GLU	G94	Q95	L101	P102	P105	D106	R109	M110	A111	E114	T119	G120	D122	E123	R133	R137	Y138	P142
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I162	I163	Y172	F177		H182	R183	V184	G185	R186	V187	P188		Q193	G194	R195		T198		A204		I209		L214	P215	D216	I217	J218	P219	A220	A221	D221	L222		G233	G234	Q235	H236	V237	I238	J239	T240	D241	S242		R245	L246	T247	H248		L249	P250		V254	V255	E256	C257		S262
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Q263	H264	K265	N266	K267	L274	R294	L298	G299	R303	R306	T309	Y310	N311	F312	P313	Q314	G315	R316	V317	T318	R321	I322	N323	T325	T326	Y327	R328	L329	V332	R333	G334	G335	R336	L337	D338	M339	L340	I341	T345	G351	L351	A352	A353	A354	A355	A356	A357	A358	A359	A360	A361	A362	A363	A364	A365	A366	A367	A368	A369	A370	A371	A372	A373	A374	A375	A376	A377	A378	A379	A380	A381	A382	A383	A384	A385	A386	A387	A388	A389	A390	A391	A392	A393	A394	A395	A396	A397	A398	A399	A400	A401	A402	A403	A404	A405	A406	A407	A408	A409	A410	A411	A412	A413	A414	A415	A416	A417	A418	A419	A420	A421	A422	A423	A424	A425	A426	A427	A428	A429	A430	A431	A432	A433	A434	A435	A436	A437	A438	A439	A440	A441	A442	A443	A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750	A751	A752	A753	A754	A755	A756	A757	A758	A759	A760	A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A8
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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
ASP	ASP	A164	H264	GLU
PRO	PRO	K165	K265	GLU
GLU	GLU	I166	N266	
MET	MET	S167	K267	
ARG	ARG		L274	
GLU	GLU	G170		
MET	MET		R286	
ALA	ALA	R174		
GLN	GLN		R294	
ASP	ASP	F177		
LEU	LEU		D302	
ARG	ARG	R183	R303	
GLU	GLU	V184	S304	
ALA	ALA	Q185	D305	
LYS	LYS	R186	R306	
GLU	GLU	V187	N307	
LYS	LYS	P188	R308	
SER	SER		T309	
GLU	GLU	Q193	V310	
GLN	GLN	G194	R311	
LEU	LEU	R195	F312	
LEU	LEU	I196	P313	
GLU	GLU	H197		
		T198	R316	
Q94	Q94	S199	V317	
		A200	T318	
L101	L101		D319	
P102	P102		R320	
K103	K103		R321	
D104	D104	E208	I322	
P105	P105	L209	N323	
D106	D106	P210	L324	
D107	D107	D211	T325	
E108	E108	A212	L326	
R109	R109	E213	Y327	
		L214	R328	
E114	E114	P215	L329	
V115	V115	I217	D330	
R116	R116		N333	
			K336	
T119	T119	L222	L337	
G120	G120	R223	D338	
G121	G121	I224	H339	
D122	D122	D225	L340	
E123	E123	T226	I341	
		F227		
G129	G129	R228		
		S229		
R133	R133	G233		
M134	M134			

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%)	32	74
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%)	18	61
6	RG	179/182 (98%)	166 (93%)	12 (7%)	1 (1%)	28	72
6	YG	179/182 (98%)	170 (95%)	8 (4%)	1 (1%)	28	72
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%)	25	68
11	YP	147/150 (98%)	142 (97%)	4 (3%)	1 (1%)	25	68
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%)	20	64
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%)	18	61
17	YV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	18	61
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	58
23	Y1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	17	58
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	14
26	Y4	67/71 (94%)	55 (82%)	9 (13%)	3 (4%)	3	21
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	48
33	XB	229/256 (90%)	205 (90%)	19 (8%)	5 (2%)	8	41
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%)	25	68
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%)	11	50
41	QJ	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	3	23
41	XJ	94/105 (90%)	84 (89%)	8 (8%)	2 (2%)	8	42
42	QK	112/129 (87%)	105 (94%)	6 (5%)	1 (1%)	20	64

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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%)	10	47
44	XM	112/126 (89%)	105 (94%)	6 (5%)	1 (1%)	20	64
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%)	18	61
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%)	15	56
50	XS	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
51	QT	94/106 (89%)	88 (94%)	5 (5%)	1 (1%)	17	58
51	XT	96/106 (91%)	89 (93%)	5 (5%)	2 (2%)	8	42
52	QU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	XU	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	20
55	QY	255/360 (71%)	224 (88%)	17 (7%)	14 (6%)	2	16
55	XY	256/360 (71%)	222 (87%)	25 (10%)	9 (4%)	4	28
All	All	11925/12848 (93%)	11396 (96%)	459 (4%)	70 (1%)	28	72

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%)	39	75
3	YD	215/218 (99%)	210 (98%)	5 (2%)	56	84
4	RE	164/166 (99%)	157 (96%)	7 (4%)	33	71
4	YE	164/166 (99%)	156 (95%)	8 (5%)	29	68
5	RF	160/166 (96%)	151 (94%)	9 (6%)	25	64
5	YF	159/166 (96%)	149 (94%)	10 (6%)	21	59
6	RG	144/156 (92%)	136 (94%)	8 (6%)	25	64
6	YG	142/156 (91%)	131 (92%)	11 (8%)	15	50
7	RH	144/148 (97%)	141 (98%)	3 (2%)	59	85
7	YH	143/148 (97%)	133 (93%)	10 (7%)	18	54
8	RI	111/124 (90%)	102 (92%)	9 (8%)	14	48
8	YI	108/124 (87%)	101 (94%)	7 (6%)	20	58
9	RN	119/119 (100%)	111 (93%)	8 (7%)	19	56
9	YN	118/119 (99%)	114 (97%)	4 (3%)	42	77
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%)	66	88
11	YP	115/116 (99%)	113 (98%)	2 (2%)	66	88
12	RQ	111/111 (100%)	108 (97%)	3 (3%)	50	82
12	YQ	111/111 (100%)	105 (95%)	6 (5%)	26	65
13	RR	101/101 (100%)	95 (94%)	6 (6%)	23	62
13	YR	101/101 (100%)	95 (94%)	6 (6%)	23	62
14	RS	87/88 (99%)	85 (98%)	2 (2%)	56	84
14	YS	85/88 (97%)	83 (98%)	2 (2%)	54	84
15	RT	115/127 (91%)	111 (96%)	4 (4%)	41	76
15	YT	113/127 (89%)	110 (97%)	3 (3%)	50	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	RU	93/94 (99%)	89 (96%)	4 (4%)	33	71
16	YU	93/94 (99%)	90 (97%)	3 (3%)	44	78
17	RV	81/82 (99%)	77 (95%)	4 (5%)	29	68
17	YV	80/82 (98%)	76 (95%)	4 (5%)	28	67
18	RW	90/92 (98%)	84 (93%)	6 (7%)	19	56
18	YW	90/92 (98%)	87 (97%)	3 (3%)	43	78
19	RX	77/78 (99%)	76 (99%)	1 (1%)	73	91
19	YX	77/78 (99%)	77 (100%)	0	100	100
20	RY	86/91 (94%)	84 (98%)	2 (2%)	56	84
20	YY	86/91 (94%)	83 (96%)	3 (4%)	41	76
21	RZ	159/179 (89%)	153 (96%)	6 (4%)	38	74
21	YZ	156/179 (87%)	150 (96%)	6 (4%)	38	74
22	R0	61/67 (91%)	59 (97%)	2 (3%)	43	78
22	Y0	61/67 (91%)	60 (98%)	1 (2%)	68	89
23	R1	79/83 (95%)	77 (98%)	2 (2%)	53	83
23	Y1	81/83 (98%)	77 (95%)	4 (5%)	29	68
24	R2	65/67 (97%)	63 (97%)	2 (3%)	45	79
24	Y2	66/67 (98%)	64 (97%)	2 (3%)	46	79
25	R3	51/52 (98%)	51 (100%)	0	100	100
25	Y3	50/52 (96%)	44 (88%)	6 (12%)	6	26
26	R4	58/63 (92%)	56 (97%)	2 (3%)	42	77
26	Y4	54/63 (86%)	46 (85%)	8 (15%)	3	16
27	R5	51/52 (98%)	49 (96%)	2 (4%)	37	74
27	Y5	50/52 (96%)	48 (96%)	2 (4%)	36	73
28	R6	51/52 (98%)	49 (96%)	2 (4%)	37	74
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%)	25	64
30	Y8	54/55 (98%)	52 (96%)	2 (4%)	39	75
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%)	23	62
33	XB	187/220 (85%)	173 (92%)	14 (8%)	16	52
34	QC	144/188 (77%)	142 (99%)	2 (1%)	71	90
34	XC	140/188 (74%)	137 (98%)	3 (2%)	59	85
35	QD	171/181 (94%)	166 (97%)	5 (3%)	48	80
35	XD	172/181 (95%)	169 (98%)	3 (2%)	66	88
36	QE	114/123 (93%)	113 (99%)	1 (1%)	82	94
36	XE	114/123 (93%)	113 (99%)	1 (1%)	82	94
37	QF	85/90 (94%)	85 (100%)	0	100	100
37	XF	85/90 (94%)	84 (99%)	1 (1%)	75	91
38	QG	120/127 (94%)	114 (95%)	6 (5%)	28	67
38	XG	119/127 (94%)	115 (97%)	4 (3%)	42	77
39	QH	116/119 (98%)	113 (97%)	3 (3%)	51	83
39	XH	114/119 (96%)	110 (96%)	4 (4%)	41	76
40	QI	91/99 (92%)	83 (91%)	8 (9%)	12	42
40	XI	88/99 (89%)	83 (94%)	5 (6%)	24	63
41	QJ	68/92 (74%)	66 (97%)	2 (3%)	48	80
41	XJ	68/92 (74%)	67 (98%)	1 (2%)	70	90
42	QK	83/99 (84%)	81 (98%)	2 (2%)	54	84
42	XK	83/99 (84%)	83 (100%)	0	100	100
43	QL	96/108 (89%)	95 (99%)	1 (1%)	80	93
43	XL	96/108 (89%)	95 (99%)	1 (1%)	80	93
44	QM	90/101 (89%)	87 (97%)	3 (3%)	43	78
44	XM	87/101 (86%)	86 (99%)	1 (1%)	78	92
45	QN	49/50 (98%)	44 (90%)	5 (10%)	8	34
45	XN	49/50 (98%)	48 (98%)	1 (2%)	60	86
46	QO	78/80 (98%)	74 (95%)	4 (5%)	28	66
46	XO	78/80 (98%)	75 (96%)	3 (4%)	38	74
47	QP	69/74 (93%)	68 (99%)	1 (1%)	71	90
47	XP	68/74 (92%)	66 (97%)	2 (3%)	48	80

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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%)	66	88
50	QS	68/80 (85%)	66 (97%)	2 (3%)	48	80
50	XS	67/80 (84%)	67 (100%)	0	100	100
51	QT	71/82 (87%)	68 (96%)	3 (4%)	34	72
51	XT	70/82 (85%)	69 (99%)	1 (1%)	71	90
52	QU	18/22 (82%)	18 (100%)	0	100	100
52	XU	18/22 (82%)	17 (94%)	1 (6%)	25	64
55	QY	210/299 (70%)	200 (95%)	10 (5%)	30	68
55	XY	211/299 (71%)	198 (94%)	13 (6%)	21	60
All	All	9765/10662 (92%)	9411 (96%)	354 (4%)	40	76

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	19,26,27	4.26	6 (31%)	20,38,41	2.76	8 (40%)
32	5MC	QA	1400	32	15,22,23	3.20	5 (33%)	17,32,35	1.12	2 (11%)
32	4OC	QA	1402	32	16,23,24	3.52	6 (37%)	19,32,35	1.64	1 (5%)
32	5MC	QA	1404	32	15,22,23	3.21	5 (33%)	17,32,35	1.17	3 (17%)
32	5MC	QA	1407	32	15,22,23	3.20	5 (33%)	17,32,35	1.13	2 (11%)
32	UR3	QA	1498	32	14,22,23	3.34	3 (21%)	16,32,35	0.77	0
32	MA6	QA	1518	32	16,26,27	1.19	2 (12%)	18,38,41	4.33	4 (22%)
32	MA6	QA	1519	32	16,26,27	1.17	2 (12%)	18,38,41	4.29	4 (22%)
32	PSU	QA	516	32,56	16,21,22	3.72	8 (50%)	20,30,33	3.51	6 (30%)
32	7MG	QA	527	32,56	20,26,27	4.88	8 (40%)	22,39,42	1.95	8 (36%)
32	M2G	QA	966	32	20,27,28	4.00	6 (30%)	21,40,43	2.65	8 (38%)
32	5MC	QA	967	32	15,22,23	3.26	5 (33%)	17,32,35	0.92	0
43	0TD	QL	92	43	5,9,10	1.53	1 (20%)	3,11,13	1.92	1 (33%)
55	MEQ	QY	235	55	9,9,10	1.03	0	7,10,12	1.50	2 (28%)
1	PSU	RA	1911	1	16,21,22	3.74	7 (43%)	20,30,33	3.71	5 (25%)
1	5MU	RA	1915	1	14,22,23	1.62	2 (14%)	16,32,35	2.72	3 (18%)
1	PSU	RA	1917	1	16,21,22	3.75	7 (43%)	20,30,33	3.85	6 (30%)
1	4OC	RA	1920	1	15,22,24	3.48	6 (40%)	19,31,35	0.88	1 (5%)
1	5MU	RA	1939	1	14,22,23	1.43	2 (14%)	16,32,35	3.00	3 (18%)
1	5MC	RA	1942	1,56	15,22,23	3.26	5 (33%)	17,32,35	1.00	1 (5%)
1	5MC	RA	1962	1,56	15,22,23	3.21	5 (33%)	17,32,35	1.01	1 (5%)
1	OMG	RA	2251	1,56,53	18,26,27	3.42	7 (38%)	22,38,41	2.39	8 (36%)
1	2MA	RA	2503	1,56	18,25,26	3.93	5 (27%)	17,37,40	2.87	4 (23%)
1	2MU	RA	2552	1,56	14,22,24	8.05	10 (71%)	18,31,36	1.56	2 (11%)
1	PSU	RA	2605	1	16,21,22	3.72	7 (43%)	20,30,33	3.45	6 (30%)
32	2MG	XA	1207	32	19,26,27	4.22	6 (31%)	20,38,41	2.61	7 (35%)
32	5MC	XA	1400	32	15,22,23	3.20	5 (33%)	17,32,35	0.95	1 (5%)
32	4OC	XA	1402	32	16,23,24	3.34	6 (37%)	19,32,35	2.69	1 (5%)
32	5MC	XA	1404	32	15,22,23	3.17	5 (33%)	17,32,35	1.12	2 (11%)
32	5MC	XA	1407	32	15,22,23	3.20	5 (33%)	17,32,35	0.99	1 (5%)
32	UR3	XA	1498	32,56	14,22,23	3.36	3 (21%)	16,32,35	0.78	0
32	MA6	XA	1518	32	16,26,27	1.11	2 (12%)	18,38,41	4.40	4 (22%)
32	MA6	XA	1519	32	16,26,27	1.15	2 (12%)	18,38,41	4.38	4 (22%)
32	PSU	XA	516	32	16,21,22	3.73	7 (43%)	20,30,33	3.61	6 (30%)
32	7MG	XA	527	32,56	20,26,27	4.91	9 (45%)	22,39,42	1.96	9 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	M2G	XA	966	32	20,27,28	3.93	6 (30%)	21,40,43	2.63	7 (33%)
32	5MC	XA	967	32	15,22,23	3.22	5 (33%)	17,32,35	1.06	2 (11%)
43	0TD	XL	92	43	5,9,10	1.62	1 (20%)	3,11,13	2.17	1 (33%)
55	MEQ	XY	235	55	9,9,10	1.11	1 (11%)	7,10,12	1.49	1 (14%)
1	PSU	YA	1911	1	16,21,22	3.73	7 (43%)	20,30,33	3.72	6 (30%)
1	5MU	YA	1915	1,56	14,22,23	1.58	2 (14%)	16,32,35	2.75	3 (18%)
1	PSU	YA	1917	1	16,21,22	3.71	7 (43%)	20,30,33	3.70	6 (30%)
1	4OC	YA	1920	1	15,22,24	3.45	6 (40%)	19,31,35	0.85	1 (5%)
1	5MU	YA	1939	1,56	14,22,23	1.39	2 (14%)	16,32,35	3.03	3 (18%)
1	5MC	YA	1942	1	15,22,23	3.25	5 (33%)	17,32,35	1.07	2 (11%)
1	5MC	YA	1962	1,56	15,22,23	3.22	5 (33%)	17,32,35	0.96	1 (5%)
1	OMG	YA	2251	1,56,53	18,26,27	3.39	6 (33%)	22,38,41	2.34	8 (36%)
1	2MA	YA	2503	1,56	18,25,26	3.97	5 (27%)	17,37,40	2.87	4 (23%)
1	2MU	YA	2552	1,56	14,22,24	8.08	10 (71%)	18,31,36	1.64	2 (11%)
1	PSU	YA	2605	1	16,21,22	3.70	7 (43%)	20,30,33	3.47	6 (30%)

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 250 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	YA	2552	2MU	C6-C5	-9.63	1.17	1.38
1	RA	2552	2MU	C6-C5	-9.61	1.17	1.38
1	YA	2552	2MU	C3'-C2'	-8.59	1.33	1.53
1	RA	2552	2MU	C3'-C2'	-8.33	1.34	1.53
1	RA	2552	2MU	C4-N3	-6.87	1.20	1.33

The worst 5 of 177 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	QA	1519	MA6	N1-C6-N6	-14.02	102.12	117.00
32	XA	1518	MA6	N1-C6-N6	-14.00	102.14	117.00
32	XA	1519	MA6	N1-C6-N6	-13.68	102.48	117.00
32	QA	1518	MA6	N1-C6-N6	-13.63	102.54	117.00
1	RA	1917	PSU	N1-C2-N3	-12.57	119.36	128.40

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.