



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 6, 2020 – 07:20 am BST

PDB ID : 6NDK
Title : Structure of ASLSufA6 A37.5 bound to the 70S A site
Authors : Nguyen, H.T.; Hoffer, E.D.; Dunham, C.M.
Deposited on : 2018-12-13
Resolution : 3.64 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

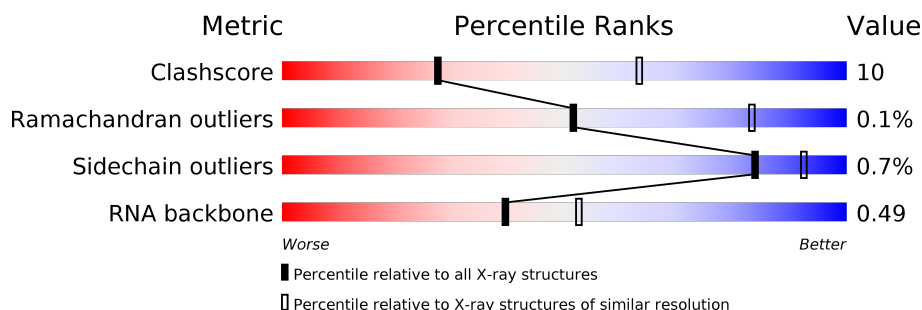
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.64 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1439 (3.78-3.50)
Ramachandran outliers	138981	1391 (3.78-3.50)
Sidechain outliers	138945	1391 (3.78-3.50)
RNA backbone	3102	1019 (4.26-3.00)


























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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	QA	1521	
1	XA	1521	
2	QB	256	
2	XB	256	
3	QC	239	
3	XC	239	
4	QD	209	

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


























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Mol	Chain	Length	Quality of chain
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	26	
23	XX	26	
24	QY	18	
24	XY	18	
25	RA	2915	
25	YA	2915	
26	RB	122	
26	YB	122	
27	RD	276	
27	YD	276	
28	RE	206	
28	YE	206	
29	RF	210	











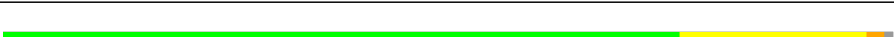


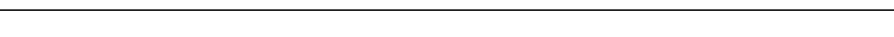











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Mol	Chain	Length	Quality of chain
29	YF	210	
30	RG	182	
30	YG	182	
31	RH	180	
31	YH	180	
32	RI	148	
32	YI	148	
33	RN	140	
33	YN	140	
34	RO	122	
34	YO	122	
35	RP	150	
35	YP	150	
36	RQ	141	
36	YQ	141	
37	RR	118	
37	YR	118	
38	RS	112	
38	YS	112	
39	RT	146	
39	YT	146	
40	RU	118	
40	YU	118	
41	RV	101	
41	YV	101	






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

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Mol	Chain	Length	Quality of chain
54	Y8	65	 72%25% . .
55	R9	37	 59%38% .
55	Y9	37	 73%27%
56	ZA	3	 67%33%
56	ZB	3	 67%33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	QN	101	-	-	X	-
57	MG	RB	203	-	-	X	-
57	MG	RD	303	-	-	X	-
58	SF4	QD	303	-	-	X	-
58	SF4	XD	302	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291822 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	QF	100	Total	C	N	O	S	0	0	0
			837	528	154	152	3			
6	XF	100	Total	C	N	O	S	0	0	0
			837	528	154	152	3			

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	114	Total	C	N	O	S	0	0	0
			844	525	158	158	3			
11	XK	114	Total	C	N	O	S	0	0	0
			844	525	158	158	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	QL	122	Total	C	N	O	S	0	0	0
			958	604	193	159	2			
12	XL	122	Total	C	N	O	S	0	0	0
			958	604	193	159	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
13	XM	114	Total	C	N	O	S	0	0	0
			916	566	189	159	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	QP	82	Total	C	N	O	S	0	0	0
			691	438	138	114	1			
16	XP	82	Total	C	N	O	S	0	0	0
			691	438	138	114	1			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	96	Total	C	N	O	S	0	0	0
			743	458	159	124	2			
20	XT	98	Total	C	N	O	S	0	0	0
			759	469	162	126	2			

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

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

- Molecule 22 is a RNA chain called P-site tRNA^{fMet}.

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

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total	C	N	O	P	0	0	0
			167	75	28	56	8			
23	XX	11	Total	C	N	O	P	0	0	0
			233	105	43	74	11			

- Molecule 24 is a RNA chain called A-site ASLSufA6 A37.5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	14	Total	C	N	O	P	0	0	0
			301	134	55	98	14			
24	XY	16	Total	C	N	O	P	0	0	0
			341	153	63	110	15			

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	RA	2870	Total	C	N	O	P	0	0	0
			61819	27519	11565	19867	2868			
25	YA	2870	Total	C	N	O	P	0	0	0
			61822	27520	11565	19869	2868			

- Molecule 26 is a RNA chain called 5S rRNA.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	RD	275	Total	C	N	O	S	0	0	0
			2144	1353	428	360	3			
27	YD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	RE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
28	YE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RP	149	Total	C	N	O	S	0	0	0
			1139	709	231	196	3			
35	YP	149	Total	C	N	O	S	0	0	0
			1139	709	231	196	3			

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RS	110	Total	C	N	O	S	0	0	0
			877	553	175	149				
38	YS	110	Total	C	N	O	S	0	0	0
			877	553	175	149				

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
39	YT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RW	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	YW	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RZ	196	Total	C	N	O	S	0	0	0
			1552	988	273	288	3			
45	YZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R0	77	Total	C	N	O	S	0	0	0
			611	378	129	103	1			
46	Y0	77	Total	C	N	O	S	0	0	0
			611	378	129	103	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
47	Y1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	R3	59	Total	C	N	O	0	0	0
			469	298	90	81			
49	Y3	59	Total	C	N	O	0	0	0
			468	298	90	80			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
51	Y5	58	Total	C	N	O	S	0	0	0
			451	283	89	74	5			

- Molecule 52 is a protein called 50S ribosomal protein L33.

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

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

- Molecule 55 is a protein called 50S ribosomal protein L36.

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

- Molecule 56 is a RNA chain called tRNA acceptor end mimic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	ZA	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
56	ZB	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	124	Total	Mg	0	0
			124	124		
57	YV	1	Total	Mg	0	0
			1	1		
57	RP	2	Total	Mg	0	0
			2	2		
57	R7	1	Total	Mg	0	0
			1	1		
57	YA	544	Total	Mg	0	0
			544	544		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QM	2	Total 2	Mg 2	0	0
57	YR	1	Total 1	Mg 1	0	0
57	Y9	1	Total 1	Mg 1	0	0
57	QD	2	Total 2	Mg 2	0	0
57	RN	2	Total 2	Mg 2	0	0
57	Y1	3	Total 3	Mg 3	0	0
57	YD	8	Total 8	Mg 8	0	0
57	XX	1	Total 1	Mg 1	0	0
57	QV	3	Total 3	Mg 3	0	0
57	RX	1	Total 1	Mg 1	0	0
57	Y8	1	Total 1	Mg 1	0	0
57	XA	128	Total 128	Mg 128	0	0
57	RQ	1	Total 1	Mg 1	0	0
57	R0	2	Total 2	Mg 2	0	0
57	QL	2	Total 2	Mg 2	0	0
57	YU	1	Total 1	Mg 1	0	0
57	RO	1	Total 1	Mg 1	0	0
57	XJ	1	Total 1	Mg 1	0	0
57	Y7	1	Total 1	Mg 1	0	0
57	Y0	1	Total 1	Mg 1	0	0
57	YG	1	Total 1	Mg 1	0	0

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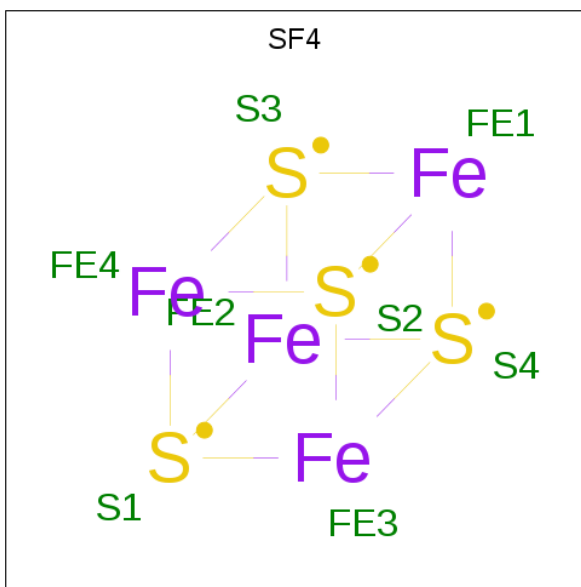
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YQ	2	Total 2	Mg 2	0	0
57	QC	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	YX	1	Total 1	Mg 1	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RD	5	Total 5	Mg 5	0	0
57	R1	1	Total 1	Mg 1	0	0
57	QO	1	Total 1	Mg 1	0	0
57	YT	1	Total 1	Mg 1	0	0
57	RV	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	RA	414	Total 414	Mg 414	0	0
57	Y3	1	Total 1	Mg 1	0	0
57	YF	1	Total 1	Mg 1	0	0
57	YP	3	Total 3	Mg 3	0	0
57	RZ	1	Total 1	Mg 1	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	R9	1	Total 1	Mg 1	0	0
57	RE	5	Total 5	Mg 5	0	0
57	XK	2	Total 2	Mg 2	0	0
57	YB	8	Total 8	Mg 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y6	1	Total 1	Mg 1	0	0
57	QN	2	Total 2	Mg 2	0	0
57	YW	1	Total 1	Mg 1	0	0
57	RW	1	Total 1	Mg 1	0	0
57	XN	1	Total 1	Mg 1	0	0
57	R6	1	Total 1	Mg 1	0	0
57	XV	1	Total 1	Mg 1	0	0
57	RB	8	Total 8	Mg 8	0	0
57	QE	2	Total 2	Mg 2	0	0
57	XD	1	Total 1	Mg 1	0	0
57	RF	5	Total 5	Mg 5	0	0
57	R3	1	Total 1	Mg 1	0	0
57	YE	7	Total 7	Mg 7	0	0

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



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

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

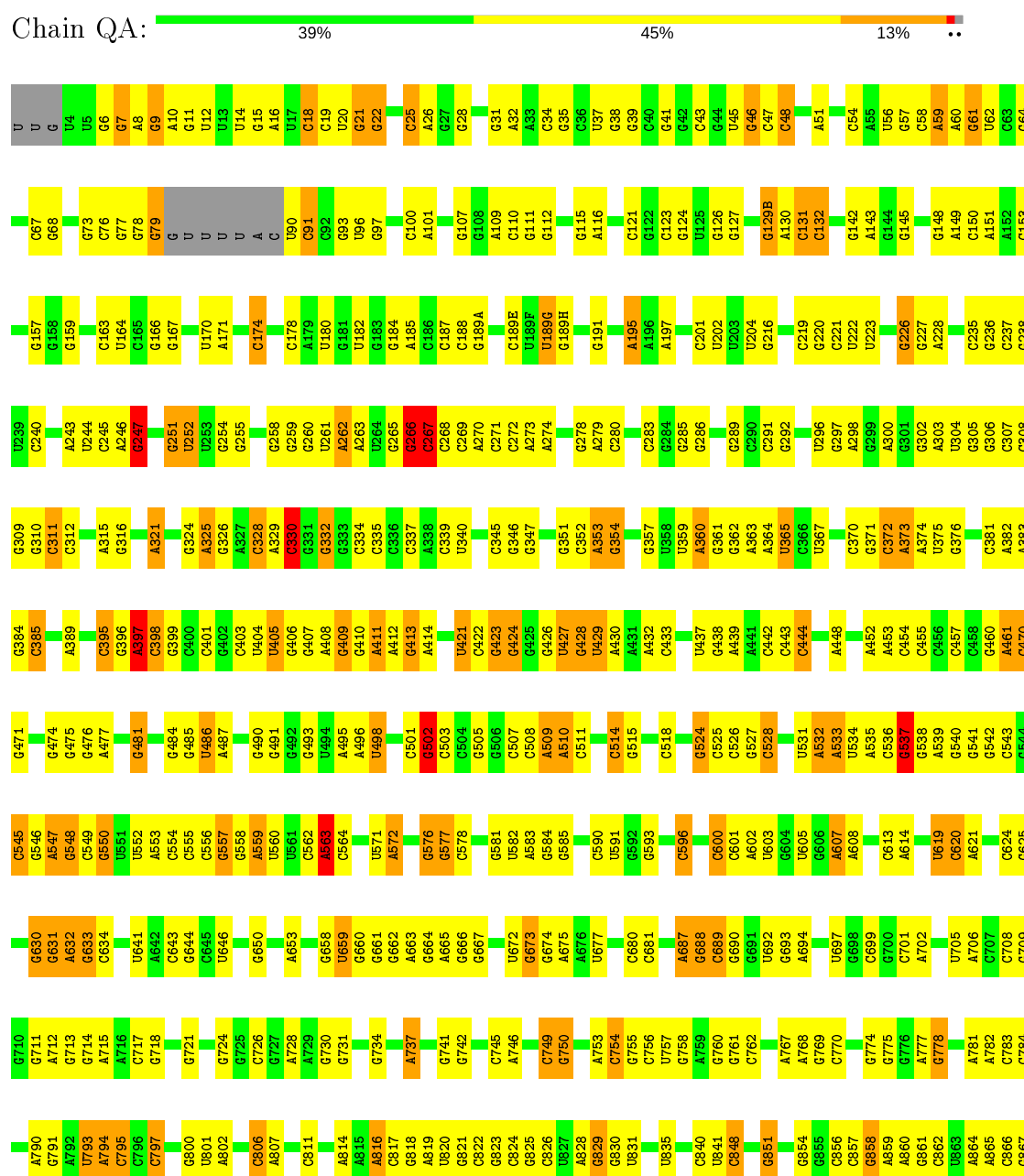
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Y4	1	Total	Zn	0	0
			1	1		
59	R4	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		
59	QN	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		

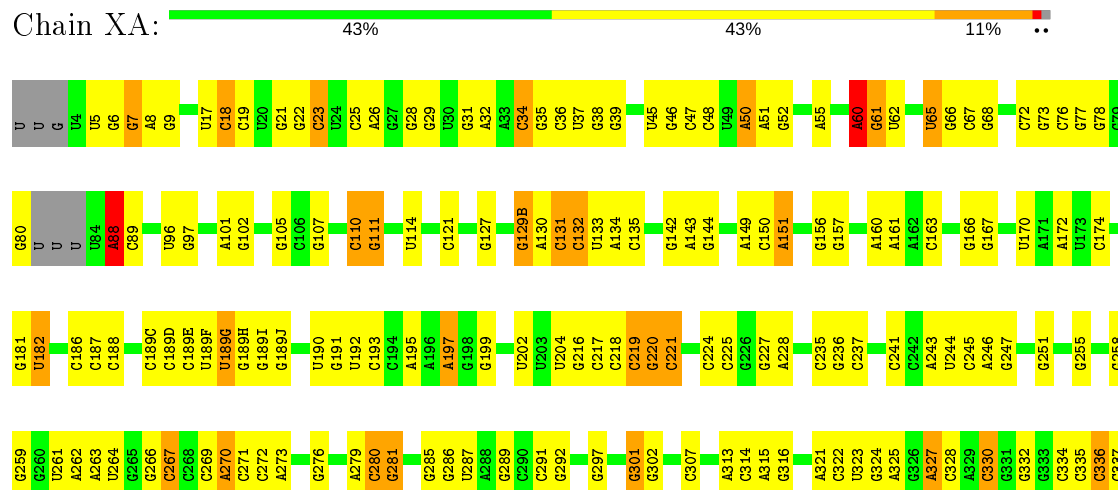
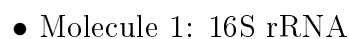
3 Residue-property plots

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

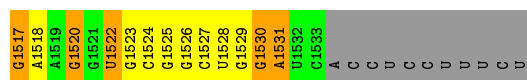
Note EDS failed to run properly.

- Molecule 1: 16S rRNA



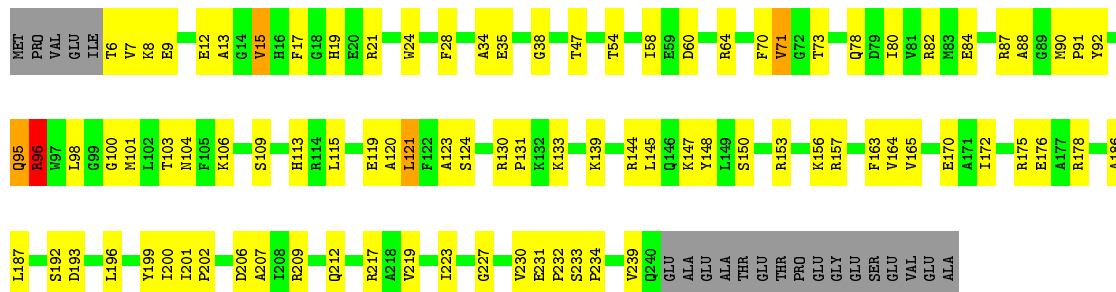


WORLDWIDE
PDB
PROTEIN DATA BANK



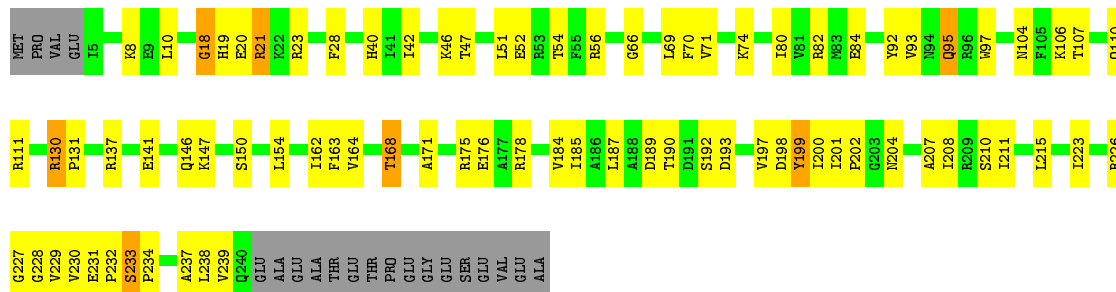
• Molecule 2: 30S ribosomal protein S2

Chain QB: 56% 34% 8%



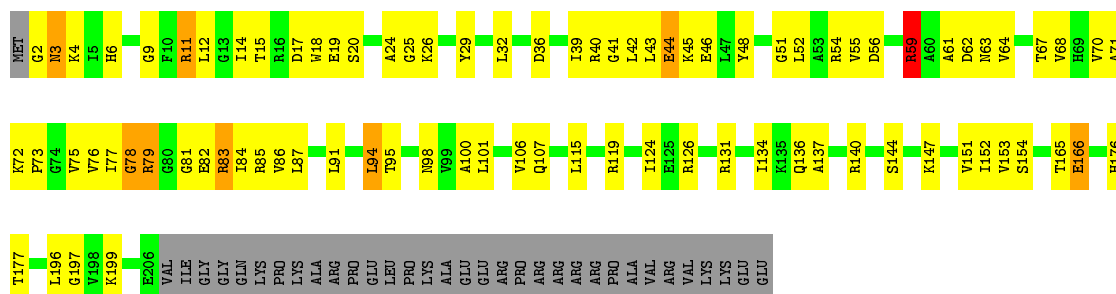
• Molecule 2: 30S ribosomal protein S2

Chain XB: 61% 29% 8%



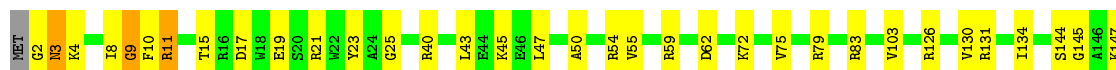
• Molecule 3: 30S ribosomal protein S3

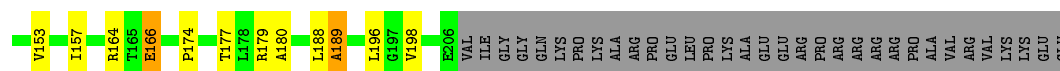
Chain QC: 50% 32% 14%



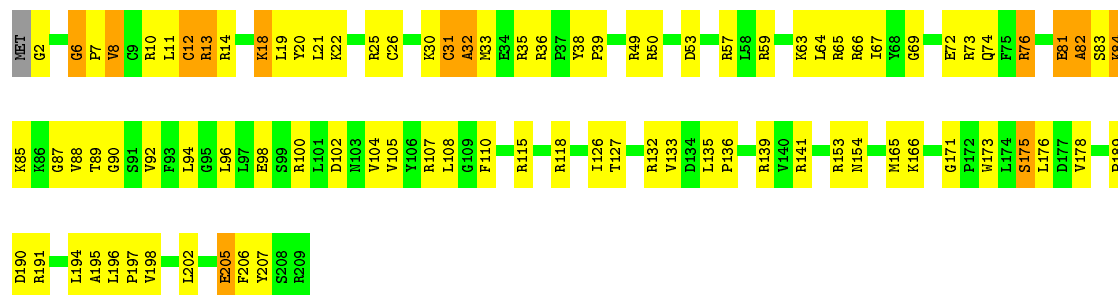
• Molecule 3: 30S ribosomal protein S3

Chain XC: 67% 17% 14%

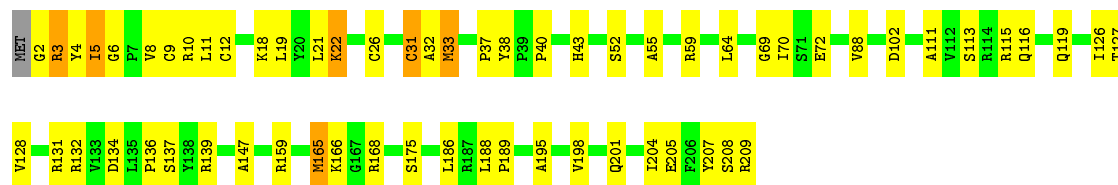




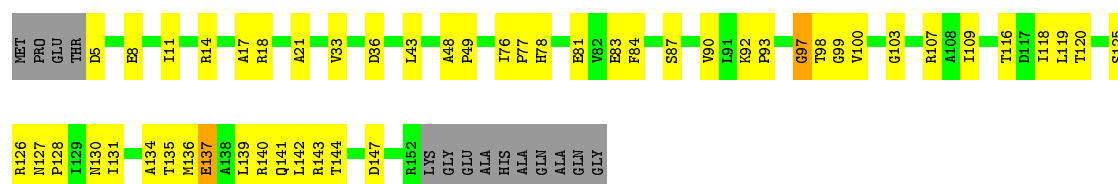
• Molecule 4: 30S ribosomal protein S4



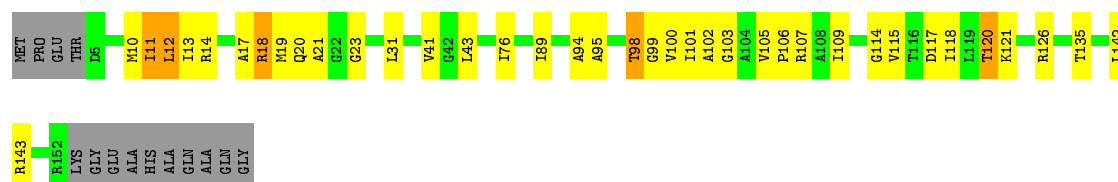
• Molecule 4: 30S ribosomal protein S4




• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5




• Molecule 6: 30S ribosomal protein S6

Chain QF:  73% 25% ..



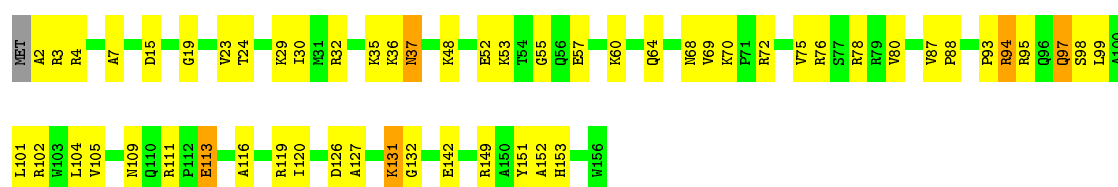
- Molecule 6: 30S ribosomal protein S6

Chain XF:  76% 23% .



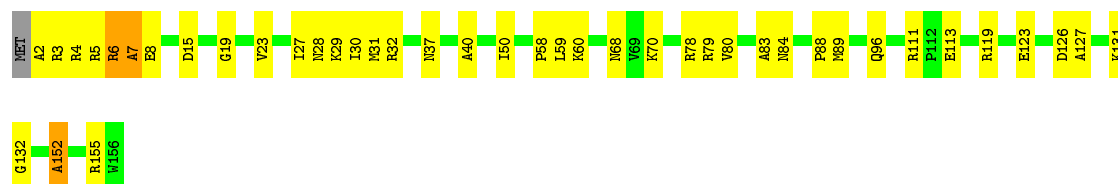
- Molecule 7: 30S ribosomal protein S7

Chain QG:  63% 33% ..



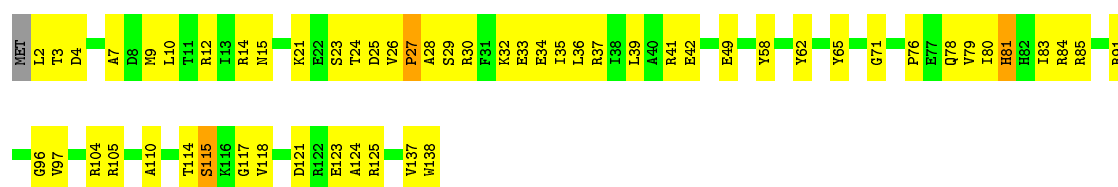
- Molecule 7: 30S ribosomal protein S7

Chain XG:  72% 25% ..



- Molecule 8: 30S ribosomal protein S8

Chain QH:  59% 38% ..



- Molecule 8: 30S ribosomal protein S8

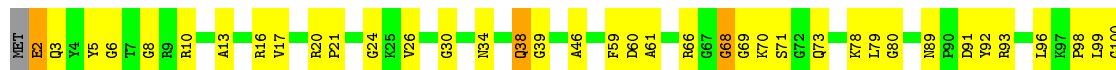
Chain XH:  68% 30% ..





- Molecule 9: 30S ribosomal protein S9

Chain QI: 53% 41% 5%



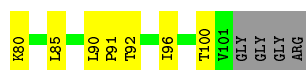
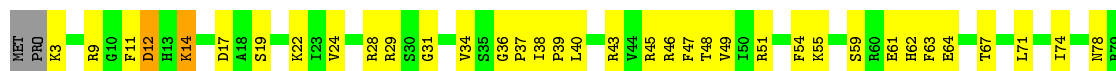
- Molecule 9: 30S ribosomal protein S9

Chain XI: 62% 35% 3%



- Molecule 10: 30S ribosomal protein S10

Chain QJ: 53% 39% 6%



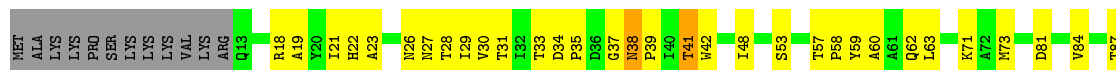
- Molecule 10: 30S ribosomal protein S10

Chain XJ: 64% 28% 9%



- Molecule 11: 30S ribosomal protein S11

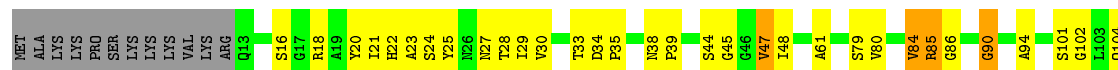
Chain QK: 57% 28% 12%





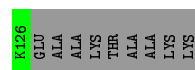
- Molecule 11: 30S ribosomal protein S11

Chain XK: 59% 26% 12%



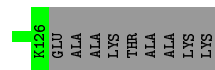
- Molecule 12: 30S ribosomal protein S12

Chain QL: 65% 23% 5% 8%



- Molecule 12: 30S ribosomal protein S12

Chain XL: 65% 26% 8%



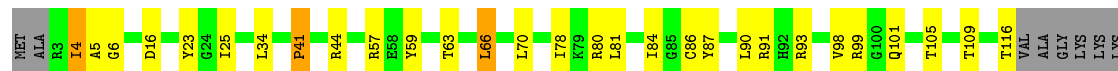
- Molecule 13: 30S ribosomal protein S13

Chain QM: 52% 36% 8%



- Molecule 13: 30S ribosomal protein S13

Chain XM: 67% 21% 10%



ALA
PRO
ARG
LYS

- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:  49% 46% ..


MET A2 R3 R4 A5 L6 L7 E8 E9 A10 A11 K11 R12 R17 V18 R19 T22 R23 G28 R29 S32 V33 V34 L39 C40 R41 T42 C43 L44 R45 E46 L47 Q52 L53 P54 G55 K58 A59 S60 M61

- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:  67% 30% ..


MET A2 R3 R4 L6 K9 A10 K11 R12 T13 A20 Y21 T22 R23 C24 C27 G28 R29 R35 C40 C43 H49 K58 M61

- Molecule 15: 30S ribosomal protein S15

Chain QO:  83% 12% ..

MET P2 Q9 K10 V11 I12 R17 F18 D21 E26 L31 D49 H50 H51 L67 R77 Y78 G86 G89

- Molecule 15: 30S ribosomal protein S15

Chain XO:  83% 15% ..

MET P2 I3 T4 K5 E6 E7 G20 D21 T22 G23 S24 T25 L34 L39 K47 R54 R88 G89

- Molecule 16: 30S ribosomal protein S16

Chain QP:  58% 34% 7%

M1 V2 K3 I4 R5 L6 M14 P15 H16 I19 V20 V21 R25 G30 I33 E34 K35 I36 G37 Y38 T45 P46 D47 K50 V51 R55 A56 S57 V62 T69 R72 L73 L74 R75 Q76 A77 G78 V79 F80 R81 Q82 GLU ALA ARG GLY GLY ALA

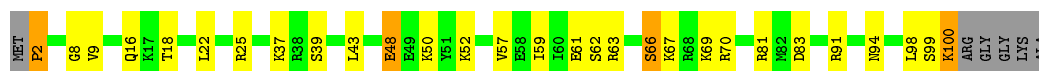
- Molecule 16: 30S ribosomal protein S16

Chain XP:  60% 32% 7%

M1 V2 K3 R5 H8 K12 P15 R18 I19 V20 R25 R28 D29 Y32 I33 E34 K35 I36 G37 D52 R57 V58 H59 L60 S61 V62 T67 A70 R71 R72 L73 L74 V79 F80 R81 Q82 GLU ALA ARG GLY GLY ALA

- Molecule 17: 30S ribosomal protein S17

Chain QQ:  67% 24% 6%



- Molecule 17: 30S ribosomal protein S17



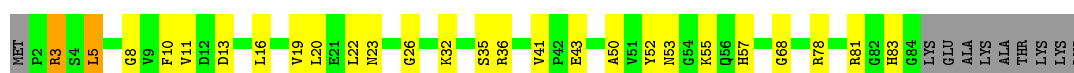
- Molecule 18: 30S ribosomal protein S18



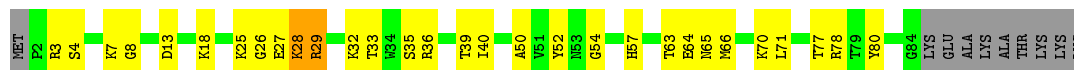
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S19

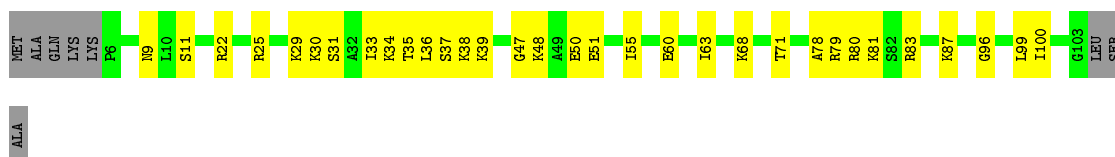


- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20





- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: P-site tRNAfMet



- Molecule 22: P-site tRNAfMet




- Molecule 23: mRNA



- Molecule 23: mRNA

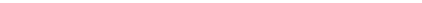


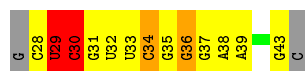
- Molecule 24: A-site ASLSufA6 A37.5

Chain QY: 



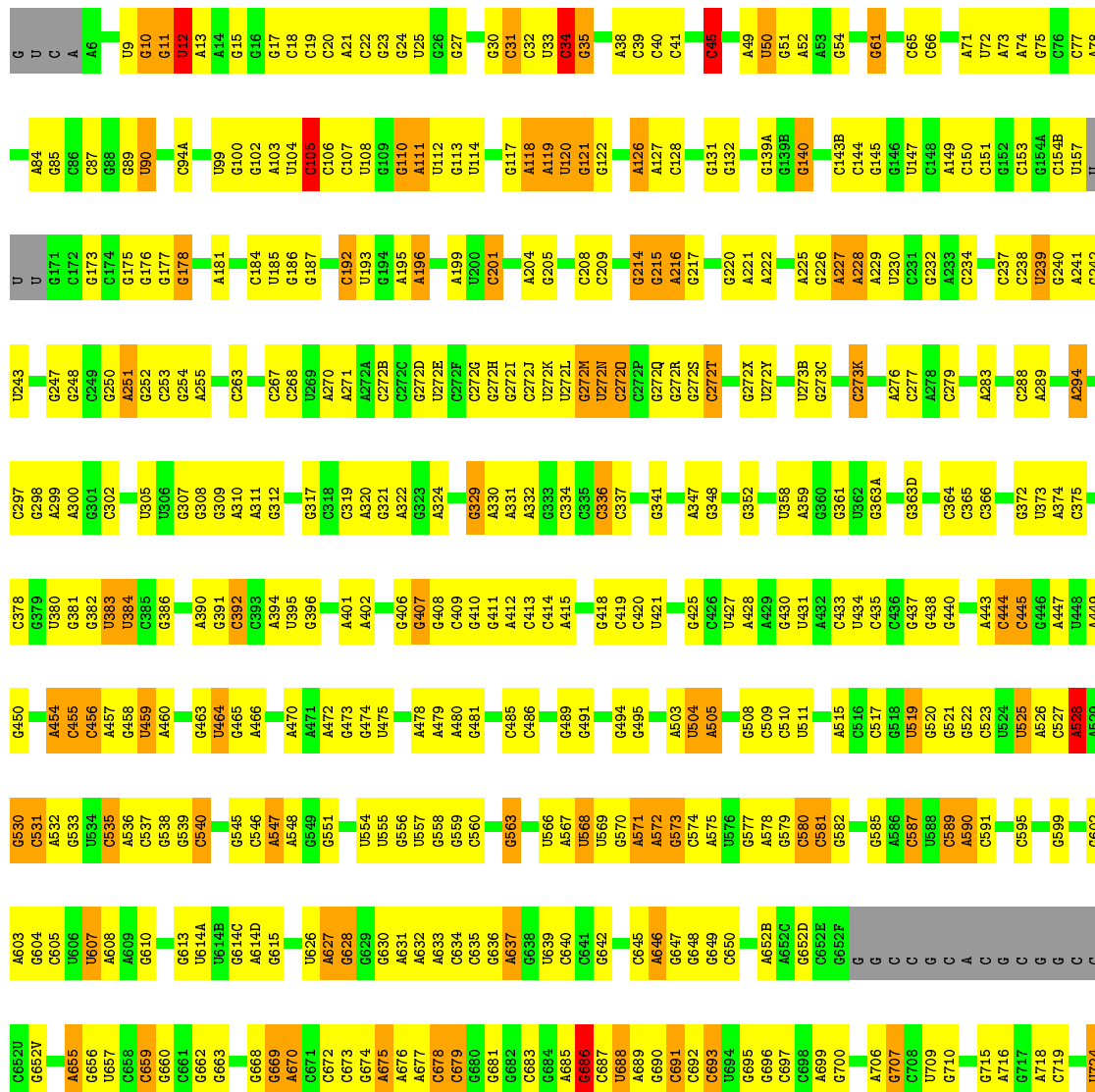
- Molecule 24: A-site ASLSufA6 A37.5

Chain XY:  17% 50% 11% 11% 11%



- Molecule 25: 23S rRNA

Chain RA: 





C	A2823	C2742	G2663	G2581	A2503	A2426	U2344	C2275	C2195	G2127	G2056	A1981	G1899
U	C2824	C2743	C2666	G2582	U2504	C2427	G2345	A2278	C2196	C2128	A2057	C1982	A1900
C	C2825	C2744	C2667	G2583	G2505	G2428	C2346	G2279	U2197	U2130	A2060	C1983	A1901
		C2745		U2584	U2506	G2429	C2347	G2280	A2198	U2131	A2061	C1984	C1902
	C2828	U2746	A2675	U2585	U2511	A2430	C2350	G2281	C2200	U2132	A2062	G1988	G1903
	C2829	C2747	C2676	C2586	C2512	A2431	G2351	G2282	C2201	G2133	C2063	G1989	C1905
		A2748	C2676	A2587	G2513	A2432	G2352	C2283	C2205	A2134	C2064	C1990	G1906
	A2835	A2749		G2588	U2514	A2434	G2353		G2206	C2136	C2065	U1991	
	U2836	A2750	A2679	A2589	U2515	A2439	G2354	A2286	G2207	G2137	C2066	G1992	A1913
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	G2838	C2752	C2681	C2591	A2519	C2441	C2356	A2288	A2208	C2139	U2068	C1994	C1919
	G2839	U2682	U2683	U2592	U2519	C2442	A2361	A2289	A2218	C2140	U2069	U1995	C1920
	C2840	C2683	C2684	U2593	G2526	C2443	G2362	G2290	G2219	G2141		C1996	
		U2756	G2685	G2595	C2527		G2363	U2291	G2220	C2142	G2072	G1997	
	G2846	A2757	G2685	U2596	U2528	G2447	C2364	C2292	G2221	C2143		G1998	A1921
	U2847	A2758		G2597	U2529	G2448	C2365	C2293	G2222	C2144	U2075	C1999	G1922
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	U2849	A2765	C2691	G2599	U2537	A2450	G2371	C2295	G2224	C2146	U2079	A2001	U1926
	A2850	C2766	C2692	G2600	C2538	A2452	C2374	U2296	G2225	G2147	G2080	G2003	A1927
	A2851			G2601	C2539			A2298	C2226	G2148	A2082	G2004	U1928
	C2852		U2696	U2611	A2542	G2455	A2377	C2299	C2231		C2084	A2005	G1930
	C2853	C2773	U2697	U2612	G2543	U2456	A2378	G2300	U2232	G2152	C2085	C2006	C1934
	C2854	C2774	U2698	U2613	G2544	U2457	G2379	G2303	U2233	G2153	C2086	G2009	G1935
	C2855	A2775	C2699	A2614	G2545	G2458	C2380	G2304	G2234	G2154	C2087	G2010	A1936
	C2856	A2776	C2700	G2615	U2546		C2381	G2305	G2235	G2155	U2096	U2011	A1937
	G2857	A2777	C2701	G2616	U2547	C2465	G2382	C2306	G2238	G2156	G2088	U2012	A1938
		A2778	U2702	C2617	G2548	C2467	G2383	G2307	G2239	A2158	U2091	A2013	
	U2865	G2782	C2703	C2620	G2549	G2468	C2384	G2308	C2240	G2159	U2092	A2014	C1941
	U2866	G2783	A2705	G2621	G2550	A2469	C2385	A2309	A2241	G2160	G2093	A2015	C1942
	G2867	C2784		G2622	U2551	G2470	U2390	U2312	G2246	C2161	U2094	U2016	U1943
	A2868	C2785	G2709	G2623	U2552	C2471	G2391	G2313	C2247	G2162	U2095	U2017	
			A2710	G2624	G2553	G2472	A2392	C2314	C2248	C2163	G2096	G2022	C1947
	G2872	C2788	U2711	G2625	U2554	G2473	A2393	C2315	C2249	G2164	U2096	U2023	A1952
	C2873	C2789	U2712	G2626	U2555	U2473	C2394	G2316	G2250	C2165	G2100	A1953	A1953
	C2874	A	A2713	G2630	C2556		C2395	C2317	G2251	G2166		A2030	U1955
	C2875	C	G2714	G2631	C2557	A2476	C2396	C2318	C2254		C2103	A2031	U1956
	G2876	G	G2715	A2632	G2558	C2477	U2398	G2319	C2255		G2104	G2032	U1957
		U	U2716	U2636	C2559	G2478	G2399	A2320	G2256	A2171	C2107	A2033	C1958
	A	C	G2717	U2637	A2561	G2481	C2402	A2322	U2257	C2172	C2108	G2036	G1959
		C	G2718	G2642	U2562	G2482	C2403	A2323	C2258	C2173	G2109	G2037	U1963
		A	U2720	G2643	A2563	C2483	C2404	A2324	G2259	C2174	G2110	G2038	G1964
				G2645	A2564	G2484	U2406	G2325	C2261	C2175	G2111	C2039	C1965
	C2889	C2723	C2724	G2646	A2565	G2485	G2407	A2326	U2262	C2176	G2112	C2041	A1966
	U2808	A2725	G2726	U2647	G2566	G2486	G2408	A2327	U2263	C2177	G2113	U2042	C1967
	A2809	U2726	G2727	U2648	G2567	G2487	A2411	G2330	C2264	C2178	G2114	A2043	G1968
	A2810	G2727		U2649	C2568	A2488	G2412	G2331	U2265	C2179	G2115	G2043	A1969
	G2811			U2653	A2572	U2493	G2413	G2332	A2266	U2180	G2116	U2047	G1970
				A2654	C2573	G2494	G2414	G2333	A2267	G2182	A2117	U2048	A1971
	C2816	G2732	A2733	G2655	G2574	G2495	G2415	G2334	A2268	C2183	C2108	G2049	A1972
	G2817	U2733		U2656	A2575	G2496	G2416	G2335	A2269	C2184	G2109	G2050	A1973
	G2818	G2737		G2657	G2576	A2497	G2421	A2336	G2270	C2185	U2121	C2051	G1974
	G2819	A2738		A2577	A2577	C2498	A2422	G2340	G2271	G2187	U2122	G2052	G1975
	A2820	U2739		G2578	C2578	C2499	U2423	G2341	U2272	C2188	G2125	C2055	G1980
	A2821	A2740		G2579	C2579	C2501	C2424	G2342	A2273	U2189			
	C	G2822		A2662	U2580	G2502	A2425	C2343	A2274				

• Molecule 25: 23S rRNA

Chain YA:



G1059	A988	G915	U839	G769	G886	A833	A567	C484	C393	C272C	G192	G
U1060	G989	G916	C340	G770	C887	C634	U688	C485	C393	C272C	G192	U
A990	A990	A917	A841	G771	U688	C635	U569	C486	G396	G272D	A195	C
G1062	C991	A918	A842	G772	A689	G636	G570	C487	G397	U272E	A196	A
G1063	G919	G919	G843	U773	G690	A637	A571	G488	U403	C272F	A197	A6
G1064	C994	U922	C346	A774	C691	G638	A572	G489	U403	C272G	U328	G10
U1065	C995	U922	U847	G775	C692	U639	G573	G494	G407	C272H	A199	G11
U1066	A996	C925	U847	G776	C693	C640	G574	G495	G407	G272I	U200	U12
G1068	C997	C925	A848	A777	U694	C641	A575	G495	G408	U272L	U202	G15
A1069	U999	G928	C850	U778	G695	G642	U576	A503	G409	G272M	C203	G16
A1070	A1000	U928	U851	U779	G696	G643	U577	U504	G410	U272N	A204	G17
G1071	A1001	G932	G852	A782	C697	C645	A578	A505	G411	G272O	G205	C18
C1072	G1002	A933	G853	A783	C698	A646	G579	A505	G412	G272P	U206	C19
A1073	C1005	C935	G854	A784	A699	G647	C581	C509	C413	G272Q	U206	
G1074	C1005	C935	G855	A785	G700	G648	G582	C510	C414	G272R	C210	
A1077	A1009	U937	C856	C786	G701	G649	G583	U511	A415	G272S	A211	G24
U1078	A1010	G938	U858	U787	G702	A652C	C587	U512	C420	G272T	A212	U25
C1079	G1011	A941	U859	A788	G717	G652D	U588	A513	C423	G272U	A213	G26
U1082	C1013	G942	U860	A793	A718	C652E	C589	A514	A428	G273B	G214	G27
U1083	U943	U943	A861	G794	C719	G652F	C590	A515	A428	G273C	G215	A28
A1084	G944	G944	G862	C795	C720	G	A590	C516	A428	G273D	A216	U29
A1085	G1017	G945	A863	C796	C721	C	C591	C517	C435	C273K	G217	G30
A1086	U1019	G946	G864	C797	A722	C	G593	G521	C435	G274	G115	C31
G1087	A1020	G947	A866	U724	G723	G	U594	G522	A443	G275	G116	C32
A1088	G1021	G948	C867	G801	G725	A	C595	C523	A443	C276	G117	U33
G1089	G1022	C949	U868	A802	G725	A	G596	C523	C445	C277	A118	C34
U1090	U1023		G869	U803	G728	C	C601	C527	C445	A278	U120	G35
G1091	U1026	A953	G870	U804	G729	C	A603	A528	A449	C279	G125	C37
C1092	A1027	G954	U871	G805	C730	C	A604	A529	G450	G27A	A126	A38
G1093	A1028	G955	A872	C806	C731	G	U606	C530	C451	G27B	A127	C39
A1096	U1029	A957	G873	U807	C737	C	C607	C534	A457	C285	G131	A43
U1097	G1030	U958	C876	U810	G738	C652U	U607	U534	A457	C286	G140	G44
U1101	A1032	A959	U877	U811	G739		G610	C535	G458	C288	A141	C45
C1102	U1033	G961	A878	C812	U740	C858	G611	G538	U459	A289	A142A	C47
A1103	C1038	G962	G880	C813	G745	C859	G612	G539	A460	G290	A142A	G51
C1104	U1039	U963	C886	C815	A746	C861	G613	C540	C462	C236	C154B	A52
G1106	G1040	C964	C887	C816	U747	G662	U614A	C546	G463	C237	U157	A53
U1107	C1041	C964	C888	C817	G748	G663	G614B	C546	G463	G301	U	G61
U1108	G1042	G968	C889	A820	A750	G664	G614C	A547	U464	C302	U	A64
C1109	C1043	U969	C890	C825	A751	G665	A614D	A548	A466	U303	G171	C65
A1111	G1044	C971	A890	A752	C753	G666	G615	G552	G467	U306	C172	C66
G1112	A1045	G972	C893	C754	C754	G669	G616	G553	G468	G307	G173	U67
U1113	A1046	A973	U827	C755	C755	G672	G618	G554	G469	G307	G178	A71
G1114	G1047	C974	U828	C756	C756	C673	G619	U555	A470	A311	G179	U72
G1115	A1048	G975A	A836	C757	U757	G674	G620	U556	A471	G312	G180	A73
C1116	C1049	G975B	C898	U758	C758	A675	A621	G557	G472	C313	A181	A74
G1122	G1050	A981	G906	C759	G759	A676	U626	G558	G473	A314	G182	A75
C1123	C1052	U907	U907	G832	G759	A676	A627	C560	A477	G315	C183	C76
G1124	A1053	A983	C908	C833	G760	A676	G628	C563	A478	C318	U185	G81
A1125	A1054	A984	A909	A835	A761	C679	G629	G563	A479	C319	U289	G82
	A1057	C985	A910	C836	A764	C683	G630	C564	A480	A320	A270	G83
	G1058	G987	C914	A885	G768	A885	A632	U566	C481	G321	A271	A84

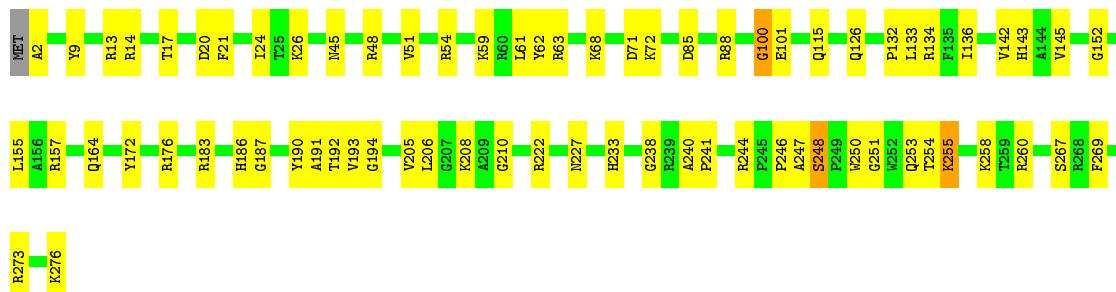
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G2055	C2055	A1912	A1819	A1912	A1819	G1744	A1646	G1573	G1500	G1421	G1343	U1273	A1204	G1131
G2056	G1980	A1913	U1820	A1913	U1820	A1749	G1647	G1574	C1501	G1422	G1344	A1274	U1205	A1132
A2059	C1981	C1914	A1821	C1914	A1821	G1752	G1648	G1575	G1505	G1423	C1345	A1275	G1206	U1133
A2060	C1982	U1915	G1822	U1915	G1822	G1753	G1649	U1576	G1506	G1424	A1276	A1276	C1135	C1135
G2061	C1983	A1916	G1823	A1916	G1823	G1754	G1651	U1577	A1507	G1425	U1352	G1280	G1210	G1136
A2062	C1988	A1917	G1826	A1917	G1826	A1755	G1652	U1578	A1508	G1426	A1353	G1281	U1211	G1137
C2063	A1919	G1756	C1827	A1919	C1827	G1756	G1653	A1579	A1509	G1427	A1354	G1282	G1212	G1138
C2064	C1920	G1757	G1828	C1920	G1828	A1760	G1654	G1581	C1509A	G1428	G1355	U1283	G1139	C1139
C2065	U1993	A1761	A1829	U1993	A1829	G1761	G1655	C1582	C1509B	G1429	G1356	G1284	G1215	G1140
C2066	C1966	A1762	C1830	C1966	C1830	A1762	G1656	C1583	A1509C	G1430	U1357	A1285	G1216	U1141
C2067	G1997	G1763	G1831	G1997	G1831	A1763	G1657	C1584	C1511	C1431	G1358	A1287	C1217	U1142
U2068	G1998	G1764	U1832	G1998	U1832	G1764	G1658	A1586	U1512	U1433	A1359	U1288	G1218	A1142B
C2070	C1999	C1765	U1833	C1999	U1833	C1765	G1659	A1587	C1513	A1434	A1360	G1291	C1221A	A1143
A2071	A1927	G1766	G1836	A1927	G1836	G1766	G1660	A1588	U1514	G1435	G1363	U1292	G1223	C1145
A2072	A1928	G1767	G1837	A1928	G1837	G1767	G1661	C1589	G1515	G1436	G1364	U1293	G1224	C1150
G2072	G1929	G1768	G1838	G1929	G1838	G1768	G1662	G1593	U1518	G1437	A1365	U1294	C1225	
C2073	G1930	G1769	G1839	G1930	G1839	G1769	G1663	G1594	U1519	G1438	A1366	C1295	G1226	C1153
G2074	G1931	G1770	G1840	G1931	G1840	G1770	G1664	G1595	G1525	U1439	A1367	C1296	A1226	G1154
U2075	C1934	G1771	G1841	U2075	G1841	G1771	G1665	G1596	G1526	G1440	G1368	C1297	G1227	A1155
C2006	G1935	A1772	C1842	C2006	G1935	A1772	G1666	A1597	G1531	A1445A	G1374	C1298	G1231	C1156
U2076	G1936	A1773	C1843	U2076	G1936	A1773	G1667	C1598	C1532	C1445B	C1375	C1299	G1232	G1157
A2077	A1937	C1774	C1844	A2077	A1937	C1774	G1668	G1599	U	C1446	C1376	A1301	C1233	C1158
	A1938	G1775	G1845		A1938	G1775	G1669	C1597	A	G1447	G1377	A1302	U1234	U1159
G2080	C2008	U1943	A1852	G2080	C2008	U1943	G1670	A1603	C1536	G1450A	A1379	C1306	G1236	G1160
C2081	U2011	U1940	A1853	C2081	U2011	U1940	G1671	C1604	G1537		G1380	A1307	G1237	G1164
A2082	G2012	G1945	G1854	A2082	G2012	G1945	G1672	C1605	G1538	A1452	A1308	G1309	G1239	U1165
C2085	A2013	U1946	G1855	C2085	A2013	U1946	G1673	C1606	G1539	U1453	G1310	G1240	A1241	G1171
A2014	G1947	A1783	G1856	A2014	G1947	A1783	G1674	C1607	U	U1454	G1311	A1242	G1243	G
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U2016	G1949	A1785	G1858	U2016	G1949	A1785	G1676	A1609	G1539		G1313	A1245		U
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G2018	G1951	A1787	G1860	G2018	G1951	A1787	G1678	C1611	A1542	G1462	C1315	A1247		A
A2019	U1955	G1788	G1861	A2019	U1955	G1788	G1679	C1612	A1544	C1463	U1316	G1250		C1178
A2020	C1957	C1795	G1862	A2020	C1957	C1795	G1680	G1613	A1545	G1464	U1317	G1251		C1179
	C1958	U1798	A1889		C1958	U1798	G1681	A1614	C1546	G1465	G1318	G1252		C1180
G2023	C2023	G1799	C1892	G2023	C2023	G1799	G1682	A1615	C1547	G1466	U1397	G1253		C1181
C2026	C2026	G1801	C1893	C2026	C2026	G1801	G1683	A1616	C1548	G1467	C1398	G1254		A1182
G2029	G2029	A1802	C1894	G2029	G2029	A1802	G1684	A1617	C1549		C1399	A1253		G1183
A2030	A2030	A1803	G1897	A2030	A2030	A1803	G1685	G1619		G1470	A1321	A1254		G1184
A2031	A2031	G1804	U1898	A2031	A2031	G1804	G1686	G1695	A1553	A1471	A1322	U1255		G1185
A2032	A2032	C1800	U1899	A2032	A2032	C1800	G1687	G1696	A1554	A1472	G1325	G1256		G1186
C2036	C2036	G1801	G1899	C2036	C2036	G1801	G1688	G1697	C1557	G1473	U1326	G1257		G1187
G2037	G2037	A1803	C1894	G2037	G2037	A1803	G1689	U1629	C1558	G1476	G1327	G1258		U1188
C2038	C2038	G1804	U1897	C2038	C2038	G1804	G1690	G1698	A1559		U1328	G1259		A1189
U2109	U2109	C1804	U1898	U2109	U2109	C1804	G1691	G1699	G1560	G1482	U1405	G1260		G1190
		A1809	G1899			A1809	G1692	G1699	G1561	G1483	C1407	A1261		G1191
U2113	U2113	A1810	A1900	U2113	U2113	A1810	G1693	G1699	U1562	G1484	C1408	A1262		G1192
A2114	A2114	G1811	A1901	A2114	A2114	G1811	G1694	G1699	G1563	G1485	C1409	G1263		C1196
G2115	G2115	U1720	G1903	G2115	G2115	U1720	G1695	G1699	G1564	G1486	G1411	A1265		A1183
G2116	G2116	G1813	G1904	G2116	G2116	G1813	G1696	G1699	A1565	G1487	A1412	G1266		G1197
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G2118	G2118	A1815	G1906	G2118	G2118	A1815	G1698	G1699	A1567	G1489	A1336	A1268		U1199
C2119	C2119	G1816	G1907	C2119	C2119	G1816	G1699	G1699	A1568	G1490	G1337	A1269		C1200
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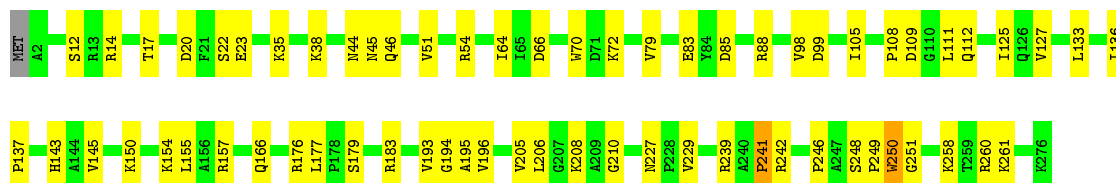
- Molecule 27: 50S ribosomal protein L2

Chain RD: 74% 25% .



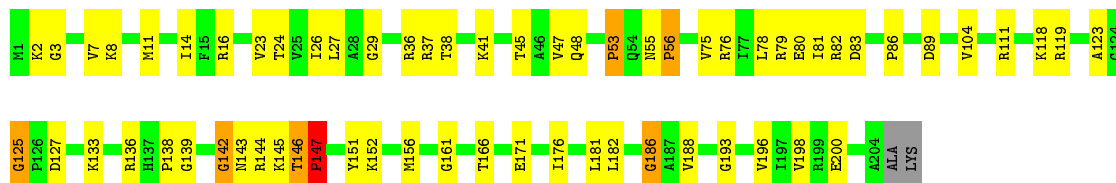
- Molecule 27: 50S ribosomal protein L2

Chain YD: 76% 23% .



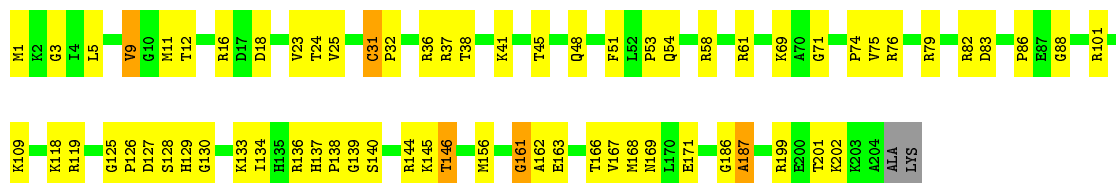
- Molecule 28: 50S ribosomal protein L3

Chain RE: 68% 28% . .



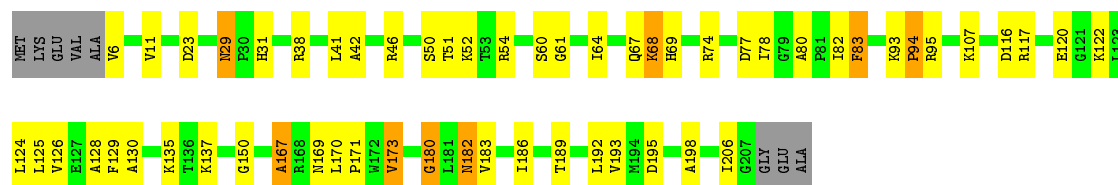
- Molecule 28: 50S ribosomal protein L3

Chain YE: 66% 31% . .



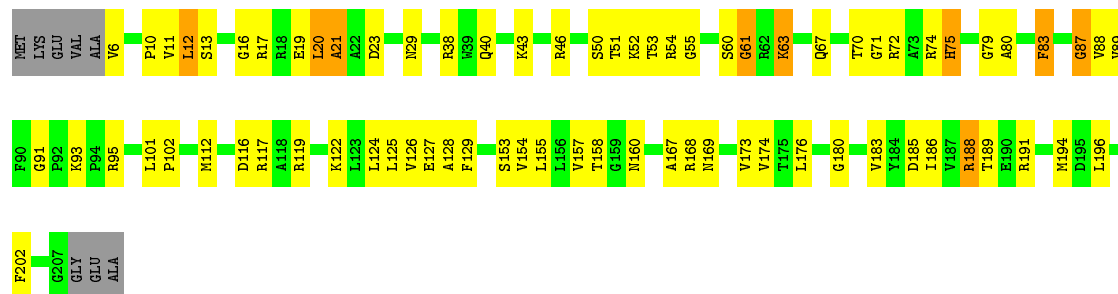
- Molecule 29: 50S ribosomal protein L4

Chain RF: 69% 23% . .



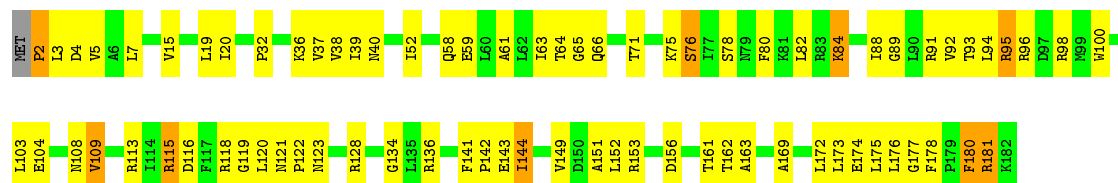
- Molecule 29: 50S ribosomal protein L4

Chain YF: 60% 31%



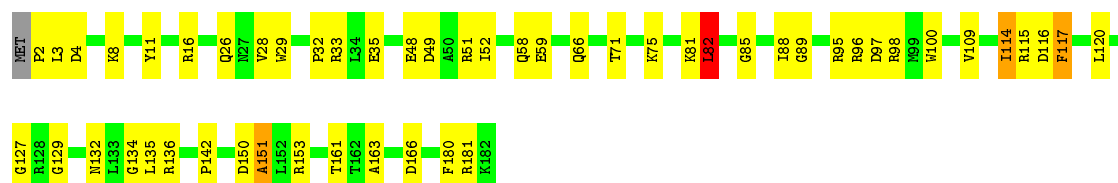
- Molecule 30: 50S ribosomal protein L5

Chain RG: 57% 37% 5%



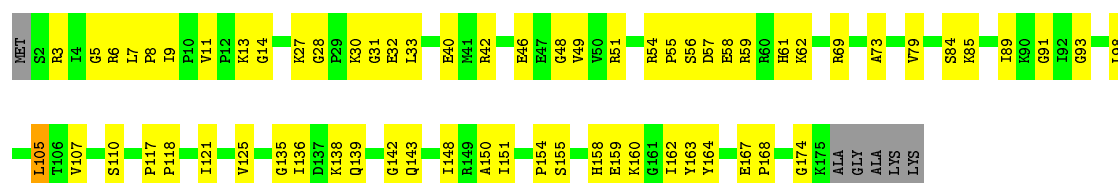
- Molecule 30: 50S ribosomal protein L5

Chain YG: 71% 26%



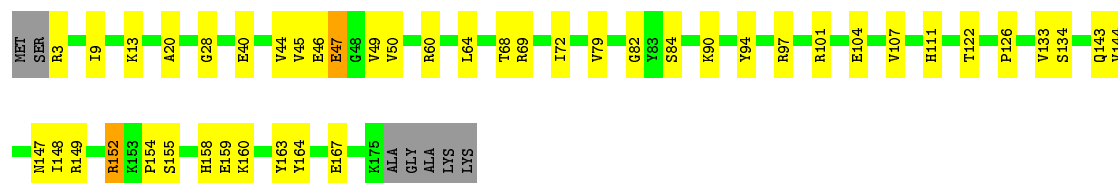
- Molecule 31: 50S ribosomal protein L6

Chain RH: 61% 36%



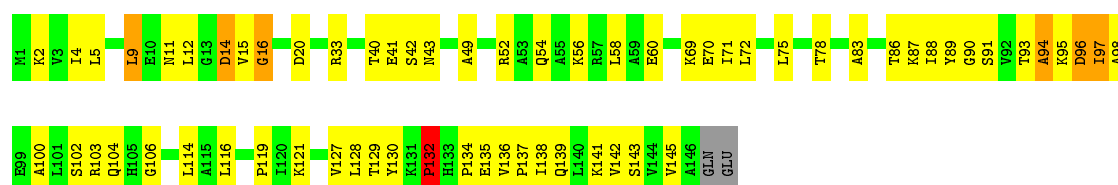
- Molecule 31: 50S ribosomal protein L6

Chain YH:  71% 24% . .



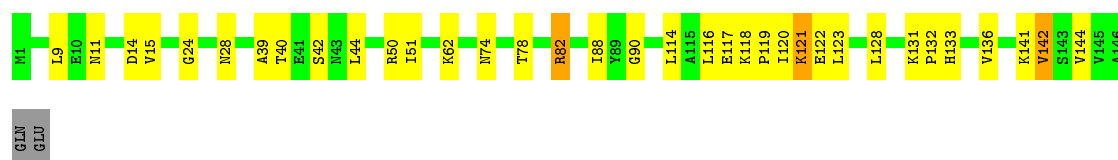
- Molecule 32: 50S ribosomal protein L9

Chain RI:  55% 39% . .



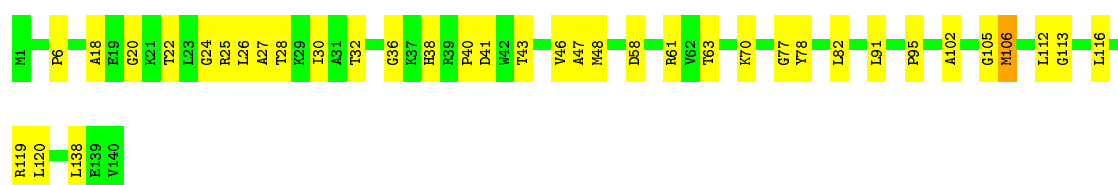
- Molecule 32: 50S ribosomal protein L9

Chain YI:  75% 22% . .




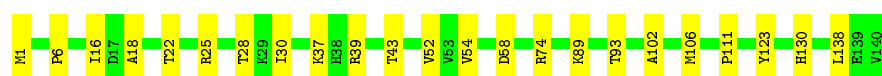
- Molecule 33: 50S ribosomal protein L13

Chain RN:  74% 26% .



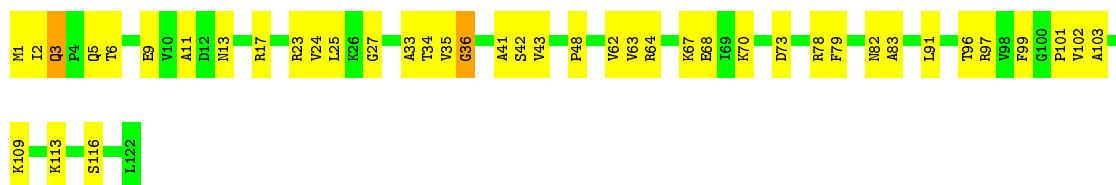
- Molecule 33: 50S ribosomal protein L13

Chain YN:  84% 16%

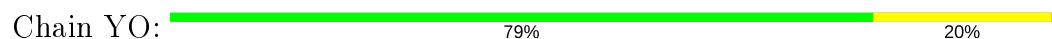


- Molecule 34: 50S ribosomal protein L14

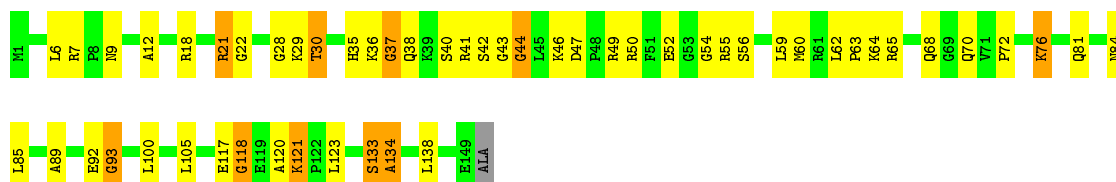
Chain RO:  66% 33% .



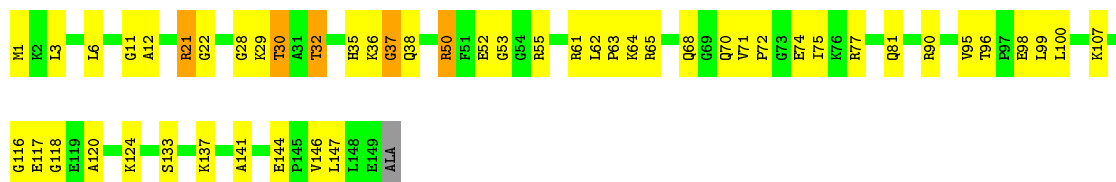
- Molecule 34: 50S ribosomal protein L14



- Molecule 35: 50S ribosomal protein L15



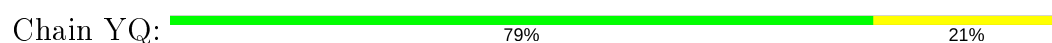
- Molecule 35: 50S ribosomal protein L15



- Molecule 36: 50S ribosomal protein L16



- Molecule 36: 50S ribosomal protein L16

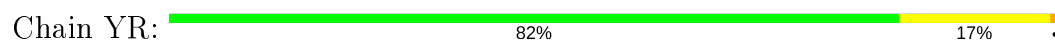




- Molecule 37: 50S ribosomal protein L17



- Molecule 37: 50S ribosomal protein L17



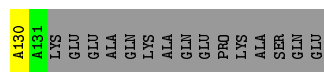
- Molecule 38: 50S ribosomal protein L18



- Molecule 38: 50S ribosomal protein L18



- Molecule 39: 50S ribosomal protein L19



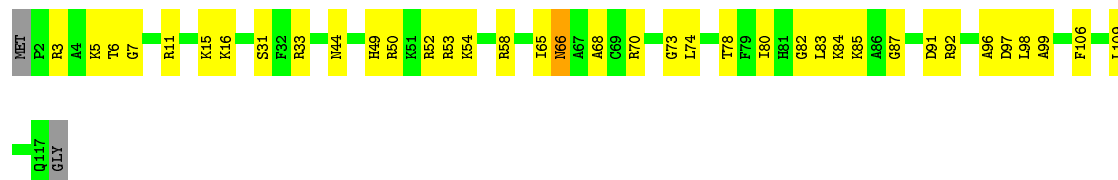
- Molecule 39: 50S ribosomal protein L19





- Molecule 40: 50S ribosomal protein L20

Chain RU: 67% 31% ..



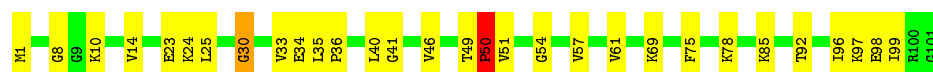
- Molecule 40: 50S ribosomal protein L20

Chain YU: 78% 20% .



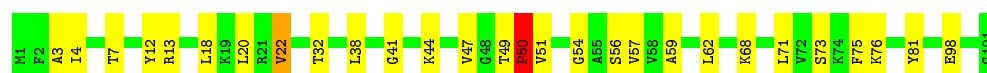
- Molecule 41: 50S ribosomal protein L21

Chain RV: 70% 28% ..



- Molecule 41: 50S ribosomal protein L21

Chain YV: 72% 26% ..



- Molecule 42: 50S ribosomal protein L22

Chain RW: 77% 22% .



- Molecule 42: 50S ribosomal protein L22

Chain YW: 79% 19% ..



- Molecule 43: 50S ribosomal protein L23

Chain RX: 72% 25% ..



- Molecule 43: 50S ribosomal protein L23

Chain YX: 86% 13% .



- Molecule 44: 50S ribosomal protein L24

Chain RY: 75% 19% . .



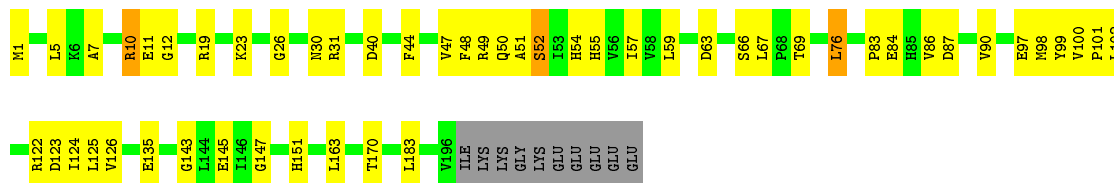
- Molecule 44: 50S ribosomal protein L24

Chain YY: 68% 27% . .



- Molecule 45: 50S ribosomal protein L25

Chain RZ: 70% 24% . 5%



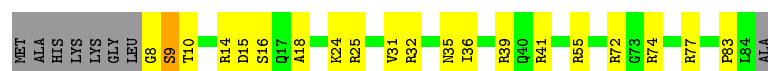
- Molecule 45: 50S ribosomal protein L25

Chain YZ: 62% 25% . 11%

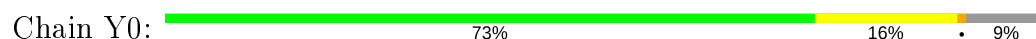




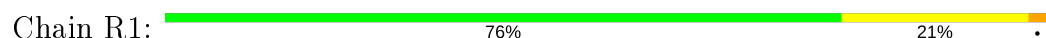
- Molecule 46: 50S ribosomal protein L27



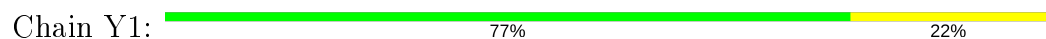
- Molecule 46: 50S ribosomal protein L27



- Molecule 47: 50S ribosomal protein L28



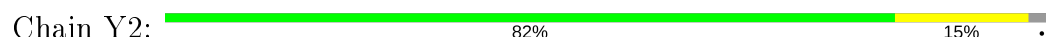
- Molecule 47: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L29

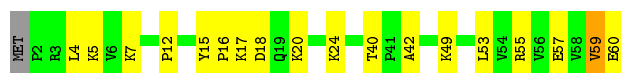


- Molecule 48: 50S ribosomal protein L29



- Molecule 49: 50S ribosomal protein L30





- Molecule 49: 50S ribosomal protein L30



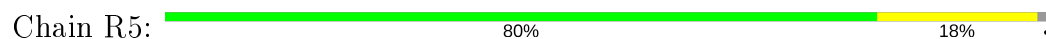
- Molecule 50: 50S ribosomal protein L31



- Molecule 50: 50S ribosomal protein L31



- Molecule 51: 50S ribosomal protein L32



- Molecule 51: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L33

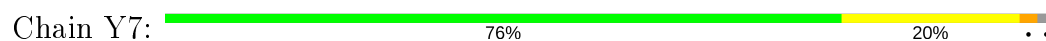




- Molecule 53: 50S ribosomal protein L34



- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: tRNA acceptor end mimic





- Molecule 56: tRNA acceptor end mimic



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	208.91Å 445.91Å 617.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.17 – 3.64	Depositor
% Data completeness (in resolution range)	93.4 (49.17-3.64)	Depositor
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.208 , 0.250	Depositor
Wilson B-factor (Å ²)	123.8	Xtriage
Anisotropy	0.381	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	291822	wwPDB-VP
Average B, all atoms (Å ²)	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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, OMC, ZN, OMG, OMU, MA6, G7M, SF4, 0TD, MG, 2MA, 2MG, 5MC, UR3, 4OC, M2G, PPU, 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	QA	0.92	1/35795 (0.0%)	1.25	264/55864 (0.5%)
1	XA	1.03	8/35890 (0.0%)	1.25	234/56012 (0.4%)
2	QB	0.36	0/1942	0.64	0/2619
2	XB	0.39	0/1950	0.59	0/2630
3	QC	0.36	0/1629	0.60	1/2195 (0.0%)
3	XC	0.42	0/1629	0.59	0/2195
4	QD	0.47	0/1733	0.66	0/2318
4	XD	0.48	0/1733	0.61	0/2318
5	QE	0.40	0/1149	0.61	0/1548
5	XE	0.47	0/1149	0.59	0/1548
6	QF	0.40	0/850	0.56	0/1147
6	XF	0.49	0/850	0.60	1/1147 (0.1%)
7	QG	0.36	0/1276	0.55	0/1709
7	XG	0.43	0/1276	0.56	0/1709
8	QH	0.43	0/1128	0.59	0/1517
8	XH	0.44	0/1128	0.59	0/1517
9	QI	0.38	0/1029	0.62	0/1379
9	XI	0.42	0/1017	0.64	0/1365
10	QJ	0.37	0/814	0.61	0/1095
10	XJ	0.40	0/790	0.52	0/1063
11	QK	0.42	0/859	0.54	0/1162
11	XK	0.41	0/859	0.52	0/1162
12	QL	0.49	0/963	0.65	0/1287
12	XL	0.52	0/963	0.60	0/1287
13	QM	0.41	0/938	0.64	0/1258
13	XM	0.45	0/926	0.61	0/1241
14	QN	0.40	0/501	0.59	0/664
14	XN	0.48	0/501	0.60	0/664
15	QO	0.38	0/745	0.55	0/992
15	XO	0.45	0/745	0.62	0/992
16	QP	0.50	0/707	0.56	0/951

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	XP	0.43	0/707	0.57	0/951
17	QQ	0.45	0/836	0.58	0/1117
17	XQ	0.45	0/836	0.56	0/1117
18	QR	0.38	0/560	0.58	0/746
18	XR	0.45	0/560	0.60	0/746
19	QS	0.33	0/680	0.57	0/915
19	XS	0.44	0/680	0.58	0/915
20	QT	0.43	0/745	0.57	0/981
20	XT	0.34	0/762	0.57	0/1003
21	QU	0.37	0/203	0.54	0/266
21	XU	0.41	0/203	0.47	0/266
22	QV	0.90	1/1836 (0.1%)	1.28	31/2859 (1.1%)
22	XV	1.16	1/1836 (0.1%)	1.40	25/2859 (0.9%)
23	QX	0.71	0/185	1.34	1/285 (0.4%)
23	XX	0.89	0/260	1.69	8/402 (2.0%)
24	QY	0.69	0/336	1.25	3/522 (0.6%)
24	XY	0.71	0/381	1.39	7/593 (1.2%)
25	RA	1.20	15/68971 (0.0%)	1.33	622/107656 (0.6%)
25	YA	1.36	49/68976 (0.1%)	1.43	918/107668 (0.9%)
26	RB	0.78	0/2876	1.27	26/4486 (0.6%)
26	YB	1.09	0/2878	1.27	18/4490 (0.4%)
27	RD	0.60	0/2194	0.59	0/2955
27	YD	0.67	0/2195	0.62	0/2955
28	RE	0.57	0/1596	0.59	0/2153
28	YE	0.61	0/1596	0.65	0/2153
29	RF	0.60	1/1620 (0.1%)	0.61	0/2194
29	YF	0.65	0/1620	0.64	1/2194 (0.0%)
30	RG	0.40	0/1499	0.69	0/2016
30	YG	0.53	0/1499	0.67	1/2016 (0.0%)
31	RH	0.38	0/1362	0.58	0/1841
31	YH	0.55	0/1356	0.58	0/1833
32	RI	0.42	0/1151	0.68	1/1558 (0.1%)
32	YI	0.44	0/1151	0.67	0/1558
33	RN	0.51	0/1148	0.55	0/1547
33	YN	0.58	0/1148	0.54	0/1547
34	RO	0.56	0/943	0.67	1/1269 (0.1%)
34	YO	0.64	0/943	0.67	2/1269 (0.2%)
35	RP	0.50	0/1156	0.60	0/1537
35	YP	0.56	0/1156	0.62	0/1537
36	RQ	0.50	0/1143	0.58	0/1527
36	YQ	0.59	0/1143	0.59	0/1527
37	RR	0.56	0/982	0.66	0/1312
37	YR	0.54	0/982	0.62	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	RS	0.39	0/887	0.63	1/1180 (0.1%)
38	YS	0.49	0/887	0.62	0/1180
39	RT	0.52	0/1105	0.57	0/1477
39	YT	0.58	0/1105	0.58	0/1477
40	RU	0.52	0/977	0.52	0/1301
40	YU	0.61	0/977	0.54	0/1301
41	RV	0.48	0/790	0.64	0/1057
41	YV	0.59	0/790	0.67	0/1057
42	RW	0.60	0/901	0.55	0/1209
42	YW	0.62	0/901	0.54	0/1209
43	RX	0.54	0/764	0.57	1/1025 (0.1%)
43	YX	0.63	0/764	0.59	0/1025
44	RY	0.49	0/831	0.59	0/1108
44	YY	0.57	0/831	0.61	0/1108
45	RZ	0.42	0/1585	0.61	1/2153 (0.0%)
45	YZ	0.50	0/1493	0.65	1/2026 (0.0%)
46	R0	0.47	0/619	0.55	0/825
46	Y0	0.59	0/619	0.57	0/825
47	R1	0.52	0/770	0.58	0/1022
47	Y1	0.59	1/770 (0.1%)	0.60	0/1022
48	R2	0.40	0/594	0.52	0/785
48	Y2	0.47	0/594	0.51	0/785
49	R3	0.52	0/474	0.61	0/635
49	Y3	0.52	0/473	0.62	0/635
50	R4	0.36	0/578	0.60	0/776
50	Y4	0.42	0/578	0.63	1/776 (0.1%)
51	R5	0.58	0/473	0.61	0/639
51	Y5	0.57	0/465	0.57	0/629
52	R6	0.32	0/460	0.56	0/613
52	Y6	0.33	0/460	0.64	0/613
53	R7	0.58	0/426	0.59	0/561
53	Y7	0.62	0/426	0.63	0/561
54	R8	0.52	0/525	0.58	0/691
54	Y8	0.59	0/525	0.65	0/691
55	R9	0.29	0/310	0.56	0/407
55	Y9	0.38	0/310	0.59	0/407
56	ZA	0.64	0/40	1.52	4/60 (6.7%)
56	ZB	1.26	0/40	1.60	0/60
All	All	1.02	77/314471 (0.0%)	1.18	2174/470119 (0.5%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	XA	0	1
2	QB	0	30
2	XB	0	23
3	QC	0	24
3	XC	0	16
4	QD	0	18
4	XD	0	8
5	QE	0	13
5	XE	0	15
6	QF	0	6
6	XF	0	5
7	QG	0	10
7	XG	0	10
8	QH	0	14
8	XH	0	6
9	QI	0	22
9	XI	0	9
10	QJ	0	10
10	XJ	0	8
11	QK	0	6
11	XK	0	11
12	QL	0	13
12	XL	0	10
13	QM	0	12
13	XM	0	7
14	QN	0	5
14	XN	0	6
15	QO	0	4
15	XO	0	3
16	QP	0	10
16	XP	0	4
17	QQ	0	7
17	XQ	0	5
18	QR	0	3
18	XR	0	1
19	QS	0	10
19	XS	0	8
20	QT	0	6
20	XT	0	4
21	QU	0	3
21	XU	0	2
25	YA	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
27	RD	0	17
27	YD	0	9
28	RE	0	14
28	YE	0	16
29	RF	0	15
29	YF	0	19
30	RG	0	29
30	YG	0	19
31	RH	0	20
31	YH	0	5
32	RI	0	26
32	YI	0	19
33	RN	0	7
33	YN	0	5
34	RO	0	5
34	YO	0	1
35	RP	0	23
35	YP	0	18
36	RQ	0	4
36	YQ	0	4
37	RR	0	5
37	YR	0	5
38	RS	0	5
38	YS	0	5
39	RT	0	5
39	YT	0	5
40	RU	0	6
40	YU	0	1
41	RV	0	8
41	YV	0	9
42	RW	0	2
42	YW	0	5
43	RX	0	4
43	YX	0	3
44	RY	0	6
44	YY	0	6
45	RZ	0	13
45	YZ	0	22
46	R0	0	5
46	Y0	0	3
47	R1	0	5
47	Y1	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
48	R2	0	3
48	Y2	0	1
49	R3	0	2
49	Y3	0	4
50	R4	0	10
50	Y4	0	11
51	R5	0	2
51	Y5	0	3
52	R6	0	5
52	Y6	0	5
53	R7	0	4
53	Y7	0	2
54	R8	0	1
54	Y8	0	4
55	R9	0	4
55	Y9	0	1
All	All	0	858

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	XA	88	A	C3'-C2'	11.98	1.66	1.52
22	XV	1	C	OP3-P	-9.54	1.49	1.61
22	QV	1	C	OP3-P	-9.31	1.50	1.61
1	XA	88	A	C1'-N9	7.29	1.59	1.48
1	XA	88	A	C4'-O4'	7.00	1.54	1.45

The worst 5 of 2174 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	88	A	O4'-C1'-C2'	16.46	122.42	107.60
1	XA	359	U	C2-N1-C1'	15.95	136.84	117.70
25	YA	2415	G	N3-C2-N2	-15.63	108.96	119.90
23	XX	19	C	N1-C2-O2	13.47	126.98	118.90
1	XA	358	U	N1-C1'-C2'	-12.81	97.35	114.00

There are no chirality outliers.

5 of 858 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	13	ALA	Peptide

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Mol	Chain	Res	Type	Group
2	QB	15	VAL	Peptide
2	QB	17	PHE	Peptide
2	QB	19	HIS	Peptide
2	QB	21	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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32246	0	16294	685	0
1	XA	32331	0	16338	595	14
2	QB	1907	0	1958	42	0
2	XB	1915	0	1969	45	0
3	QC	1605	0	1668	48	0
3	XC	1605	0	1668	20	1
4	QD	1703	0	1762	81	0
4	XD	1703	0	1763	52	6
5	QE	1133	0	1190	32	0
5	XE	1133	0	1191	23	0
6	QF	837	0	852	11	1
6	XF	837	0	852	15	0
7	QG	1257	0	1296	34	0
7	XG	1257	0	1296	26	0
8	QH	1108	0	1165	33	0
8	XH	1108	0	1165	27	0
9	QI	1010	0	1037	36	0
9	XI	998	0	1024	29	0
10	QJ	801	0	849	29	0
10	XJ	777	0	815	16	0
11	QK	844	0	855	29	1
11	XK	844	0	855	22	0
12	QL	958	0	1047	23	0
12	XL	958	0	1047	19	0
13	QM	928	0	987	37	0
13	XM	916	0	973	20	0
14	QN	492	0	530	30	0
14	XN	492	0	528	11	0
15	QO	734	0	771	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	XO	734	0	771	10	0
16	QP	691	0	714	17	0
16	XP	691	0	714	19	0
17	QQ	823	0	891	24	0
17	XQ	823	0	891	20	0
18	QR	555	0	618	11	0
18	XR	555	0	618	8	0
19	QS	665	0	686	13	0
19	XS	665	0	686	20	0
20	QT	743	0	840	22	0
20	XT	759	0	861	24	0
21	QU	199	0	208	10	0
21	XU	199	0	208	8	0
22	QV	1644	0	835	29	0
22	XV	1644	0	836	26	0
23	QX	167	0	86	2	0
23	XX	233	0	120	4	0
24	QY	301	0	152	5	0
24	XY	341	0	175	8	0
25	RA	61819	0	31179	950	3
25	YA	61822	0	31176	961	3
26	RB	2572	0	1305	44	0
26	YB	2573	0	1306	28	0
27	RD	2144	0	2233	57	3
27	YD	2145	0	2234	53	0
28	RE	1563	0	1629	44	0
28	YE	1563	0	1628	44	0
29	RF	1585	0	1632	35	0
29	YF	1585	0	1632	43	0
30	RG	1474	0	1535	40	0
30	YG	1474	0	1535	29	0
31	RH	1336	0	1418	30	0
31	YH	1330	0	1413	28	13
32	RI	1136	0	1223	26	14
32	YI	1136	0	1223	13	0
33	RN	1121	0	1195	25	0
33	YN	1121	0	1195	16	0
34	RO	933	0	996	32	0
34	YO	933	0	996	22	0
35	RP	1139	0	1222	35	0
35	YP	1139	0	1222	36	0
36	RQ	1122	0	1179	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	YQ	1122	0	1179	20	0
37	RR	968	0	1033	22	0
37	YR	968	0	1033	17	0
38	RS	877	0	938	26	0
38	YS	877	0	938	28	0
39	RT	1091	0	1151	25	0
39	YT	1091	0	1151	32	0
40	RU	959	0	1019	28	0
40	YU	959	0	1019	25	0
41	RV	779	0	852	16	0
41	YV	779	0	852	13	6
42	RW	890	0	951	17	1
42	YW	890	0	951	17	0
43	RX	750	0	814	16	0
43	YX	750	0	814	7	0
44	RY	818	0	913	13	0
44	YY	818	0	911	15	14
45	RZ	1552	0	1573	31	0
45	YZ	1461	0	1493	24	0
46	R0	611	0	631	13	0
46	Y0	611	0	631	12	0
47	R1	763	0	848	15	0
47	Y1	763	0	848	11	0
48	R2	592	0	654	10	0
48	Y2	592	0	654	6	1
49	R3	469	0	518	12	0
49	Y3	468	0	518	15	0
50	R4	565	0	556	14	0
50	Y4	565	0	557	13	0
51	R5	459	0	480	8	0
51	Y5	451	0	471	6	3
52	R6	453	0	477	6	0
52	Y6	453	0	477	8	0
53	R7	418	0	467	12	0
53	Y7	418	0	467	8	0
54	R8	517	0	582	15	0
54	Y8	517	0	582	12	0
55	R9	307	0	335	10	0
55	Y9	307	0	338	8	0
56	ZA	74	0	51	13	0
56	ZB	74	0	51	5	0
57	QA	124	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	QC	1	0	0	0	0
57	QD	2	0	0	0	0
57	QE	2	0	0	0	0
57	QL	2	0	0	0	0
57	QM	2	0	0	0	0
57	QN	2	0	0	2	0
57	QO	1	0	0	0	0
57	QV	3	0	0	0	0
57	R0	2	0	0	0	0
57	R1	1	0	0	0	0
57	R3	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R7	1	0	0	0	0
57	R8	1	0	0	0	0
57	R9	1	0	0	0	0
57	RA	414	0	0	2	0
57	RB	8	0	0	2	0
57	RD	5	0	0	2	0
57	RE	5	0	0	2	0
57	RF	5	0	0	0	0
57	RN	2	0	0	0	0
57	RO	1	0	0	0	0
57	RP	2	0	0	0	0
57	RQ	1	0	0	0	0
57	RR	1	0	0	0	0
57	RV	1	0	0	0	0
57	RW	1	0	0	0	0
57	RX	1	0	0	0	0
57	RZ	1	0	0	0	0
57	XA	128	0	0	0	0
57	XD	1	0	0	0	0
57	XJ	1	0	0	0	0
57	XK	2	0	0	0	0
57	XN	1	0	0	0	0
57	XV	1	0	0	0	0
57	XX	1	0	0	0	0
57	Y0	1	0	0	0	0
57	Y1	3	0	0	0	0
57	Y3	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	Y7	1	0	0	0	0
57	Y8	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YA	544	0	0	1	0
57	YB	8	0	0	0	0
57	YD	8	0	0	0	0
57	YE	7	0	0	1	0
57	YF	1	0	0	0	0
57	YG	1	0	0	0	0
57	YP	3	0	0	0	0
57	YQ	2	0	0	0	0
57	YR	1	0	0	0	0
57	YT	1	0	0	0	0
57	YU	1	0	0	0	0
57	YV	1	0	0	0	0
57	YW	1	0	0	0	0
57	YX	1	0	0	0	0
58	QD	8	0	0	6	0
58	XD	8	0	0	4	0
59	QN	1	0	0	1	0
59	R4	1	0	0	0	0
59	R9	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y4	1	0	0	0	0
All	All	291822	0	197739	4729	42

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 10.

The worst 5 of 4729 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)
28:RE:152:LYS:HG3	33:RN:77:GLY:O	1.40	1.18
49:Y3:10:LYS:NZ	49:Y3:15:TYR:OH	1.81	1.13
25:YA:2228:G:OP1	27:YD:261:LYS:NZ	1.83	1.12
1:QA:982:U:H3	1:QA:1223:C:N4	1.52	1.08
1:QA:1055:A:H62	1:QA:1200:C:N4	1.56	1.04

The worst 5 of 42 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)
31:YH:46:GLU:CG	44:YY:22:GLY:O[4_445]	1.23	0.97
31:YH:46:GLU:CB	44:YY:22:GLY:O[4_445]	1.41	0.79
32:RI:89:TYR:CD2	1:XA:55:A:C2[4_555]	1.42	0.78
27:RD:134:ARG:NE	4:XD:166:LYS:NZ[4_555]	1.53	0.67
32:RI:89:TYR:CE2	1:XA:55:A:N3[4_555]	1.58	0.62

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	204 (88%)	29 (12%)	0	100	100
2	XB	234/256 (91%)	204 (87%)	30 (13%)	0	100	100
3	QC	203/239 (85%)	184 (91%)	19 (9%)	0	100	100
3	XC	203/239 (85%)	183 (90%)	20 (10%)	0	100	100
4	QD	206/209 (99%)	183 (89%)	21 (10%)	2 (1%)	15	54
4	XD	206/209 (99%)	196 (95%)	10 (5%)	0	100	100
5	QE	146/162 (90%)	134 (92%)	12 (8%)	0	100	100
5	XE	146/162 (90%)	134 (92%)	12 (8%)	0	100	100
6	QF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
6	XF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
8	QH	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
8	XH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
9	QI	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
9	XI	124/128 (97%)	110 (89%)	14 (11%)	0	100	100
10	QJ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
10	XJ	94/105 (90%)	83 (88%)	11 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	QK	112/129 (87%)	105 (94%)	7 (6%)	0	100	100
11	XK	112/129 (87%)	104 (93%)	8 (7%)	0	100	100
12	QL	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
12	XL	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
13	QM	114/126 (90%)	108 (95%)	6 (5%)	0	100	100
13	XM	112/126 (89%)	102 (91%)	10 (9%)	0	100	100
14	QN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
14	XN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
15	QO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
15	XO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
16	QP	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
16	XP	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
17	QQ	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
17	XQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
18	QR	66/88 (75%)	66 (100%)	0	0	100	100
18	XR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
19	QS	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
19	XS	81/93 (87%)	78 (96%)	3 (4%)	0	100	100
20	QT	94/106 (89%)	89 (95%)	5 (5%)	0	100	100
20	XT	96/106 (91%)	91 (95%)	5 (5%)	0	100	100
21	QU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
21	XU	21/27 (78%)	21 (100%)	0	0	100	100
27	RD	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
27	YD	273/276 (99%)	252 (92%)	21 (8%)	0	100	100
28	RE	202/206 (98%)	184 (91%)	17 (8%)	1 (0%)	29	67
28	YE	202/206 (98%)	181 (90%)	21 (10%)	0	100	100
29	RF	200/210 (95%)	192 (96%)	8 (4%)	0	100	100
29	YF	200/210 (95%)	188 (94%)	12 (6%)	0	100	100
30	RG	179/182 (98%)	156 (87%)	23 (13%)	0	100	100
30	YG	179/182 (98%)	151 (84%)	27 (15%)	1 (1%)	25	63
31	RH	172/180 (96%)	166 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	YH	171/180 (95%)	162 (95%)	8 (5%)	1 (1%)	25	63
32	RI	144/148 (97%)	115 (80%)	28 (19%)	1 (1%)	22	61
32	YI	144/148 (97%)	125 (87%)	19 (13%)	0	100	100
33	RN	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
33	YN	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
34	RO	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
34	YO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
35	RP	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	22	61
35	YP	147/150 (98%)	135 (92%)	12 (8%)	0	100	100
36	RQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
36	YQ	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
37	RR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
37	YR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
38	RS	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
38	YS	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
39	RT	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
39	YT	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
40	RU	114/118 (97%)	107 (94%)	7 (6%)	0	100	100
40	YU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
41	RV	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	54
41	YV	99/101 (98%)	88 (89%)	10 (10%)	1 (1%)	15	54
42	RW	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
42	YW	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
43	RX	93/96 (97%)	84 (90%)	9 (10%)	0	100	100
43	YX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
44	RY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
44	YY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
45	RZ	194/206 (94%)	181 (93%)	13 (7%)	0	100	100
45	YZ	181/206 (88%)	154 (85%)	27 (15%)	0	100	100
46	R0	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
46	Y0	75/85 (88%)	72 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	R1	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
47	Y1	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
48	R2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
48	Y2	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
49	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
49	Y3	57/60 (95%)	57 (100%)	0	0	100	100
50	R4	67/71 (94%)	53 (79%)	14 (21%)	0	100	100
50	Y4	67/71 (94%)	53 (79%)	14 (21%)	0	100	100
51	R5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
51	Y5	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
52	R6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
52	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
53	R7	46/49 (94%)	42 (91%)	4 (9%)	0	100	100
53	Y7	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
54	R8	62/65 (95%)	55 (89%)	7 (11%)	0	100	100
54	Y8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
55	R9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
55	Y9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
All	All	11420/12128 (94%)	10610 (93%)	801 (7%)	9 (0%)	51	83

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	QD	32	ALA
4	QD	31	CYS
30	YG	81	LYS
32	RI	132	PRO
41	RV	50	PRO

5.3.2 Protein sidechains ⓘ

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

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

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	203/220 (92%)	201 (99%)	2 (1%)	76	88
2	XB	204/220 (93%)	201 (98%)	3 (2%)	65	83
3	QC	159/188 (85%)	158 (99%)	1 (1%)	86	94
3	XC	159/188 (85%)	157 (99%)	2 (1%)	69	85
4	QD	180/181 (99%)	175 (97%)	5 (3%)	43	71
4	XD	180/181 (99%)	175 (97%)	5 (3%)	43	71
5	QE	114/123 (93%)	114 (100%)	0	100	100
5	XE	114/123 (93%)	113 (99%)	1 (1%)	78	89
6	QF	90/90 (100%)	89 (99%)	1 (1%)	73	87
6	XF	90/90 (100%)	89 (99%)	1 (1%)	73	87
7	QG	126/127 (99%)	123 (98%)	3 (2%)	49	74
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	118/119 (99%)	118 (100%)	0	100	100
8	XH	118/119 (99%)	117 (99%)	1 (1%)	81	91
9	QI	98/99 (99%)	98 (100%)	0	100	100
9	XI	97/99 (98%)	96 (99%)	1 (1%)	76	88
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	86/99 (87%)	85 (99%)	1 (1%)	71	86
11	XK	86/99 (87%)	86 (100%)	0	100	100
12	QL	102/108 (94%)	102 (100%)	0	100	100
12	XL	102/108 (94%)	102 (100%)	0	100	100
13	QM	94/101 (93%)	93 (99%)	1 (1%)	73	87
13	XM	93/101 (92%)	93 (100%)	0	100	100
14	QN	49/50 (98%)	47 (96%)	2 (4%)	30	63
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	78 (99%)	1 (1%)	69	85
15	XO	79/80 (99%)	78 (99%)	1 (1%)	69	85
16	QP	71/74 (96%)	71 (100%)	0	100	100
16	XP	71/74 (96%)	71 (100%)	0	100	100
17	QQ	94/97 (97%)	93 (99%)	1 (1%)	73	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	XQ	94/97 (97%)	93 (99%)	1 (1%)	73	87
18	QR	59/77 (77%)	59 (100%)	0	100	100
18	XR	59/77 (77%)	58 (98%)	1 (2%)	60	81
19	QS	72/80 (90%)	72 (100%)	0	100	100
19	XS	72/80 (90%)	72 (100%)	0	100	100
20	QT	74/82 (90%)	74 (100%)	0	100	100
20	XT	76/82 (93%)	75 (99%)	1 (1%)	69	85
21	QU	18/22 (82%)	18 (100%)	0	100	100
21	XU	18/22 (82%)	18 (100%)	0	100	100
27	RD	217/218 (100%)	217 (100%)	0	100	100
27	YD	217/218 (100%)	217 (100%)	0	100	100
28	RE	165/166 (99%)	165 (100%)	0	100	100
28	YE	165/166 (99%)	163 (99%)	2 (1%)	71	86
29	RF	161/166 (97%)	161 (100%)	0	100	100
29	YF	161/166 (97%)	160 (99%)	1 (1%)	86	94
30	RG	155/156 (99%)	155 (100%)	0	100	100
30	YG	155/156 (99%)	154 (99%)	1 (1%)	86	94
31	RH	145/148 (98%)	145 (100%)	0	100	100
31	YH	144/148 (97%)	142 (99%)	2 (1%)	67	84
32	RI	122/124 (98%)	122 (100%)	0	100	100
32	YI	122/124 (98%)	122 (100%)	0	100	100
33	RN	119/119 (100%)	117 (98%)	2 (2%)	60	81
33	YN	119/119 (100%)	119 (100%)	0	100	100
34	RO	100/100 (100%)	100 (100%)	0	100	100
34	YO	100/100 (100%)	100 (100%)	0	100	100
35	RP	116/116 (100%)	116 (100%)	0	100	100
35	YP	116/116 (100%)	115 (99%)	1 (1%)	78	89
36	RQ	111/111 (100%)	111 (100%)	0	100	100
36	YQ	111/111 (100%)	110 (99%)	1 (1%)	78	89
37	RR	101/101 (100%)	99 (98%)	2 (2%)	55	78
37	YR	101/101 (100%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	RS	87/88 (99%)	86 (99%)	1 (1%)	73	87
38	YS	87/88 (99%)	87 (100%)	0	100	100
39	RT	115/127 (91%)	115 (100%)	0	100	100
39	YT	115/127 (91%)	115 (100%)	0	100	100
40	RU	93/94 (99%)	93 (100%)	0	100	100
40	YU	93/94 (99%)	92 (99%)	1 (1%)	73	87
41	RV	82/82 (100%)	82 (100%)	0	100	100
41	YV	82/82 (100%)	81 (99%)	1 (1%)	71	86
42	RW	91/92 (99%)	91 (100%)	0	100	100
42	YW	91/92 (99%)	91 (100%)	0	100	100
43	RX	77/78 (99%)	77 (100%)	0	100	100
43	YX	77/78 (99%)	77 (100%)	0	100	100
44	RY	88/91 (97%)	87 (99%)	1 (1%)	73	87
44	YY	88/91 (97%)	88 (100%)	0	100	100
45	RZ	170/179 (95%)	169 (99%)	1 (1%)	86	94
45	YZ	162/179 (90%)	160 (99%)	2 (1%)	71	86
46	R0	62/67 (92%)	61 (98%)	1 (2%)	62	82
46	Y0	62/67 (92%)	62 (100%)	0	100	100
47	R1	82/83 (99%)	82 (100%)	0	100	100
47	Y1	82/83 (99%)	82 (100%)	0	100	100
48	R2	66/67 (98%)	65 (98%)	1 (2%)	65	83
48	Y2	66/67 (98%)	66 (100%)	0	100	100
49	R3	51/52 (98%)	49 (96%)	2 (4%)	32	64
49	Y3	51/52 (98%)	51 (100%)	0	100	100
50	R4	62/63 (98%)	62 (100%)	0	100	100
50	Y4	62/63 (98%)	61 (98%)	1 (2%)	62	82
51	R5	51/52 (98%)	50 (98%)	1 (2%)	55	78
51	Y5	50/52 (96%)	49 (98%)	1 (2%)	55	78
52	R6	51/52 (98%)	50 (98%)	1 (2%)	55	78
52	Y6	51/52 (98%)	48 (94%)	3 (6%)	19	54
53	R7	41/42 (98%)	40 (98%)	1 (2%)	49	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	Y7	41/42 (98%)	41 (100%)	0	100	100
54	R8	54/55 (98%)	54 (100%)	0	100	100
54	Y8	54/55 (98%)	54 (100%)	0	100	100
55	R9	34/34 (100%)	33 (97%)	1 (3%)	42	71
55	Y9	34/34 (100%)	34 (100%)	0	100	100
All	All	9676/10064 (96%)	9608 (99%)	68 (1%)	84	92

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

Mol	Chain	Res	Type
52	R6	44	ARG
4	XD	12	CYS
45	YZ	59	LEU
53	R7	47	ARG
2	XB	137	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
14	XN	52	GLN
15	XO	9	GLN
30	YG	58	GLN
35	RP	9	ASN
27	YD	166	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1494/1521 (98%)	292 (19%)	14 (0%)
1	XA	1498/1521 (98%)	287 (19%)	14 (0%)
22	QV	76/77 (98%)	18 (23%)	0
22	XV	76/77 (98%)	17 (22%)	1 (1%)
23	QX	7/26 (26%)	1 (14%)	1 (14%)
23	XX	10/26 (38%)	7 (70%)	1 (10%)
24	QY	13/18 (72%)	5 (38%)	2 (15%)
24	XY	15/18 (83%)	9 (60%)	1 (6%)
25	RA	2860/2915 (98%)	599 (20%)	21 (0%)
25	YA	2861/2915 (98%)	580 (20%)	19 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	RB	119/122 (97%)	17 (14%)	0
26	YB	119/122 (97%)	24 (20%)	0
56	ZA	1/3 (33%)	0	0
56	ZB	1/3 (33%)	1 (100%)	0
All	All	9150/9364 (97%)	1857 (20%)	74 (0%)

5 of 1857 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	11	G
1	QA	21	G
1	QA	22	G
1	QA	32	A
1	QA	39	G

5 of 74 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2321	G
1	XA	358	U
25	YA	2126	A
25	RA	2406	U
25	RA	2689	U

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
1	UR3	QA	1498	1	14,22,23	0.89	1 (7%)	15,32,35	0.79	1 (6%)
25	PSU	YA	2605	25	17,21,22	1.61	6 (35%)	20,30,33	3.18	9 (45%)
25	PSU	RA	1911	25	17,21,22	2.05	5 (29%)	20,30,33	3.14	7 (35%)
25	OMU	YA	2552	25,57	14,22,23	1.23	2 (14%)	14,31,34	1.00	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	QA	1404	1	15,22,23	1.18	1 (6%)	19,32,35	1.42	2 (10%)
25	5MU	YA	1915	25	15,22,23	1.05	2 (13%)	16,32,35	1.95	2 (12%)
1	MA6	QA	1519	1	19,26,27	0.93	1 (5%)	18,38,41	1.95	6 (33%)
56	PPU	ZB	3	25,56	32,40,41	0.89	0	33,57,60	1.57	7 (21%)
25	PSU	RA	1917	25	17,21,22	1.60	5 (29%)	20,30,33	2.91	5 (25%)
25	OMG	RA	2251	25,57,22	18,26,27	0.94	2 (11%)	20,38,41	2.00	5 (25%)
1	PSU	QA	516	1	17,21,22	1.90	5 (29%)	20,30,33	3.17	7 (35%)
1	4OC	QA	1402	1	16,23,24	0.77	0	17,32,35	1.33	1 (5%)
25	5MC	RA	1942	25	15,22,23	1.10	1 (6%)	19,32,35	1.72	4 (21%)
1	4OC	XA	1402	1	16,23,24	0.98	1 (6%)	17,32,35	1.28	2 (11%)
56	PPU	ZA	3	25,57,56	32,40,41	0.96	1 (3%)	33,57,60	1.82	7 (21%)
1	G7M	XA	527	1	20,26,27	2.53	4 (20%)	20,39,42	1.98	4 (20%)
1	2MG	QA	1207	1	19,26,27	1.02	2 (10%)	21,38,41	2.05	6 (28%)
25	PSU	YA	1917	25	17,21,22	1.72	5 (29%)	20,30,33	2.89	6 (30%)
1	5MC	QA	1400	1	15,22,23	1.23	1 (6%)	19,32,35	1.33	3 (15%)
25	2MA	RA	2503	25,57	17,25,26	1.22	1 (5%)	19,37,40	2.10	3 (15%)
25	PSU	RA	2605	25	17,21,22	2.61	6 (35%)	20,30,33	2.90	6 (30%)
12	0TD	XL	92	12	4,9,10	0.55	0	3,11,13	1.75	1 (33%)
1	5MC	QA	967	1	15,22,23	1.23	1 (6%)	19,32,35	1.44	3 (15%)
25	OMU	RA	2552	25	14,22,23	1.19	2 (14%)	14,31,34	1.46	2 (14%)
25	PSU	YA	1911	25	17,21,22	2.41	5 (29%)	20,30,33	3.24	8 (40%)
1	5MC	XA	967	1	15,22,23	1.13	1 (6%)	19,32,35	1.45	4 (21%)
1	PSU	XA	516	1,57	17,21,22	1.60	5 (29%)	20,30,33	3.47	7 (35%)
1	5MC	XA	1404	1	15,22,23	1.12	1 (6%)	19,32,35	1.56	4 (21%)
1	MA6	XA	1518	1	19,26,27	1.00	1 (5%)	18,38,41	1.77	4 (22%)
25	2MA	YA	2503	25,57	17,25,26	1.28	1 (5%)	19,37,40	2.20	3 (15%)
1	MA6	QA	1518	1	19,26,27	0.88	1 (5%)	18,38,41	1.97	7 (38%)
1	MA6	XA	1519	1	19,26,27	0.82	0	18,38,41	2.10	6 (33%)
1	G7M	QA	527	1	20,26,27	2.58	4 (20%)	20,39,42	1.97	4 (20%)
25	5MC	YA	1962	25	15,22,23	1.01	1 (6%)	19,32,35	1.81	4 (21%)
1	UR3	XA	1498	1	14,22,23	0.98	1 (7%)	15,32,35	0.71	0
25	OMG	YA	2251	25,57,22	18,26,27	1.04	1 (5%)	20,38,41	2.06	7 (35%)
1	M2G	QA	966	1	20,27,28	1.16	3 (15%)	22,40,43	2.04	6 (27%)
25	5MC	YA	1942	25	15,22,23	1.19	1 (6%)	19,32,35	1.87	4 (21%)
25	OMC	RA	1920	25	15,22,23	0.92	0	17,31,34	2.06	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	QA	1407	1	15,22,23	1.10	1 (6%)	19,32,35	1.44	2 (10%)
25	OMC	YA	1920	25	15,22,23	0.93	0	17,31,34	1.88	4 (23%)
25	5MU	RA	1915	25	15,22,23	1.06	2 (13%)	16,32,35	2.01	1 (6%)
1	5MC	XA	1400	1	15,22,23	1.17	1 (6%)	19,32,35	1.42	3 (15%)
12	0TD	QL	92	12	4,9,10	0.62	0	3,11,13	1.79	1 (33%)
1	5MC	XA	1407	1	15,22,23	1.12	2 (13%)	19,32,35	1.61	5 (26%)
1	M2G	XA	966	1	20,27,28	1.15	2 (10%)	22,40,43	2.20	7 (31%)
25	5MU	RA	1939	25,57	15,22,23	0.95	2 (13%)	16,32,35	1.88	2 (12%)
25	5MC	RA	1962	25,57	15,22,23	0.95	1 (6%)	19,32,35	1.79	4 (21%)
1	2MG	XA	1207	1	19,26,27	0.98	1 (5%)	21,38,41	2.24	6 (28%)
25	5MU	YA	1939	25,57	15,22,23	1.24	3 (20%)	16,32,35	1.84	2 (12%)

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
1	UR3	QA	1498	1	-	2/5/25/26	0/2/2/2
25	PSU	YA	2605	25	-	0/7/25/26	0/2/2/2
25	PSU	RA	1911	25	-	0/7/25/26	0/2/2/2
25	OMU	YA	2552	25,57	-	2/7/27/28	0/2/2/2
1	5MC	QA	1404	1	-	0/5/25/26	0/2/2/2
25	5MU	YA	1915	25	-	3/5/25/26	0/2/2/2
1	MA6	QA	1519	1	-	5/7/29/30	0/3/3/3
56	PPU	ZB	3	25,56	-	5/21/43/44	0/4/4/4
25	PSU	RA	1917	25	-	1/7/25/26	0/2/2/2
25	OMG	RA	2251	25,57,22	-	0/5/27/28	0/3/3/3
1	PSU	QA	516	1	-	0/7/25/26	0/2/2/2
1	4OC	QA	1402	1	-	2/9/29/30	0/2/2/2
25	5MC	RA	1942	25	-	0/5/25/26	0/2/2/2
1	4OC	XA	1402	1	-	2/9/29/30	0/2/2/2
56	PPU	ZA	3	25,57,56	-	5/21/43/44	0/4/4/4
1	G7M	XA	527	1	-	2/3/25/26	0/3/3/3
1	2MG	QA	1207	1	-	0/5/27/28	0/3/3/3
25	PSU	YA	1917	25	-	0/7/25/26	0/2/2/2
1	5MC	QA	1400	1	-	3/5/25/26	0/2/2/2
25	2MA	RA	2503	25,57	-	1/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PSU	RA	2605	25	-	0/7/25/26	0/2/2/2
12	0TD	XL	92	12	-	1/3/12/14	-
1	5MC	QA	967	1	-	0/5/25/26	0/2/2/2
25	OMU	RA	2552	25	-	3/7/27/28	0/2/2/2
25	PSU	YA	1911	25	-	0/7/25/26	0/2/2/2
1	5MC	XA	967	1	-	0/5/25/26	0/2/2/2
1	PSU	XA	516	1,57	-	1/7/25/26	0/2/2/2
1	5MC	XA	1404	1	-	0/5/25/26	0/2/2/2
1	MA6	XA	1518	1	-	1/7/29/30	0/3/3/3
25	2MA	YA	2503	25,57	-	2/3/25/26	0/3/3/3
1	MA6	QA	1518	1	-	1/7/29/30	0/3/3/3
1	MA6	XA	1519	1	-	6/7/29/30	0/3/3/3
1	G7M	QA	527	1	-	2/3/25/26	0/3/3/3
25	5MC	YA	1962	25	-	2/5/25/26	0/2/2/2
1	UR3	XA	1498	1	-	0/5/25/26	0/2/2/2
25	OMG	YA	2251	25,57,22	-	0/5/27/28	0/3/3/3
1	M2G	QA	966	1	-	0/7/29/30	0/3/3/3
25	5MC	YA	1942	25	-	0/5/25/26	0/2/2/2
25	OMC	RA	1920	25	-	3/7/27/28	0/2/2/2
1	5MC	QA	1407	1	-	0/5/25/26	0/2/2/2
25	OMC	YA	1920	25	-	3/7/27/28	0/2/2/2
25	5MU	RA	1915	25	-	2/5/25/26	0/2/2/2
1	5MC	XA	1400	1	-	4/5/25/26	0/2/2/2
12	0TD	QL	92	12	-	3/3/12/14	-
1	5MC	XA	1407	1	-	0/5/25/26	0/2/2/2
1	M2G	XA	966	1	-	2/7/29/30	0/3/3/3
25	5MU	RA	1939	25,57	-	0/5/25/26	0/2/2/2
25	5MC	RA	1962	25,57	-	2/5/25/26	0/2/2/2
1	2MG	XA	1207	1	-	0/5/27/28	0/3/3/3
25	5MU	YA	1939	25,57	-	0/5/25/26	0/2/2/2

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	RA	2605	PSU	C5-C1'	-8.78	1.44	1.52
25	YA	1911	PSU	C5-C1'	-8.22	1.45	1.52
1	QA	527	G7M	C8-N9	7.01	1.46	1.33
1	XA	527	G7M	C8-N9	6.96	1.46	1.33
1	QA	527	G7M	C8-N7	6.54	1.45	1.33

The worst 5 of 211 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	516	PSU	N1-C2-N3	-10.36	120.19	128.43
1	QA	516	PSU	N1-C2-N3	-9.17	121.14	128.43
25	YA	1911	PSU	N1-C2-N3	-8.55	121.63	128.43
25	YA	2605	PSU	N1-C2-N3	-8.24	121.88	128.43
25	YA	1917	PSU	N1-C2-N3	-8.02	122.06	128.43

There are no chirality outliers.

5 of 71 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	QA	1498	UR3	C3'-C4'-C5'-O5'
25	YA	1915	5MU	C2'-C1'-N1-C6
1	QA	1519	MA6	O4'-C4'-C5'-O5'
1	QA	1519	MA6	C3'-C4'-C5'-O5'
1	QA	1519	MA6	C5-C6-N6-C10

There are no ring outliers.

26 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	YA	2552	OMU	2	0
1	QA	1519	MA6	1	0
56	ZB	3	PPU	4	0
25	RA	2251	OMG	2	0
1	QA	1402	4OC	1	0
25	RA	1942	5MC	1	0
1	XA	1402	4OC	1	0
56	ZA	3	PPU	10	0
25	YA	1917	PSU	1	0
1	QA	1400	5MC	1	0
25	RA	2503	2MA	2	0
12	XL	92	0TD	1	0
25	RA	2552	OMU	3	0
1	XA	967	5MC	1	0
1	XA	1404	5MC	2	0
1	XA	1518	MA6	1	0
25	YA	2503	2MA	1	0
25	YA	1962	5MC	1	0
25	YA	2251	OMG	1	0
1	QA	966	M2G	1	0
25	RA	1920	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	YA	1920	OMC	2	0
12	QL	92	0TD	1	0
1	XA	1407	5MC	1	0
1	XA	1207	2MG	2	0
25	YA	1939	5MU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1328 ligands modelled in this entry, 1326 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	XD	302	4	0,12,12	0.00	-	-		
58	SF4	QD	303	4	0,12,12	0.00	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	XD	302	4	-	-	0/6/5/5
58	SF4	QD	303	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	XD	302	SF4	4	0
58	QD	303	SF4	6	0

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.