



wwPDB X-ray Structure Validation Summary Report

Nov 6, 2023 – 08:47 PM EST

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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)
Xtrriage (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) : 2.36

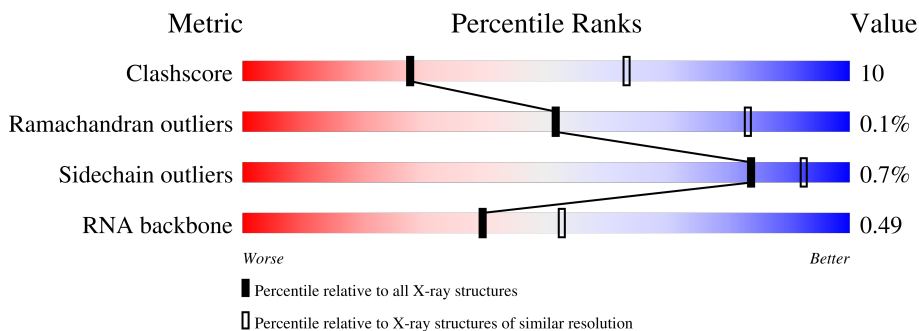
1 Overall quality at a glance

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 of 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	

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Mol	Chain	Length	Quality of chain
4	QD	209	56% 37% 6%
4	XD	209	70% 27%
5	QE	162	60% 30% 9%
5	XE	162	68% 20% 9%
6	QF	101	73% 25%
6	XF	101	76% 23%
7	QG	156	63% 33%
7	XG	156	72% 25%
8	QH	138	59% 38%
8	XH	138	68% 30%
9	QI	128	53% 41% 5%
9	XI	128	62% 35%
10	QJ	105	53% 39% 6%
10	XJ	105	64% 28% 9%
11	QK	129	57% 28% 12%
11	XK	129	59% 26% 12%
12	QL	132	65% 23% 8%
12	XL	132	65% 25% 8%
13	QM	126	52% 36% 8%
13	XM	126	67% 21% 10%
14	QN	61	49% 46%
14	XN	61	67% 30%
15	QO	89	83% 12%
15	XO	89	83% 15%
16	QP	88	58% 34% 7%

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Mol	Chain	Length	Quality of chain
16	XP	88	60% 32% 7%
17	QQ	105	67% 24% 6%
17	XQ	105	65% 29% 6%
18	QR	88	56% 22% 23%
18	XR	88	61% 15% 23%
19	QS	93	61% 26% 11%
19	XS	93	57% 30% 11%
20	QT	106	64% 24% 9%
20	XT	106	62% 30% 8%
21	QU	27	41% 37% 7% 15%
21	XU	27	44% 41% 15%
22	QV	77	44% 40% 10% 5%
22	XV	77	40% 48% 10% 2%
23	QX	26	12% 19% 69%
23	XX	26	12% 15% 12% 58%
24	QY	18	33% 11% 33% 22%
24	XY	18	17% 50% 11% 11% 11%
25	RA	2915	41% 43% 13% 2%
25	YA	2915	41% 40% 15% 4%
26	RB	122	44% 45% 9% 2%
26	YB	122	58% 29% 10% 3%
27	RD	276	74% 25% 1%
27	YD	276	76% 23% 1%
28	RE	206	68% 28% 4%
28	YE	206	66% 31% 3%

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Mol	Chain	Length	Quality of chain
29	RF	210	
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	


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Mol	Chain	Length	Quality of chain
41	YV	101	72% 26% ..
42	RW	113	77% 22% .
42	YW	113	79% 19% ..
43	RX	96	72% 25% ..
43	YX	96	86% 12% .
44	RY	110	75% 19% . .
44	YY	110	68% 27% . .
45	RZ	206	70% 24% . 5%
45	YZ	206	62% 25% . 11%
46	R0	85	67% 22% . 9%
46	Y0	85	73% 16% . 9%
47	R1	98	76% 21% ..
47	Y1	98	77% 22% .
48	R2	72	72% 25% .
48	Y2	72	82% 15% .
49	R3	60	68% 28% ..
49	Y3	60	68% 27% ..
50	R4	71	58% 38% ..
50	Y4	71	58% 37% . .
51	R5	60	80% 18% .
51	Y5	60	80% 17% .
52	R6	54	70% 28% .
52	Y6	54	65% 31% ..
53	R7	49	59% 37% ..
53	Y7	49	76% 20% ..

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Mol	Chain	Length	Quality of chain
54	R8	65	 72% 26% .
54	Y8	65	 72% 25% ..
55	R9	37	 59% 38% .
55	Y9	37	 73% 27%
56	ZA	3	 33% 67%
56	ZB	3	 33% 67%

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
			Total	C	N	O	P			
1	QA	1500	Total 32246	C 14358	N 5975	O 10413	P 1500	0	0	0
1	XA	1504	Total 32331	C 14396	N 5990	O 10441	P 1504	0	0	0

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

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

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

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

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

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

- 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
			Total	C	N	O	S			
10	XJ	96	777	487	153	136	1	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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 tRNAfMet.

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
			Total	C	N	O	P			
26	YB	120	2573	1146	476	832	119	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S			
42	YW	112	890	560	175	153	2	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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	QC	1	Total	Mg	0	0
			1	1		
57	QD	2	Total	Mg	0	0
			2	2		
57	QE	2	Total	Mg	0	0
			2	2		
57	QL	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QM	2	Total 2	Mg 2	0	0
57	QN	2	Total 2	Mg 2	0	0
57	QO	1	Total 1	Mg 1	0	0
57	QV	3	Total 3	Mg 3	0	0
57	RA	414	Total 414	Mg 414	0	0
57	RB	8	Total 8	Mg 8	0	0
57	RD	5	Total 5	Mg 5	0	0
57	RE	5	Total 5	Mg 5	0	0
57	RF	5	Total 5	Mg 5	0	0
57	RN	2	Total 2	Mg 2	0	0
57	RO	1	Total 1	Mg 1	0	0
57	RP	2	Total 2	Mg 2	0	0
57	RQ	1	Total 1	Mg 1	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RV	1	Total 1	Mg 1	0	0
57	RW	1	Total 1	Mg 1	0	0
57	RX	1	Total 1	Mg 1	0	0
57	RZ	1	Total 1	Mg 1	0	0
57	R0	2	Total 2	Mg 2	0	0
57	R1	1	Total 1	Mg 1	0	0
57	R3	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	R5	1	Total 1	Mg 1	0	0
57	R6	1	Total 1	Mg 1	0	0
57	R7	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	R9	1	Total 1	Mg 1	0	0
57	XA	128	Total 128	Mg 128	0	0
57	XD	1	Total 1	Mg 1	0	0
57	XJ	1	Total 1	Mg 1	0	0
57	XK	2	Total 2	Mg 2	0	0
57	XN	1	Total 1	Mg 1	0	0
57	XV	1	Total 1	Mg 1	0	0
57	XX	1	Total 1	Mg 1	0	0
57	YA	544	Total 544	Mg 544	0	0
57	YB	8	Total 8	Mg 8	0	0
57	YD	8	Total 8	Mg 8	0	0
57	YE	7	Total 7	Mg 7	0	0
57	YF	1	Total 1	Mg 1	0	0
57	YG	1	Total 1	Mg 1	0	0
57	YP	3	Total 3	Mg 3	0	0
57	YQ	2	Total 2	Mg 2	0	0
57	YR	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	YT	1	Total Mg 1 1	0	0
57	YU	1	Total Mg 1 1	0	0
57	YV	1	Total Mg 1 1	0	0
57	YW	1	Total Mg 1 1	0	0
57	YX	1	Total Mg 1 1	0	0
57	Y0	1	Total Mg 1 1	0	0
57	Y1	3	Total Mg 3 3	0	0
57	Y3	1	Total Mg 1 1	0	0
57	Y5	1	Total Mg 1 1	0	0
57	Y6	1	Total Mg 1 1	0	0
57	Y7	1	Total Mg 1 1	0	0
57	Y8	1	Total Mg 1 1	0	0
57	Y9	1	Total Mg 1 1	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	QN	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	XN	1	Total	Zn	0	0
			1	1		
59	Y4	1	Total	Zn	0	0
			1	1		

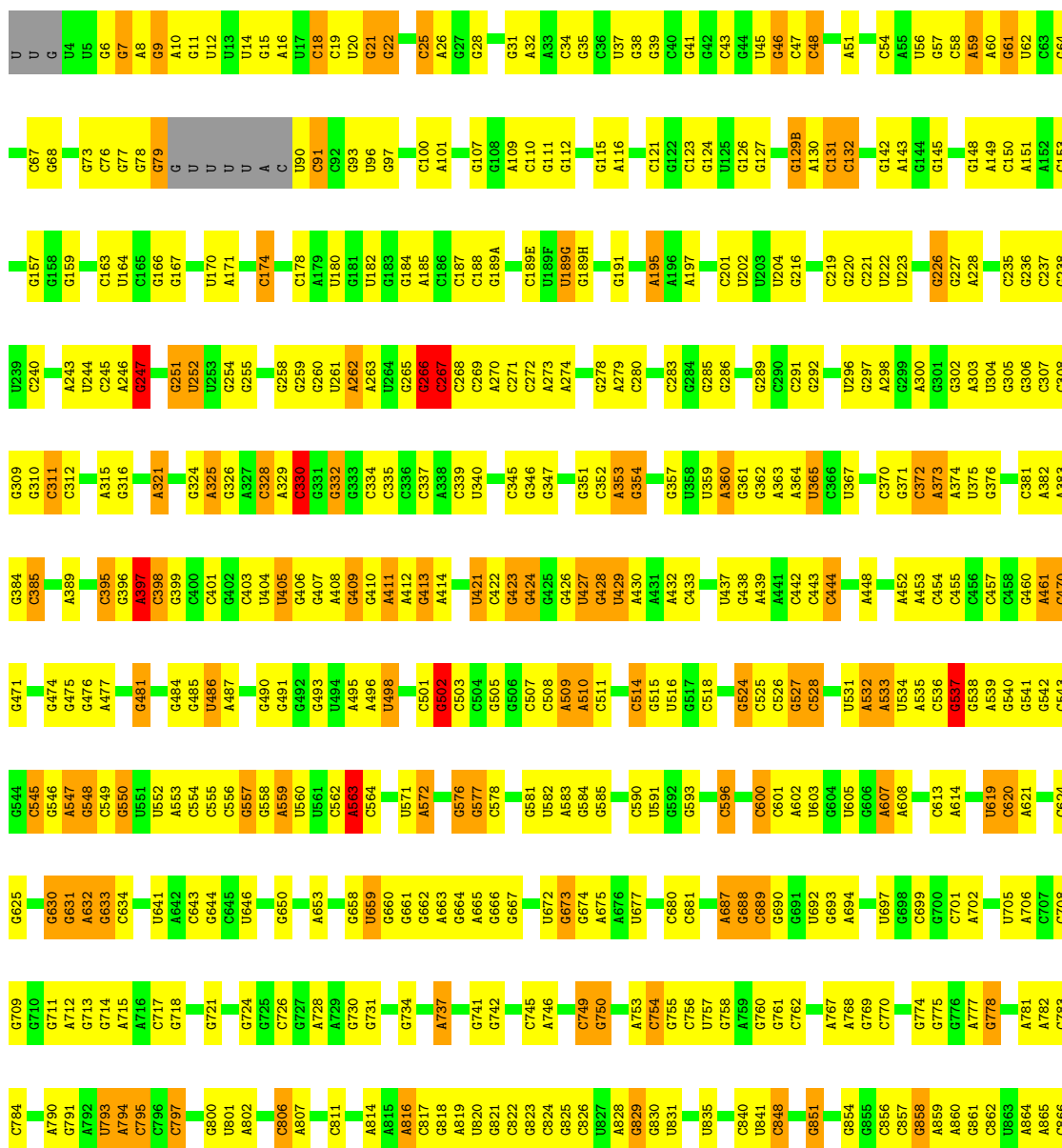
3 Residue-property plots [i](#)

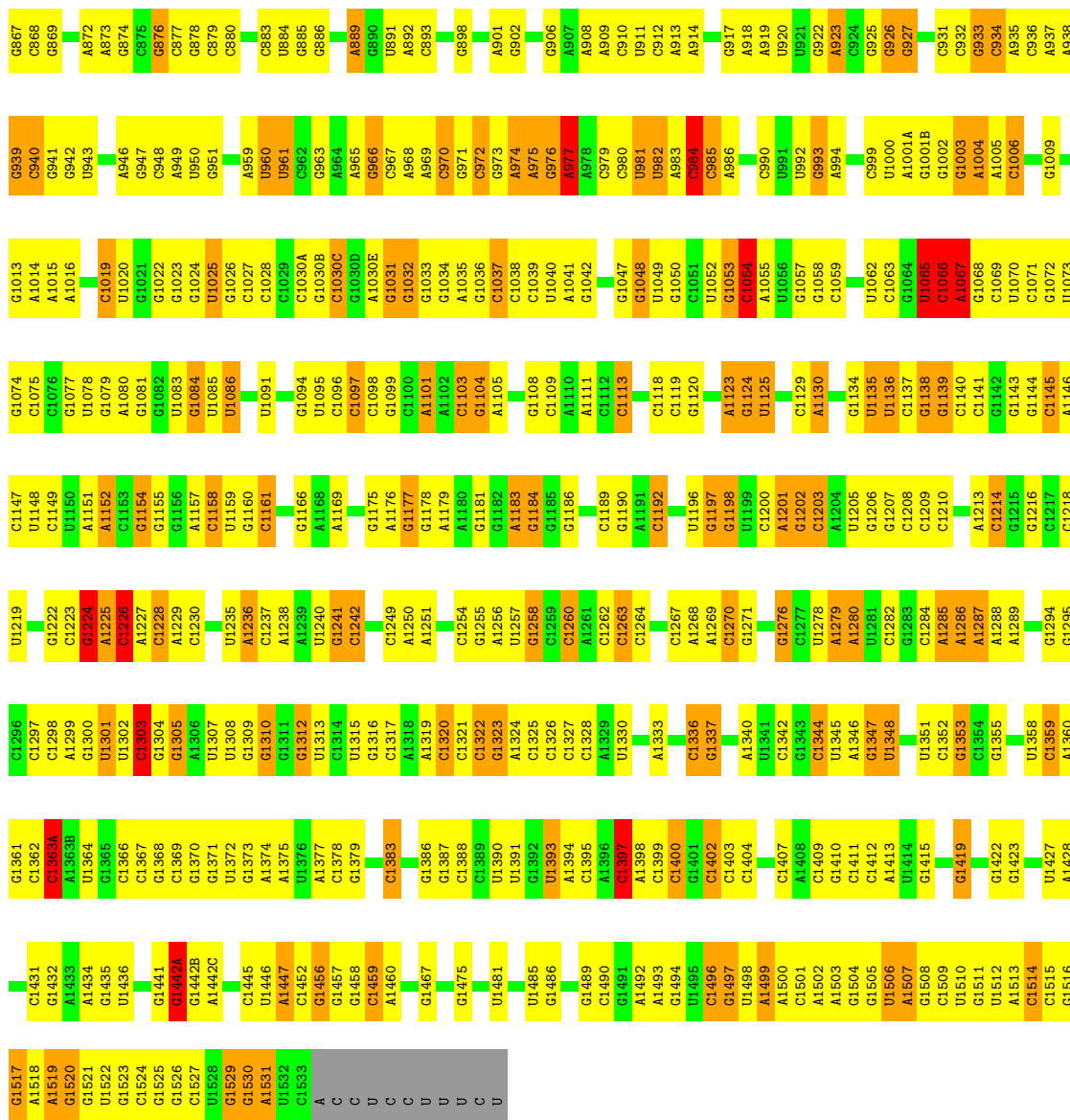
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

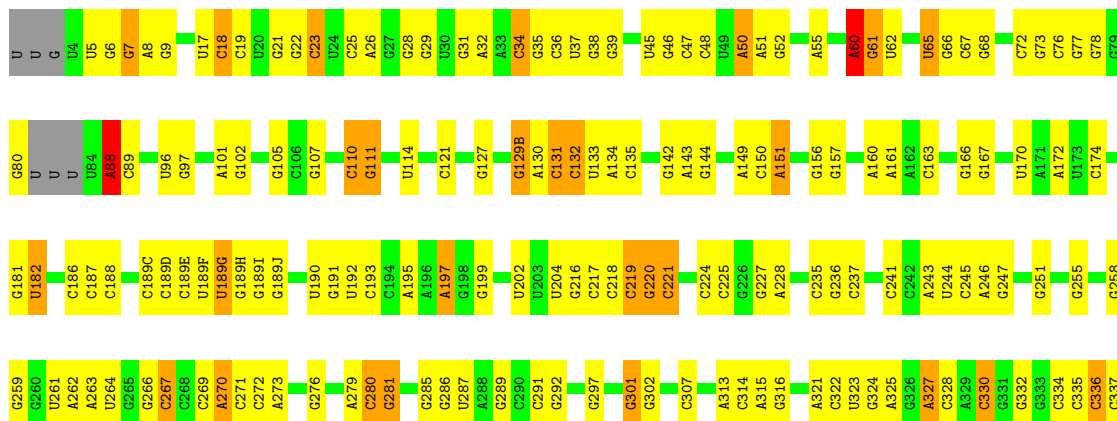
- Molecule 1: 16S rRNA

Chain QA: 





• Molecule 1: 16S rRNA

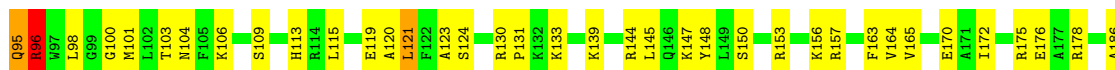


C1430	C1431	C1432	A1363A	A1363B	A1433	A1434	G1365	G1366	G1367	G1368	G1369	G1370	G1371	G1372	G1373	A1447	A1448	G1452	G1456	G1457	G1458	G1459	G1464	G1469	G1470	G1475	G1476	G1487	G1488	G1489	G1490	G1491	G1492	G1493	G1494	G1497	G1498	G1499	A1500	A1501	A1502	A1503	G1504	G1505	A1506	A1507	U1510	G1511	A1512	A1513	C1514						
C1218	U1219	G1220	G1221	G1222	G1223	G1224	A1225	G1226	A1227	G1228	G1229	G1230	G1231	A1236	A1237	A1238	A1239	U1240	G1241	G1244	A1245	G1246	U1247	A1248	G1249	G1250	G1251	G1255	A1256	G1257	G1258	G1259	A1260	A1261	G1262	G1263	G1264	G1265	G1266	G1267	A1268	A1269	G1270	G1271	G1272	G1273	G1274	A1275	G1276	G1277	A1278	A1279	A1280	G1281	G1282	A1285	A1286
A1287	A1288	A1289	A1363B	U1290	U1291	U1292	G1293	G1294	G1295	G1296	G1297	G1298	G1299	G1300	U1301	U1302	G1303	G1304	G1305	A1306	U1307	U1308	G1309	G1312	U1313	U1314	U1315	U1316	U1317	U1318	U1319	A1320	G1323	G1324	G1325	G1326	A1329	U1330	G1331	A1340	G1343	G1344	U1345	U1346	G1347	U1348	G1352	G1353	G1422	G1423	C1424	U1427	A1428	C1429			
G1361	C1362	C1363A	A1363B	U1364	U1365	U1366	G1367	G1368	G1369	G1370	G1371	G1372	G1373	A1374	A1375	U1380	U1381	U1382	C1383	C1384	C1385	C1386	C1387	U1390	U1391	G1392	C1395	A1396	A1397	A1398	G1399	C1400	G1488	G1489	C1402	C1403	G1404	G1405	U1406	C1407	C1408	C1409	G1410	G1411	C1412	C1413	U1414	G1419	G1422	G1423	C1424	U1427	A1428	C1429			
U1126	G1127	C1128	G1129	A1130	C1131	G1132	G1133	G1134	G1135	G1136	G1137	G1138	G1139	G1140	G1141	G1142	G1143	C1147	U1148	A1152	C1158	U1159	G1160	C1161	G1164	A1170	G1178	A1179	A1183	G1184	G1185	G1186	G1187	G1188	G1189	A1190	A1191	A1192	U1196	G1197	C1200	A1201	G1202	G1203	A1204	G1207	C1208	C1209	C1210	U1211	U1212	A1213	G1214	G1215			
C1054	A1055	G1056	A1057	C1058	G1059	G1060	G1061	U1062	U1065	C1066	C1067	G1068	C1069	U1070	C1071	G1072	U1073	G1074	C1075	U1078	U1079	A1080	G1081	U1085	U1086	A1092	A1093	G1094	U1095	C1096	C1097	C1098	C1099	C1100	A1101	A1102	C1103	G1104	G1108	C1109	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	G1120	U1121	U1122	A1123	G1124	U1125			
G902	G903	G906	A907	A908	A909	G910	G911	G912	A913	A914	A918	A919	A920	U921	U922	U923	C924	G925	G926	G927	G928	G929	C931	C932	G933	C934	A935	C936	A946	G947	A948	U949	U950	C951	U952	G953	G954	U955	U960	U961	G966	A968	A969	C970	G971	C972	G973	A974	A975	U976	A977	A978	C979	C980			
C811	C812	U813	A814	C817	C818	A819	U820	G821	G822	A823	C824	A828	G829	U833	C834	U835	G836	C840	U841	C848	G851	A852	G853	G854	A855	A859	A860	G861	C862	U863	A864	A865	C866	C867	G868	G869	A870	U871	A872	A873	A874	C877	G878	C883	U884	U889	A891	A892	C893	A900	A901						
A737	C738	U739	G740	G741	G742	U743	G744	G745	A746	G747	G748	G750	G754	G755	G756	U757	G761	G762	G763	A766	A767	A694	A695	U603	U609	A610	A611	C618	A619	C620	A621	A622	C623	G714	A715	A716	G717	G718	A721	G722	A723	U724	G725	A728	G803	U804	C805	G806	A807	G808	G809	C810					
A653	A653	G661	G662	A663	G664	A665	G666	G673	G674	A675	A676	U677	U678	G679	C680	G683	A687	G688	G689	U692	G693	G694	G695	A696	A697	A698	A699	A702	C707	G711	A712	G713	G714	A715	A716	G717	G718	A721	G722	A723	U724	G725	A728	G803	U804	C805	G806	A807	G808	G809	C810						
A338	C339	C342	U343	A344	C345	C346	G347	G348	A349	G350	G351	C352	A353	C354	C355	A356	G357	U358	U359	A360	G361	U365	C366	U367	U368	G371	C372	A373	A374	U375	G376	G377	G378	C379	G380	C381	A382	A383	G384	C385	C386	U387	G388	A389	C390	G391	G392	G396	A397	C398	G399	C400	C401	G402	C403		
U404	U405	G406	G407	G408	G409	G410	A411	G412	G413	G416	C417	U421	C422	G423	G424	G425	G426	G428	U429	A430	A431	A432	C433	U434	C435	C436	U437	G438	A439	U442	A443	A444	A448	A449	A452	A453	C454	G455	A461	C470	G471	A472	G473	G474	G475	G476	A477	C479	A480	G481	A482	G483	G485				
U486	A487	C488	G489	G490	A495	G496	U498	C501	A501	G502	C503	C504	G505	A509	A510	G511	U512	C513	C514	A515	U516	C517	C518	C519	A520	G521	G524	C525	C526	G527	C528	A532	A533	U534	A535	A539	G540	C543	G544	C545	G546	A547	U552	A553	C554	C555	C556	G557	G558	A559	U560	C561					



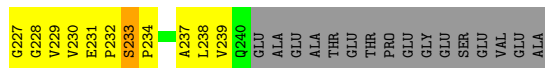
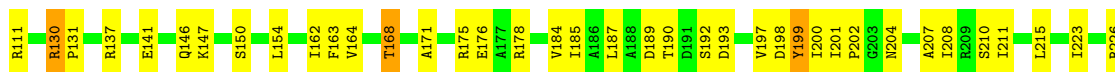
- Molecule 2: 30S ribosomal protein S2

Chain QB: 56% 34% 8%



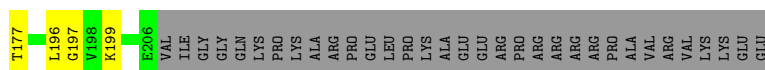
- Molecule 2: 30S ribosomal protein S2

Chain XB: 61% 29% 8%



- Molecule 3: 30S ribosomal protein S3

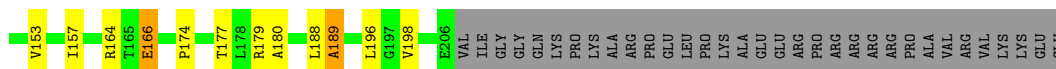
Chain QC: 50% 32% 14%



- Molecule 3: 30S ribosomal protein S3

Chain XC: 67% 17% 14%

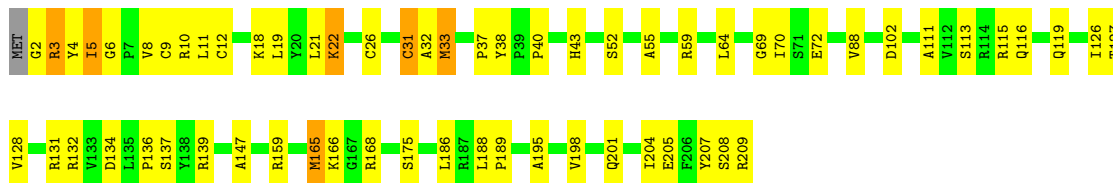




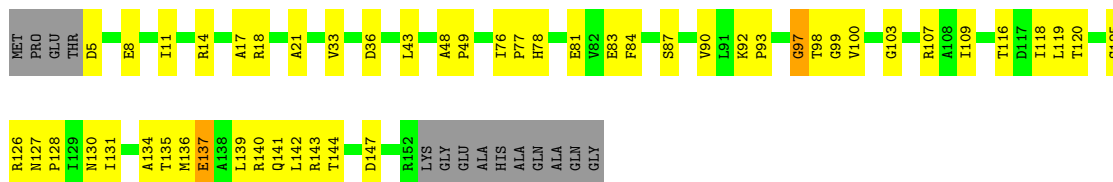
- Molecule 4: 30S ribosomal protein S4



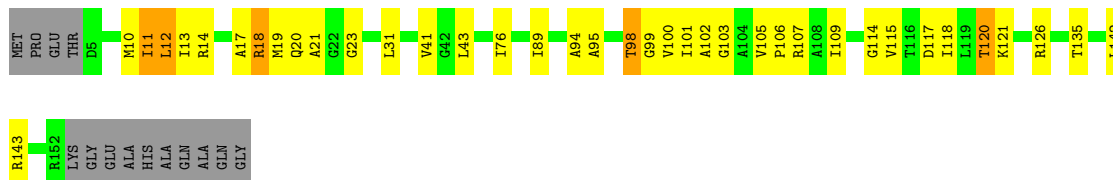
- Molecule 4: 30S ribosomal protein S4



- Molecule 5: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S5




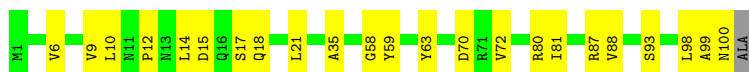
- Molecule 6: 30S ribosomal protein S6

Chain QF:  73% 25% ..



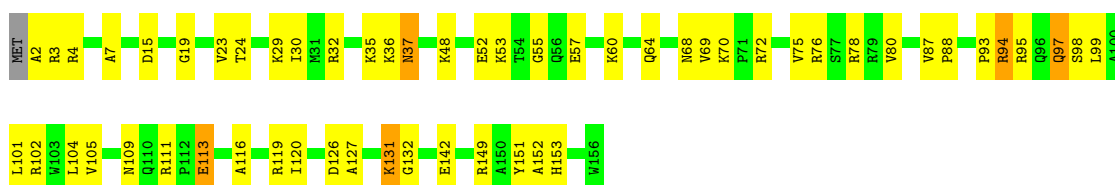
- Molecule 6: 30S ribosomal protein S6

Chain XF:  76% 23% ..



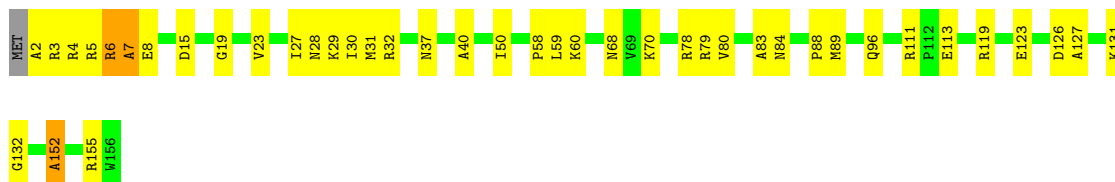
- Molecule 7: 30S ribosomal protein S7

Chain QG:  63% 33% ..



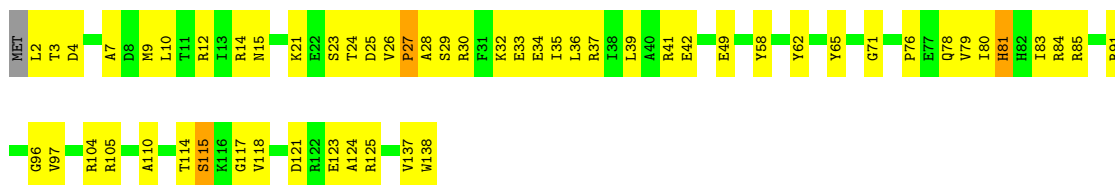
- Molecule 7: 30S ribosomal protein S7

Chain XG:  72% 25% ..



- Molecule 8: 30S ribosomal protein S8

Chain QH:  59% 38% ..



- Molecule 8: 30S ribosomal protein S8

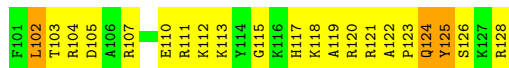
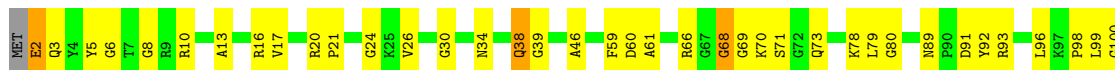
Chain XH:  68% 30% ..





- Molecule 9: 30S ribosomal protein S9

Chain QI: 53% 41% 5%



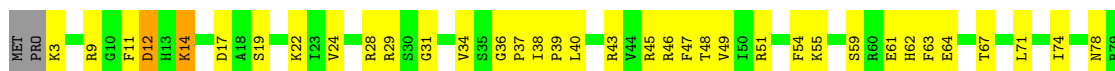
- Molecule 9: 30S ribosomal protein S9

Chain XI: 62% 35% ...



- Molecule 10: 30S ribosomal protein S10

Chain QJ: 53% 39% 6%



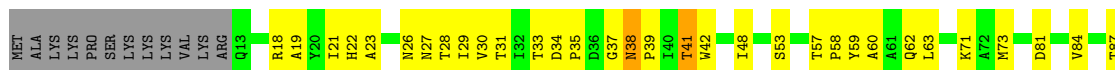
- Molecule 10: 30S ribosomal protein S10

Chain XJ: 64% 28% 9%



- Molecule 11: 30S ribosomal protein S11

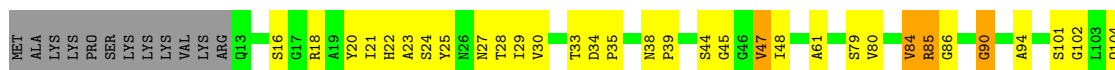
Chain QK: 57% 28% 12%





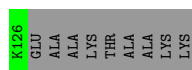
- Molecule 11: 30S ribosomal protein S11

Chain XK: 59% 26% 12%



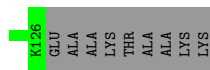
- Molecule 12: 30S ribosomal protein S12

Chain QL: 65% 23% 8%



- Molecule 12: 30S ribosomal protein S12

Chain XL: 65% 25% 8%



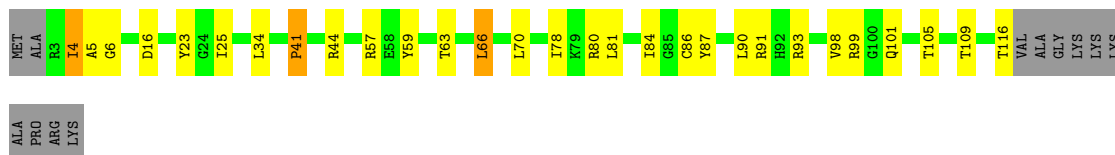
- Molecule 13: 30S ribosomal protein S13

Chain QM: 52% 36% 8%



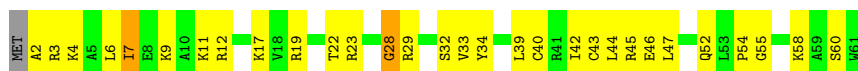
- Molecule 13: 30S ribosomal protein S13

Chain XM: 67% 21% 10%



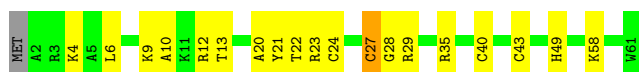
- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN: 49% 46%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN: 67% 30%



- Molecule 15: 30S ribosomal protein S15

Chain QO: 83% 12%



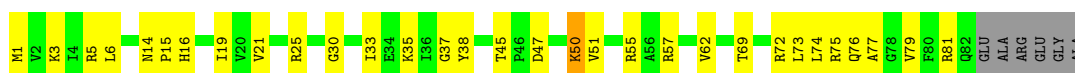
- Molecule 15: 30S ribosomal protein S15

Chain XO: 83% 15%



- Molecule 16: 30S ribosomal protein S16

Chain QP: 58% 34% 7%



- Molecule 16: 30S ribosomal protein S16

Chain XP: 60% 32% 7%



- Molecule 17: 30S ribosomal protein S17

Chain QQ:  67% 24% 6%



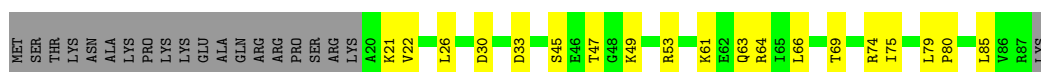
- Molecule 17: 30S ribosomal protein S17

Chain XQ:  65% 29% 6%



- Molecule 18: 30S ribosomal protein S18

Chain QR:  56% 22% 23%



- Molecule 18: 30S ribosomal protein S18

Chain XR:  61% 15% 23%



- Molecule 19: 30S ribosomal protein S19

Chain QS:  61% 26% 11%



- Molecule 19: 30S ribosomal protein S19

Chain XS:  57% 30% 11%



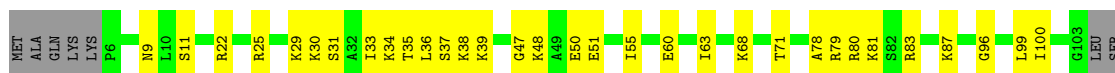
- Molecule 20: 30S ribosomal protein S20

Chain QT:  64% 24% 9%



- Molecule 20: 30S ribosomal protein S20

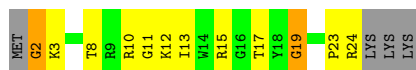
Chain XT:  62% 30% 8%



ALA

- Molecule 21: 30S ribosomal protein Thx

Chain QU:  41% 37% 7% 15%



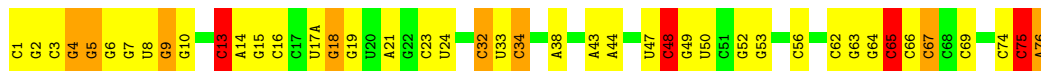
- Molecule 21: 30S ribosomal protein Thx

Chain XU:  44% 41% 15%



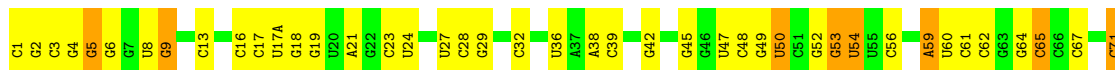
- Molecule 22: P-site tRNAfMet

Chain QV:  44% 40% 10% 5%



- Molecule 22: P-site tRNAfMet

Chain XV:  40% 48% 10% 2%



A72, A73, C74, C75, A76

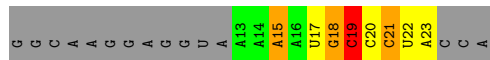
- Molecule 23: mRNA

Chain QX:  12% 19% 69%

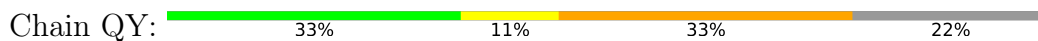


- Molecule 23: mRNA

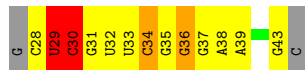
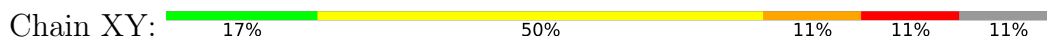
Chain XX:  12% 15% 12% 58%



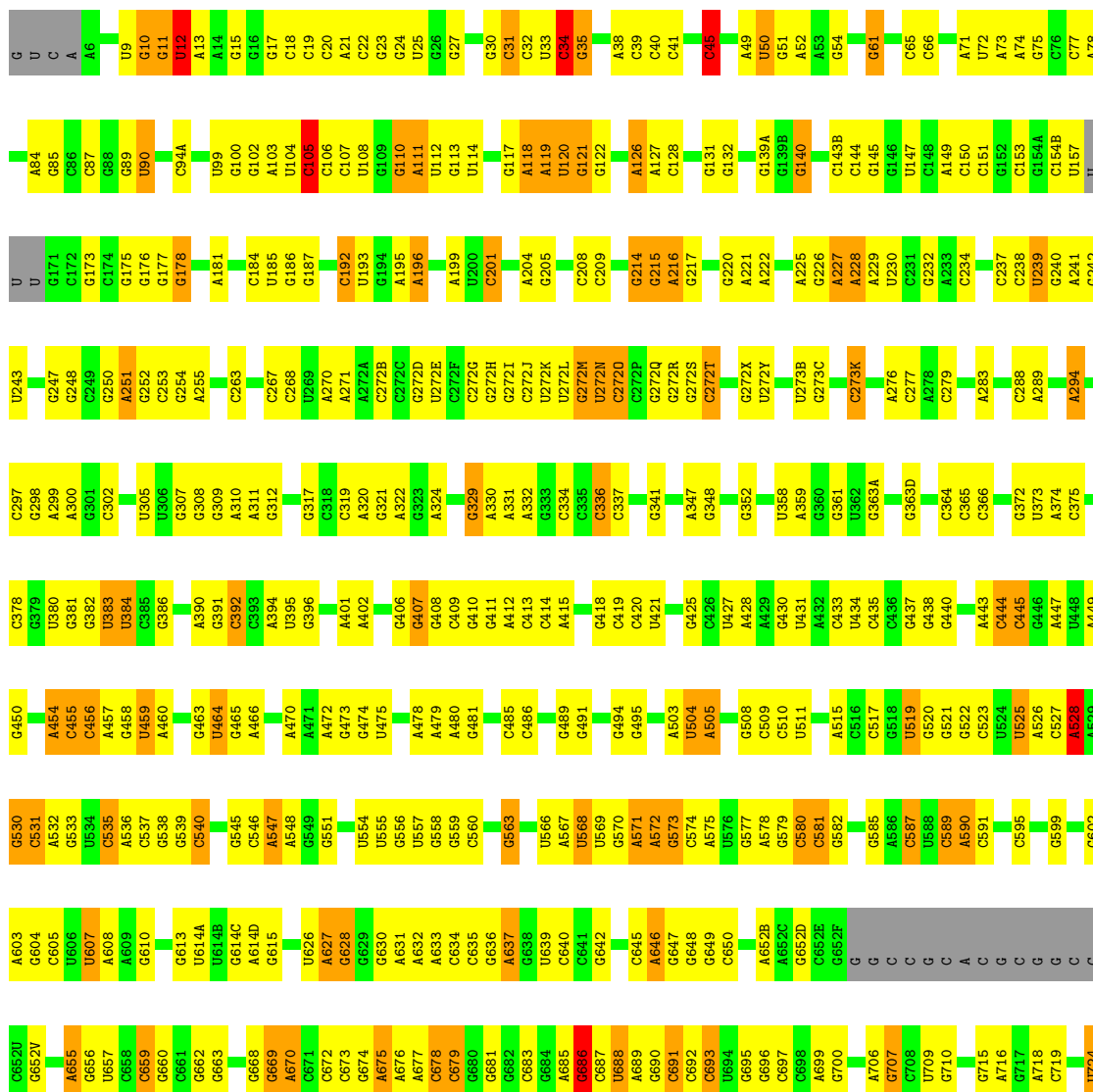
• Molecule 24: A-site ASLSufA6 A37.5



• Molecule 24: A-site ASLSufA6 A37.5

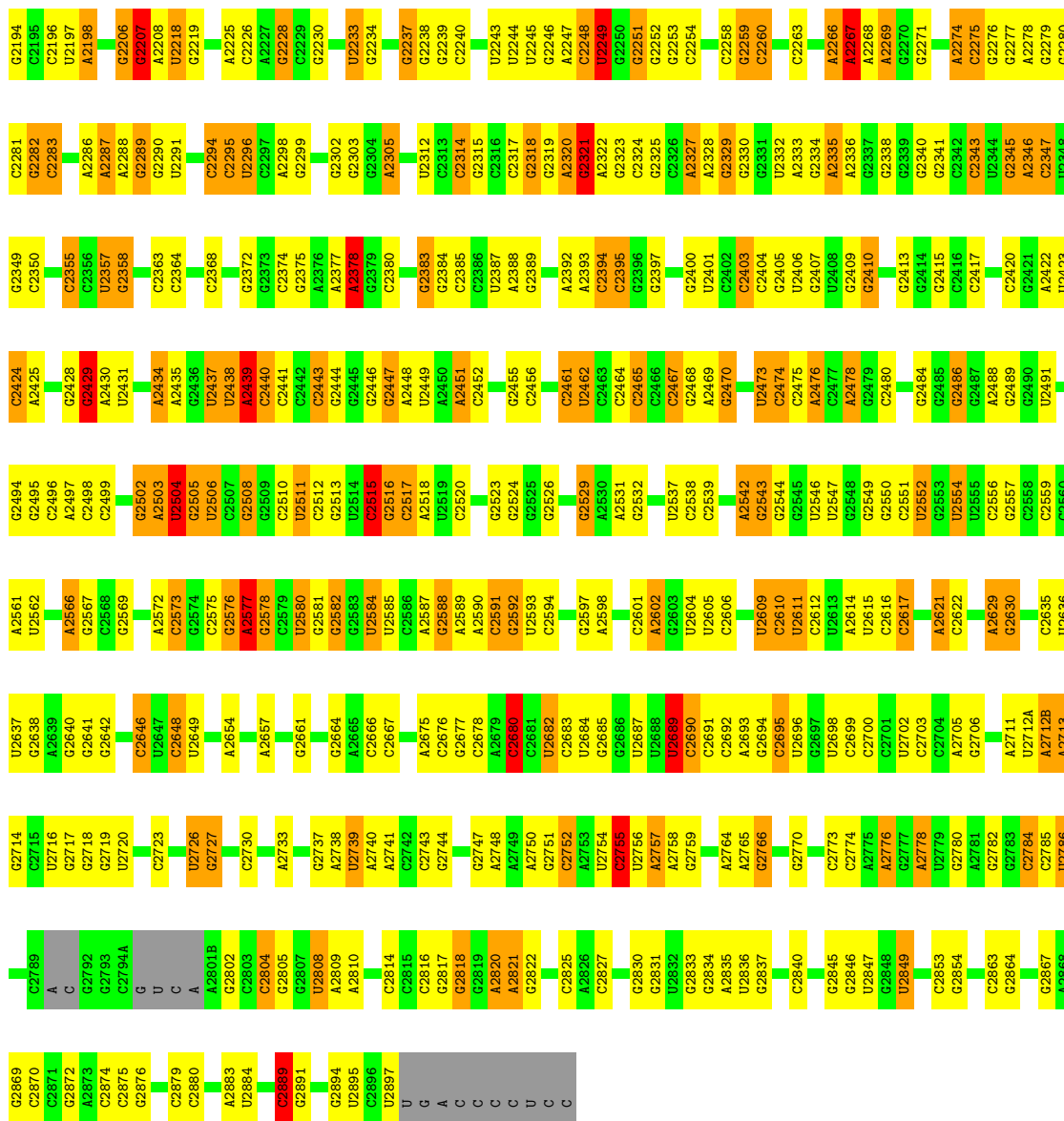


• Molecule 25: 23S rRNA

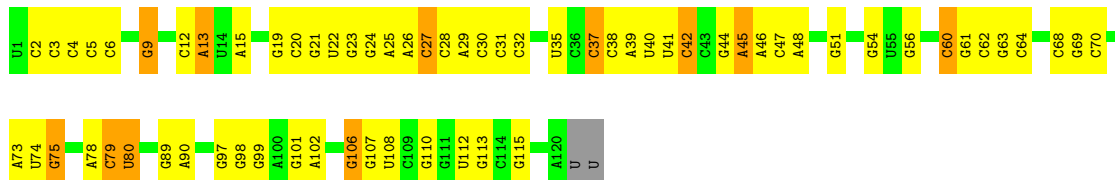


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G1814	G1699	C1615	G1458	G1371	C1221A	C1147	U1082	C1013	G942	C865	G798	G729
G1815	A1700	A1616	G1459	C1375	C1221B	C1146	U1083	G1017	U943	A866	G799	C730
G1816	A1701	A1542	G1459	C1375	C1222	A1148	A1084	C1018	A945	C867	A800	G801
G1817	G1702	A1543	C1376	C1377	G1223	G1149	A1085	U1019	G946	U868	G801	C731
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A1821	U1629	C1463	C1304	C1304	G1225	G1151	G1087	A1021	G948	U871	G805	G733
G1824	G1630	C1464	A1379	G1380	A1226	C1152	A1088	G1022	G952	C806	A735	A734
A1825	C1631A	G1466	G1380	C1306	G1227	C1153	U1089	G1023	G956	A736	A735	C736
G1826	A1632	C1467	A1384	G1309	G1231	A1155	G1091	G1024	G957	G809	G808	G739
A1829	G1633	A1471	G1385	G1309	C1232	A1156	C1092	U1026	A958	U810	U811	G742
C1830	C1638	C1474	G1389	U1312	G1233	G1157	G1093	A1027	U959	C886	C812	G743
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G1850	A1663	G1500	A1419	G1335	U1254	C1178	C1109	U1044	C975A	C903	A831	G763
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A1854	A1669	A1495	G1415	C1337	G1256	C1181	G1111	A1046	C976	C908	U833	G765
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C1886	A1686	A1528B	G1442	A1353	C1271	U1198	A1126	U	A989	G919	U846	
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							G1139	C1072	A1000	G932	U858	U858
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G2110	C2039	A1966	A1900	A1809	G1635	G1563	G1563	A1491	C1410	G1333	G1263	G1192
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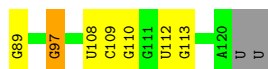


• Molecule 26: 5S rRNA



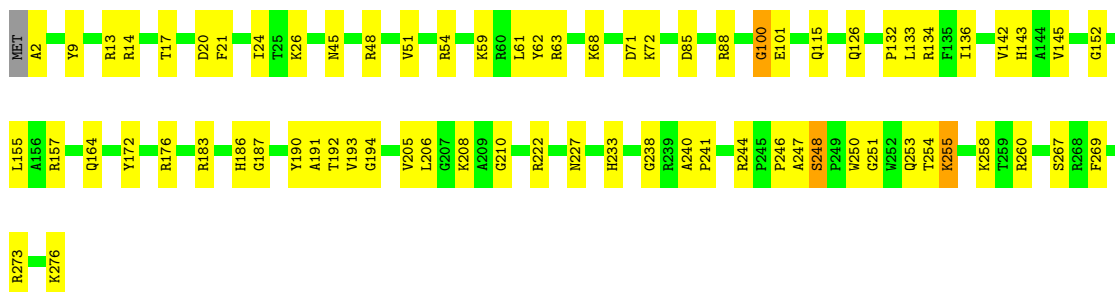
• Molecule 26: 5S rRNA





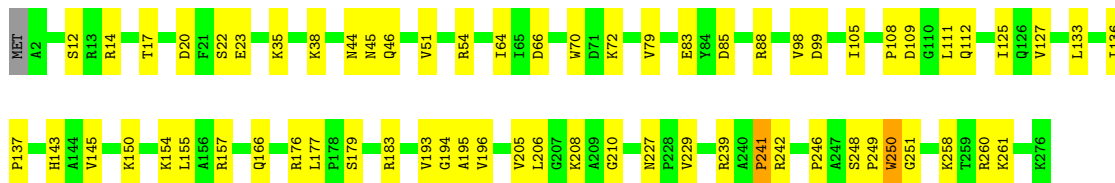
- Molecule 27: 50S ribosomal protein L2

Chain RD: 74% 25%



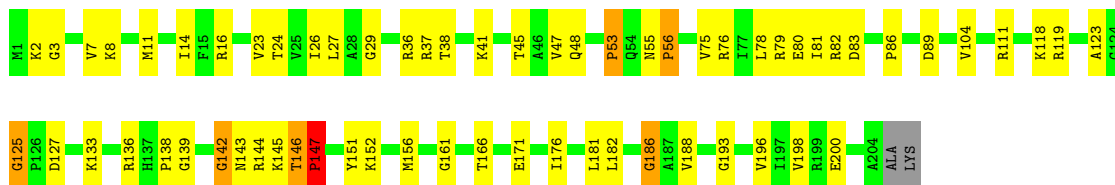
- Molecule 27: 50S ribosomal protein L2

Chain YD: 76% 23%



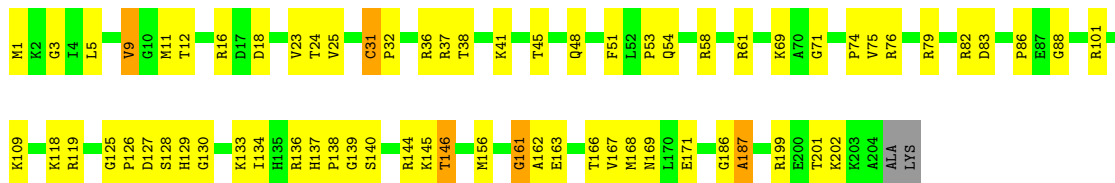
- Molecule 28: 50S ribosomal protein L3

Chain RE: 68% 28%



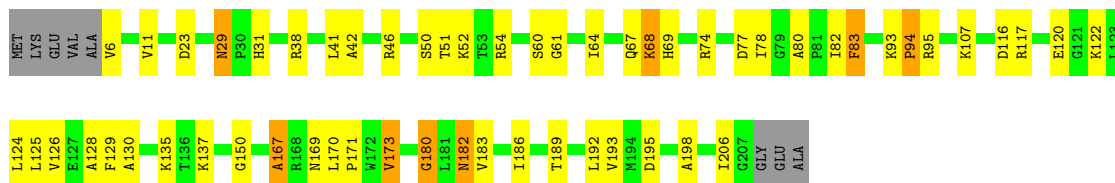
- Molecule 28: 50S ribosomal protein L3

Chain YE: 66% 31%



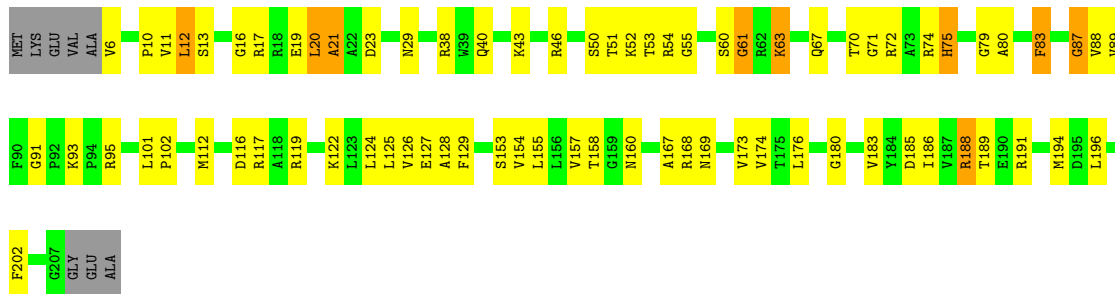
- Molecule 29: 50S ribosomal protein L4

Chain RF: 69% 23%



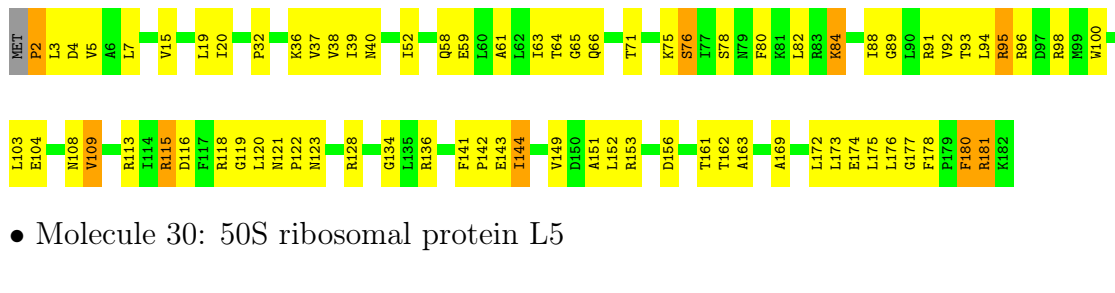
- Molecule 29: 50S ribosomal protein L4

Chain YF: 60% 31%



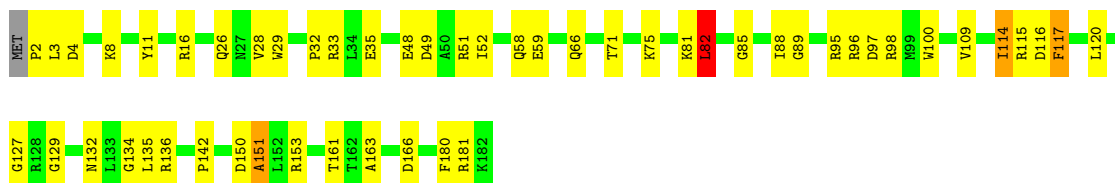
- Molecule 30: 50S ribosomal protein L5

Chain RG: 57% 37% 5%



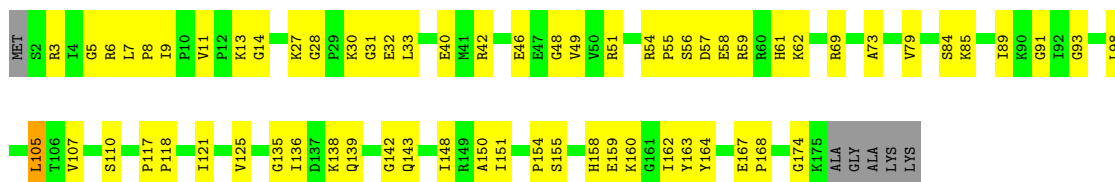
- Molecule 30: 50S ribosomal protein L5

Chain YG: 71% 26%



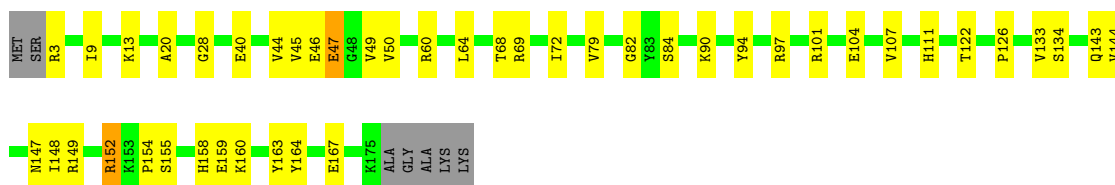
- Molecule 31: 50S ribosomal protein L6

Chain RH: 61% 36%



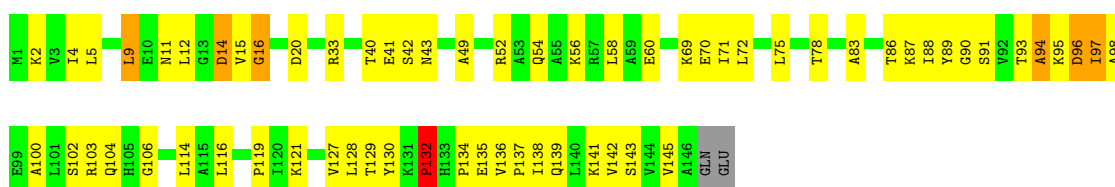
- Molecule 31: 50S ribosomal protein L6

Chain YH:  71% 24% ..




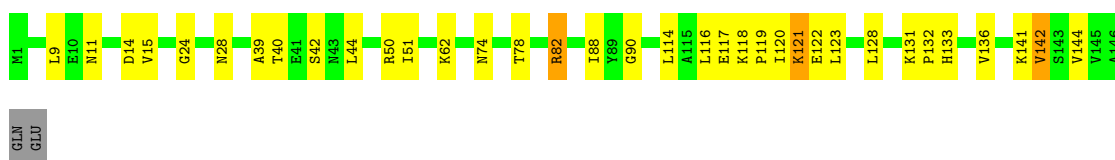
- Molecule 32: 50S ribosomal protein L9

Chain RI:  55% 39% ..



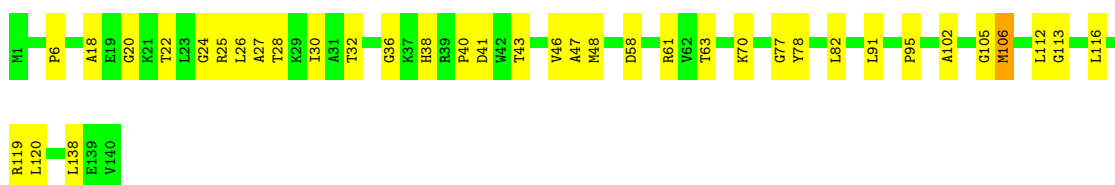
- Molecule 32: 50S ribosomal protein L9

Chain YI:  75% 22% ..




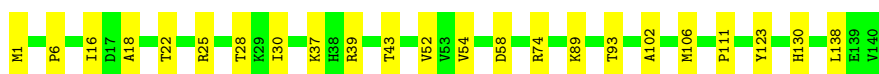
- Molecule 33: 50S ribosomal protein L13

Chain RN:  74% 26%



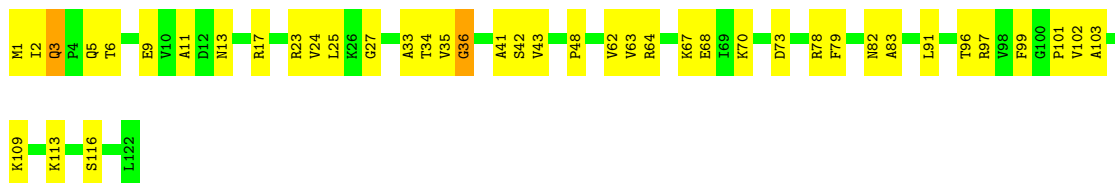
- Molecule 33: 50S ribosomal protein L13

Chain YN:  84% 16%



- Molecule 34: 50S ribosomal protein L14

Chain RO:  66% 33%



- Molecule 34: 50S ribosomal protein L14

Chain YO: 79% 20%



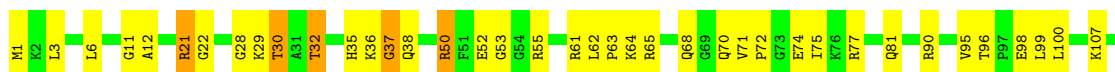
- Molecule 35: 50S ribosomal protein L15

Chain RP: 64% 29% 7%



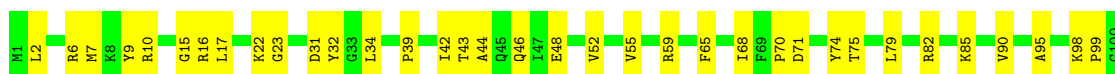
- Molecule 35: 50S ribosomal protein L15

Chain YP: 66% 30%



- Molecule 36: 50S ribosomal protein L16

Chain RQ: 67% 33%

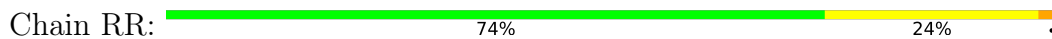


- Molecule 36: 50S ribosomal protein L16

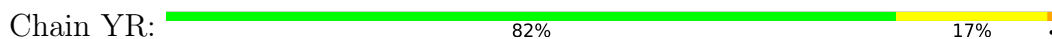
Chain YQ: 79% 21%



- Molecule 37: 50S ribosomal protein L17



- Molecule 37: 50S ribosomal protein L17



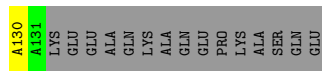
- Molecule 38: 50S ribosomal protein L18



- Molecule 38: 50S ribosomal protein L18



- Molecule 39: 50S ribosomal protein L19

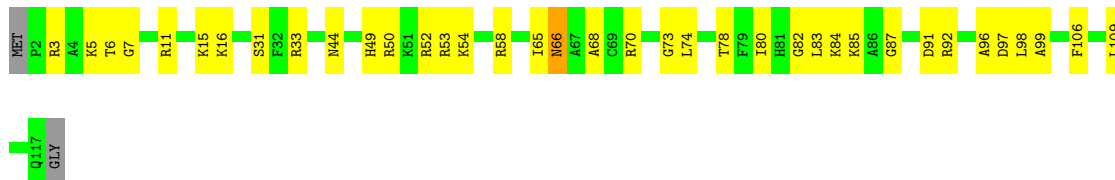


- Molecule 39: 50S ribosomal protein L19

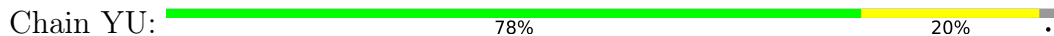




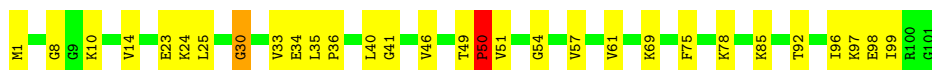
• Molecule 40: 50S ribosomal protein L20



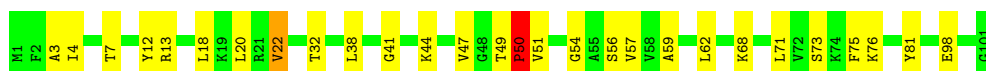
• Molecule 40: 50S ribosomal protein L20



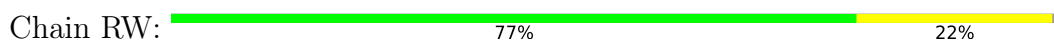
• Molecule 41: 50S ribosomal protein L21



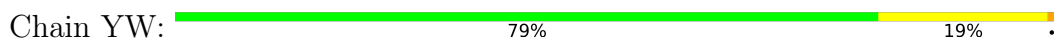
• Molecule 41: 50S ribosomal protein L21



• Molecule 42: 50S ribosomal protein L22



• Molecule 42: 50S ribosomal protein L22

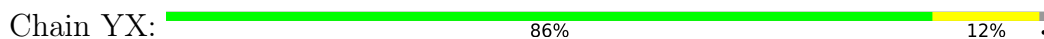




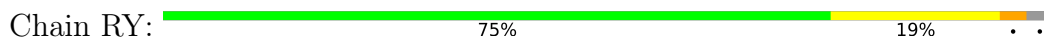
- Molecule 43: 50S ribosomal protein L23



- Molecule 43: 50S ribosomal protein L23



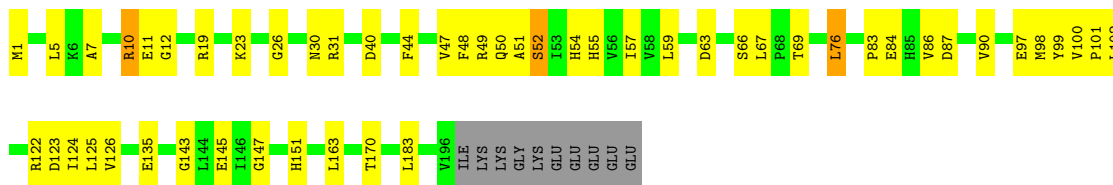
- Molecule 44: 50S ribosomal protein L24



- Molecule 44: 50S ribosomal protein L24



- Molecule 45: 50S ribosomal protein L25

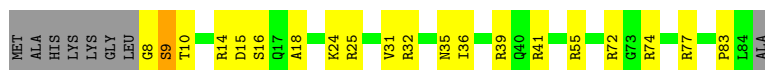


- Molecule 45: 50S ribosomal protein L25

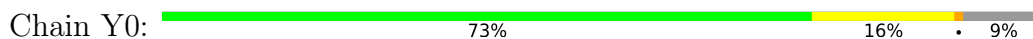




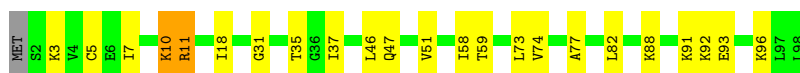
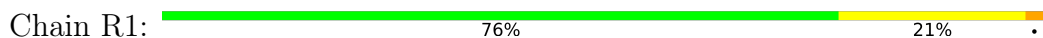
- Molecule 46: 50S ribosomal protein L27



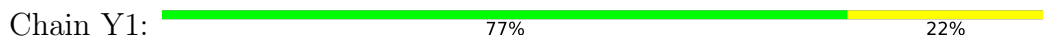
- Molecule 46: 50S ribosomal protein L27



- Molecule 47: 50S ribosomal protein L28



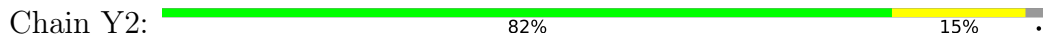
- Molecule 47: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L29

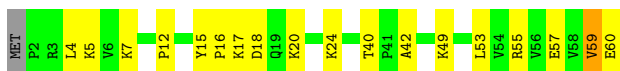


- Molecule 48: 50S ribosomal protein L29



- Molecule 49: 50S ribosomal protein L30

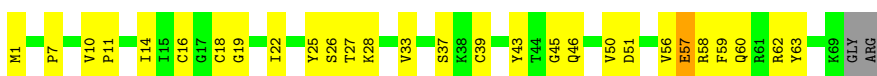




- Molecule 49: 50S ribosomal protein L30



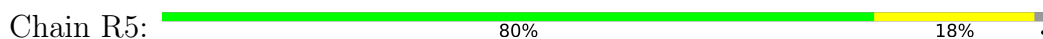
- Molecule 50: 50S ribosomal protein L31



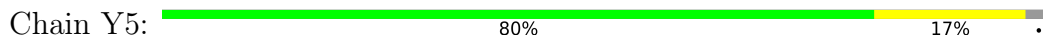
- Molecule 50: 50S ribosomal protein L31



- Molecule 51: 50S ribosomal protein L32



- Molecule 51: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L33

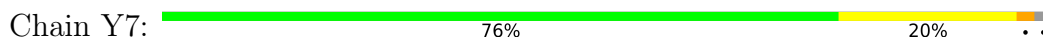




- Molecule 53: 50S ribosomal protein L34



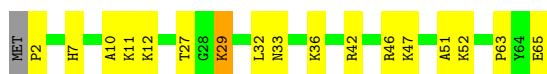
- Molecule 53: 50S ribosomal protein L34



- 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, UR3, OMC, 5MU, 5MC, 2MG, 4OC, OMU, MG, MA6, M2G, ZN, PSU, SF4, 0TD, PPU, 2MA, G7M

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	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 [i](#)

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
35	YP	32	THR
40	YU	95	LEU
52	Y6	6	ARG
45	RZ	55	HIS
44	RY	99	CYS

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

Mol	Chain	Res	Type
30	YG	58	GLN
32	YI	133	HIS
52	Y6	49	HIS
35	RP	9	ASN
14	XN	52	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	YA	752	A
25	YA	2439	A
25	YA	856	C
25	YA	1900	A
25	RA	1073	A

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

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	5MC	QA	1400	1	18,22,23	0.93	1 (5%)	26,32,35	1.22	1 (3%)
1	PSU	QA	516	1	18,21,22	1.37	3 (16%)	22,30,33	1.91	5 (22%)
25	5MU	RA	1915	25	19,22,23	1.57	5 (26%)	28,32,35	2.43	9 (32%)
25	5MC	YA	1942	25	18,22,23	1.17	2 (11%)	26,32,35	1.54	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	OMG	YA	2251	25,22,57	18,26,27	1.19	1 (5%)	19,38,41	1.21	4 (21%)
1	5MC	XA	1400	1	18,22,23	0.99	2 (11%)	26,32,35	1.25	2 (7%)
25	5MU	YA	1915	25	19,22,23	1.52	5 (26%)	28,32,35	2.51	9 (32%)
25	OMC	YA	1920	25	19,22,23	0.92	1 (5%)	26,31,34	1.81	5 (19%)
12	0TD	QL	92	12	7,9,10	1.40	1 (14%)	6,11,13	2.18	3 (50%)
1	5MC	XA	1404	1	18,22,23	1.02	1 (5%)	26,32,35	1.35	3 (11%)
25	OMG	RA	2251	25,22,57	18,26,27	1.13	1 (5%)	19,38,41	1.19	2 (10%)
1	4OC	QA	1402	1	20,23,24	0.78	0	26,32,35	0.95	1 (3%)
1	5MC	XA	967	1	18,22,23	0.96	1 (5%)	26,32,35	1.33	2 (7%)
1	5MC	QA	967	1	18,22,23	0.96	2 (11%)	26,32,35	1.30	2 (7%)
56	PPU	ZB	3	25,56	32,40,41	0.89	0	33,57,60	1.57	7 (21%)
25	2MA	YA	2503	25,57	17,25,26	1.26	2 (11%)	17,37,40	0.96	1 (5%)
1	MA6	XA	1518	1	19,26,27	1.00	1 (5%)	18,38,41	1.77	4 (22%)
25	OMU	YA	2552	25,57	19,22,23	1.41	3 (15%)	26,31,34	2.01	7 (26%)
25	PSU	RA	1911	25	18,21,22	1.55	5 (27%)	22,30,33	2.01	4 (18%)
25	OMC	RA	1920	25	19,22,23	0.95	1 (5%)	26,31,34	1.87	8 (30%)
1	G7M	XA	527	1	20,26,27	2.49	4 (20%)	17,39,42	1.00	1 (5%)
25	PSU	YA	1917	25	18,21,22	1.44	3 (16%)	22,30,33	2.01	4 (18%)
1	PSU	XA	516	1,57	18,21,22	1.37	4 (22%)	22,30,33	1.82	5 (22%)
1	2MG	QA	1207	1	18,26,27	1.00	1 (5%)	16,38,41	1.16	3 (18%)
25	5MC	RA	1942	25	18,22,23	1.07	1 (5%)	26,32,35	1.39	2 (7%)
1	UR3	QA	1498	1	19,22,23	0.96	2 (10%)	26,32,35	1.34	2 (7%)
25	PSU	RA	2605	25	18,21,22	1.71	4 (22%)	22,30,33	2.10	5 (22%)
1	MA6	XA	1519	1	19,26,27	0.82	0	18,38,41	2.10	6 (33%)
1	M2G	XA	966	1	20,27,28	1.21	2 (10%)	22,40,43	1.11	3 (13%)
1	MA6	QA	1519	1	19,26,27	0.93	1 (5%)	18,38,41	1.95	6 (33%)
1	M2G	QA	966	1	20,27,28	1.34	3 (15%)	22,40,43	0.99	2 (9%)
1	5MC	XA	1407	1	18,22,23	0.96	2 (11%)	26,32,35	1.39	5 (19%)
1	UR3	XA	1498	1	19,22,23	1.01	2 (10%)	26,32,35	1.39	2 (7%)
1	5MC	QA	1407	1	18,22,23	0.88	2 (11%)	26,32,35	1.10	3 (11%)
12	0TD	XL	92	12	7,9,10	1.38	2 (28%)	6,11,13	1.40	1 (16%)
1	MA6	QA	1518	1	19,26,27	0.88	1 (5%)	18,38,41	1.97	7 (38%)
25	PSU	YA	2605	25	18,21,22	1.60	4 (22%)	22,30,33	2.19	4 (18%)
25	2MA	RA	2503	25,57	17,25,26	1.10	1 (5%)	17,37,40	0.98	2 (11%)
1	G7M	QA	527	1	20,26,27	2.53	4 (20%)	17,39,42	1.04	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	5MU	YA	1939	25,57	19,22,23	1.55	4 (21%)	28,32,35	2.20	6 (21%)
1	4OC	XA	1402	1	20,23,24	0.85	1 (5%)	26,32,35	0.95	2 (7%)
25	5MC	YA	1962	25	18,22,23	1.00	1 (5%)	26,32,35	2.27	8 (30%)
1	5MC	QA	1404	1	18,22,23	0.92	1 (5%)	26,32,35	1.42	4 (15%)
25	PSU	YA	1911	25	18,21,22	1.56	5 (27%)	22,30,33	1.89	4 (18%)
25	PSU	RA	1917	25	18,21,22	1.47	4 (22%)	22,30,33	2.08	4 (18%)
56	PPU	ZA	3	25,57,56	32,40,41	0.96	1 (3%)	33,57,60	1.82	7 (21%)
25	5MU	RA	1939	25,57	19,22,23	1.45	4 (21%)	28,32,35	2.31	6 (21%)
25	5MC	RA	1962	25,57	18,22,23	0.98	1 (5%)	26,32,35	1.60	7 (26%)
25	OMU	RA	2552	25	19,22,23	1.38	3 (15%)	26,31,34	1.95	6 (23%)
1	2MG	XA	1207	1	18,26,27	1.08	1 (5%)	16,38,41	1.25	3 (18%)

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	5MC	QA	1400	1	-	5/7/25/26	0/2/2/2
1	PSU	QA	516	1	-	0/7/25/26	0/2/2/2
25	5MU	RA	1915	25	-	3/7/25/26	0/2/2/2
25	5MC	YA	1942	25	-	0/7/25/26	0/2/2/2
25	OMG	YA	2251	25,22,57	-	0/5/27/28	0/3/3/3
1	5MC	XA	1400	1	-	4/7/25/26	0/2/2/2
25	5MU	YA	1915	25	-	4/7/25/26	0/2/2/2
25	OMC	YA	1920	25	-	4/9/27/28	0/2/2/2
12	0TD	QL	92	12	-	4/7/12/14	-
1	5MC	XA	1404	1	-	0/7/25/26	0/2/2/2
25	OMG	RA	2251	25,22,57	-	0/5/27/28	0/3/3/3
1	4OC	QA	1402	1	-	2/9/29/30	0/2/2/2
1	5MC	XA	967	1	-	0/7/25/26	0/2/2/2
1	5MC	QA	967	1	-	0/7/25/26	0/2/2/2
56	PPU	ZB	3	25,56	-	5/21/43/44	0/4/4/4
25	2MA	YA	2503	25,57	-	2/3/25/26	0/3/3/3
1	MA6	XA	1518	1	-	1/7/29/30	0/3/3/3
25	OMU	YA	2552	25,57	-	2/9/27/28	0/2/2/2
25	PSU	RA	1911	25	-	0/7/25/26	0/2/2/2
25	OMC	RA	1920	25	-	4/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	G7M	XA	527	1	-	2/3/25/26	0/3/3/3
25	PSU	YA	1917	25	-	0/7/25/26	0/2/2/2
1	PSU	XA	516	1,57	-	0/7/25/26	0/2/2/2
1	2MG	QA	1207	1	-	0/5/27/28	0/3/3/3
25	5MC	RA	1942	25	-	0/7/25/26	0/2/2/2
1	UR3	QA	1498	1	-	2/7/25/26	0/2/2/2
25	PSU	RA	2605	25	-	0/7/25/26	0/2/2/2
1	MA6	XA	1519	1	-	6/7/29/30	0/3/3/3
1	M2G	XA	966	1	-	2/7/29/30	0/3/3/3
1	MA6	QA	1519	1	-	5/7/29/30	0/3/3/3
1	M2G	QA	966	1	-	0/7/29/30	0/3/3/3
1	5MC	XA	1407	1	-	0/7/25/26	0/2/2/2
1	UR3	XA	1498	1	-	0/7/25/26	0/2/2/2
1	5MC	QA	1407	1	-	0/7/25/26	0/2/2/2
12	0TD	XL	92	12	-	4/7/12/14	-
1	MA6	QA	1518	1	-	1/7/29/30	0/3/3/3
25	PSU	YA	2605	25	-	0/7/25/26	0/2/2/2
25	2MA	RA	2503	25,57	-	1/3/25/26	0/3/3/3
1	G7M	QA	527	1	-	2/3/25/26	0/3/3/3
25	5MU	YA	1939	25,57	-	0/7/25/26	0/2/2/2
1	4OC	XA	1402	1	-	2/9/29/30	0/2/2/2
25	5MC	YA	1962	25	-	4/7/25/26	0/2/2/2
1	5MC	QA	1404	1	-	0/7/25/26	0/2/2/2
25	PSU	YA	1911	25	-	0/7/25/26	0/2/2/2
25	PSU	RA	1917	25	-	0/7/25/26	0/2/2/2
56	PPU	ZA	3	25,57,56	-	5/21/43/44	0/4/4/4
25	5MU	RA	1939	25,57	-	0/7/25/26	0/2/2/2
25	5MC	RA	1962	25,57	-	0/7/25/26	0/2/2/2
25	OMU	RA	2552	25	-	3/9/27/28	0/2/2/2
1	2MG	XA	1207	1	-	0/5/27/28	0/3/3/3

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	QA	527	G7M	C8-N9	7.06	1.46	1.33
1	XA	527	G7M	C8-N9	7.02	1.46	1.33
1	QA	527	G7M	C8-N7	6.58	1.45	1.33
1	XA	527	G7M	C8-N7	6.18	1.44	1.33
25	RA	1915	5MU	C4-N3	-3.96	1.31	1.38

The worst 5 of 202 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	RA	1917	PSU	N1-C2-N3	6.22	122.18	115.13
25	RA	1915	5MU	N3-C2-N1	6.21	123.14	114.89
25	RA	2605	PSU	N1-C2-N3	6.14	122.09	115.13
25	RA	1911	PSU	N1-C2-N3	6.13	122.08	115.13
25	YA	1917	PSU	N1-C2-N3	6.11	122.06	115.13

There are no chirality outliers.

5 of 79 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	QL	92	0TD	O-C-CA-CB
12	QL	92	0TD	CA-CB-SB-CSB
12	QL	92	0TD	CG-CB-SB-CSB
1	QA	527	G7M	O4'-C4'-C5'-O5'
1	QA	527	G7M	C3'-C4'-C5'-O5'

There are no ring outliers.

26 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	QA	1400	5MC	1	0
25	YA	2251	OMG	1	0
25	YA	1920	OMC	2	0
12	QL	92	0TD	1	0
1	XA	1404	5MC	2	0
25	RA	2251	OMG	2	0
1	QA	1402	4OC	1	0
1	XA	967	5MC	1	0
56	ZB	3	PPU	4	0
25	YA	2503	2MA	1	0
1	XA	1518	MA6	1	0
25	YA	2552	OMU	2	0
25	RA	1920	OMC	1	0
25	YA	1917	PSU	1	0
25	RA	1942	5MC	1	0
1	QA	1519	MA6	1	0
1	QA	966	M2G	1	0
1	XA	1407	5MC	1	0
12	XL	92	0TD	1	0
25	RA	2503	2MA	2	0
25	YA	1939	5MU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	XA	1402	4OC	1	0
25	YA	1962	5MC	1	0
56	ZA	3	PPU	10	0
25	RA	2552	OMU	3	0
1	XA	1207	2MG	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	QD	303	4	0,12,12	-	-	-		
58	SF4	XD	302	4	0,12,12	-	-	-		

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
58	SF4	QD	303	4	-	-	0/6/5/5
58	SF4	XD	302	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	QD	303	SF4	6	0
58	XD	302	SF4	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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