



wwPDB EM Model Validation Summary Report ⓘ

Apr 13, 2020 – 04:31 PM EDT

PDB ID : 6TB3
EMDB ID : EMD-10431
Title : yeast 80S ribosome in complex with the Not5 subunit of the CCR4-NOT complex
Authors : Buschauer, R.; Cheng, J.; Berninghausen, O.; Tesina, P.; Becker, T.; Beckmann, R.
Deposited on : 2019-10-31
Resolution : 2.80 Å(reported)

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB entry.

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

A user guide is available at

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

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)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.10.1

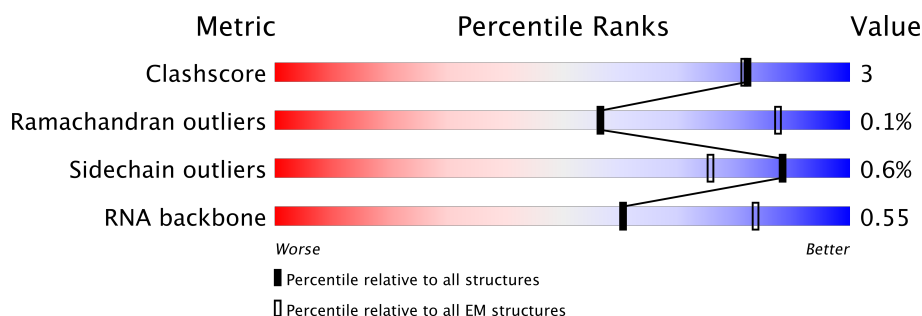
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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.








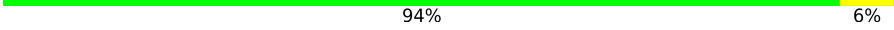

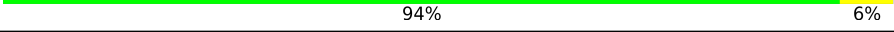



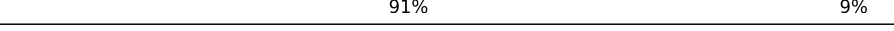
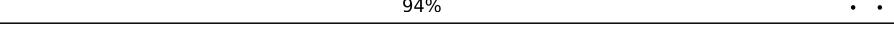


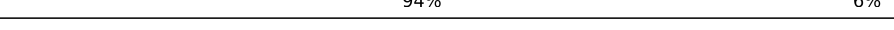

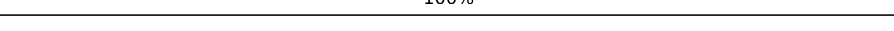
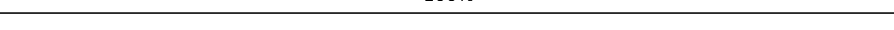
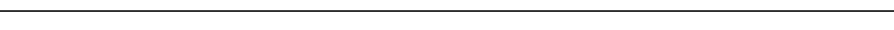

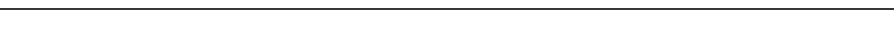
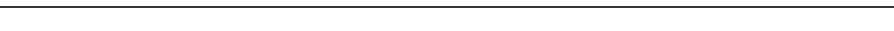


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	2	1798	64% 28% 6% .
2	1	3	100%
3	P	206	89% 11%
4	Q	232	88% 9% .
5	E	117	85% 15%
6	R	216	93% 7%
7	A	222	95% 5%

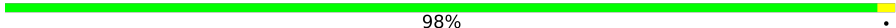



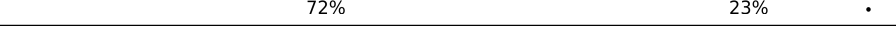
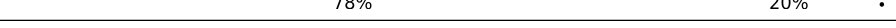

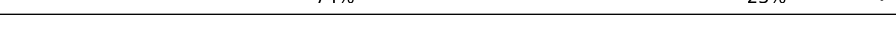
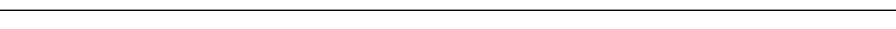
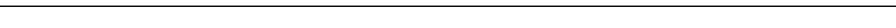









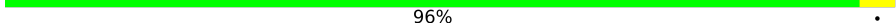
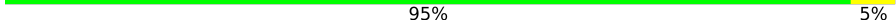
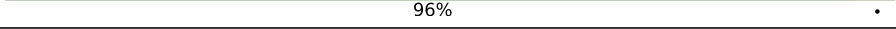



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Mol	Chain	Length	Quality of chain
8	S	258	 91% 9%
9	B	206	 90% 10%
10	T	228	 90% 10%
11	U	184	 88% 13%
12	V	187	 88% 12%
13	W	184	 94% 6%
14	C	92	 87% 13%
15	X	142	 94% 6%
16	D	121	 80% 18% .
17	Y	150	 91% 9%
18	Z	127	 89% 11%
19	F	141	 91% 9%
20	G	125	 94% . .
21	H	145	 90% 10%
22	I	143	 83% 17%
23	J	100	 94% 6%
24	n	75	 77% 23%
25	a	87	 100%
26	b	129	 100%
27	c	144	 99% .
28	d	134	 100%
29	K	82	 95% . .
30	e	97	 100%
31	f	81	 99% .
32	M	53	 89% 11%



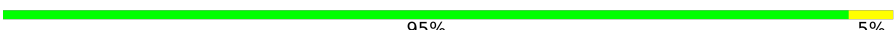

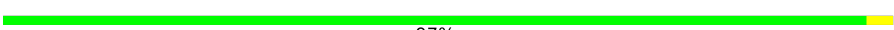





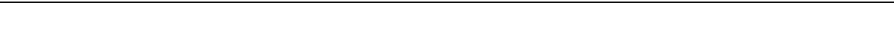

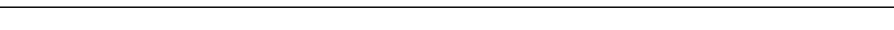
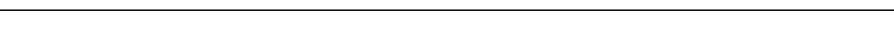


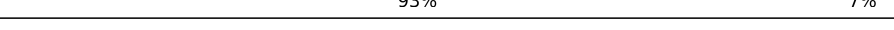
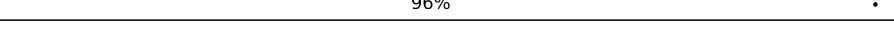







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Mol	Chain	Length	Quality of chain
33	g	60	 98% .
34	N	73	 84% 15% .
35	O	312	 89% 11%
36	L	63	 81% 19%
37	BQ	3223	 72% 23% .
38	BT	204	 78% 20% .
39	BR	121	 83% 14% .
40	BS	158	 74% 23% .
41	AW	251	 92% 8%
42	BA	386	 93% 7%
43	BE	361	 93% 6%
44	BI	294	 93% 7%
45	BM	175	 87% 7% . 5%
46	BO	222	 94% 6%
47	AA	233	 93% 7%
48	AD	191	 90% 10%
49	BD	218	 91% 8%
50	AG	169	 92% 8%
51	AJ	193	 92% 8%
52	AM	136	 85% 15%
53	AQ	203	 96% .
54	AU	197	 95% 5%
55	AX	183	 96% .
56	BB	185	 91% 9%
57	BF	188	 88% 11% .

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Mol	Chain	Length	Quality of chain
58	BH	171	 89% 11%
59	BJ	159	 92% 8%
60	BL	100	 95% 5%
61	AB	136	 92% 8%
62	AE	126	 97% .
63	AH	121	 95% 5%
64	AK	125	 96% . .
65	AN	135	 93% 7%
66	AR	148	 90% 10%
67	AV	58	 91% 7% .
68	AY	96	 91% 9%
69	BC	109	 89% 11%
70	BG	127	 92% 8%
71	BK	106	 90% 10%
72	BN	112	 90% 9% .
73	BP	119	 93% 7%
74	AC	99	 96% .
75	AF	81	 89% 11%
76	AI	77	 88% 12%
77	AL	50	 86% 14%
78	AO	52	 90% 10%
79	AS	25	 92% 8%
80	AP	103	 93% 7%
81	AT	91	 92% 8%
82	BV	22	 73% 27%

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Mol	Chain	Length	Quality of chain
83	BW	112	<div><div></div><div>86%</div><div>13%</div><div></div></div>

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 205032 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 *Saccharomyces cerevisiae* S288C 18S ribosomal RNA (RDN18-1), rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1771	Total	C	N	O	P	0	0
			37739	16872	6683	12413	1771		

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	3	Total	C	N	O	P	0	0
			65	29	12	21	3		

- Molecule 3 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	206	Total	C	N	O	S	0	0
			1603	1030	284	287	2		

- Molecule 4 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	226	Total	C	N	O	S	0	0
			1798	1139	330	325	4		

- Molecule 5 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	117	Total	C	N	O	S	0	0
			916	583	171	155	7		

- Molecule 6 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	216	Total	C	N	O	S	0	0
			1626	1042	287	295	2		

- Molecule 7 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	222	Total	C	N	O	S	0	0
			1729	1098	312	313	6		

- Molecule 8 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	258	Total	C	N	O	S	0	0
			2056	1308	387	358	3		

- Molecule 9 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	206	Total	C	N	O	S	0	0
			1605	1005	299	298	3		

- Molecule 10 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	228	Total	C	N	O	S	0	0
			1815	1138	351	323	3		

- Molecule 11 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	U	184	Total	C	N	O	S	0	0
			1473	946	263	264			

- Molecule 12 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	V	187	Total	C	N	O	S	0	0
			1476	916	295	263	2		

- Molecule 13 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	184	Total	C	N	O	S	0	0
			1479	935	285	258	1		

- Molecule 14 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	92	Total	C	N	O	S	0	0
			752	487	122	141	2		

- Molecule 15 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	142	Total	C	N	O	S	0	0
			1142	733	217	189	3		

- Molecule 16 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	121	Total	C	N	O	S	0	0
			875	551	153	169	2		

- Molecule 17 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 18 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	127	Total	C	N	O	S	0	0
			923	568	185	167	3		

- Molecule 19 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	F	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 20 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	G	121	Total	C	N	O	S	0	0
			948	596	179	171	2		

- Molecule 21 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	145	Total	C	N	O	S	0	0
			1188	741	237	208	2		

- Molecule 22 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	I	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 23 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	J	100	Total	C	N	O	S	0	0
			797	506	144	146	1		

- Molecule 24 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	n	75	Total	C	N	O	P	0	0
			1624	728	298	523	75		

- Molecule 25 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	87	Total	C	N	O	S	0	0
			673	415	125	131	2		

- Molecule 26 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 27 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 28 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	d	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 29 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	K	82	Total	C	N	O	0	0
			651	416	123	112		

- Molecule 30 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	97	Total	C	N	O	S	0	0
			765	473	160	127	5		

- Molecule 31 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 32 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	M	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 33 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	60	Total	C	N	O	S	0	0
			472	298	97	76	1		

- Molecule 34 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	N	73	Total	C	N	O	S	0	0
			556	352	105	95	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	97	ALA	LYS	conflict	UNP P05759

- Molecule 35 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	O	312	Total	C	N	O	S	0	0
			2383	1514	409	452	8		

- Molecule 36 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	L	63	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 37 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BQ	3223	Total	C	N	O	P	0	0
			68931	30790	12416	22502	3223		

- Molecule 38 is a protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BT	204	Total	C	N	O	S	0	0
			1609	1031	279	290	9		

- Molecule 39 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BR	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 40 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BS	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 41 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AW	251	Total	C	N	O	S	0	0
			1899	1182	385	331	1		

- Molecule 42 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BA	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 43 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BE	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 44 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BI	294	Total	C	N	O	S	0	0
			2351	1484	410	455	2		

- Molecule 45 is a protein called 60S ribosomal protein L6-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	BM	167	Total	C	N	O	0	0
			1307	843	234	230		

- Molecule 46 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BO	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 47 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AA	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 48 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AD	191	Total	C	N	O	S	0	0
			1508	957	274	273	4		

- Molecule 49 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BD	218	Total	C	N	O	S	0	0
			1764	1117	334	306	7		

- Molecule 50 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AG	169	Total	C	N	O	S	0	0
			1346	843	252	247	4		

- Molecule 51 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AJ	193	Total	C	N	O		0	0
			1543	962	315	266			

- Molecule 52 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AM	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 53 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AQ	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 54 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AU	197	Total	C	N	O	S	197	0
			1555	1003	289	262	1		

- Molecule 55 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	AX	183	Total	C	N	O	0	0
			1416	879	284	253		

- Molecule 56 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	BB	185	Total	C	N	O	S	0
			1441	908	290	241	2	0

- Molecule 57 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	BF	188	Total	C	N	O		0
			1515	932	323	260		0

- Molecule 58 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	BH	171	Total	C	N	O	S	0
			1437	925	266	243	3	0

- Molecule 59 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	BJ	159	Total	C	N	O	S	0
			1272	802	245	221	4	0

- Molecule 60 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
60	BL	100	Total	C	N	O		0
			796	516	131	149		0

- Molecule 61 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	AB	136	Total	C	N	O	S	0
			1003	628	189	179	7	0

- Molecule 62 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AE	126	Total	C	N	O	S	0	0
			836	525	165	145	1		

- Molecule 63 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AH	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 64 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AK	125	Total	C	N	O		0	0
			984	620	191	173			

- Molecule 65 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AN	135	Total	C	N	O		0	0
			1080	701	199	180			

- Molecule 66 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AR	148	Total	C	N	O	S	0	0
			1169	747	231	188	3		

- Molecule 67 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AV	58	Total	C	N	O		0	0
			462	289	100	73			

- Molecule 68 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AY	96	Total	C	N	O	S	0	0
			737	476	123	137	1		

- Molecule 69 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	BC	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 70 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	BG	127	Total	C	N	O	S	0	0
			1013	642	205	165	1		

- Molecule 71 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	BK	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 72 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	BN	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 73 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	BP	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 74 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AC	99	Total	C	N	O	S	0	0
			766	478	154	132	2		

- Molecule 75 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	AF	81	Total	C	N	O	S	0	0
			645	393	141	106	5		

- Molecule 76 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
76	AI	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 77 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AL	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 78 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AO	52	Total	C	N	O	S	0	0
			410	254	86	65	5		

- Molecule 79 is a protein called 60S ribosomal protein L41-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AS	25	Total	C	N	O	S	0	0
			229	139	62	27	1		

- Molecule 80 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	AP	103	Total	C	N	O	S	0	0
			824	517	167	135	5		

- Molecule 81 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	AT	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 82 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	BV	22	Total	C	N	O	S	0	0
			207	127	56	23	1		

- Molecule 83 is a protein called General negative regulator of transcription subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	BW	112	Total	C	N	O	S	0	0
			940	585	170	182	3		

- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	BO	1	Total	Mg	0
			1	1	
84	AQ	1	Total	Mg	0
			1	1	
84	BA	3	Total	Mg	0
			3	3	
84	BN	1	Total	Mg	0
			1	1	
84	AW	2	Total	Mg	0
			2	2	
84	B	1	Total	Mg	0
			1	1	
84	BF	1	Total	Mg	0
			1	1	
84	BG	1	Total	Mg	0
			1	1	
84	BR	1	Total	Mg	0
			1	1	
84	BQ	220	Total	Mg	0
			220	220	
84	n	3	Total	Mg	0
			3	3	
84	AX	1	Total	Mg	0
			1	1	
84	2	89	Total	Mg	0
			89	89	
84	S	1	Total	Mg	0
			1	1	
84	AB	1	Total	Mg	0
			1	1	

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

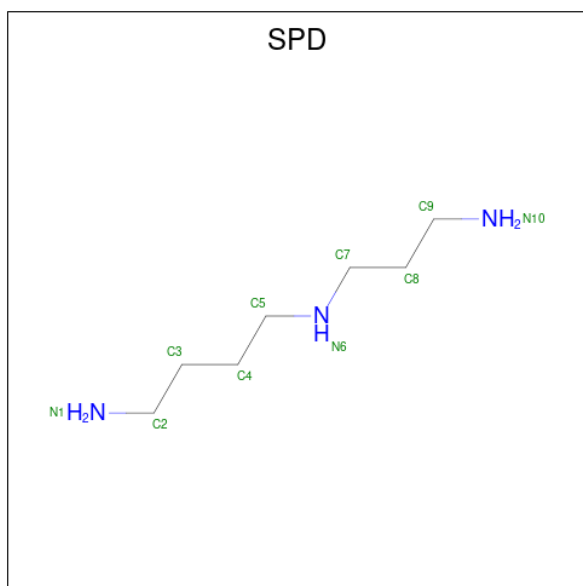
Mol	Chain	Residues	Atoms		AltConf
85	AP	1	Total	Zn	0
			1	1	
85	BN	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
85	AT	1	Total	Zn	0
			1	1	
85	N	1	Total	Zn	0
			1	1	
85	AO	1	Total	Zn	0
			1	1	
85	AF	1	Total	Zn	0
			1	1	
85	M	1	Total	Zn	0
			1	1	

- Molecule 86 is SPERMIDINE (three-letter code: SPD) (formula: C₇H₁₉N₃).

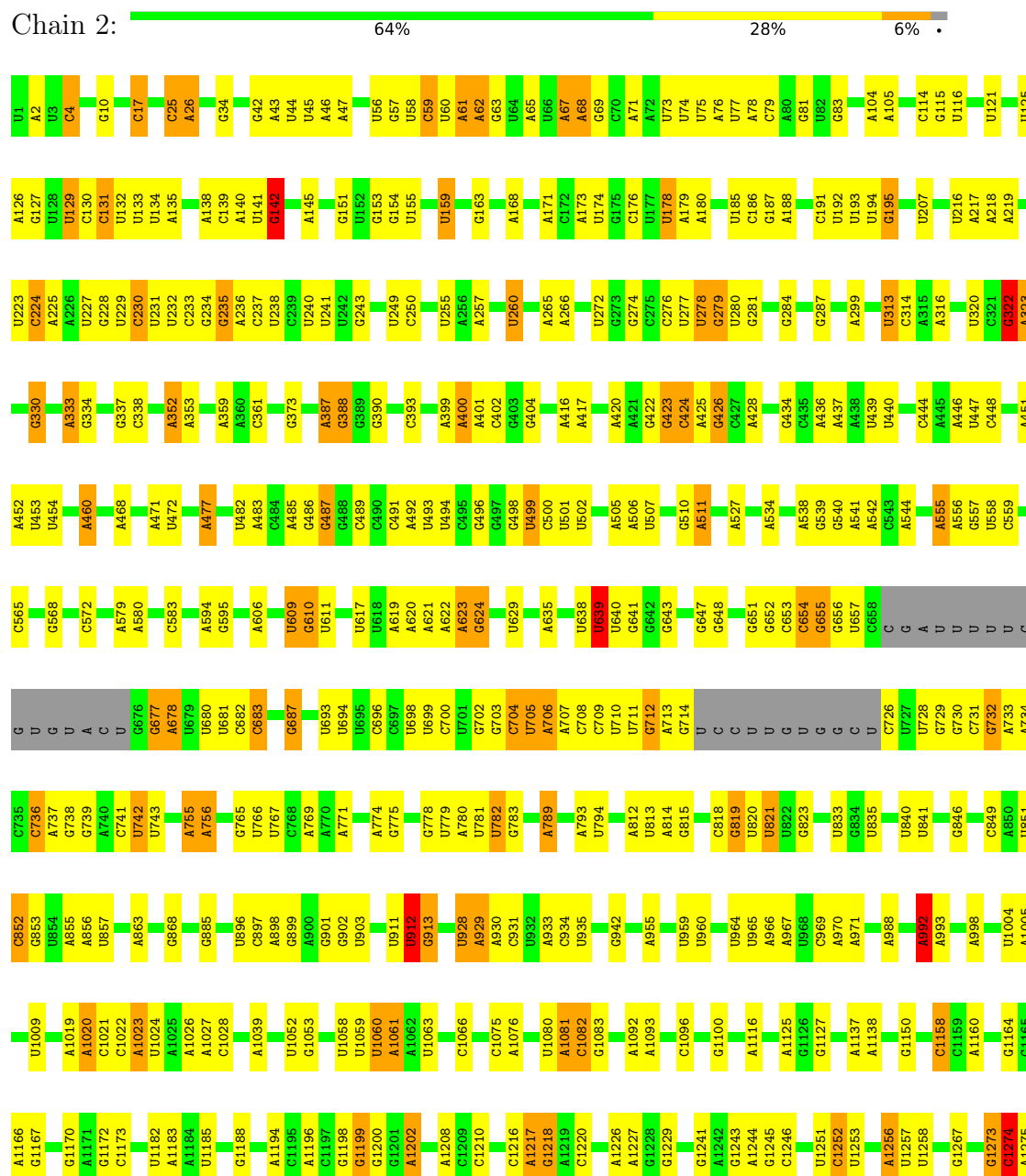


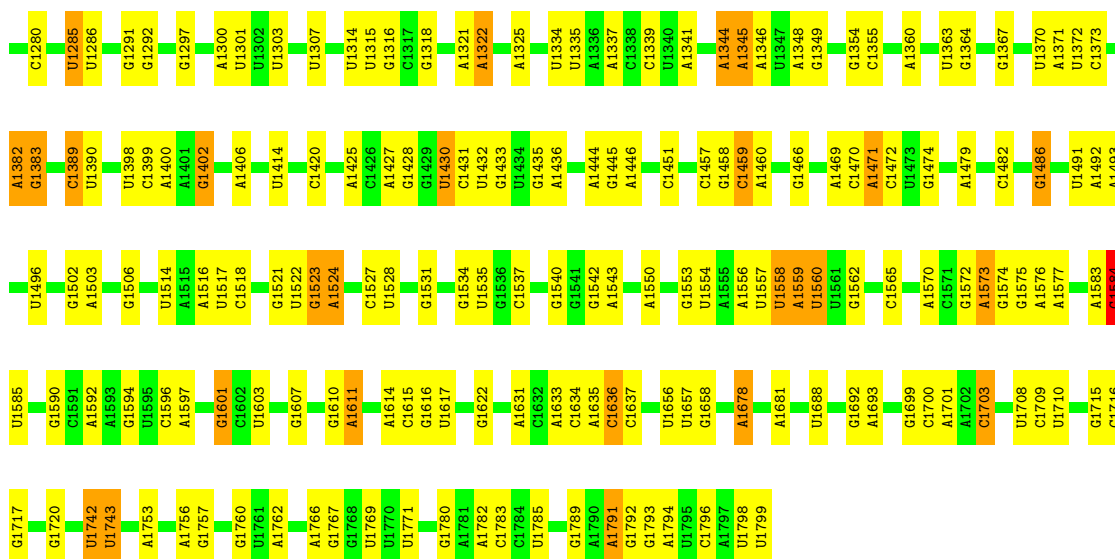
Mol	Chain	Residues	Atoms			AltConf
86	BQ	1	Total	C	N	0
			10	7	3	

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.

- Molecule 1: *Saccharomyces cerevisiae* S288C 18S ribosomal RNA (RDN18-1), rRNA





- Molecule 2: mRNA

Chain I: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: 40S ribosomal protein S0-A

Chain P: 89% 11%



- Molecule 4: 40S ribosomal protein S1-A

Chain Q: 88% 9%



- Molecule 5: 40S ribosomal protein S15

Chain E: 85%



- Molecule 6: 40S ribosomal protein S2

Chain R: 93%




- Molecule 7: 40S ribosomal protein S3

Chain A:  95% 5%




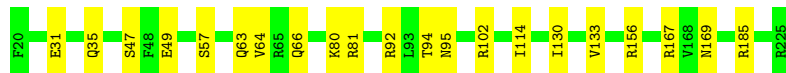
- Molecule 8: 40S ribosomal protein S4-A

Chain S:  91% 9%




- Molecule 9: 40S ribosomal protein S5

Chain B:  90% 10%




- Molecule 10: 40S ribosomal protein S6-A

Chain T:  90% 10%




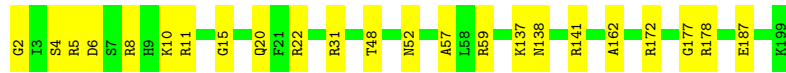
- Molecule 11: 40S ribosomal protein S7-A

Chain U:  88% 13%



- Molecule 12: 40S ribosomal protein S8

Chain V:  88% 12%




- Molecule 13: 40S ribosomal protein S9-A

Chain W:  94% 6%



- Molecule 14: 40S ribosomal protein S10-A

Chain C:  87% 13%



- Molecule 15: 40S ribosomal protein S11-A

Chain X:  94% 6%



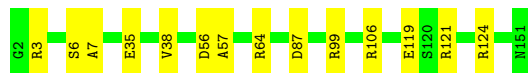
- Molecule 16: 40S ribosomal protein S12

Chain D:  80% 18%



- Molecule 17: 40S ribosomal protein S13

Chain Y:  91% 9%



- Molecule 18: 40S ribosomal protein S14-B

Chain Z:  89% 11%



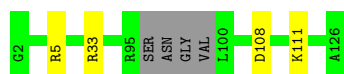
- Molecule 19: 40S ribosomal protein S16-A

Chain F:  91% 9%




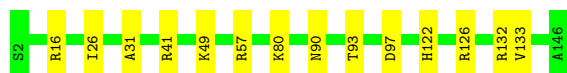
- Molecule 20: 40S ribosomal protein S17-B

Chain G:  94%




- Molecule 21: 40S ribosomal protein S18-A

Chain H:  90% 10%



- Molecule 22: 40S ribosomal protein S19-A

Chain I:  83% 17%




- Molecule 23: 40S ribosomal protein S20

Chain J:  94% 6%



- Molecule 24: tRNA

Chain n:  77% 23%



- Molecule 25: 40S ribosomal protein S21-A

Chain a:  100%

There are no outlier residues recorded for this chain.

- Molecule 26: 40S ribosomal protein S22-A

Chain b:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: 40S ribosomal protein S23-A

Chain c:  99%



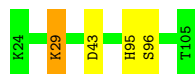
- Molecule 28: 40S ribosomal protein S24-A

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 29: 40S ribosomal protein S25-A

Chain K:  95% ..



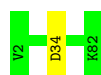
- Molecule 30: 40S ribosomal protein S26-B

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 31: 40S ribosomal protein S27-A

Chain f:  99% .



- Molecule 32: 40S ribosomal protein S29-A

Chain M:  89% 11%




- Molecule 33: 40S ribosomal protein S30-A

Chain g:  98% .




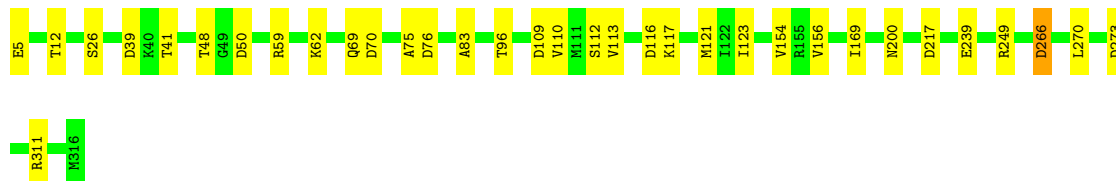
- Molecule 34: Ubiquitin-40S ribosomal protein S31

Chain N:  84% 15% .

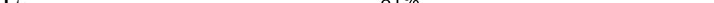


- Molecule 35: Guanine nucleotide-binding protein subunit beta-like protein

Chain O:  89% 11%




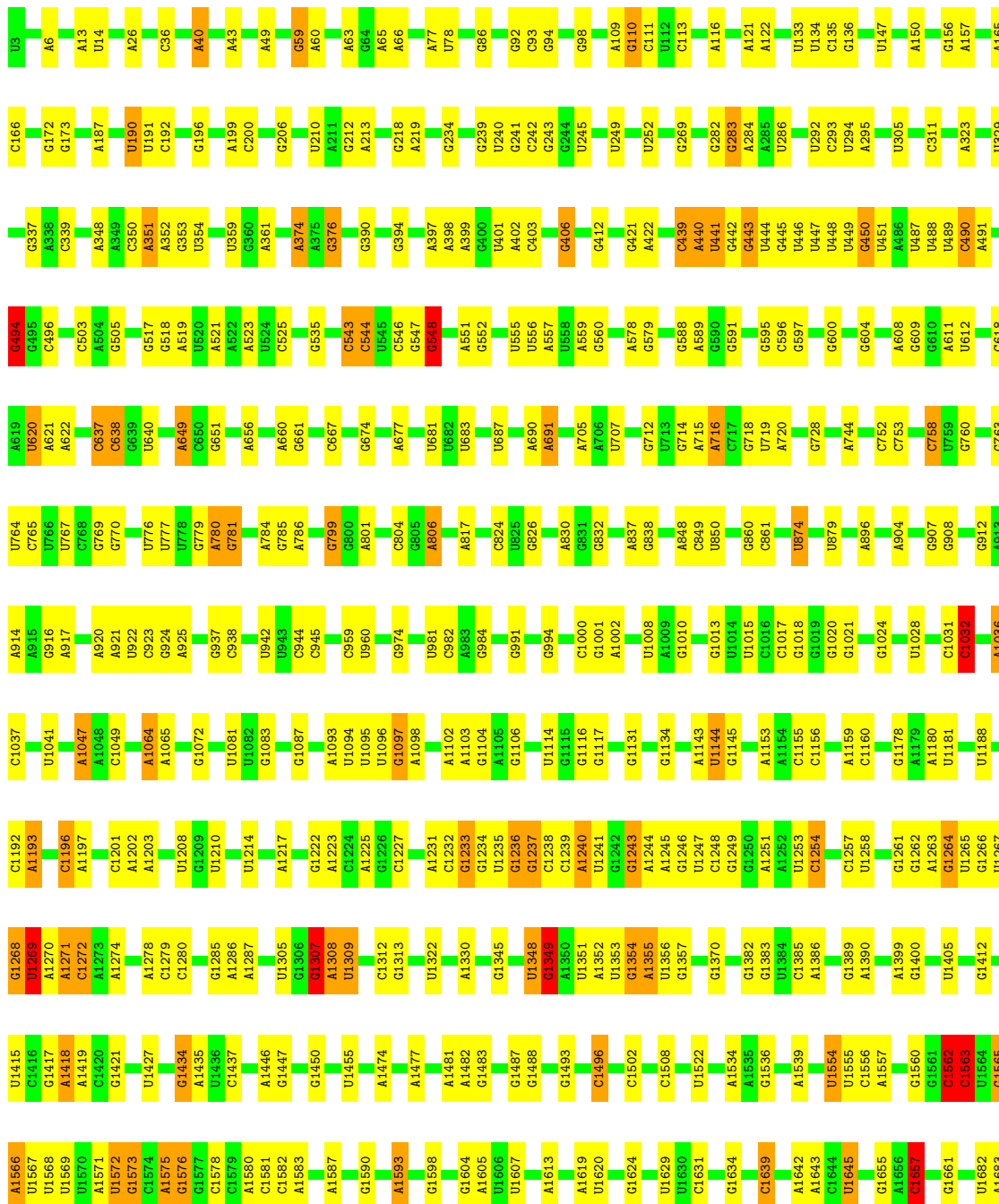
- Molecule 36: 40S ribosomal protein S28-A

Chain L:  81% 19%




- Molecule 37: 25S rRNA

Chain BQ:  72% 23% 5%




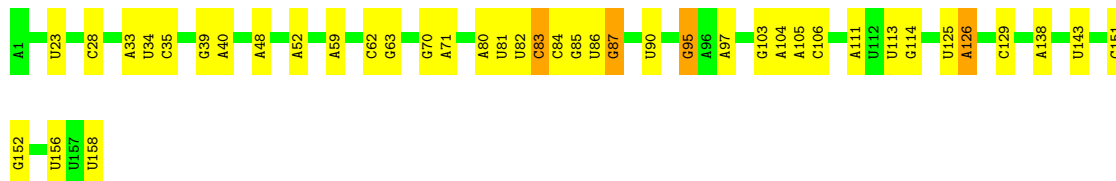
- Molecule 39: 5S rRNA

Chain BR:  83% 14%



- Molecule 40: 5.8S rRNA

Chain BS:  74% 23%



- Molecule 41: 60S ribosomal protein L2-A

Chain AW:  92% 8%



- Molecule 42: 60S ribosomal protein L3

Chain BA:  93% 7%



- Molecule 43: 60S ribosomal protein L4-A

Chain BE:  93% 6%



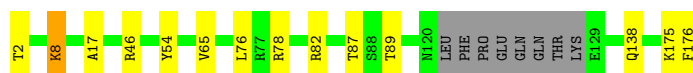
- Molecule 44: 60S ribosomal protein L5

Chain BI:  93% 7%



- Molecule 45: 60S ribosomal protein L6-B

Chain BM:  87% 7% 5%



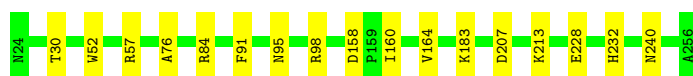
- Molecule 46: 60S ribosomal protein L7-A

Chain BO: 94% 6%



- Molecule 47: 60S ribosomal protein L8-A

Chain AA: 93% 7%



- Molecule 48: 60S ribosomal protein L9-A

Chain AD: 90% 10%



- Molecule 49: 60S ribosomal protein L10

Chain BD: 91% 8%



- Molecule 50: 60S ribosomal protein L11-B

Chain AG: 92% 8%



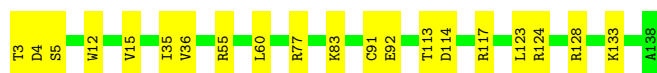
- Molecule 51: 60S ribosomal protein L13-A

Chain AJ: 92% 8%



- Molecule 52: 60S ribosomal protein L14-A

Chain AM: 85% 15%



- Molecule 53: 60S ribosomal protein L15-A

Chain AQ: 96%



- Molecule 54: 60S ribosomal protein L16-A

Chain AU: 95%



- Molecule 55: 60S ribosomal protein L17-A

Chain AX: 96%



- Molecule 56: 60S ribosomal protein L18-A

Chain BB: 91%



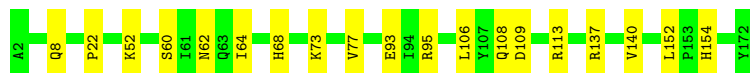
- Molecule 57: 60S ribosomal protein L19-A

Chain BF: 88%



- Molecule 58: 60S ribosomal protein L20-A

Chain BH: 89%



- Molecule 59: 60S ribosomal protein L21-A

Chain BJ: 92%



- Molecule 60: 60S ribosomal protein L22-A

Chain BL: 95% 5%



- Molecule 61: 60S ribosomal protein L23-A

Chain AB: 92% 8%



- Molecule 62: 60S ribosomal protein L24-A

Chain AE: 97% 3%



- Molecule 63: 60S ribosomal protein L25

Chain AH: 95% 5%



- Molecule 64: 60S ribosomal protein L26-A

Chain AK: 96% 4%



- Molecule 65: 60S ribosomal protein L27-A

Chain AN: 93% 7%



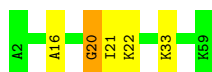
- Molecule 66: 60S ribosomal protein L28

Chain AR: 90% 10%



- Molecule 67: 60S ribosomal protein L29

Chain AV: 91% 7%



- Molecule 68: 60S ribosomal protein L30

Chain AY: 91% 9%



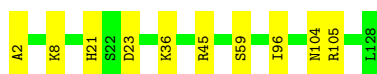
- Molecule 69: 60S ribosomal protein L31-A

Chain BC: 89% 11%



- Molecule 70: 60S ribosomal protein L32

Chain BG: 92% 8%



- Molecule 71: 60S ribosomal protein L33-A

Chain BK: 90% 10%



- Molecule 72: 60S ribosomal protein L34-A

Chain BN: 90% 9%



- Molecule 73: 60S ribosomal protein L35-A

Chain BP: 93% 7%



- Molecule 74: 60S ribosomal protein L36-A

Chain AC: 96%



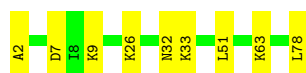
- Molecule 75: 60S ribosomal protein L37-A

Chain AF: 89%



- Molecule 76: 60S ribosomal protein L38

Chain AI: 88%



- Molecule 77: 60S ribosomal protein L39

Chain AL: 86%



- Molecule 78: Ubiquitin-60S ribosomal protein L40

Chain AO: 90%



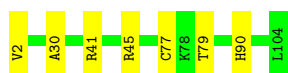
- Molecule 79: 60S ribosomal protein L41-B

Chain AS: 92%



- Molecule 80: 60S ribosomal protein L42-A

Chain AP: 93%



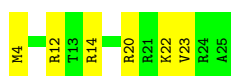
- Molecule 81: 60S ribosomal protein L43-A

Chain AT: 92% 8%



- Molecule 82: 60S ribosomal protein L41-A

Chain BV: 73% 27%



- Molecule 83: General negative regulator of transcription subunit 5

Chain BW: 86% 13%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	176111	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, H2U, T6A, MG, 7MG, 2MG, 5MC, 1MA, M2G, SPD, 1MG

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	2	0.49	0/42211	0.93	63/65773 (0.1%)
2	l	0.50	0/72	0.79	0/110
3	P	0.33	0/1644	0.60	0/2249
4	Q	0.33	0/1823	0.71	1/2447 (0.0%)
5	E	0.33	0/936	0.64	0/1259
6	R	0.36	0/1656	0.64	0/2251
7	A	0.33	0/1754	0.66	1/2361 (0.0%)
8	S	0.33	0/2097	0.64	0/2823
9	B	0.32	0/1625	0.63	0/2197
10	T	0.32	0/1839	0.68	0/2460
11	U	0.33	0/1498	0.68	0/2019
12	V	0.33	0/1501	0.66	0/2006
13	W	0.32	0/1504	0.68	0/2016
14	C	0.35	0/769	0.61	0/1039
15	X	0.36	0/1168	0.64	0/1575
16	D	0.34	0/883	0.74	0/1199
17	Y	0.36	0/1215	0.69	0/1638
18	Z	0.35	0/934	0.71	0/1257
19	F	0.35	0/1125	0.68	1/1510 (0.1%)
20	G	0.31	0/957	0.64	0/1283
21	H	0.32	0/1207	0.69	0/1623
22	I	0.36	0/1130	0.69	1/1517 (0.1%)
23	J	0.33	0/807	0.63	0/1091
24	n	0.50	1/1577 (0.1%)	0.94	1/2457 (0.0%)
25	a	0.34	0/682	0.67	0/921
26	b	0.36	0/1038	0.65	0/1395
27	c	0.35	0/1139	0.68	0/1518
28	d	0.33	0/1087	0.64	0/1449
29	K	0.33	0/661	0.68	0/888
30	e	0.35	0/778	0.69	0/1042
31	f	0.32	0/620	0.60	0/838
32	M	0.33	0/452	0.69	0/600

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.33	0/480	0.80	1/639 (0.2%)
34	N	0.33	0/567	0.69	0/764
35	O	0.30	0/2436	0.62	0/3318
36	L	0.34	0/493	0.78	1/663 (0.2%)
37	BQ	0.57	0/77157	0.93	86/120295 (0.1%)
38	BT	0.42	0/1634	1.00	5/2195 (0.2%)
39	BR	0.50	0/2883	0.85	0/4491
40	BS	0.57	0/3746	0.89	0/5832
41	AW	0.40	0/1933	0.68	0/2598
42	BA	0.38	0/3146	0.65	2/4228 (0.0%)
43	BE	0.37	0/2800	0.63	0/3790
44	BI	0.36	0/2400	0.65	1/3239 (0.0%)
45	BM	0.35	0/1329	0.61	0/1794
46	BO	0.39	0/1821	0.61	0/2451
47	AA	0.35	0/1836	0.58	0/2481
48	AD	0.34	0/1529	0.61	0/2060
49	BD	0.35	0/1801	0.64	0/2416
50	AG	0.33	0/1367	0.71	1/1834 (0.1%)
51	AJ	0.38	0/1568	0.70	0/2106
52	AM	0.33	0/1068	0.68	0/1438
53	AQ	0.42	0/1757	0.72	0/2354
54	AU	0.38	0/1585	0.60	0/2128
55	AX	0.37	0/1439	0.67	0/1938
56	BB	0.36	0/1465	0.69	0/1965
57	BF	0.36	0/1532	0.72	1/2043 (0.0%)
58	BH	0.38	0/1473	0.62	0/1980
59	BJ	0.38	0/1296	0.61	0/1739
60	BL	0.37	0/812	0.61	0/1099
61	AB	0.35	0/1018	0.61	0/1369
62	AE	0.32	0/850	0.58	0/1152
63	AH	0.37	0/979	0.59	0/1321
64	AK	0.33	0/995	0.64	0/1329
65	AN	0.38	0/1106	0.62	0/1485
66	AR	0.37	0/1200	0.62	0/1607
67	AV	0.34	0/473	0.64	0/629
68	AY	0.35	0/745	0.58	0/1001
69	BC	0.36	0/890	0.63	0/1196
70	BG	0.36	0/1034	0.61	0/1385
71	BK	0.41	0/868	0.63	0/1168
72	BN	0.37	0/890	0.70	1/1189 (0.1%)
73	BP	0.34	0/978	0.65	0/1301
74	AC	0.33	0/772	0.66	0/1026
75	AF	0.41	0/660	0.74	0/875

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	AI	0.32	0/618	0.64	0/826
77	AL	0.34	0/443	0.65	0/588
78	AO	0.36	0/416	0.72	1/553 (0.2%)
79	AS	0.34	0/230	0.79	0/296
80	AP	0.36	0/836	0.66	0/1104
81	AT	0.38	0/701	0.71	0/934
82	BV	0.31	0/208	0.98	0/267
83	BW	0.36	0/950	0.66	0/1260
All	All	0.47	1/219602 (0.0%)	0.83	168/322550 (0.1%)

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
11	U	0	1
12	V	0	1
16	D	0	2
19	F	0	1
34	N	0	1
35	O	0	2
38	BT	0	1
43	BE	0	2
47	AA	0	2
48	AD	0	1
52	AM	0	1
67	AV	0	1
69	BC	0	1
73	BP	0	1
All	All	0	18

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	61	C	O3'-P	7.05	1.69	1.61

The worst 5 of 168 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BQ	1254	C	N1-C2-O2	22.03	132.12	118.90
37	BQ	1254	C	N3-C2-O2	-19.43	108.30	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BQ	1234	G	N3-C2-N2	11.76	128.13	119.90
37	BQ	1254	C	C6-N1-C2	-10.62	116.05	120.30
37	BQ	1234	G	N1-C2-N2	-10.18	107.04	116.20

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	D	110	GLY	Peptide
16	D	84	ASN	Peptide
19	F	40	GLU	Peptide
11	U	64	VAL	Peptide
12	V	187	GLU	Sidechain

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	2	37739	0	18988	164	0
2	l	65	0	33	0	0
3	P	1603	0	1610	12	0
4	Q	1798	0	1890	15	0
5	E	916	0	941	12	0
6	R	1626	0	1715	10	0
7	A	1729	0	1812	6	0
8	S	2056	0	2140	16	0
9	B	1605	0	1669	13	0
10	T	1815	0	1894	17	0
11	U	1473	0	1555	13	0
12	V	1476	0	1501	16	0
13	W	1479	0	1556	6	0
14	C	752	0	719	8	0
15	X	1142	0	1209	4	0
16	D	875	0	878	13	0
17	Y	1192	0	1255	10	0
18	Z	923	0	948	12	0
19	F	1105	0	1166	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	G	948	0	990	4	0
21	H	1188	0	1218	13	0
22	I	1112	0	1124	15	0
23	J	797	0	863	5	0
24	n	1624	0	841	0	0
25	a	673	0	662	0	0
26	b	1021	0	1060	0	0
27	c	1121	0	1196	0	0
28	d	1073	0	1132	0	0
29	K	651	0	682	3	0
30	e	765	0	814	0	0
31	f	610	0	633	0	0
32	M	442	0	428	7	0
33	g	472	0	521	0	0
34	N	556	0	550	7	0
35	O	2383	0	2332	21	0
36	L	491	0	524	7	0
37	BQ	68931	0	34632	269	0
38	BT	1609	0	1701	25	0
39	BR	2579	0	1303	9	0
40	BS	3353	0	1695	15	0
41	AW	1899	0	1957	15	0
42	BA	3075	0	3142	21	0
43	BE	2748	0	2859	15	0
44	BI	2351	0	2294	13	0
45	BM	1307	0	1377	12	0
46	BO	1784	0	1862	10	0
47	AA	1804	0	1877	9	0
48	AD	1508	0	1572	15	0
49	BD	1764	0	1804	12	0
50	AG	1346	0	1370	9	0
51	AJ	1543	0	1608	11	0
52	AM	1053	0	1149	16	0
53	AQ	1720	0	1779	8	0
54	AU	1555	0	1659	8	0
55	AX	1416	0	1433	7	0
56	BB	1441	0	1543	13	0
57	BF	1515	0	1606	16	0
58	BH	1437	0	1475	13	0
59	BJ	1272	0	1312	9	0
60	BL	796	0	812	3	0
61	AB	1003	0	1048	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	AE	836	0	706	3	0
63	AH	964	0	1025	3	0
64	AK	984	0	1075	8	0
65	AN	1080	0	1122	7	0
66	AR	1169	0	1211	14	0
67	AV	462	0	491	3	0
68	AY	737	0	792	6	0
69	BC	876	0	912	7	0
70	BG	1013	0	1077	10	0
71	BK	850	0	880	8	0
72	BN	880	0	942	9	0
73	BP	969	0	1078	5	0
74	AC	766	0	844	4	0
75	AF	645	0	645	9	0
76	AI	612	0	682	6	0
77	AL	436	0	475	9	0
78	AO	410	0	442	5	0
79	AS	229	0	273	2	0
80	AP	824	0	888	5	0
81	AT	694	0	734	7	0
82	BV	207	0	250	5	0
83	BW	940	0	973	10	0
84	2	89	0	0	0	0
84	AB	1	0	0	0	0
84	AQ	1	0	0	0	0
84	AW	2	0	0	0	0
84	AX	1	0	0	0	0
84	B	1	0	0	0	0
84	BA	3	0	0	0	0
84	BF	1	0	0	0	0
84	BG	1	0	0	0	0
84	BN	1	0	0	0	0
84	BO	1	0	0	0	0
84	BQ	220	0	0	0	0
84	BR	1	0	0	0	0
84	S	1	0	0	0	0
84	n	3	0	0	0	0
85	AF	1	0	0	0	0
85	AO	1	0	0	0	0
85	AP	1	0	0	0	0
85	AT	1	0	0	0	0
85	BN	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	M	1	0	0	0	0
85	N	1	0	0	0	0
86	BQ	10	0	19	2	0
All	All	205032	0	151454	842	0

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 3.

The worst 5 of 842 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)
83:BW:53:ILE:O	83:BW:57:GLN:HG3	1.69	0.92
67:AV:16:ALA:O	67:AV:20:GLY:HA3	1.75	0.85
38:BT:60:ARG:NH2	38:BT:166:ALA:O	2.10	0.85
37:BQ:687:U:OP2	51:AJ:36:ARG:NH2	2.13	0.81
37:BQ:2883:U:OP1	42:BA:10:ARG:NH2	2.14	0.80

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	204/206 (99%)	188 (92%)	16 (8%)	0	100	100
4	Q	222/232 (96%)	202 (91%)	20 (9%)	0	100	100
5	E	115/117 (98%)	107 (93%)	8 (7%)	0	100	100
6	R	214/216 (99%)	195 (91%)	19 (9%)	0	100	100
7	A	220/222 (99%)	209 (95%)	11 (5%)	0	100	100
8	S	256/258 (99%)	237 (93%)	19 (7%)	0	100	100
9	B	204/206 (99%)	186 (91%)	18 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	T	226/228 (99%)	212 (94%)	14 (6%)	0	100	100
11	U	182/184 (99%)	171 (94%)	11 (6%)	0	100	100
12	V	183/187 (98%)	174 (95%)	9 (5%)	0	100	100
13	W	182/184 (99%)	174 (96%)	8 (4%)	0	100	100
14	C	90/92 (98%)	75 (83%)	15 (17%)	0	100	100
15	X	140/142 (99%)	131 (94%)	9 (6%)	0	100	100
16	D	119/121 (98%)	93 (78%)	23 (19%)	3 (2%)	6	21
17	Y	148/150 (99%)	141 (95%)	7 (5%)	0	100	100
18	Z	125/127 (98%)	113 (90%)	12 (10%)	0	100	100
19	F	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	24	57
20	G	117/125 (94%)	111 (95%)	6 (5%)	0	100	100
21	H	143/145 (99%)	137 (96%)	6 (4%)	0	100	100
22	I	141/143 (99%)	136 (96%)	5 (4%)	0	100	100
23	J	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
25	a	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
26	b	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
27	c	142/144 (99%)	129 (91%)	12 (8%)	1 (1%)	24	57
28	d	132/134 (98%)	127 (96%)	5 (4%)	0	100	100
29	K	80/82 (98%)	72 (90%)	8 (10%)	0	100	100
30	e	95/97 (98%)	89 (94%)	6 (6%)	0	100	100
31	f	79/81 (98%)	72 (91%)	7 (9%)	0	100	100
32	M	51/53 (96%)	51 (100%)	0	0	100	100
33	g	58/60 (97%)	51 (88%)	7 (12%)	0	100	100
34	N	71/73 (97%)	50 (70%)	21 (30%)	0	100	100
35	O	310/312 (99%)	276 (89%)	34 (11%)	0	100	100
36	L	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
38	BT	202/204 (99%)	140 (69%)	62 (31%)	0	100	100
41	AW	249/251 (99%)	234 (94%)	15 (6%)	0	100	100
42	BA	384/386 (100%)	358 (93%)	26 (7%)	0	100	100
43	BE	359/361 (99%)	331 (92%)	27 (8%)	1 (0%)	43	75
44	BI	292/294 (99%)	276 (94%)	16 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BM	163/175 (93%)	154 (94%)	9 (6%)	0	100	100
46	BO	220/222 (99%)	208 (94%)	12 (6%)	0	100	100
47	AA	231/233 (99%)	218 (94%)	13 (6%)	0	100	100
48	AD	189/191 (99%)	175 (93%)	14 (7%)	0	100	100
49	BD	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
50	AG	167/169 (99%)	156 (93%)	10 (6%)	1 (1%)	27	60
51	AJ	191/193 (99%)	174 (91%)	16 (8%)	1 (0%)	31	65
52	AM	134/136 (98%)	125 (93%)	9 (7%)	0	100	100
53	AQ	201/203 (99%)	188 (94%)	13 (6%)	0	100	100
54	AU	195/197 (99%)	192 (98%)	3 (2%)	0	100	100
55	AX	181/183 (99%)	170 (94%)	11 (6%)	0	100	100
56	BB	183/185 (99%)	171 (93%)	12 (7%)	0	100	100
57	BF	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
58	BH	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
59	BJ	157/159 (99%)	150 (96%)	7 (4%)	0	100	100
60	BL	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
61	AB	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
62	AE	124/126 (98%)	112 (90%)	12 (10%)	0	100	100
63	AH	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
64	AK	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
65	AN	133/135 (98%)	127 (96%)	6 (4%)	0	100	100
66	AR	146/148 (99%)	134 (92%)	12 (8%)	0	100	100
67	AV	56/58 (97%)	49 (88%)	6 (11%)	1 (2%)	9	30
68	AY	94/96 (98%)	94 (100%)	0	0	100	100
69	BC	107/109 (98%)	98 (92%)	9 (8%)	0	100	100
70	BG	125/127 (98%)	123 (98%)	2 (2%)	0	100	100
71	BK	104/106 (98%)	101 (97%)	3 (3%)	0	100	100
72	BN	110/112 (98%)	106 (96%)	4 (4%)	0	100	100
73	BP	117/119 (98%)	112 (96%)	5 (4%)	0	100	100
74	AC	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
75	AF	79/81 (98%)	75 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
76	AI	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
77	AL	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
78	AO	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
79	AS	23/25 (92%)	23 (100%)	0	0	100	100
80	AP	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
81	AT	89/91 (98%)	84 (94%)	5 (6%)	0	100	100
82	BV	20/22 (91%)	18 (90%)	2 (10%)	0	100	100
83	BW	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
All	All	11310/11490 (98%)	10528 (93%)	773 (7%)	9 (0%)	56	84

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	D	85	LYS
16	D	126	TRP
16	D	109	GLU
43	BE	4	PRO
67	AV	21	ILE

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	170/173 (98%)	170 (100%)	0	100	100
4	Q	200/205 (98%)	200 (100%)	0	100	100
5	E	95/98 (97%)	95 (100%)	0	100	100
6	R	175/175 (100%)	173 (99%)	2 (1%)	76	93
7	A	182/182 (100%)	180 (99%)	2 (1%)	76	93
8	S	220/220 (100%)	218 (99%)	2 (1%)	81	95
9	B	172/173 (99%)	171 (99%)	1 (1%)	87	96
10	T	189/195 (97%)	188 (100%)	1 (0%)	90	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	U	163/165 (99%)	163 (100%)	0	100	100
12	V	148/149 (99%)	148 (100%)	0	100	100
13	W	156/157 (99%)	154 (99%)	2 (1%)	71	92
14	C	77/85 (91%)	77 (100%)	0	100	100
15	X	126/127 (99%)	125 (99%)	1 (1%)	83	95
16	D	88/98 (90%)	88 (100%)	0	100	100
17	Y	127/127 (100%)	126 (99%)	1 (1%)	83	95
18	Z	90/96 (94%)	89 (99%)	1 (1%)	76	93
19	F	117/117 (100%)	117 (100%)	0	100	100
20	G	101/113 (89%)	101 (100%)	0	100	100
21	H	127/128 (99%)	127 (100%)	0	100	100
22	I	115/115 (100%)	114 (99%)	1 (1%)	81	95
23	J	93/93 (100%)	93 (100%)	0	100	100
25	a	71/74 (96%)	71 (100%)	0	100	100
26	b	110/110 (100%)	110 (100%)	0	100	100
27	c	119/119 (100%)	119 (100%)	0	100	100
28	d	112/112 (100%)	112 (100%)	0	100	100
29	K	67/73 (92%)	66 (98%)	1 (2%)	67	91
30	e	82/83 (99%)	82 (100%)	0	100	100
31	f	70/70 (100%)	69 (99%)	1 (1%)	69	91
32	M	47/47 (100%)	47 (100%)	0	100	100
33	g	50/51 (98%)	50 (100%)	0	100	100
34	N	56/63 (89%)	55 (98%)	1 (2%)	62	88
35	O	250/257 (97%)	248 (99%)	2 (1%)	83	95
36	L	55/56 (98%)	55 (100%)	0	100	100
38	BT	185/185 (100%)	179 (97%)	6 (3%)	42	76
41	AW	190/193 (98%)	190 (100%)	0	100	100
42	BA	321/322 (100%)	318 (99%)	3 (1%)	81	95
43	BE	288/288 (100%)	287 (100%)	1 (0%)	93	98
44	BI	241/243 (99%)	241 (100%)	0	100	100
45	BM	139/154 (90%)	138 (99%)	1 (1%)	85	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	BO	186/186 (100%)	186 (100%)	0	100	100
47	AA	187/191 (98%)	185 (99%)	2 (1%)	76	93
48	AD	168/171 (98%)	168 (100%)	0	100	100
49	BD	185/185 (100%)	184 (100%)	1 (0%)	90	97
50	AG	145/147 (99%)	145 (100%)	0	100	100
51	AJ	154/154 (100%)	151 (98%)	3 (2%)	60	87
52	AM	107/107 (100%)	107 (100%)	0	100	100
53	AQ	175/175 (100%)	175 (100%)	0	100	100
54	AU	160/160 (100%)	159 (99%)	1 (1%)	87	96
55	AX	138/145 (95%)	138 (100%)	0	100	100
56	BB	150/150 (100%)	149 (99%)	1 (1%)	85	96
57	BF	152/153 (99%)	150 (99%)	2 (1%)	71	92
58	BH	155/155 (100%)	155 (100%)	0	100	100
59	BJ	135/136 (99%)	134 (99%)	1 (1%)	85	96
60	BL	87/87 (100%)	87 (100%)	0	100	100
61	AB	104/104 (100%)	104 (100%)	0	100	100
62	AE	56/108 (52%)	56 (100%)	0	100	100
63	AH	104/105 (99%)	103 (99%)	1 (1%)	78	94
64	AK	108/108 (100%)	107 (99%)	1 (1%)	81	95
65	AN	112/115 (97%)	111 (99%)	1 (1%)	81	95
66	AR	117/118 (99%)	117 (100%)	0	100	100
67	AV	46/46 (100%)	45 (98%)	1 (2%)	55	85
68	AY	81/81 (100%)	81 (100%)	0	100	100
69	BC	92/96 (96%)	92 (100%)	0	100	100
70	BG	107/109 (98%)	107 (100%)	0	100	100
71	BK	90/90 (100%)	90 (100%)	0	100	100
72	BN	95/95 (100%)	94 (99%)	1 (1%)	76	93
73	BP	104/104 (100%)	104 (100%)	0	100	100
74	AC	80/81 (99%)	80 (100%)	0	100	100
75	AF	67/67 (100%)	67 (100%)	0	100	100
76	AI	68/68 (100%)	66 (97%)	2 (3%)	45	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	AL	45/45 (100%)	45 (100%)	0	100	100
78	AO	45/47 (96%)	45 (100%)	0	100	100
79	AS	22/23 (96%)	22 (100%)	0	100	100
80	AP	87/88 (99%)	87 (100%)	0	100	100
81	AT	71/71 (100%)	71 (100%)	0	100	100
82	BV	20/20 (100%)	19 (95%)	1 (5%)	27	60
83	BW	109/109 (100%)	105 (96%)	4 (4%)	37	71
All	All	9498/9691 (98%)	9445 (99%)	53 (1%)	88	96

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	BT	118	LYS
45	BM	8	LYS
82	BV	22	LYS
38	BT	161	LYS
42	BA	369	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
38	BT	40	ASN
83	BW	104	GLN
41	AW	7	ASN
21	H	25	ASN
38	BT	197	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1768/1798 (98%)	472 (26%)	39 (2%)
2	1	2/3 (66%)	0	0
24	n	74/75 (98%)	16 (21%)	0
37	BQ	3220/3223 (99%)	654 (20%)	35 (1%)
39	BR	120/121 (99%)	11 (9%)	1 (0%)
40	BS	157/158 (99%)	28 (17%)	1 (0%)
All	All	5341/5378 (99%)	1181 (22%)	76 (1%)

5 of 1181 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A

5 of 76 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1573	A
37	BQ	439	C
37	BQ	3269	U
1	2	1633	A
1	2	1791	A

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

9 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	$\# Z > 2$
24	7MG	n	46	24	22,26,27	3.88	11 (50%)	28,39,42	1.74	8 (28%)
24	5MC	n	48	24	15,22,23	2.96	5 (33%)	19,32,35	1.27	1 (5%)
24	T6A	n	37	24,84	24,34,35	2.50	6 (25%)	24,49,52	2.44	7 (29%)
24	M2G	n	26	24	20,27,28	3.62	7 (35%)	22,40,43	2.06	5 (22%)
24	1MA	n	58	24	15,25,26	4.31	3 (20%)	15,37,40	3.30	2 (13%)
24	H2U	n	16	24	18,21,22	3.51	3 (16%)	21,30,33	2.03	5 (23%)
24	2MG	n	10	24	19,26,27	4.28	7 (36%)	21,38,41	1.90	7 (33%)
24	H2U	n	47	24	18,21,22	3.62	3 (16%)	21,30,33	2.04	5 (23%)
24	1MG	n	9	24	18,26,27	3.66	6 (33%)	19,39,42	1.50	3 (15%)

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
24	7MG	n	46	24	-	0/7/37/38	0/3/3/3
24	5MC	n	48	24	-	2/5/25/26	0/2/2/2
24	T6A	n	37	24,84	-	2/15/41/42	0/3/3/3
24	M2G	n	26	24	-	0/7/29/30	0/3/3/3
24	1MA	n	58	24	-	0/3/25/26	0/3/3/3
24	H2U	n	16	24	-	0/7/38/39	0/2/2/2
24	2MG	n	10	24	-	0/5/27/28	0/3/3/3
24	H2U	n	47	24	-	6/7/38/39	0/2/2/2
24	1MG	n	9	24	-	0/3/25/26	0/3/3/3

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	10	2MG	C2-N2	12.80	1.44	1.34
24	n	47	H2U	C2-N1	12.60	1.53	1.35
24	n	16	H2U	C2-N1	12.10	1.52	1.35
24	n	58	1MA	C4-N3	11.00	1.50	1.35
24	n	46	7MG	C4-N3	9.85	1.46	1.34

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	n	58	1MA	C1'-N9-C4	12.17	148.03	126.64
24	n	16	H2U	C4-N3-C2	-7.17	119.84	125.79
24	n	37	T6A	N6-C10-N11	7.07	123.63	113.76
24	n	47	H2U	C4-N3-C2	-6.97	120.01	125.79
24	n	26	M2G	C1'-N9-C4	5.58	136.44	126.64

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	n	48	5MC	O4'-C4'-C5'-O5'
24	n	48	5MC	C3'-C4'-C5'-O5'
24	n	47	H2U	O4'-C4'-C5'-O5'
24	n	47	H2U	C3'-C4'-C5'-O5'
24	n	47	H2U	O4'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 335 ligands modelled in this entry, 334 are monoatomic - leaving 1 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	$\# Z > 2$
86	SPD	BQ	3621	-	9,9,9	0.30	0	8,8,8	0.61	0

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
86	SPD	BQ	3621	-	-	6/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	BQ	3621	SPD	C3-C4-C5-N6
86	BQ	3621	SPD	N6-C7-C8-C9
86	BQ	3621	SPD	C2-C3-C4-C5
86	BQ	3621	SPD	C7-C8-C9-N10
86	BQ	3621	SPD	C4-C5-N6-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	BQ	3621	SPD	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
37	BQ	2
12	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BQ	1955:U	O3'	2093:A	P	26.76
1	V	123:LYS	C	135:LYS	N	21.11
1	BQ	451:U	O3'	486:A	P	9.87