Full wwPDB EM Validation Report ⓘ

Mar 2, 2025 – 02:38 PM JST

PDB ID	:	8ZDB
EMDB ID	:	EMD-39956
Title	:	Cryo-EM structure of the human ubiquitylated 40S ribosome with RIOK3
Authors	:	Huang, Z.; Wang, M.; Li, Y.; Beckmann, R.; Cheng, J.
Deposited on	:	2024-05-01
Resolution	:	3.60 Å(reported)

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

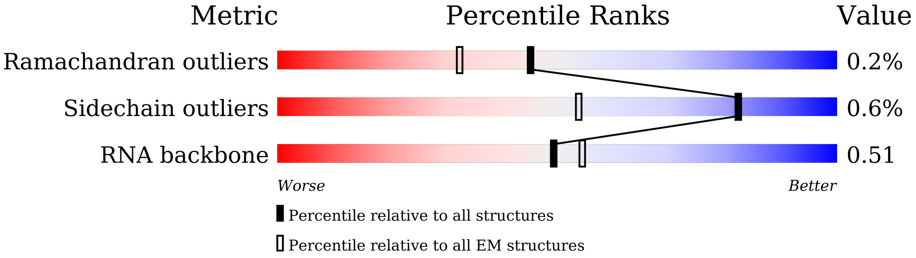
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

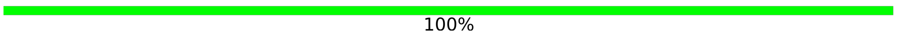
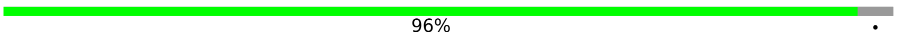
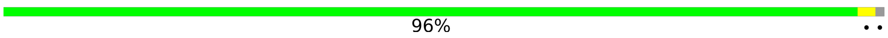
The reported resolution of this entry is 3.60 Å.

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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 of 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 <=5%

Mol	Chain	Length	Quality of chain
1	2	1869	
2	A	295	
3	B	264	
4	C	293	
5	E	263	
6	G	249	
7	H	194	
8	I	208	
9	J	194	

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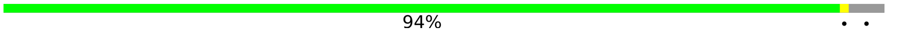
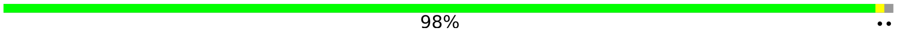
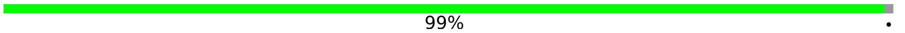
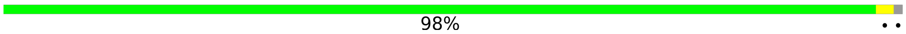
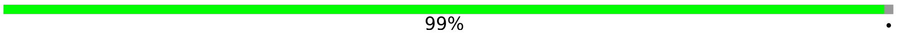
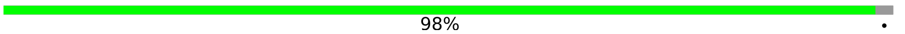
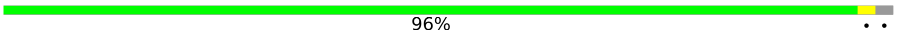
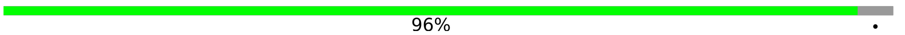
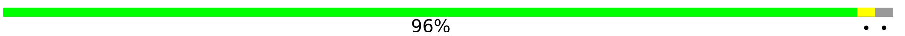
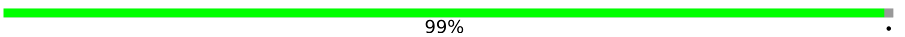
Mol	Chain	Length	Quality of chain
10	L	158	
11	N	151	
12	O	151	
13	V	83	
14	W	130	
15	X	143	
16	Y	133	
17	a	115	
18	b	84	
19	d	56	
20	e	59	
21	h	25	
22	D	243	
23	F	204	
24	K	165	
25	M	132	
26	P	145	
27	Q	146	
28	R	135	
29	S	152	
30	T	145	
31	U	119	
32	Z	125	
33	c	69	
34	f	156	

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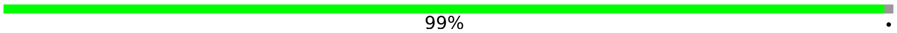
Mol	Chain	Length	Quality of chain
34	i	156	
34	j	156	
35	g	317	
36	p	519	

2 Entry composition ⓘ

There are 37 unique types of molecules in this entry. The entry contains 77772 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1665	35552	15869	6386	11632	1665	0	0

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	206	1624	1035	287	294	8	0	0

- Molecule 3 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	213	1729	1098	309	308	14	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	218	1690	1094	289	297	10	0	0

- Molecule 5 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	262	2076	1324	386	358	8	0	0

- Molecule 6 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	230	1862	1164	371	320	7	0	0

- Molecule 7 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	186	1501	957	276	267	1	0	0

- Molecule 8 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	205	1682	1056	331	290	5	0	0

- Molecule 9 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	180	1499	955	300	242	2	0	0

- Molecule 10 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	151	1229	782	230	211	6	0	0

- Molecule 11 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	N	149	1202	770	228	203	1	0	0

- Molecule 12 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	O	126	948	580	188	174	6	0	0

- Molecule 13 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	V	82	625	384	116	120	5	0	0

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	129	Total 1034	C 659	N 193	O 176	S 6	0	0

- Molecule 15 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	141	Total 1098	C 693	N 219	O 183	S 3	0	0

- Molecule 16 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	124	Total 1014	C 641	N 198	O 170	S 5	0	0

- Molecule 17 is a protein called Small ribosomal subunit protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	101	Total 814	C 507	N 170	O 132	S 5	0	0

- Molecule 18 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	82	Total 640	C 402	N 118	O 113	S 7	0	0

- Molecule 19 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	d	55	Total 459	C 286	N 94	O 74	S 5	0	0

- Molecule 20 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	e	46	Total 368	C 223	N 83	O 61	S 1	0	0

- Molecule 21 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	h	24	231	140	63	26	2	0	0

- Molecule 22 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	D	225	1752	1117	315	313	7	0	0

- Molecule 23 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	F	180	1427	894	266	260	7	0	0

- Molecule 24 is a protein called Small ribosomal subunit protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	K	95	800	522	142	131	5	0	0

- Molecule 25 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	M	123	953	598	169	177	9	0	0

- Molecule 26 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	P	120	984	625	184	168	7	0	0

- Molecule 27 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Q	139	1109	704	210	192	3	0	0

- Molecule 28 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	R	132	1066	669	199	194	4	0	0

- Molecule 29 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	S	143	1184	743	240	200	1	0	0

- Molecule 30 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	T	144	1122	703	217	199	3	0	0

- Molecule 31 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	U	101	803	504	153	142	4	0	0

- Molecule 32 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Z	72	574	368	104	101	1	0	0

- Molecule 33 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	c	61	479	292	95	90	2	0	0

- Molecule 34 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	29	Total 248	C 162	N 51	O 35		0	0
34	i	73	Total 582	C 368	N 99	O 114	S 1	0	0
34	j	73	Total 574	C 364	N 99	O 110	S 1	0	0

- Molecule 35 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	g	314	2440	1537	425	466	12	0	0

- Molecule 36 is a protein called Serine/threonine-protein kinase RIO3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	p	342	2796	1767	497	510	22	0	0

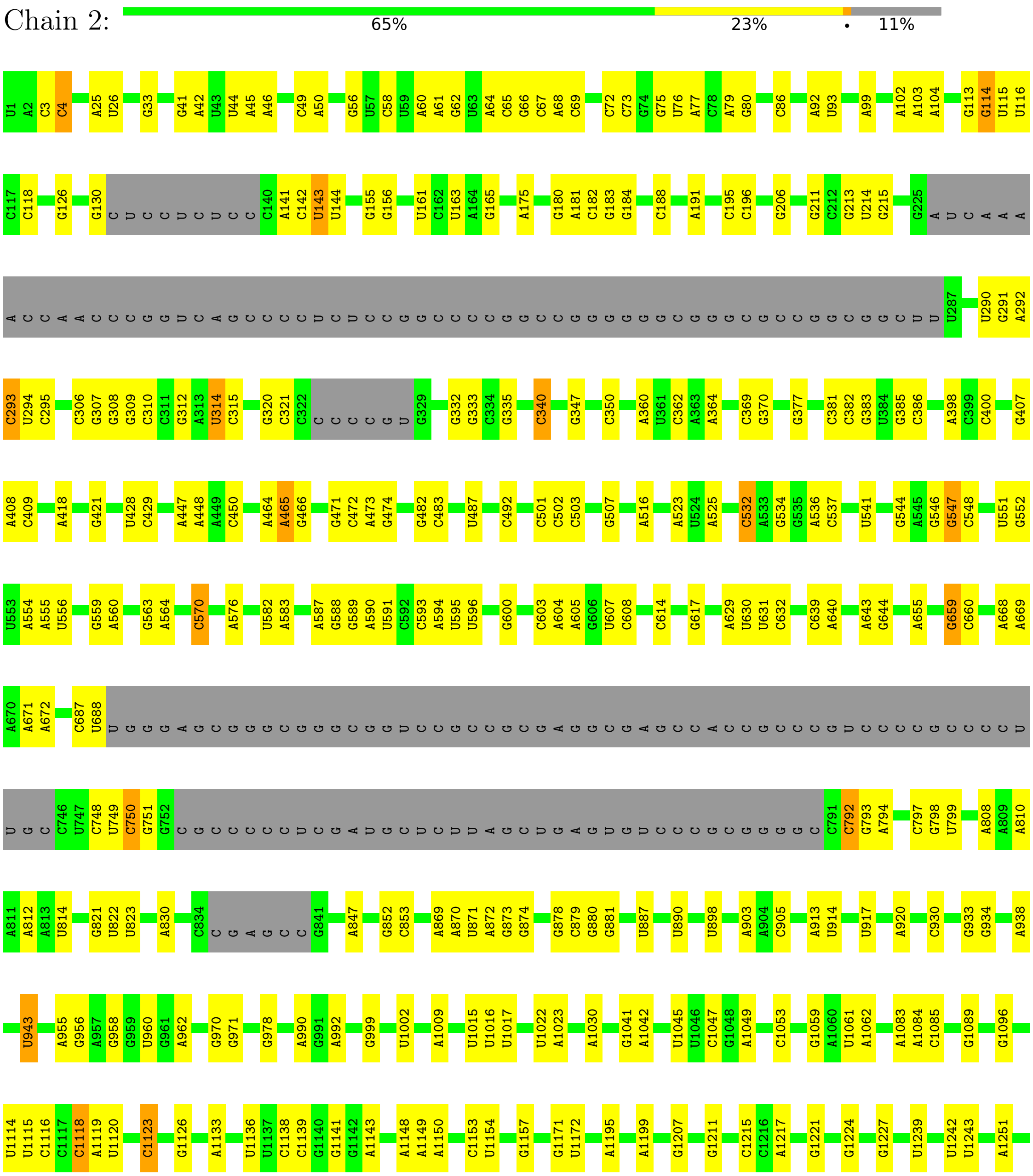
- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

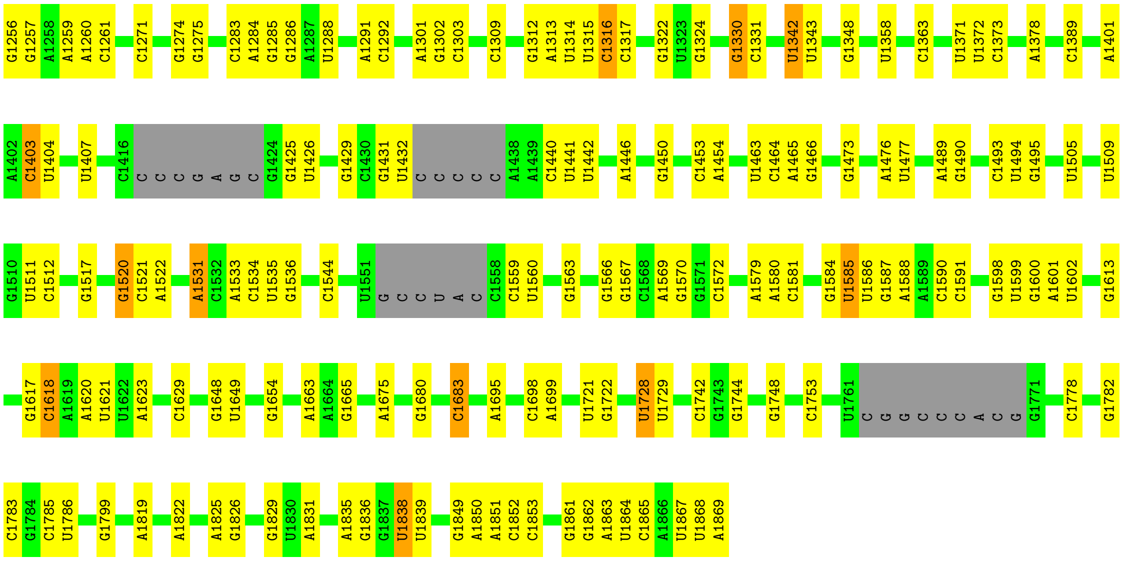
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
37	a	1	1	1	0
			Total	Zn	
37	d	1	1	1	0

3 Residue-property plots (i)

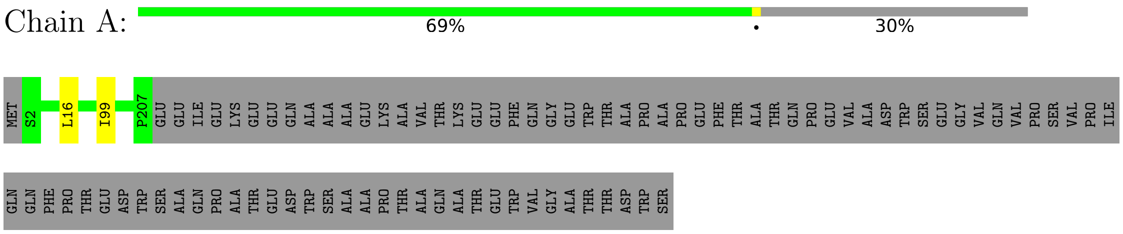
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

- Molecule 1: 18S rRNA

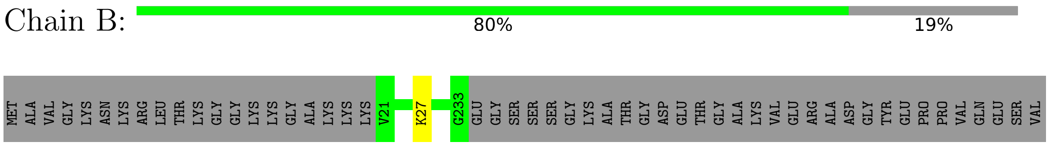




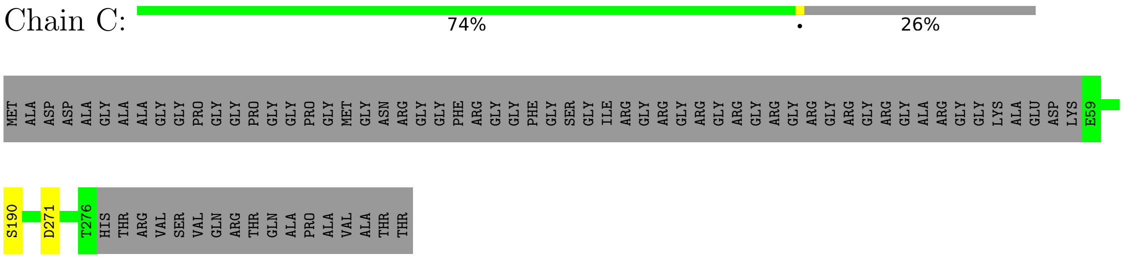
- Molecule 2: Small ribosomal subunit protein uS2



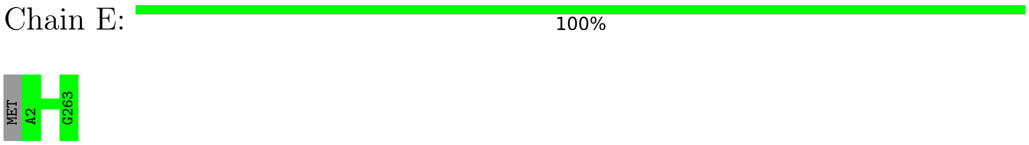
- Molecule 3: Small ribosomal subunit protein eS1



- Molecule 4: Small ribosomal subunit protein uS5

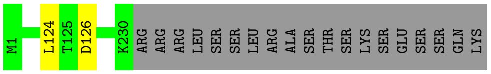


- Molecule 5: Small ribosomal subunit protein eS4, X isoform



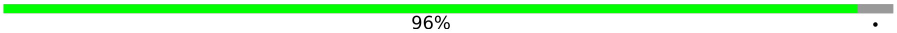
- Molecule 6: Small ribosomal subunit protein eS6

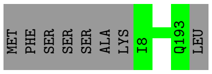
Chain G:



- Molecule 7: Small ribosomal subunit protein eS7

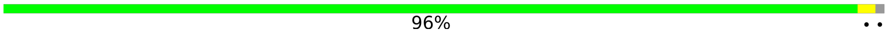
Chain H:

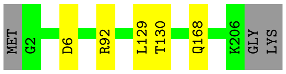




- Molecule 8: Small ribosomal subunit protein eS8

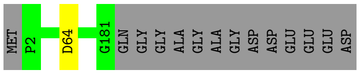
Chain I:





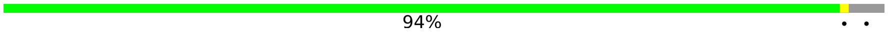
- Molecule 9: Small ribosomal subunit protein uS4

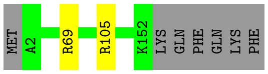
Chain J:



- Molecule 10: Small ribosomal subunit protein uS17

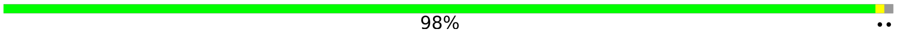
Chain L:

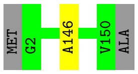




- Molecule 11: Small ribosomal subunit protein uS15

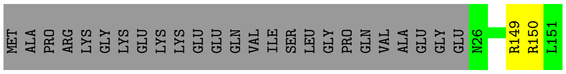
Chain N:





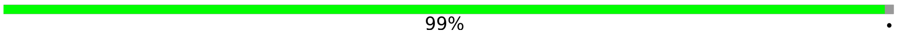
- Molecule 12: Small ribosomal subunit protein uS11

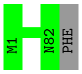
Chain O:



- Molecule 13: Small ribosomal subunit protein eS21

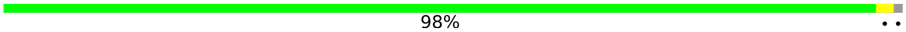
Chain V:

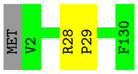




- Molecule 14: Small ribosomal subunit protein uS8

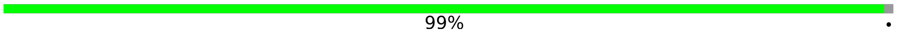
Chain W:

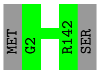




- Molecule 15: Small ribosomal subunit protein uS12

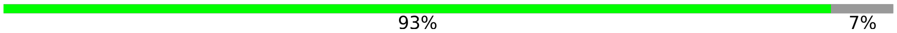
Chain X:





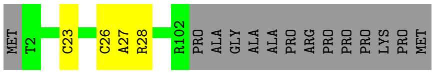
- Molecule 16: Small ribosomal subunit protein eS24

Chain Y:



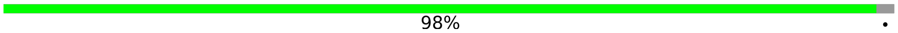
- Molecule 17: Small ribosomal subunit protein eS26

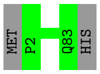
Chain a:



- Molecule 18: Small ribosomal subunit protein eS27

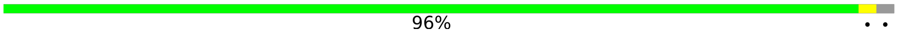
Chain b:

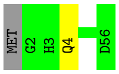




- Molecule 19: Small ribosomal subunit protein uS14

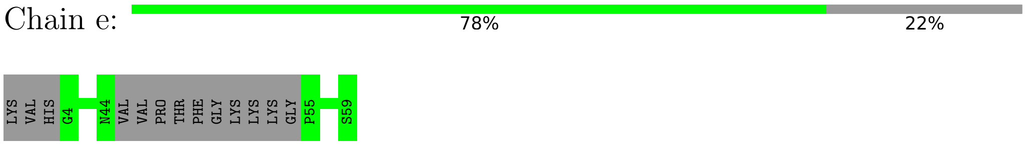
Chain d:





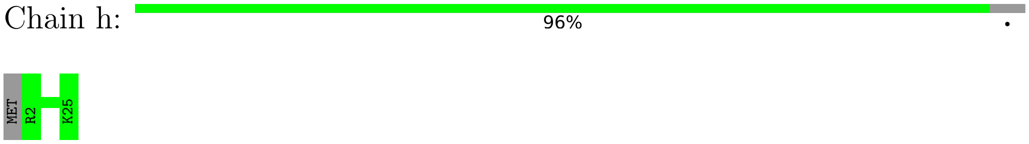
- Molecule 20: Small ribosomal subunit protein eS30

Chain e:



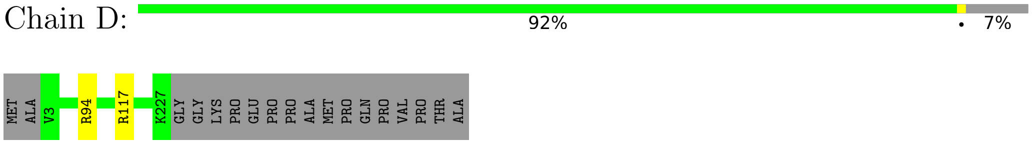
- Molecule 21: Small ribosomal subunit protein eS32

Chain h:



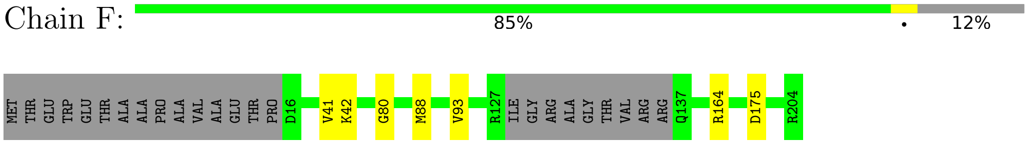
- Molecule 22: Small ribosomal subunit protein uS3

Chain D:



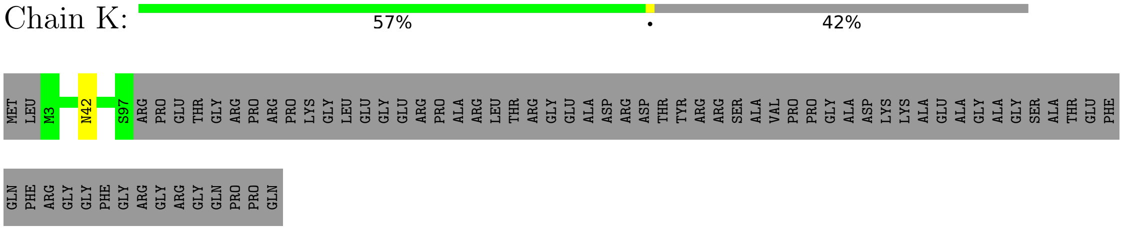
- Molecule 23: Small ribosomal subunit protein uS7

Chain F:



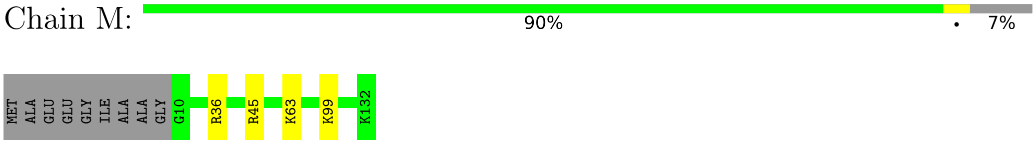
- Molecule 24: Small ribosomal subunit protein eS10

Chain K:



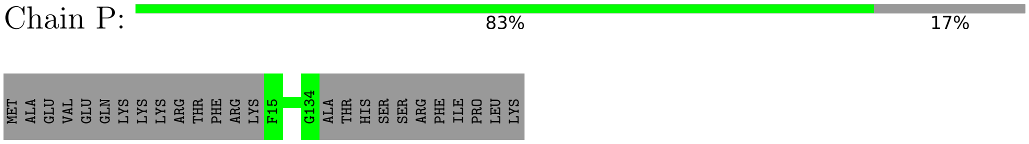
- Molecule 25: Small ribosomal subunit protein eS12

Chain M:



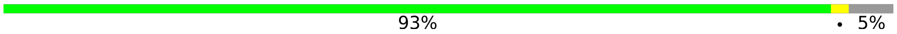
- Molecule 26: Small ribosomal subunit protein uS19

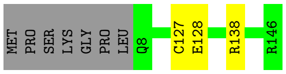
Chain P:



- Molecule 27: Small ribosomal subunit protein uS9

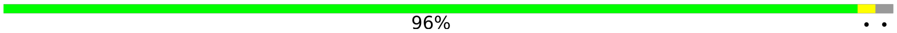
Chain Q:

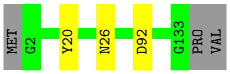




- Molecule 28: Small ribosomal subunit protein eS17

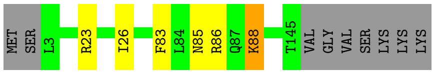
Chain R:





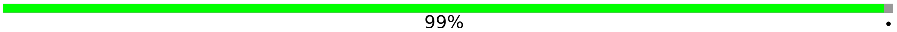
- Molecule 29: Small ribosomal subunit protein uS13

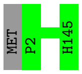
Chain S:



- Molecule 30: Small ribosomal subunit protein eS19

Chain T:



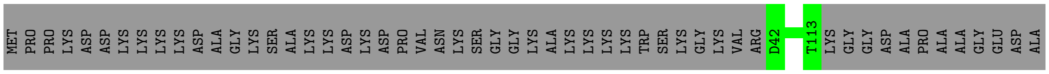


- Molecule 31: Small ribosomal subunit protein uS10

Chain U:

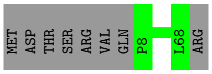
- Molecule 32: Small ribosomal subunit protein eS25

Chain Z:

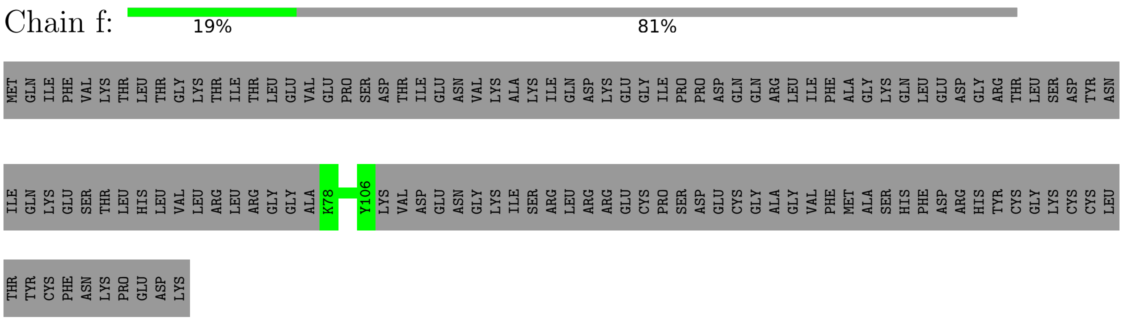


- Molecule 33: Small ribosomal subunit protein eS28

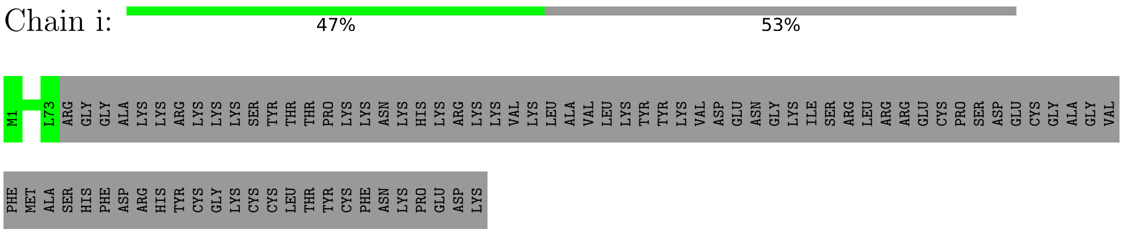
Chain c:



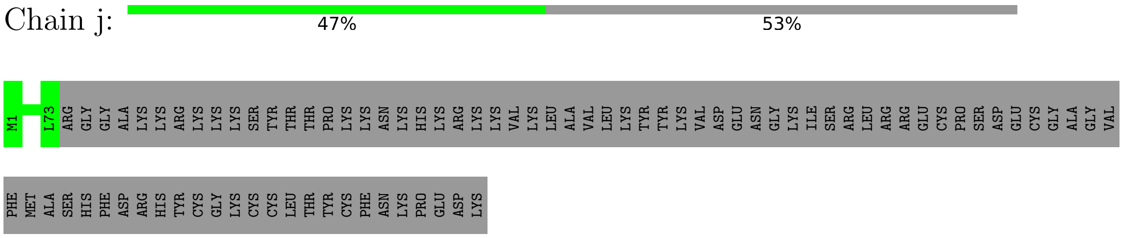
- Molecule 34: Ubiquitin



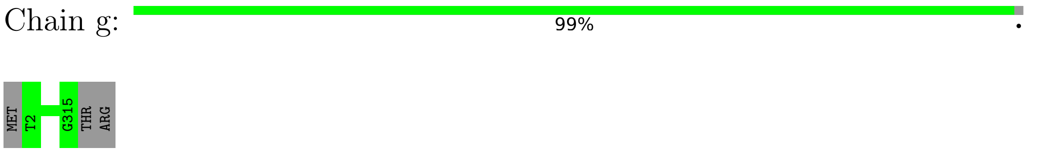
- Molecule 34: Ubiquitin



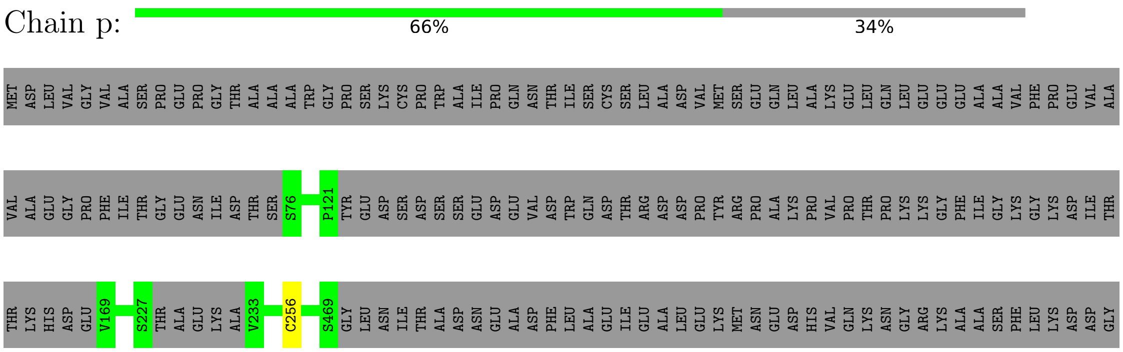
- Molecule 34: Ubiquitin



- Molecule 35: Small ribosomal subunit protein RACK1



- Molecule 36: Serine/threonine-protein kinase RIO3




ASP
PRO
PRO
LEU
LEU
TYR
ASP
GLU

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20179	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 $(e^-/\text{Å}^2)$	44	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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: ZN

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	0.36	0/39755	0.97	107/61954 (0.2%)
2	A	0.28	0/1661	0.59	2/2259 (0.1%)
3	B	0.26	0/1756	0.62	0/2350
4	C	0.29	0/1726	0.58	1/2332 (0.0%)
5	E	0.28	0/2118	0.57	0/2849
6	G	0.28	0/1885	0.64	1/2510 (0.0%)
7	H	0.30	0/1524	0.65	0/2042
8	I	0.31	0/1711	0.67	1/2282 (0.0%)
9	J	0.28	0/1524	0.63	1/2035 (0.0%)
10	L	0.32	0/1250	0.63	0/1673
11	N	0.25	0/1226	0.55	0/1649
12	O	0.30	0/960	0.68	0/1286
13	V	0.30	0/631	0.60	0/844
14	W	0.28	0/1051	0.58	0/1406
15	X	0.29	0/1116	0.60	0/1490
16	Y	0.27	0/1031	0.62	0/1370
17	a	0.42	0/828	0.76	1/1109 (0.1%)
18	b	0.30	0/653	0.64	0/876
19	d	0.29	0/470	0.70	0/623
20	e	0.27	0/370	0.62	0/482
21	h	0.23	0/232	0.76	0/295
22	D	0.28	0/1780	0.63	0/2397
23	F	0.28	0/1447	0.66	2/1944 (0.1%)
24	K	0.29	0/824	0.66	0/1112
25	M	0.27	0/963	0.54	0/1291
26	P	0.33	0/1003	0.68	0/1341
27	Q	0.31	0/1126	0.66	0/1506
28	R	0.29	0/1080	0.71	1/1449 (0.1%)
29	S	0.38	0/1202	0.78	1/1610 (0.1%)
30	T	0.28	0/1142	0.62	0/1530
31	U	0.28	0/813	0.65	0/1092
32	Z	0.28	0/580	0.74	0/780

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	c	0.27	0/481	0.72	0/643
34	f	0.31	0/251	0.61	0/326
34	i	0.25	0/588	0.55	0/792
34	j	0.25	0/580	0.55	0/782
35	g	0.26	0/2497	0.56	0/3399
36	p	0.28	0/2853	0.57	0/3824
All	All	0.32	0/82688	0.82	118/119534 (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
14	W	0	1
23	F	0	1
All	All	0	2

There are no bond length outliers.

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	293	C	N1-C2-O2	11.46	125.78	118.90
1	2	293	C	C2-N1-C1’	10.28	130.11	118.80
1	2	501	C	N1-C2-O2	9.88	124.83	118.90
1	2	1453	C	N1-C2-O2	9.61	124.67	118.90
1	2	501	C	C2-N1-C1’	9.51	129.26	118.80
1	2	1453	C	C2-N1-C1’	9.48	129.23	118.80
1	2	1618	C	N1-C2-O2	8.57	124.04	118.90
1	2	853	C	C2-N1-C1’	8.48	128.13	118.80
1	2	293	C	N3-C2-O2	-8.21	116.16	121.90
1	2	501	C	N3-C2-O2	-7.95	116.34	121.90
1	2	1022	U	C2-N1-C1’	7.81	127.07	117.70
1	2	196	C	N3-C2-O2	-7.71	116.50	121.90
1	2	1453	C	N3-C2-O2	-7.58	116.59	121.90
1	2	853	C	N1-C2-O2	7.48	123.39	118.90
1	2	293	C	C6-N1-C1’	-7.43	111.89	120.80
1	2	1292	C	N1-C2-O2	7.33	123.30	118.90
1	2	1520	G	C4-N9-C1’	7.22	135.89	126.50
1	2	1531	A	P-O3’-C3’	7.20	128.33	119.70
1	2	547	G	P-O3’-C3’	7.12	128.25	119.70
1	2	1590	C	N1-C2-O2	7.00	123.10	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1618	C	N3-C2-O2	-7.00	117.00	121.90
1	2	630	U	C2-N1-C1'	6.95	126.04	117.70
1	2	1118	C	N1-C2-O2	6.92	123.06	118.90
1	2	501	C	C6-N1-C2	-6.88	117.55	120.30
1	2	853	C	N3-C2-O2	-6.77	117.16	121.90
1	2	1618	C	C2-N1-C1'	6.76	126.23	118.80
1	2	1520	G	C8-N9-C1'	-6.66	118.34	127.00
1	2	1453	C	C6-N1-C1'	-6.58	112.90	120.80
1	2	1016	U	N1-C2-O2	6.58	127.40	122.80
1	2	630	U	N1-C2-O2	6.52	127.36	122.80
1	2	1172	U	C2-N1-C1'	6.50	125.51	117.70
1	2	853	C	C6-N1-C2	-6.49	117.71	120.30
1	2	1016	U	N3-C2-O2	-6.44	117.69	122.20
1	2	1389	C	C2-N1-C1'	6.43	125.88	118.80
1	2	930	C	N1-C2-O2	6.42	122.75	118.90
1	2	1520	G	P-O3'-C3'	6.39	127.37	119.70
1	2	501	C	C6-N1-C1'	-6.38	113.14	120.80
1	2	570	C	N1-C2-O2	6.34	122.71	118.90
1	2	630	U	N3-C2-O2	-6.29	117.80	122.20
1	2	130	G	C4-N9-C1'	6.28	134.66	126.50
1	2	1123	C	N1-C2-O2	6.24	122.64	118.90
17	a	28	ARG	CB-CA-C	-6.23	97.94	110.40
1	2	1838	U	P-O3'-C3'	6.17	127.10	119.70
1	2	1016	U	C2-N1-C1'	6.17	125.10	117.70
1	2	1520	G	N3-C4-N9	6.15	129.69	126.00
4	C	271	ASP	CB-CG-OD1	6.15	123.83	118.30
1	2	532	C	C2-N1-C1'	6.14	125.56	118.80
1	2	195	C	N1-C2-O2	6.13	122.58	118.90
23	F	175	ASP	CB-CG-OD1	6.07	123.77	118.30
1	2	1453	C	C6-N1-C2	-6.07	117.87	120.30
1	2	1172	U	N1-C2-O2	6.04	127.03	122.80
1	2	1591	C	N1-C2-O2	5.97	122.48	118.90
1	2	814	U	N1-C2-O2	5.89	126.92	122.80
1	2	659	G	C4-N9-C1'	5.88	134.15	126.50
1	2	196	C	C6-N1-C2	-5.88	117.95	120.30
1	2	1292	C	N3-C2-O2	-5.87	117.79	121.90
1	2	930	C	C2-N1-C1'	5.87	125.25	118.80
1	2	293	C	C5-C6-N1	5.86	123.93	121.00
1	2	340	C	N1-C2-O2	5.82	122.39	118.90
1	2	814	U	N3-C2-O2	-5.81	118.13	122.20
1	2	570	C	C2-N1-C1'	5.79	125.17	118.80
1	2	541	U	N1-C2-O2	5.76	126.83	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1292	C	C2-N1-C1’	5.75	125.13	118.80
2	A	16	LEU	CA-CB-CG	5.74	128.51	115.30
1	2	114	G	P-O3’-C3’	5.74	126.59	119.70
1	2	293	C	C6-N1-C2	-5.74	118.00	120.30
1	2	130	G	N3-C4-C5	-5.73	125.74	128.60
1	2	1118	C	N3-C2-O2	-5.70	117.91	121.90
1	2	1407	U	C5-C4-O4	-5.70	122.48	125.90
1	2	1590	C	N3-C2-O2	-5.70	117.91	121.90
1	2	1585	U	P-O3’-C3’	5.69	126.53	119.70
1	2	1022	U	N1-C2-O2	5.64	126.75	122.80
1	2	1728	U	C2-N1-C1’	5.62	124.45	117.70
1	2	130	G	N3-C4-N9	5.60	129.36	126.00
1	2	823	U	C2-N1-C1’	5.57	124.38	117.70
1	2	501	C	C5-C6-N1	5.55	123.78	121.00
1	2	4	C	C2-N1-C1’	5.54	124.89	118.80
1	2	853	C	C6-N1-C1’	-5.54	114.16	120.80
28	R	92	ASP	CB-CG-OD1	5.52	123.27	118.30
1	2	314	U	N3-C2-O2	-5.52	118.34	122.20
1	2	1172	U	C5-C6-N1	5.51	125.45	122.70
1	2	1389	C	N1-C2-O2	5.46	122.18	118.90
1	2	4	C	C6-N1-C2	-5.46	118.12	120.30
29	S	85	ASN	CB-CA-C	-5.45	99.49	110.40
2	A	99	ILE	CG1-CB-CG2	-5.45	99.41	111.40
1	2	750	C	P-O3’-C3’	5.42	126.21	119.70
1	2	1342	U	P-O3’-C3’	5.40	126.18	119.70
1	2	1261	C	N1-C2-O2	5.39	122.14	118.90
1	2	541	U	C2-N1-C1’	5.39	124.16	117.70
1	2	1403	C	P-O3’-C3’	5.38	126.16	119.70
1	2	1618	C	C6-N1-C2	-5.38	118.15	120.30
1	2	823	U	N3-C2-O2	-5.38	118.44	122.20
1	2	1453	C	C5-C6-N1	5.37	123.69	121.00
1	2	1123	C	N3-C2-O2	-5.36	118.15	121.90
1	2	1022	U	C6-N1-C1’	-5.34	113.72	121.20
1	2	943	U	C2-N1-C1’	5.32	124.08	117.70
1	2	465	A	P-O3’-C3’	5.31	126.08	119.70
1	2	86	C	C2-N1-C1’	5.30	124.64	118.80
1	2	905	C	N3-C2-O2	-5.30	118.19	121.90
6	G	124	LEU	CA-CB-CG	5.29	127.46	115.30
1	2	309	G	O4’-C1’-N9	5.28	112.42	108.20
1	2	118	C	N1-C2-O2	5.28	122.06	118.90
8	I	6	ASP	CB-CG-OD1	5.28	123.05	118.30
23	F	88	MET	CA-CB-CG	5.23	122.19	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1590	C	C2-N1-C1'	5.19	124.51	118.80
1	2	130	G	C8-N9-C1'	-5.17	120.27	127.00
1	2	792	C	C2-N1-C1'	5.17	124.48	118.80
1	2	314	U	P-O3'-C3'	5.14	125.87	119.70
9	J	64	ASP	CB-CG-OD1	5.14	122.93	118.30
1	2	541	U	N3-C2-O2	-5.13	118.61	122.20
1	2	143	U	P-O3'-C3'	5.12	125.85	119.70
1	2	1683	C	N1-C2-O2	5.12	121.97	118.90
1	2	165	G	C4-N9-C1'	5.12	133.15	126.50
1	2	1330	G	P-O3'-C3'	5.10	125.82	119.70
1	2	1389	C	C6-N1-C2	-5.08	118.27	120.30
1	2	1590	C	C6-N1-C2	-5.08	118.27	120.30
1	2	92	A	OP2-P-O3'	5.02	116.24	105.20
1	2	1316	C	P-O3'-C3'	5.01	125.71	119.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	F	93	VAL	Peptide
14	W	28	ARG	Peptide

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
2	A	204/295 (69%)	189 (93%)	15 (7%)	0	100	100
3	B	211/264 (80%)	200 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	216/293 (74%)	201 (93%)	14 (6%)	1 (0%)	25	59
5	E	260/263 (99%)	248 (95%)	12 (5%)	0	100	100
6	G	228/249 (92%)	216 (95%)	11 (5%)	1 (0%)	30	63
7	H	184/194 (95%)	175 (95%)	9 (5%)	0	100	100
8	I	203/208 (98%)	190 (94%)	13 (6%)	0	100	100
9	J	178/194 (92%)	168 (94%)	10 (6%)	0	100	100
10	L	149/158 (94%)	142 (95%)	7 (5%)	0	100	100
11	N	147/151 (97%)	142 (97%)	4 (3%)	1 (1%)	19	53
12	O	124/151 (82%)	117 (94%)	6 (5%)	1 (1%)	16	51
13	V	80/83 (96%)	77 (96%)	3 (4%)	0	100	100
14	W	127/130 (98%)	123 (97%)	3 (2%)	1 (1%)	16	51
15	X	139/143 (97%)	125 (90%)	14 (10%)	0	100	100
16	Y	122/133 (92%)	118 (97%)	4 (3%)	0	100	100
17	a	99/115 (86%)	92 (93%)	6 (6%)	1 (1%)	13	46
18	b	80/84 (95%)	76 (95%)	4 (5%)	0	100	100
19	d	53/56 (95%)	52 (98%)	0	1 (2%)	6	35
20	e	42/59 (71%)	40 (95%)	2 (5%)	0	100	100
21	h	22/25 (88%)	22 (100%)	0	0	100	100
22	D	223/243 (92%)	217 (97%)	6 (3%)	0	100	100
23	F	176/204 (86%)	153 (87%)	20 (11%)	3 (2%)	7	37
24	K	93/165 (56%)	90 (97%)	3 (3%)	0	100	100
25	M	121/132 (92%)	115 (95%)	6 (5%)	0	100	100
26	P	118/145 (81%)	115 (98%)	3 (2%)	0	100	100
27	Q	137/146 (94%)	125 (91%)	12 (9%)	0	100	100
28	R	130/135 (96%)	118 (91%)	11 (8%)	1 (1%)	16	51
29	S	141/152 (93%)	131 (93%)	9 (6%)	1 (1%)	19	53
30	T	142/145 (98%)	140 (99%)	2 (1%)	0	100	100
31	U	99/119 (83%)	95 (96%)	4 (4%)	0	100	100
32	Z	70/125 (56%)	67 (96%)	3 (4%)	0	100	100
33	c	59/69 (86%)	55 (93%)	4 (7%)	0	100	100
34	f	27/156 (17%)	22 (82%)	5 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	i	71/156 (46%)	70 (99%)	1 (1%)	0	100	100
34	j	71/156 (46%)	70 (99%)	1 (1%)	0	100	100
35	g	312/317 (98%)	293 (94%)	19 (6%)	0	100	100
36	p	336/519 (65%)	318 (95%)	18 (5%)	0	100	100
All	All	5194/6332 (82%)	4907 (94%)	275 (5%)	12 (0%)	45	73

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	190	SER
6	G	126	ASP
11	N	146	ALA
28	R	20	TYR
17	a	27	ALA
19	d	4	GLN
23	F	80	GLY
23	F	42	LYS
12	O	149	ARG
29	S	88	LYS
23	F	41	VAL
14	W	29	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
2	A	172/243 (71%)	172 (100%)	0	100	100
3	B	194/231 (84%)	193 (100%)	1 (0%)	86	93
4	C	184/225 (82%)	184 (100%)	0	100	100
5	E	224/225 (100%)	224 (100%)	0	100	100
6	G	200/218 (92%)	200 (100%)	0	100	100
7	H	167/174 (96%)	167 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	178/180 (99%)	174 (98%)	4 (2%)	47	69
9	J	160/168 (95%)	160 (100%)	0	100	100
10	L	135/142 (95%)	133 (98%)	2 (2%)	60	78
11	N	130/131 (99%)	130 (100%)	0	100	100
12	O	99/119 (83%)	98 (99%)	1 (1%)	73	85
13	V	66/67 (98%)	66 (100%)	0	100	100
14	W	112/113 (99%)	112 (100%)	0	100	100
15	X	113/115 (98%)	113 (100%)	0	100	100
16	Y	108/115 (94%)	108 (100%)	0	100	100
17	a	88/98 (90%)	86 (98%)	2 (2%)	45	68
18	b	74/76 (97%)	74 (100%)	0	100	100
19	d	48/49 (98%)	48 (100%)	0	100	100
20	e	37/48 (77%)	37 (100%)	0	100	100
21	h	23/24 (96%)	23 (100%)	0	100	100
22	D	189/202 (94%)	187 (99%)	2 (1%)	70	83
23	F	153/170 (90%)	152 (99%)	1 (1%)	81	90
24	K	86/136 (63%)	85 (99%)	1 (1%)	67	82
25	M	104/108 (96%)	100 (96%)	4 (4%)	28	57
26	P	107/130 (82%)	107 (100%)	0	100	100
27	Q	115/121 (95%)	112 (97%)	3 (3%)	41	65
28	R	118/122 (97%)	117 (99%)	1 (1%)	79	88
29	S	124/132 (94%)	119 (96%)	5 (4%)	27	56
30	T	114/115 (99%)	114 (100%)	0	100	100
31	U	93/107 (87%)	93 (100%)	0	100	100
32	Z	64/103 (62%)	64 (100%)	0	100	100
33	c	54/62 (87%)	54 (100%)	0	100	100
34	f	27/140 (19%)	27 (100%)	0	100	100
34	i	67/140 (48%)	67 (100%)	0	100	100
34	j	65/140 (46%)	65 (100%)	0	100	100
35	g	272/275 (99%)	272 (100%)	0	100	100
36	p	308/454 (68%)	307 (100%)	1 (0%)	91	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4572/5418 (84%)	4544 (99%)	28 (1%)	82 92

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	27	LYS
8	I	92	ARG
8	I	129	LEU
8	I	130	THR
8	I	168	GLN
10	L	69	ARG
10	L	105	ARG
12	O	150	ARG
17	a	23	CYS
17	a	26	CYS
22	D	94	ARG
22	D	117	ARG
23	F	164	ARG
24	K	42	ASN
25	M	36	ARG
25	M	45	ARG
25	M	63	LYS
25	M	99	LYS
27	Q	127	CYS
27	Q	128	GLU
27	Q	138	ARG
28	R	26	ASN
29	S	23	ARG
29	S	26	ILE
29	S	83	PHE
29	S	86	ARG
29	S	88	LYS
36	p	256	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	115	GLN
4	C	120	GLN
6	G	59	GLN
17	a	25	ASN

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Mol	Chain	Res	Type
22	D	101	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1654/1869 (88%)	418 (25%)	40 (2%)

All (418) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	C
1	2	4	C
1	2	25	A
1	2	26	U
1	2	33	G
1	2	41	G
1	2	42	A
1	2	44	U
1	2	45	A
1	2	46	A
1	2	49	C
1	2	50	A
1	2	56	G
1	2	58	C
1	2	61	A
1	2	62	G
1	2	64	A
1	2	65	C
1	2	66	G
1	2	67	C
1	2	68	A
1	2	69	C
1	2	72	C
1	2	73	C
1	2	75	G
1	2	76	U
1	2	77	A
1	2	79	A
1	2	80	G
1	2	93	U
1	2	99	A

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Mol	Chain	Res	Type
1	2	103	A
1	2	104	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	116	U
1	2	126	G
1	2	141	A
1	2	142	C
1	2	143	U
1	2	144	U
1	2	155	G
1	2	156	G
1	2	161	U
1	2	163	U
1	2	175	A
1	2	181	A
1	2	182	C
1	2	183	G
1	2	184	G
1	2	188	C
1	2	191	A
1	2	206	G
1	2	211	G
1	2	213	G
1	2	214	U
1	2	215	G
1	2	290	U
1	2	291	G
1	2	292	A
1	2	293	C
1	2	294	U
1	2	295	C
1	2	306	C
1	2	307	G
1	2	308	G
1	2	310	C
1	2	312	G
1	2	315	C
1	2	320	G
1	2	321	C
1	2	332	G

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Mol	Chain	Res	Type
1	2	333	G
1	2	335	G
1	2	340	C
1	2	347	G
1	2	350	C
1	2	360	A
1	2	362	C
1	2	364	A
1	2	369	C
1	2	370	G
1	2	377	G
1	2	381	C
1	2	383	G
1	2	385	G
1	2	386	C
1	2	398	A
1	2	400	C
1	2	407	G
1	2	408	A
1	2	409	C
1	2	418	A
1	2	421	G
1	2	428	U
1	2	429	C
1	2	447	A
1	2	448	A
1	2	450	C
1	2	464	A
1	2	465	A
1	2	466	G
1	2	471	G
1	2	472	C
1	2	473	A
1	2	474	G
1	2	482	G
1	2	483	C
1	2	487	U
1	2	492	C
1	2	502	C
1	2	503	C
1	2	507	G
1	2	516	A

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Mol	Chain	Res	Type
1	2	523	A
1	2	525	A
1	2	532	C
1	2	534	G
1	2	536	A
1	2	537	C
1	2	544	G
1	2	546	G
1	2	548	C
1	2	551	U
1	2	552	G
1	2	554	A
1	2	555	A
1	2	556	U
1	2	559	G
1	2	560	A
1	2	563	G
1	2	564	A
1	2	570	C
1	2	576	A
1	2	582	U
1	2	583	A
1	2	587	A
1	2	588	G
1	2	589	G
1	2	590	A
1	2	591	U
1	2	593	C
1	2	595	U
1	2	596	U
1	2	600	G
1	2	603	C
1	2	604	A
1	2	605	A
1	2	607	U
1	2	608	C
1	2	614	C
1	2	617	G
1	2	629	A
1	2	631	U
1	2	632	C
1	2	639	C

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Mol	Chain	Res	Type
1	2	640	A
1	2	643	A
1	2	644	G
1	2	655	A
1	2	659	G
1	2	660	C
1	2	668	A
1	2	669	A
1	2	671	A
1	2	672	A
1	2	687	C
1	2	688	U
1	2	748	C
1	2	749	U
1	2	750	C
1	2	751	G
1	2	792	C
1	2	793	G
1	2	794	A
1	2	798	G
1	2	799	U
1	2	808	A
1	2	810	A
1	2	812	A
1	2	821	G
1	2	822	U
1	2	830	A
1	2	847	A
1	2	852	G
1	2	869	A
1	2	870	A
1	2	871	U
1	2	872	A
1	2	873	G
1	2	874	G
1	2	878	G
1	2	879	C
1	2	880	G
1	2	881	G
1	2	887	U
1	2	890	U
1	2	898	U

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Mol	Chain	Res	Type
1	2	903	A
1	2	913	A
1	2	914	U
1	2	917	U
1	2	920	A
1	2	933	G
1	2	934	G
1	2	938	A
1	2	943	U
1	2	955	A
1	2	956	G
1	2	958	G
1	2	960	U
1	2	962	A
1	2	970	G
1	2	971	G
1	2	978	G
1	2	990	A
1	2	992	A
1	2	999	G
1	2	1002	U
1	2	1009	A
1	2	1015	U
1	2	1017	U
1	2	1023	A
1	2	1030	A
1	2	1041	G
1	2	1042	A
1	2	1045	U
1	2	1047	C
1	2	1049	A
1	2	1053	C
1	2	1059	G
1	2	1061	U
1	2	1062	A
1	2	1083	A
1	2	1084	A
1	2	1085	C
1	2	1089	G
1	2	1096	G
1	2	1114	U
1	2	1115	U

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Mol	Chain	Res	Type
1	2	1116	C
1	2	1118	C
1	2	1119	A
1	2	1120	U
1	2	1123	C
1	2	1126	G
1	2	1133	A
1	2	1136	U
1	2	1138	C
1	2	1139	C
1	2	1141	G
1	2	1143	A
1	2	1148	A
1	2	1149	A
1	2	1150	A
1	2	1153	C
1	2	1154	U
1	2	1157	G
1	2	1171	G
1	2	1195	A
1	2	1199	A
1	2	1207	G
1	2	1211	G
1	2	1215	C
1	2	1217	A
1	2	1221	G
1	2	1224	G
1	2	1227	G
1	2	1239	U
1	2	1242	U
1	2	1243	U
1	2	1251	A
1	2	1256	G
1	2	1257	G
1	2	1259	A
1	2	1260	A
1	2	1271	C
1	2	1274	G
1	2	1275	G
1	2	1283	C
1	2	1284	A
1	2	1285	G

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Mol	Chain	Res	Type
1	2	1286	G
1	2	1288	U
1	2	1291	A
1	2	1301	A
1	2	1302	G
1	2	1303	C
1	2	1309	C
1	2	1312	G
1	2	1313	A
1	2	1314	U
1	2	1315	U
1	2	1317	C
1	2	1322	G
1	2	1324	G
1	2	1330	G
1	2	1331	C
1	2	1343	U
1	2	1348	G
1	2	1358	U
1	2	1363	C
1	2	1371	U
1	2	1372	U
1	2	1373	C
1	2	1378	A
1	2	1401	A
1	2	1404	U
1	2	1426	U
1	2	1429	G
1	2	1431	G
1	2	1432	U
1	2	1441	U
1	2	1442	U
1	2	1446	A
1	2	1450	G
1	2	1454	A
1	2	1463	U
1	2	1464	C
1	2	1465	A
1	2	1466	G
1	2	1473	G
1	2	1476	A
1	2	1477	U

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Mol	Chain	Res	Type
1	2	1489	A
1	2	1490	G
1	2	1493	C
1	2	1494	U
1	2	1495	G
1	2	1505	U
1	2	1509	U
1	2	1512	C
1	2	1517	G
1	2	1520	G
1	2	1521	C
1	2	1522	A
1	2	1531	A
1	2	1533	A
1	2	1534	C
1	2	1535	U
1	2	1536	G
1	2	1544	C
1	2	1559	C
1	2	1560	U
1	2	1563	G
1	2	1566	G
1	2	1567	G
1	2	1569	A
1	2	1570	G
1	2	1572	C
1	2	1579	A
1	2	1580	A
1	2	1581	C
1	2	1584	G
1	2	1585	U
1	2	1586	U
1	2	1587	G
1	2	1588	A
1	2	1598	G
1	2	1599	U
1	2	1600	G
1	2	1601	A
1	2	1602	U
1	2	1613	G
1	2	1617	G
1	2	1618	C

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Mol	Chain	Res	Type
1	2	1621	U
1	2	1623	A
1	2	1629	C
1	2	1648	G
1	2	1649	U
1	2	1654	G
1	2	1663	A
1	2	1665	G
1	2	1675	A
1	2	1680	G
1	2	1683	C
1	2	1695	A
1	2	1698	C
1	2	1699	A
1	2	1721	U
1	2	1722	G
1	2	1728	U
1	2	1729	U
1	2	1742	C
1	2	1744	G
1	2	1748	G
1	2	1753	C
1	2	1778	C
1	2	1782	G
1	2	1783	C
1	2	1785	C
1	2	1786	U
1	2	1799	G
1	2	1819	A
1	2	1822	A
1	2	1825	A
1	2	1826	G
1	2	1829	G
1	2	1831	A
1	2	1835	A
1	2	1836	G
1	2	1838	U
1	2	1839	U
1	2	1849	G
1	2	1850	A
1	2	1851	A
1	2	1852	C

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Mol	Chain	Res	Type
1	2	1853	C
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1864	U
1	2	1865	C
1	2	1867	U
1	2	1868	U
1	2	1869	A

All (40) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	60	A
1	2	65	C
1	2	102	A
1	2	114	G
1	2	143	U
1	2	180	G
1	2	291	G
1	2	314	U
1	2	332	G
1	2	382	C
1	2	465	A
1	2	547	G
1	2	554	A
1	2	594	A
1	2	604	A
1	2	750	C
1	2	793	G
1	2	797	C
1	2	870	A
1	2	1148	A
1	2	1274	G
1	2	1302	G
1	2	1316	C
1	2	1330	G
1	2	1342	U
1	2	1403	C
1	2	1425	G
1	2	1431	G
1	2	1440	C

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Mol	Chain	Res	Type
1	2	1464	C
1	2	1511	U
1	2	1520	G
1	2	1534	C
1	2	1585	U
1	2	1587	G
1	2	1599	U
1	2	1601	A
1	2	1620	A
1	2	1648	G
1	2	1838	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.