



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:21 PM UTC

PDB ID : 6EM5 / pdb_00006em5
EMDB ID : EMD-3890
Title : State D architectural model (Nsa1-TAP Flag-Ytm1) - Visualizing the assembly pathway of nucleolar pre-60S ribosomes
Authors : Kater, L.; Cheng, J.; Barrio-Garcia, C.; Hurt, E.; Beckmann, R.
Deposited on : 2017-10-01
Resolution : 4.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

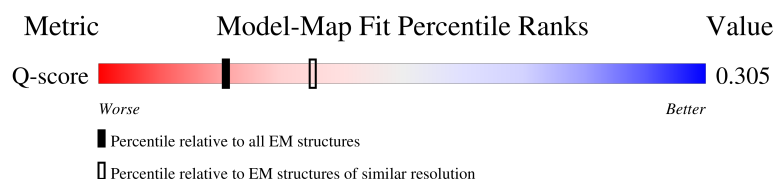
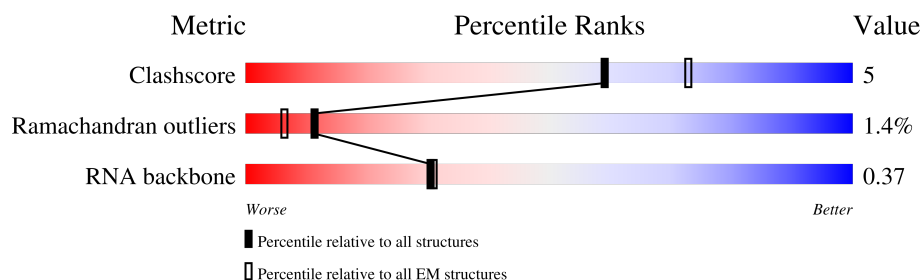
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.30 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.



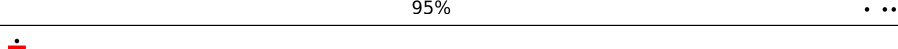
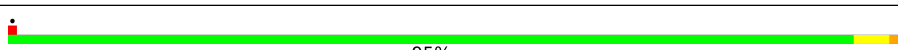
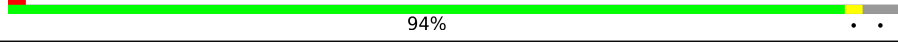
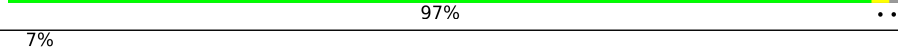
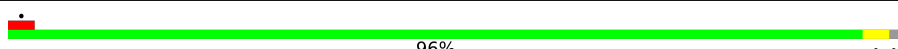
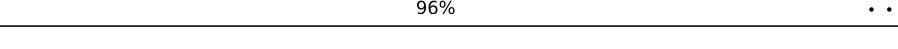
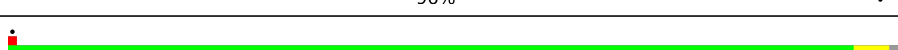
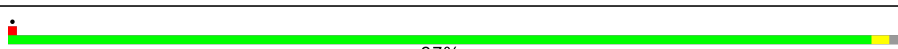
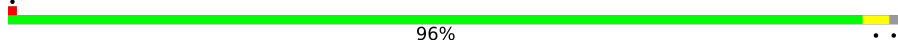
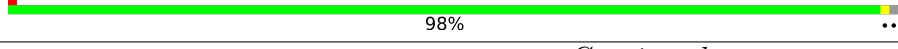
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
RNA backbone	8273	3508	-
Q-score	-	25397	5410 (3.70 - 4.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	158	 67% 30% .
2	6	232	 12% 12% . 72%
3	L	199	 58% . 39%
4	M	138	 96% ..

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Mol	Chain	Length	Quality of chain
5	N	204	
6	Q	186	
7	R	189	
8	S	172	
9	T	160	
10	U	121	
11	Z	136	
12	c	105	
13	d	113	
14	e	130	
15	f	107	
16	g	121	
17	i	100	
18	j	88	
19	k	78	
20	E	176	
21	G	256	
22	O	199	
23	V	137	
24	X	142	
25	Y	127	
26	h	120	
27	B	387	
28	C	362	
29	H	191	

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Mol	Chain	Length	Quality of chain
30	A	291	
31	K	376	
32	m	807	
33	D	505	
34	W	236	
35	l	181	
36	b	647	
37	o	220	
38	n	605	
39	r	261	
40	s	520	
41	t	322	
42	y	245	
43	z	106	
44	p	460	
45	q	618	
46	u	199	
47	v	231	
48	w	841	
49	I	663	
50	J	427	
51	x	295	
52	3	306	
53	4	278	
54	5	463	

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Mol	Chain	Length	Quality of chain
55	1	3396	5% 45% 24% • 28%
56	F	244	96% ••
57	P	184	70% • 26%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 74285 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 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	2	158	Total	C	O	P	0	0
			1896	790	948	158		

- Molecule 2 is a RNA chain called Internal Transcribed Spacer 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	6	65	Total	C	O	P	0	0
			780	325	390	65		

- Molecule 3 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	L	122	Total	C	N	O	0	0
			488	244	122	122		

- Molecule 4 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	M	136	Total	C	N	O	0	0
			544	272	136	136		

- Molecule 5 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	N	186	Total	C	N	O	0	0
			744	372	186	186		

- Molecule 6 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	Q	134	Total	C	N	O	0	0
			536	268	134	134		

- Molecule 7 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	R	120	Total	C	N	O	0	0
			480	240	120	120		

- Molecule 8 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	S	170	Total	C	N	O	0	0
			680	340	170	170		

- Molecule 9 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	T	22	Total	C	N	O	0	0
			88	44	22	22		

- Molecule 10 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	U	98	Total	C	N	O	0	0
			392	196	98	98		

- Molecule 11 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	Z	135	Total	C	N	O	0	0
			540	270	135	135		

- Molecule 12 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	c	97	Total	C	N	O	0	0
			388	194	97	97		

- Molecule 13 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	d	107	Total	C	N	O	0	0
			428	214	107	107		

- Molecule 14 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	e	125	Total	C	N	O	0	0
			500	250	125	125		

- Molecule 15 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	f	106	Total	C	N	O	0	0
			424	212	106	106		

- Molecule 16 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	g	112	Total	C	N	O	0	0
			448	224	112	112		

- Molecule 17 is a protein called 60S ribosomal protein L36-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	i	72	Total	C	N	O	0	0
			288	144	72	72		

- Molecule 18 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	j	73	Total	C	N	O	0	0
			292	146	73	73		

- Molecule 19 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	k	77	Total	C	N	O	0	0
			308	154	77	77		

- Molecule 20 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	E	156	Total	C	N	O	0	0
			624	312	156	156		

- Molecule 21 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	G	184	Total	C	N	O	0	0
			736	368	184	184		

- Molecule 22 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	O	197	Total	C	N	O	0	0
			788	394	197	197		

- Molecule 23 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	V	134	Total	C	N	O	0	0
			536	268	134	134		

- Molecule 24 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	141	Total	C	N	O	0	0
			564	282	141	141		

- Molecule 25 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	126	Total	C	N	O	0	0
			504	252	126	126		

- Molecule 26 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	h	119	Total	C	N	O	0	0
			476	238	119	119		

- Molecule 27 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	B	341	Total	C	N	O	0	0
			1364	682	341	341		

- Molecule 28 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	C	359	Total	C	N	O	0	0
			1436	718	359	359		

- Molecule 29 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	H	190	Total	C	N	O	0	0
			760	380	190	190		

- Molecule 30 is a protein called Ribosome biogenesis protein BRX1.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	A	198	Total	C	N	O	0	0
			792	396	198	198		

- Molecule 31 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	K	257	Total	C	N	O	0	0
			1028	514	257	257		

- Molecule 32 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	m	645	Total	C	N	O	0	0
			2580	1290	645	645		

- Molecule 33 is a protein called ATP-dependent RNA helicase HAS1.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	D	194	Total	C	N	O	0	0
			776	388	194	194		

- Molecule 34 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	W	232	Total	C	N	O	0	0
			928	464	232	232		

- Molecule 35 is a protein called 60S ribosome subunit biogenesis protein NIP7.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	l	174	Total	C	N	O	0	0
			696	348	174	174		

- Molecule 36 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	b	421	Total	C	N	O	0	0
			1684	842	421	421		

- Molecule 37 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	o	133	Total	C	N	O	0	0
			532	266	133	133		

- Molecule 38 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	n	411	Total	C	N	O	0	0
			1644	822	411	411		

- Molecule 39 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	r	176	Total	C	N	O	0	0
			704	352	176	176		

- Molecule 40 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	s	36	Total	C	N	O	0	0
			144	72	36	36		

- Molecule 41 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	t	290	Total	C	N	O	0	0
			1160	580	290	290		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	y	225	Total	C	N	O	0	0
			900	450	225	225		

- Molecule 43 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	z	55	Total	C	N	O	0	0
			220	110	55	55		

- Molecule 44 is a protein called Ribosome biogenesis protein YTM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	p	298	Total	C	N	O	0	0
			1192	596	298	298		

- Molecule 45 is a protein called 25S rRNA (cytosine(2870)-C(5))-methyltransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	q	317	Total	C	N	O	0	0
			1268	634	317	317		

- Molecule 46 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	u	116	Total	C	N	O	0	0
			464	232	116	116		

- Molecule 47 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	v	130	Total	C	N	O	0	0
			520	260	130	130		

- Molecule 48 is a protein called 27S pre-rRNA (guanosine(2922)-2'-O)-methyltransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	w	436	Total	C	N	O	0	0
			1744	872	436	436		

- Molecule 49 is a protein called Nucleolar complex-associated protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	I	451	Total	C	N	O	0	0
			1804	902	451	451		

- Molecule 50 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	J	132	Total	C	N	O	0	0
			528	264	132	132		

- Molecule 51 is a protein called Ribosome production factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	x	267	Total	C	N	O	0	0
			1068	534	267	267		

- Molecule 52 is a protein called Protein MAK16.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	3	173	Total	C	N	O	0	0
			692	346	173	173		

- Molecule 53 is a protein called Ribosomal RNA-processing protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	4	220	Total	C	N	O	0	0
			880	440	220	220		

- Molecule 54 is a protein called Ribosome biogenesis protein NSA1.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	5	385	Total	C	N	O	0	0
			1540	770	385	385		

- Molecule 55 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	1	2438	Total	C	O	P	0	0
			29253	12190	14626	2437		

- Molecule 56 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	F	241	Total 964	C 482	N 241	O 241	0	0

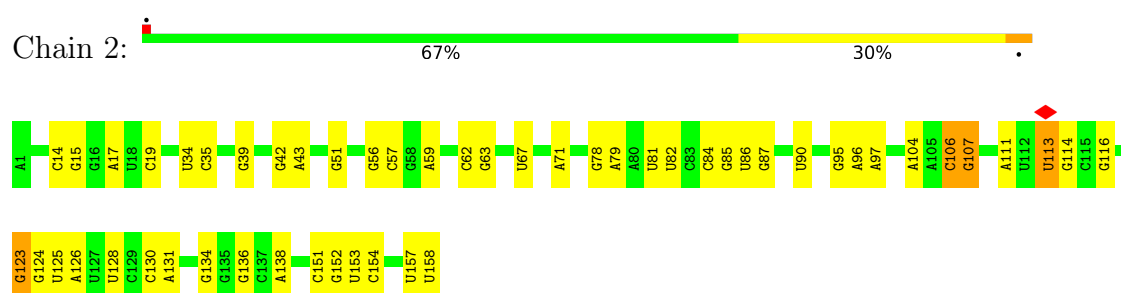
- Molecule 57 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	P	137	Total 548	C 274	N 137	O 137	0	0

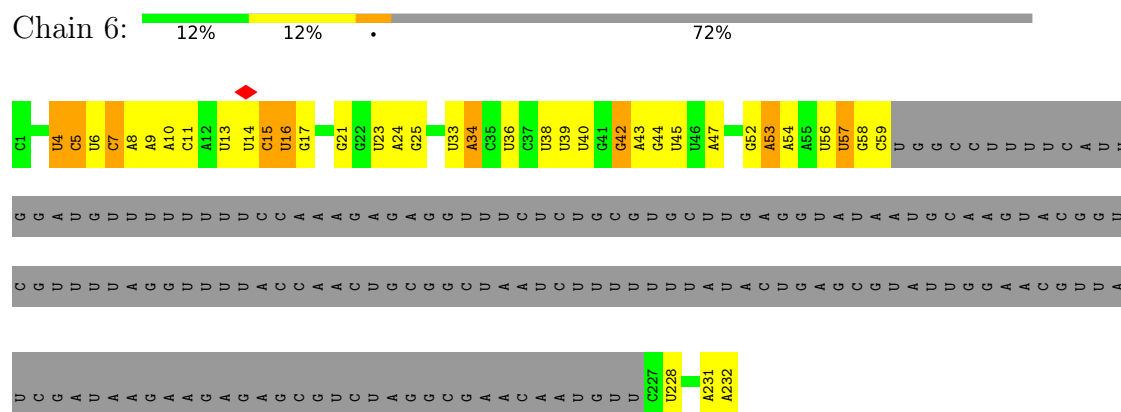
3 Residue-property plots [i](#)

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

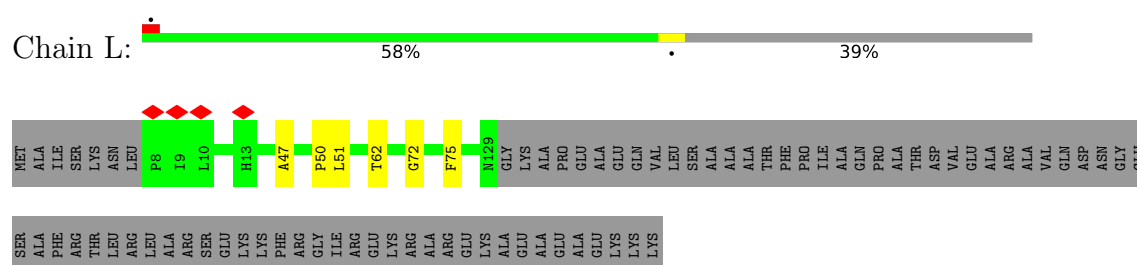
- Molecule 1: 5.8S ribosomal RNA



- Molecule 2: Internal Transcribed Spacer 2

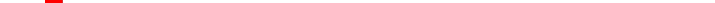


- Molecule 3: 60S ribosomal protein L13-A

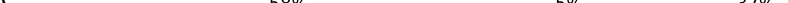


- Molecule 4: 60S ribosomal protein L14-A

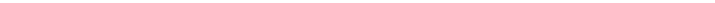
- Chain N: 88% 9%

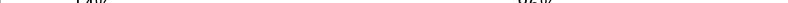
- Chain Q:  68% 28%

[illegible]

- Chain R: 

ARG	GLU	LYS	ALA	LEU	ASN	GLU	GLU	ALA	ALA	GLY	ALA	ARG	ARG	LEU	LYS	THR	ARG	ALA	ALA	ALA	GLN	SER	LYS	ARG	ARG	GLU	GLY	ARG	HIS	GLY	GLY	LYS	GLY	THR	ARG	ARG	GLU	ALA	ALA	ARG	LYS	ASP	ASP	GLU	GLY	LYS	THR	LYS	LEU	LEU	ALA	LEU	ASP	ALA	
MET	A2	L24	K53	A54	V57	S59	LYS	SER	ARG	THR	ARG	ALA	HIS	ALA	GLN	SER	LYS	ARG	ARG	GLU	GLY	ARG	ARG	HIS	GLY	GLY	LYS	THR	GLY	LYS	LYS	LYS	GLY	THR	ARG	ARG	GLU	ALA	ALA	ARG	I49	I96	K117	H118	L119	Y120	H121	G129	I142	A145	K146	A147	D148	A149	S150

- Chain S:  95% ..

- Chain T:  14% 86%

[illegible]

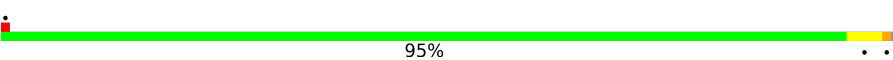
GLN PRO ARG GLU SER ARG TLE VAL SER THR GLU GLY ASN VAL PRO GLN THR LEU ALA PRO VAL TYR GLU THR PHE TLE

- Molecule 10: 60S ribosomal protein L22-A

Chain U:  7% 80% 19%

MET ALA PRO ASN THR SER ARG LYS LYS I11 G26 E44 N52 G60 A69 K70 D91 S97 Y108 GLN VAL THR PRO GLU GLU ASP GLU GLU ASP GLU

- Molecule 11: 60S ribosomal protein L27-A

Chain Z:  95%

MET A2 K3 G16 R17 Y18 Q103 G125 R135 F136

- Molecule 12: 60S ribosomal protein L30

Chain c:  5% 90% 8%

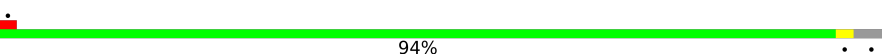
MET ALA PRO VAL LYS SER GLN GLU S9 I10 H11 I18 Q36 G37 G78 G88 L104 A105

- Molecule 13: 60S ribosomal protein L31-A

Chain d:  5% 88% 6% 5%

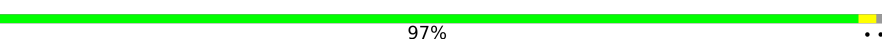
MET ALA GLY LEU LYS D6 T13 G45 R62 E83 D84 A85 K86 N87 P88 A99 G103 L104 Q105 T106 D112 ALA

- Molecule 14: 60S ribosomal protein L32

Chain e:  94%

MET ALA SER L4 R27 G56 A127 L128 GLU ALA

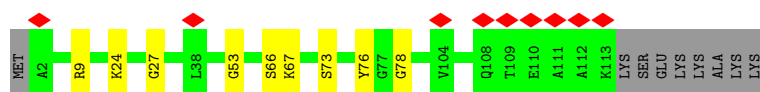
- Molecule 15: 60S ribosomal protein L33-A

Chain f:  97%

MET A2 R6 L45 I107

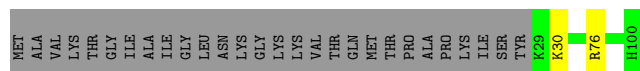
- Molecule 16: 60S ribosomal protein L34-A

Chain g:  7% 85% 7% 7%



- Molecule 17: 60S ribosomal protein L36-B

Chain i: 70% 28%



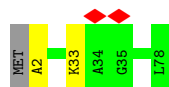
- Molecule 18: 60S ribosomal protein L37-A

Chain j: 78% 17%



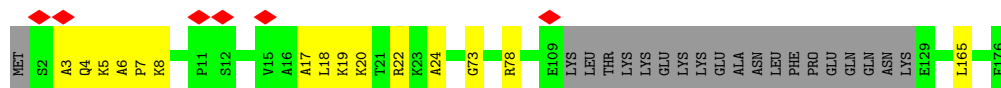
- Molecule 19: 60S ribosomal protein L38

Chain k: 96%



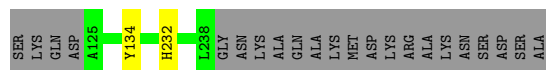
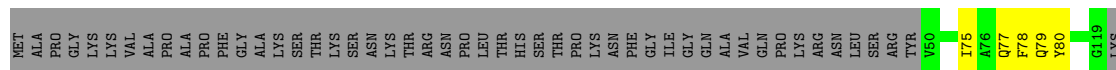
- Molecule 20: 60S ribosomal protein L6-A

Chain E: 80% 9% 11%



- Molecule 21: 60S ribosomal protein L8-A

Chain G: 69% 28%

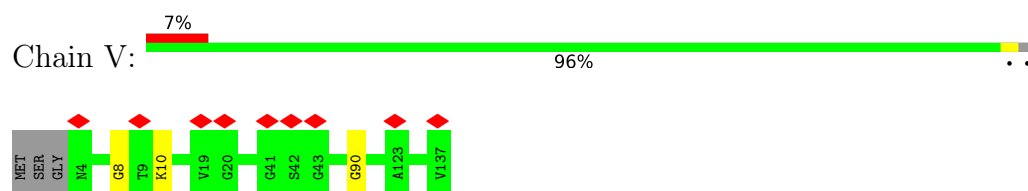


- Molecule 22: 60S ribosomal protein L16-A

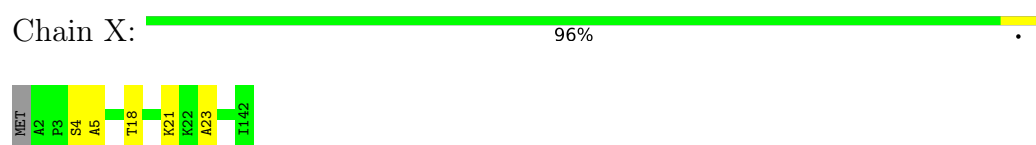
Chain O: 82% 17%



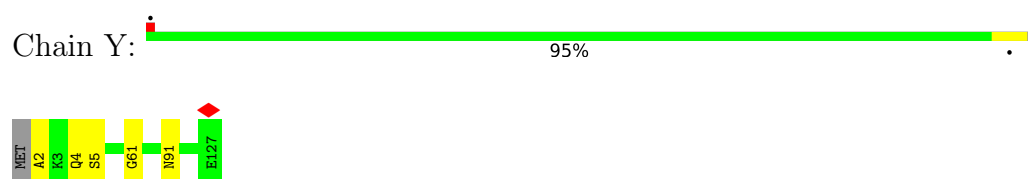
- Molecule 23: 60S ribosomal protein L23-A



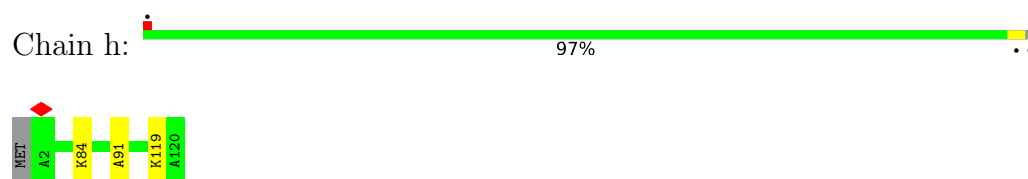
- Molecule 24: 60S ribosomal protein L25



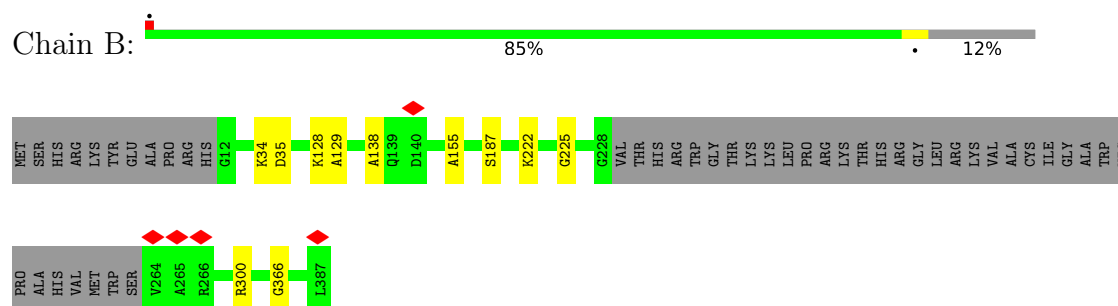
- Molecule 25: 60S ribosomal protein L26-A



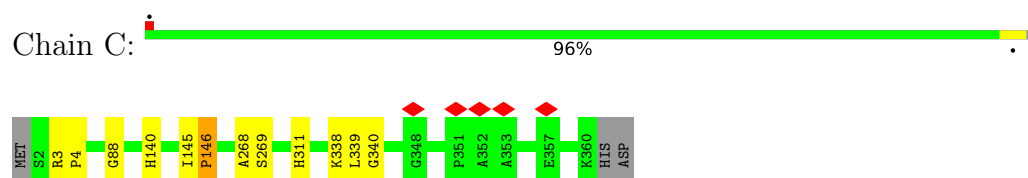
- Molecule 26: 60S ribosomal protein L35-A



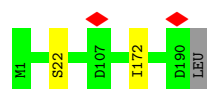
- Molecule 27: 60S ribosomal protein L3



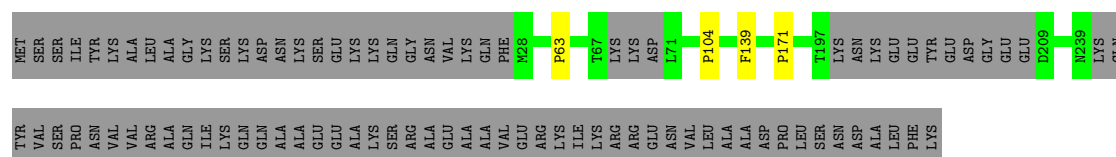
- Molecule 28: 60S ribosomal protein L4-A

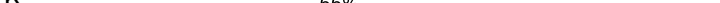


- Molecule 29: 60S ribosomal protein L9-A



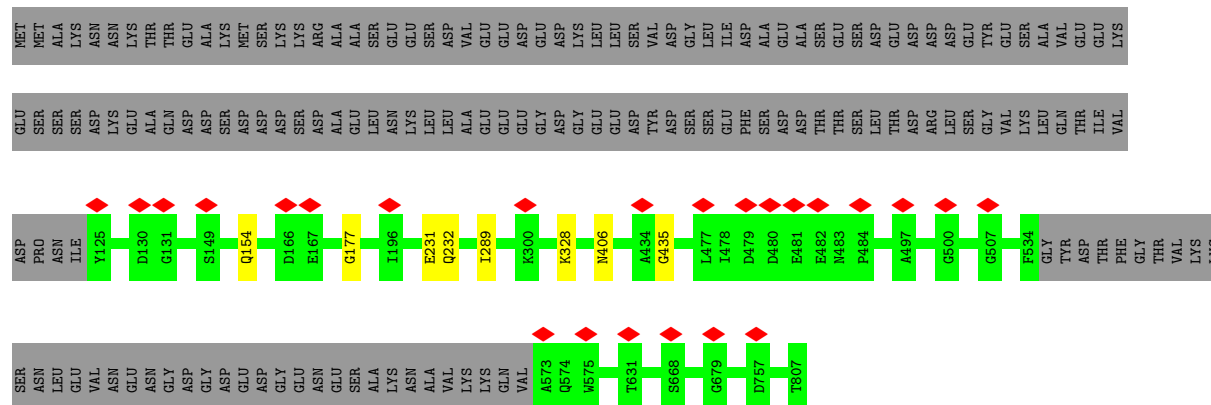
- Chain A: 67% . 32%



- Chain K:  66% 1% 32%

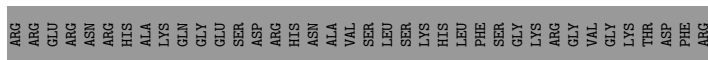


- Chain m: 79% 20%

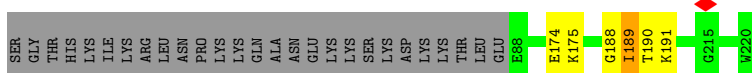


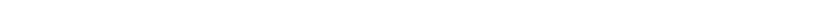
- Chain D: 38% 62%

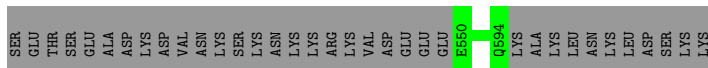


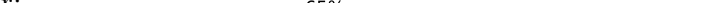


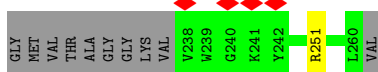
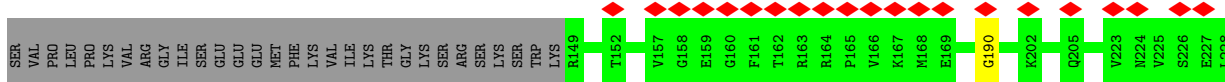
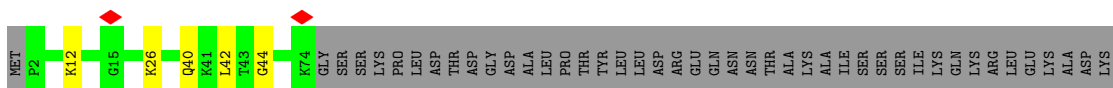
Chain o: 58% . 40%



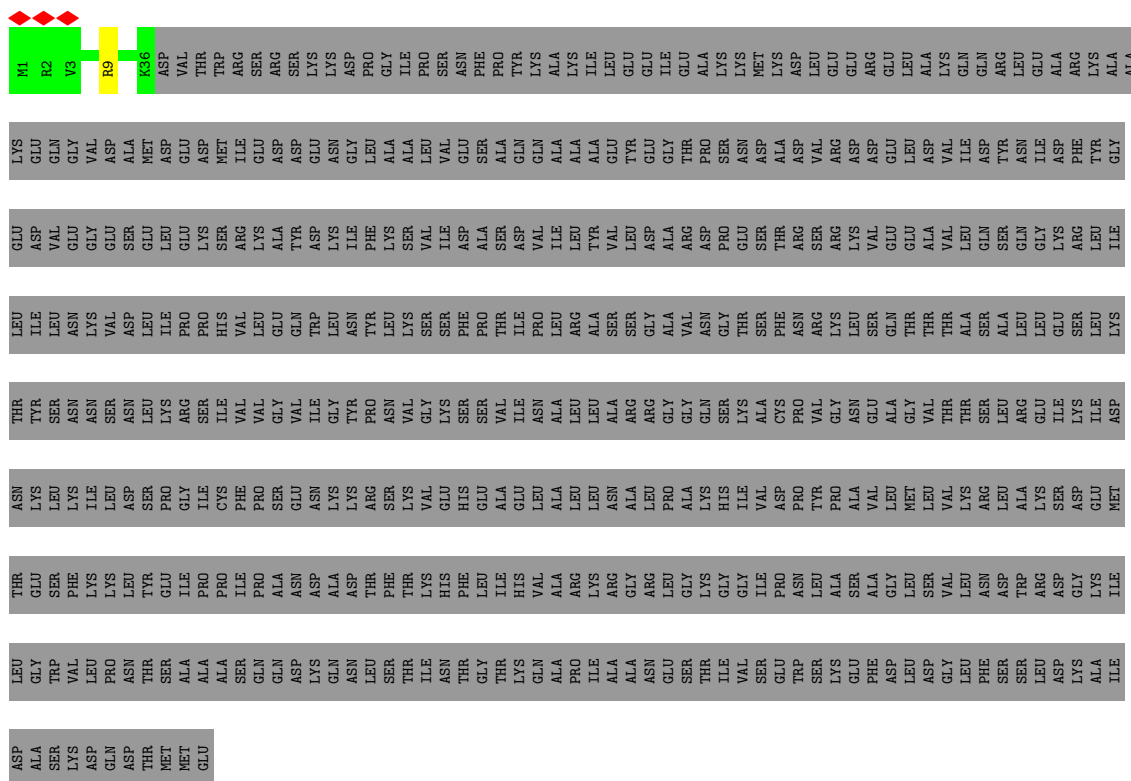
Chain n:  67% . 32%



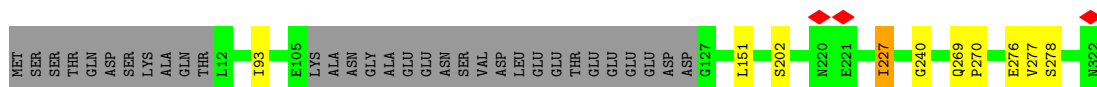
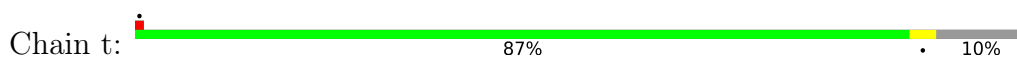
Chain r:  10% 65% 25%



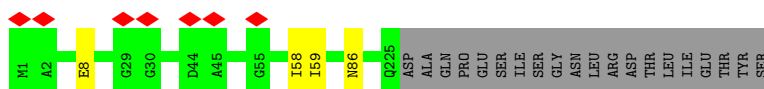
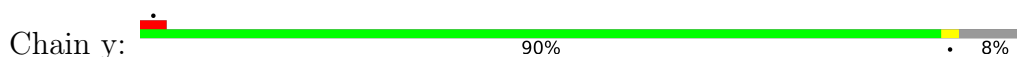
Chain s: 7% 93%



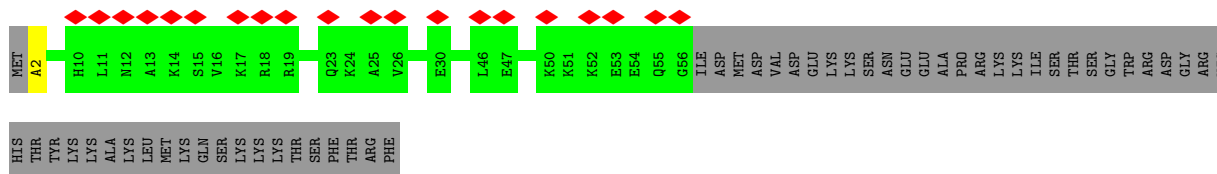
- Molecule 41: Ribosome biogenesis protein RLP7



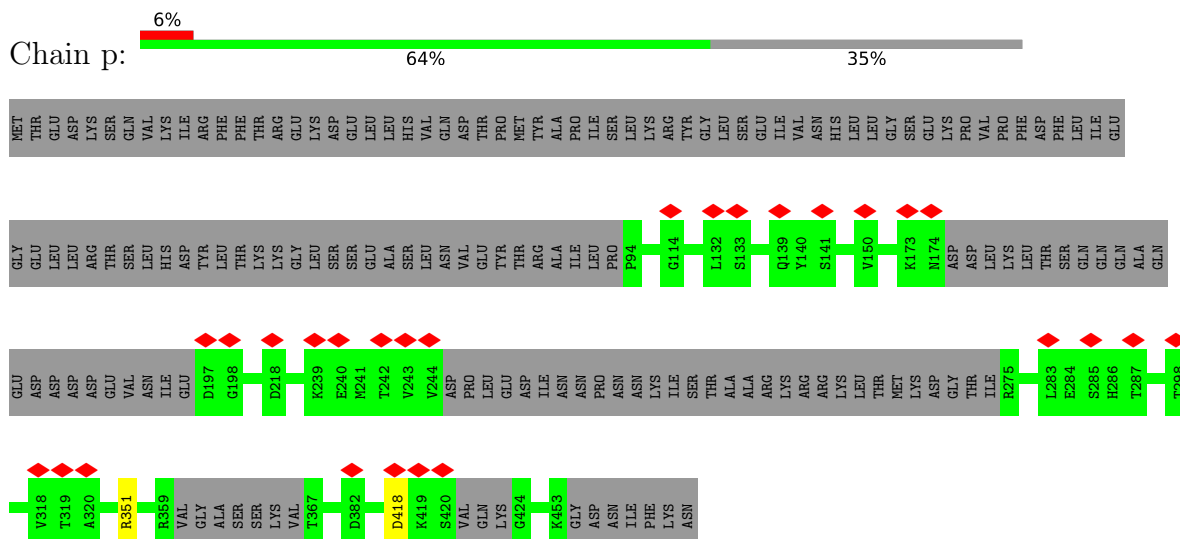
- Molecule 42: Eukaryotic translation initiation factor 6



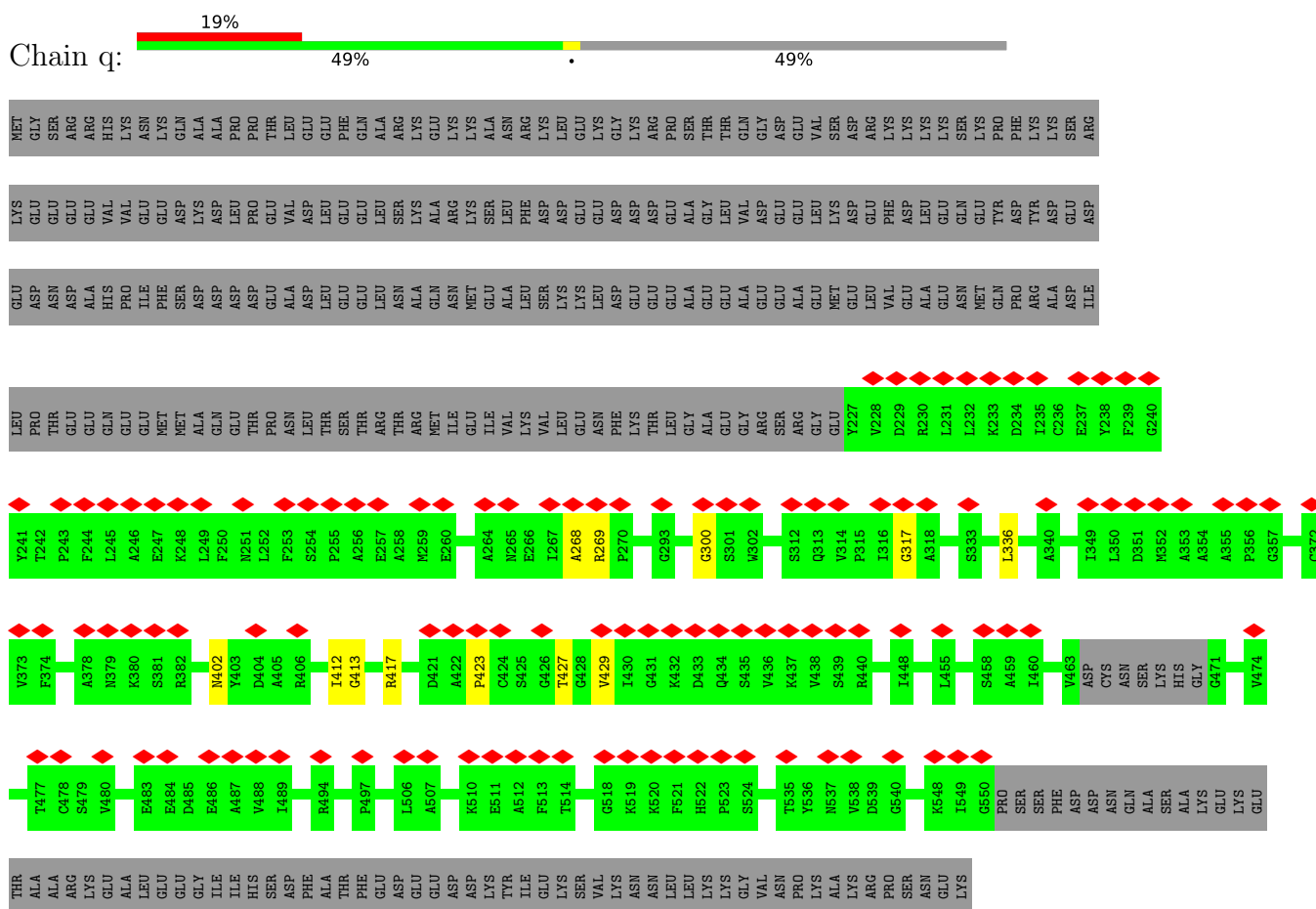
- Molecule 43: UPF0642 protein YBL028C



- Molecule 44: Ribosome biogenesis protein YTM1

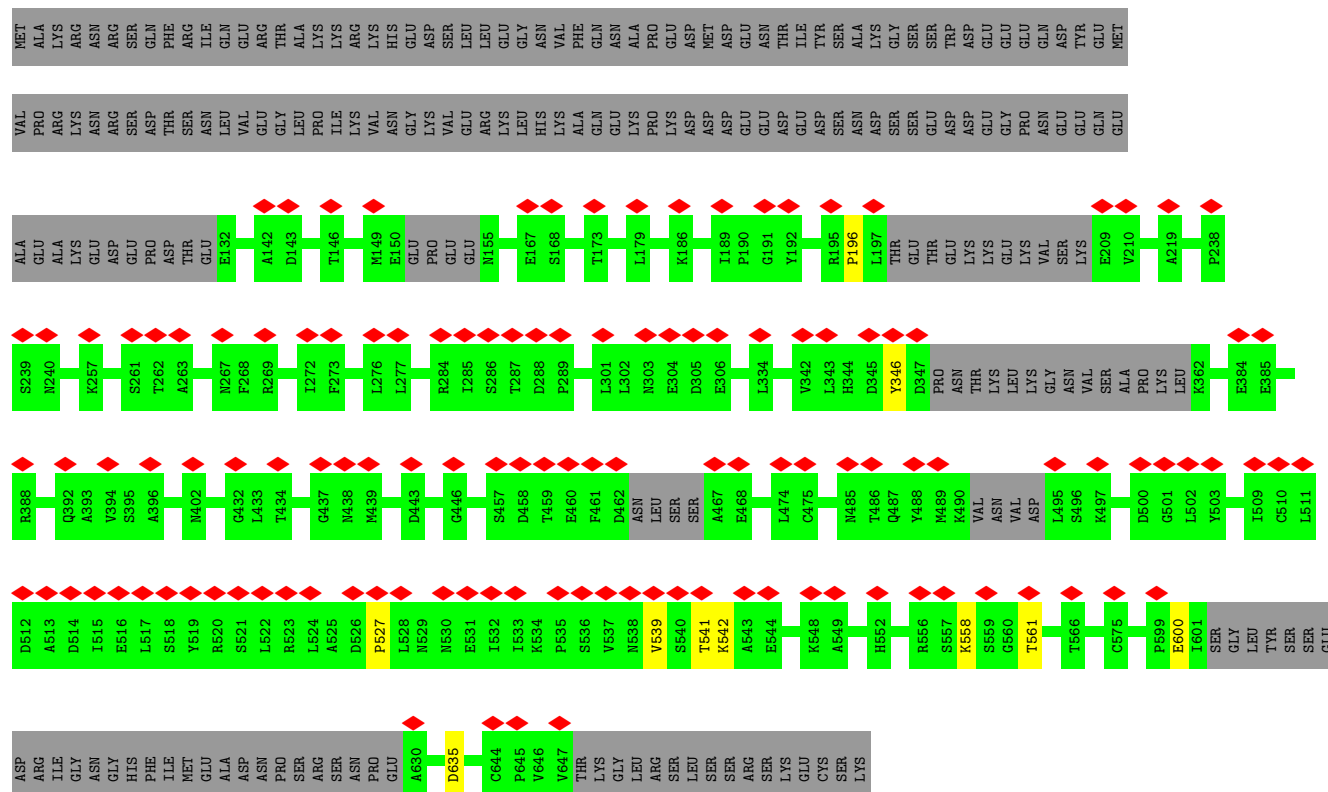


- Molecule 45: 25S rRNA (cytosine(2870)-C(5))-methyltransferase

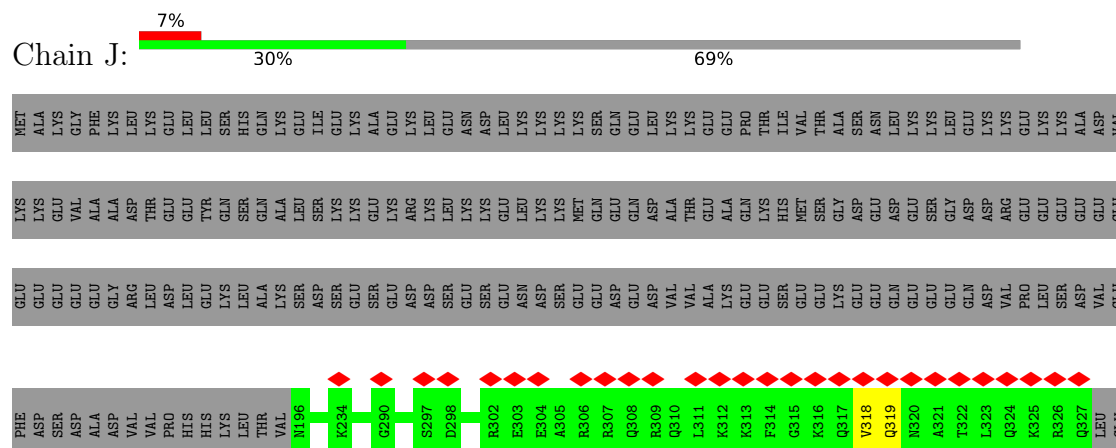


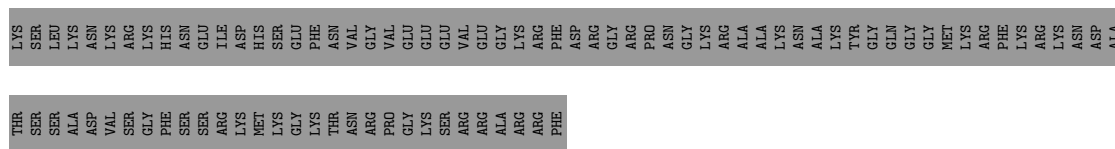
- Molecule 46: Ribosome biogenesis protein RLP24



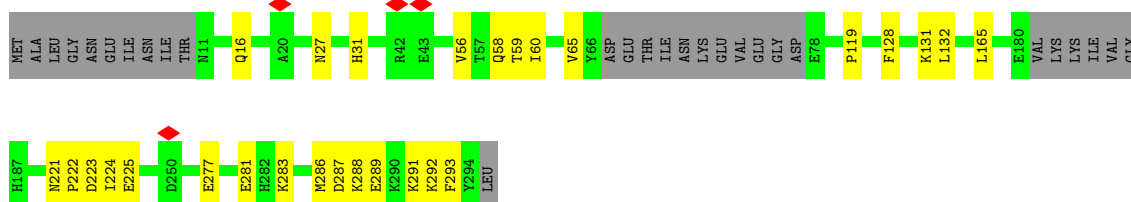
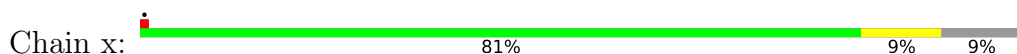


- Molecule 50: rRNA-processing protein EBP2

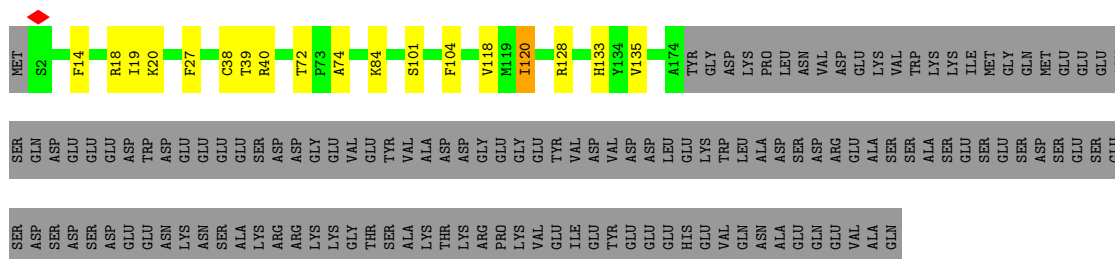




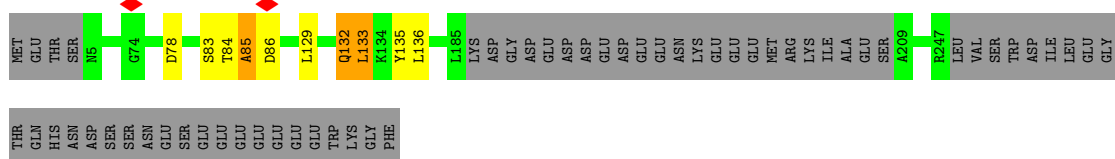
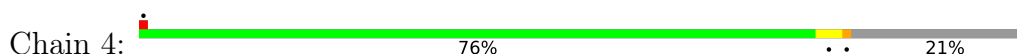
- Molecule 51: Ribosome production factor 1



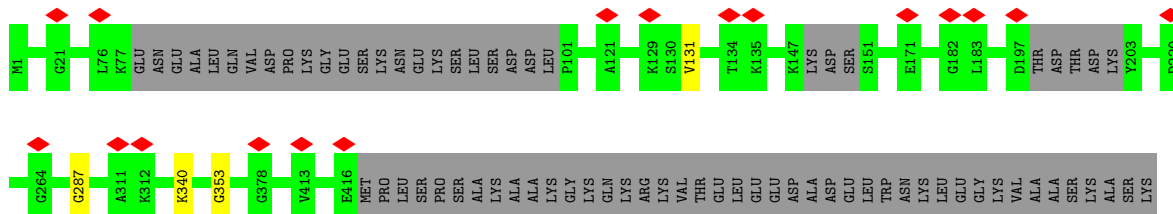
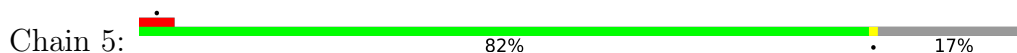
- Molecule 52: Protein MAK16



- Molecule 53: Ribosomal RNA-processing protein 1

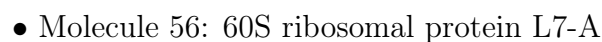


- Molecule 54: Ribosome biogenesis protein NSA1





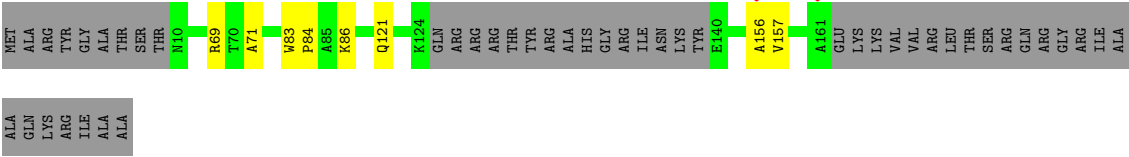




96%



• Molecule 57: 60S ribosomal protein L17-A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37251	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.124	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	455.28, 455.28, 455.28	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.084, 1.084, 1.084	Depositor

5 Model quality

5.1 Standard geometry

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	0/2053	0.99	1/3156 (0.0%)
2	6	0.55	0/843	1.15	4/1292 (0.3%)
3	L	0.61	0/486	1.28	1/604 (0.2%)
4	M	0.58	0/543	1.24	0/677
5	N	0.56	0/742	1.19	2/924 (0.2%)
6	Q	0.65	0/535	1.24	0/667
7	R	0.63	0/478	1.39	0/594
8	S	0.62	0/679	1.22	1/847 (0.1%)
9	T	0.63	0/87	1.27	0/107
10	U	0.67	0/391	1.15	0/487
11	Z	0.62	0/539	1.25	0/672
12	c	0.65	0/387	1.27	0/482
13	d	0.59	0/427	1.11	0/532
14	e	0.59	0/499	1.17	0/622
15	f	0.52	0/423	1.00	0/527
16	g	0.62	0/447	1.19	1/557 (0.2%)
17	i	0.59	0/287	1.46	0/357
18	j	0.57	0/291	1.20	0/362
19	k	0.63	0/307	1.18	0/382
20	E	0.61	0/622	1.18	0/774
21	G	0.65	0/734	1.34	1/914 (0.1%)
22	O	0.40	0/787	0.85	0/982
23	V	0.63	0/535	1.11	0/667
24	X	0.61	0/563	1.17	1/702 (0.1%)
25	Y	0.61	0/503	1.17	0/627
26	h	0.59	0/475	1.33	0/592
27	B	0.65	0/1362	1.15	1/1699 (0.1%)
28	C	0.62	0/1435	1.23	3/1792 (0.2%)
29	H	0.58	0/759	1.10	1/947 (0.1%)
30	A	0.60	0/789	1.15	2/981 (0.2%)
31	K	0.67	0/1026	1.29	3/1279 (0.2%)
32	m	0.65	0/2578	1.18	2/3219 (0.1%)
33	D	0.67	0/773	1.24	1/961 (0.1%)
34	W	0.69	0/927	1.21	1/1157 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	l	0.69	0/694	1.18	1/864 (0.1%)
36	b	0.66	0/1680	1.30	1/2093 (0.0%)
37	o	0.63	0/531	1.24	1/662 (0.2%)
38	n	0.62	1/1640 (0.1%)	1.26	0/2043
39	r	0.59	0/701	1.16	0/871
40	s	0.55	0/143	1.34	0/177
41	t	0.64	0/1158	1.25	1/1444 (0.1%)
42	y	0.66	0/899	1.19	1/1122 (0.1%)
43	z	0.61	0/219	1.42	0/272
44	p	0.68	0/1187	1.14	0/1475
45	q	0.72	0/1266	1.26	2/1579 (0.1%)
46	u	0.62	0/463	1.16	0/577
47	v	0.56	0/517	1.24	0/641
48	w	0.65	0/1739	1.23	0/2165
49	I	0.66	0/1797	1.38	3/2234 (0.1%)
50	J	0.60	0/527	1.40	0/657
51	x	0.69	0/1064	1.39	5/1323 (0.4%)
52	3	0.59	0/691	1.30	1/862 (0.1%)
53	4	0.33	0/878	1.17	7/1094 (0.6%)
54	5	0.61	0/1536	1.02	1/1913 (0.1%)
55	1	0.61	4/31669 (0.0%)	1.04	48/48668 (0.1%)
56	F	0.60	0/963	1.32	0/1202
57	P	0.59	0/546	1.22	1/679 (0.1%)
All	All	0.62	5/76820 (0.0%)	1.13	99/105758 (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
5	N	0	1
53	4	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1	3263	G	O3'-P	-43.51	0.95	1.61
55	1	3301	U	O3'-P	29.71	2.05	1.61
55	1	3176	G	O3'-P	23.26	1.96	1.61
55	1	3145	C	O3'-P	-12.36	1.42	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	n	454	PRO	CA-C	5.12	1.54	1.51

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1	3263	G	P-O3'-C3'	-22.81	85.99	120.20
53	4	132	GLN	N-CA-C	-19.79	76.70	109.96
55	1	3263	G	O3'-P-O5'	17.70	130.55	104.00
55	1	3263	G	OP1-P-O3'	-14.67	64.00	108.00
55	1	3145	C	P-O3'-C3'	-14.36	98.66	120.20
55	1	3301	U	P-O3'-C3'	-12.82	100.97	120.20
55	1	649	A	C2'-C3'-O3'	9.38	127.77	113.70
53	4	133	LEU	N-CA-C	-7.86	94.06	110.80
55	1	3176	G	P-O3'-C3'	7.34	131.22	120.20
30	A	104	PRO	N-CA-C	7.28	119.58	110.70
55	1	1227	C	C2'-C3'-O3'	7.16	124.44	113.70
55	1	3145	C	OP2-P-O3'	7.06	129.17	108.00
55	1	1203	A	C4'-C3'-O3'	-6.97	102.54	113.00
53	4	78	ASP	CA-C-N	6.91	127.06	119.87
53	4	78	ASP	C-N-CA	6.91	127.06	119.87
55	1	2940	A	C4'-C3'-O3'	6.83	123.25	113.00
55	1	3176	G	OP2-P-O3'	-6.83	87.52	108.00
52	3	120	ILE	N-CA-C	-6.83	106.07	112.83
55	1	3301	U	OP2-P-O3'	6.82	128.47	108.00
55	1	3145	C	OP1-P-O3'	-6.79	87.64	108.00
55	1	644	G	C2'-C3'-O3'	6.76	123.85	113.70
55	1	2922	G	C2'-C3'-O3'	6.71	123.77	113.70
55	1	898	U	C4'-C3'-O3'	-6.64	103.05	113.00
5	N	93	LYS	N-CA-C	6.62	119.48	111.40
55	1	1560	G	C2'-C3'-O3'	-6.61	103.79	113.70
55	1	374	A	C2'-C3'-O3'	-6.57	103.84	113.70
55	1	977	C	C4'-C3'-O3'	6.54	122.81	113.00
55	1	59	G	C2'-C3'-O3'	-6.42	104.07	113.70
55	1	436	A	C4'-C3'-O3'	-6.42	103.38	113.00
31	K	255	ARG	CA-C-N	6.39	127.82	119.84
31	K	255	ARG	C-N-CA	6.39	127.82	119.84
1	2	123	G	C2'-C3'-O3'	6.35	123.23	113.70
5	N	177	GLY	N-CA-C	6.28	119.89	110.97
55	1	3301	U	OP1-P-O3'	-6.24	89.28	108.00
55	1	1307	G	C2'-C3'-O3'	6.23	123.05	113.70
21	G	134	TYR	N-CA-C	6.23	122.31	113.02
55	1	1278	A	C1'-C2'-O2'	6.22	117.73	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1	239	G	C2'-C3'-O3'	6.19	122.98	113.70
49	I	539	VAL	N-CA-C	6.03	116.21	110.42
53	4	83	SER	N-CA-C	5.98	118.90	110.23
55	1	2954	U	C2'-C3'-O3'	5.91	122.57	113.70
2	6	33	U	C3'-C2'-O2'	5.85	119.47	110.70
35	l	142	GLY	N-CA-C	5.83	118.72	110.74
2	6	53	A	C4'-C3'-O3'	-5.82	104.28	113.00
34	W	98	GLY	N-CA-C	5.79	115.48	110.21
36	b	71	ILE	N-CA-C	5.78	116.43	110.36
33	D	341	GLY	N-CA-C	5.74	119.94	112.25
28	C	3	ARG	CA-C-N	5.65	126.91	119.84
28	C	3	ARG	C-N-CA	5.65	126.91	119.84
55	1	352	A	C2'-C3'-O3'	-5.65	105.23	113.70
55	1	1796	G	C4'-C3'-O3'	-5.63	104.56	113.00
55	1	1507	G	C2'-C3'-O3'	-5.59	105.31	113.70
8	S	23	LYS	N-CA-C	5.59	119.84	113.19
55	1	1154	A	C4'-C3'-O3'	-5.57	104.64	113.00
55	1	3021	A	C4'-C3'-O3'	-5.57	104.65	113.00
51	x	221	ASN	CA-C-N	5.53	126.75	119.84
51	x	221	ASN	C-N-CA	5.53	126.75	119.84
29	H	172	ILE	N-CA-C	-5.53	107.06	111.81
32	m	289	ILE	CA-C-N	5.52	123.69	119.66
32	m	289	ILE	C-N-CA	5.52	123.69	119.66
24	X	18	THR	N-CA-C	5.51	119.83	113.38
37	o	189	ILE	N-CA-C	5.51	115.96	110.23
55	1	720	A	C2'-C3'-O3'	5.49	121.93	113.70
55	1	282	G	C2'-C3'-O3'	-5.46	105.50	113.70
45	q	417	ARG	N-CA-C	5.46	117.58	110.43
55	1	551	A	C3'-C2'-O2'	5.43	118.85	110.70
55	1	1861	G	C2'-C3'-O3'	5.42	121.83	113.70
16	g	73	SER	N-CA-C	5.42	119.15	112.54
31	K	114	SER	N-CA-C	-5.37	106.73	113.28
53	4	83	SER	CA-C-N	5.37	129.76	122.19
53	4	83	SER	C-N-CA	5.37	129.76	122.19
55	1	1111	U	C3'-C2'-O2'	5.35	118.72	110.70
55	1	1561	G	C3'-C2'-O2'	5.35	118.72	110.70
28	C	88	GLY	N-CA-C	5.34	117.60	111.36
55	1	1716	U	C2'-C3'-O3'	5.32	121.68	113.70
55	1	1820	U	C2'-C3'-O3'	5.31	121.67	113.70
41	t	227	ILE	N-CA-C	5.30	120.37	109.34
49	I	346	TYR	N-CA-C	5.29	118.89	111.90
55	1	1418	A	C4'-C3'-O3'	-5.29	105.07	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	P	157	VAL	N-CA-C	5.29	115.98	108.42
55	1	3185	U	C4'-C3'-O3'	-5.28	105.07	113.00
55	1	109	A	C2'-C3'-O3'	-5.28	105.79	113.70
55	1	1329	U	C3'-C2'-O2'	5.28	118.61	110.70
2	6	7	C	C3'-C2'-O2'	5.27	118.60	110.70
42	y	59	ILE	N-CA-C	5.25	115.47	110.53
55	1	268	A	C4'-C3'-O3'	-5.23	105.15	113.00
51	x	165	LEU	CA-C-N	-5.22	114.60	120.14
51	x	165	LEU	C-N-CA	-5.22	114.60	120.14
2	6	42	G	C4'-C3'-O3'	-5.21	105.18	113.00
3	L	47	ALA	N-CA-C	5.21	121.32	109.81
54	5	287	GLY	N-CA-C	5.20	118.34	110.75
55	1	1895	A	C1'-C2'-O2'	5.17	116.15	108.40
55	1	2986	U	C2'-C3'-O3'	5.14	121.40	113.70
27	B	300	ARG	N-CA-C	5.12	118.66	111.90
51	x	131	LYS	N-CA-C	5.09	117.23	111.02
30	A	139	PHE	N-CA-C	5.07	114.97	108.34
45	q	336	LEU	N-CA-C	5.07	121.00	109.81
49	I	542	LYS	N-CA-C	-5.05	108.39	114.75
55	1	1299	U	C4'-C3'-O3'	5.04	120.57	113.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
53	4	135	TYR	Peptide
53	4	136	LEU	Peptide
5	N	92	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	1896	0	949	16	0
2	6	780	0	392	16	0
3	L	488	0	125	1	0
4	M	544	0	145	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	N	744	0	202	0	0
6	Q	536	0	140	25	0
7	R	480	0	126	30	0
8	S	680	0	170	2	0
9	T	88	0	21	0	0
10	U	392	0	107	2	0
11	Z	540	0	144	13	0
12	c	388	0	112	13	0
13	d	428	0	112	16	0
14	e	500	0	133	3	0
15	f	424	0	117	2	0
16	g	448	0	121	38	0
17	i	288	0	78	1	0
18	j	292	0	85	4	0
19	k	308	0	79	1	0
20	E	624	0	160	66	0
21	G	736	0	189	2	0
22	O	788	0	214	1	0
23	V	536	0	158	2	0
24	X	564	0	144	7	0
25	Y	504	0	134	5	0
26	h	476	0	118	0	0
27	B	1364	0	384	5	0
28	C	1436	0	397	3	0
29	H	760	0	214	0	0
30	A	792	0	203	0	0
31	K	1028	0	259	7	0
32	m	2580	0	660	0	0
33	D	776	0	199	0	0
34	W	928	0	246	5	0
35	l	696	0	193	3	0
36	b	1684	0	436	11	0
37	o	532	0	147	6	0
38	n	1644	0	417	4	0
39	r	704	0	186	9	0
40	s	144	0	40	1	0
41	t	1160	0	304	3	0
42	y	900	0	258	8	0
43	z	220	0	58	2	0
44	p	1192	0	324	0	0
45	q	1268	0	342	5	0
46	u	464	0	122	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	v	520	0	139	1	0
48	w	1744	0	457	0	0
49	I	1804	0	452	0	0
50	J	528	0	132	6	0
51	x	1068	0	271	27	0
52	3	692	0	174	45	0
53	4	880	0	223	5	0
54	5	1540	0	421	2	0
55	1	29253	0	14649	358	0
56	F	964	0	259	2	0
57	P	548	0	144	9	0
All	All	74285	0	27185	462	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 5.

All (462) 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)
11:Z:2:ALA:CA	12:c:37:GLY:CA	1.85	1.50
20:E:6:ALA:CA	52:3:27:PHE:H	1.22	1.44
20:E:17:ALA:O	55:1:592:A:C5'	1.66	1.44
11:Z:2:ALA:N	12:c:37:GLY:CA	1.81	1.37
7:R:129:GLY:CA	55:1:840:C:O2'	1.73	1.34
11:Z:2:ALA:CA	12:c:37:GLY:HA2	1.50	1.32
6:Q:74:GLU:O	55:1:741:U:C4'	1.78	1.31
7:R:117:LYS:O	55:1:1718:G:H5'	1.27	1.28
27:B:129:ALA:O	55:1:3150:A:H5'	1.18	1.27
51:x:60:ILE:N	55:1:392:G:OP1	1.66	1.27
55:1:2352:A:H5''	57:P:83:TRP:O	1.15	1.27
16:g:76:TYR:N	55:1:1806:A:OP1	1.67	1.26
20:E:8:LYS:O	52:3:39:THR:CA	1.84	1.26
13:d:13:THR:O	55:1:3324:C:H4'	1.34	1.25
20:E:6:ALA:H	52:3:19:ILE:N	1.31	1.25
11:Z:2:ALA:N	12:c:37:GLY:HA2	0.91	1.22
11:Z:2:ALA:CA	12:c:37:GLY:HA3	1.55	1.22
16:g:67:LYS:N	55:1:1821:U:O2'	1.72	1.22
20:E:17:ALA:O	55:1:592:A:H5'	1.10	1.22
16:g:24:LYS:O	55:1:1696:A:H5'	1.30	1.22
20:E:6:ALA:N	52:3:19:ILE:N	1.85	1.21
2:6:45:U:O2'	31:K:243:THR:O	1.57	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:d:104:LEU:O	55:1:3325:G:H5'	1.39	1.20
7:R:129:GLY:HA3	55:1:840:C:O2'	1.26	1.19
50:J:319:GLN:CA	55:1:2406:C:O2'	1.92	1.17
55:1:2352:A:C5'	57:P:83:TRP:O	1.92	1.17
20:E:6:ALA:CA	52:3:27:PHE:N	1.89	1.16
51:x:60:ILE:CA	55:1:392:G:OP1	1.95	1.15
7:R:129:GLY:N	55:1:840:C:O2'	1.79	1.15
20:E:3:ALA:H	55:1:1422:G:C1'	1.58	1.14
55:1:3301:U:O3'	55:1:3302:U:P	2.05	1.13
7:R:117:LYS:O	55:1:1718:G:C5'	1.95	1.13
51:x:27:ASN:O	55:1:385:A:O3'	1.65	1.13
16:g:24:LYS:O	55:1:1696:A:C5'	1.98	1.12
20:E:5:LYS:C	52:3:19:ILE:C	2.17	1.12
20:E:20:LYS:N	55:1:593:C:OP1	1.84	1.11
53:4:84:THR:O	53:4:86:ASP:N	1.83	1.09
7:R:118:HIS:O	55:1:1718:G:OP1	1.72	1.07
52:3:101:SER:CA	55:1:1350:A:H2'	1.85	1.07
54:5:353:GLY:HA2	55:1:193:C:H5'	1.26	1.06
42:y:8:GLU:CA	55:1:3019:U:OP1	2.03	1.05
13:d:104:LEU:O	55:1:3325:G:C5'	2.05	1.04
6:Q:74:GLU:O	55:1:741:U:H4'	0.87	1.04
7:R:117:LYS:C	55:1:1718:G:H5'	1.80	1.03
20:E:17:ALA:C	55:1:592:A:H5'	1.83	1.03
6:Q:134:GLY:O	55:1:729:C:H5''	1.58	1.02
20:E:6:ALA:H	52:3:18:ARG:C	1.68	1.02
27:B:129:ALA:O	55:1:3150:A:C5'	2.07	1.01
51:x:27:ASN:O	55:1:386:A:P	2.09	1.00
2:6:44:G:O2'	31:K:241:GLY:CA	2.10	0.99
24:X:21:LYS:CA	55:1:2:U:OP2	2.11	0.99
51:x:31:HIS:CA	55:1:385:A:H5''	1.93	0.98
51:x:27:ASN:CA	55:1:386:A:H5''	1.92	0.98
16:g:53:GLY:HA2	55:1:1640:G:OP1	1.63	0.97
39:r:40:GLN:O	55:1:1298:C:O2'	1.83	0.96
13:d:103:GLY:HA2	55:1:3326:G:P	2.06	0.96
50:J:319:GLN:N	55:1:2406:C:O2'	1.97	0.95
20:E:5:LYS:C	52:3:20:LYS:N	2.25	0.95
55:1:249:U:H3'	55:1:250:U:H5''	1.48	0.95
7:R:118:HIS:C	55:1:1718:G:OP1	2.10	0.95
7:R:118:HIS:CA	55:1:1718:G:H5'	1.97	0.94
6:Q:136:ASN:H	55:1:730:C:P	1.91	0.94
16:g:78:GLY:O	55:1:1804:A:O2'	1.86	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:E:17:ALA:O	55:1:592:A:O5'	1.85	0.93
11:Z:2:ALA:C	12:c:37:GLY:CA	2.43	0.92
6:Q:74:GLU:C	55:1:741:U:H4'	1.94	0.92
11:Z:2:ALA:C	12:c:37:GLY:N	2.29	0.91
45:q:412:ILE:O	55:1:2428:U:O2'	1.88	0.90
20:E:8:LYS:O	52:3:38:CYS:O	1.90	0.90
20:E:3:ALA:N	55:1:1422:G:C1'	2.33	0.90
51:x:27:ASN:CA	55:1:386:A:C5'	2.51	0.89
20:E:19:LYS:CA	55:1:593:C:OP1	2.22	0.88
36:b:131:ALA:CA	55:1:2830:G:C1'	2.51	0.88
13:d:103:GLY:CA	55:1:3326:G:OP1	2.22	0.87
16:g:27:GLY:CA	55:1:1598:G:C5'	2.52	0.87
24:X:21:LYS:O	55:1:2:U:OP2	1.91	0.87
24:X:21:LYS:C	55:1:2:U:OP2	2.17	0.86
24:X:21:LYS:N	55:1:2:U:OP2	2.08	0.86
54:5:353:GLY:HA2	55:1:193:C:C5'	2.05	0.86
16:g:66:SER:CA	55:1:1821:U:O3'	2.23	0.86
34:W:15:THR:C	55:1:1279:C:H5''	2.00	0.86
20:E:17:ALA:C	55:1:592:A:C5'	2.45	0.86
39:r:44:GLY:N	55:1:1300:G:OP1	2.08	0.86
16:g:27:GLY:HA3	55:1:1598:G:C5'	2.06	0.85
20:E:24:ALA:H	55:1:607:A:P	1.98	0.85
20:E:7:PRO:O	52:3:38:CYS:O	1.94	0.85
53:4:129:LEU:O	53:4:132:GLN:O	1.94	0.85
6:Q:143:PRO:CA	55:1:745:C:OP1	2.24	0.85
11:Z:3:LYS:N	12:c:37:GLY:N	2.25	0.85
16:g:27:GLY:CA	55:1:1598:G:H5''	2.06	0.85
20:E:5:LYS:CA	52:3:18:ARG:C	2.49	0.85
51:x:56:VAL:O	55:1:379:C:O2'	1.94	0.84
55:1:986:U:O2'	56:F:122:ALA:O	1.95	0.84
16:g:53:GLY:HA3	55:1:1640:G:OP2	1.77	0.84
16:g:67:LYS:H	55:1:1821:U:HO2'	1.25	0.84
55:1:3263:G:H2'	55:1:3264:G:C5'	2.06	0.84
12:c:88:GLY:N	55:1:1729:A:OP2	2.12	0.83
7:R:118:HIS:CA	55:1:1718:G:OP1	2.27	0.82
4:M:13:ARG:N	8:S:172:TYR:O	2.13	0.82
6:Q:141:ARG:O	55:1:744:A:C4'	2.28	0.82
2:6:44:G:O2'	31:K:241:GLY:HA3	1.80	0.81
25:Y:61:GLY:HA2	55:1:198:A:H4'	1.61	0.81
16:g:27:GLY:HA3	55:1:1598:G:H5''	1.60	0.81
7:R:129:GLY:HA3	55:1:840:C:C2'	2.10	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:d:103:GLY:HA2	55:1:3326:G:OP1	1.81	0.80
20:E:6:ALA:N	52:3:19:ILE:C	2.39	0.80
51:x:27:ASN:C	55:1:385:A:O3'	2.25	0.79
55:1:3263:G:O2'	55:1:3264:G:H5'	1.81	0.79
15:f:6:ARG:O	20:E:165:LEU:N	2.14	0.79
7:R:118:HIS:CA	55:1:1718:G:C5'	2.60	0.79
36:b:421:LEU:N	42:y:86:ASN:O	2.17	0.78
20:E:6:ALA:H	52:3:19:ILE:H	1.26	0.78
34:W:15:THR:O	55:1:1279:C:H5''	1.84	0.78
20:E:8:LYS:C	52:3:38:CYS:O	2.27	0.78
55:1:3301:U:C3'	55:1:3302:U:P	2.71	0.78
6:Q:137:THR:H	55:1:729:C:H4'	1.48	0.78
55:1:3263:G:C2'	55:1:3264:G:H5'	2.12	0.78
20:E:24:ALA:N	55:1:607:A:OP1	2.17	0.77
20:E:4:GLN:N	55:1:1422:G:O2'	2.17	0.77
7:R:117:LYS:O	55:1:1718:G:C4'	2.33	0.76
13:d:104:LEU:H	55:1:3325:G:H5''	1.49	0.76
20:E:6:ALA:N	52:3:19:ILE:H	1.75	0.76
52:3:40:ARG:O	55:1:1353:U:H4'	1.85	0.76
16:g:78:GLY:CA	55:1:1805:C:H5'	2.14	0.76
6:Q:136:ASN:N	55:1:729:C:O3'	2.18	0.76
20:E:6:ALA:H	52:3:18:ARG:CA	1.99	0.76
55:1:3158:G:OP1	55:1:3395:G:O2'	2.02	0.75
55:1:2352:A:OP1	57:P:83:TRP:C	2.29	0.75
16:g:27:GLY:HA3	55:1:1598:G:OP1	1.87	0.75
7:R:121:HIS:N	55:1:1719:G:OP2	2.19	0.75
19:k:2:ALA:N	55:1:1613:A:OP1	2.20	0.74
51:x:58:GLN:O	55:1:391:A:O2'	2.06	0.73
16:g:27:GLY:CA	55:1:1598:G:H5'	2.17	0.73
51:x:31:HIS:O	55:1:385:A:OP1	2.06	0.73
2:6:57:U:O2'	37:o:174:GLU:O	2.05	0.73
45:q:412:ILE:O	55:1:2428:U:C1'	2.37	0.72
13:d:103:GLY:HA3	55:1:3326:G:OP1	1.88	0.72
20:E:19:LYS:C	55:1:593:C:OP1	2.31	0.72
39:r:42:LEU:O	55:1:1299:U:O2'	2.06	0.72
55:1:3263:G:H2'	55:1:3264:G:H5'	1.70	0.72
20:E:78:ARG:O	55:1:3272:C:H4'	1.90	0.72
1:2:19:C:H4'	55:1:1395:G:H4'	1.72	0.72
42:y:8:GLU:CA	55:1:3019:U:P	2.79	0.71
16:g:76:TYR:CA	55:1:1805:C:O3'	2.37	0.71
53:4:84:THR:O	53:4:85:ALA:C	2.33	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:44:G:O2'	31:K:241:GLY:HA2	1.90	0.71
24:X:23:ALA:N	55:1:2:U:H4'	2.05	0.70
35:l:62:ASN:O	45:q:402:ASN:N	2.23	0.70
53:4:84:THR:C	53:4:86:ASP:N	2.48	0.70
51:x:56:VAL:C	55:1:379:C:O2'	2.35	0.70
6:Q:141:ARG:O	55:1:744:A:H4'	1.90	0.69
7:R:129:GLY:CA	55:1:840:C:C2'	2.67	0.69
51:x:283:LYS:O	51:x:286:MET:N	2.25	0.69
11:Z:3:LYS:N	12:c:36:GLN:C	2.50	0.69
7:R:118:HIS:N	55:1:1718:G:H5'	2.08	0.69
55:1:249:U:H3'	55:1:250:U:C5'	2.21	0.69
52:3:101:SER:N	55:1:1350:A:H2'	2.08	0.69
55:1:3263:G:C2'	55:1:3264:G:C5'	2.70	0.69
51:x:56:VAL:C	55:1:379:C:HO2'	2.00	0.68
16:g:53:GLY:HA2	55:1:1640:G:P	2.34	0.68
4:M:132:LYS:C	55:1:3229:G:O2'	2.36	0.68
53:4:84:THR:C	53:4:86:ASP:H	2.01	0.68
20:E:3:ALA:H	55:1:1422:G:C2'	2.07	0.68
55:1:873:C:H3'	55:1:874:U:H4'	1.74	0.68
51:x:16:GLN:CA	55:1:402:A:OP2	2.42	0.68
16:g:53:GLY:CA	55:1:1640:G:P	2.82	0.67
16:g:24:LYS:O	55:1:1696:A:H5''	1.92	0.67
13:d:104:LEU:C	55:1:3325:G:H4'	2.18	0.67
1:2:15:G:H4'	55:1:1441:G:O3'	1.95	0.67
55:1:144:A:H2'	55:1:145:G:O4'	1.96	0.66
13:d:104:LEU:N	55:1:3325:G:H5''	2.10	0.66
20:E:5:LYS:O	52:3:20:LYS:CA	2.43	0.66
51:x:31:HIS:CA	55:1:385:A:C5'	2.70	0.66
13:d:106:THR:O	55:1:3384:U:O2'	2.09	0.66
1:2:114:G:OP1	55:1:1831:U:O2'	2.12	0.66
20:E:3:ALA:CA	55:1:1422:G:O2'	2.43	0.66
20:E:8:LYS:O	52:3:38:CYS:C	2.38	0.66
24:X:21:LYS:CA	55:1:2:U:P	2.83	0.65
55:1:3301:U:H3'	55:1:3302:U:P	2.36	0.65
10:U:97:SER:N	55:1:1678:G:OP1	2.28	0.65
20:E:5:LYS:O	52:3:20:LYS:N	2.30	0.65
20:E:73:GLY:HA3	55:1:3267:A:O2'	1.96	0.65
16:g:27:GLY:HA2	55:1:1598:G:H5''	1.76	0.65
2:6:38:U:H5'	37:o:188:GLY:O	1.97	0.65
10:U:97:SER:H	55:1:1678:G:P	2.19	0.65
6:Q:137:THR:N	55:1:729:C:H4'	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:146:PRO:O	52:3:72:THR:CA	2.46	0.64
34:W:178:GLY:HA2	39:r:12:LYS:O	1.96	0.64
4:M:132:LYS:C	55:1:3229:G:HO2'	2.05	0.64
20:E:6:ALA:N	52:3:19:ILE:CA	2.60	0.64
20:E:8:LYS:O	55:1:1353:U:O2'	2.16	0.64
24:X:23:ALA:CA	55:1:2:U:H4'	2.28	0.64
16:g:78:GLY:H	55:1:1805:C:C5'	2.10	0.64
36:b:421:LEU:O	42:y:86:ASN:O	2.15	0.63
20:E:5:LYS:CA	52:3:19:ILE:CA	2.77	0.63
43:z:2:ALA:N	55:1:2891:U:HO2'	1.97	0.63
55:1:1253:U:H5''	55:1:1254:C:H5'	1.80	0.63
20:E:3:ALA:CA	55:1:1422:G:C1'	2.77	0.63
51:x:60:ILE:N	55:1:392:G:P	2.72	0.62
55:1:240:U:H4'	55:1:241:G:H5'	1.80	0.62
16:g:76:TYR:H	55:1:1806:A:P	2.14	0.62
52:3:101:SER:CA	55:1:1350:A:C2'	2.72	0.61
1:2:113:U:OP1	55:1:1832:C:O2'	2.17	0.61
55:1:40:A:H4'	55:1:41:G:OP1	2.00	0.61
20:E:6:ALA:CA	52:3:19:ILE:O	2.49	0.61
52:3:104:PHE:N	55:1:1351:U:O4'	2.33	0.61
16:g:27:GLY:HA2	55:1:1598:G:C5'	2.30	0.61
20:E:5:LYS:C	52:3:19:ILE:N	2.57	0.60
6:Q:136:ASN:N	55:1:730:C:OP1	2.35	0.60
20:E:73:GLY:CA	55:1:3267:A:O2'	2.50	0.60
55:1:2979:U:H5'	55:1:2980:U:H5'	1.82	0.60
16:g:78:GLY:H	55:1:1805:C:H5''	1.65	0.60
20:E:17:ALA:O	55:1:592:A:P	2.60	0.60
16:g:78:GLY:HA3	55:1:1805:C:H5'	1.84	0.59
6:Q:143:PRO:CA	55:1:745:C:P	2.90	0.59
7:R:118:HIS:CA	55:1:1718:G:O5'	2.50	0.59
20:E:17:ALA:C	55:1:592:A:C4'	2.75	0.59
40:s:9:ARG:N	55:1:1309:U:OP2	2.34	0.58
55:1:1764:U:H4'	55:1:1765:U:H5''	1.84	0.58
55:1:3117:C:H2'	55:1:3118:C:O4'	2.02	0.58
2:6:15:C:H4'	2:6:16:U:OP2	2.04	0.58
20:E:5:LYS:CA	52:3:18:ARG:O	2.51	0.58
36:b:421:LEU:CA	42:y:86:ASN:O	2.52	0.58
13:d:104:LEU:O	55:1:3325:G:C4'	2.51	0.58
20:E:6:ALA:N	52:3:18:ARG:C	2.41	0.58
39:r:44:GLY:H	55:1:1300:G:P	2.24	0.58
43:z:2:ALA:N	55:1:3015:G:OP2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:76:ARG:O	55:1:293:C:O2'	2.19	0.57
55:1:3064:U:H2'	55:1:3065:G:O4'	2.05	0.57
7:R:120:TYR:C	55:1:1719:G:OP2	2.48	0.57
27:B:366:GLY:HA3	55:1:3330:A:H4'	1.87	0.57
20:E:5:LYS:C	52:3:19:ILE:CA	2.78	0.57
55:1:2604:U:H2'	55:1:2605:G:O4'	2.04	0.57
13:d:13:THR:O	55:1:3324:C:C4'	2.29	0.56
7:R:118:HIS:CA	55:1:1718:G:P	2.94	0.56
6:Q:74:GLU:O	55:1:741:U:C5'	2.51	0.56
20:E:5:LYS:CA	52:3:19:ILE:C	2.72	0.56
50:J:319:GLN:CA	55:1:2406:C:C2'	2.84	0.56
51:x:59:THR:CA	55:1:391:A:O3'	2.53	0.56
51:x:60:ILE:H	55:1:392:G:P	2.27	0.56
51:x:286:MET:C	51:x:288:LYS:H	2.12	0.56
6:Q:136:ASN:CA	55:1:730:C:H5'	2.36	0.56
16:g:66:SER:C	55:1:1821:U:O2'	2.46	0.56
7:R:118:HIS:O	55:1:1718:G:P	2.64	0.56
55:1:3294:A:H2'	55:1:3295:A:O4'	2.06	0.56
36:b:128:LEU:CA	39:r:251:ARG:O	2.53	0.55
20:E:78:ARG:O	55:1:3272:C:C4'	2.53	0.55
16:g:53:GLY:HA3	55:1:1640:G:P	2.45	0.55
42:y:8:GLU:C	55:1:3019:U:P	2.89	0.55
11:Z:2:ALA:C	12:c:37:GLY:HA2	2.21	0.55
36:b:130:ARG:O	55:1:2830:G:O4'	2.24	0.55
55:1:3078:U:OP1	55:1:3080:G:H5'	2.07	0.55
2:6:10:A:H2'	2:6:11:C:O4'	2.07	0.55
20:E:18:LEU:O	55:1:592:A:H4'	2.07	0.55
2:6:38:U:OP1	37:o:189:ILE:O	2.25	0.55
55:1:3308:C:O2'	57:P:69:ARG:O	2.14	0.55
39:r:44:GLY:CA	55:1:1300:G:OP1	2.54	0.54
20:E:5:LYS:CA	52:3:19:ILE:N	2.70	0.54
55:1:1611:G:H2'	55:1:1612:A:O4'	2.08	0.54
6:Q:143:PRO:CA	55:1:744:A:O3'	2.56	0.54
7:R:57:VAL:CA	55:1:1690:C:H4'	2.36	0.54
55:1:3223:A:H2'	55:1:3224:G:O4'	2.07	0.54
20:E:17:ALA:O	55:1:591:G:O3'	2.26	0.54
20:E:8:LYS:O	52:3:39:THR:N	2.37	0.54
20:E:18:LEU:C	55:1:592:A:H5'	2.33	0.54
55:1:2909:U:H2'	55:1:2910:A:O4'	2.08	0.54
6:Q:142:GLY:C	55:1:744:A:H4'	2.33	0.54
16:g:66:SER:CA	55:1:1821:U:O2'	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:g:78:GLY:C	55:1:1804:A:O2'	2.49	0.54
16:g:76:TYR:CA	55:1:1806:A:OP1	2.54	0.54
20:E:4:GLN:CA	52:3:20:LYS:O	2.56	0.54
2:6:34:A:OP1	31:K:287:PRO:CA	2.56	0.53
45:q:412:ILE:O	55:1:2428:U:C2'	2.55	0.53
51:x:56:VAL:N	55:1:379:C:O2'	2.41	0.53
55:1:3158:G:P	55:1:3395:G:O2'	2.65	0.53
55:1:310:U:H2'	55:1:311:C:O4'	2.09	0.53
2:6:21:G:O2'	41:t:93:ILE:O	2.25	0.53
16:g:76:TYR:CA	55:1:1806:A:P	2.97	0.53
16:g:78:GLY:N	55:1:1805:C:H5'	2.22	0.53
7:R:58:HIS:H	55:1:1690:C:C5'	2.21	0.53
35:l:53:LYS:O	55:1:2427:U:H5'	2.07	0.53
14:e:56:GLY:HA3	55:1:1161:G:O2'	2.09	0.53
55:1:3027:A:H2'	55:1:3028:G:O4'	2.09	0.53
55:1:3129:A:H2'	55:1:3130:A:H5''	1.91	0.53
55:1:3158:G:P	55:1:3395:G:HO2'	2.29	0.53
1:2:96:A:H5'	18:j:81:GLY:O	2.08	0.52
55:1:29:C:H4'	55:1:62:A:H4'	1.91	0.52
55:1:3045:G:H2'	55:1:3046:A:O4'	2.10	0.52
50:J:318:VAL:C	55:1:2406:C:O2'	2.53	0.52
6:Q:74:GLU:H	55:1:742:G:P	2.33	0.51
22:O:66:LYS:O	55:1:3008:A:H4'	2.10	0.51
11:Z:2:ALA:N	12:c:37:GLY:C	2.64	0.51
16:g:27:GLY:N	55:1:1598:G:H5'	2.24	0.51
13:d:104:LEU:O	55:1:3325:G:H4'	2.11	0.51
28:C:338:LYS:O	28:C:340:GLY:N	2.41	0.51
14:e:127:ALA:O	52:3:135:VAL:O	2.29	0.51
36:b:33:ILE:N	55:1:2826:U:O2'	2.33	0.51
55:1:3375:A:O2'	55:1:3378:C:OP2	2.26	0.51
55:1:3145:C:O2'	55:1:3146:G:H5'	2.10	0.51
16:g:78:GLY:N	55:1:1805:C:C5'	2.73	0.51
55:1:596:C:H2'	55:1:597:G:O4'	2.11	0.51
55:1:2352:A:H5'	57:P:83:TRP:O	2.04	0.51
38:n:254:LYS:O	41:t:202:SER:N	2.43	0.50
51:x:31:HIS:C	55:1:385:A:H5'	2.36	0.50
1:2:106:C:H4'	1:2:107:G:H5''	1.92	0.50
27:B:128:LYS:O	55:1:3150:A:H4'	2.11	0.50
38:n:6:LYS:CA	55:1:1618:G:OP1	2.59	0.50
52:3:118:VAL:C	52:3:120:ILE:H	2.18	0.50
55:1:1324:U:H2'	55:1:1325:U:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:g:76:TYR:N	55:1:1806:A:P	2.80	0.50
23:V:10:LYS:O	55:1:3039:C:O2'	2.24	0.50
28:C:145:ILE:O	52:3:74:ALA:N	2.44	0.50
55:1:759:U:H3'	55:1:760:G:H5''	1.93	0.50
34:W:15:THR:O	55:1:1279:C:C5'	2.58	0.49
55:1:2353:G:OP1	57:P:86:LYS:N	2.44	0.49
1:2:42:G:OP2	18:j:64:MET:N	2.42	0.49
1:2:19:C:C4'	55:1:1395:G:H4'	2.41	0.49
6:Q:141:ARG:O	55:1:744:A:O4'	2.30	0.49
55:1:238:A:H2'	55:1:239:G:O4'	2.12	0.49
55:1:990:U:H3'	55:1:991:G:H5''	1.95	0.49
25:Y:2:ALA:N	55:1:212:G:OP2	2.46	0.49
55:1:884:A:H4'	55:1:885:U:H5'	1.95	0.49
2:6:57:U:O3'	37:o:175:LYS:O	2.30	0.49
7:R:24:LEU:O	55:1:1473:G:H5'	2.13	0.48
6:Q:74:GLU:N	55:1:742:G:OP1	2.37	0.48
55:1:1806:A:H2'	55:1:1807:G:O4'	2.14	0.48
55:1:1449:A:H2'	55:1:1450:G:O4'	2.14	0.48
25:Y:5:SER:N	55:1:229:G:OP1	2.44	0.48
55:1:514:G:H2'	55:1:515:C:O4'	2.14	0.47
55:1:3118:C:H2'	55:1:3119:U:O4'	2.14	0.47
55:1:548:G:H2'	55:1:549:U:O4'	2.14	0.47
20:E:8:LYS:CA	52:3:38:CYS:O	2.62	0.47
36:b:131:ALA:CA	55:1:2830:G:O4'	2.62	0.47
21:G:75:ILE:C	21:G:77:GLN:H	2.23	0.47
39:r:26:LYS:CA	55:1:3119:U:H5''	2.45	0.47
51:x:286:MET:O	51:x:288:LYS:N	2.45	0.47
55:1:3308:C:H2'	55:1:3309:G:O4'	2.15	0.47
16:g:9:ARG:CA	55:1:1527:C:O2'	2.62	0.47
55:1:1581:C:H4'	55:1:1582:C:OP1	2.15	0.47
1:2:14:C:H5'	57:P:121:GLN:O	2.14	0.46
7:R:96:ILE:O	55:1:1722:U:H5'	2.15	0.46
55:1:1697:A:H2'	55:1:1698:C:O4'	2.15	0.46
55:1:2352:A:OP1	57:P:84:PRO:N	2.47	0.46
7:R:117:LYS:O	55:1:1718:G:O3'	2.32	0.46
55:1:1883:A:H2'	55:1:1884:A:O4'	2.15	0.46
55:1:2933:A:OP1	55:1:3015:G:H4'	2.16	0.46
20:E:22:ARG:O	55:1:607:A:C5'	2.63	0.46
55:1:2998:U:H2'	55:1:2999:U:O4'	2.16	0.46
20:E:6:ALA:CA	52:3:19:ILE:H	2.27	0.46
25:Y:4:GLN:N	55:1:229:G:OP1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:1:355:A:H2'	55:1:356:C:O4'	2.15	0.46
41:t:276:GLU:O	41:t:278:SER:N	2.49	0.46
50:J:319:GLN:N	55:1:2406:C:HO2'	2.10	0.46
55:1:220:G:O2'	55:1:221:A:H5'	2.15	0.46
55:1:551:A:O2'	55:1:552:G:O5'	2.31	0.46
47:v:17:ALA:O	55:1:333:G:H4'	2.16	0.46
13:d:62:ARG:CA	55:1:3075:G:H5''	2.45	0.46
13:d:104:LEU:C	55:1:3325:G:C5'	2.87	0.46
36:b:130:ARG:O	55:1:2830:G:C4'	2.64	0.45
1:2:107:G:H4'	1:2:138:A:H5'	1.98	0.45
37:o:189:ILE:O	37:o:191:LYS:N	2.49	0.45
50:J:319:GLN:O	55:1:2406:C:H4'	2.16	0.45
25:Y:91:ASN:CA	55:1:378:A:C1'	2.95	0.45
1:2:67:U:H5''	18:j:85:LYS:CA	2.46	0.45
55:1:3006:A:H2'	55:1:3007:U:O4'	2.16	0.45
2:6:44:G:O2'	31:K:241:GLY:N	2.48	0.45
8:S:14:LEU:H	8:S:56:GLY:HA2	1.82	0.45
7:R:117:LYS:O	55:1:1718:G:C3'	2.64	0.45
51:x:27:ASN:C	55:1:386:A:C5'	2.89	0.45
55:1:543:C:O2'	55:1:544:C:O4'	2.29	0.45
55:1:1339:C:H2'	55:1:1340:G:O4'	2.17	0.45
55:1:1619:A:H5'	55:1:1620:U:OP2	2.17	0.45
55:1:208:C:H2'	55:1:209:A:O4'	2.16	0.45
55:1:674:G:H2'	55:1:675:C:O4'	2.17	0.45
55:1:814:U:H2'	55:1:815:G:O4'	2.17	0.44
55:1:1439:U:H2'	55:1:1440:G:O4'	2.17	0.44
55:1:2422:C:H2'	55:1:2423:U:O4'	2.16	0.44
36:b:128:LEU:N	39:r:251:ARG:O	2.50	0.44
55:1:16:A:H2'	55:1:17:G:O4'	2.17	0.44
55:1:370:U:H4'	55:1:404:G:H5'	1.98	0.44
45:q:413:GLY:O	55:1:2428:U:O3'	2.35	0.44
55:1:3305:A:H2'	55:1:3306:U:O4'	2.17	0.44
11:Z:2:ALA:C	12:c:37:GLY:H	2.19	0.44
36:b:134:GLY:CA	55:1:2829:U:O3'	2.66	0.44
52:3:101:SER:N	55:1:1350:A:C2'	2.79	0.44
55:1:3310:A:OP1	57:P:71:ALA:CA	2.65	0.44
55:1:1551:C:H2'	55:1:1552:G:O4'	2.18	0.44
20:E:17:ALA:C	55:1:592:A:H4'	2.43	0.44
55:1:496:C:H2'	55:1:497:C:O4'	2.17	0.44
55:1:497:C:H2'	55:1:498:A:O4'	2.18	0.44
2:6:4:U:H3'	2:6:5:C:H5'	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:129:GLY:H	55:1:840:C:HO2'	1.62	0.43
23:V:8:GLY:HA2	55:1:3017:A:O2'	2.17	0.43
1:2:130:C:H2'	1:2:131:A:O4'	2.18	0.43
20:E:5:LYS:O	52:3:19:ILE:C	2.57	0.43
21:G:78:PHE:C	21:G:80:TYR:H	2.26	0.43
20:E:3:ALA:N	55:1:1422:G:C2'	2.76	0.43
55:1:3057:U:H3'	55:1:3058:U:H4'	1.99	0.43
16:g:27:GLY:HA3	55:1:1598:G:P	2.58	0.43
55:1:3072:C:H5'	55:1:3336:A:H5''	1.99	0.43
55:1:3388:C:H5''	55:1:3389:U:H5'	2.01	0.43
55:1:1895:A:O2'	55:1:3053:G:H4'	2.18	0.43
55:1:3347:A:H2'	55:1:3348:G:O4'	2.18	0.43
38:n:4:LYS:O	55:1:1617:G:H4'	2.19	0.43
6:Q:141:ARG:O	55:1:744:A:H5'	2.19	0.43
55:1:715:A:H4'	55:1:752:C:O2'	2.19	0.43
55:1:1141:C:H2'	55:1:1142:G:O4'	2.18	0.43
27:B:225:GLY:HA2	55:1:3306:U:OP1	2.19	0.42
55:1:195:U:H2'	55:1:196:G:O4'	2.19	0.42
55:1:1734:G:H2'	55:1:1735:G:O4'	2.19	0.42
1:2:17:A:H4'	55:1:656:A:O2'	2.19	0.42
11:Z:16:GLY:C	11:Z:18:TYR:H	2.26	0.42
38:n:6:LYS:C	55:1:1618:G:OP1	2.62	0.42
55:1:772:U:H2'	55:1:773:G:O4'	2.20	0.42
6:Q:137:THR:O	55:1:729:C:O4'	2.38	0.42
7:R:96:ILE:CA	55:1:1722:U:C4'	2.97	0.42
55:1:216:G:H2'	55:1:217:U:O4'	2.19	0.42
6:Q:141:ARG:O	55:1:744:A:C5'	2.66	0.42
20:E:6:ALA:N	52:3:18:ARG:CA	2.75	0.42
55:1:221:A:O2'	55:1:223:U:OP2	2.37	0.42
7:R:129:GLY:HA2	55:1:840:C:C1'	2.49	0.42
3:L:72:GLY:HA2	55:1:76:G:OP1	2.19	0.42
55:1:811:U:H2'	55:1:812:G:O4'	2.20	0.42
55:1:3141:A:H3'	55:1:3142:A:H4'	2.00	0.42
55:1:3237:U:H2'	55:1:3238:G:O4'	2.19	0.41
51:x:289:GLU:C	51:x:291:LYS:H	2.27	0.41
55:1:357:A:H2'	55:1:358:G:O4'	2.19	0.41
55:1:2363:A:H2'	55:1:2364:G:O4'	2.20	0.41
55:1:2929:C:O2'	55:1:2930:A:O5'	2.37	0.41
6:Q:144:ARG:H	55:1:745:C:H5'	1.84	0.41
34:W:3:ARG:C	55:1:1210:U:OP2	2.63	0.41
51:x:31:HIS:C	55:1:385:A:C5'	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:45:LEU:C	55:1:584:G:H4'	2.45	0.41
20:E:22:ARG:O	55:1:607:A:H5'	2.19	0.41
55:1:3077:A:H2'	55:1:3080:G:O4'	2.21	0.41
14:e:27:ARG:N	55:1:655:C:OP1	2.54	0.41
42:y:8:GLU:C	55:1:3019:U:OP1	2.62	0.41
55:1:1870:C:O2'	55:1:3067:C:H5'	2.20	0.41
6:Q:137:THR:O	55:1:729:C:C1'	2.69	0.41
7:R:121:HIS:CA	55:1:1719:G:OP2	2.68	0.41
42:y:8:GLU:C	55:1:3019:U:OP2	2.64	0.41
55:1:1317:A:O2'	55:1:1318:A:H3'	2.21	0.41
55:1:1333:C:O2'	56:F:207:LEU:O	2.38	0.41
55:1:1837:U:H2'	55:1:1838:G:O4'	2.21	0.41
55:1:2902:A:H2'	55:1:2903:A:O4'	2.21	0.41
55:1:1167:U:H2'	55:1:1168:U:O4'	2.21	0.41
55:1:1231:A:H5''	55:1:1232:C:H5'	2.02	0.41
1:2:43:A:OP2	18:j:62:GLY:HA3	2.20	0.40
2:6:57:U:O2'	37:o:175:LYS:O	2.39	0.40
55:1:940:G:O2'	55:1:1435:A:H4'	2.20	0.40
55:1:1137:C:H2'	55:1:1138:U:O4'	2.21	0.40
1:2:56:G:H2'	1:2:57:C:O4'	2.21	0.40
1:2:153:U:H2'	1:2:154:C:O4'	2.21	0.40
51:x:223:ASP:O	51:x:225:GLU:N	2.53	0.40
55:1:106:A:H2'	55:1:107:A:O4'	2.21	0.40
55:1:254:A:H2'	55:1:255:A:O4'	2.21	0.40
55:1:798:G:H2'	55:1:799:G:O4'	2.22	0.40
20:E:5:LYS:C	52:3:18:ARG:C	2.90	0.40
55:1:643:U:H2'	55:1:644:G:H3'	2.03	0.40
55:1:821:U:H2'	55:1:822:G:O4'	2.21	0.40
35:l:100:LYS:CA	55:1:879:U:OP1	2.70	0.40
2:6:25:G:H4'	31:K:191:PRO:O	2.21	0.40

There are no symmetry-related clashes.

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	
3	L	119/199 (60%)	107 (90%)	8 (7%)	4 (3%)	3	21
4	M	134/138 (97%)	123 (92%)	10 (8%)	1 (1%)	18	55
5	N	182/204 (89%)	166 (91%)	13 (7%)	3 (2%)	7	37
6	Q	132/186 (71%)	123 (93%)	9 (7%)	0	100	100
7	R	116/189 (61%)	109 (94%)	6 (5%)	1 (1%)	14	49
8	S	168/172 (98%)	151 (90%)	13 (8%)	4 (2%)	4	27
9	T	20/160 (12%)	20 (100%)	0	0	100	100
10	U	96/121 (79%)	90 (94%)	6 (6%)	0	100	100
11	Z	133/136 (98%)	117 (88%)	13 (10%)	3 (2%)	5	28
12	c	95/105 (90%)	92 (97%)	3 (3%)	0	100	100
13	d	105/113 (93%)	96 (91%)	7 (7%)	2 (2%)	6	32
14	e	123/130 (95%)	120 (98%)	3 (2%)	0	100	100
15	f	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
16	g	110/121 (91%)	106 (96%)	4 (4%)	0	100	100
17	i	70/100 (70%)	61 (87%)	8 (11%)	1 (1%)	9	39
18	j	71/88 (81%)	67 (94%)	3 (4%)	1 (1%)	9	39
19	k	75/78 (96%)	69 (92%)	5 (7%)	1 (1%)	9	41
20	E	152/176 (86%)	131 (86%)	21 (14%)	0	100	100
21	G	180/256 (70%)	166 (92%)	12 (7%)	2 (1%)	11	45
22	O	195/199 (98%)	125 (64%)	38 (20%)	32 (16%)	0	2
23	V	132/137 (96%)	123 (93%)	8 (6%)	1 (1%)	16	52
24	X	139/142 (98%)	122 (88%)	15 (11%)	2 (1%)	9	39
25	Y	124/127 (98%)	115 (93%)	9 (7%)	0	100	100
26	h	117/120 (98%)	108 (92%)	6 (5%)	3 (3%)	4	25
27	B	337/387 (87%)	293 (87%)	38 (11%)	6 (2%)	6	33
28	C	357/362 (99%)	317 (89%)	33 (9%)	7 (2%)	6	31
29	H	188/191 (98%)	172 (92%)	15 (8%)	1 (0%)	24	62
30	A	192/291 (66%)	174 (91%)	16 (8%)	2 (1%)	12	47
31	K	253/376 (67%)	231 (91%)	20 (8%)	2 (1%)	16	52
32	m	641/807 (79%)	577 (90%)	57 (9%)	7 (1%)	11	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	D	188/505 (37%)	167 (89%)	21 (11%)	0	100	100
34	W	230/236 (98%)	214 (93%)	14 (6%)	2 (1%)	14	49
35	l	170/181 (94%)	156 (92%)	14 (8%)	0	100	100
36	b	413/647 (64%)	387 (94%)	24 (6%)	2 (0%)	24	62
37	o	131/220 (60%)	121 (92%)	9 (7%)	1 (1%)	16	52
38	n	403/605 (67%)	373 (93%)	28 (7%)	2 (0%)	24	62
39	r	170/261 (65%)	149 (88%)	20 (12%)	1 (1%)	21	58
40	s	34/520 (6%)	33 (97%)	1 (3%)	0	100	100
41	t	286/322 (89%)	260 (91%)	20 (7%)	6 (2%)	5	30
42	y	223/245 (91%)	211 (95%)	11 (5%)	1 (0%)	30	66
43	z	53/106 (50%)	53 (100%)	0	0	100	100
44	p	288/460 (63%)	262 (91%)	24 (8%)	2 (1%)	18	55
45	q	313/618 (51%)	270 (86%)	36 (12%)	7 (2%)	5	29
46	u	114/199 (57%)	107 (94%)	6 (5%)	1 (1%)	14	49
47	v	124/231 (54%)	118 (95%)	6 (5%)	0	100	100
48	w	426/841 (51%)	389 (91%)	37 (9%)	0	100	100
49	I	437/663 (66%)	392 (90%)	38 (9%)	7 (2%)	7	37
50	J	130/427 (30%)	122 (94%)	8 (6%)	0	100	100
51	x	259/295 (88%)	220 (85%)	28 (11%)	11 (4%)	2	17
52	3	171/306 (56%)	148 (86%)	19 (11%)	4 (2%)	5	28
53	4	216/278 (78%)	197 (91%)	17 (8%)	2 (1%)	14	49
54	5	377/463 (81%)	356 (94%)	19 (5%)	2 (0%)	24	62
56	F	239/244 (98%)	227 (95%)	8 (3%)	4 (2%)	7	35
57	P	133/184 (72%)	127 (96%)	5 (4%)	1 (1%)	16	52
All	All	10388/14975 (69%)	9430 (91%)	816 (8%)	142 (1%)	11	39

All (142) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	51	LEU
5	N	145	ASP
8	S	13	ARG
11	Z	103	GLN
19	k	33	LYS

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Mol	Chain	Res	Type
22	O	28	LEU
22	O	47	PHE
22	O	48	PHE
22	O	62	THR
22	O	63	ALA
22	O	86	GLY
22	O	89	SER
22	O	113	ASP
22	O	114	LYS
22	O	137	THR
22	O	145	VAL
22	O	162	VAL
22	O	189	ASP
23	V	90	GLY
26	h	91	ALA
27	B	34	LYS
27	B	222	LYS
28	C	4	PRO
28	C	140	HIS
28	C	339	LEU
32	m	231	GLU
37	o	190	THR
41	t	227	ILE
41	t	269	GLN
49	I	558	LYS
51	x	128	PHE
51	x	222	PRO
51	x	277	GLU
52	3	133	HIS
53	4	85	ALA
53	4	133	LEU
3	L	50	PRO
4	M	29	ALA
5	N	144	ARG
11	Z	125	GLY
13	d	87	ASN
17	i	30	LYS
22	O	13	GLY
22	O	16	VAL
22	O	17	GLY
22	O	27	LEU
22	O	77	SER

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Mol	Chain	Res	Type
22	O	190	VAL
22	O	191	ALA
22	O	198	GLY
27	B	35	ASP
27	B	138	ALA
28	C	269	SER
29	H	22	SER
32	m	177	GLY
32	m	232	GLN
32	m	328	LYS
41	t	277	VAL
45	q	300	GLY
45	q	427	THR
45	q	429	VAL
51	x	281	GLU
51	x	287	ASP
54	5	340	LYS
56	F	159	GLN
56	F	164	SER
3	L	62	THR
3	L	75	PHE
7	R	53	LYS
21	G	232	HIS
22	O	11	GLY
22	O	168	TYR
22	O	169	ALA
22	O	192	LYS
24	X	4	SER
26	h	119	LYS
27	B	187	SER
30	A	171	PRO
32	m	406	ASN
36	b	198	ALA
46	u	81	TYR
49	I	541	THR
51	x	65	VAL
51	x	292	LYS
56	F	157	ASN
57	P	156	ALA
5	N	94	TYR
8	S	24	LEU
18	j	85	LYS

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Mol	Chain	Res	Type
22	O	24	ALA
22	O	37	ARG
22	O	85	ARG
22	O	152	VAL
24	X	5	ALA
26	h	84	LYS
27	B	155	ALA
28	C	268	ALA
30	A	63	PRO
31	K	284	ASN
32	m	154	GLN
32	m	435	GLY
41	t	270	PRO
45	q	317	GLY
49	I	600	GLU
49	I	635	ASP
51	x	293	PHE
56	F	163	LEU
8	S	14	LEU
13	d	88	PRO
21	G	79	GLN
28	C	311	HIS
31	K	256	PRO
36	b	432	MET
38	n	196	GLU
38	n	456	HIS
41	t	151	LEU
41	t	240	GLY
44	p	351	ARG
44	p	418	ASP
49	I	527	PRO
49	I	561	THR
51	x	132	LEU
51	x	224	ILE
52	3	14	PHE
52	3	128	ARG
22	O	46	GLU
45	q	268	ALA
51	x	119	PRO
52	3	84	LYS
22	O	43	ILE
34	W	146	GLY

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Mol	Chain	Res	Type
45	q	269	ARG
11	Z	16	GLY
28	C	146	PRO
34	W	101	GLY
49	I	196	PRO
8	S	167	ARG
39	r	190	GLY
42	y	58	ILE
45	q	423	PRO
54	5	131	VAL
22	O	153	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	157/158 (99%)	36 (22%)	0
2	6	63/232 (27%)	30 (47%)	0
55	1	2416/3396 (71%)	725 (30%)	0
All	All	2636/3786 (69%)	791 (30%)	0

All (791) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	34	U
1	2	35	C
1	2	39	G
1	2	51	G
1	2	59	A
1	2	62	C
1	2	63	G
1	2	71	A
1	2	78	G
1	2	79	A
1	2	81	U
1	2	82	U
1	2	84	C
1	2	85	G

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Mol	Chain	Res	Type
1	2	86	U
1	2	87	G
1	2	90	U
1	2	95	G
1	2	97	A
1	2	104	A
1	2	106	C
1	2	107	G
1	2	111	A
1	2	113	U
1	2	116	G
1	2	123	G
1	2	124	G
1	2	125	U
1	2	126	A
1	2	128	U
1	2	134	G
1	2	136	G
1	2	151	C
1	2	152	G
1	2	157	U
1	2	158	U
2	6	4	U
2	6	5	C
2	6	6	U
2	6	7	C
2	6	8	A
2	6	9	A
2	6	13	U
2	6	14	U
2	6	15	C
2	6	16	U
2	6	17	G
2	6	23	U
2	6	24	A
2	6	34	A
2	6	36	U
2	6	39	U
2	6	40	U
2	6	42	G
2	6	43	A
2	6	47	A

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Mol	Chain	Res	Type
2	6	52	G
2	6	53	A
2	6	54	A
2	6	56	U
2	6	57	U
2	6	58	G
2	6	59	C
2	6	228	U
2	6	231	A
2	6	232	A
55	1	2	U
55	1	7	C
55	1	14	U
55	1	22	G
55	1	40	A
55	1	41	G
55	1	42	C
55	1	43	A
55	1	44	U
55	1	48	A
55	1	49	A
55	1	57	A
55	1	59	G
55	1	60	A
55	1	65	A
55	1	66	A
55	1	72	C
55	1	73	C
55	1	74	G
55	1	75	G
55	1	77	A
55	1	85	A
55	1	92	G
55	1	94	G
55	1	96	G
55	1	110	G
55	1	111	C
55	1	113	C
55	1	117	U
55	1	118	U
55	1	120	G
55	1	121	A

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Mol	Chain	Res	Type
55	1	122	A
55	1	135	C
55	1	136	G
55	1	143	G
55	1	148	G
55	1	150	A
55	1	154	U
55	1	155	G
55	1	156	G
55	1	157	A
55	1	164	A
55	1	165	A
55	1	166	C
55	1	170	G
55	1	173	G
55	1	190	U
55	1	191	U
55	1	196	G
55	1	197	G
55	1	200	C
55	1	205	C
55	1	206	G
55	1	210	U
55	1	211	A
55	1	212	G
55	1	213	A
55	1	218	G
55	1	219	A
55	1	220	G
55	1	234	G
55	1	240	U
55	1	241	G
55	1	243	G
55	1	249	U
55	1	250	U
55	1	251	G
55	1	252	U
55	1	264	G
55	1	265	A
55	1	266	A
55	1	268	A
55	1	269	G

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Mol	Chain	Res	Type
55	1	283	G
55	1	284	A
55	1	285	A
55	1	295	A
55	1	298	U
55	1	299	G
55	1	305	U
55	1	311	C
55	1	323	A
55	1	329	U
55	1	338	A
55	1	339	C
55	1	352	A
55	1	368	G
55	1	370	U
55	1	376	G
55	1	390	G
55	1	398	A
55	1	399	A
55	1	401	U
55	1	403	C
55	1	404	G
55	1	421	G
55	1	422	A
55	1	437	G
55	1	438	A
55	1	439	C
55	1	440	A
55	1	495	G
55	1	496	C
55	1	498	A
55	1	503	C
55	1	510	G
55	1	515	C
55	1	517	G
55	1	518	G
55	1	519	A
55	1	520	U
55	1	521	A
55	1	523	A
55	1	533	A
55	1	534	U

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Mol	Chain	Res	Type
55	1	535	G
55	1	536	U
55	1	542	G
55	1	543	C
55	1	547	G
55	1	550	A
55	1	551	A
55	1	552	G
55	1	555	U
55	1	556	U
55	1	557	A
55	1	558	U
55	1	559	A
55	1	569	A
55	1	578	A
55	1	579	G
55	1	588	G
55	1	589	A
55	1	592	A
55	1	593	C
55	1	597	G
55	1	603	A
55	1	604	G
55	1	609	G
55	1	611	A
55	1	620	U
55	1	621	A
55	1	622	A
55	1	623	U
55	1	634	C
55	1	636	C
55	1	643	U
55	1	644	G
55	1	645	A
55	1	649	A
55	1	650	C
55	1	660	A
55	1	676	G
55	1	677	A
55	1	681	U
55	1	690	A
55	1	691	A

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Mol	Chain	Res	Type
55	1	705	A
55	1	710	A
55	1	720	A
55	1	721	G
55	1	722	G
55	1	733	G
55	1	734	C
55	1	735	A
55	1	742	G
55	1	743	C
55	1	757	C
55	1	759	U
55	1	760	G
55	1	761	A
55	1	770	G
55	1	772	U
55	1	774	G
55	1	775	A
55	1	776	U
55	1	777	U
55	1	779	G
55	1	780	A
55	1	781	G
55	1	784	A
55	1	785	G
55	1	786	A
55	1	799	G
55	1	801	A
55	1	806	A
55	1	808	A
55	1	813	G
55	1	815	G
55	1	818	C
55	1	819	U
55	1	820	A
55	1	822	G
55	1	826	G
55	1	830	A
55	1	849	C
55	1	854	G
55	1	857	G
55	1	859	G

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Mol	Chain	Res	Type
55	1	860	G
55	1	861	C
55	1	864	G
55	1	871	U
55	1	874	U
55	1	875	G
55	1	877	C
55	1	878	G
55	1	879	U
55	1	880	G
55	1	881	C
55	1	882	A
55	1	883	A
55	1	884	A
55	1	886	C
55	1	887	G
55	1	891	G
55	1	892	U
55	1	893	C
55	1	894	G
55	1	895	A
55	1	896	A
55	1	898	U
55	1	899	U
55	1	900	G
55	1	904	A
55	1	906	A
55	1	909	G
55	1	910	G
55	1	918	C
55	1	919	U
55	1	920	A
55	1	921	A
55	1	932	U
55	1	936	A
55	1	938	C
55	1	944	C
55	1	957	C
55	1	958	C
55	1	959	C
55	1	960	U
55	1	961	C

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Mol	Chain	Res	Type
55	1	962	A
55	1	963	G
55	1	964	G
55	1	970	A
55	1	977	C
55	1	978	G
55	1	979	U
55	1	980	A
55	1	981	U
55	1	982	C
55	1	984	G
55	1	985	U
55	1	991	G
55	1	992	A
55	1	1059	G
55	1	1060	U
55	1	1098	A
55	1	1103	A
55	1	1104	G
55	1	1105	A
55	1	1108	U
55	1	1111	U
55	1	1112	A
55	1	1116	G
55	1	1117	G
55	1	1126	G
55	1	1127	G
55	1	1128	U
55	1	1129	A
55	1	1132	C
55	1	1135	A
55	1	1136	A
55	1	1139	G
55	1	1142	G
55	1	1144	U
55	1	1151	U
55	1	1153	A
55	1	1155	C
55	1	1159	A
55	1	1160	C
55	1	1174	G
55	1	1177	G

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Mol	Chain	Res	Type
55	1	1180	A
55	1	1181	U
55	1	1186	G
55	1	1192	C
55	1	1193	A
55	1	1196	C
55	1	1197	A
55	1	1198	C
55	1	1199	C
55	1	1200	A
55	1	1201	C
55	1	1204	A
55	1	1213	G
55	1	1217	A
55	1	1218	U
55	1	1221	A
55	1	1222	G
55	1	1227	C
55	1	1228	C
55	1	1233	G
55	1	1235	U
55	1	1237	G
55	1	1241	U
55	1	1242	G
55	1	1244	A
55	1	1245	A
55	1	1250	G
55	1	1251	A
55	1	1252	A
55	1	1253	U
55	1	1258	U
55	1	1259	A
55	1	1262	G
55	1	1263	A
55	1	1264	G
55	1	1266	G
55	1	1272	C
55	1	1273	A
55	1	1277	C
55	1	1278	A
55	1	1279	C
55	1	1283	C

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Mol	Chain	Res	Type
55	1	1284	C
55	1	1286	A
55	1	1287	A
55	1	1299	U
55	1	1300	G
55	1	1302	A
55	1	1303	A
55	1	1304	A
55	1	1305	U
55	1	1307	G
55	1	1308	A
55	1	1309	U
55	1	1325	U
55	1	1330	A
55	1	1331	U
55	1	1332	A
55	1	1348	U
55	1	1349	G
55	1	1350	A
55	1	1351	U
55	1	1352	A
55	1	1353	U
55	1	1354	G
55	1	1355	A
55	1	1356	U
55	1	1357	G
55	1	1364	C
55	1	1367	G
55	1	1380	G
55	1	1386	A
55	1	1391	C
55	1	1397	C
55	1	1399	A
55	1	1400	G
55	1	1419	A
55	1	1421	G
55	1	1429	G
55	1	1434	G
55	1	1437	C
55	1	1443	G
55	1	1446	A
55	1	1450	G

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Mol	Chain	Res	Type
55	1	1452	A
55	1	1453	A
55	1	1454	A
55	1	1455	U
55	1	1477	A
55	1	1481	A
55	1	1483	G
55	1	1484	U
55	1	1485	G
55	1	1487	G
55	1	1495	U
55	1	1503	A
55	1	1508	C
55	1	1512	U
55	1	1533	U
55	1	1536	G
55	1	1539	A
55	1	1544	G
55	1	1546	A
55	1	1547	G
55	1	1555	U
55	1	1556	C
55	1	1557	A
55	1	1560	G
55	1	1561	G
55	1	1562	C
55	1	1566	A
55	1	1567	U
55	1	1568	U
55	1	1569	U
55	1	1571	A
55	1	1573	G
55	1	1574	C
55	1	1575	A
55	1	1580	A
55	1	1581	C
55	1	1582	C
55	1	1587	A
55	1	1589	A
55	1	1590	G
55	1	1593	A
55	1	1596	C

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Mol	Chain	Res	Type
55	1	1605	A
55	1	1608	C
55	1	1613	A
55	1	1619	A
55	1	1620	U
55	1	1627	U
55	1	1628	C
55	1	1630	U
55	1	1639	C
55	1	1641	U
55	1	1642	A
55	1	1643	A
55	1	1647	A
55	1	1656	A
55	1	1657	C
55	1	1658	G
55	1	1683	A
55	1	1685	C
55	1	1687	U
55	1	1688	U
55	1	1713	G
55	1	1715	A
55	1	1716	U
55	1	1717	U
55	1	1724	U
55	1	1725	C
55	1	1730	G
55	1	1736	G
55	1	1741	A
55	1	1742	U
55	1	1743	G
55	1	1749	A
55	1	1750	A
55	1	1751	G
55	1	1756	C
55	1	1764	U
55	1	1765	U
55	1	1766	G
55	1	1768	U
55	1	1770	G
55	1	1775	G
55	1	1780	G

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Mol	Chain	Res	Type
55	1	1792	C
55	1	1794	G
55	1	1795	U
55	1	1796	G
55	1	1797	A
55	1	1808	G
55	1	1813	A
55	1	1814	A
55	1	1815	U
55	1	1816	A
55	1	1817	G
55	1	1820	U
55	1	1821	U
55	1	1852	G
55	1	1853	U
55	1	1862	U
55	1	1865	A
55	1	1866	C
55	1	1867	A
55	1	1868	G
55	1	1869	C
55	1	1871	U
55	1	1878	G
55	1	1879	A
55	1	1880	U
55	1	1881	A
55	1	1884	A
55	1	1886	A
55	1	1900	A
55	1	1906	G
55	1	1947	G
55	1	1948	G
55	1	1951	C
55	1	1952	G
55	1	1953	G
55	1	2095	G
55	1	2098	C
55	1	2100	A
55	1	2101	C
55	1	2123	G
55	1	2130	G
55	1	2322	C

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Mol	Chain	Res	Type
55	1	2323	G
55	1	2324	A
55	1	2325	G
55	1	2334	U
55	1	2335	G
55	1	2336	U
55	1	2347	U
55	1	2363	A
55	1	2370	G
55	1	2371	G
55	1	2372	A
55	1	2373	A
55	1	2374	C
55	1	2377	G
55	1	2385	G
55	1	2388	U
55	1	2392	C
55	1	2393	G
55	1	2394	G
55	1	2395	G
55	1	2405	C
55	1	2410	U
55	1	2411	U
55	1	2412	G
55	1	2414	G
55	1	2418	G
55	1	2419	A
55	1	2434	U
55	1	2597	U
55	1	2606	G
55	1	2607	G
55	1	2805	G
55	1	2807	U
55	1	2811	A
55	1	2812	C
55	1	2813	A
55	1	2818	U
55	1	2819	A
55	1	2820	A
55	1	2821	C
55	1	2822	U
55	1	2823	G

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Mol	Chain	Res	Type
55	1	2824	G
55	1	2825	C
55	1	2826	U
55	1	2836	C
55	1	2837	A
55	1	2838	A
55	1	2841	G
55	1	2842	U
55	1	2845	A
55	1	2846	U
55	1	2849	C
55	1	2855	U
55	1	2857	C
55	1	2858	U
55	1	2877	G
55	1	2878	G
55	1	2879	C
55	1	2880	U
55	1	2887	A
55	1	2889	C
55	1	2898	G
55	1	2899	C
55	1	2911	A
55	1	2916	U
55	1	2919	A
55	1	2920	U
55	1	2921	U
55	1	2922	G
55	1	2923	U
55	1	2924	U
55	1	2925	C
55	1	2926	A
55	1	2927	C
55	1	2929	C
55	1	2930	A
55	1	2935	U
55	1	2936	A
55	1	2941	A
55	1	2942	C
55	1	2943	G
55	1	2944	U
55	1	2945	G

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Mol	Chain	Res	Type
55	1	2946	A
55	1	2947	G
55	1	2949	U
55	1	2950	G
55	1	2951	G
55	1	2952	G
55	1	2953	U
55	1	2954	U
55	1	2955	U
55	1	2956	A
55	1	2964	G
55	1	2965	U
55	1	2966	G
55	1	2967	A
55	1	2968	G
55	1	2969	A
55	1	2970	C
55	1	2971	A
55	1	2972	G
55	1	2975	U
55	1	2976	A
55	1	2977	G
55	1	2979	U
55	1	2980	U
55	1	2981	U
55	1	2982	A
55	1	2983	C
55	1	2984	C
55	1	2987	A
55	1	2990	G
55	1	2992	U
55	1	2996	U
55	1	2997	G
55	1	3003	G
55	1	3012	A
55	1	3017	A
55	1	3019	U
55	1	3020	U
55	1	3021	A
55	1	3022	G
55	1	3023	U
55	1	3026	G

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Mol	Chain	Res	Type
55	1	3029	A
55	1	3030	G
55	1	3032	A
55	1	3037	U
55	1	3046	A
55	1	3056	U
55	1	3057	U
55	1	3058	U
55	1	3065	G
55	1	3069	G
55	1	3070	A
55	1	3071	U
55	1	3072	C
55	1	3074	G
55	1	3076	C
55	1	3078	U
55	1	3079	U
55	1	3086	A
55	1	3090	U
55	1	3092	C
55	1	3093	C
55	1	3094	A
55	1	3099	C
55	1	3100	U
55	1	3102	G
55	1	3104	U
55	1	3109	G
55	1	3116	G
55	1	3117	C
55	1	3122	A
55	1	3124	G
55	1	3129	A
55	1	3130	A
55	1	3131	U
55	1	3141	A
55	1	3142	A
55	1	3143	C
55	1	3173	G
55	1	3174	A
55	1	3176	G
55	1	3179	U
55	1	3180	A

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Mol	Chain	Res	Type
55	1	3181	C
55	1	3186	A
55	1	3187	A
55	1	3188	G
55	1	3196	U
55	1	3199	G
55	1	3206	C
55	1	3207	U
55	1	3216	G
55	1	3217	C
55	1	3218	A
55	1	3219	G
55	1	3227	A
55	1	3228	C
55	1	3229	G
55	1	3242	G
55	1	3243	A
55	1	3244	A
55	1	3245	A
55	1	3247	G
55	1	3249	C
55	1	3252	G
55	1	3256	G
55	1	3259	U
55	1	3263	G
55	1	3270	U
55	1	3275	U
55	1	3276	G
55	1	3286	G
55	1	3288	G
55	1	3289	G
55	1	3290	G
55	1	3294	A
55	1	3303	G
55	1	3304	U
55	1	3306	U
55	1	3307	A
55	1	3309	G
55	1	3313	U
55	1	3316	A
55	1	3317	U
55	1	3319	U

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Mol	Chain	Res	Type
55	1	3324	C
55	1	3328	G
55	1	3341	U
55	1	3342	A
55	1	3344	A
55	1	3345	G
55	1	3350	C
55	1	3351	U
55	1	3352	U
55	1	3353	G
55	1	3355	U
55	1	3356	G
55	1	3363	U
55	1	3366	G
55	1	3369	G
55	1	3375	A
55	1	3378	C
55	1	3386	G
55	1	3387	U
55	1	3390	G
55	1	3396	U

There are no RNA pucker outliers to report.

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
55	1	5
35	1	1
3	L	1
51	x	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	135:ALA	C	136:MET	N	6.21
1	1	1792:C	O3'	1793:C	P	5.60
1	L	8:PRO	C	9:ILE	N	4.88
1	1	966:U	O3'	967:A	P	4.55
1	x	285:GLU	C	286:MET	N	3.36
1	1	3301:U	O3'	3302:U	P	2.05
1	1	3176:G	O3'	3177:G	P	1.96
1	1	3263:G	O3'	3264:G	P	0.95

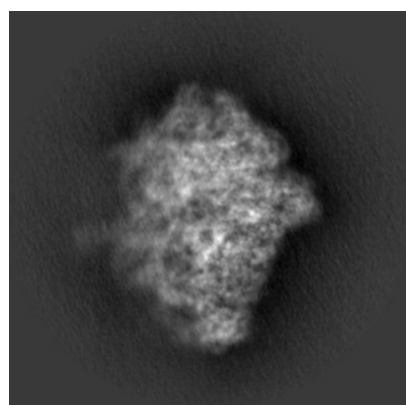
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3890. These allow visual inspection of the internal detail of the map and identification of artifacts.

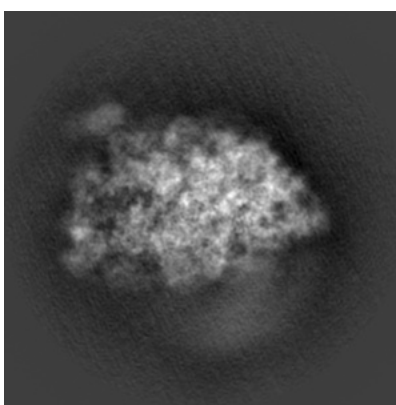
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

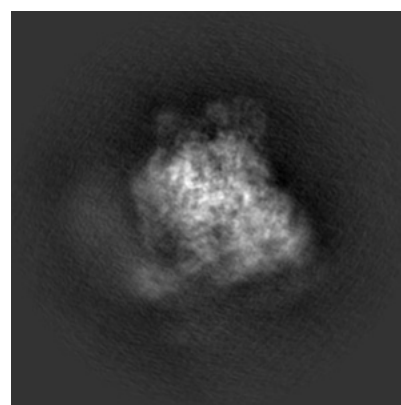
6.1.1 Primary map



X



Y

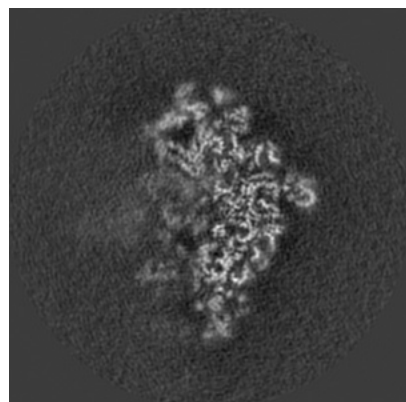


Z

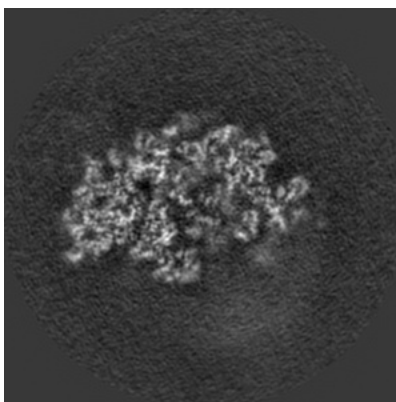
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

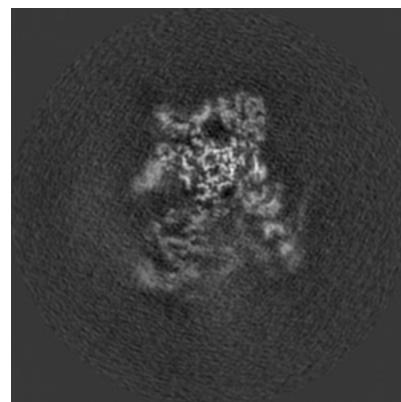
6.2.1 Primary map



X Index: 210



Y Index: 210

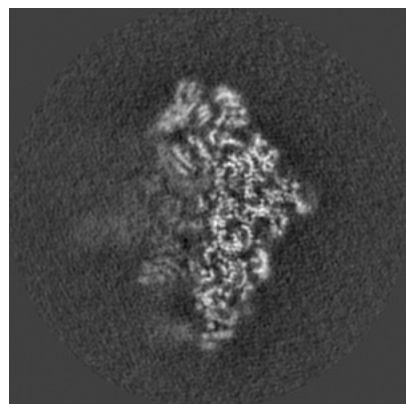


Z Index: 210

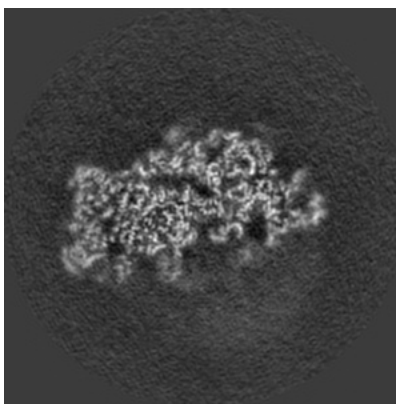
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

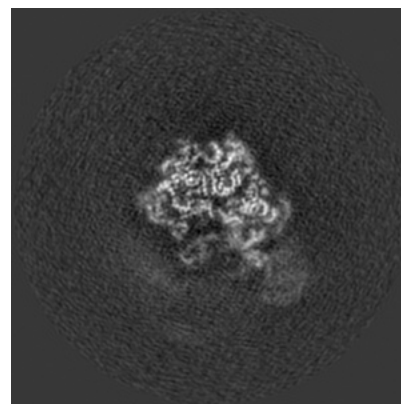
6.3.1 Primary map



X Index: 203



Y Index: 224

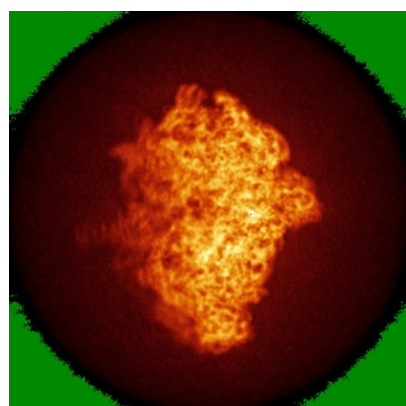


Z Index: 167

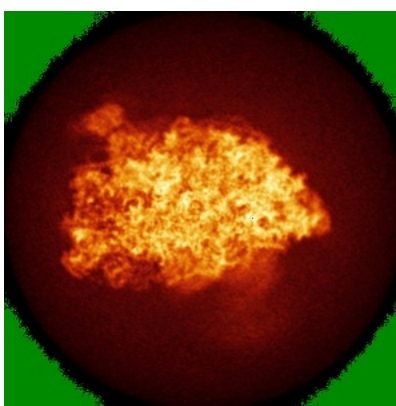
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

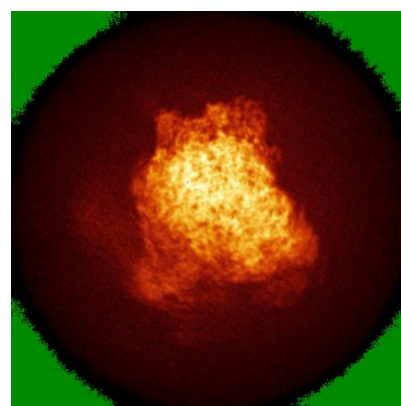
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

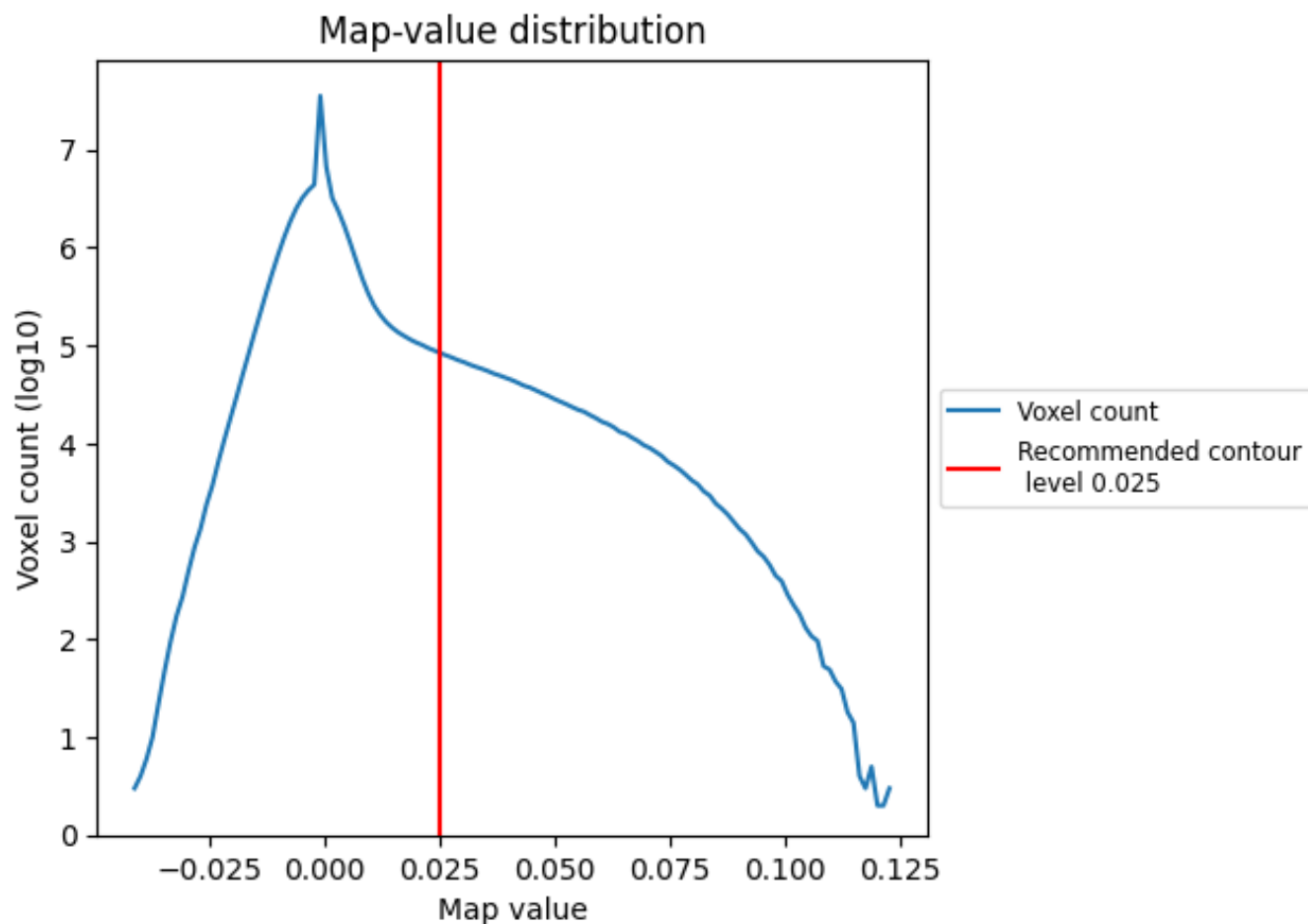
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

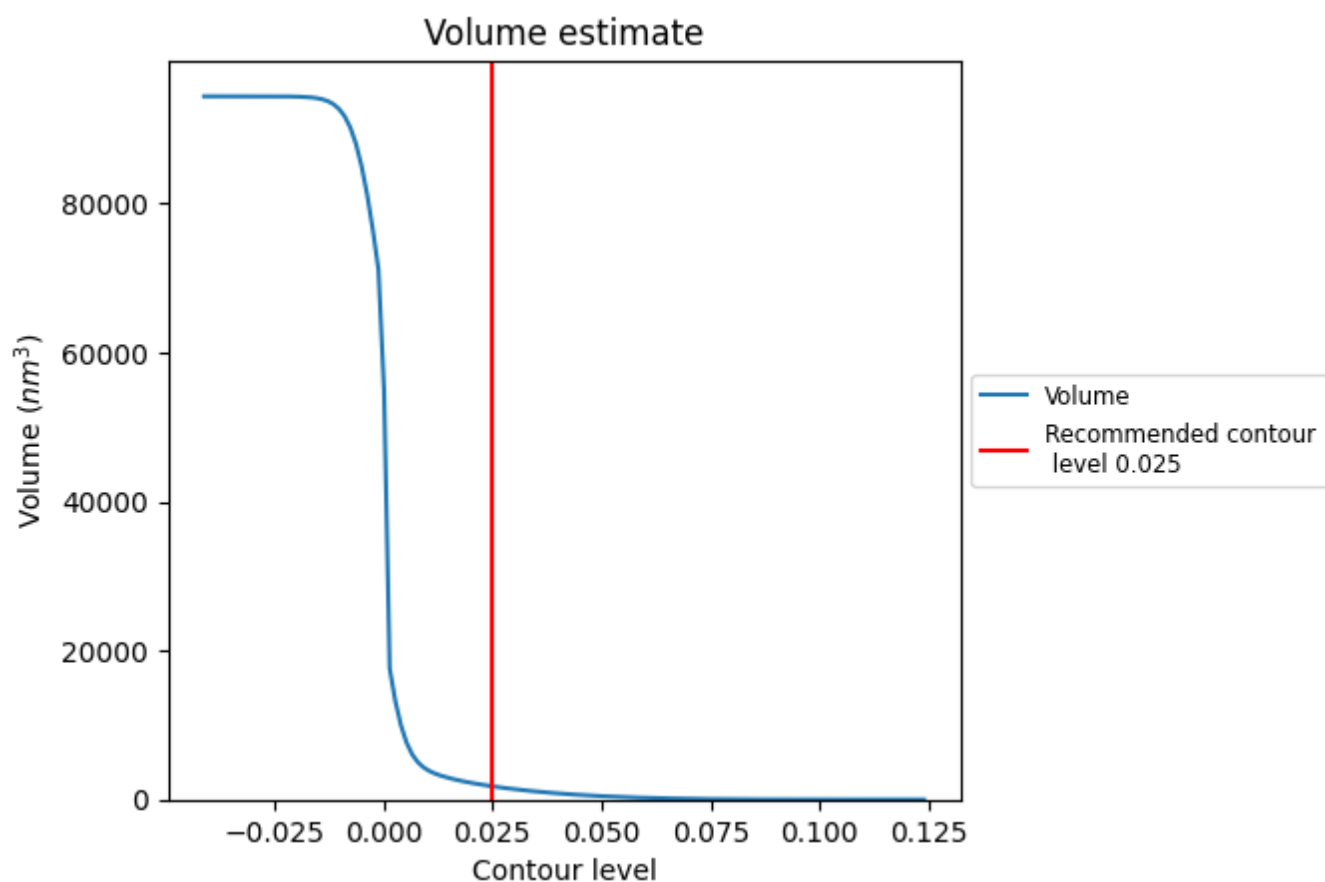
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

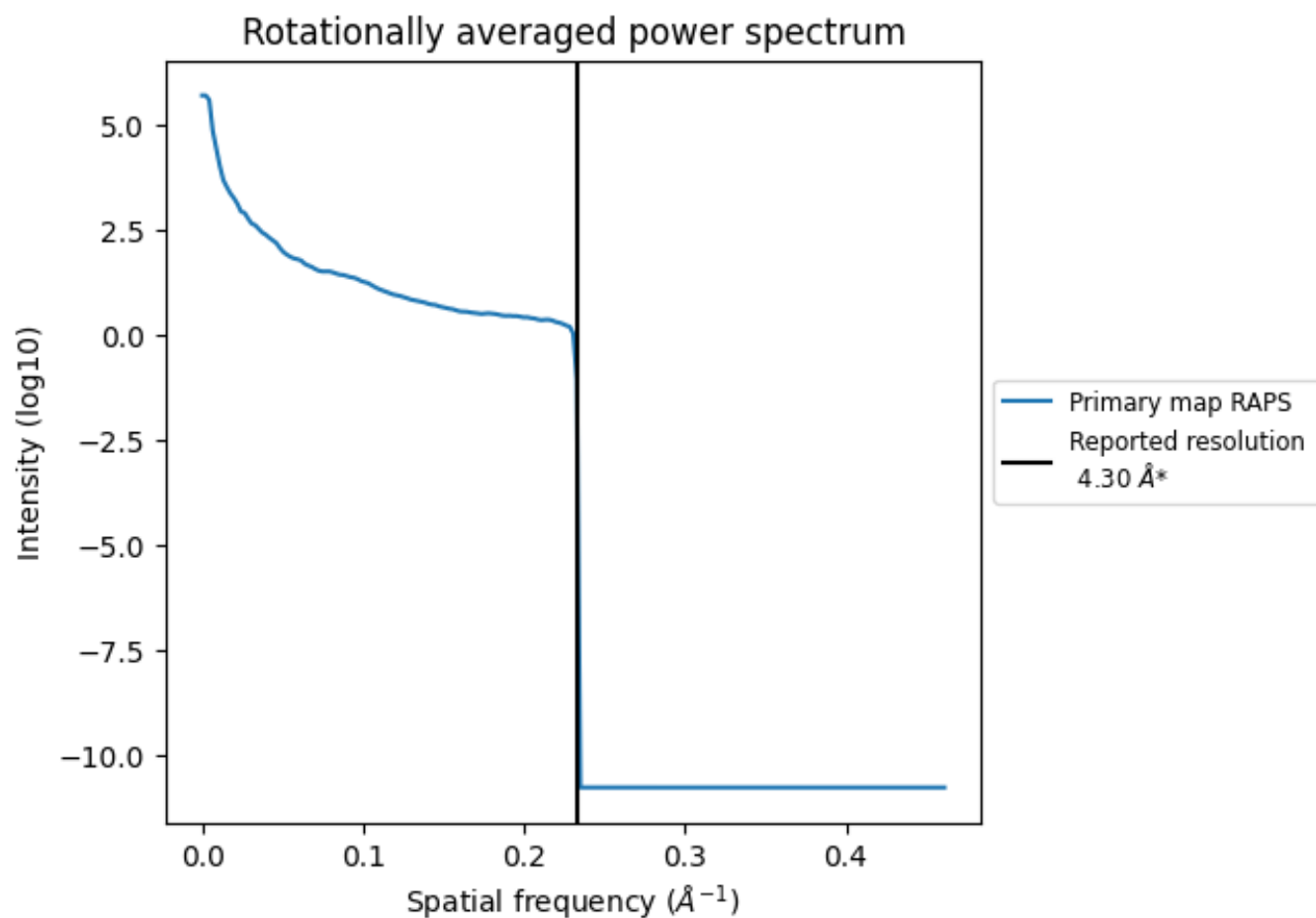
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1775 nm³; this corresponds to an approximate mass of 1603 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

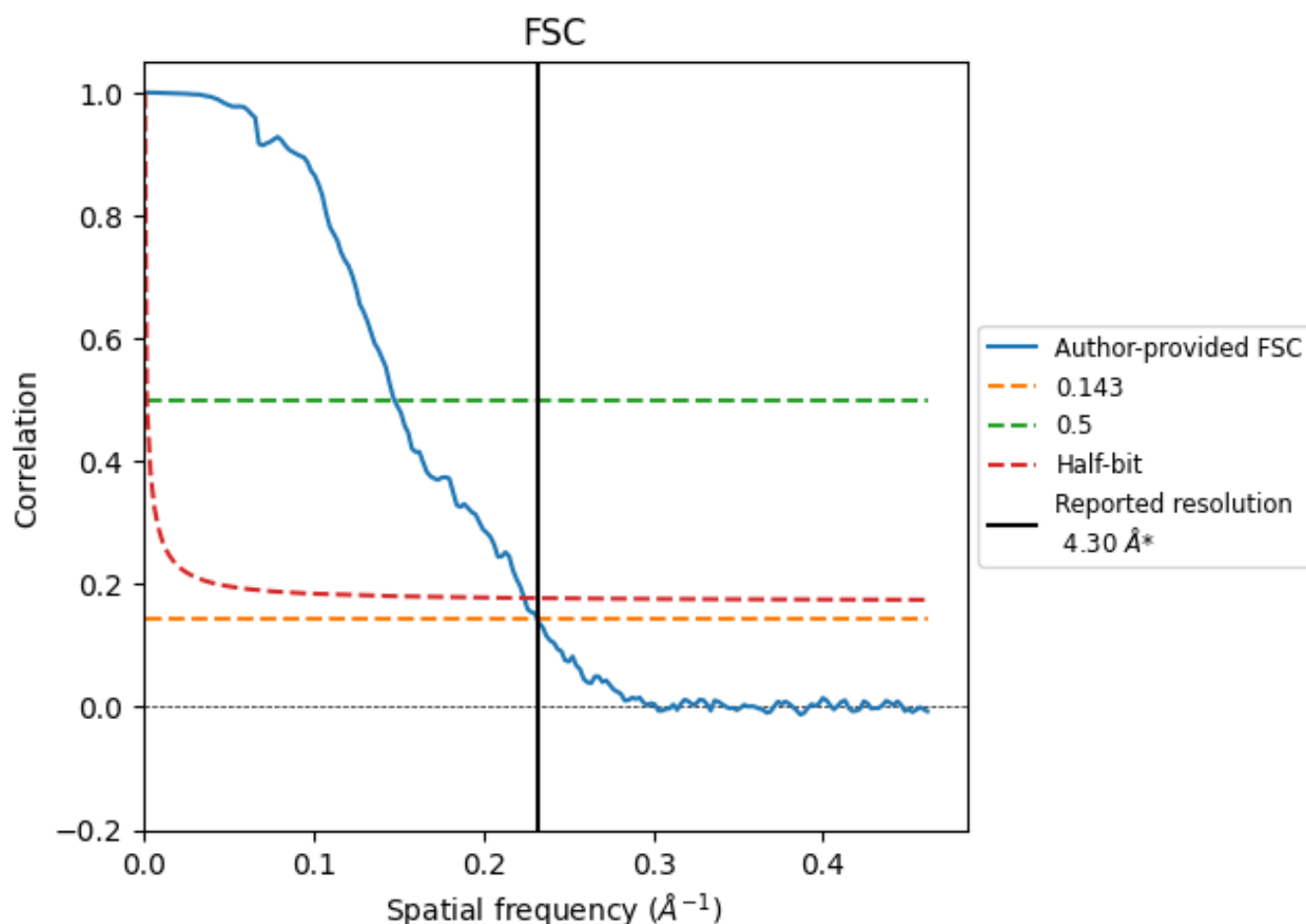


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

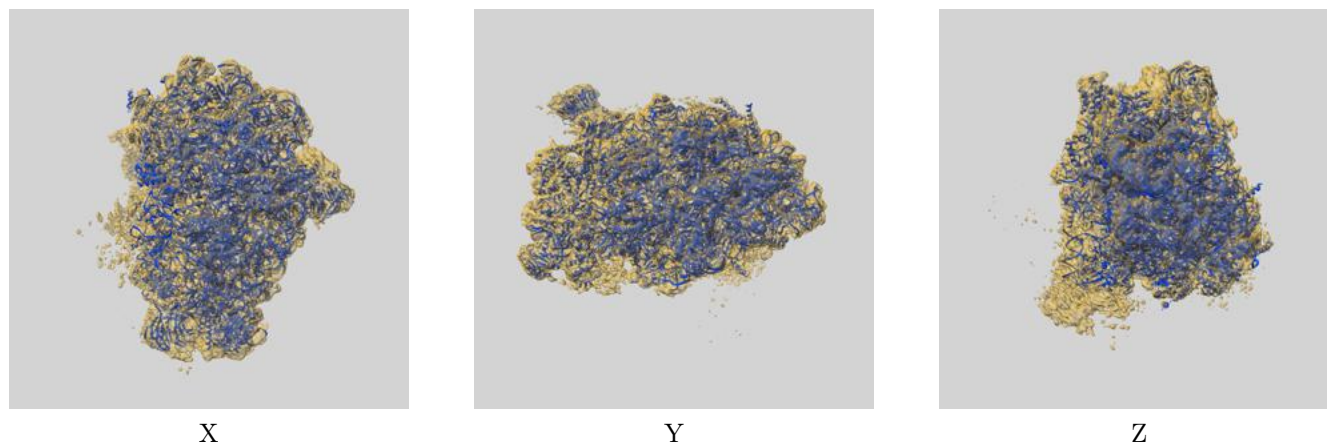
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.31	6.77	4.46
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

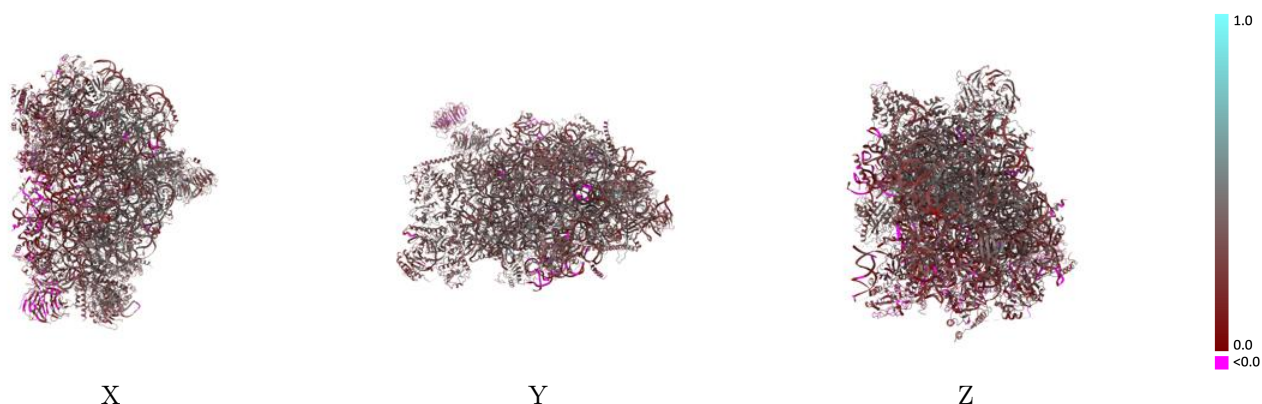
This section contains information regarding the fit between EMDB map EMD-3890 and PDB model 6EM5. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



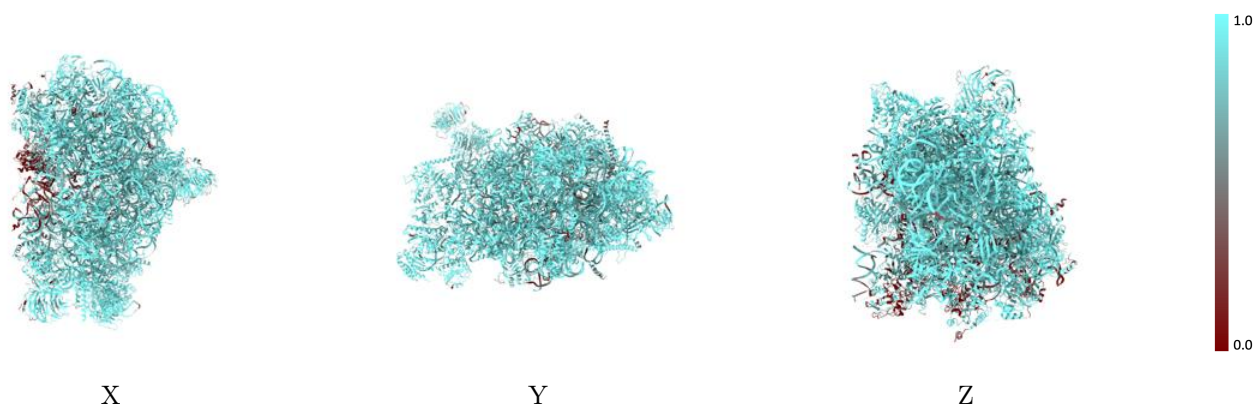
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



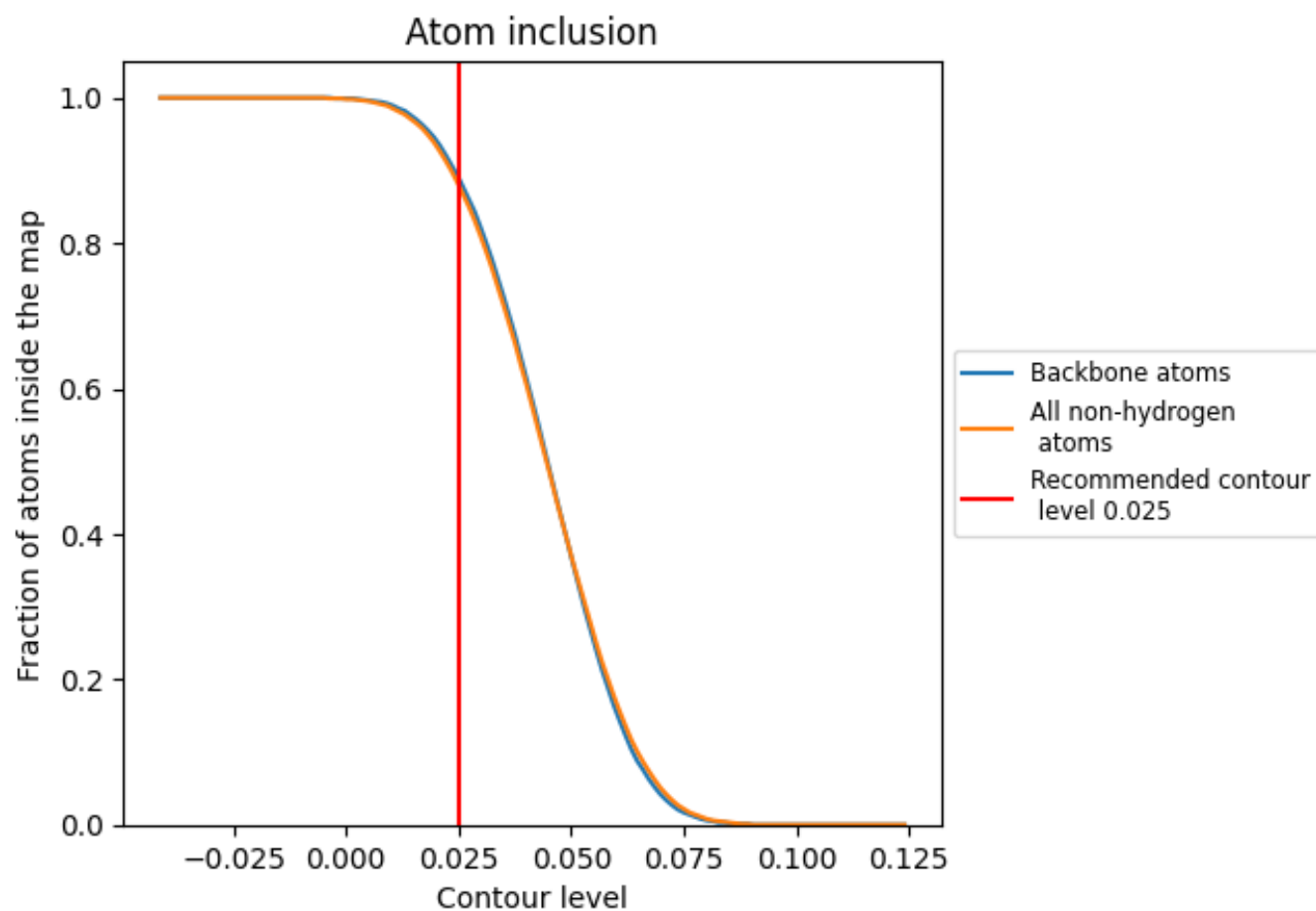
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8800	 0.3050
1	 0.8650	 0.2710
2	 0.9710	 0.3480
3	 0.9670	 0.4000
4	 0.9640	 0.3490
5	 0.8900	 0.3590
6	 0.9510	 0.2910
A	 0.9700	 0.3530
B	 0.9710	 0.3790
C	 0.9560	 0.4000
D	 0.9560	 0.3220
E	 0.9520	 0.3460
F	 0.9930	 0.3810
G	 0.9770	 0.3820
H	 0.9790	 0.3770
I	 0.6240	 0.2580
J	 0.7500	 0.2780
K	 0.9670	 0.3120
L	 0.9530	 0.3870
M	 0.9870	 0.3800
N	 0.9440	 0.3970
O	 0.9820	 0.4130
P	 0.9710	 0.4030
Q	 0.9680	 0.3850
R	 0.8850	 0.2870
S	 0.9810	 0.3820
T	 0.6930	 0.1620
U	 0.8800	 0.2410
V	 0.8790	 0.3330
W	 0.9290	 0.2700
X	 0.9660	 0.3760
Y	 0.9860	 0.4140
Z	 0.9740	 0.3100
b	 0.7950	 0.2730
c	 0.8690	 0.1730



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Chain	Atom inclusion	Q-score
d	 0.9210	 0.3090
e	 0.9500	 0.4180
f	 0.9810	 0.4380
g	 0.8820	 0.3330
h	 0.9790	 0.3760
i	 0.9760	 0.3120
j	 0.9900	 0.4050
k	 0.9680	 0.3380
l	 0.6490	 0.2710
m	 0.9280	 0.3140
n	 0.9790	 0.3400
o	 0.9720	 0.3460
p	 0.8580	 0.1620
q	 0.5580	 0.2020
r	 0.8170	 0.3080
s	 0.8610	 0.3110
t	 0.9850	 0.3440
u	 0.9660	 0.3250
v	 0.9770	 0.3700
w	 0.4550	 0.2510
x	 0.9530	 0.3680
y	 0.9400	 0.2740
z	 0.5270	 0.2410