Full wwPDB EM Validation Report (i)

Jul 3, 2024 – 06:18 am BST

PDB ID	:	6S0K
EMDB ID	:	EMD-10073
Title	:	Ribosome nascent chain in complex with SecA
Authors	:	Jomaa, A.; Wang, S.; Shan, S.; Ban, N.
Deposited on	:	2019-06-17
Resolution	:	3.10 Å(reported)
Based on initial model	:	5GAG

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 (i) 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 (i)) were used in the production of this report:

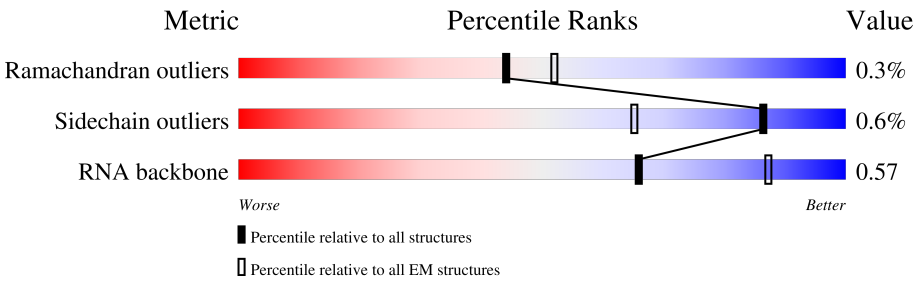
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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% 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	3	67% 33%
2	A	2883	83% 17%
3	B	120	84% 16%
4	C	273	99%
5	D	209	100%
6	E	201	100%
7	F	179	98%
8	G	177	99%

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Mol	Chain	Length	Quality of chain
9	H	149	25% 99%
10	I	165	65% 72% 24%
11	J	142	77% 94% 6%
12	K	142	100%
13	L	123	100%
14	M	144	100%
15	N	136	100%
16	O	127	98%
17	P	117	100%
18	Q	115	99%
19	R	118	99%
20	S	103	99%
21	T	110	100%
22	U	100	92% 8%
23	V	104	99%
24	W	94	100%
25	X	85	89% 11%
26	Y	78	99%
27	Z	63	98%
28	a	59	97%
29	b	57	98%
30	c	55	75% 91% 7%
31	d	46	100%
32	e	65	94% 5%
33	f	38	100%

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Mol	Chain	Length	Quality of chain
34	h	838	61% 97%
35	k	57	53% 100%

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 98708 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 tRNA-CCA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	3	62	28	11	20	3	0	0

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	A	2883	61902	27613	11397	20009	2883	0	0

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	B	120	2569	1144	468	837	120	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	272	2083	1288	424	364	7	0	1

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	209	1565	979	288	294	4	0	0

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	201	1552	974	283	290	5	0	0

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	F	178	1411	899	250	256	6	0	1

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	G	176	1323	832	243	246	2	0	0

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	H	149	1110	699	197	213	1	0	0

- Molecule 10 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	I	125	946	598	169	175	4	0	0

- Molecule 11 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	J	134	979	619	169	185	6	0	0

- Molecule 12 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	K	142	1129	714	212	199	4	0	0

- Molecule 13 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	L	123	946	593	181	166	6	0	0

- Molecule 14 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	M	144	1053	654	207	190	2	0	0

- Molecule 15 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	N	136	1074	686	205	177	6	0	0

- Molecule 16 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	O	125	993	613	202	173	5	0	0

- Molecule 17 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	P	117	900	557	179	163	1	0	0

- Molecule 18 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Q	114	917	574	179	163	1	0	0

- Molecule 19 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	R	117	947	604	192	151	0	0

- Molecule 20 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	S	103	816	516	153	145	2	0	0

- Molecule 21 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	T	110	857	532	166	156	3	0	0

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	U	92	730	461	138	130	1	0	0

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	V	103	780	492	147	141	0	1

- Molecule 24 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	W	94	753	479	137	134	3	0	0

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	X	76	580	359	117	103	1	0	0

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Y	77	625	388	129	106	2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Z	62	501	308	98	94	1	0	0

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	a	58	449	281	87	79	2	0	0

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	b	56	444	269	94	80	1	0	0

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	c	51	414	266	76	72	0	0

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	d	46	377	228	90	57	2	0	0

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	e	64	504	323	105	74	2	0	0

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	f	38	302	185	65	48	4	0	0

- Molecule 34 is a protein called Protein translocase subunit SecA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	h	838	6672	4181	1181	1276	34	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	-3	GLN	-	expression tag	UNP A0A037YQ84
h	-2	GLY	-	expression tag	UNP A0A037YQ84
h	-1	HIS	-	expression tag	UNP A0A037YQ84
h	0	MET	-	expression tag	UNP A0A037YQ84
h	12	CYS	SER	conflict	UNP A0A037YQ84

- Molecule 35 is a protein called Cytoskeleton protein RodZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	k	57	374	247	63	63	1	0	0

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
36	A	65	65	65	0
36	B	2	2	2	0
36	b	1	1	1	0

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
37	f	1	1	1	0

3 Residue-property plots (i)

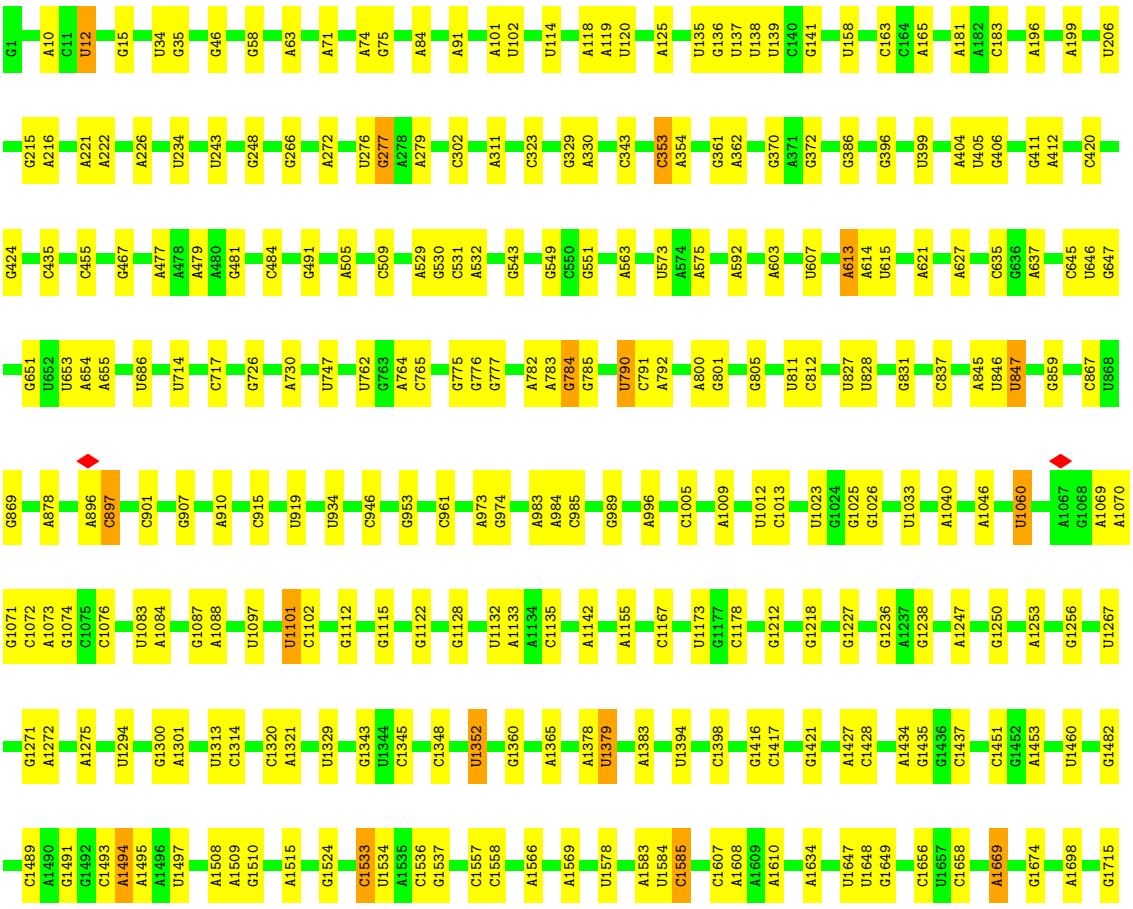
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

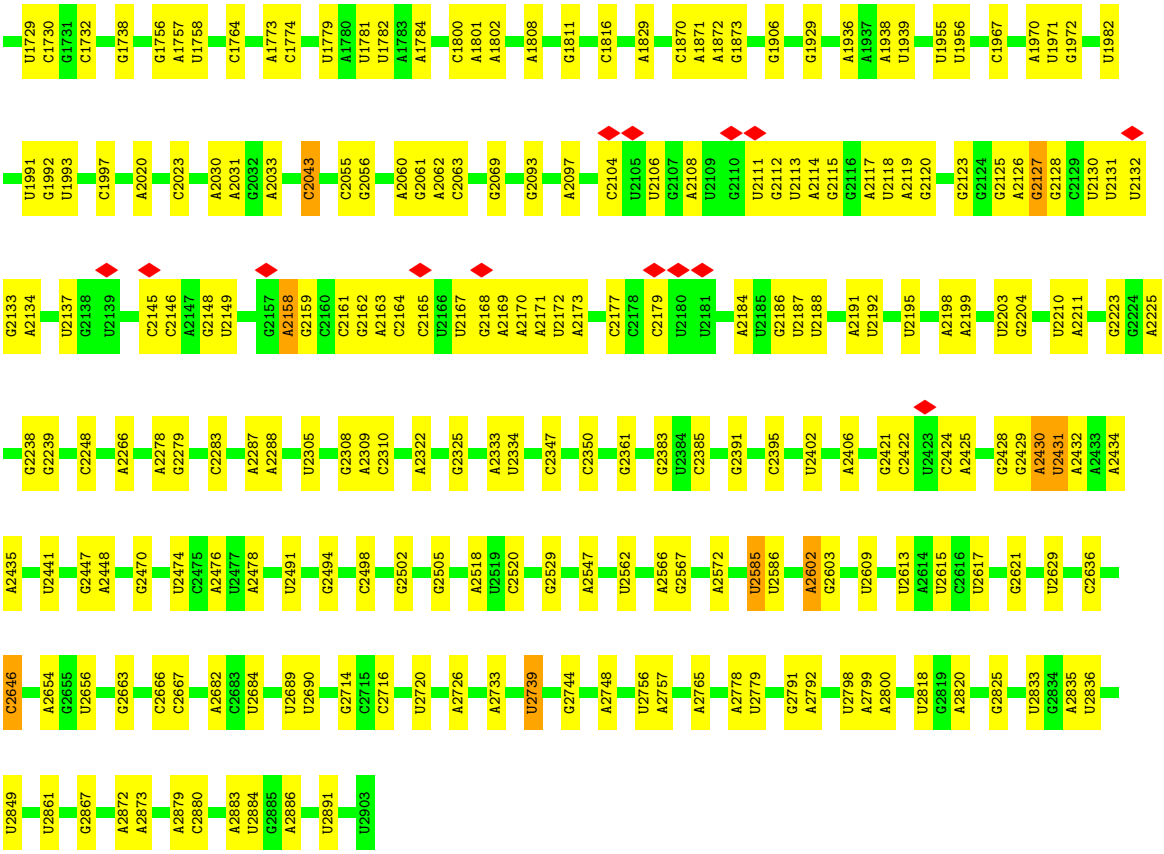
- Molecule 1: tRNA-CCA

Chain 2: 67% 33%

- Molecule 2: 23S ribosomal RNA

Chain A: 83% 17%



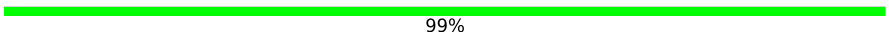


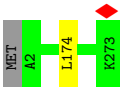
- Molecule 3: 5S ribosomal RNA

Chain B:

- Molecule 4: 50S ribosomal protein L2

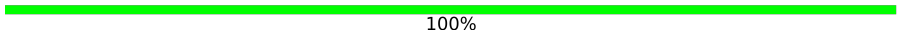
Chain C:





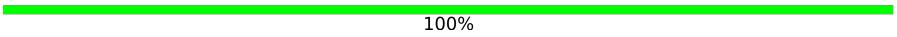
- Molecule 5: 50S ribosomal protein L3

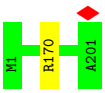
Chain D:



- Molecule 6: 50S ribosomal protein L4

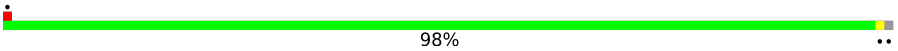
Chain E:

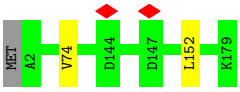




• Molecule 7: 50S ribosomal protein L5

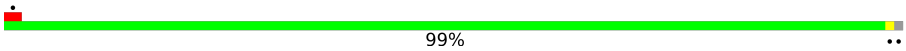
Chain F:

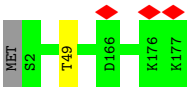




• Molecule 8: 50S ribosomal protein L6

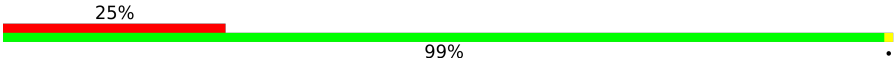
Chain G:

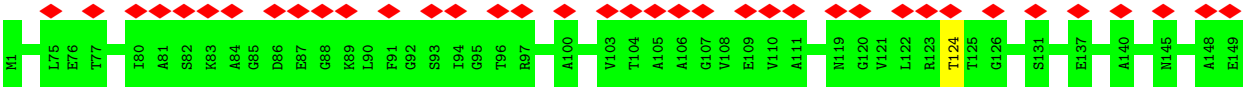




• Molecule 9: 50S ribosomal protein L9

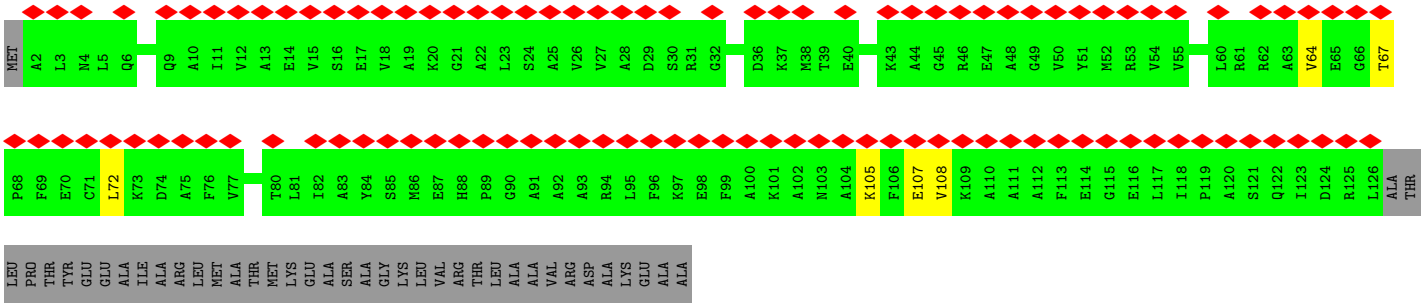
Chain H:





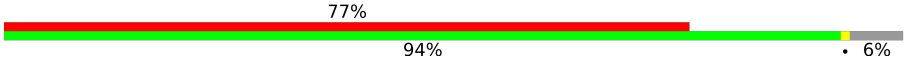
• Molecule 10: 50S ribosomal protein L10

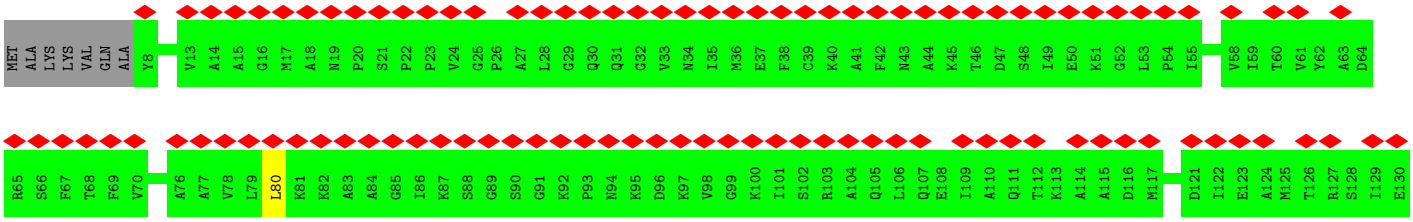
Chain I:

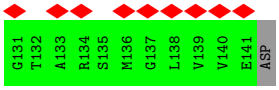


• Molecule 11: 50S ribosomal protein L11

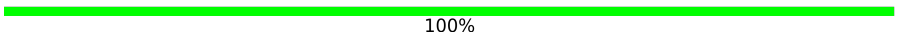
Chain J:







• Molecule 12: 50S ribosomal protein L13

Chain K: 

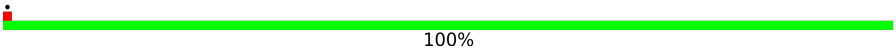
There are no outlier residues recorded for this chain.

• Molecule 13: 50S ribosomal protein L14

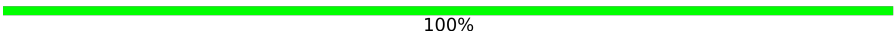
Chain L:

There are no outlier residues recorded for this chain.

• Molecule 14: 50S ribosomal protein L15

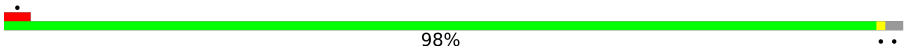
Chain M: 

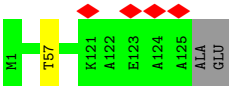
• Molecule 15: 50S ribosomal protein L16

Chain N: 

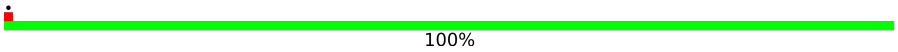
There are no outlier residues recorded for this chain.

• Molecule 16: 50S ribosomal protein L17

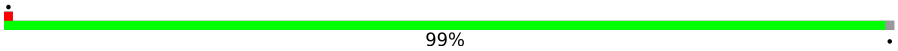
Chain O: 

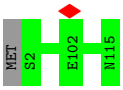


• Molecule 17: 50S ribosomal protein L18

Chain P: 

• Molecule 18: 50S ribosomal protein L19

Chain Q: 



• Molecule 19: 50S ribosomal protein L20

Chain R: 99%

• Molecule 20: 50S ribosomal protein L21

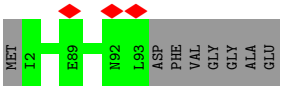
Chain S: 99%

• Molecule 21: 50S ribosomal protein L22

Chain T: 100%

• Molecule 22: 50S ribosomal protein L23

Chain U: 92% 8%



• Molecule 23: 50S ribosomal protein L24

Chain V: 99%

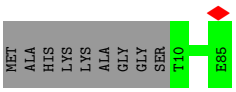
• Molecule 24: 50S ribosomal protein L25

Chain W: 100%

There are no outlier residues recorded for this chain.

• Molecule 25: 50S ribosomal protein L27

Chain X: 89% 11%

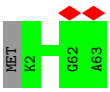


• Molecule 26: 50S ribosomal protein L28

Chain Y: 99%

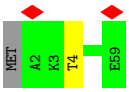
• Molecule 27: 50S ribosomal protein L29

Chain Z: 98%



• Molecule 28: 50S ribosomal protein L30

Chain a: 97%

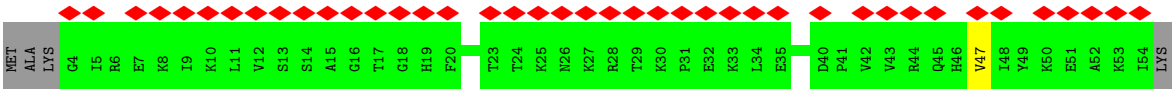


• Molecule 29: 50S ribosomal protein L32

Chain b: 98%

• Molecule 30: 50S ribosomal protein L33

Chain c: 75% 91% 7%

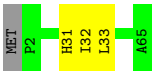


• Molecule 31: 50S ribosomal protein L34

Chain d: 100%

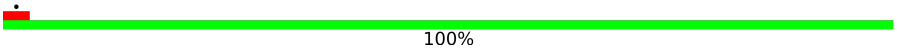
• Molecule 32: 50S ribosomal protein L35

Chain e: 94% 5%



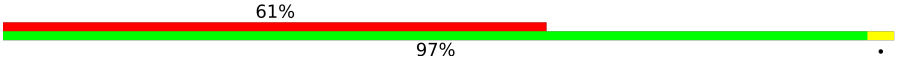
• Molecule 33: 50S ribosomal protein L36

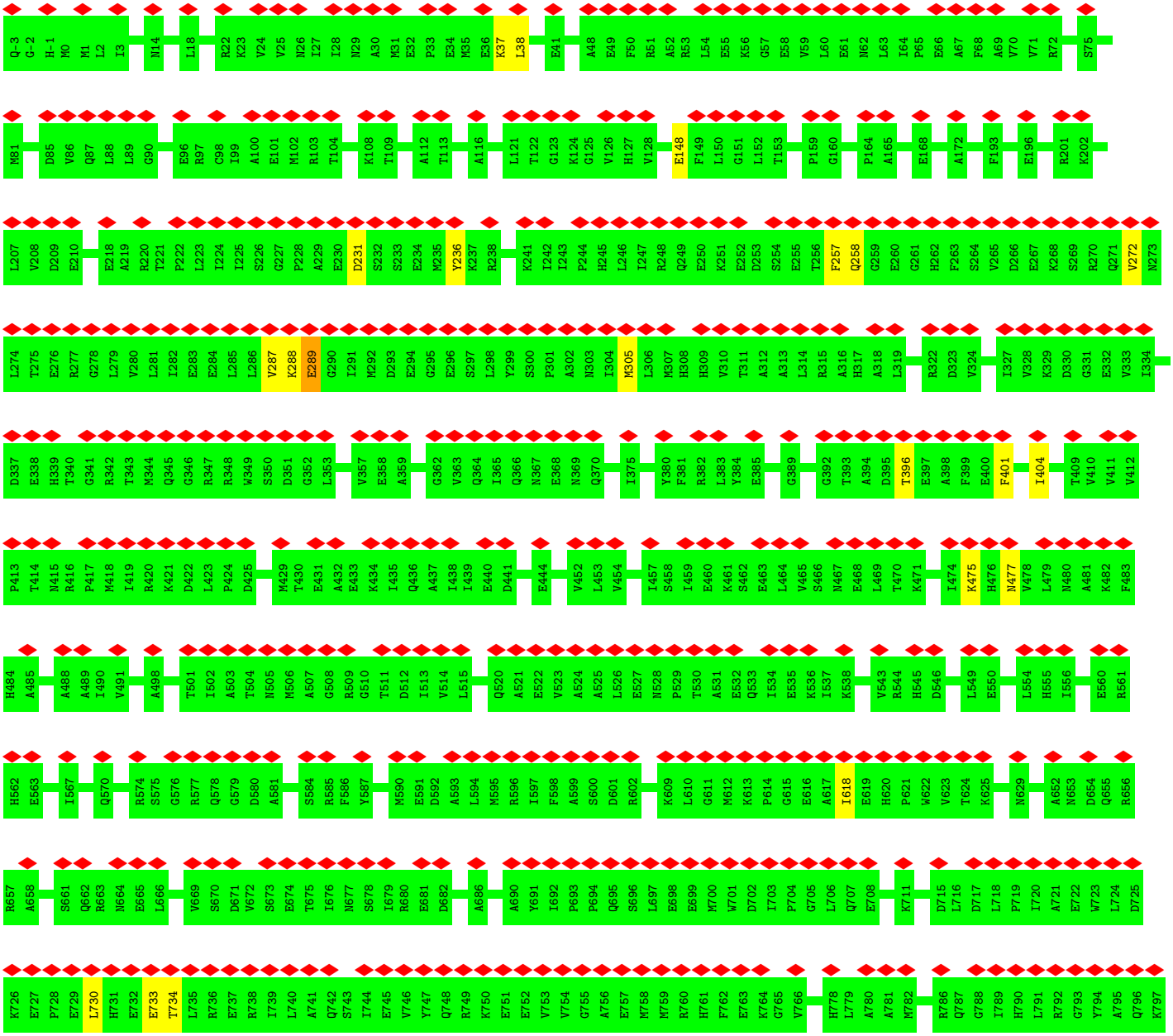
Chain f:

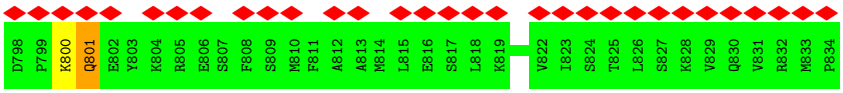


• Molecule 34: Protein translocase subunit SecA

Chain h:

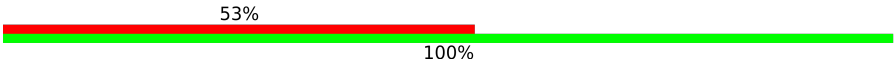


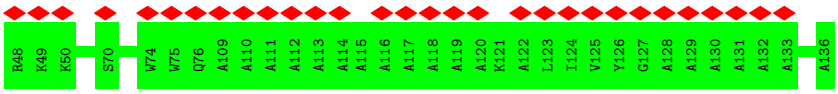




• Molecule 35: Cytoskeleton protein RodZ

Chain k:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37334	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	6.126	Depositor
Minimum map value	-2.568	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.411	Depositor
Recommended contour level	0.82	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	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, MG

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	0.42	0/68	1.13	0/103
2	A	0.57	0/69329	1.00	144/108152 (0.1%)
3	B	0.49	0/2872	1.02	8/4478 (0.2%)
4	C	0.35	0/2122	0.53	0/2854
5	D	0.35	0/1586	0.51	0/2134
6	E	0.33	0/1571	0.47	0/2113
7	F	0.29	0/1435	0.50	1/1928 (0.1%)
8	G	0.30	0/1343	0.49	0/1816
9	H	0.30	0/1121	0.53	0/1515
10	I	0.32	0/958	0.65	0/1290
11	J	0.31	0/993	0.60	0/1341
12	K	0.35	0/1152	0.47	0/1551
13	L	0.34	0/955	0.54	0/1279
14	M	0.32	0/1062	0.52	0/1413
15	N	0.34	0/1093	0.51	0/1460
16	O	0.33	0/1006	0.51	0/1345
17	P	0.31	0/910	0.48	0/1219
18	Q	0.34	0/929	0.47	0/1242
19	R	0.34	0/960	0.41	0/1278
20	S	0.35	0/829	0.55	0/1107
21	T	0.32	0/864	0.51	0/1156
22	U	0.34	0/736	0.51	0/984
23	V	0.33	0/788	0.51	0/1053
24	W	0.31	0/766	0.49	0/1025
25	X	0.34	0/587	0.46	0/776
26	Y	0.34	0/635	0.51	0/848
27	Z	0.30	0/502	0.45	0/667
28	a	0.31	0/453	0.45	0/605
29	b	0.32	0/450	0.47	0/599
30	c	0.29	0/421	0.51	0/561
31	d	0.32	0/380	0.51	0/498
32	e	0.33	0/513	0.62	0/676

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	f	0.33	0/303	0.47	0/397
34	h	0.31	0/6782	0.60	3/9146 (0.0%)
35	k	0.27	0/384	0.58	0/531
All	All	0.50	0/106858	0.89	156/159140 (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
10	I	0	2
32	e	0	1
34	h	0	3
All	All	0	6

There are no bond length outliers.

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1313	U	C2-N1-C1'	10.24	129.99	117.70
2	A	1313	U	N1-C2-O2	9.89	129.72	122.80
2	A	1533	C	C2-N1-C1'	9.56	129.32	118.80
2	A	1313	U	N3-C2-O2	-9.54	115.52	122.20
2	A	1314	C	C2-N1-C1'	8.66	128.33	118.80
2	A	1348	C	N1-C2-O2	8.54	124.03	118.90
2	A	837	C	N3-C2-O2	-7.70	116.51	121.90
2	A	1956	U	N1-C2-O2	7.67	128.17	122.80
2	A	837	C	N1-C2-O2	7.66	123.50	118.90
2	A	1774	C	N3-C2-O2	-7.66	116.54	121.90
2	A	1314	C	C6-N1-C2	-7.61	117.25	120.30
2	A	1956	U	N3-C2-O2	-7.54	116.92	122.20
2	A	897	C	N1-C2-O2	7.49	123.39	118.90
2	A	234	U	N3-C2-O2	-7.12	117.22	122.20
3	B	31	C	C2-N1-C1'	7.11	126.62	118.80
2	A	1348	C	N3-C2-O2	-7.09	116.93	121.90
2	A	2666	C	N1-C2-O2	7.09	123.16	118.90
2	A	2430	A	C2-N3-C4	6.98	114.09	110.60
2	A	1314	C	C5-C6-N1	6.89	124.44	121.00
2	A	1313	U	C6-N1-C1'	-6.86	111.59	121.20
2	A	1774	C	N1-C2-O2	6.86	123.01	118.90
2	A	2617	U	N3-C2-O2	-6.86	117.40	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	31	C	C6-N1-C2	-6.85	117.56	120.30
2	A	607	U	N3-C2-O2	-6.71	117.50	122.20
2	A	2063	C	C6-N1-C2	-6.67	117.63	120.30
2	A	2063	C	C2-N1-C1'	6.64	126.10	118.80
2	A	1533	C	C6-N1-C2	-6.61	117.66	120.30
2	A	1060	U	N3-C4-O4	6.57	124.00	119.40
2	A	1533	C	C6-N1-C1'	-6.54	112.95	120.80
2	A	1101	U	N1-C2-O2	6.54	127.38	122.80
2	A	1533	C	N1-C2-O2	6.53	122.82	118.90
2	A	2063	C	N1-C2-O2	6.50	122.80	118.90
2	A	353	C	N1-C2-O2	6.50	122.80	118.90
2	A	613	A	P-O3'-C3'	6.48	127.48	119.70
2	A	897	C	C6-N1-C2	-6.48	117.71	120.30
2	A	1060	U	C5-C4-O4	-6.46	122.02	125.90
2	A	901	C	N1-C2-O2	6.42	122.75	118.90
2	A	1072	C	C6-N1-C2	-6.34	117.76	120.30
2	A	897	C	C2-N1-C1'	6.31	125.74	118.80
2	A	1294	U	N3-C2-O2	-6.27	117.81	122.20
2	A	1101	U	N3-C2-O2	-6.27	117.81	122.20
2	A	2395	C	C5-C6-N1	6.24	124.12	121.00
3	B	30	C	C6-N1-C2	-6.21	117.81	120.30
2	A	1489	C	N3-C2-O2	-6.20	117.56	121.90
2	A	1533	C	C5-C6-N1	6.17	124.08	121.00
2	A	2474	U	N1-C2-O2	6.14	127.09	122.80
2	A	985	C	C2-N1-C1'	6.13	125.54	118.80
2	A	114	U	C2-N1-C1'	6.12	125.04	117.70
2	A	2063	C	N3-C2-O2	-6.07	117.65	121.90
34	h	288	LYS	C-N-CA	6.06	136.85	121.70
2	A	2617	U	N1-C2-O2	6.06	127.04	122.80
2	A	867	C	N1-C2-O2	6.02	122.51	118.90
2	A	897	C	N3-C2-O2	-5.99	117.71	121.90
2	A	2666	C	N3-C2-O2	-5.98	117.71	121.90
2	A	2195	U	N1-C2-O2	5.98	126.98	122.80
2	A	2149	U	N1-C2-O2	5.97	126.98	122.80
2	A	1489	C	N1-C2-O2	5.97	122.48	118.90
2	A	1320	C	N3-C2-O2	-5.93	117.75	121.90
2	A	1348	C	C2-N1-C1'	5.92	125.32	118.80
2	A	1343	G	C4-N9-C1'	5.88	134.15	126.50
2	A	2158	A	P-O3'-C3'	5.84	126.71	119.70
2	A	370	G	O4'-C1'-N9	-5.80	103.56	108.20
2	A	919	U	N1-C2-O2	5.78	126.84	122.80
2	A	2474	U	N3-C2-O2	-5.78	118.16	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	837	C	C6-N1-C2	-5.77	117.99	120.30
2	A	790	U	C2-N1-C1'	5.76	124.61	117.70
2	A	12	U	N3-C2-O2	-5.76	118.17	122.20
2	A	2149	U	C2-N1-C1'	5.75	124.60	117.70
2	A	2667	C	C6-N1-C2	-5.74	118.00	120.30
2	A	1267	U	N1-C2-O2	5.70	126.79	122.80
2	A	1294	U	N1-C2-O2	5.68	126.77	122.80
2	A	2602	A	P-O3'-C3'	5.67	126.51	119.70
3	B	26	C	N1-C2-O2	5.67	122.30	118.90
2	A	2656	U	N1-C2-O2	5.66	126.76	122.80
7	F	152	LEU	CA-CB-CG	5.66	128.31	115.30
2	A	2149	U	N3-C2-O2	-5.65	118.24	122.20
2	A	607	U	N1-C2-O2	5.64	126.75	122.80
2	A	2474	U	C2-N1-C1'	5.64	124.47	117.70
3	B	31	C	N3-C2-O2	-5.64	117.95	121.90
2	A	135	U	N1-C2-O2	5.63	126.74	122.80
2	A	234	U	N1-C2-O2	5.62	126.74	122.80
2	A	2248	C	C2-N1-C1'	5.62	124.98	118.80
2	A	1398	C	C2-N1-C1'	5.60	124.96	118.80
2	A	353	C	N3-C2-O2	-5.60	117.98	121.90
2	A	2195	U	N3-C2-O2	-5.59	118.28	122.20
3	B	25	U	N1-C2-O2	5.59	126.72	122.80
2	A	135	U	C2-N1-C1'	5.59	124.41	117.70
2	A	784	G	P-O3'-C3'	5.59	126.41	119.70
2	A	897	C	C5-C6-N1	5.59	123.79	121.00
3	B	31	C	N1-C2-O2	5.58	122.25	118.90
2	A	783	A	C2-N3-C4	5.57	113.39	110.60
34	h	733	GLU	C-N-CA	5.56	135.60	121.70
2	A	1494	A	P-O3'-C3'	5.55	126.36	119.70
2	A	2127	G	P-O3'-C3'	5.53	126.33	119.70
2	A	1352	U	N3-C2-O2	-5.51	118.34	122.20
2	A	1267	U	C2-N1-C1'	5.50	124.30	117.70
2	A	243	U	N1-C2-O2	5.49	126.65	122.80
2	A	343	C	C6-N1-C2	-5.49	118.10	120.30
2	A	1314	C	C6-N1-C1'	-5.48	114.22	120.80
2	A	1314	C	N1-C2-O2	5.47	122.18	118.90
2	A	2431	U	N3-C2-O2	-5.47	118.37	122.20
2	A	1102	C	N1-C2-O2	5.46	122.18	118.90
2	A	1115	G	O4'-C1'-N9	5.46	112.57	108.20
2	A	1343	G	C8-N9-C1'	-5.44	119.93	127.00
2	A	2395	C	C6-N1-C2	-5.44	118.13	120.30
2	A	323	C	N1-C2-O2	5.42	122.15	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	635	C	C6-N1-C2	-5.42	118.13	120.30
2	A	1585	C	N1-C2-O2	5.39	122.13	118.90
2	A	323	C	C2-N1-C1'	5.38	124.72	118.80
2	A	1267	U	N3-C2-O2	-5.38	118.43	122.20
2	A	984	A	C2-N3-C4	5.37	113.28	110.60
2	A	847	U	N3-C2-O2	-5.36	118.45	122.20
2	A	2195	U	C2-N1-C1'	5.33	124.10	117.70
2	A	183	C	N1-C2-O2	5.31	122.08	118.90
2	A	1956	U	C2-N1-C1'	5.31	124.07	117.70
2	A	1320	C	C6-N1-C2	-5.30	118.18	120.30
2	A	1509	A	O4'-C1'-N9	5.29	112.43	108.20
2	A	2720	U	N3-C2-O2	-5.29	118.50	122.20
34	h	800	LYS	C-N-CA	5.29	134.93	121.70
2	A	2421	G	N3-C4-N9	5.27	129.16	126.00
2	A	901	C	N3-C2-O2	-5.27	118.21	121.90
2	A	2656	U	C2-N1-C1'	5.26	124.02	117.70
2	A	919	U	N3-C2-O2	-5.26	118.52	122.20
2	A	1167	C	C2-N1-C1'	5.25	124.58	118.80
2	A	1379	U	N3-C2-O2	-5.25	118.53	122.20
2	A	1669	A	C4-N9-C1'	5.25	135.75	126.30
2	A	867	C	N3-C2-O2	-5.20	118.26	121.90
2	A	135	U	N3-C2-O2	-5.19	118.57	122.20
2	A	2656	U	N3-C2-O2	-5.19	118.57	122.20
2	A	1779	U	C2-N1-C1'	5.18	123.92	117.70
2	A	1313	U	C5-C6-N1	5.18	125.29	122.70
2	A	2739	U	N3-C2-O2	-5.17	118.58	122.20
2	A	2430	A	N3-C4-N9	5.17	131.54	127.40
2	A	353	C	C2-N1-C1'	5.15	124.46	118.80
2	A	2043	C	C6-N1-C2	-5.14	118.25	120.30
2	A	985	C	N1-C2-O2	5.13	121.98	118.90
2	A	2585	U	N3-C2-O2	-5.13	118.61	122.20
2	A	243	U	N3-C2-O2	-5.12	118.61	122.20
2	A	2636	C	C2-N1-C1'	5.10	124.41	118.80
2	A	1076	C	C6-N1-C2	-5.09	118.26	120.30
2	A	1394	U	C6-N1-C1'	5.09	128.33	121.20
2	A	915	C	C2-N1-C1'	5.08	124.39	118.80
3	B	70	C	C6-N1-C2	-5.08	118.27	120.30
2	A	1352	U	N1-C2-O2	5.08	126.36	122.80
2	A	484	C	C5-C6-N1	5.07	123.54	121.00
2	A	1658	C	C6-N1-C2	-5.05	118.28	120.30
2	A	2430	A	N3-C4-C5	-5.05	123.27	126.80
2	A	783	A	C4-N9-C1'	5.05	135.38	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	206	U	N1-C2-O2	5.04	126.33	122.80
2	A	1656	C	C5-C6-N1	5.04	123.52	121.00
2	A	343	C	C2-N1-C1'	5.03	124.33	118.80
2	A	985	C	C6-N1-C2	-5.03	118.29	120.30
2	A	277	G	N3-C4-C5	-5.02	126.09	128.60
2	A	2667	C	N1-C2-O2	5.02	121.91	118.90
2	A	158	U	C2-N1-C1'	5.02	123.72	117.70
2	A	2646	C	C5-C6-N1	5.01	123.51	121.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	I	105	LYS	Peptide
10	I	107	GLU	Peptide
32	e	31	HIS	Peptide
34	h	289	GLU	Peptide
34	h	618	ILE	Peptide
34	h	801	GLN	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	270/273 (99%)	262 (97%)	8 (3%)	0	100	100
5	D	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
6	E	199/201 (99%)	197 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	F	176/179 (98%)	169 (96%)	7 (4%)	0	100	100
8	G	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
9	H	147/149 (99%)	141 (96%)	6 (4%)	0	100	100
10	I	123/165 (74%)	114 (93%)	7 (6%)	2 (2%)	9	37
11	J	132/142 (93%)	122 (92%)	10 (8%)	0	100	100
12	K	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
13	L	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
14	M	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
15	N	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
16	O	123/127 (97%)	119 (97%)	4 (3%)	0	100	100
17	P	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
18	Q	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
19	R	115/118 (98%)	115 (100%)	0	0	100	100
20	S	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
21	T	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
22	U	90/100 (90%)	86 (96%)	4 (4%)	0	100	100
23	V	101/104 (97%)	94 (93%)	7 (7%)	0	100	100
24	W	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
25	X	74/85 (87%)	70 (95%)	4 (5%)	0	100	100
26	Y	75/78 (96%)	75 (100%)	0	0	100	100
27	Z	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
28	a	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
29	b	54/57 (95%)	54 (100%)	0	0	100	100
30	c	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
31	d	44/46 (96%)	44 (100%)	0	0	100	100
32	e	62/65 (95%)	55 (89%)	5 (8%)	2 (3%)	4	22
33	f	36/38 (95%)	36 (100%)	0	0	100	100
34	h	836/838 (100%)	753 (90%)	75 (9%)	8 (1%)	15	49
35	k	53/57 (93%)	46 (87%)	7 (13%)	0	100	100
All	All	4321/4469 (97%)	4123 (95%)	186 (4%)	12 (0%)	44	73

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	e	32	ILE
34	h	734	THR
32	e	33	LEU
34	h	38	LEU
34	h	258	GLN
34	h	231	ASP
34	h	257	PHE
34	h	801	GLN
34	h	404	ILE
34	h	287	VAL
10	I	108	VAL
10	I	67	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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
4	C	216/218 (99%)	215 (100%)	1 (0%)	88 94
5	D	164/164 (100%)	164 (100%)	0	100 100
6	E	165/165 (100%)	164 (99%)	1 (1%)	86 94
7	F	148/150 (99%)	147 (99%)	1 (1%)	84 93
8	G	137/138 (99%)	136 (99%)	1 (1%)	84 93
9	H	114/114 (100%)	113 (99%)	1 (1%)	78 91
10	I	95/123 (77%)	93 (98%)	2 (2%)	53 79
11	J	104/110 (94%)	103 (99%)	1 (1%)	76 90
12	K	116/116 (100%)	116 (100%)	0	100 100
13	L	104/104 (100%)	104 (100%)	0	100 100
14	M	103/103 (100%)	103 (100%)	0	100 100
15	N	109/109 (100%)	109 (100%)	0	100 100
16	O	102/103 (99%)	101 (99%)	1 (1%)	76 90
17	P	87/87 (100%)	87 (100%)	0	100 100
18	Q	99/100 (99%)	99 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	R	89/90 (99%)	89 (100%)	0	100	100
20	S	84/84 (100%)	83 (99%)	1 (1%)	71	88
21	T	93/93 (100%)	93 (100%)	0	100	100
22	U	79/84 (94%)	79 (100%)	0	100	100
23	V	83/85 (98%)	83 (100%)	0	100	100
24	W	78/78 (100%)	78 (100%)	0	100	100
25	X	57/63 (90%)	57 (100%)	0	100	100
26	Y	67/68 (98%)	67 (100%)	0	100	100
27	Z	54/55 (98%)	54 (100%)	0	100	100
28	a	48/49 (98%)	47 (98%)	1 (2%)	53	79
29	b	47/48 (98%)	47 (100%)	0	100	100
30	c	45/49 (92%)	44 (98%)	1 (2%)	52	78
31	d	38/38 (100%)	38 (100%)	0	100	100
32	e	51/52 (98%)	51 (100%)	0	100	100
33	f	34/34 (100%)	34 (100%)	0	100	100
34	h	714/714 (100%)	703 (98%)	11 (2%)	65	85
35	k	21/30 (70%)	21 (100%)	0	100	100
All	All	3545/3618 (98%)	3522 (99%)	23 (1%)	86	94

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	174	LEU
6	E	170	ARG
7	F	74	VAL
8	G	49	THR
9	H	124	THR
10	I	64	VAL
10	I	72	LEU
11	J	80	LEU
16	O	57	THR
20	S	63	VAL
28	a	4	THR
30	c	47	VAL
34	h	37	LYS
34	h	148	GLU

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Mol	Chain	Res	Type
34	h	236	TYR
34	h	272	VAL
34	h	289	GLU
34	h	305	MET
34	h	396	THR
34	h	401	PHE
34	h	475	LYS
34	h	477	ASN
34	h	730	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	260	ASN
5	D	49	GLN
5	D	173	GLN
6	E	136	GLN
7	F	23	ASN
7	F	63	GLN
8	G	38	ASN
9	H	33	GLN
9	H	135	HIS
10	I	103	ASN
11	J	12	GLN
11	J	30	GLN
14	M	54	GLN
15	N	3	GLN
16	O	18	GLN
16	O	62	ASN
18	Q	41	GLN
18	Q	75	GLN
19	R	44	GLN
19	R	72	ASN
19	R	81	ASN
20	S	82	HIS
22	U	48	GLN
22	U	92	ASN
23	V	74	ASN
26	Y	6	GLN
27	Z	27	ASN
27	Z	39	GLN
34	h	29	ASN

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Mol	Chain	Res	Type
34	h	87	GLN
34	h	354	HIS
34	h	415	ASN
34	h	520	GLN
34	h	533	GLN
34	h	629	ASN
34	h	662	GLN
34	h	731	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	2/3 (66%)	1 (50%)	0
2	A	2878/2883 (99%)	446 (15%)	8 (0%)
3	B	119/120 (99%)	14 (11%)	0
All	All	2999/3006 (99%)	461 (15%)	8 (0%)

All (461) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	76	A
2	A	10	A
2	A	12	U
2	A	15	G
2	A	34	U
2	A	35	G
2	A	46	G
2	A	58	G
2	A	63	A
2	A	71	A
2	A	74	A
2	A	75	G
2	A	84	A
2	A	91	A
2	A	101	A
2	A	102	U
2	A	118	A
2	A	119	A
2	A	120	U
2	A	125	A
2	A	136	G

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Mol	Chain	Res	Type
2	A	137	U
2	A	138	U
2	A	139	U
2	A	141	G
2	A	163	C
2	A	165	A
2	A	181	A
2	A	196	A
2	A	199	A
2	A	215	G
2	A	216	A
2	A	221	A
2	A	222	A
2	A	226	A
2	A	248	G
2	A	266	G
2	A	272	A
2	A	276	U
2	A	277	G
2	A	279	A
2	A	302	C
2	A	311	A
2	A	329	G
2	A	330	A
2	A	353	C
2	A	354	A
2	A	361	G
2	A	362	A
2	A	372	G
2	A	386	G
2	A	396	G
2	A	399	U
2	A	404	A
2	A	405	U
2	A	406	G
2	A	411	G
2	A	412	A
2	A	420	C
2	A	424	G
2	A	435	C
2	A	455	C
2	A	467	G

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Mol	Chain	Res	Type
2	A	477	A
2	A	479	A
2	A	481	G
2	A	491	G
2	A	505	A
2	A	509	C
2	A	529	A
2	A	530	G
2	A	531	C
2	A	532	A
2	A	543	G
2	A	549	G
2	A	551	G
2	A	563	A
2	A	573	U
2	A	575	A
2	A	592	A
2	A	603	A
2	A	613	A
2	A	614	A
2	A	615	U
2	A	621	A
2	A	627	A
2	A	637	A
2	A	645	C
2	A	646	U
2	A	647	G
2	A	651	G
2	A	653	U
2	A	654	A
2	A	655	A
2	A	686	U
2	A	714	U
2	A	717	C
2	A	726	G
2	A	730	A
2	A	747	U
2	A	762	U
2	A	764	A
2	A	765	C
2	A	775	G
2	A	776	G

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Mol	Chain	Res	Type
2	A	777	G
2	A	782	A
2	A	784	G
2	A	785	G
2	A	790	U
2	A	791	C
2	A	792	A
2	A	800	A
2	A	801	G
2	A	805	G
2	A	811	U
2	A	812	C
2	A	827	U
2	A	828	U
2	A	831	G
2	A	845	A
2	A	846	U
2	A	847	U
2	A	859	G
2	A	869	G
2	A	878	A
2	A	896	A
2	A	897	C
2	A	907	G
2	A	910	A
2	A	934	U
2	A	946	C
2	A	953	G
2	A	961	C
2	A	973	A
2	A	974	G
2	A	983	A
2	A	989	G
2	A	996	A
2	A	1005	C
2	A	1009	A
2	A	1012	U
2	A	1013	C
2	A	1023	U
2	A	1025	G
2	A	1026	G
2	A	1033	U

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Mol	Chain	Res	Type
2	A	1040	A
2	A	1046	A
2	A	1060	U
2	A	1069	A
2	A	1070	A
2	A	1071	G
2	A	1073	A
2	A	1074	G
2	A	1083	U
2	A	1084	A
2	A	1087	G
2	A	1088	A
2	A	1097	U
2	A	1101	U
2	A	1112	G
2	A	1122	G
2	A	1128	G
2	A	1132	U
2	A	1133	A
2	A	1135	C
2	A	1142	A
2	A	1155	A
2	A	1173	U
2	A	1178	C
2	A	1212	G
2	A	1218	G
2	A	1227	G
2	A	1236	G
2	A	1238	G
2	A	1247	A
2	A	1250	G
2	A	1253	A
2	A	1256	G
2	A	1271	G
2	A	1272	A
2	A	1275	A
2	A	1300	G
2	A	1301	A
2	A	1321	A
2	A	1329	U
2	A	1345	C
2	A	1352	U

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Mol	Chain	Res	Type
2	A	1360	G
2	A	1365	A
2	A	1378	A
2	A	1379	U
2	A	1383	A
2	A	1416	G
2	A	1417	C
2	A	1421	G
2	A	1427	A
2	A	1428	C
2	A	1434	A
2	A	1435	G
2	A	1437	C
2	A	1451	C
2	A	1453	A
2	A	1460	U
2	A	1482	G
2	A	1491	G
2	A	1493	C
2	A	1494	A
2	A	1495	A
2	A	1497	U
2	A	1508	A
2	A	1510	G
2	A	1515	A
2	A	1524	G
2	A	1533	C
2	A	1534	U
2	A	1536	C
2	A	1537	G
2	A	1557	C
2	A	1558	C
2	A	1566	A
2	A	1569	A
2	A	1578	U
2	A	1583	A
2	A	1584	U
2	A	1585	C
2	A	1607	C
2	A	1608	A
2	A	1610	A
2	A	1634	A

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Mol	Chain	Res	Type
2	A	1647	U
2	A	1648	U
2	A	1649	G
2	A	1669	A
2	A	1674	G
2	A	1698	A
2	A	1715	G
2	A	1729	U
2	A	1730	C
2	A	1732	C
2	A	1738	G
2	A	1756	G
2	A	1757	A
2	A	1758	U
2	A	1764	C
2	A	1773	A
2	A	1781	U
2	A	1782	U
2	A	1784	A
2	A	1800	C
2	A	1801	A
2	A	1802	A
2	A	1808	A
2	A	1811	G
2	A	1816	C
2	A	1829	A
2	A	1870	C
2	A	1871	A
2	A	1872	A
2	A	1873	G
2	A	1906	G
2	A	1929	G
2	A	1936	A
2	A	1938	A
2	A	1939	U
2	A	1955	U
2	A	1967	C
2	A	1970	A
2	A	1971	U
2	A	1972	G
2	A	1982	U
2	A	1991	U

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Mol	Chain	Res	Type
2	A	1992	G
2	A	1993	U
2	A	1997	C
2	A	2020	A
2	A	2023	C
2	A	2030	A
2	A	2031	A
2	A	2033	A
2	A	2043	C
2	A	2055	C
2	A	2056	G
2	A	2060	A
2	A	2061	G
2	A	2062	A
2	A	2069	G
2	A	2093	G
2	A	2097	A
2	A	2104	C
2	A	2106	U
2	A	2108	A
2	A	2111	U
2	A	2112	G
2	A	2113	U
2	A	2114	A
2	A	2115	G
2	A	2117	A
2	A	2118	U
2	A	2119	A
2	A	2120	G
2	A	2123	G
2	A	2125	G
2	A	2126	A
2	A	2128	G
2	A	2130	U
2	A	2131	U
2	A	2132	U
2	A	2133	G
2	A	2134	A
2	A	2137	U
2	A	2145	C
2	A	2146	C
2	A	2148	G

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Mol	Chain	Res	Type
2	A	2158	A
2	A	2159	G
2	A	2161	C
2	A	2162	G
2	A	2163	A
2	A	2164	C
2	A	2165	C
2	A	2167	U
2	A	2168	G
2	A	2169	A
2	A	2170	A
2	A	2171	A
2	A	2172	U
2	A	2173	A
2	A	2177	C
2	A	2179	C
2	A	2184	A
2	A	2186	G
2	A	2187	U
2	A	2188	U
2	A	2191	A
2	A	2192	U
2	A	2198	A
2	A	2199	A
2	A	2203	U
2	A	2204	G
2	A	2210	U
2	A	2211	A
2	A	2223	G
2	A	2225	A
2	A	2238	G
2	A	2239	G
2	A	2266	A
2	A	2278	A
2	A	2279	G
2	A	2283	C
2	A	2287	A
2	A	2288	A
2	A	2305	U
2	A	2308	G
2	A	2309	A
2	A	2310	C

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Mol	Chain	Res	Type
2	A	2322	A
2	A	2325	G
2	A	2333	A
2	A	2334	U
2	A	2347	C
2	A	2350	C
2	A	2361	G
2	A	2383	G
2	A	2385	C
2	A	2391	G
2	A	2402	U
2	A	2406	A
2	A	2422	C
2	A	2424	C
2	A	2425	A
2	A	2428	G
2	A	2429	G
2	A	2430	A
2	A	2431	U
2	A	2432	A
2	A	2434	A
2	A	2435	A
2	A	2441	U
2	A	2447	G
2	A	2448	A
2	A	2470	G
2	A	2476	A
2	A	2478	A
2	A	2491	U
2	A	2494	G
2	A	2498	C
2	A	2502	G
2	A	2505	G
2	A	2518	A
2	A	2520	C
2	A	2529	G
2	A	2547	A
2	A	2562	U
2	A	2566	A
2	A	2567	G
2	A	2572	A
2	A	2585	U

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Mol	Chain	Res	Type
2	A	2586	U
2	A	2602	A
2	A	2603	G
2	A	2609	U
2	A	2613	U
2	A	2615	U
2	A	2621	G
2	A	2629	U
2	A	2646	C
2	A	2654	A
2	A	2663	G
2	A	2682	A
2	A	2684	U
2	A	2689	U
2	A	2690	U
2	A	2714	G
2	A	2716	C
2	A	2726	A
2	A	2733	A
2	A	2739	U
2	A	2744	G
2	A	2748	A
2	A	2757	A
2	A	2765	A
2	A	2778	A
2	A	2779	U
2	A	2791	G
2	A	2792	A
2	A	2798	U
2	A	2799	A
2	A	2800	A
2	A	2818	U
2	A	2820	A
2	A	2825	G
2	A	2833	U
2	A	2835	A
2	A	2836	U
2	A	2849	U
2	A	2861	U
2	A	2867	G
2	A	2872	A
2	A	2873	A

Continued on next page...

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Mol	Chain	Res	Type
2	A	2879	A
2	A	2880	C
2	A	2883	A
2	A	2884	U
2	A	2886	A
2	A	2891	U
3	B	9	G
3	B	13	G
3	B	24	G
3	B	35	C
3	B	41	G
3	B	56	G
3	B	66	A
3	B	67	G
3	B	88	C
3	B	89	U
3	B	90	C
3	B	105	G
3	B	109	A
3	B	120	U

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	613	A
2	A	784	G
2	A	1494	A
2	A	2112	G
2	A	2127	G
2	A	2158	A
2	A	2602	A
2	A	2756	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 69 ligands modelled in this entry, 69 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	A	4
35	k	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	k	76:GLN	C	109:ALA	N	27.78
1	A	882:G	O3'	894:U	P	15.86
1	A	1912:A	O3'	1917:U	P	14.04
1	A	545:U	O3'	548:G	P	13.58
1	A	1173:U	O3'	1177:G	P	13.39

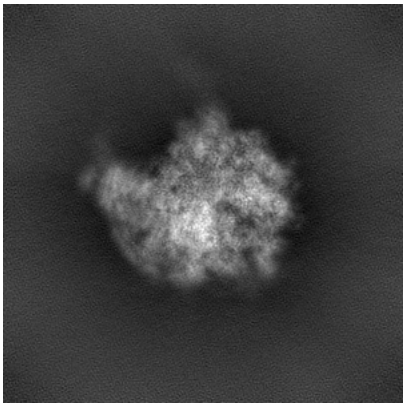
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10073. These allow visual inspection of the internal detail of the map and identification of artifacts.

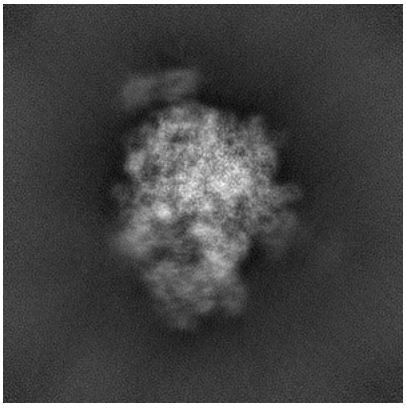
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

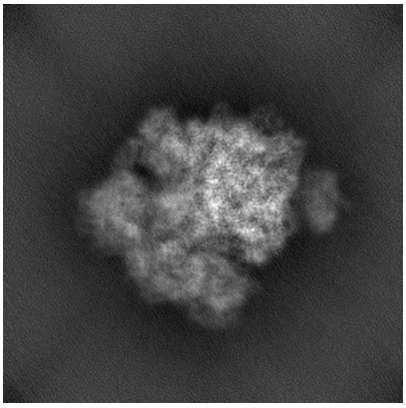
6.1.1 Primary map



X



Y

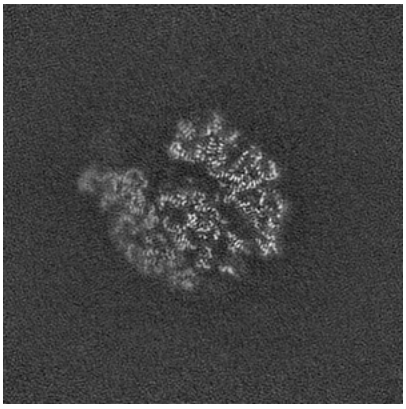


Z

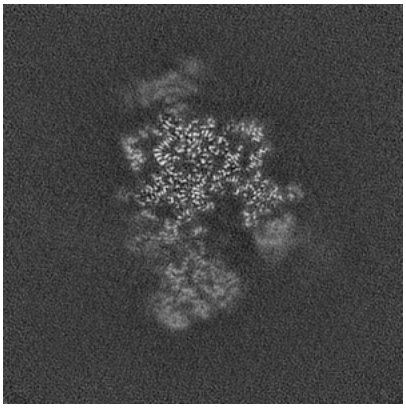
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

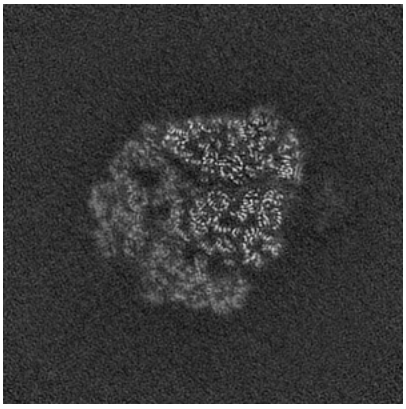
6.2.1 Primary map



X Index: 160



Y Index: 160

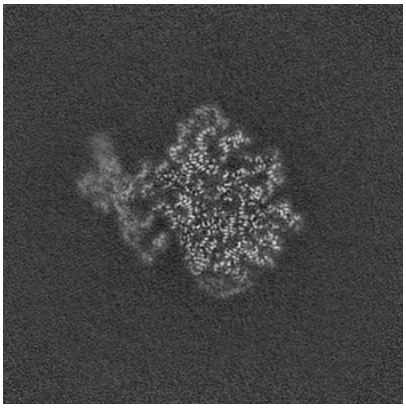


Z Index: 160

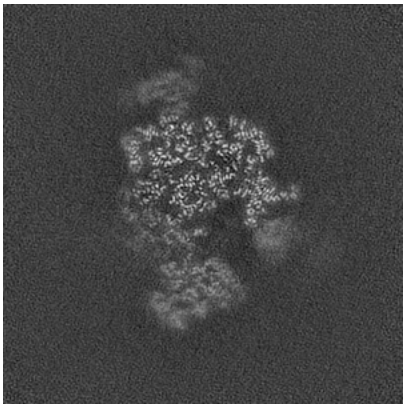
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

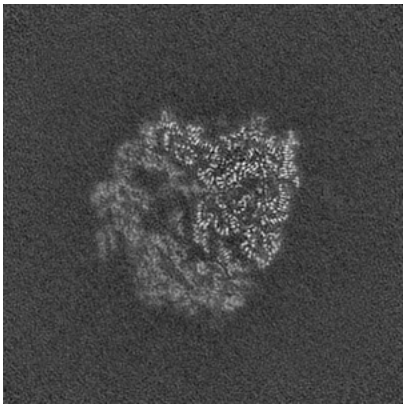
6.3.1 Primary map



X Index: 170



Y Index: 157

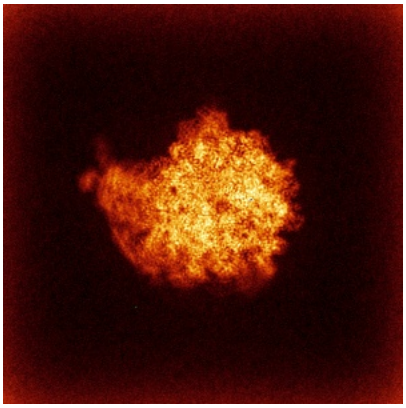


Z Index: 165

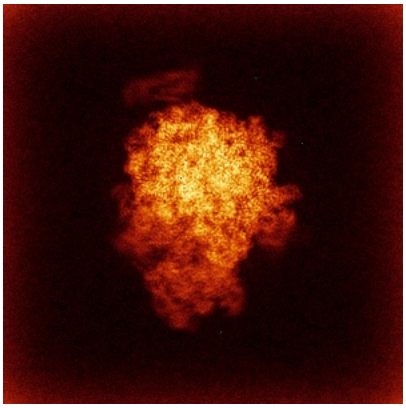
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

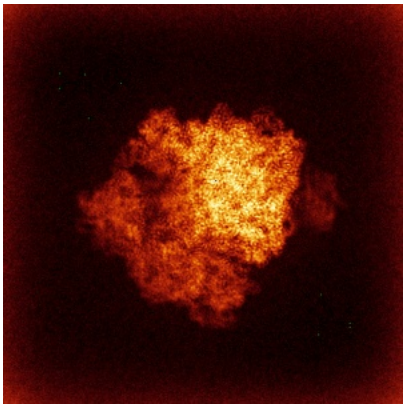
6.4.1 Primary map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.82. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

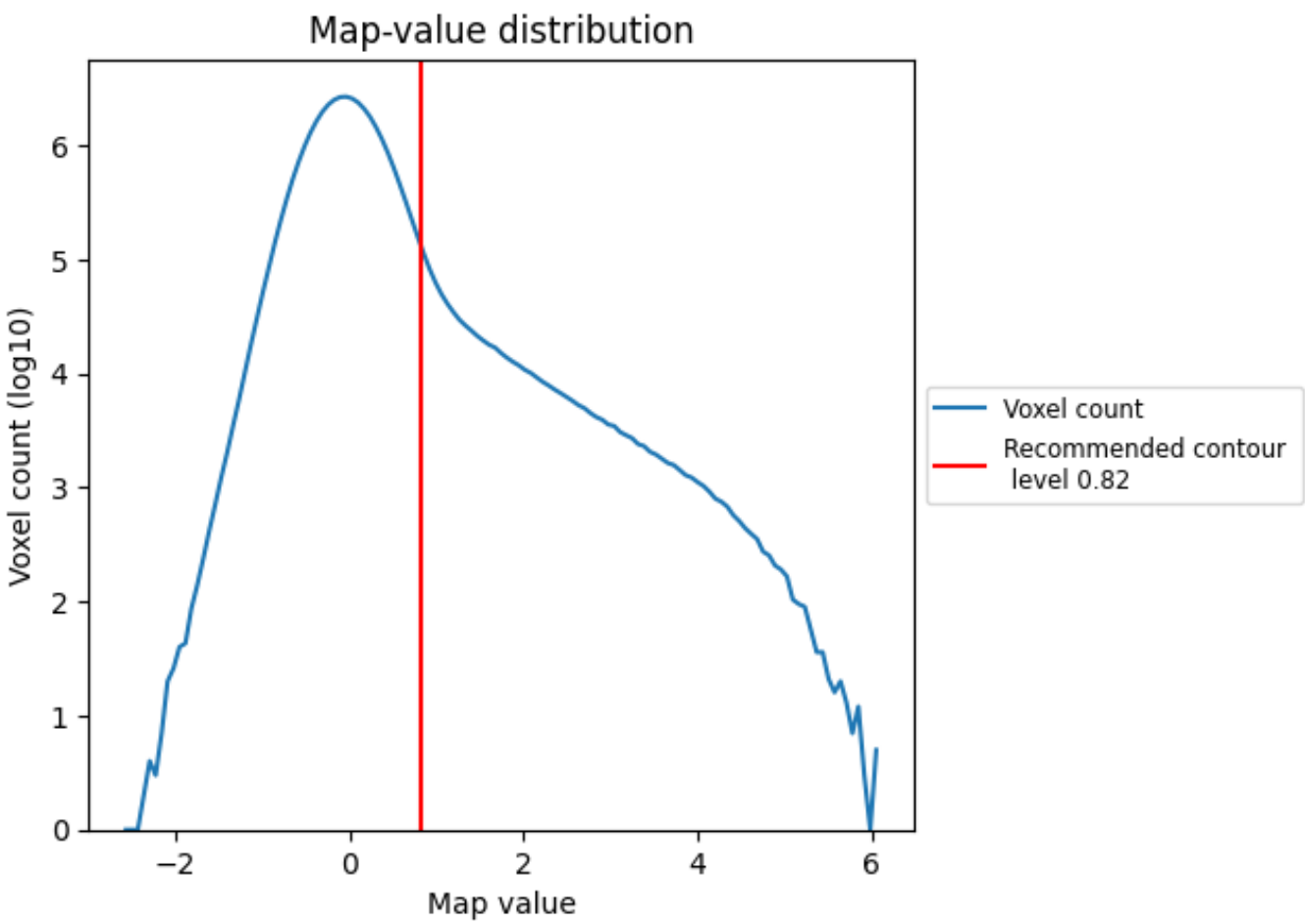
6.6 Mask visualisation (i)

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

7 Map analysis (i)

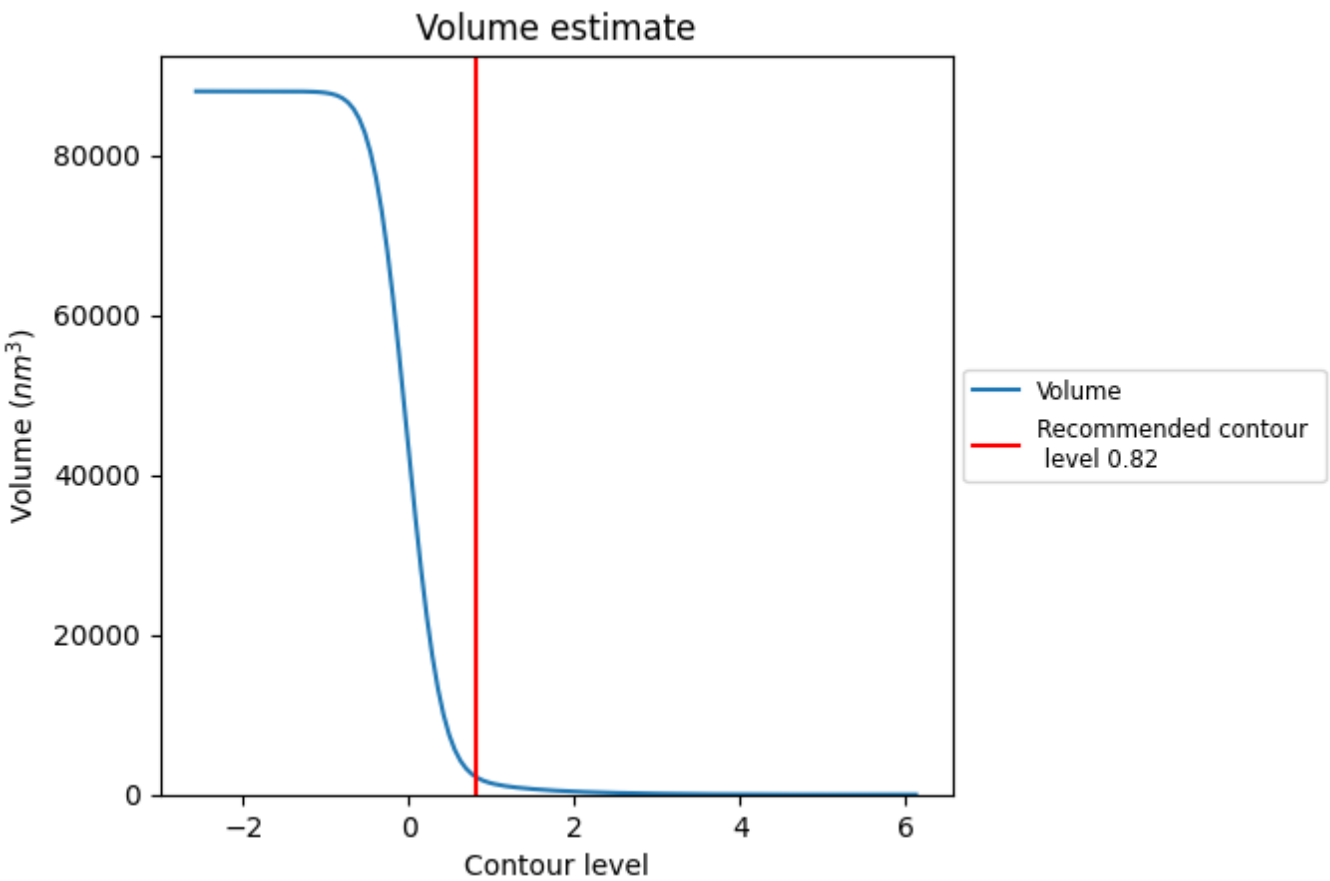
This section contains the results of statistical analysis of the map.

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.

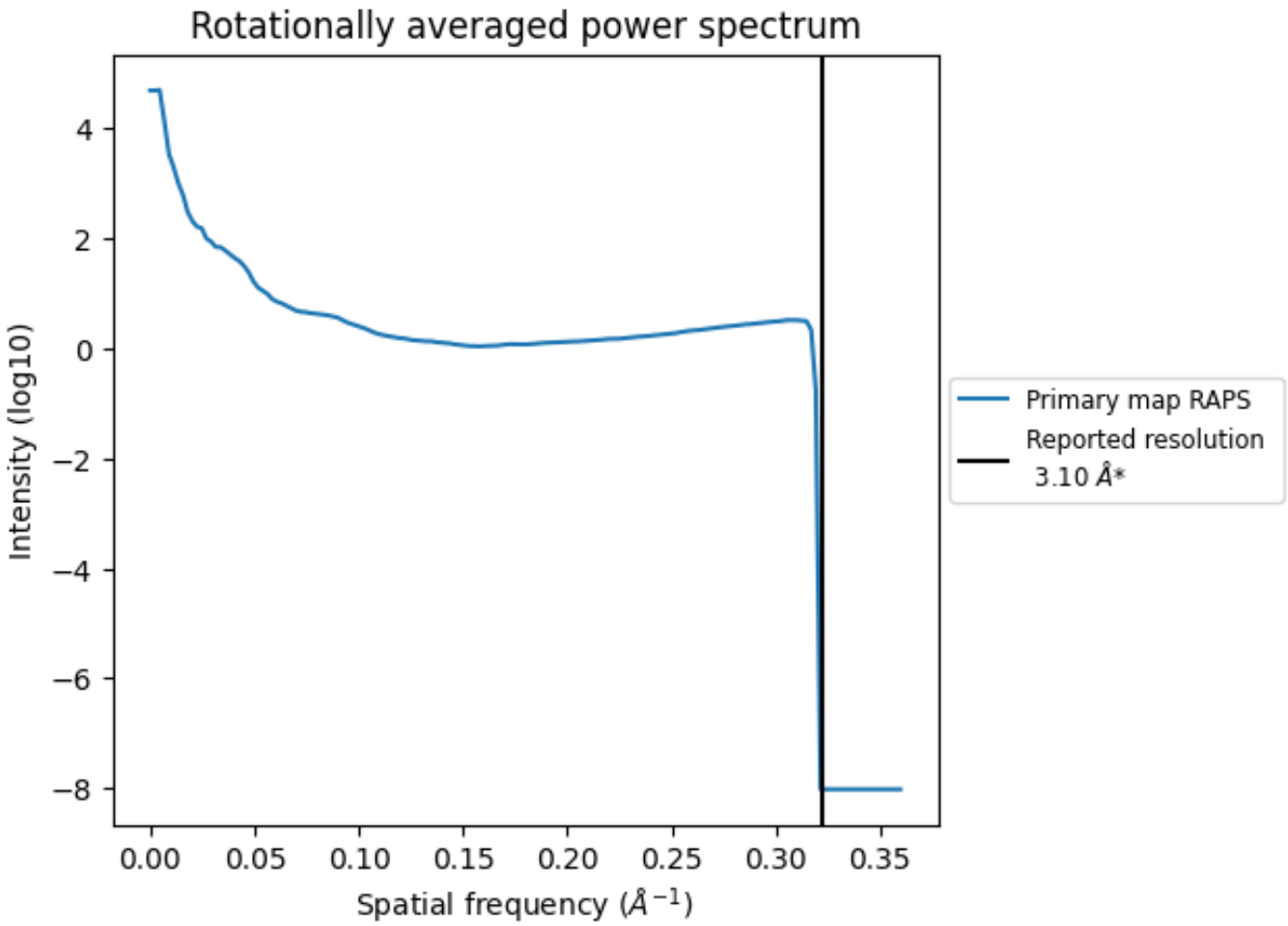
7.2 Volume estimate (i)



The volume at the recommended contour level is 2156 nm^3; this corresponds to an approximate mass of 1948 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 (i)



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

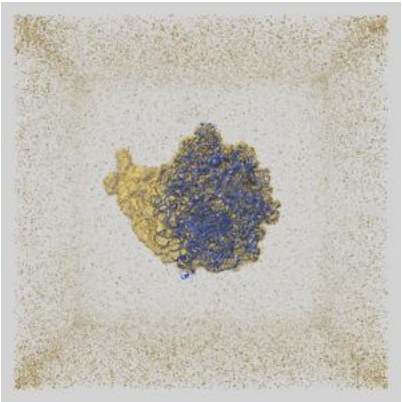
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

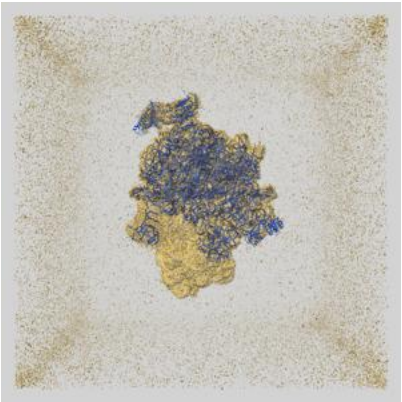
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10073 and PDB model 6S0K. Per-residue inclusion information can be found in section 3 on page 11.

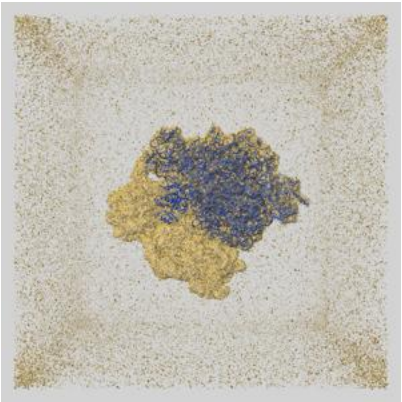
9.1 Map-model overlay (i)



X



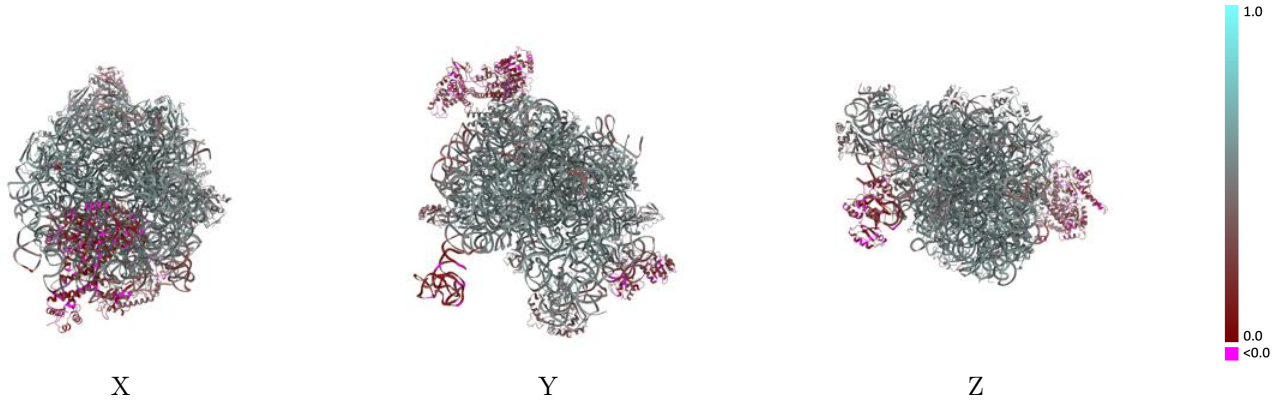
Y



Z

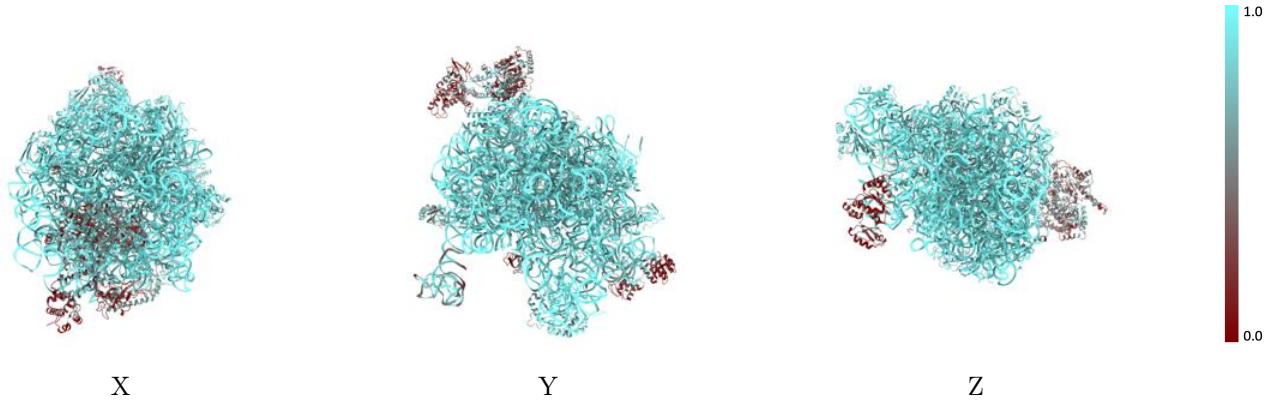
The images above show the 3D surface view of the map at the recommended contour level 0.82 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



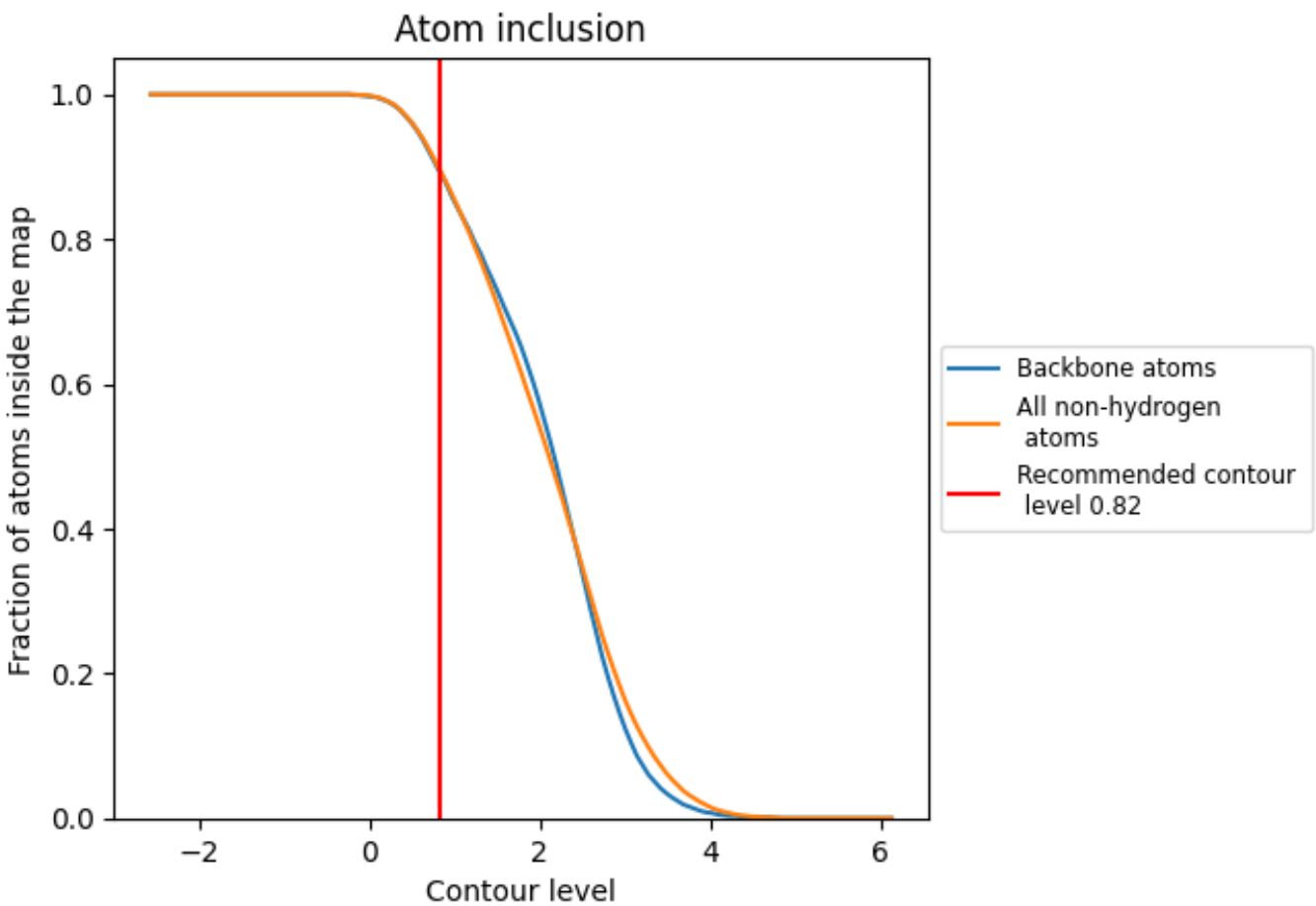
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.82).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.82) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8960	0.4800
2	0.9190	0.5050
A	0.9780	0.5100
B	0.9900	0.4970
C	0.9230	0.5540
D	0.9250	0.5420
E	0.9060	0.5090
F	0.8530	0.4200
G	0.9070	0.4680
H	0.5930	0.3700
I	0.1720	0.1650
J	0.2120	0.1100
K	0.9370	0.5470
L	0.8840	0.5390
M	0.9340	0.5410
N	0.9210	0.5420
O	0.9210	0.5330
P	0.9400	0.4950
Q	0.9010	0.5330
R	0.9380	0.5330
S	0.9250	0.5250
T	0.8930	0.5240
U	0.8590	0.5130
V	0.9150	0.4960
W	0.9250	0.5170
X	0.9330	0.5570
Y	0.9070	0.5330
Z	0.8510	0.4730
a	0.9110	0.5310
b	0.9020	0.5380
c	0.2360	0.4130
d	0.9180	0.5580
e	0.9330	0.5520
f	0.9320	0.5440
h	0.3510	0.1690
k	0.4930	0.3020