



## Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 01:40 PM EST

PDB ID : 3J80  
EMDB ID : EMD-2764  
Title : CryoEM structure of 40S-eIF1-eIF1A preinitiation complex  
Authors : Hussain, T.; Llacer, J.L.; Fernandez, I.S.; Savva, C.G.; Ramakrishnan, V.  
Deposited on : 2014-08-28  
Resolution : 3.75 Å(reported)  
Based on initial models : 3U5B, 3U5C

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

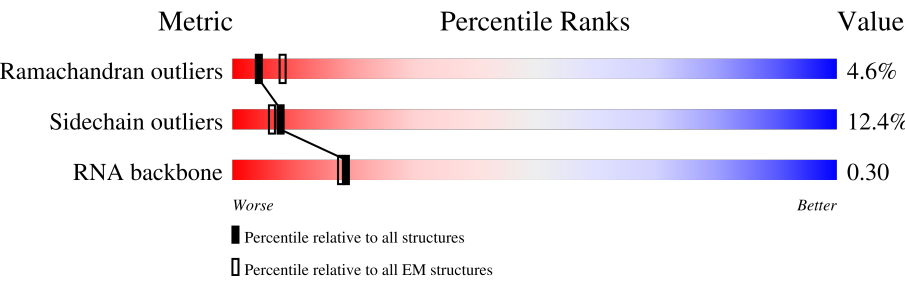


# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.75 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







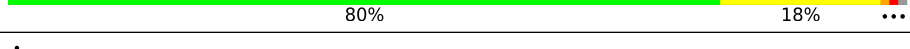
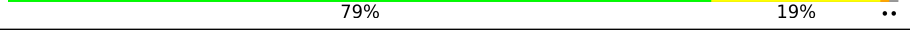
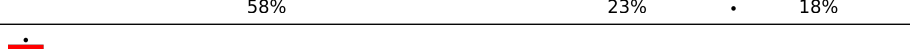
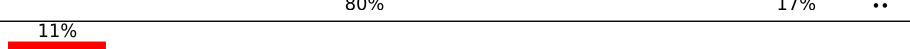
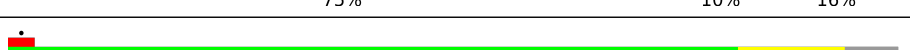

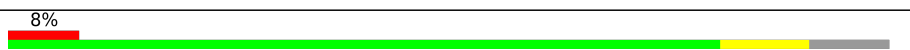

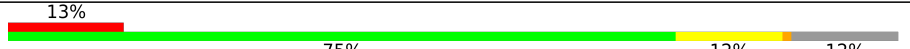





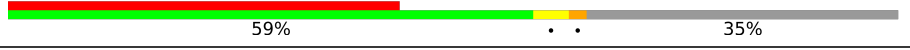
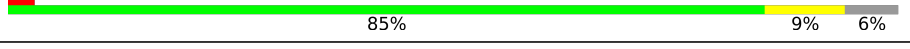



The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey 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	1799	
2	A	254	
3	B	255	
4	C	259	
5	E	261	
6	G	236	
7	H	190	
8	I	201	

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Mol	Chain	Length	Quality of chain
9	J	188	
10	L	156	
11	N	151	
12	O	137	
13	V	87	
14	W	130	
15	X	145	
16	Y	135	
17	a	119	
18	b	82	
19	e	63	
20	D	237	
21	F	227	
22	K	106	
23	M	134	
24	P	140	
25	Q	143	
26	R	136	
27	S	146	
28	T	144	
29	U	117	
30	Z	108	
31	c	67	
32	d	56	
33	f	150	

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Mol	Chain	Length	Quality of chain
34	g	326	<div><div></div><div>7%</div><div>91%</div><div>6%</div><div></div></div>
35	h	25	<div><div></div><div>36%</div><div>88%</div><div>12%</div><div></div></div>
36	i	153	<div><div></div><div>20%</div><div>58%</div><div>5%</div><div>37%</div><div></div></div>
37	j	108	<div><div></div><div>9%</div><div>74%</div><div>6%</div><div>20%</div><div></div></div>



## 2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 77716 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1779	Total	C	N	O	P	0	0
			37775	16882	6653	12461	1779		

- Molecule 2 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	206	Total	C	N	O	S	0	0
			1616	1035	285	294	2		

- Molecule 3 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	214	Total	C	N	O	S	0	0
			1722	1089	313	317	3		

- Molecule 4 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	217	Total	C	N	O	S	0	0
			1629	1041	287	297	4		

- Molecule 5 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 6 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	226	Total	C	N	O	S	0	0
			1812	1134	348	326	4		



- Molecule 7 is a protein called eS7.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	184	Total	C	N	O	0	0
			1483	950	270	263		

- Molecule 8 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	188	Total	C	N	O	S	0	0
			1493	926	301	265	1		

- Molecule 9 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 10 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 11 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	150	Total	C	N	O	S	0	0
			1187	756	223	206	2		

- Molecule 12 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	127	Total	C	N	O	S	0	0
			942	578	188	173	3		

- Molecule 13 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 14 is a protein called uS8.



Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 15 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	144	Total	C	N	O	S	0	0
			1119	708	218	191	2		

- Molecule 16 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	134	Total	C	N	O	S	0	0
			1061	665	207	189			

- Molecule 17 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	97	Total	C	N	O	S	0	0
			770	475	163	127	5		

- Molecule 18 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	81	Total	C	N	O	S	0	0
			609	379	112	113	5		

- Molecule 19 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	53	Total	C	N	O	S	0	0
			428	268	87	72	1		

- Molecule 20 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	D	223	Total	C	N	O	S	0	0
			1744	1108	313	318	5		

- Molecule 21 is a protein called uS7.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 22 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 23 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	122	Total	C	N	O		0	0
			922	575	167	180			

- Molecule 24 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	123	Total	C	N	O	S	0	0
			980	628	179	168	5		

- Molecule 25 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	141	Total	C	N	O		0	0
			1105	709	204	192			

- Molecule 26 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	120	Total	C	N	O	S	0	0
			959	598	178	180	3		

- Molecule 27 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	145	Total	C	N	O	S	0	0
			1193	741	240	210	2		

- Molecule 28 is a protein called eS19.



Mol	Chain	Residues	Atoms				AltConf	Trace
28	T	143	Total	C	N	O	0	0
			1110	693	210	207		

- Molecule 29 is a protein called uS10.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	U	106	Total	C	N	O	S	0
			845	540	152	152	1	0

- Molecule 30 is a protein called eS25.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Z	70	Total	C	N	O	S	0
			558	355	104	98	1	0

- Molecule 31 is a protein called eS28.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	c	63	Total	C	N	O	S	0
			494	305	98	90	1	0

- Molecule 32 is a protein called uS14.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	d	53	Total	C	N	O	S	0
			446	280	89	76	1	0

- Molecule 33 is a protein called eS31.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	f	69	Total	C	N	O	S	0
			549	352	102	91	4	0

- Molecule 34 is a protein called RACK1.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	g	318	Total	C	N	O	S	0
			2466	1561	430	470	5	0

- Molecule 35 is a protein called eL41.



Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 36 is a protein called eIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	96	Total	C	N	O	S	0	0
			778	482	144	147	5		

- Molecule 37 is a protein called eIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	86	Total	C	N	O	S	0	0
			695	439	128	124	4		

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	2	67	Total	Mg	0
			67	67	

- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
39	a	1	Total	Zn	0
			1	1	
39	b	1	Total	Zn	0
			1	1	
39	f	1	Total	Zn	0
			1	1	



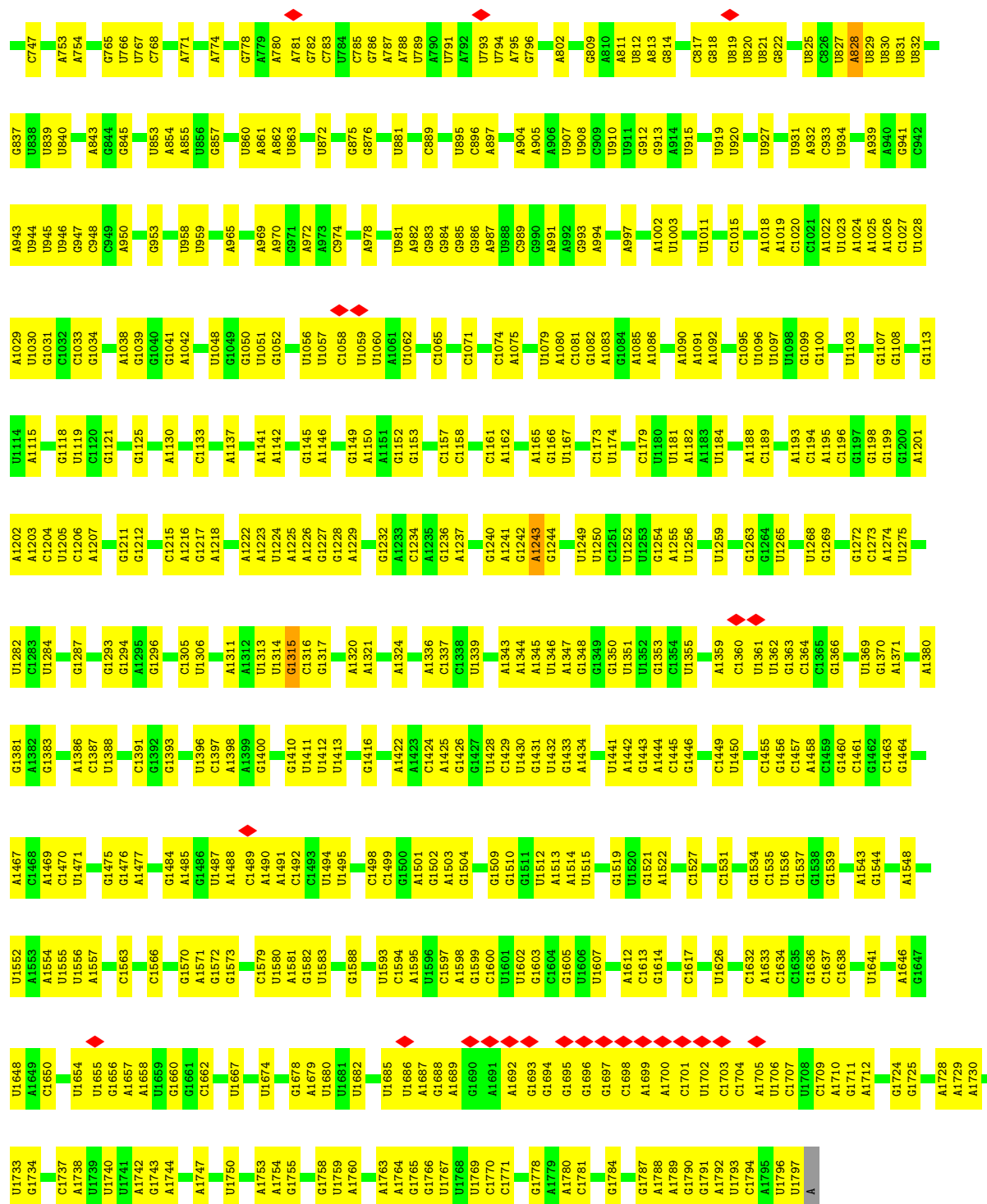
### 3 Residue-property plots

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: 18S rRNA





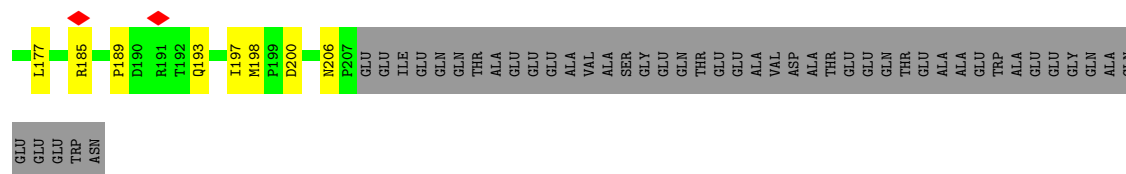


• Molecule 2: uS2

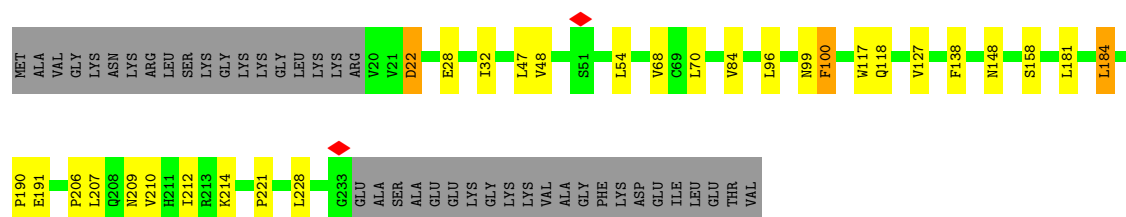
Chain A: 66% 15% 19%



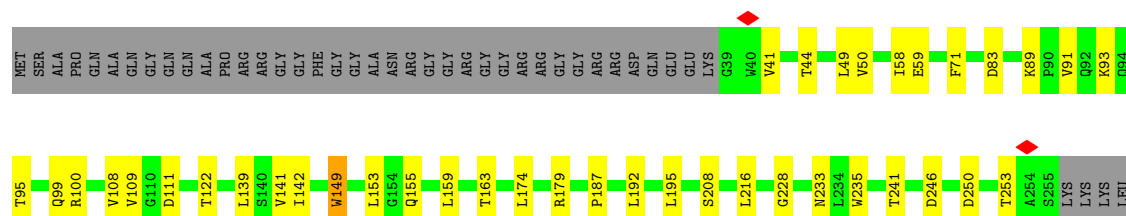




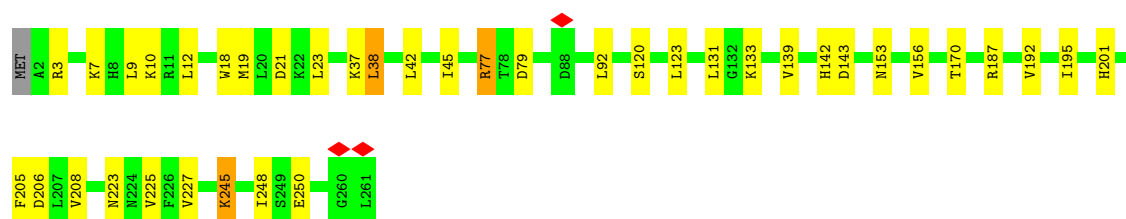
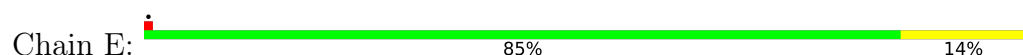
• Molecule 3: eS1



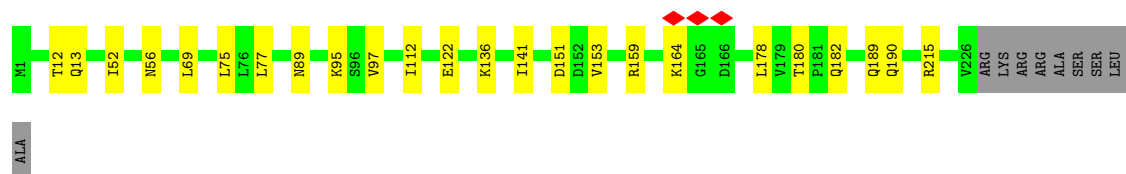
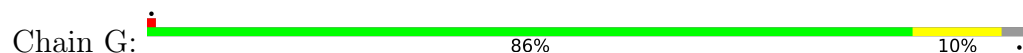
• Molecule 4: uS5



• Molecule 5: eS4




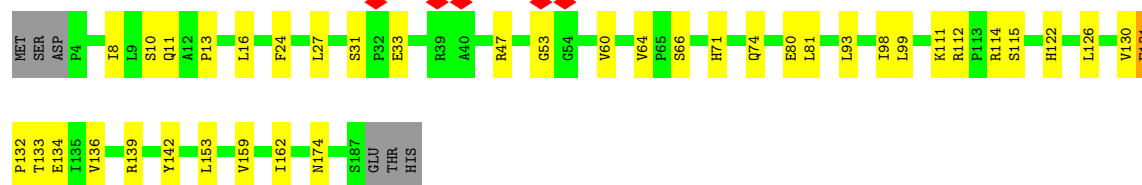
• Molecule 6: eS6




• Molecule 7: eS7

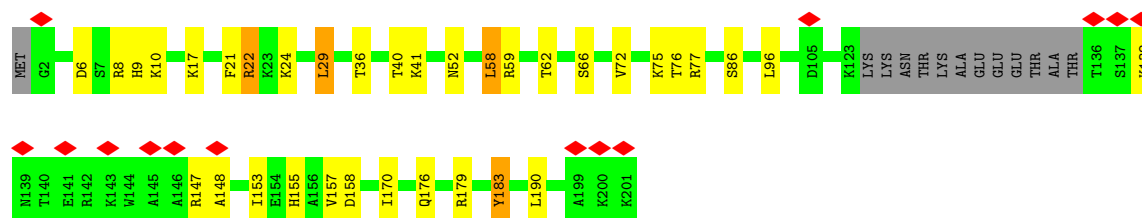


Chain H:  76% 20% ..




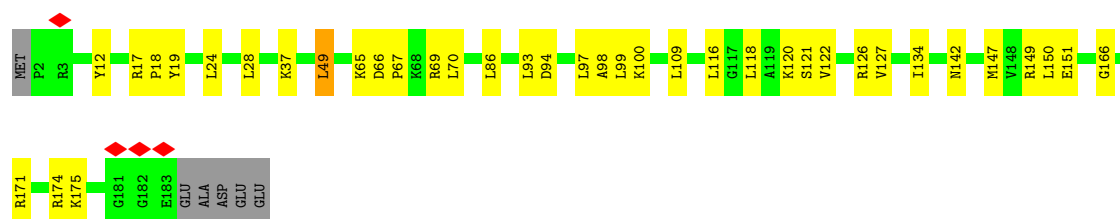
• Molecule 8: eS8

Chain I:  7% 76% 15% • 6%




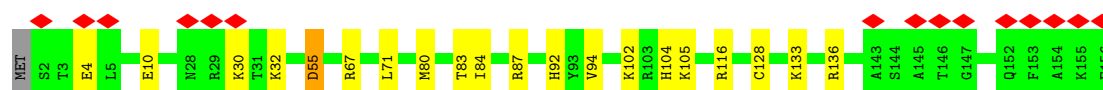
• Molecule 9: uS4

Chain J:  77% 20% ..




• Molecule 10: uS17

Chain L:  10% 87% 12% ..




• Molecule 11: uS15

Chain N:  88% 11% ..



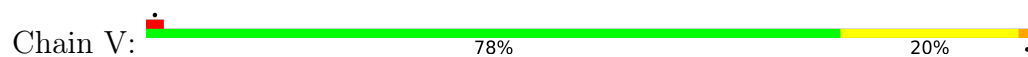
• Molecule 12: uS11

Chain O:  83% 9% 7%

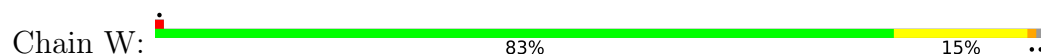




• Molecule 13: eS21



• Molecule 14: uS8



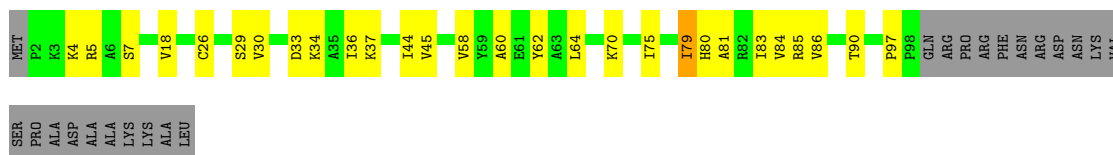
• Molecule 15: uS12



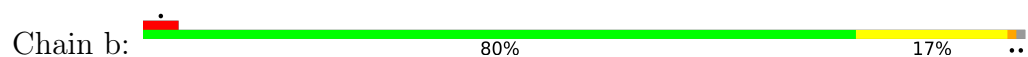
• Molecule 16: eS24



• Molecule 17: eS26

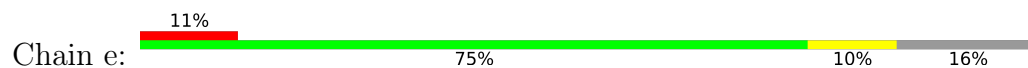


• Molecule 18: eS27

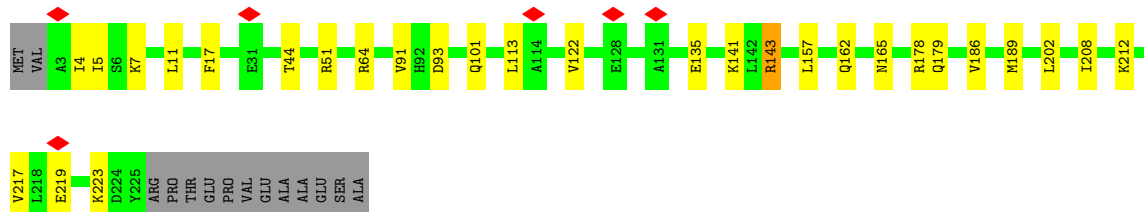
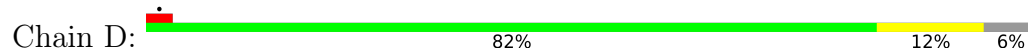




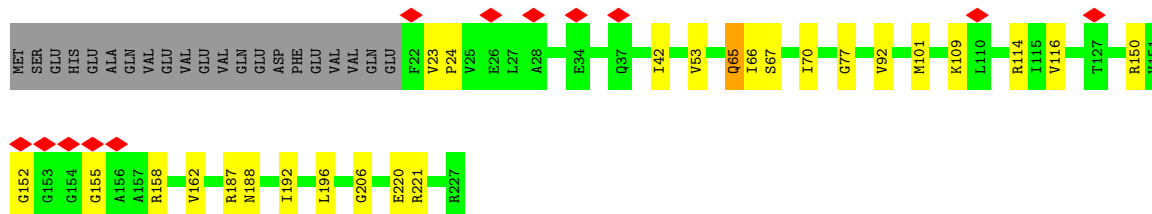
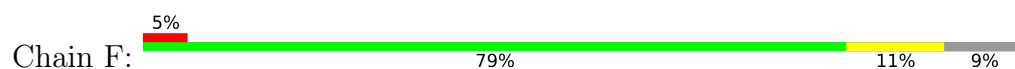
- Molecule 19: eS30



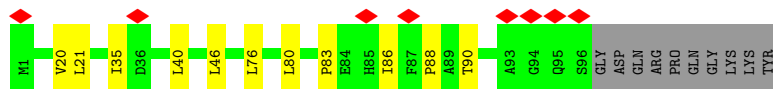
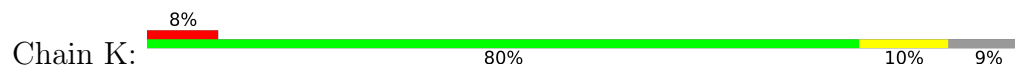
- Molecule 20: uS3



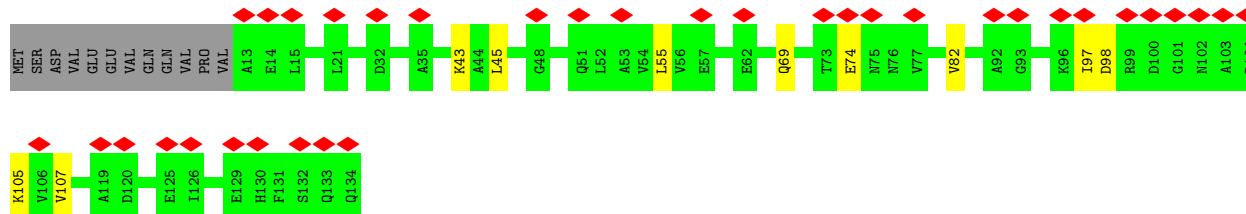
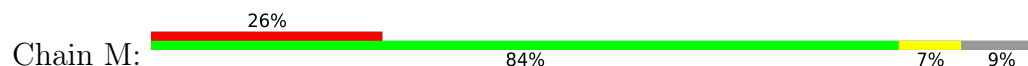
- Molecule 21: uS7



- Molecule 22: eS10

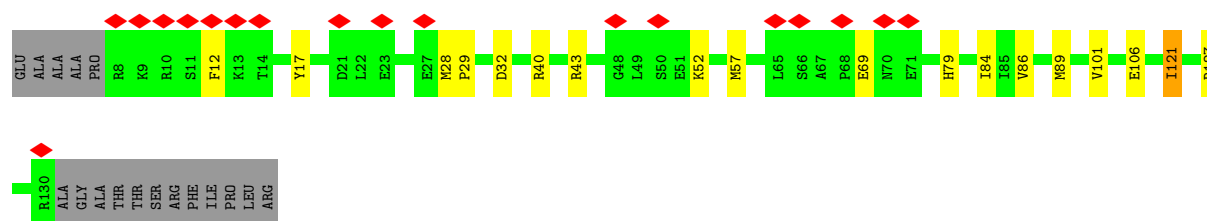
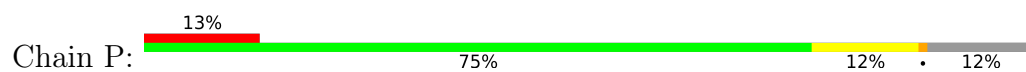


- Molecule 23: eS12

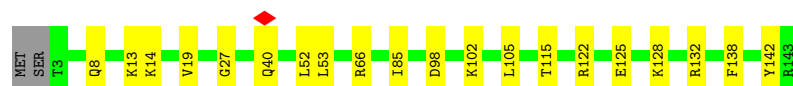
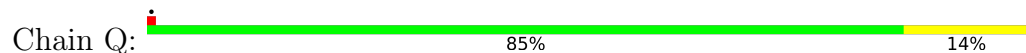


- Molecule 24: uS19

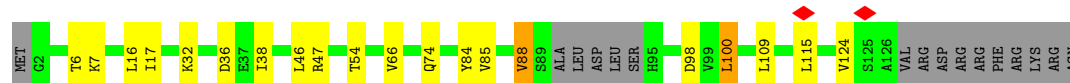
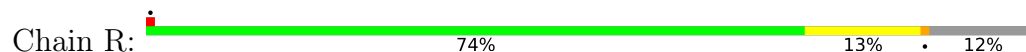




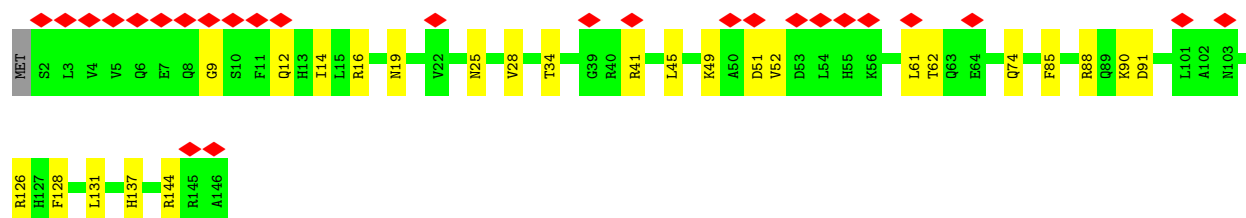
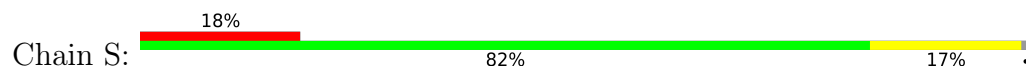
• Molecule 25: uS9



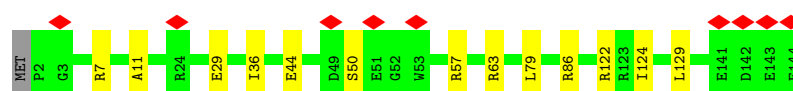
• Molecule 26: eS17



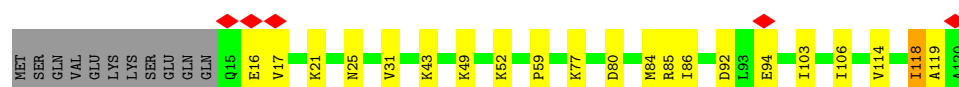
• Molecule 27: uS13



• Molecule 28: eS19

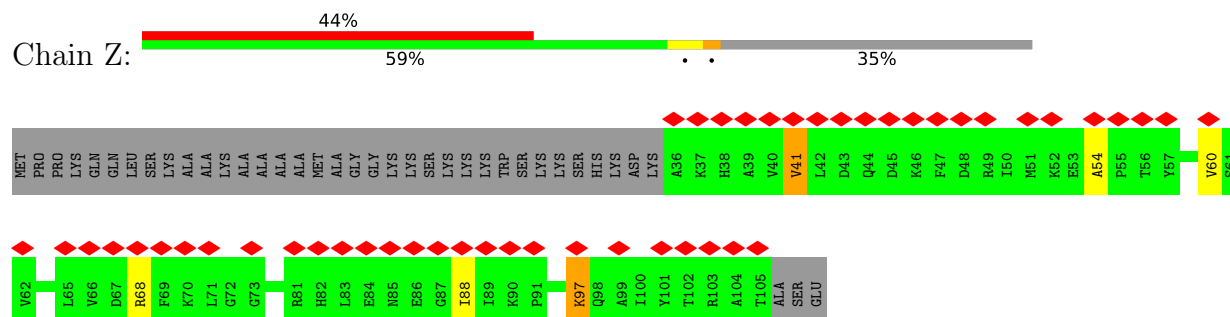


• Molecule 29: uS10

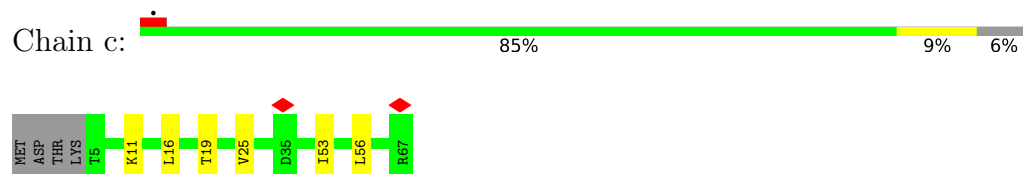




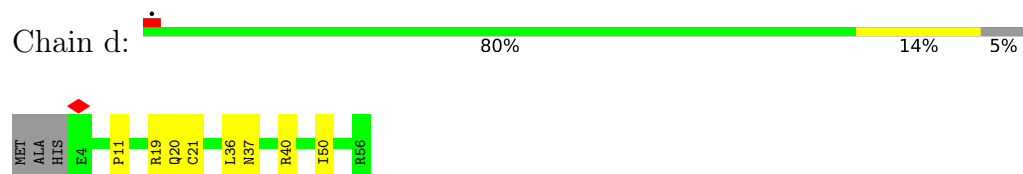
- Molecule 30: eS25



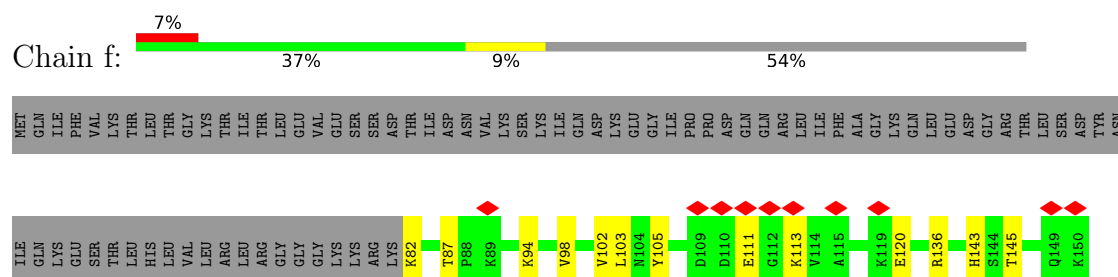
- Molecule 31: eS28



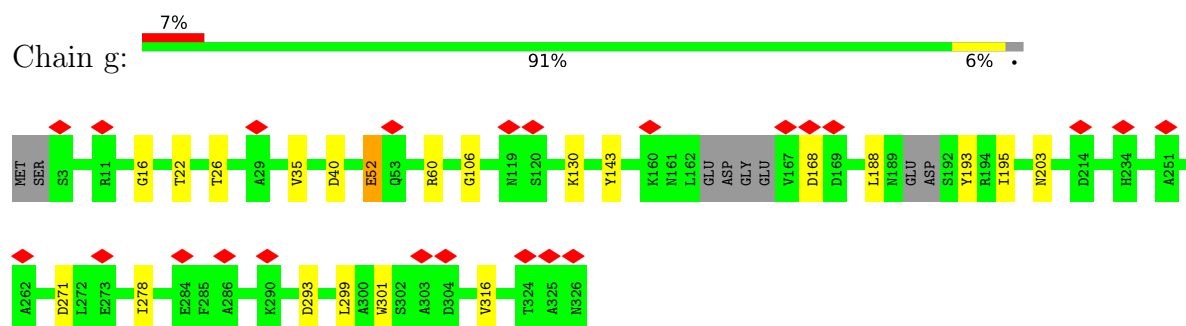
- Molecule 32: uS14



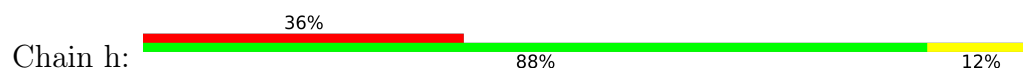
- Molecule 33: eS31



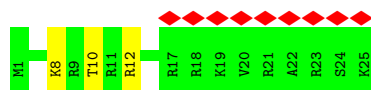
- Molecule 34: RACK1



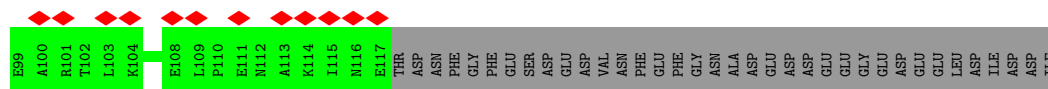
- Molecule 35: eL41



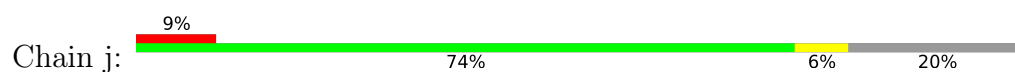




• Molecule 36: eIF1A



• Molecule 37: eIF1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	100709	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	28	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.602	Depositor
Minimum map value	-0.221	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.065	Depositor
Map size ( $\text{\AA}$ )	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.34, 1.34, 1.34	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	2	0.30	0/42244	0.70	5/65823 (0.0%)
2	A	0.43	0/1656	0.78	0/2264
3	B	0.40	0/1747	0.72	1/2353 (0.0%)
4	C	0.45	0/1659	0.79	3/2252 (0.1%)
5	E	0.41	0/2122	0.71	1/2861 (0.0%)
6	G	0.39	0/1835	0.68	0/2451
7	H	0.43	0/1507	0.74	0/2028
8	I	0.44	0/1519	0.74	2/2033 (0.1%)
9	J	0.45	0/1495	0.82	2/2001 (0.1%)
10	L	0.45	0/1276	0.70	0/1718
11	N	0.45	0/1210	0.78	1/1628 (0.1%)
12	O	0.40	0/953	0.72	0/1279
13	V	0.43	0/696	0.73	0/938
14	W	0.50	0/1039	0.82	0/1399
15	X	0.48	0/1137	0.80	0/1516
16	Y	0.42	0/1075	0.72	0/1433
17	a	0.44	0/782	0.82	0/1047
18	b	0.40	0/619	0.70	0/837
19	e	0.39	0/435	0.70	0/579
20	D	0.43	0/1769	0.70	0/2378
21	F	0.40	0/1628	0.71	0/2198
22	K	0.46	0/831	0.67	0/1123
23	M	0.40	0/929	0.69	0/1255
24	P	0.43	0/1000	0.65	0/1343
25	Q	0.41	0/1125	0.69	0/1510
26	R	0.44	0/969	0.73	0/1299
27	S	0.39	0/1212	0.68	0/1629
28	T	0.39	0/1129	0.68	0/1520
29	U	0.43	0/857	0.73	0/1158
30	Z	0.43	0/567	0.64	0/762
31	c	0.39	0/496	0.72	0/666
32	d	0.47	0/457	0.66	0/607



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	f	0.47	0/562	0.65	0/751
34	g	0.41	0/2521	0.61	0/3431
35	h	0.39	0/234	0.81	0/300
36	i	0.38	0/788	0.62	0/1051
37	j	0.41	0/703	0.66	0/938
All	All	0.37	0/82783	0.71	15/120359 (0.0%)

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
7	H	0	1
9	J	0	1
14	W	0	1
15	X	0	2
16	Y	0	1
17	a	0	1
25	Q	0	1
All	All	0	8

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1315	G	C2'-C3'-O3'	7.15	125.23	109.50
9	J	49	LEU	CA-CB-CG	7.12	131.67	115.30
4	C	139	LEU	CA-CB-CG	6.41	130.05	115.30
3	B	184	LEU	CA-CB-CG	6.33	129.86	115.30
8	I	29	LEU	CA-CB-CG	6.22	129.61	115.30
1	2	1243	A	C2'-C3'-O3'	5.86	123.07	113.70
4	C	192	LEU	CA-CB-CG	5.75	128.51	115.30
1	2	279	U	C2'-C3'-O3'	5.60	122.66	113.70
1	2	828	A	C2'-C3'-O3'	5.43	122.39	113.70
5	E	38	LEU	CA-CB-CG	5.26	127.41	115.30
1	2	700	C	C2'-C3'-O3'	5.24	122.09	113.70
11	N	128	TYR	CB-CA-C	5.21	120.83	110.40
4	C	216	LEU	CA-CB-CG	-5.13	103.49	115.30
8	I	183	TYR	CA-CB-CG	-5.13	103.65	113.40
9	J	24	LEU	CA-CB-CG	5.12	127.09	115.30



There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	H	131	PHE	Peptide
9	J	12	TYR	Peptide
25	Q	40	GLN	Peptide
14	W	75	ILE	Peptide
15	X	11	SER	Peptide
15	X	63	GLN	Peptide
16	Y	29	HIS	Peptide
17	a	79	ILE	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	
2	A	204/254 (80%)	167 (82%)	24 (12%)	13 (6%)	1	19
3	B	212/255 (83%)	175 (82%)	25 (12%)	12 (6%)	1	20
4	C	215/259 (83%)	182 (85%)	23 (11%)	10 (5%)	2	24
5	E	258/261 (99%)	215 (83%)	36 (14%)	7 (3%)	5	35
6	G	224/236 (95%)	196 (88%)	24 (11%)	4 (2%)	8	42
7	H	182/190 (96%)	152 (84%)	15 (8%)	15 (8%)	1	12
8	I	184/201 (92%)	146 (79%)	26 (14%)	12 (6%)	1	19
9	J	180/188 (96%)	148 (82%)	20 (11%)	12 (7%)	1	18
10	L	153/156 (98%)	129 (84%)	18 (12%)	6 (4%)	3	28
11	N	148/151 (98%)	127 (86%)	17 (12%)	4 (3%)	5	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	O	125/137 (91%)	98 (78%)	20 (16%)	7 (6%)	2	21
13	V	85/87 (98%)	67 (79%)	11 (13%)	7 (8%)	1	12
14	W	127/130 (98%)	109 (86%)	13 (10%)	5 (4%)	3	28
15	X	142/145 (98%)	115 (81%)	13 (9%)	14 (10%)	0	9
16	Y	132/135 (98%)	114 (86%)	10 (8%)	8 (6%)	1	19
17	a	95/119 (80%)	64 (67%)	21 (22%)	10 (10%)	0	8
18	b	79/82 (96%)	62 (78%)	12 (15%)	5 (6%)	1	19
19	e	51/63 (81%)	47 (92%)	3 (6%)	1 (2%)	7	41
20	D	221/237 (93%)	197 (89%)	18 (8%)	6 (3%)	5	35
21	F	204/227 (90%)	169 (83%)	25 (12%)	10 (5%)	2	23
22	K	94/106 (89%)	81 (86%)	11 (12%)	2 (2%)	7	40
23	M	120/134 (90%)	96 (80%)	20 (17%)	4 (3%)	4	32
24	P	121/140 (86%)	99 (82%)	16 (13%)	6 (5%)	2	23
25	Q	139/143 (97%)	120 (86%)	15 (11%)	4 (3%)	4	34
26	R	116/136 (85%)	93 (80%)	18 (16%)	5 (4%)	2	26
27	S	143/146 (98%)	113 (79%)	23 (16%)	7 (5%)	2	23
28	T	141/144 (98%)	123 (87%)	15 (11%)	3 (2%)	7	40
29	U	104/117 (89%)	91 (88%)	5 (5%)	8 (8%)	1	14
30	Z	68/108 (63%)	53 (78%)	10 (15%)	5 (7%)	1	15
31	c	61/67 (91%)	55 (90%)	6 (10%)	0	100	100
32	d	51/56 (91%)	41 (80%)	9 (18%)	1 (2%)	7	41
33	f	67/150 (45%)	43 (64%)	17 (25%)	7 (10%)	0	8
34	g	312/326 (96%)	256 (82%)	48 (15%)	8 (3%)	5	36
35	h	23/25 (92%)	23 (100%)	0	0	100	100
36	i	94/153 (61%)	86 (92%)	8 (8%)	0	100	100
37	j	84/108 (78%)	75 (89%)	8 (10%)	1 (1%)	13	49
All	All	4959/5572 (89%)	4127 (83%)	603 (12%)	229 (5%)	4	24

All (229) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	26	ALA
2	A	95	ALA

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Mol	Chain	Res	Type
3	B	100	PHE
3	B	117	TRP
4	C	141	VAL
4	C	153	LEU
5	E	201	HIS
6	G	122	GLU
7	H	13	PRO
7	H	31	SER
7	H	64	VAL
7	H	74	GLN
8	I	52	ASN
8	I	153	ILE
9	J	98	ALA
10	L	133	LYS
11	N	47	PRO
13	V	44	ARG
15	X	42	PRO
15	X	64	PRO
15	X	144	ARG
16	Y	30	PRO
17	a	75	ILE
17	a	83	ILE
21	F	67	SER
22	K	83	PRO
22	K	88	PRO
23	M	74	GLU
24	P	29	PRO
26	R	85	VAL
26	R	88	VAL
28	T	11	ALA
37	j	72	PRO
2	A	49	ASN
2	A	81	TYR
3	B	158	SER
4	C	149	TRP
7	H	111	LYS
7	H	136	VAL
8	I	9	HIS
8	I	22	ARG
8	I	40	THR
8	I	58	LEU
8	I	147	ARG

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Mol	Chain	Res	Type
9	J	118	LEU
10	L	30	LYS
10	L	105	LYS
12	O	124	ASP
14	W	29	PRO
14	W	83	ILE
14	W	98	GLN
15	X	67	ALA
15	X	115	GLY
16	Y	52	LYS
17	a	81	ALA
17	a	86	VAL
18	b	21	LEU
18	b	75	GLU
20	D	93	ASP
21	F	65	GLN
21	F	206	GLY
24	P	28	MET
24	P	121	ILE
27	S	28	VAL
27	S	51	ASP
29	U	49	LYS
29	U	106	ILE
29	U	118	ILE
30	Z	41	VAL
33	f	102	VAL
33	f	143	HIS
34	g	130	LYS
2	A	43	ASP
3	B	207	LEU
3	B	209	ASN
3	B	210	VAL
3	B	221	PRO
4	C	111	ASP
5	E	12	LEU
5	E	245	LYS
7	H	10	SER
7	H	159	VAL
8	I	148	ALA
8	I	155	HIS
10	L	55	ASP
10	L	104	HIS

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Mol	Chain	Res	Type
11	N	3	ARG
11	N	24	ALA
12	O	40	ALA
12	O	114	ARG
13	V	4	ASP
13	V	30	SER
13	V	42	GLU
14	W	30	SER
15	X	3	LYS
15	X	7	ARG
15	X	63	GLN
15	X	89	ASN
15	X	90	ASP
15	X	128	SER
15	X	131	SER
16	Y	36	SER
16	Y	60	PHE
16	Y	61	ARG
17	a	60	ALA
17	a	64	LEU
20	D	44	THR
20	D	143	ARG
20	D	217	VAL
21	F	155	GLY
24	P	12	PHE
27	S	61	LEU
28	T	50	SER
29	U	16	GLU
30	Z	54	ALA
30	Z	97	LYS
33	f	111	GLU
33	f	145	THR
34	g	106	GLY
34	g	168	ASP
34	g	278	ILE
34	g	301	TRP
2	A	35	PRO
2	A	82	GLY
2	A	158	VAL
2	A	193	GLN
2	A	197	ILE
3	B	54	LEU

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Mol	Chain	Res	Type
3	B	206	PRO
4	C	41	VAL
4	C	155	GLN
5	E	120	SER
5	E	195	ILE
5	E	205	PHE
6	G	153	VAL
7	H	115	SER
7	H	132	PRO
9	J	65	LYS
9	J	120	LYS
9	J	121	SER
9	J	147	MET
12	O	24	ASN
12	O	42	VAL
13	V	10	GLU
15	X	5	LYS
16	Y	63	GLN
19	e	47	VAL
20	D	4	ILE
20	D	219	GLU
21	F	66	ILE
23	M	82	VAL
23	M	98	ASP
24	P	69	GLU
24	P	101	VAL
25	Q	138	PHE
26	R	115	LEU
27	S	90	LYS
29	U	21	LYS
29	U	59	PRO
33	f	94	LYS
33	f	98	VAL
34	g	193	TYR
2	A	185	ARG
2	A	189	PRO
4	C	44	THR
4	C	228	GLY
5	E	77	ARG
7	H	134	GLU
8	I	10	LYS
8	I	41	LYS

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Mol	Chain	Res	Type
8	I	59	ARG
9	J	18	PRO
9	J	67	PRO
9	J	134	ILE
9	J	171	ARG
10	L	4	GLU
11	N	27	LYS
13	V	7	GLN
13	V	12	TYR
14	W	57	ARG
16	Y	51	GLU
17	a	36	ILE
18	b	24	LEU
18	b	62	VAL
21	F	23	VAL
23	M	97	ILE
26	R	100	LEU
26	R	124	VAL
27	S	14	ILE
27	S	19	ASN
28	T	29	GLU
29	U	119	ALA
30	Z	68	ARG
34	g	16	GLY
34	g	52	GLU
2	A	103	THR
3	B	22	ASP
3	B	148	ASN
4	C	253	THR
6	G	89	ASN
7	H	131	PHE
9	J	99	LEU
12	O	25	ASP
15	X	53	VAL
17	a	62	TYR
25	Q	14	LYS
25	Q	27	GLY
25	Q	115	THR
30	Z	88	ILE
3	B	190	PRO
12	O	88	GLY
21	F	53	VAL

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Mol	Chain	Res	Type
7	H	8	ILE
7	H	53	GLY
18	b	39	GLY
21	F	24	PRO
21	F	152	GLY
27	S	9	GLY
32	d	11	PRO
33	f	87	THR
4	C	187	PRO
7	H	98	ILE
16	Y	5	ILE
29	U	17	VAL
6	G	69	LEU
9	J	166	GLY
21	F	77	GLY
17	a	84	VAL
17	a	97	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	174/211 (82%)	146 (84%)	28 (16%)	2	16
3	B	196/228 (86%)	176 (90%)	20 (10%)	7	32
4	C	176/203 (87%)	148 (84%)	28 (16%)	2	16
5	E	223/224 (100%)	189 (85%)	34 (15%)	3	18
6	G	192/200 (96%)	172 (90%)	20 (10%)	7	31
7	H	164/170 (96%)	140 (85%)	24 (15%)	3	19
8	I	148/159 (93%)	123 (83%)	25 (17%)	2	14
9	J	153/158 (97%)	129 (84%)	24 (16%)	2	17
10	L	136/137 (99%)	121 (89%)	15 (11%)	6	29
11	N	127/128 (99%)	114 (90%)	13 (10%)	7	32
12	O	96/104 (92%)	90 (94%)	6 (6%)	18	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	V	73/73 (100%)	59 (81%)	14 (19%)	1	9
14	W	110/111 (99%)	94 (86%)	16 (14%)	3	19
15	X	119/120 (99%)	104 (87%)	15 (13%)	4	24
16	Y	108/109 (99%)	88 (82%)	20 (18%)	1	10
17	a	82/100 (82%)	64 (78%)	18 (22%)	1	6
18	b	71/72 (99%)	60 (84%)	11 (16%)	2	17
19	e	47/55 (86%)	42 (89%)	5 (11%)	6	30
20	D	185/196 (94%)	161 (87%)	24 (13%)	4	23
21	F	174/194 (90%)	157 (90%)	17 (10%)	8	33
22	K	88/96 (92%)	79 (90%)	9 (10%)	7	32
23	M	97/109 (89%)	91 (94%)	6 (6%)	18	50
24	P	105/117 (90%)	92 (88%)	13 (12%)	4	24
25	Q	117/119 (98%)	102 (87%)	15 (13%)	4	23
26	R	109/124 (88%)	92 (84%)	17 (16%)	2	17
27	S	128/129 (99%)	110 (86%)	18 (14%)	3	21
28	T	117/118 (99%)	107 (92%)	10 (8%)	10	40
29	U	96/107 (90%)	82 (85%)	14 (15%)	3	19
30	Z	60/88 (68%)	57 (95%)	3 (5%)	24	55
31	c	55/59 (93%)	49 (89%)	6 (11%)	6	29
32	d	46/48 (96%)	39 (85%)	7 (15%)	3	18
33	f	58/133 (44%)	52 (90%)	6 (10%)	7	31
34	g	265/272 (97%)	251 (95%)	14 (5%)	22	54
35	h	23/23 (100%)	20 (87%)	3 (13%)	4	23
36	i	83/130 (64%)	76 (92%)	7 (8%)	11	41
37	j	77/96 (80%)	72 (94%)	5 (6%)	17	49
All	All	4278/4720 (91%)	3748 (88%)	530 (12%)	8	24

All (530) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	6	THR
2	A	8	ASP
2	A	9	LEU

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Mol	Chain	Res	Type
2	A	13	ASP
2	A	24	LEU
2	A	33	GLN
2	A	37	VAL
2	A	43	ASP
2	A	47	VAL
2	A	56	LYS
2	A	57	ILE
2	A	59	LEU
2	A	79	ARG
2	A	81	TYR
2	A	84	ARG
2	A	93	THR
2	A	108	THR
2	A	109	ASN
2	A	134	LYS
2	A	135	GLU
2	A	137	SER
2	A	146	LEU
2	A	147	THR
2	A	173	ILE
2	A	177	LEU
2	A	198	MET
2	A	200	ASP
2	A	206	ASN
3	B	22	ASP
3	B	28	GLU
3	B	32	ILE
3	B	47	LEU
3	B	48	VAL
3	B	68	VAL
3	B	70	LEU
3	B	84	VAL
3	B	96	LEU
3	B	99	ASN
3	B	100	PHE
3	B	118	GLN
3	B	127	VAL
3	B	138	PHE
3	B	181	LEU
3	B	184	LEU
3	B	191	GLU

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Mol	Chain	Res	Type
3	B	212	ILE
3	B	214	LYS
3	B	228	LEU
4	C	49	LEU
4	C	50	VAL
4	C	58	ILE
4	C	59	GLU
4	C	71	PHE
4	C	83	ASP
4	C	89	LYS
4	C	91	VAL
4	C	93	LYS
4	C	95	THR
4	C	99	GLN
4	C	100	ARG
4	C	108	VAL
4	C	109	VAL
4	C	122	THR
4	C	142	ILE
4	C	149	TRP
4	C	159	LEU
4	C	163	THR
4	C	174	LEU
4	C	179	ARG
4	C	195	LEU
4	C	208	SER
4	C	233	ASN
4	C	235	TRP
4	C	241	THR
4	C	246	ASP
4	C	250	ASP
5	E	3	ARG
5	E	7	LYS
5	E	9	LEU
5	E	10	LYS
5	E	18	TRP
5	E	19	MET
5	E	21	ASP
5	E	23	LEU
5	E	37	LYS
5	E	38	LEU
5	E	42	LEU

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Mol	Chain	Res	Type
5	E	45	ILE
5	E	77	ARG
5	E	79	ASP
5	E	92	LEU
5	E	123	LEU
5	E	131	LEU
5	E	133	LYS
5	E	139	VAL
5	E	142	HIS
5	E	143	ASP
5	E	153	ASN
5	E	156	VAL
5	E	170	THR
5	E	187	ARG
5	E	192	VAL
5	E	206	ASP
5	E	208	VAL
5	E	223	ASN
5	E	225	VAL
5	E	227	VAL
5	E	245	LYS
5	E	248	ILE
5	E	250	GLU
6	G	12	THR
6	G	13	GLN
6	G	52	ILE
6	G	56	ASN
6	G	75	LEU
6	G	77	LEU
6	G	95	LYS
6	G	97	VAL
6	G	112	ILE
6	G	136	LYS
6	G	141	ILE
6	G	151	ASP
6	G	159	ARG
6	G	164	LYS
6	G	178	LEU
6	G	180	THR
6	G	182	GLN
6	G	189	GLN
6	G	190	GLN

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Mol	Chain	Res	Type
6	G	215	ARG
7	H	11	GLN
7	H	16	LEU
7	H	24	PHE
7	H	27	LEU
7	H	33	GLU
7	H	47	ARG
7	H	60	VAL
7	H	66	SER
7	H	71	HIS
7	H	80	GLU
7	H	81	LEU
7	H	93	LEU
7	H	99	LEU
7	H	112	ARG
7	H	114	ARG
7	H	122	HIS
7	H	126	LEU
7	H	130	VAL
7	H	133	THR
7	H	139	ARG
7	H	142	TYR
7	H	153	LEU
7	H	162	ILE
7	H	174	ASN
8	I	6	ASP
8	I	8	ARG
8	I	17	LYS
8	I	21	PHE
8	I	22	ARG
8	I	24	LYS
8	I	29	LEU
8	I	36	THR
8	I	58	LEU
8	I	62	THR
8	I	66	SER
8	I	72	VAL
8	I	75	LYS
8	I	76	THR
8	I	77	ARG
8	I	86	SER
8	I	96	LEU

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Mol	Chain	Res	Type
8	I	138	LYS
8	I	157	VAL
8	I	158	ASP
8	I	170	ILE
8	I	176	GLN
8	I	179	ARG
8	I	183	TYR
8	I	190	LEU
9	J	17	ARG
9	J	19	TYR
9	J	28	LEU
9	J	37	LYS
9	J	49	LEU
9	J	66	ASP
9	J	69	ARG
9	J	70	LEU
9	J	86	LEU
9	J	93	LEU
9	J	94	ASP
9	J	97	LEU
9	J	100	LYS
9	J	109	LEU
9	J	116	LEU
9	J	122	VAL
9	J	126	ARG
9	J	127	VAL
9	J	142	ASN
9	J	149	ARG
9	J	150	LEU
9	J	151	GLU
9	J	174	ARG
9	J	175	LYS
10	L	10	GLU
10	L	32	LYS
10	L	55	ASP
10	L	67	ARG
10	L	71	LEU
10	L	80	MET
10	L	83	THR
10	L	84	ILE
10	L	87	ARG
10	L	92	HIS

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Mol	Chain	Res	Type
10	L	94	VAL
10	L	102	LYS
10	L	116	ARG
10	L	128	CYS
10	L	136	ARG
11	N	3	ARG
11	N	49	GLN
11	N	64	LYS
11	N	72	LEU
11	N	75	LEU
11	N	88	LEU
11	N	89	TYR
11	N	99	ARG
11	N	105	ASN
11	N	121	ARG
11	N	125	LEU
11	N	139	TRP
11	N	142	GLU
12	O	61	MET
12	O	67	VAL
12	O	81	ILE
12	O	83	ILE
12	O	86	THR
12	O	102	LEU
13	V	1	MET
13	V	4	ASP
13	V	8	LEU
13	V	12	TYR
13	V	24	ILE
13	V	28	ASP
13	V	32	VAL
13	V	34	ILE
13	V	40	ASP
13	V	59	ILE
13	V	60	ARG
13	V	64	GLU
13	V	66	ASP
13	V	69	LEU
14	W	3	ARG
14	W	7	LEU
14	W	14	ILE
14	W	19	LYS

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Mol	Chain	Res	Type
14	W	23	ARG
14	W	24	GLN
14	W	25	VAL
14	W	28	ARG
14	W	35	ILE
14	W	55	ASP
14	W	63	VAL
14	W	66	ASN
14	W	70	ASN
14	W	81	VAL
14	W	83	ILE
14	W	130	TYR
15	X	5	LYS
15	X	17	VAL
15	X	19	ARG
15	X	22	ASN
15	X	23	ARG
15	X	55	GLU
15	X	63	GLN
15	X	77	ILE
15	X	84	THR
15	X	100	ASP
15	X	107	PHE
15	X	109	ARG
15	X	117	ILE
15	X	132	LEU
15	X	142	LYS
16	Y	5	ILE
16	Y	6	THR
16	Y	8	ARG
16	Y	20	ARG
16	Y	35	VAL
16	Y	38	ASP
16	Y	46	GLU
16	Y	51	GLU
16	Y	53	ASP
16	Y	57	VAL
16	Y	62	THR
16	Y	64	TYR
16	Y	69	SER
16	Y	74	LEU
16	Y	81	ASP

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Mol	Chain	Res	Type
16	Y	98	GLU
16	Y	110	GLN
16	Y	112	LYS
16	Y	121	THR
16	Y	125	ILE
17	a	4	LYS
17	a	5	ARG
17	a	7	SER
17	a	18	VAL
17	a	26	CYS
17	a	29	SER
17	a	30	VAL
17	a	33	ASP
17	a	34	LYS
17	a	37	LYS
17	a	44	ILE
17	a	45	VAL
17	a	58	VAL
17	a	70	LYS
17	a	79	ILE
17	a	80	HIS
17	a	85	ARG
17	a	90	THR
18	b	7	LEU
18	b	8	LEU
18	b	9	HIS
18	b	21	LEU
18	b	34	ASP
18	b	35	VAL
18	b	43	ILE
18	b	44	THR
18	b	54	VAL
18	b	56	CYS
18	b	81	ARG
19	e	14	VAL
19	e	22	GLU
19	e	33	ARG
19	e	37	ARG
19	e	38	LEU
20	D	5	ILE
20	D	7	LYS
20	D	11	LEU

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Mol	Chain	Res	Type
20	D	17	PHE
20	D	51	ARG
20	D	64	ARG
20	D	91	VAL
20	D	101	GLN
20	D	113	LEU
20	D	122	VAL
20	D	135	GLU
20	D	141	LYS
20	D	143	ARG
20	D	157	LEU
20	D	162	GLN
20	D	165	ASN
20	D	178	ARG
20	D	179	GLN
20	D	186	VAL
20	D	189	MET
20	D	202	LEU
20	D	208	ILE
20	D	212	LYS
20	D	223	LYS
21	F	42	ILE
21	F	65	GLN
21	F	70	ILE
21	F	92	VAL
21	F	101	MET
21	F	109	LYS
21	F	114	ARG
21	F	116	VAL
21	F	150	ARG
21	F	158	ARG
21	F	162	VAL
21	F	187	ARG
21	F	188	ASN
21	F	192	ILE
21	F	196	LEU
21	F	220	GLU
21	F	221	ARG
22	K	20	VAL
22	K	21	LEU
22	K	35	ILE
22	K	40	LEU

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Mol	Chain	Res	Type
22	K	46	LEU
22	K	76	LEU
22	K	80	LEU
22	K	86	ILE
22	K	90	THR
23	M	43	LYS
23	M	45	LEU
23	M	55	LEU
23	M	69	GLN
23	M	105	LYS
23	M	107	VAL
24	P	17	TYR
24	P	32	ASP
24	P	40	ARG
24	P	43	ARG
24	P	52	LYS
24	P	57	MET
24	P	79	HIS
24	P	84	ILE
24	P	86	VAL
24	P	89	MET
24	P	106	GLU
24	P	121	ILE
24	P	127	ARG
25	Q	8	GLN
25	Q	13	LYS
25	Q	19	VAL
25	Q	52	LEU
25	Q	53	LEU
25	Q	66	ARG
25	Q	85	ILE
25	Q	98	ASP
25	Q	102	LYS
25	Q	105	LEU
25	Q	122	ARG
25	Q	125	GLU
25	Q	128	LYS
25	Q	132	ARG
25	Q	142	TYR
26	R	6	THR
26	R	7	LYS
26	R	16	LEU

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Mol	Chain	Res	Type
26	R	17	ILE
26	R	32	LYS
26	R	36	ASP
26	R	38	ILE
26	R	46	LEU
26	R	47	ARG
26	R	54	THR
26	R	66	VAL
26	R	74	GLN
26	R	84	TYR
26	R	88	VAL
26	R	98	ASP
26	R	100	LEU
26	R	109	LEU
27	S	12	GLN
27	S	16	ARG
27	S	25	ASN
27	S	34	THR
27	S	41	ARG
27	S	45	LEU
27	S	49	LYS
27	S	52	VAL
27	S	62	THR
27	S	74	GLN
27	S	85	PHE
27	S	88	ARG
27	S	91	ASP
27	S	126	ARG
27	S	128	PHE
27	S	131	LEU
27	S	137	HIS
27	S	144	ARG
28	T	7	ARG
28	T	36	ILE
28	T	44	GLU
28	T	57	ARG
28	T	63	ARG
28	T	79	LEU
28	T	86	ARG
28	T	122	ARG
28	T	124	ILE
28	T	129	LEU

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Mol	Chain	Res	Type
29	U	25	ASN
29	U	31	VAL
29	U	43	LYS
29	U	52	LYS
29	U	77	LYS
29	U	80	ASP
29	U	84	MET
29	U	85	ARG
29	U	86	ILE
29	U	92	ASP
29	U	94	GLU
29	U	103	ILE
29	U	114	VAL
29	U	118	ILE
30	Z	41	VAL
30	Z	60	VAL
30	Z	97	LYS
31	c	11	LYS
31	c	16	LEU
31	c	19	THR
31	c	25	VAL
31	c	53	ILE
31	c	56	LEU
32	d	19	ARG
32	d	20	GLN
32	d	21	CYS
32	d	36	LEU
32	d	37	ASN
32	d	40	ARG
32	d	50	ILE
33	f	82	LYS
33	f	103	LEU
33	f	105	TYR
33	f	113	LYS
33	f	120	GLU
33	f	136	ARG
34	g	22	THR
34	g	26	THR
34	g	35	VAL
34	g	40	ASP
34	g	52	GLU
34	g	60	ARG

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Mol	Chain	Res	Type
34	g	143	TYR
34	g	188	LEU
34	g	195	ILE
34	g	203	ASN
34	g	271	ASP
34	g	293	ASP
34	g	299	LEU
34	g	316	VAL
35	h	8	LYS
35	h	10	THR
35	h	12	ARG
36	i	31	GLU
36	i	39	THR
36	i	46	ARG
36	i	62	ARG
36	i	70	TRP
36	i	75	ASP
36	i	97	LEU
37	j	24	ASN
37	j	40	THR
37	j	53	ARG
37	j	71	ASP
37	j	87	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	30	GLN
2	A	33	GLN
2	A	92	HIS
2	A	109	ASN
3	B	124	ASN
3	B	149	GLN
3	B	183	GLN
4	C	64	HIS
5	E	50	ASN
5	E	57	ASN
5	E	142	HIS
5	E	216	ASN
5	E	224	ASN
6	G	4	ASN
6	G	81	HIS

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Mol	Chain	Res	Type
6	G	139	ASN
7	H	108	GLN
8	I	116	HIS
8	I	160	GLN
9	J	112	GLN
10	L	8	GLN
10	L	14	GLN
10	L	104	HIS
11	N	49	GLN
11	N	62	GLN
12	O	99	GLN
13	V	74	GLN
14	W	15	ASN
14	W	24	GLN
15	X	22	ASN
15	X	79	ASN
16	Y	15	ASN
16	Y	29	HIS
19	e	57	ASN
20	D	159	HIS
21	F	102	ASN
21	F	106	ASN
21	F	188	ASN
24	P	114	HIS
25	Q	74	HIS
25	Q	83	GLN
25	Q	94	GLN
27	S	27	ASN
27	S	99	HIS
27	S	136	GLN
28	T	70	GLN
30	Z	95	HIS
32	d	10	HIS
34	g	226	GLN
36	i	112	ASN
37	j	43	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1777/1799 (98%)	836 (47%)	132 (7%)



All (836) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	U
1	2	4	C
1	2	5	U
1	2	11	A
1	2	16	G
1	2	17	C
1	2	22	A
1	2	25	C
1	2	26	A
1	2	31	C
1	2	32	U
1	2	34	G
1	2	36	C
1	2	40	A
1	2	42	G
1	2	45	U
1	2	46	A
1	2	47	A
1	2	48	G
1	2	50	C
1	2	51	A
1	2	55	A
1	2	56	U
1	2	57	G
1	2	58	U
1	2	59	C
1	2	60	U
1	2	61	A
1	2	62	A
1	2	63	G
1	2	67	A
1	2	68	A
1	2	69	G
1	2	71	A
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	76	A
1	2	77	U
1	2	78	A

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Mol	Chain	Res	Type
1	2	79	C
1	2	80	A
1	2	81	G
1	2	84	A
1	2	86	A
1	2	90	C
1	2	93	A
1	2	104	A
1	2	105	A
1	2	109	G
1	2	111	U
1	2	114	C
1	2	115	G
1	2	123	G
1	2	124	A
1	2	125	U
1	2	126	A
1	2	127	G
1	2	129	U
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	137	U
1	2	139	C
1	2	140	A
1	2	141	U
1	2	142	G
1	2	143	G
1	2	144	A
1	2	145	U
1	2	146	A
1	2	147	U
1	2	148	C
1	2	150	G
1	2	154	U
1	2	157	U
1	2	158	U
1	2	159	C
1	2	160	U

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Mol	Chain	Res	Type
1	2	161	A
1	2	167	A
1	2	168	A
1	2	169	U
1	2	173	U
1	2	178	A
1	2	187	A
1	2	189	C
1	2	190	C
1	2	191	U
1	2	194	G
1	2	195	G
1	2	199	A
1	2	200	G
1	2	203	G
1	2	209	A
1	2	210	U
1	2	217	A
1	2	218	A
1	2	220	A
1	2	225	A
1	2	226	U
1	2	228	U
1	2	230	U
1	2	231	U
1	2	232	C
1	2	233	G
1	2	234	G
1	2	237	U
1	2	239	C
1	2	240	U
1	2	241	U
1	2	245	G
1	2	248	U
1	2	249	C
1	2	251	U
1	2	256	A
1	2	258	U
1	2	260	U
1	2	264	A
1	2	265	A
1	2	266	U

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Mol	Chain	Res	Type
1	2	270	A
1	2	272	G
1	2	273	G
1	2	275	C
1	2	276	U
1	2	278	G
1	2	279	U
1	2	280	G
1	2	282	U
1	2	287	A
1	2	288	U
1	2	289	G
1	2	292	U
1	2	294	A
1	2	298	A
1	2	300	A
1	2	301	U
1	2	308	C
1	2	311	A
1	2	313	C
1	2	314	A
1	2	315	A
1	2	318	U
1	2	319	U
1	2	320	C
1	2	321	G
1	2	322	A
1	2	328	G
1	2	332	A
1	2	336	G
1	2	337	C
1	2	345	G
1	2	347	U
1	2	349	U
1	2	351	A
1	2	358	A
1	2	359	A
1	2	360	C
1	2	362	G
1	2	368	A
1	2	369	A
1	2	371	G

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Mol	Chain	Res	Type
1	2	372	G
1	2	373	U
1	2	374	U
1	2	377	A
1	2	378	U
1	2	380	C
1	2	382	G
1	2	384	A
1	2	385	G
1	2	386	A
1	2	387	G
1	2	389	G
1	2	390	A
1	2	392	C
1	2	399	A
1	2	400	A
1	2	401	C
1	2	403	G
1	2	411	A
1	2	412	U
1	2	415	A
1	2	416	A
1	2	417	G
1	2	421	G
1	2	422	G
1	2	423	C
1	2	424	A
1	2	425	G
1	2	427	A
1	2	433	G
1	2	434	C
1	2	438	U
1	2	439	U
1	2	440	A
1	2	442	C
1	2	443	C
1	2	444	A
1	2	447	C
1	2	448	C
1	2	452	U
1	2	453	U
1	2	456	G

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Mol	Chain	Res	Type
1	2	458	G
1	2	459	A
1	2	460	G
1	2	467	A
1	2	468	C
1	2	469	A
1	2	473	A
1	2	474	A
1	2	476	A
1	2	477	A
1	2	478	C
1	2	479	G
1	2	480	A
1	2	481	U
1	2	483	C
1	2	489	C
1	2	491	A
1	2	492	U
1	2	493	U
1	2	495	G
1	2	496	G
1	2	499	C
1	2	502	G
1	2	504	A
1	2	505	A
1	2	506	U
1	2	507	U
1	2	508	G
1	2	512	U
1	2	513	G
1	2	514	A
1	2	515	G
1	2	516	U
1	2	517	A
1	2	518	C
1	2	521	U
1	2	522	G
1	2	523	U
1	2	524	A
1	2	525	A
1	2	526	A
1	2	532	U

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Mol	Chain	Res	Type
1	2	533	A
1	2	534	A
1	2	536	G
1	2	537	A
1	2	538	G
1	2	539	G
1	2	540	A
1	2	541	A
1	2	542	C
1	2	543	A
1	2	544	A
1	2	545	C
1	2	547	G
1	2	554	A
1	2	557	U
1	2	558	C
1	2	563	G
1	2	564	C
1	2	565	C
1	2	566	A
1	2	567	G
1	2	568	C
1	2	571	C
1	2	573	G
1	2	577	U
1	2	578	A
1	2	580	U
1	2	581	U
1	2	584	A
1	2	587	U
1	2	593	A
1	2	594	G
1	2	600	A
1	2	605	A
1	2	607	U
1	2	608	U
1	2	609	G
1	2	610	U
1	2	614	A
1	2	618	A
1	2	619	A
1	2	622	A

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Mol	Chain	Res	Type
1	2	623	G
1	2	628	U
1	2	634	A
1	2	635	A
1	2	637	U
1	2	638	U
1	2	640	G
1	2	641	G
1	2	642	G
1	2	646	G
1	2	648	U
1	2	649	U
1	2	651	U
1	2	653	C
1	2	654	G
1	2	655	G
1	2	656	U
1	2	657	C
1	2	684	A
1	2	687	C
1	2	691	U
1	2	692	C
1	2	693	U
1	2	694	U
1	2	695	U
1	2	696	C
1	2	697	C
1	2	698	U
1	2	701	U
1	2	702	G
1	2	704	C
1	2	705	U
1	2	706	A
1	2	707	A
1	2	709	C
1	2	710	U
1	2	712	U
1	2	714	C
1	2	715	U
1	2	717	C
1	2	718	U
1	2	719	U

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Mol	Chain	Res	Type
1	2	720	G
1	2	721	U
1	2	722	G
1	2	723	G
1	2	724	G
1	2	725	U
1	2	727	C
1	2	728	A
1	2	732	G
1	2	734	A
1	2	735	C
1	2	736	C
1	2	738	G
1	2	741	C
1	2	742	U
1	2	743	U
1	2	747	C
1	2	753	A
1	2	754	A
1	2	765	G
1	2	766	U
1	2	767	U
1	2	768	C
1	2	771	A
1	2	774	A
1	2	778	G
1	2	780	A
1	2	781	A
1	2	782	G
1	2	783	C
1	2	785	C
1	2	786	G
1	2	787	A
1	2	788	A
1	2	789	U
1	2	791	U
1	2	793	U
1	2	794	U
1	2	795	A
1	2	796	G
1	2	802	A
1	2	811	A

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Mol	Chain	Res	Type
1	2	812	U
1	2	813	A
1	2	814	G
1	2	817	C
1	2	818	G
1	2	819	U
1	2	820	U
1	2	821	U
1	2	822	G
1	2	825	U
1	2	827	U
1	2	828	A
1	2	829	U
1	2	830	U
1	2	831	U
1	2	832	U
1	2	837	G
1	2	839	U
1	2	840	U
1	2	843	A
1	2	845	G
1	2	853	U
1	2	855	A
1	2	857	G
1	2	860	U
1	2	861	A
1	2	862	A
1	2	863	U
1	2	872	U
1	2	875	G
1	2	876	G
1	2	881	U
1	2	889	C
1	2	895	U
1	2	896	C
1	2	897	A
1	2	904	A
1	2	905	A
1	2	907	U
1	2	908	U
1	2	910	U
1	2	912	G

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Mol	Chain	Res	Type
1	2	913	G
1	2	915	U
1	2	919	U
1	2	920	U
1	2	927	U
1	2	931	U
1	2	932	A
1	2	933	C
1	2	934	U
1	2	939	A
1	2	941	G
1	2	943	A
1	2	944	U
1	2	945	U
1	2	946	U
1	2	947	G
1	2	948	C
1	2	950	A
1	2	953	G
1	2	958	U
1	2	959	U
1	2	965	A
1	2	969	A
1	2	970	A
1	2	972	A
1	2	974	C
1	2	978	A
1	2	981	U
1	2	982	A
1	2	983	G
1	2	984	G
1	2	985	G
1	2	986	G
1	2	987	A
1	2	989	C
1	2	991	A
1	2	993	G
1	2	994	A
1	2	997	A
1	2	1002	A
1	2	1003	U
1	2	1011	U

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Mol	Chain	Res	Type
1	2	1015	C
1	2	1018	A
1	2	1019	A
1	2	1020	C
1	2	1022	A
1	2	1023	U
1	2	1024	A
1	2	1025	A
1	2	1026	A
1	2	1027	C
1	2	1028	U
1	2	1029	A
1	2	1030	U
1	2	1031	G
1	2	1033	C
1	2	1034	G
1	2	1038	A
1	2	1039	G
1	2	1041	G
1	2	1042	A
1	2	1048	U
1	2	1050	G
1	2	1051	U
1	2	1052	G
1	2	1057	U
1	2	1058	C
1	2	1059	U
1	2	1060	U
1	2	1062	U
1	2	1065	C
1	2	1071	C
1	2	1074	C
1	2	1075	A
1	2	1079	U
1	2	1080	A
1	2	1081	C
1	2	1082	G
1	2	1083	A
1	2	1085	A
1	2	1086	A
1	2	1090	A
1	2	1091	A

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Mol	Chain	Res	Type
1	2	1092	A
1	2	1095	C
1	2	1096	U
1	2	1097	U
1	2	1099	G
1	2	1100	G
1	2	1103	U
1	2	1108	G
1	2	1113	G
1	2	1115	A
1	2	1118	G
1	2	1119	U
1	2	1121	G
1	2	1125	G
1	2	1130	A
1	2	1133	C
1	2	1137	A
1	2	1141	A
1	2	1142	A
1	2	1145	G
1	2	1146	A
1	2	1149	G
1	2	1150	A
1	2	1152	G
1	2	1153	G
1	2	1157	C
1	2	1158	C
1	2	1161	C
1	2	1162	A
1	2	1165	A
1	2	1166	G
1	2	1167	U
1	2	1173	C
1	2	1174	U
1	2	1179	C
1	2	1181	U
1	2	1182	A
1	2	1184	U
1	2	1188	A
1	2	1189	C
1	2	1193	A
1	2	1194	C

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Mol	Chain	Res	Type
1	2	1195	A
1	2	1196	C
1	2	1198	G
1	2	1199	G
1	2	1201	A
1	2	1202	A
1	2	1203	A
1	2	1204	C
1	2	1205	U
1	2	1206	C
1	2	1207	A
1	2	1211	G
1	2	1212	G
1	2	1215	C
1	2	1216	A
1	2	1217	G
1	2	1218	A
1	2	1222	A
1	2	1223	A
1	2	1224	U
1	2	1225	A
1	2	1226	A
1	2	1227	G
1	2	1228	G
1	2	1229	A
1	2	1232	G
1	2	1234	C
1	2	1236	G
1	2	1237	A
1	2	1240	G
1	2	1241	A
1	2	1242	G
1	2	1243	A
1	2	1244	G
1	2	1249	U
1	2	1250	U
1	2	1254	G
1	2	1255	A
1	2	1256	U
1	2	1259	U
1	2	1263	G
1	2	1265	U

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Mol	Chain	Res	Type
1	2	1268	U
1	2	1269	G
1	2	1272	G
1	2	1274	A
1	2	1275	U
1	2	1282	U
1	2	1284	U
1	2	1287	G
1	2	1293	G
1	2	1294	G
1	2	1296	G
1	2	1305	C
1	2	1306	U
1	2	1311	A
1	2	1313	U
1	2	1314	U
1	2	1316	C
1	2	1317	G
1	2	1320	A
1	2	1321	A
1	2	1324	A
1	2	1336	A
1	2	1337	C
1	2	1339	U
1	2	1343	A
1	2	1344	A
1	2	1345	A
1	2	1346	U
1	2	1347	A
1	2	1348	G
1	2	1350	G
1	2	1351	U
1	2	1353	G
1	2	1355	U
1	2	1359	A
1	2	1360	C
1	2	1361	U
1	2	1362	U
1	2	1363	G
1	2	1364	C
1	2	1366	G
1	2	1369	U

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Mol	Chain	Res	Type
1	2	1370	G
1	2	1371	A
1	2	1380	A
1	2	1381	G
1	2	1383	G
1	2	1386	A
1	2	1387	C
1	2	1388	U
1	2	1391	C
1	2	1393	G
1	2	1396	U
1	2	1397	C
1	2	1398	A
1	2	1400	G
1	2	1410	G
1	2	1411	U
1	2	1412	U
1	2	1413	U
1	2	1416	G
1	2	1422	A
1	2	1425	A
1	2	1426	G
1	2	1428	U
1	2	1429	C
1	2	1430	U
1	2	1431	G
1	2	1432	U
1	2	1433	G
1	2	1434	A
1	2	1441	U
1	2	1442	A
1	2	1443	G
1	2	1444	A
1	2	1446	G
1	2	1449	C
1	2	1450	U
1	2	1455	C
1	2	1456	G
1	2	1457	C
1	2	1458	A
1	2	1460	G
1	2	1461	C

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Mol	Chain	Res	Type
1	2	1463	C
1	2	1464	G
1	2	1467	A
1	2	1469	A
1	2	1470	C
1	2	1471	U
1	2	1475	G
1	2	1476	G
1	2	1477	A
1	2	1484	G
1	2	1485	A
1	2	1487	U
1	2	1488	A
1	2	1489	C
1	2	1490	A
1	2	1491	A
1	2	1492	C
1	2	1494	U
1	2	1495	U
1	2	1498	C
1	2	1499	C
1	2	1502	G
1	2	1503	A
1	2	1504	G
1	2	1509	G
1	2	1510	G
1	2	1512	U
1	2	1513	A
1	2	1514	A
1	2	1515	U
1	2	1519	G
1	2	1521	G
1	2	1522	A
1	2	1527	C
1	2	1531	C
1	2	1534	G
1	2	1535	C
1	2	1536	U
1	2	1537	G
1	2	1539	G
1	2	1543	A
1	2	1544	G

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Mol	Chain	Res	Type
1	2	1548	A
1	2	1552	U
1	2	1554	A
1	2	1555	U
1	2	1557	A
1	2	1563	C
1	2	1566	C
1	2	1570	G
1	2	1571	A
1	2	1572	G
1	2	1573	G
1	2	1579	C
1	2	1580	U
1	2	1581	A
1	2	1582	G
1	2	1583	U
1	2	1588	G
1	2	1593	U
1	2	1594	C
1	2	1595	A
1	2	1597	C
1	2	1598	A
1	2	1599	G
1	2	1600	C
1	2	1602	U
1	2	1603	G
1	2	1605	G
1	2	1607	U
1	2	1612	A
1	2	1614	G
1	2	1617	C
1	2	1626	U
1	2	1633	A
1	2	1634	C
1	2	1636	G
1	2	1637	C
1	2	1638	C
1	2	1641	U
1	2	1646	A
1	2	1648	U
1	2	1650	C
1	2	1654	U

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Mol	Chain	Res	Type
1	2	1655	U
1	2	1656	G
1	2	1657	A
1	2	1658	A
1	2	1660	G
1	2	1662	C
1	2	1667	U
1	2	1674	U
1	2	1678	G
1	2	1679	A
1	2	1680	U
1	2	1682	U
1	2	1685	U
1	2	1686	U
1	2	1687	A
1	2	1688	G
1	2	1689	A
1	2	1692	A
1	2	1693	G
1	2	1694	G
1	2	1695	G
1	2	1696	G
1	2	1697	G
1	2	1698	C
1	2	1699	A
1	2	1700	A
1	2	1701	C
1	2	1702	U
1	2	1703	C
1	2	1704	C
1	2	1705	A
1	2	1706	U
1	2	1707	C
1	2	1709	C
1	2	1710	A
1	2	1711	G
1	2	1712	A
1	2	1724	G
1	2	1725	G
1	2	1728	A
1	2	1729	A
1	2	1730	A

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Mol	Chain	Res	Type
1	2	1733	U
1	2	1734	G
1	2	1737	C
1	2	1738	A
1	2	1740	U
1	2	1742	A
1	2	1743	G
1	2	1744	A
1	2	1747	A
1	2	1750	U
1	2	1753	A
1	2	1754	A
1	2	1755	G
1	2	1758	G
1	2	1759	U
1	2	1760	A
1	2	1763	A
1	2	1764	A
1	2	1765	G
1	2	1766	G
1	2	1767	U
1	2	1769	U
1	2	1770	C
1	2	1771	C
1	2	1778	G
1	2	1780	A
1	2	1781	C
1	2	1784	G
1	2	1787	G
1	2	1788	A
1	2	1789	A
1	2	1790	G
1	2	1791	G
1	2	1792	A
1	2	1793	U
1	2	1794	C
1	2	1796	U
1	2	1797	U

All (132) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	2	3	U
1	2	25	C
1	2	44	U
1	2	45	U
1	2	66	U
1	2	68	A
1	2	72	A
1	2	73	U
1	2	80	A
1	2	103	A
1	2	129	U
1	2	130	C
1	2	131	C
1	2	135	A
1	2	139	C
1	2	140	A
1	2	141	U
1	2	145	U
1	2	146	A
1	2	157	U
1	2	186	G
1	2	190	C
1	2	209	A
1	2	216	A
1	2	217	A
1	2	230	U
1	2	231	U
1	2	232	C
1	2	239	C
1	2	266	U
1	2	275	C
1	2	277	U
1	2	279	U
1	2	300	A
1	2	318	U
1	2	320	C
1	2	321	G
1	2	398	A
1	2	422	G
1	2	437	A
1	2	451	A

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Mol	Chain	Res	Type
1	2	452	U
1	2	453	U
1	2	497	G
1	2	538	G
1	2	542	C
1	2	564	C
1	2	566	A
1	2	577	U
1	2	593	A
1	2	695	U
1	2	700	C
1	2	704	C
1	2	720	G
1	2	721	U
1	2	724	G
1	2	737	A
1	2	740	A
1	2	742	U
1	2	747	C
1	2	809	G
1	2	812	U
1	2	818	G
1	2	827	U
1	2	828	A
1	2	839	U
1	2	854	A
1	2	896	C
1	2	907	U
1	2	912	G
1	2	1015	C
1	2	1025	A
1	2	1051	U
1	2	1056	U
1	2	1080	A
1	2	1081	C
1	2	1095	C
1	2	1099	G
1	2	1107	G
1	2	1149	G
1	2	1157	C
1	2	1161	C
1	2	1173	C

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Mol	Chain	Res	Type
1	2	1195	A
1	2	1203	A
1	2	1206	C
1	2	1216	A
1	2	1226	A
1	2	1241	A
1	2	1243	A
1	2	1244	G
1	2	1252	U
1	2	1255	A
1	2	1273	C
1	2	1315	G
1	2	1320	A
1	2	1343	A
1	2	1346	U
1	2	1380	A
1	2	1412	U
1	2	1424	C
1	2	1432	U
1	2	1445	C
1	2	1460	G
1	2	1469	A
1	2	1470	C
1	2	1491	A
1	2	1501	A
1	2	1515	U
1	2	1519	G
1	2	1521	G
1	2	1534	G
1	2	1535	C
1	2	1555	U
1	2	1556	U
1	2	1570	G
1	2	1571	A
1	2	1580	U
1	2	1598	A
1	2	1613	C
1	2	1632	C
1	2	1655	U
1	2	1678	G
1	2	1711	G
1	2	1725	G

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Mol	Chain	Res	Type
1	2	1743	G
1	2	1759	U
1	2	1765	G
1	2	1770	C
1	2	1778	G
1	2	1788	A
1	2	1792	A

## 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 70 ligands modelled in this entry, 70 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



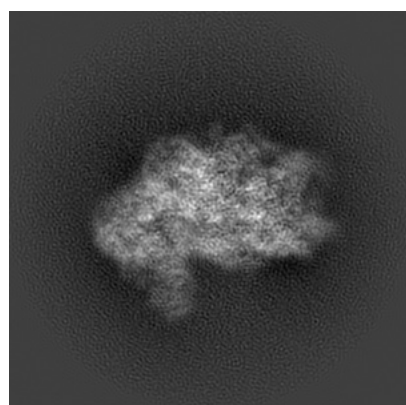
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2764. These allow visual inspection of the internal detail of the map and identification of artifacts.

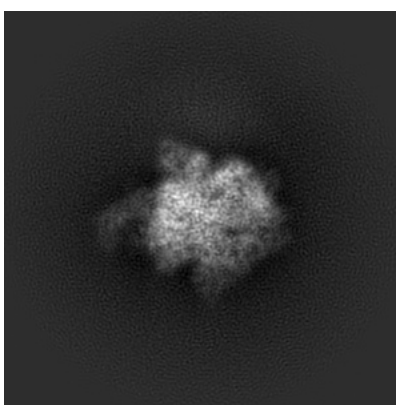
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

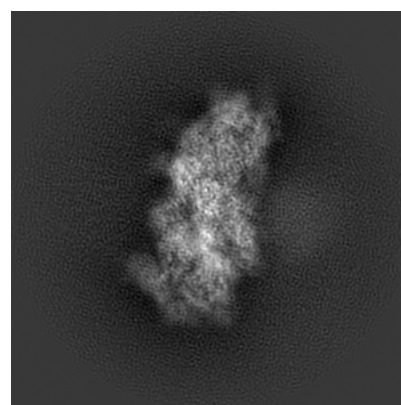
#### 6.1.1 Primary map



X



Y

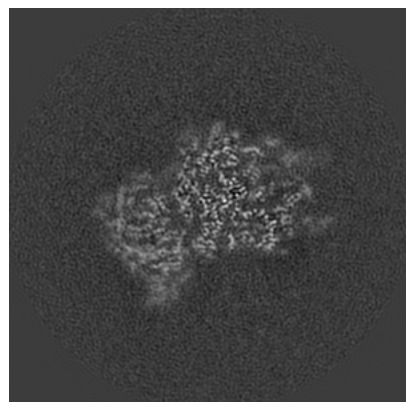


Z

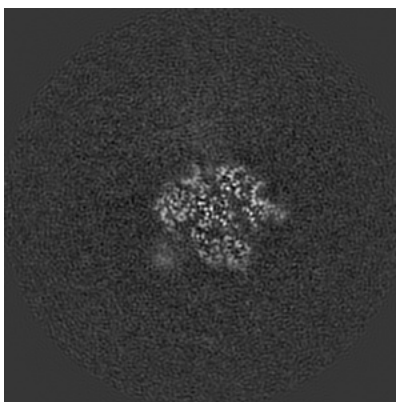
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

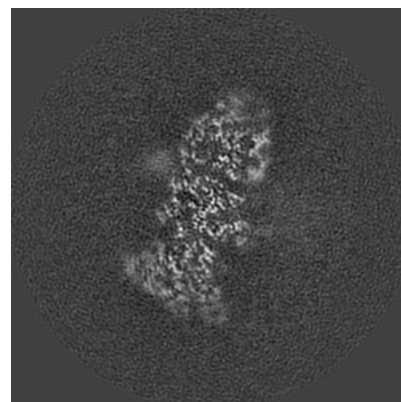
#### 6.2.1 Primary map



X Index: 150



Y Index: 150



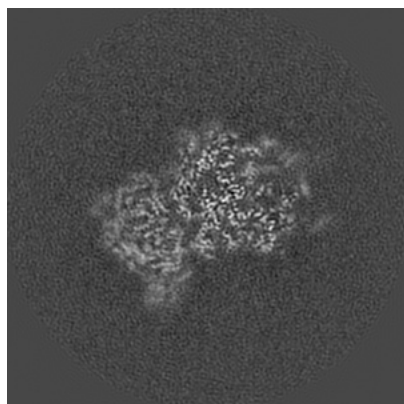
Z Index: 150



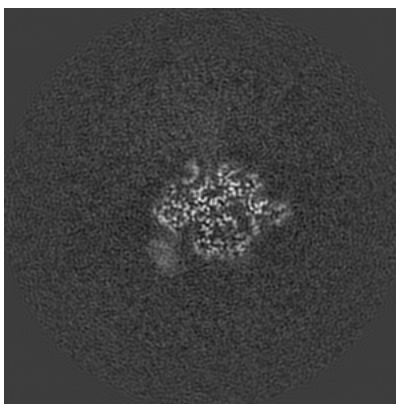
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

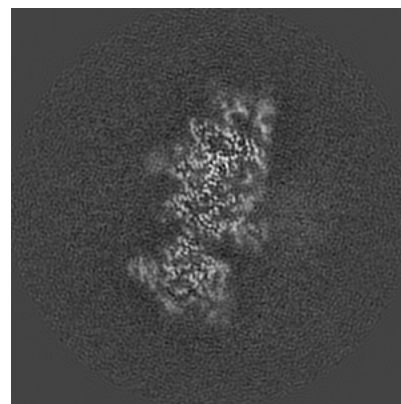
### 6.3.1 Primary map



X Index: 149



Y Index: 153



Z Index: 145

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

## 6.4 Orthogonal surface views [i](#)

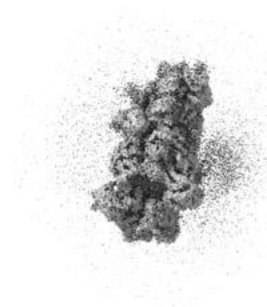
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



## 6.5 Mask visualisation

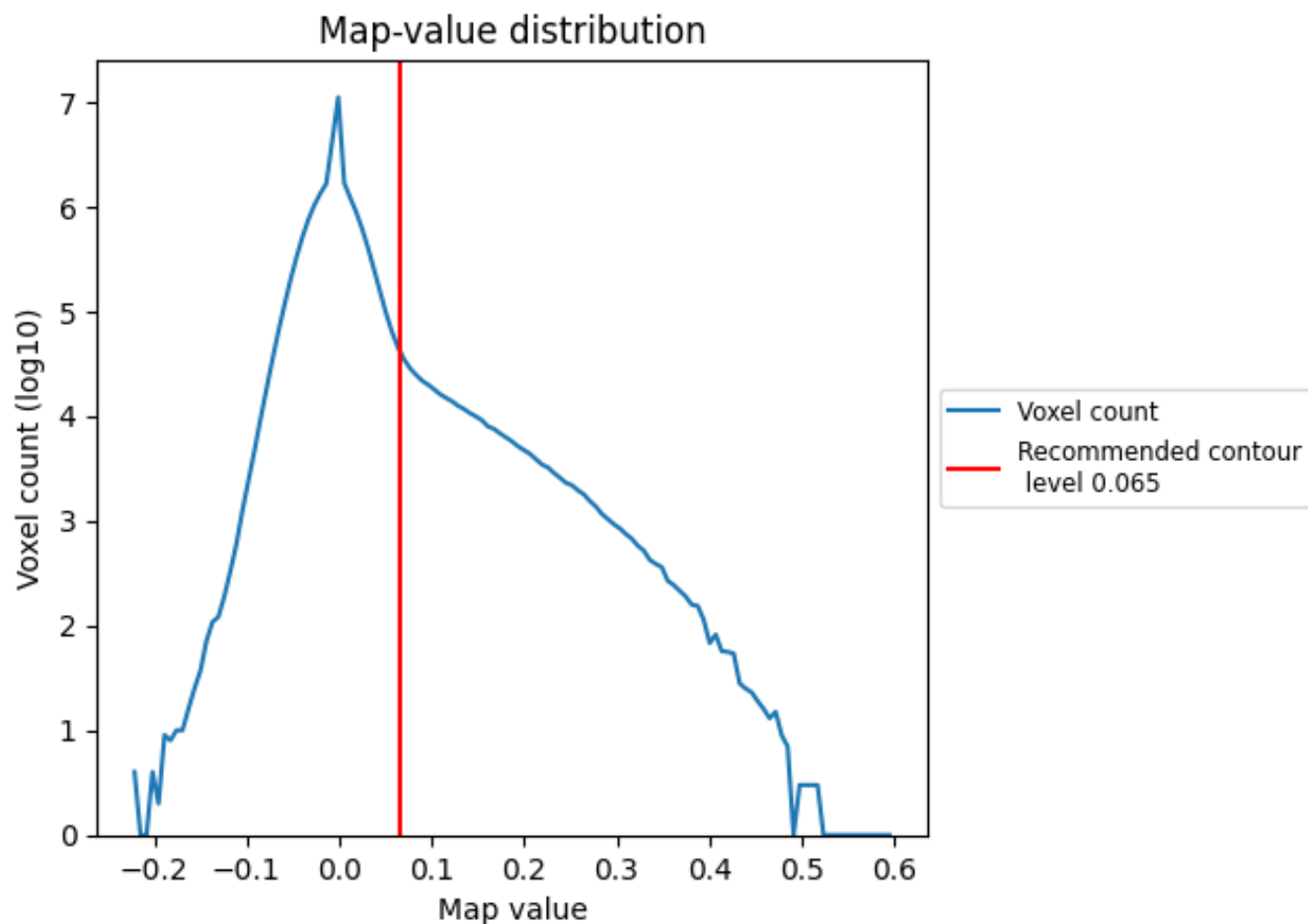
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

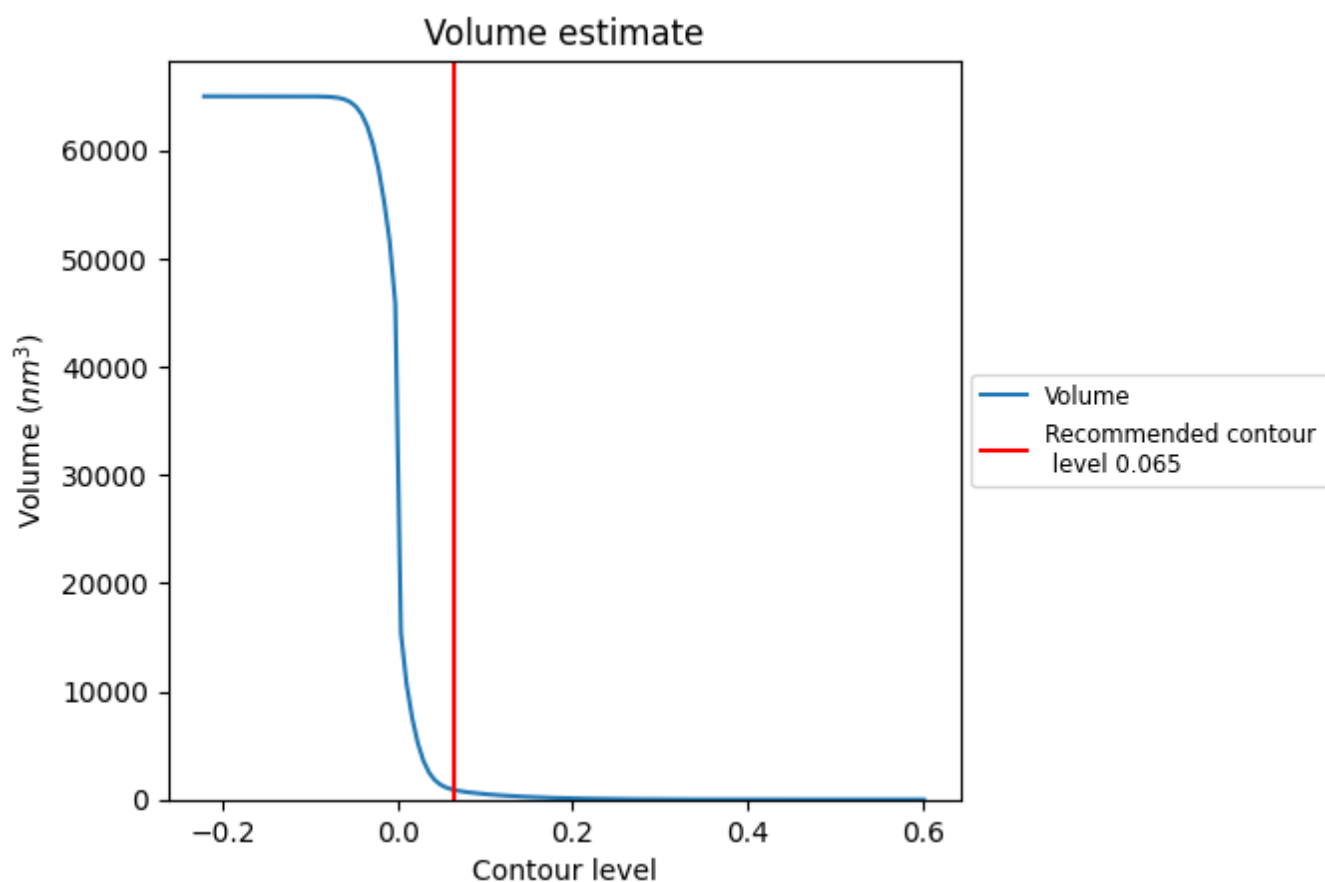
### 7.1 Map-value distribution [i](#)



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](#)

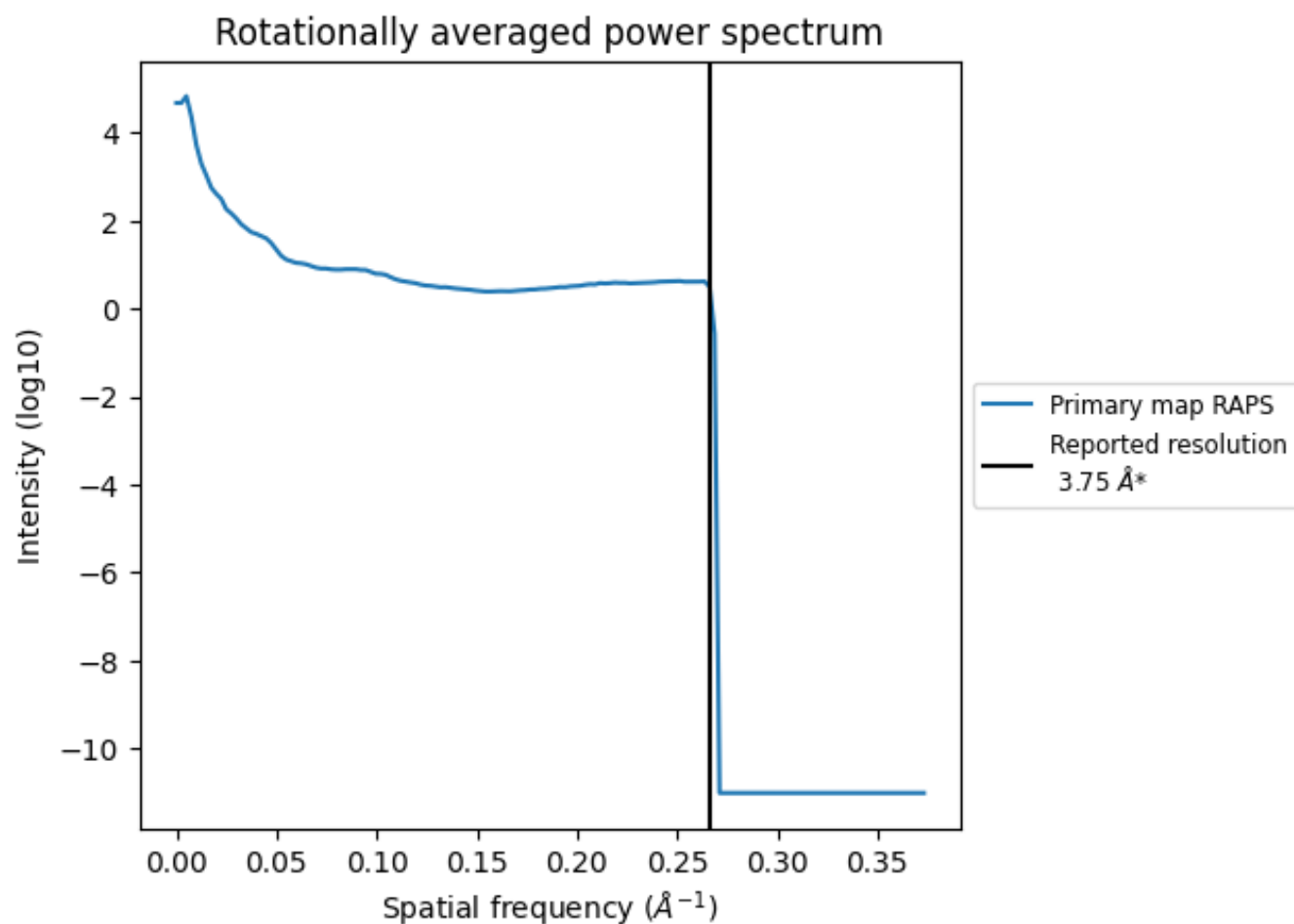


The volume at the recommended contour level is 888 nm<sup>3</sup>; this corresponds to an approximate mass of 802 kDa.

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 ⓘ



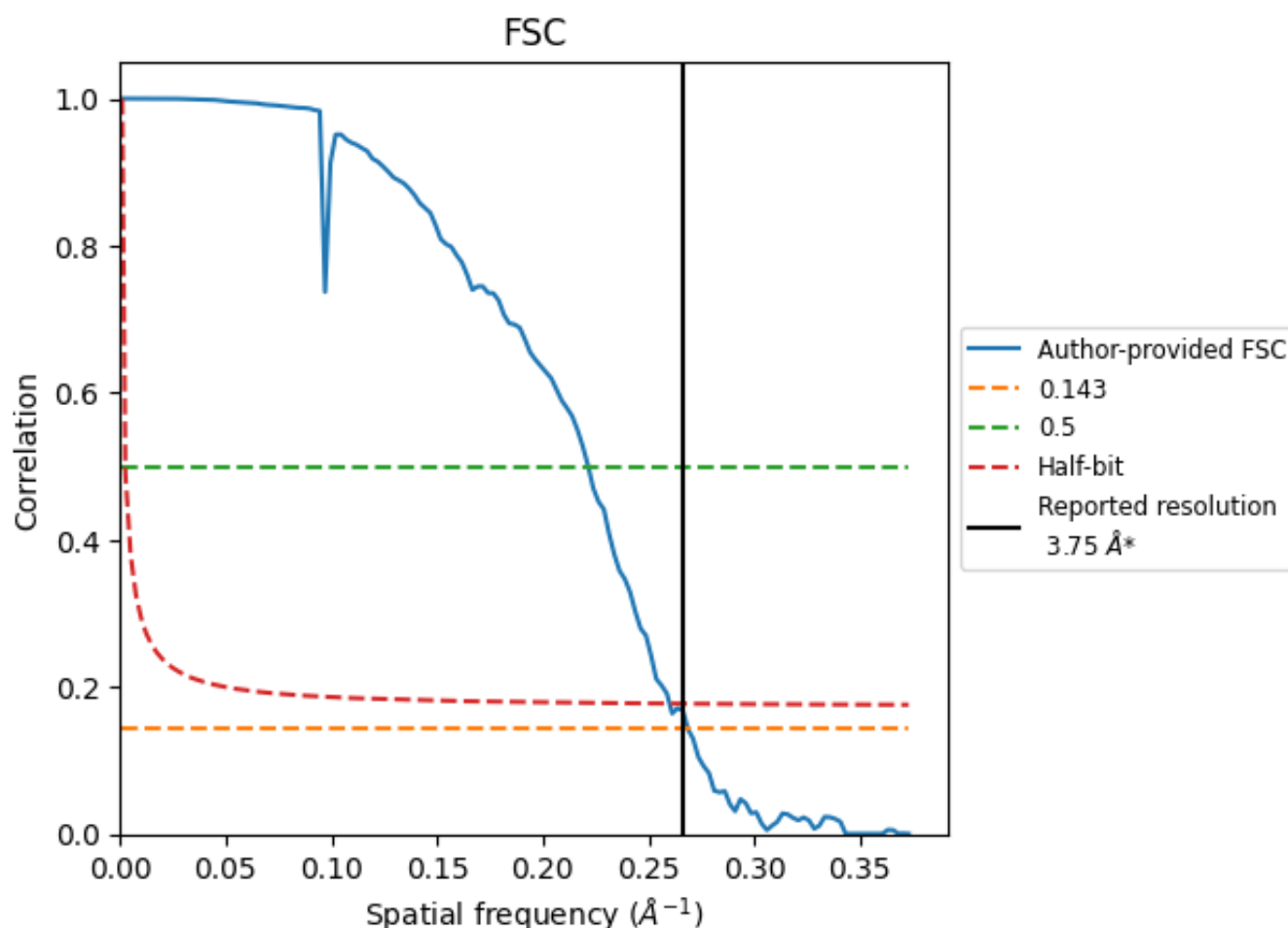
\*Reported resolution corresponds to spatial frequency of 0.267  $\text{\AA}^{-1}$



## 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  $0.267 \text{ \AA}^{-1}$



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.75	-	-
Author-provided FSC curve	3.72	4.51	3.85
Unmasked-calculated*	-	-	-

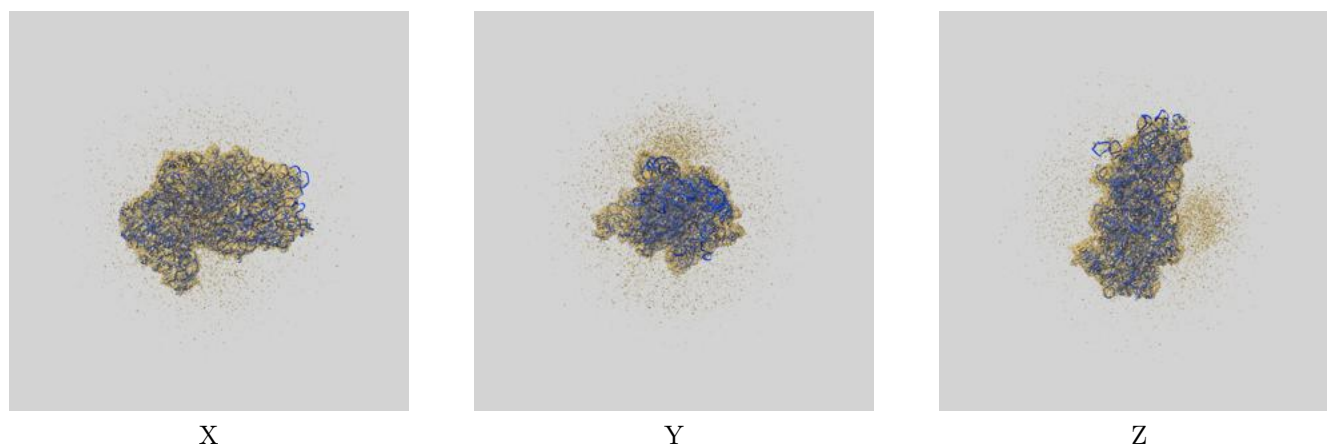
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2764 and PDB model 3J80. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

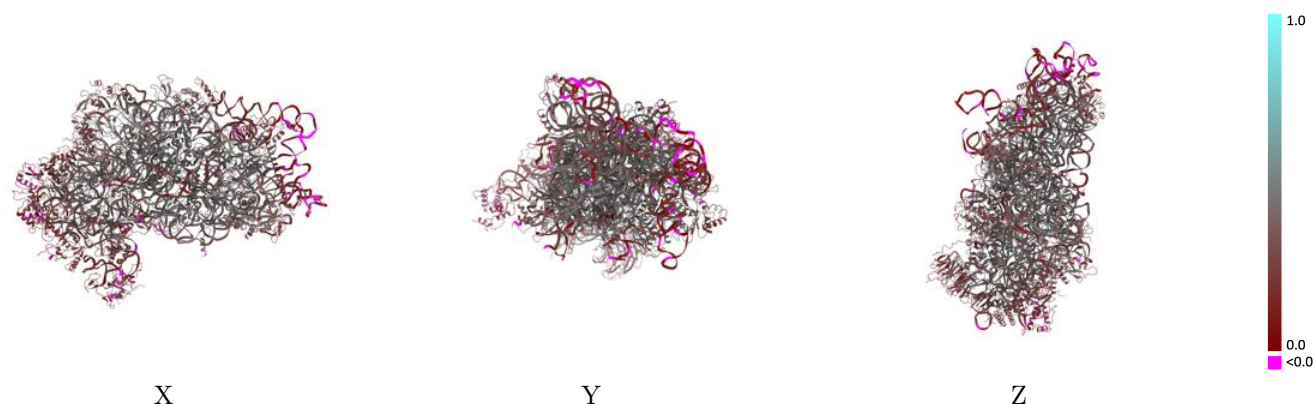
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.065 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.

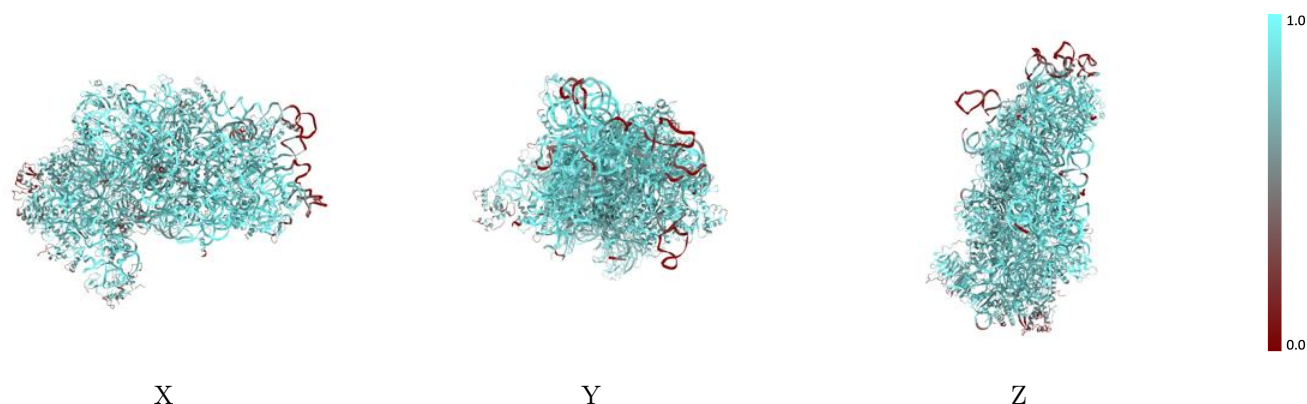


## 9.2 Q-score mapped to coordinate model [i](#)



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.

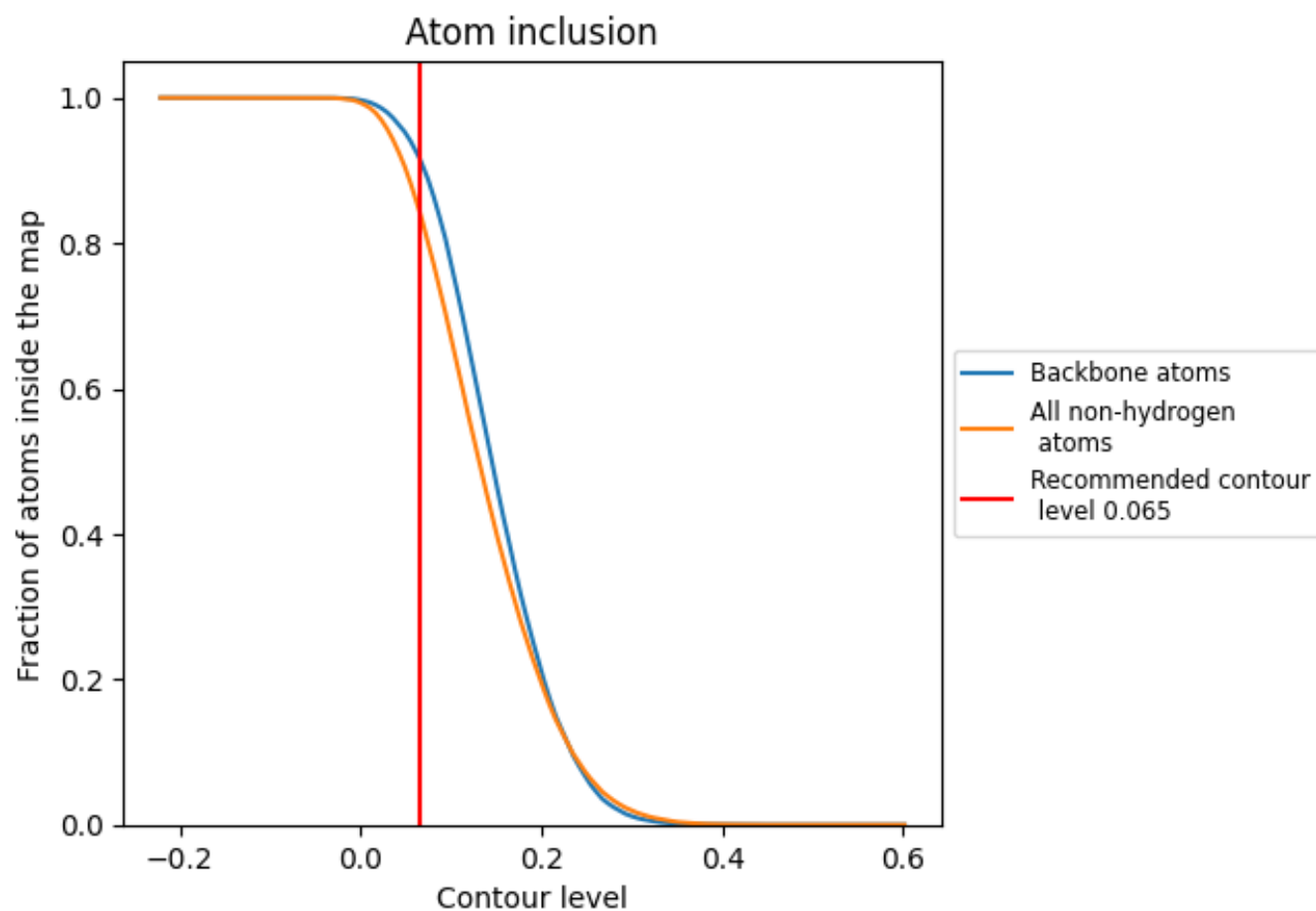
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.065).



## 9.4 Atom inclusion ⓘ









































































At the recommended contour level, 92% of all backbone atoms, 84% 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 (0.065) and Q-score for the entire model and for each chain.







Chain	Atom inclusion	Q-score
All	 0.8448	 0.3520
2	 0.9051	 0.3540
A	 0.8570	 0.3850
B	 0.8538	 0.3740
C	 0.8301	 0.4160
D	 0.7948	 0.3480
E	 0.8204	 0.4300
F	 0.7525	 0.3020
G	 0.8221	 0.3550
H	 0.8349	 0.3620
I	 0.8136	 0.3700
J	 0.8496	 0.4050
K	 0.7701	 0.3070
L	 0.7967	 0.4240
M	 0.5662	 0.1740
N	 0.8309	 0.3940
O	 0.8299	 0.3670
P	 0.6999	 0.2230
Q	 0.8009	 0.3540
R	 0.8096	 0.3420
S	 0.6331	 0.1820
T	 0.7556	 0.2730
U	 0.7687	 0.3710
V	 0.8276	 0.3890
W	 0.8720	 0.4450
X	 0.8883	 0.4490
Y	 0.8473	 0.3980
Z	 0.2818	 0.1170
a	 0.8657	 0.4390
b	 0.8605	 0.4120
c	 0.7722	 0.3420
d	 0.8689	 0.4280
e	 0.8068	 0.3920
f	 0.6926	 0.1990
g	 0.7808	 0.2890



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Chain	Atom inclusion	Q-score
h	 0.5425	 0.3260
i	 0.5329	 0.2640
j	 0.6925	 0.3040