



Full wwPDB EM Validation Report ⓘ

Dec 26, 2024 – 04:07 AM EST

PDB ID : 3J81
EMDB ID : EMD-2763
Title : CryoEM structure of a partial yeast 48S preinitiation complex
Authors : Hussain, T.; Llacer, J.L.; Fernandez, I.S.; Savva, C.G.; Ramakrishnan, V.
Deposited on : 2014-08-29
Resolution : 4.00 Å(reported)
Based on initial models : 3U5C, 3V11, 3U5B

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

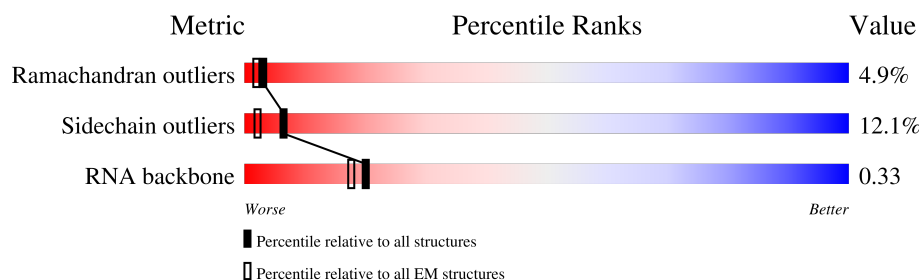
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.









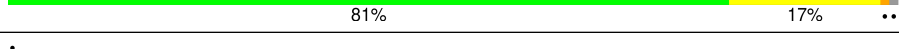
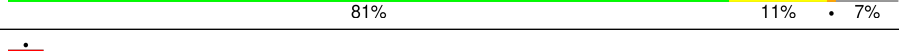
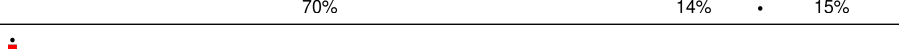
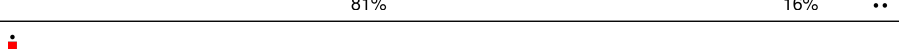
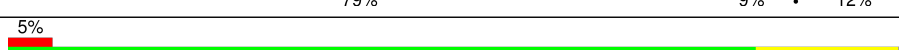

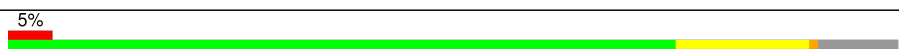

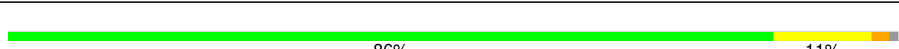





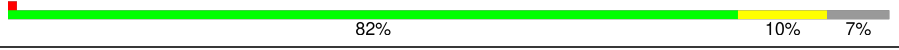




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	D	237	
6	E	261	
7	F	227	
8	G	236	


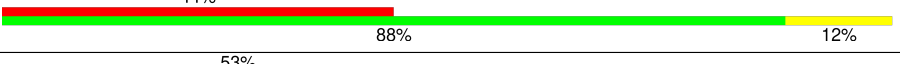

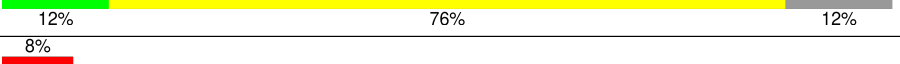



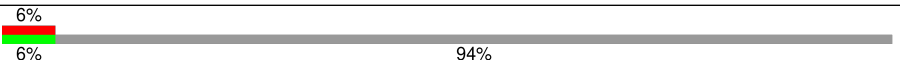

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Mol	Chain	Length	Quality of chain
9	H	190	
10	I	201	
11	J	188	
12	K	106	
13	L	156	
14	M	134	
15	N	151	
16	O	137	
17	P	140	
18	Q	143	
19	R	136	
20	S	146	
21	T	144	
22	U	117	
23	V	87	
24	W	130	
25	X	145	
26	Y	135	
27	Z	108	
28	a	119	
29	b	82	
30	c	67	
31	f	150	
32	g	326	
33	d	56	

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Mol	Chain	Length	Quality of chain
34	e	63	
35	h	25	
36	1	75	
37	3	25	
38	i	153	
39	j	300	
40	m	108	
41	k	527	
42	l	285	

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 83760 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	1780	Total	C	N	O	P	0	0
			37797	16892	6658	12467	1780		

- Molecule 2 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	207	Total	C	N	O	S	0	0
			1625	1040	286	297	2		

- Molecule 3 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	215	Total	C	N	O	S	0	0
			1727	1092	314	318	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 uS3.

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

- Molecule 6 is a protein called eS4.

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

- Molecule 7 is a protein called uS7.

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

- Molecule 8 is a protein called eS6.

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

- Molecule 9 is a protein called eS7.

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

- Molecule 10 is a protein called eS8.

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

- Molecule 11 is a protein called uS4.

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

- Molecule 12 is a protein called eS10.

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

- Molecule 13 is a protein called uS17.

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

- Molecule 14 is a protein called eS12.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	M	117	Total	C	N	O	0	0
			885	553	161	171		

- Molecule 15 is a protein called uS15.

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

- Molecule 16 is a protein called uS11.

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

- Molecule 17 is a protein called uS19.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	P	119	Total	C	N	O	S	0
			943	604	171	163	5	0

- Molecule 18 is a protein called uS9.

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

- Molecule 19 is a protein called eS17.

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

- Molecule 20 is a protein called uS13.

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

- Molecule 21 is a protein called eS19.

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

- Molecule 22 is a protein called uS10.

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

- Molecule 23 is a protein called eS21.

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

- Molecule 24 is a protein called uS8.

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

- Molecule 25 is a protein called uS12.

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

- Molecule 26 is a protein called eS24.

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

- Molecule 27 is a protein called eS25.

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

- Molecule 28 is a protein called eS26.

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

- Molecule 29 is a protein called eS27.

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

- Molecule 30 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	62	Total	C	N	O	S	0	0
			487	301	97	88	1		

- Molecule 31 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	69	Total	C	N	O	S	0	0
			546	351	101	90	4		

- Molecule 32 is a protein called RACK1.

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

- Molecule 33 is a protein called uS14.

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

- Molecule 34 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	54	Total	C	N	O	S	0	0
			433	271	88	73	1		

- 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 RNA chain called Met-tRNAi.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1	74	Total	C	N	O	P	0	0
			1584	706	291	513	74		

- Molecule 37 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	3	22	Total	C	N	O	P	0	0
			447	201	62	162	22		

- Molecule 38 is a protein called eIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	111	Total	C	N	O	S	0	0
			884	542	170	167	5		

- Molecule 39 is a protein called eIF2 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	252	Total	C	N	O	S	0	0
			2025	1294	336	386	9		

- Molecule 40 is a protein called eIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	m	90	Total	C	N	O	S	0	0
			716	452	132	128	4		

- Molecule 41 is a protein called eIF2 gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	365	Total	C	N	O		0	0
			1798	1068	365	365			

- Molecule 42 is a protein called eIF2 beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	1	17	Total	C	N	O	0	0
			84	50	17	17		

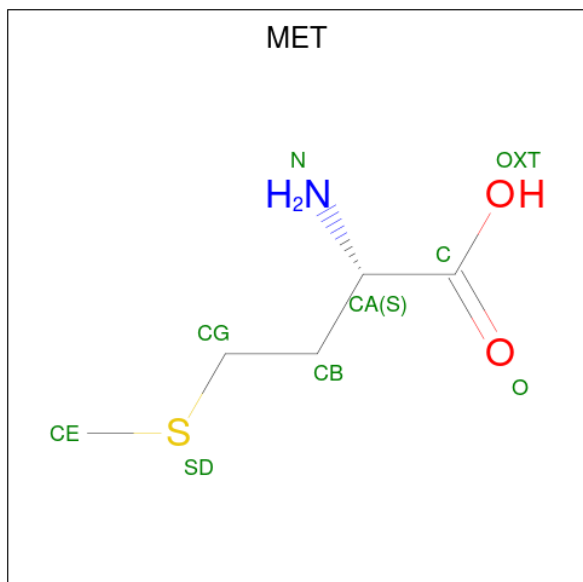
- Molecule 43 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
43	2	80	Total	Mg	0
			80	80	
43	G	1	Total	Mg	0
			1	1	

- Molecule 44 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 45 is METHIONINE (three-letter code: MET) (formula: C₅H₁₁NO₂S).



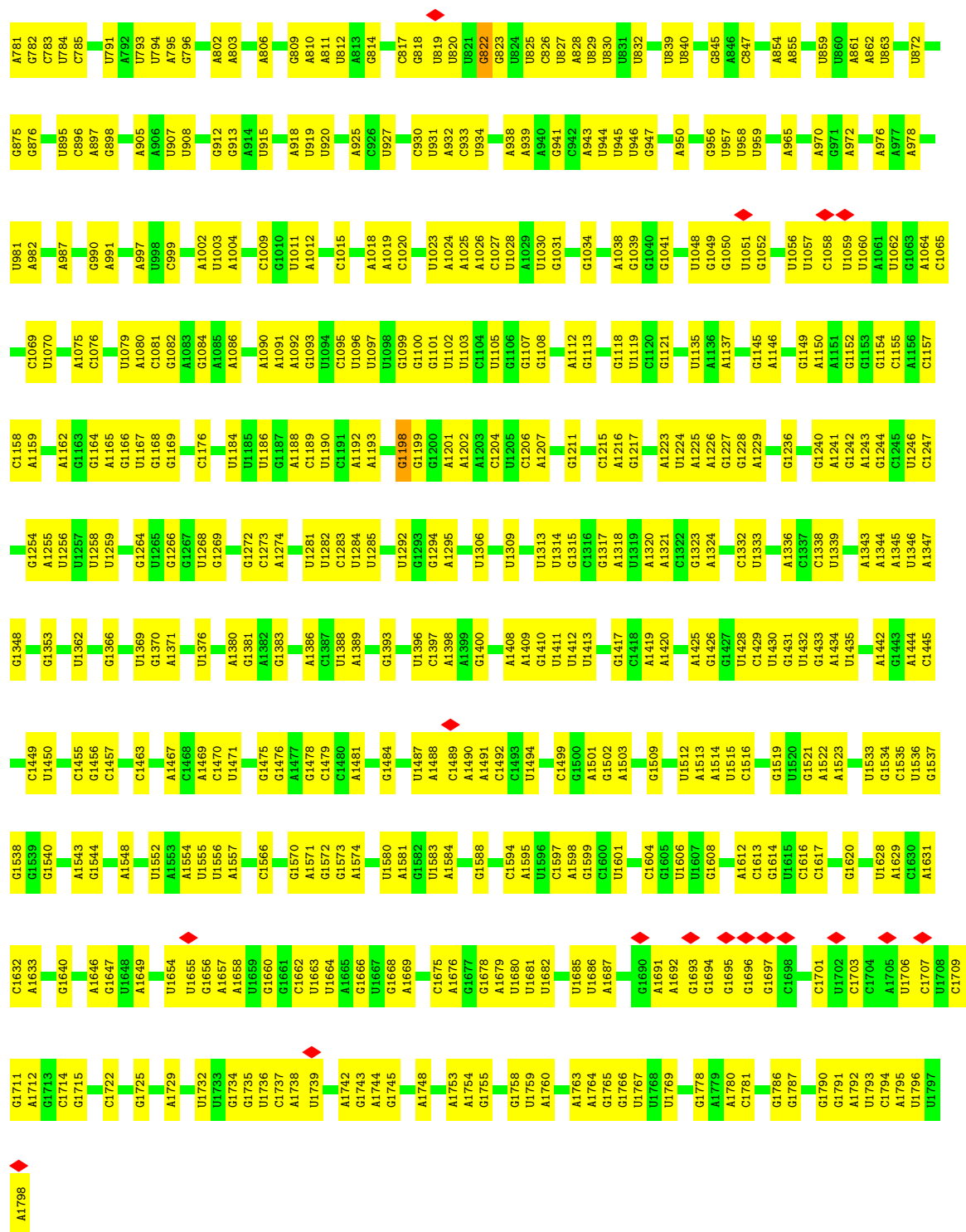
Mol	Chain	Residues	Atoms					AltConf
45	k	1	Total	C	N	O	S	0
			8	5	1	1	1	

3 Residue-property plots

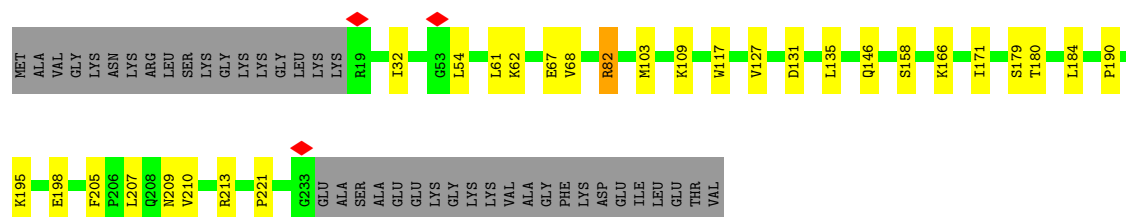
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

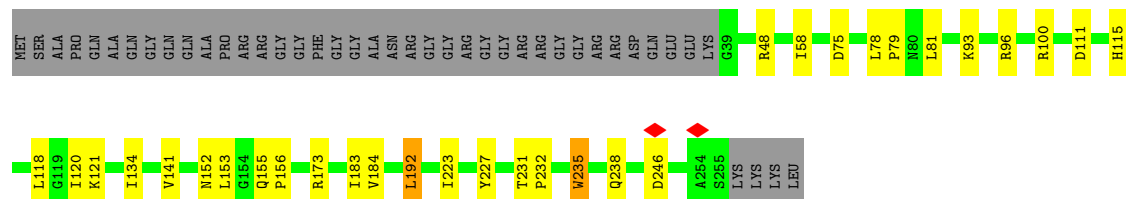




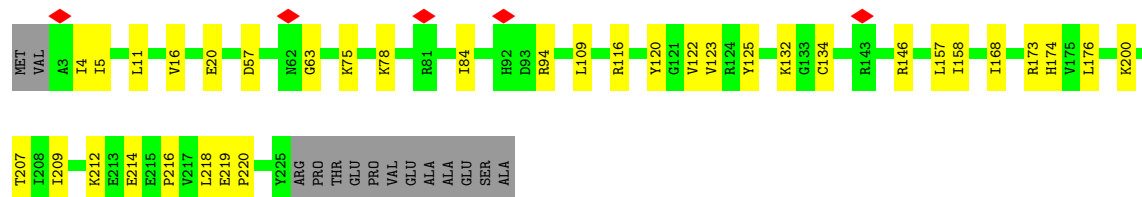
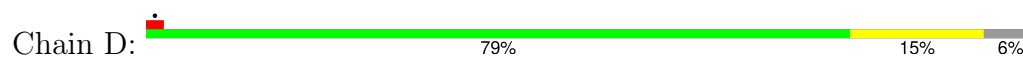
- Molecule 3: eS1



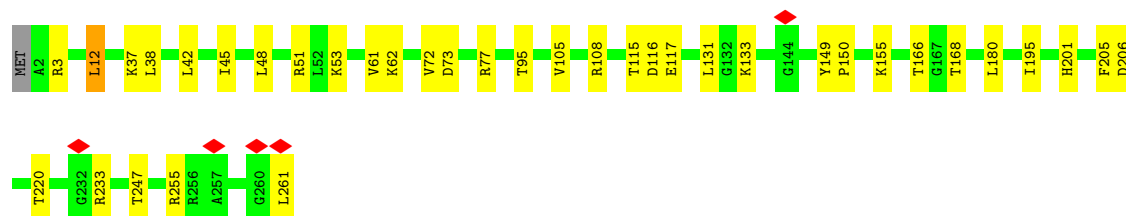
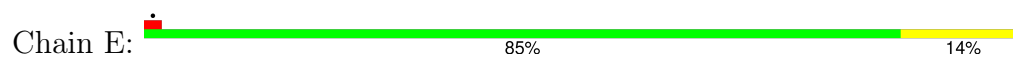
- Molecule 4: uS5



- Molecule 5: uS3

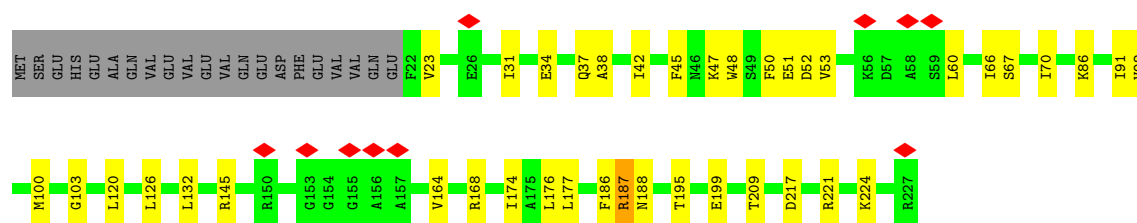


- Molecule 6: eS4




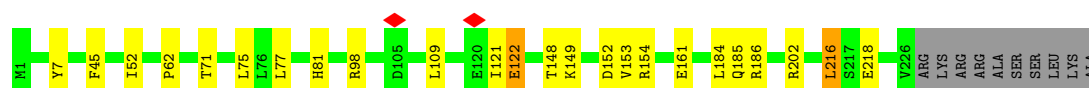
- Molecule 7: uS7

Chain F: 




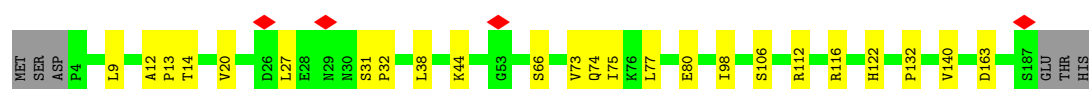
- Molecule 8: eS6

Chain G: 




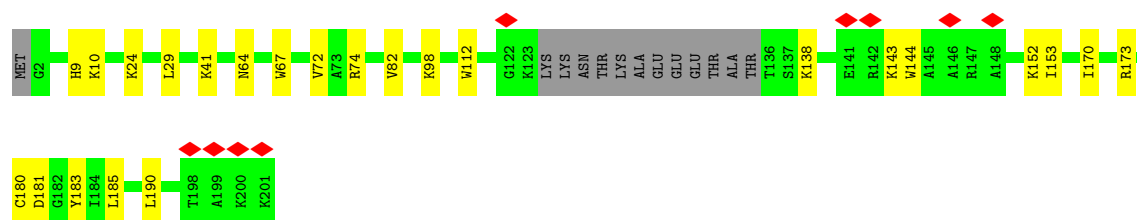
- Molecule 9: eS7

Chain H: 




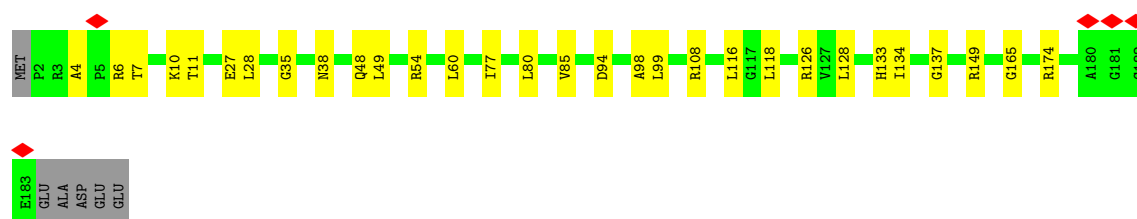
- Molecule 10: eS8

Chain I: 



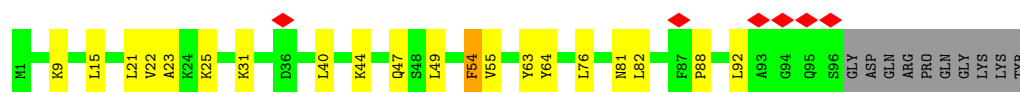
- Molecule 11: uS4

Chain J: 

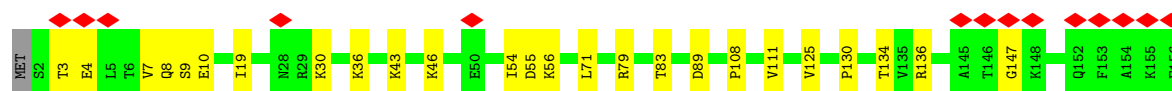
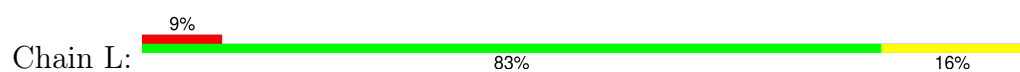


- Molecule 12: eS10

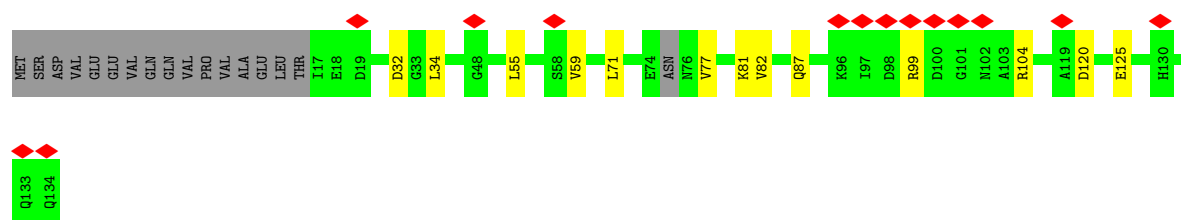
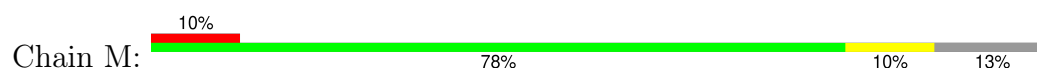
Chain K: 



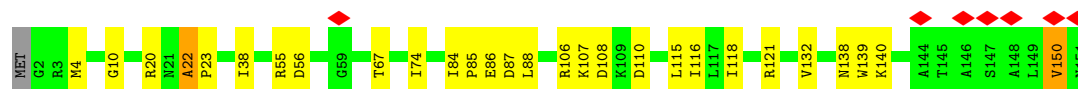
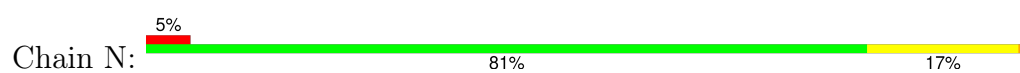
• Molecule 13: uS17



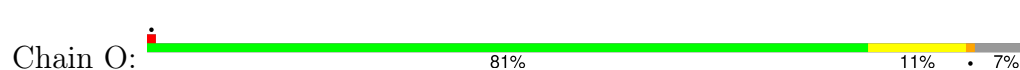
• Molecule 14: eS12



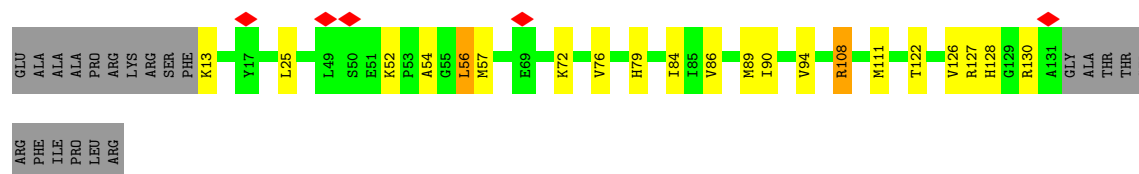
• Molecule 15: uS15



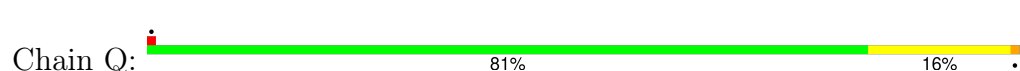
• Molecule 16: uS11

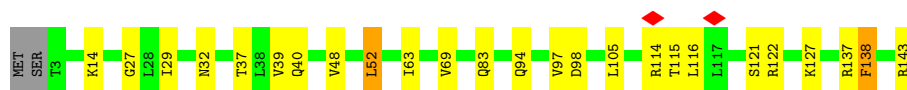


• Molecule 17: uS19

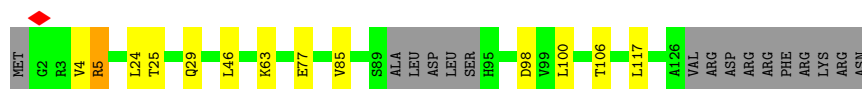
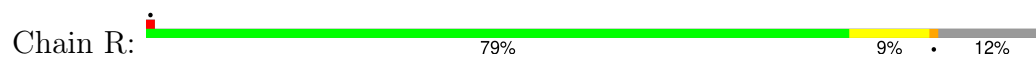


• Molecule 18: uS9

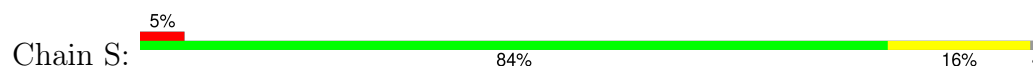




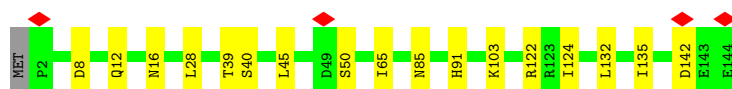
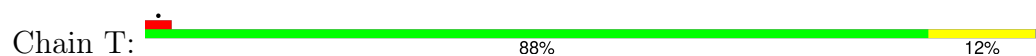
• Molecule 19: eS17



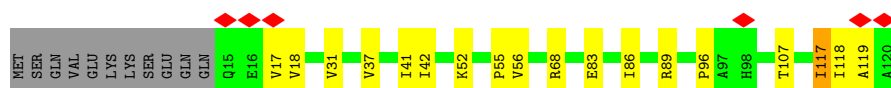
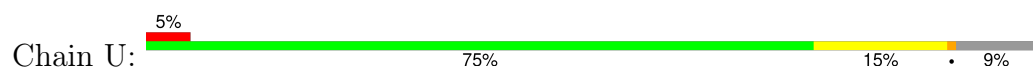
• Molecule 20: uS13



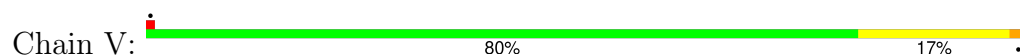
• Molecule 21: eS19



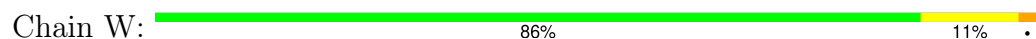
• Molecule 22: uS10



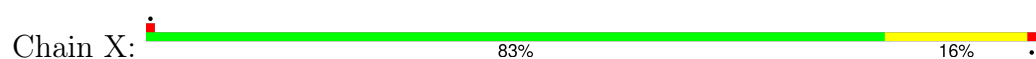
• Molecule 23: eS21



• Molecule 24: uS8

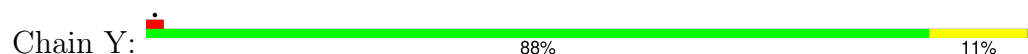


• Molecule 25: uS12

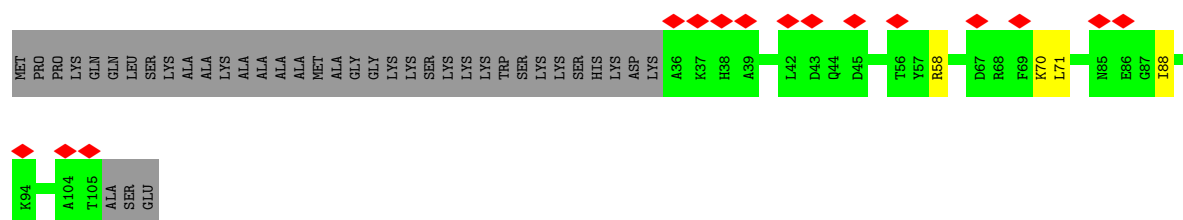




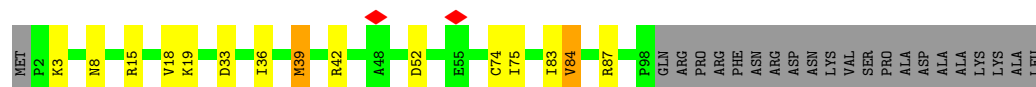
• Molecule 26: eS24



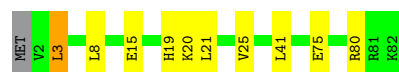
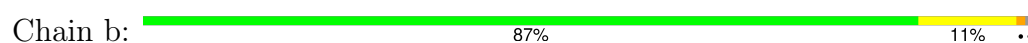
• Molecule 27: eS25



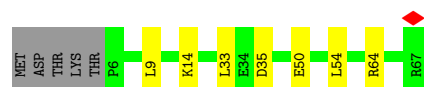
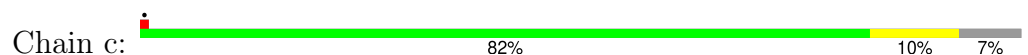
• Molecule 28: eS26



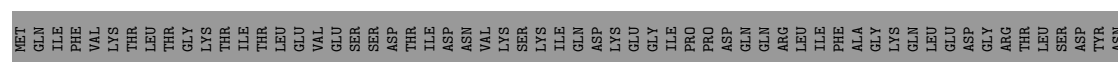
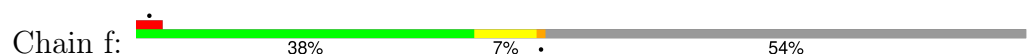
• Molecule 29: eS27



• Molecule 30: eS28



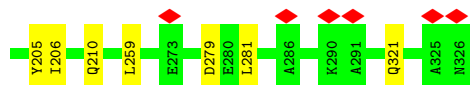
• Molecule 31: eS31





• Molecule 32: RACK1

Chain g: 88% 9%



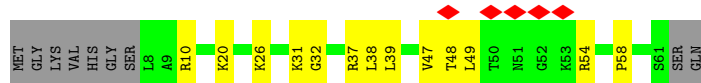
• Molecule 33: uS14

Chain d: 79% 16% 5%



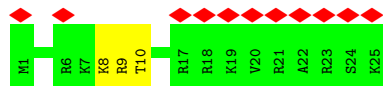
• Molecule 34: eS30

Chain e: 8% 65% 21% 14%



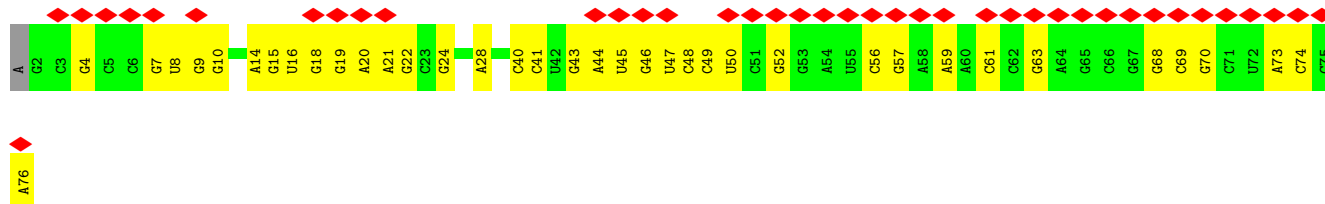
• Molecule 35: eL41

Chain h: 44% 88% 12%

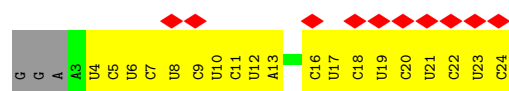


• Molecule 36: Met-tRNAi

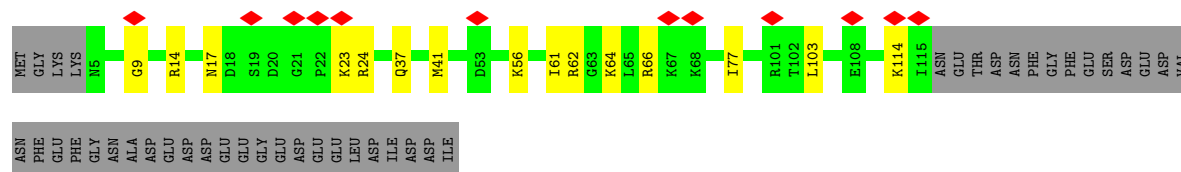
Chain 1: 53% 49% 49%



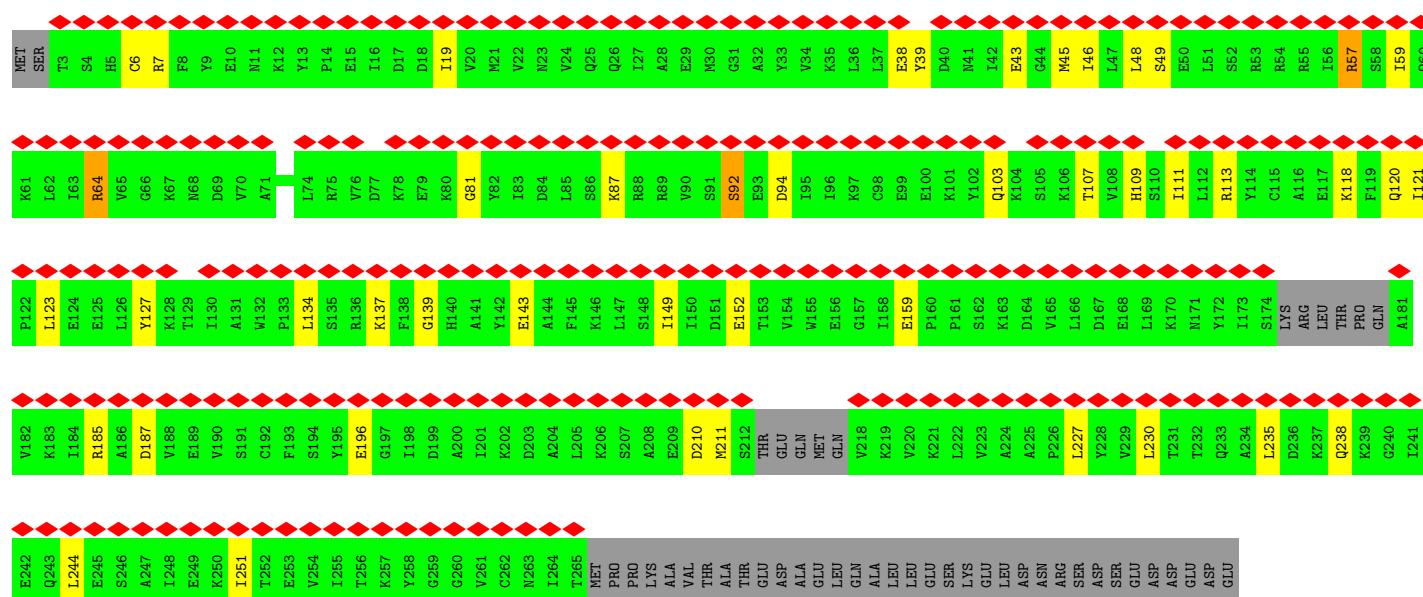
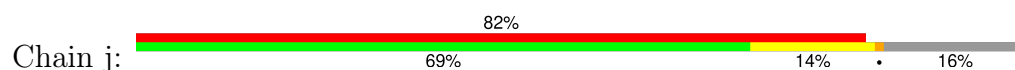
• Molecule 37: mRNA



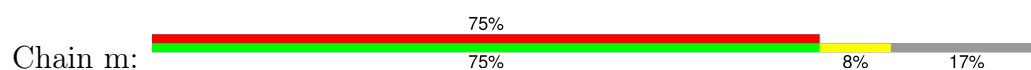
• Molecule 38: eIF1A



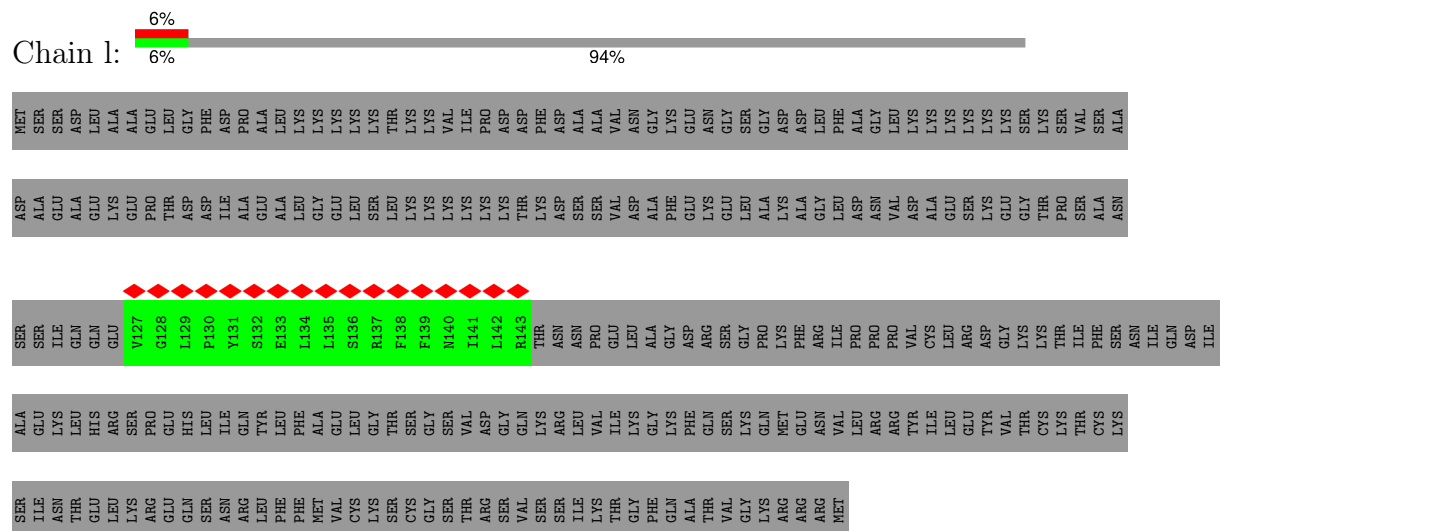
• Molecule 39: eIF2 alpha



• Molecule 40: eIF1



• Molecule 41: eIF2 gamma



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29698	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	0.467	Depositor
Minimum map value	-0.164	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.065	Depositor
Map size (\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 (\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	0.25	0/42269	0.67	6/65862 (0.0%)
2	A	0.42	0/1665	0.73	1/2276 (0.0%)
3	B	0.40	0/1752	0.67	1/2360 (0.0%)
4	C	0.39	0/1659	0.68	1/2252 (0.0%)
5	D	0.41	0/1769	0.69	0/2378
6	E	0.39	0/2122	0.66	2/2861 (0.1%)
7	F	0.41	0/1628	0.75	1/2198 (0.0%)
8	G	0.39	0/1835	0.66	2/2451 (0.1%)
9	H	0.40	0/1507	0.69	0/2028
10	I	0.40	0/1519	0.66	1/2033 (0.0%)
11	J	0.41	0/1495	0.73	0/2001
12	K	0.47	0/831	0.72	0/1123
13	L	0.40	0/1276	0.64	0/1718
14	M	0.41	0/891	0.69	0/1201
15	N	0.42	0/1210	0.75	1/1628 (0.1%)
16	O	0.38	0/953	0.67	0/1279
17	P	0.41	0/962	0.69	1/1294 (0.1%)
18	Q	0.42	0/1125	0.70	1/1510 (0.1%)
19	R	0.41	0/969	0.70	0/1299
20	S	0.40	0/1212	0.73	0/1629
21	T	0.39	0/1129	0.68	0/1520
22	U	0.39	0/857	0.66	0/1158
23	V	0.39	0/696	0.69	0/938
24	W	0.39	0/1039	0.69	0/1399
25	X	0.41	0/1137	0.71	0/1516
26	Y	0.38	0/1075	0.64	0/1433
27	Z	0.41	0/567	0.65	0/762
28	a	0.38	0/782	0.71	0/1047
29	b	0.38	0/619	0.66	0/837
30	c	0.36	0/489	0.67	0/655
31	f	0.43	0/559	0.70	1/747 (0.1%)
32	g	0.40	0/2521	0.61	0/3431

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.44	0/457	0.65	0/607
34	e	0.42	0/440	0.69	0/586
35	h	0.35	0/234	0.79	0/300
36	1	0.25	0/1771	0.65	0/2760
37	3	0.28	0/493	0.71	0/761
38	i	0.38	0/894	0.67	0/1188
39	j	0.41	0/2053	0.66	0/2762
40	m	0.39	0/724	0.65	0/968
41	k	0.47	1/1791 (0.1%)	0.74	1/2480 (0.0%)
42	l	0.42	0/83	0.69	0/114
All	All	0.34	1/89059 (0.0%)	0.67	20/129350 (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
10	I	0	1
15	N	0	1
25	X	0	1
41	k	0	2
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	k	497	GLU	N-CA	5.42	1.57	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	k	497	GLU	N-CA-C	8.38	133.61	111.00
1	2	685	A	C2'-C3'-O3'	7.22	125.38	109.50
17	P	56	LEU	CA-CB-CG	5.95	128.98	115.30
1	2	1198	G	C2'-C3'-O3'	5.93	123.19	113.70
4	C	192	LEU	CA-CB-CG	5.91	128.90	115.30
1	2	822	G	C2'-C3'-O3'	5.91	123.16	113.70
8	G	216	LEU	CA-CB-CG	5.82	128.70	115.30
6	E	38	LEU	CA-CB-CG	5.78	128.59	115.30
31	f	100	LEU	CA-CB-CG	5.75	128.51	115.30
1	2	279	U	C2'-C3'-O3'	5.64	122.72	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	693	U	C4'-C3'-O3'	5.60	124.20	113.00
2	A	59	LEU	CA-CB-CG	5.50	127.94	115.30
7	F	177	LEU	CA-CB-CG	5.49	127.93	115.30
3	B	184	LEU	CA-CB-CG	5.32	127.54	115.30
1	2	700	C	C2'-C3'-O3'	5.21	122.04	113.70
18	Q	52	LEU	CA-CB-CG	5.21	127.27	115.30
8	G	109	LEU	CA-CB-CG	5.17	127.20	115.30
6	E	42	LEU	CA-CB-CG	5.16	127.17	115.30
15	N	115	LEU	CA-CB-CG	5.08	126.98	115.30
10	I	29	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	I	183	TYR	Peptide
15	N	22	ALA	Peptide
25	X	63	GLN	Peptide
41	k	179	CYS	Peptide
41	k	495	ILE	Mainchain

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	205/254 (81%)	168 (82%)	26 (13%)	11 (5%)	1	19
3	B	213/255 (84%)	176 (83%)	23 (11%)	14 (7%)	1	15
4	C	215/259 (83%)	182 (85%)	23 (11%)	10 (5%)	2	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	D	221/237 (93%)	202 (91%)	13 (6%)	6 (3%)	4	29
6	E	258/261 (99%)	223 (86%)	25 (10%)	10 (4%)	2	23
7	F	204/227 (90%)	169 (83%)	24 (12%)	11 (5%)	1	19
8	G	224/236 (95%)	194 (87%)	24 (11%)	6 (3%)	4	29
9	H	182/190 (96%)	145 (80%)	23 (13%)	14 (8%)	1	13
10	I	184/201 (92%)	159 (86%)	21 (11%)	4 (2%)	5	32
11	J	180/188 (96%)	150 (83%)	21 (12%)	9 (5%)	1	19
12	K	94/106 (89%)	74 (79%)	12 (13%)	8 (8%)	0	11
13	L	153/156 (98%)	128 (84%)	16 (10%)	9 (6%)	1	17
14	M	113/134 (84%)	86 (76%)	21 (19%)	6 (5%)	1	19
15	N	148/151 (98%)	127 (86%)	11 (7%)	10 (7%)	1	15
16	O	125/137 (91%)	96 (77%)	24 (19%)	5 (4%)	2	22
17	P	117/140 (84%)	95 (81%)	15 (13%)	7 (6%)	1	16
18	Q	139/143 (97%)	115 (83%)	13 (9%)	11 (8%)	1	12
19	R	116/136 (85%)	101 (87%)	11 (10%)	4 (3%)	3	25
20	S	143/146 (98%)	119 (83%)	16 (11%)	8 (6%)	1	18
21	T	141/144 (98%)	129 (92%)	9 (6%)	3 (2%)	5	33
22	U	104/117 (89%)	88 (85%)	8 (8%)	8 (8%)	1	13
23	V	85/87 (98%)	69 (81%)	9 (11%)	7 (8%)	1	11
24	W	127/130 (98%)	107 (84%)	14 (11%)	6 (5%)	2	20
25	X	142/145 (98%)	111 (78%)	22 (16%)	9 (6%)	1	16
26	Y	132/135 (98%)	115 (87%)	13 (10%)	4 (3%)	3	27
27	Z	68/108 (63%)	58 (85%)	9 (13%)	1 (2%)	8	40
28	a	95/119 (80%)	71 (75%)	17 (18%)	7 (7%)	1	13
29	b	79/82 (96%)	65 (82%)	11 (14%)	3 (4%)	2	23
30	c	60/67 (90%)	55 (92%)	4 (7%)	1 (2%)	7	37
31	f	67/150 (45%)	47 (70%)	14 (21%)	6 (9%)	0	11
32	g	312/326 (96%)	270 (86%)	32 (10%)	10 (3%)	3	26
33	d	51/56 (91%)	39 (76%)	10 (20%)	2 (4%)	2	23
34	e	52/63 (82%)	40 (77%)	8 (15%)	4 (8%)	1	13
35	h	23/25 (92%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	i	109/153 (71%)	90 (83%)	16 (15%)	3 (3%)	4	28
39	j	246/300 (82%)	213 (87%)	21 (8%)	12 (5%)	2	19
40	m	88/108 (82%)	80 (91%)	6 (7%)	2 (2%)	5	32
41	k	351/527 (67%)	270 (77%)	56 (16%)	25 (7%)	1	14
42	l	15/285 (5%)	11 (73%)	4 (27%)	0	100	100
All	All	5581/6684 (84%)	4660 (84%)	645 (12%)	276 (5%)	3	19

All (276) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	29	VAL
4	C	96	ARG
4	C	141	VAL
4	C	235	TRP
5	D	4	ILE
5	D	216	PRO
5	D	220	PRO
7	F	38	ALA
8	G	122	GLU
9	H	31	SER
9	H	132	PRO
11	J	4	ALA
11	J	85	VAL
12	K	82	LEU
12	K	88	PRO
13	L	3	THR
14	M	82	VAL
15	N	23	PRO
15	N	86	GLU
15	N	150	VAL
16	O	42	VAL
16	O	132	ARG
17	P	126	VAL
18	Q	39	VAL
18	Q	97	VAL
19	R	85	VAL
20	S	40	ARG
21	T	50	SER
22	U	96	PRO
23	V	12	TYR

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Mol	Chain	Res	Type
25	X	63	GLN
25	X	64	PRO
25	X	139	LYS
28	a	18	VAL
29	b	20	LYS
31	f	102	VAL
33	d	23	ILE
34	e	47	VAL
38	i	64	LYS
39	j	57	ARG
39	j	92	SER
39	j	94	ASP
39	j	120	GLN
41	k	175	GLN
41	k	177	PRO
41	k	224	CYS
41	k	240	LYS
41	k	270	ILE
41	k	276	ASP
41	k	410	ASP
41	k	424	PRO
41	k	507	LYS
41	k	515	ALA
2	A	31	VAL
2	A	158	VAL
3	B	180	THR
3	B	213	ARG
4	C	111	ASP
4	C	183	ILE
6	E	12	LEU
6	E	73	ASP
7	F	67	SER
7	F	100	MET
7	F	103	GLY
8	G	153	VAL
9	H	32	PRO
9	H	75	ILE
9	H	163	ASP
10	I	98	LYS
10	I	152	LYS
10	I	153	ILE
11	J	35	GLY

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Mol	Chain	Res	Type
12	K	23	ALA
12	K	54	PHE
12	K	81	ASN
13	L	9	SER
13	L	55	ASP
15	N	10	GLY
16	O	32	ASP
16	O	124	ASP
17	P	54	ALA
18	Q	116	LEU
18	Q	138	PHE
20	S	28	VAL
20	S	102	ALA
22	U	117	ILE
23	V	82	VAL
28	a	84	VAL
31	f	93	HIS
32	g	147	GLY
34	e	32	GLY
38	i	17	ASN
40	m	85	ARG
41	k	136	ILE
41	k	181	GLY
41	k	223	SER
2	A	103	THR
2	A	109	ASN
2	A	124	THR
3	B	54	LEU
3	B	117	TRP
3	B	158	SER
3	B	207	LEU
4	C	152	ASN
6	E	3	ARG
6	E	77	ARG
6	E	205	PHE
7	F	66	ILE
9	H	12	ALA
9	H	66	SER
9	H	106	SER
10	I	10	LYS
11	J	98	ALA
11	J	99	LEU

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Mol	Chain	Res	Type
11	J	165	GLY
12	K	64	TYR
13	L	4	GLU
13	L	30	LYS
13	L	147	GLY
14	M	81	LYS
14	M	99	ARG
14	M	120	ASP
15	N	108	ASP
16	O	90	ARG
17	P	90	ILE
18	Q	14	LYS
18	Q	40	GLN
18	Q	115	THR
20	S	7	GLU
20	S	51	ASP
20	S	82	PRO
22	U	55	PRO
23	V	7	GLN
23	V	30	SER
23	V	81	ASN
24	W	29	PRO
24	W	32	LYS
26	Y	52	LYS
28	a	8	ASN
28	a	15	ARG
28	a	39	MET
28	a	75	ILE
29	b	3	LEU
29	b	75	GLU
32	g	4	SER
32	g	16	GLY
32	g	52	GLU
32	g	130	LYS
32	g	201	GLY
32	g	205	TYR
34	e	26	LYS
39	j	48	LEU
39	j	49	SER
39	j	64	ARG
40	m	73	GLU
41	k	172	PRO

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Mol	Chain	Res	Type
41	k	198	ASP
41	k	213	ALA
41	k	302	ILE
2	A	35	PRO
3	B	61	LEU
3	B	62	LYS
3	B	209	ASN
4	C	79	PRO
4	C	155	GLN
5	D	78	LYS
5	D	219	GLU
6	E	195	ILE
7	F	52	ASP
8	G	154	ARG
9	H	44	LYS
9	H	73	VAL
9	H	112	ARG
11	J	137	GLY
12	K	25	LYS
13	L	130	PRO
14	M	32	ASP
14	M	77	VAL
15	N	4	MET
15	N	138	ASN
17	P	108	ARG
17	P	128	HIS
18	Q	27	GLY
18	Q	32	ASN
18	Q	121	SER
19	R	5	ARG
19	R	24	LEU
19	R	98	ASP
20	S	87	ASN
22	U	17	VAL
22	U	89	ARG
22	U	119	ALA
23	V	74	GLN
25	X	3	LYS
25	X	41	SER
25	X	97	ASP
25	X	138	GLU
26	Y	5	ILE

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Mol	Chain	Res	Type
26	Y	36	SER
28	a	36	ILE
31	f	85	TYR
31	f	94	LYS
31	f	111	GLU
32	g	64	GLY
38	i	9	GLY
41	k	135	ASN
41	k	179	CYS
41	k	227	PRO
2	A	26	ALA
2	A	189	PRO
2	A	204	TYR
2	A	206	ASN
3	B	82	ARG
3	B	179	SER
5	D	63	GLY
6	E	150	PRO
7	F	51	GLU
7	F	60	LEU
7	F	187	ARG
8	G	121	ILE
9	H	14	THR
9	H	98	ILE
11	J	11	THR
11	J	118	LEU
13	L	54	ILE
15	N	22	ALA
15	N	85	PRO
17	P	89	MET
18	Q	122	ARG
20	S	14	ILE
21	T	39	THR
21	T	85	ASN
22	U	107	THR
22	U	118	ILE
23	V	10	GLU
24	W	31	SER
24	W	75	ILE
25	X	70	LYS
26	Y	45	ALA
30	c	35	ASP

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Mol	Chain	Res	Type
31	f	98	VAL
39	j	211	MET
41	k	412	LEU
41	k	443	VAL
4	C	153	LEU
6	E	149	TYR
6	E	201	HIS
8	G	62	PRO
8	G	148	THR
9	H	13	PRO
24	W	95	PRO
25	X	44	GLY
32	g	120	SER
39	j	6	CYS
39	j	81	GLY
41	k	377	ILE
41	k	495	ILE
4	C	232	PRO
15	N	132	VAL
27	Z	88	ILE
34	e	58	PRO
39	j	139	GLY
7	F	53	VAL
12	K	22	VAL
32	g	106	GLY
39	j	121	ILE
41	k	393	GLY
3	B	190	PRO
3	B	210	VAL
3	B	221	PRO
6	E	105	VAL
7	F	23	VAL
13	L	7	VAL
17	P	52	LYS
24	W	74	VAL
33	d	17	GLY

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	
2	A	175/211 (83%)	145 (83%)	30 (17%)	1	11
3	B	196/228 (86%)	181 (92%)	15 (8%)	10	33
4	C	176/203 (87%)	154 (88%)	22 (12%)	3	18
5	D	185/196 (94%)	156 (84%)	29 (16%)	2	14
6	E	223/224 (100%)	197 (88%)	26 (12%)	4	19
7	F	174/194 (90%)	145 (83%)	29 (17%)	2	12
8	G	192/200 (96%)	174 (91%)	18 (9%)	7	25
9	H	164/170 (96%)	154 (94%)	10 (6%)	15	39
10	I	148/159 (93%)	130 (88%)	18 (12%)	4	19
11	J	153/158 (97%)	132 (86%)	21 (14%)	3	17
12	K	88/96 (92%)	75 (85%)	13 (15%)	2	15
13	L	136/137 (99%)	120 (88%)	16 (12%)	4	19
14	M	93/109 (85%)	86 (92%)	7 (8%)	11	33
15	N	127/128 (99%)	109 (86%)	18 (14%)	2	16
16	O	96/104 (92%)	84 (88%)	12 (12%)	3	18
17	P	101/117 (86%)	86 (85%)	15 (15%)	2	14
18	Q	117/119 (98%)	102 (87%)	15 (13%)	3	18
19	R	109/124 (88%)	99 (91%)	10 (9%)	7	26
20	S	128/129 (99%)	113 (88%)	15 (12%)	4	19
21	T	117/118 (99%)	103 (88%)	14 (12%)	4	19
22	U	96/107 (90%)	85 (88%)	11 (12%)	4	20
23	V	73/73 (100%)	61 (84%)	12 (16%)	2	12
24	W	110/111 (99%)	96 (87%)	14 (13%)	3	18
25	X	119/120 (99%)	103 (87%)	16 (13%)	3	17
26	Y	108/109 (99%)	97 (90%)	11 (10%)	6	23
27	Z	60/88 (68%)	57 (95%)	3 (5%)	20	44
28	a	82/100 (82%)	72 (88%)	10 (12%)	4	19
29	b	71/72 (99%)	63 (89%)	8 (11%)	4	20
30	c	54/59 (92%)	48 (89%)	6 (11%)	5	21
31	f	57/133 (43%)	50 (88%)	7 (12%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	g	265/272 (97%)	245 (92%)	20 (8%)	11	33
33	d	46/48 (96%)	39 (85%)	7 (15%)	2	14
34	e	47/55 (86%)	38 (81%)	9 (19%)	1	8
35	h	23/23 (100%)	20 (87%)	3 (13%)	3	17
38	i	93/130 (72%)	81 (87%)	12 (13%)	3	17
39	j	226/270 (84%)	190 (84%)	36 (16%)	2	13
40	m	77/96 (80%)	70 (91%)	7 (9%)	7	26
All	All	4505/4990 (90%)	3960 (88%)	545 (12%)	6	19

All (545) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	6	THR
2	A	10	THR
2	A	13	ASP
2	A	22	VAL
2	A	29	VAL
2	A	32	HIS
2	A	41	ARG
2	A	45	VAL
2	A	50	VAL
2	A	72	ASP
2	A	79	ARG
2	A	84	ARG
2	A	88	LYS
2	A	92	HIS
2	A	98	ILE
2	A	112	THR
2	A	116	LYS
2	A	120	LEU
2	A	125	ASP
2	A	127	ARG
2	A	154	GLU
2	A	172	LEU
2	A	177	LEU
2	A	182	LEU
2	A	184	LEU
2	A	188	LEU
2	A	189	PRO
2	A	191	ARG

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Mol	Chain	Res	Type
2	A	201	LEU
2	A	204	TYR
3	B	32	ILE
3	B	67	GLU
3	B	68	VAL
3	B	82	ARG
3	B	103	MET
3	B	109	LYS
3	B	127	VAL
3	B	131	ASP
3	B	135	LEU
3	B	146	GLN
3	B	166	LYS
3	B	171	ILE
3	B	195	LYS
3	B	198	GLU
3	B	205	PHE
4	C	48	ARG
4	C	58	ILE
4	C	75	ASP
4	C	78	LEU
4	C	81	LEU
4	C	93	LYS
4	C	100	ARG
4	C	115	HIS
4	C	118	LEU
4	C	120	ILE
4	C	121	LYS
4	C	134	ILE
4	C	156	PRO
4	C	173	ARG
4	C	184	VAL
4	C	192	LEU
4	C	223	ILE
4	C	227	TYR
4	C	231	THR
4	C	235	TRP
4	C	238	GLN
4	C	246	ASP
5	D	5	ILE
5	D	11	LEU
5	D	16	VAL

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Mol	Chain	Res	Type
5	D	20	GLU
5	D	57	ASP
5	D	75	LYS
5	D	84	ILE
5	D	94	ARG
5	D	109	LEU
5	D	116	ARG
5	D	120	TYR
5	D	122	VAL
5	D	123	VAL
5	D	125	TYR
5	D	132	LYS
5	D	134	CYS
5	D	146	ARG
5	D	157	LEU
5	D	158	ILE
5	D	168	ILE
5	D	173	ARG
5	D	174	HIS
5	D	176	LEU
5	D	200	LYS
5	D	207	THR
5	D	209	ILE
5	D	212	LYS
5	D	214	GLU
5	D	218	LEU
6	E	12	LEU
6	E	37	LYS
6	E	45	ILE
6	E	48	LEU
6	E	51	ARG
6	E	53	LYS
6	E	61	VAL
6	E	62	LYS
6	E	72	VAL
6	E	95	THR
6	E	108	ARG
6	E	115	THR
6	E	116	ASP
6	E	117	GLU
6	E	131	LEU
6	E	133	LYS

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Mol	Chain	Res	Type
6	E	155	LYS
6	E	166	THR
6	E	168	THR
6	E	180	LEU
6	E	206	ASP
6	E	220	THR
6	E	233	ARG
6	E	247	THR
6	E	255	ARG
6	E	261	LEU
7	F	31	ILE
7	F	34	GLU
7	F	37	GLN
7	F	42	ILE
7	F	45	PHE
7	F	47	LYS
7	F	48	TRP
7	F	50	PHE
7	F	70	ILE
7	F	86	LYS
7	F	91	ILE
7	F	92	VAL
7	F	120	LEU
7	F	126	LEU
7	F	132	LEU
7	F	145	ARG
7	F	164	VAL
7	F	168	ARG
7	F	174	ILE
7	F	176	LEU
7	F	186	PHE
7	F	187	ARG
7	F	188	ASN
7	F	195	THR
7	F	199	GLU
7	F	209	THR
7	F	217	ASP
7	F	221	ARG
7	F	224	LYS
8	G	7	TYR
8	G	45	PHE
8	G	52	ILE

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Mol	Chain	Res	Type
8	G	71	THR
8	G	75	LEU
8	G	77	LEU
8	G	81	HIS
8	G	98	ARG
8	G	122	GLU
8	G	149	LYS
8	G	152	ASP
8	G	161	GLU
8	G	184	LEU
8	G	185	GLN
8	G	186	ARG
8	G	202	ARG
8	G	216	LEU
8	G	218	GLU
9	H	9	LEU
9	H	20	VAL
9	H	27	LEU
9	H	38	LEU
9	H	74	GLN
9	H	77	LEU
9	H	80	GLU
9	H	116	ARG
9	H	122	HIS
9	H	140	VAL
10	I	9	HIS
10	I	24	LYS
10	I	41	LYS
10	I	64	ASN
10	I	67	TRP
10	I	72	VAL
10	I	74	ARG
10	I	82	VAL
10	I	112	TRP
10	I	138	LYS
10	I	143	LYS
10	I	144	TRP
10	I	170	ILE
10	I	173	ARG
10	I	180	CYS
10	I	181	ASP
10	I	185	LEU

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Mol	Chain	Res	Type
10	I	190	LEU
11	J	6	ARG
11	J	7	THR
11	J	10	LYS
11	J	27	GLU
11	J	28	LEU
11	J	38	ASN
11	J	48	GLN
11	J	49	LEU
11	J	54	ARG
11	J	60	LEU
11	J	77	ILE
11	J	80	LEU
11	J	94	ASP
11	J	108	ARG
11	J	116	LEU
11	J	126	ARG
11	J	128	LEU
11	J	133	HIS
11	J	134	ILE
11	J	149	ARG
11	J	174	ARG
12	K	9	LYS
12	K	15	LEU
12	K	21	LEU
12	K	31	LYS
12	K	40	LEU
12	K	44	LYS
12	K	47	GLN
12	K	49	LEU
12	K	54	PHE
12	K	55	VAL
12	K	63	TYR
12	K	76	LEU
12	K	92	LEU
13	L	8	GLN
13	L	10	GLU
13	L	19	ILE
13	L	36	LYS
13	L	43	LYS
13	L	46	LYS
13	L	56	LYS

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Mol	Chain	Res	Type
13	L	71	LEU
13	L	79	ARG
13	L	83	THR
13	L	89	ASP
13	L	108	PRO
13	L	111	VAL
13	L	125	VAL
13	L	134	THR
13	L	136	ARG
14	M	34	LEU
14	M	55	LEU
14	M	59	VAL
14	M	71	LEU
14	M	87	GLN
14	M	104	ARG
14	M	125	GLU
15	N	20	ARG
15	N	38	ILE
15	N	55	ARG
15	N	56	ASP
15	N	67	THR
15	N	74	ILE
15	N	84	ILE
15	N	87	ASP
15	N	88	LEU
15	N	106	ARG
15	N	107	LYS
15	N	110	ASP
15	N	116	ILE
15	N	118	ILE
15	N	121	ARG
15	N	139	TRP
15	N	140	LYS
15	N	150	VAL
16	O	47	LYS
16	O	52	ARG
16	O	66	ASP
16	O	67	VAL
16	O	72	LYS
16	O	74	VAL
16	O	84	ARG
16	O	90	ARG

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Mol	Chain	Res	Type
16	O	102	LEU
16	O	103	ARG
16	O	128	LYS
16	O	129	LYS
17	P	13	LYS
17	P	25	LEU
17	P	56	LEU
17	P	57	MET
17	P	72	LYS
17	P	76	VAL
17	P	79	HIS
17	P	84	ILE
17	P	86	VAL
17	P	94	VAL
17	P	108	ARG
17	P	111	MET
17	P	122	THR
17	P	127	ARG
17	P	130	ARG
18	Q	29	ILE
18	Q	37	THR
18	Q	48	VAL
18	Q	52	LEU
18	Q	63	ILE
18	Q	69	VAL
18	Q	83	GLN
18	Q	94	GLN
18	Q	98	ASP
18	Q	105	LEU
18	Q	114	ARG
18	Q	127	LYS
18	Q	137	ARG
18	Q	138	PHE
18	Q	143	ARG
19	R	4	VAL
19	R	5	ARG
19	R	25	THR
19	R	29	GLN
19	R	46	LEU
19	R	63	LYS
19	R	77	GLU
19	R	100	LEU

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Mol	Chain	Res	Type
19	R	106	THR
19	R	117	LEU
20	S	6	GLN
20	S	18	LEU
20	S	25	ASN
20	S	26	ILE
20	S	54	LEU
20	S	81	ILE
20	S	86	LEU
20	S	88	ARG
20	S	96	LYS
20	S	97	ASP
20	S	105	LEU
20	S	110	ARG
20	S	114	GLU
20	S	126	ARG
20	S	140	THR
21	T	8	ASP
21	T	12	GLN
21	T	16	ASN
21	T	28	LEU
21	T	40	SER
21	T	45	LEU
21	T	65	ILE
21	T	91	HIS
21	T	103	LYS
21	T	122	ARG
21	T	124	ILE
21	T	132	LEU
21	T	135	ILE
21	T	142	ASP
22	U	18	VAL
22	U	31	VAL
22	U	37	VAL
22	U	41	ILE
22	U	42	ILE
22	U	52	LYS
22	U	56	VAL
22	U	68	ARG
22	U	83	GLU
22	U	86	ILE
22	U	117	ILE

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Mol	Chain	Res	Type
23	V	7	GLN
23	V	22	ARG
23	V	27	LYS
23	V	34	ILE
23	V	36	ILE
23	V	50	TYR
23	V	58	TYR
23	V	69	LEU
23	V	71	ARG
23	V	78	LEU
23	V	82	VAL
23	V	87	ARG
24	W	2	THR
24	W	18	GLU
24	W	26	LEU
24	W	32	LYS
24	W	33	VAL
24	W	52	TYR
24	W	65	LEU
24	W	74	VAL
24	W	75	ILE
24	W	97	ARG
24	W	98	GLN
24	W	111	MET
24	W	112	ASP
24	W	125	ILE
25	X	9	LEU
25	X	19	ARG
25	X	24	TRP
25	X	63	GLN
25	X	69	ARG
25	X	78	LYS
25	X	90	ASP
25	X	93	LEU
25	X	98	GLU
25	X	100	ASP
25	X	107	PHE
25	X	109	ARG
25	X	117	ILE
25	X	135	LEU
25	X	142	LYS
25	X	144	ARG

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Mol	Chain	Res	Type
26	Y	8	ARG
26	Y	10	ARG
26	Y	40	LEU
26	Y	49	LYS
26	Y	53	ASP
26	Y	93	ARG
26	Y	98	GLU
26	Y	107	GLN
26	Y	112	LYS
26	Y	118	ILE
26	Y	131	ARG
27	Z	58	ARG
27	Z	70	LYS
27	Z	71	LEU
28	a	3	LYS
28	a	19	LYS
28	a	33	ASP
28	a	39	MET
28	a	42	ARG
28	a	52	ASP
28	a	74	CYS
28	a	83	ILE
28	a	84	VAL
28	a	87	ARG
29	b	3	LEU
29	b	8	LEU
29	b	15	GLU
29	b	19	HIS
29	b	21	LEU
29	b	25	VAL
29	b	41	LEU
29	b	80	ARG
30	c	9	LEU
30	c	14	LYS
30	c	33	LEU
30	c	50	GLU
30	c	54	LEU
30	c	64	ARG
31	f	92	ARG
31	f	97	LYS
31	f	100	LEU
31	f	111	GLU

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Mol	Chain	Res	Type
31	f	119	LYS
31	f	138	TYR
31	f	148	THR
32	g	8	LEU
32	g	18	ASN
32	g	39	ARG
32	g	50	GLU
32	g	70	GLN
32	g	100	SER
32	g	112	LEU
32	g	119	ASN
32	g	124	ILE
32	g	129	ASP
32	g	146	LEU
32	g	151	TRP
32	g	188	LEU
32	g	198	ASP
32	g	206	ILE
32	g	210	GLN
32	g	259	LEU
32	g	279	ASP
32	g	281	LEU
32	g	321	GLN
33	d	10	HIS
33	d	16	LYS
33	d	20	GLN
33	d	31	ILE
33	d	34	TYR
33	d	41	GLN
33	d	44	ARG
34	e	10	ARG
34	e	20	LYS
34	e	31	LYS
34	e	37	ARG
34	e	38	LEU
34	e	39	LEU
34	e	48	THR
34	e	49	LEU
34	e	54	ARG
35	h	8	LYS
35	h	9	ARG
35	h	10	THR

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Mol	Chain	Res	Type
38	i	14	ARG
38	i	23	LYS
38	i	24	ARG
38	i	37	GLN
38	i	41	MET
38	i	56	LYS
38	i	61	ILE
38	i	62	ARG
38	i	66	ARG
38	i	77	ILE
38	i	103	LEU
38	i	114	LYS
39	j	7	ARG
39	j	19	ILE
39	j	38	GLU
39	j	39	TYR
39	j	43	GLU
39	j	45	MET
39	j	46	ILE
39	j	57	ARG
39	j	59	ILE
39	j	64	ARG
39	j	87	LYS
39	j	92	SER
39	j	103	GLN
39	j	107	THR
39	j	109	HIS
39	j	111	ILE
39	j	113	ARG
39	j	118	LYS
39	j	123	LEU
39	j	127	TYR
39	j	134	LEU
39	j	137	LYS
39	j	143	GLU
39	j	149	ILE
39	j	152	GLU
39	j	159	GLU
39	j	185	ARG
39	j	187	ASP
39	j	196	GLU
39	j	210	ASP

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Mol	Chain	Res	Type
39	j	227	LEU
39	j	230	LEU
39	j	235	LEU
39	j	238	GLN
39	j	244	LEU
39	j	251	ILE
40	m	41	THR
40	m	51	LEU
40	m	74	MET
40	m	83	ASP
40	m	87	LYS
40	m	92	MET
40	m	98	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	109	ASN
3	B	42	ASN
3	B	146	GLN
4	C	94	GLN
4	C	115	HIS
4	C	214	ASN
6	E	142	HIS
7	F	37	GLN
7	F	81	ASN
7	F	160	GLN
7	F	188	ASN
7	F	226	ASN
8	G	59	GLN
9	H	110	GLN
10	I	9	HIS
10	I	32	GLN
11	J	38	ASN
11	J	110	GLN
11	J	133	HIS
13	L	22	ASN
16	O	29	HIS
16	O	99	GLN
17	P	104	GLN
17	P	128	HIS
18	Q	40	GLN

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Mol	Chain	Res	Type
18	Q	74	HIS
18	Q	77	GLN
18	Q	93	HIS
18	Q	100	GLN
18	Q	139	GLN
19	R	29	GLN
19	R	111	ASN
20	S	78	HIS
20	S	87	ASN
20	S	136	GLN
24	W	12	ASN
24	W	56	HIS
24	W	92	ASN
24	W	113	HIS
25	X	65	ASN
26	Y	29	HIS
26	Y	34	ASN
27	Z	98	GLN
28	a	11	ASN
30	c	27	GLN
31	f	133	HIS
32	g	136	ASN
32	g	210	GLN
32	g	292	GLN
33	d	20	GLN
33	d	27	HIS
34	e	17	GLN
38	i	44	ASN
39	j	26	GLN
39	j	238	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1778/1799 (98%)	807 (45%)	139 (7%)
36	1	73/75 (97%)	34 (46%)	6 (8%)
37	3	21/25 (84%)	18 (85%)	6 (28%)
All	All	1872/1899 (98%)	859 (45%)	151 (8%)

All (859) 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	8	U
1	2	11	A
1	2	19	A
1	2	23	G
1	2	24	U
1	2	25	C
1	2	26	A
1	2	27	U
1	2	31	C
1	2	32	U
1	2	34	G
1	2	35	U
1	2	36	C
1	2	37	U
1	2	39	A
1	2	42	G
1	2	45	U
1	2	46	A
1	2	47	A
1	2	50	C
1	2	51	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	64	U
1	2	65	A
1	2	66	U
1	2	67	A
1	2	68	A
1	2	69	G
1	2	70	C
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U

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Mol	Chain	Res	Type
1	2	76	A
1	2	77	U
1	2	79	C
1	2	80	A
1	2	81	G
1	2	87	C
1	2	104	A
1	2	111	U
1	2	114	C
1	2	115	G
1	2	116	U
1	2	123	G
1	2	124	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	152	G
1	2	157	U
1	2	158	U
1	2	159	C
1	2	160	U
1	2	161	A
1	2	165	C
1	2	167	A
1	2	168	A
1	2	169	U

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Mol	Chain	Res	Type
1	2	172	A
1	2	173	U
1	2	176	U
1	2	177	U
1	2	183	C
1	2	187	A
1	2	189	C
1	2	190	C
1	2	191	U
1	2	192	U
1	2	194	G
1	2	195	G
1	2	199	A
1	2	214	A
1	2	217	A
1	2	218	A
1	2	225	A
1	2	226	U
1	2	227	G
1	2	228	U
1	2	230	U
1	2	231	U
1	2	232	C
1	2	234	G
1	2	235	A
1	2	237	U
1	2	239	C
1	2	240	U
1	2	248	U
1	2	249	C
1	2	256	A
1	2	260	U
1	2	262	C
1	2	264	A
1	2	265	A
1	2	266	U
1	2	267	C
1	2	270	A
1	2	271	U
1	2	272	G
1	2	274	C
1	2	276	U

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Mol	Chain	Res	Type
1	2	277	U
1	2	278	G
1	2	279	U
1	2	280	G
1	2	282	U
1	2	287	A
1	2	291	U
1	2	298	A
1	2	300	A
1	2	301	U
1	2	303	U
1	2	309	C
1	2	310	U
1	2	313	C
1	2	314	A
1	2	315	A
1	2	319	U
1	2	320	C
1	2	321	G
1	2	322	A
1	2	328	G
1	2	335	G
1	2	336	G
1	2	337	C
1	2	342	C
1	2	345	G
1	2	349	U
1	2	351	A
1	2	352	A
1	2	358	A
1	2	359	A
1	2	360	C
1	2	364	G
1	2	368	A
1	2	372	G
1	2	377	A
1	2	378	U
1	2	379	U
1	2	380	C
1	2	382	G
1	2	384	A
1	2	385	G

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Mol	Chain	Res	Type
1	2	386	A
1	2	387	G
1	2	389	G
1	2	390	A
1	2	391	G
1	2	397	G
1	2	398	A
1	2	399	A
1	2	400	A
1	2	401	C
1	2	403	G
1	2	413	C
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	443	C
1	2	444	A
1	2	447	C
1	2	448	C
1	2	452	U
1	2	453	U
1	2	454	C
1	2	455	A
1	2	456	G
1	2	457	G
1	2	458	G
1	2	459	A
1	2	460	G
1	2	469	A
1	2	473	A
1	2	474	A

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Mol	Chain	Res	Type
1	2	476	A
1	2	478	C
1	2	479	G
1	2	480	A
1	2	481	U
1	2	482	A
1	2	483	C
1	2	486	G
1	2	489	C
1	2	490	C
1	2	491	A
1	2	492	U
1	2	493	U
1	2	495	G
1	2	496	G
1	2	497	G
1	2	498	U
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	509	G
1	2	512	U
1	2	513	G
1	2	514	A
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	527	U
1	2	531	U
1	2	533	A
1	2	534	A
1	2	535	C
1	2	536	G
1	2	538	G

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Mol	Chain	Res	Type
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	548	G
1	2	554	A
1	2	556	G
1	2	557	U
1	2	560	G
1	2	564	C
1	2	565	C
1	2	566	A
1	2	567	G
1	2	568	C
1	2	569	A
1	2	570	G
1	2	571	C
1	2	573	G
1	2	577	U
1	2	578	A
1	2	579	A
1	2	580	U
1	2	581	U
1	2	593	A
1	2	594	G
1	2	596	G
1	2	600	A
1	2	605	A
1	2	610	U
1	2	612	G
1	2	614	A
1	2	618	A
1	2	619	A
1	2	621	A
1	2	622	A
1	2	623	G
1	2	631	U
1	2	634	A
1	2	640	G

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Mol	Chain	Res	Type
1	2	641	G
1	2	642	G
1	2	647	G
1	2	649	U
1	2	651	U
1	2	652	C
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	686	C
1	2	687	C
1	2	691	U
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	700	C
1	2	701	U
1	2	702	G
1	2	703	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	711	G
1	2	712	U
1	2	713	A
1	2	714	C
1	2	717	C
1	2	718	U
1	2	719	U
1	2	720	G
1	2	721	U
1	2	722	G
1	2	723	G

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Mol	Chain	Res	Type
1	2	725	U
1	2	727	C
1	2	728	A
1	2	731	C
1	2	733	A
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	744	U
1	2	745	U
1	2	747	C
1	2	753	A
1	2	755	A
1	2	762	A
1	2	765	G
1	2	766	U
1	2	767	U
1	2	768	C
1	2	771	A
1	2	772	G
1	2	774	A
1	2	778	G
1	2	779	A
1	2	780	A
1	2	781	A
1	2	782	G
1	2	783	C
1	2	784	U
1	2	785	C
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	803	A
1	2	806	A
1	2	809	G
1	2	811	A

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Mol	Chain	Res	Type
1	2	812	U
1	2	814	G
1	2	817	C
1	2	818	G
1	2	819	U
1	2	820	U
1	2	822	G
1	2	823	G
1	2	825	U
1	2	826	C
1	2	827	U
1	2	828	A
1	2	829	U
1	2	830	U
1	2	832	U
1	2	839	U
1	2	840	U
1	2	845	G
1	2	847	C
1	2	855	A
1	2	859	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	895	U
1	2	897	A
1	2	898	G
1	2	905	A
1	2	907	U
1	2	908	U
1	2	912	G
1	2	913	G
1	2	915	U
1	2	918	A
1	2	919	U
1	2	920	U
1	2	925	A
1	2	927	U
1	2	930	C

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Mol	Chain	Res	Type
1	2	931	U
1	2	932	A
1	2	933	C
1	2	934	U
1	2	938	A
1	2	939	A
1	2	941	G
1	2	944	U
1	2	945	U
1	2	946	U
1	2	947	G
1	2	950	A
1	2	956	G
1	2	957	U
1	2	958	U
1	2	959	U
1	2	965	A
1	2	970	A
1	2	972	A
1	2	976	A
1	2	978	A
1	2	981	U
1	2	982	A
1	2	987	A
1	2	990	G
1	2	991	A
1	2	997	A
1	2	999	C
1	2	1002	A
1	2	1003	U
1	2	1004	A
1	2	1009	C
1	2	1011	U
1	2	1012	A
1	2	1015	C
1	2	1018	A
1	2	1019	A
1	2	1020	C
1	2	1023	U
1	2	1024	A
1	2	1025	A
1	2	1026	A

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Mol	Chain	Res	Type
1	2	1027	C
1	2	1028	U
1	2	1030	U
1	2	1031	G
1	2	1034	G
1	2	1038	A
1	2	1039	G
1	2	1041	G
1	2	1048	U
1	2	1049	G
1	2	1050	G
1	2	1051	U
1	2	1052	G
1	2	1056	U
1	2	1057	U
1	2	1058	C
1	2	1059	U
1	2	1060	U
1	2	1062	U
1	2	1064	A
1	2	1065	C
1	2	1069	C
1	2	1070	U
1	2	1075	A
1	2	1076	C
1	2	1079	U
1	2	1080	A
1	2	1081	C
1	2	1082	G
1	2	1084	G
1	2	1086	A
1	2	1090	A
1	2	1091	A
1	2	1092	A
1	2	1093	G
1	2	1095	C
1	2	1096	U
1	2	1097	U
1	2	1099	G
1	2	1100	G
1	2	1101	G
1	2	1102	U

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Mol	Chain	Res	Type
1	2	1103	U
1	2	1105	U
1	2	1107	G
1	2	1108	G
1	2	1112	A
1	2	1113	G
1	2	1118	G
1	2	1119	U
1	2	1121	G
1	2	1135	U
1	2	1137	A
1	2	1145	G
1	2	1146	A
1	2	1149	G
1	2	1150	A
1	2	1152	G
1	2	1154	G
1	2	1155	C
1	2	1157	C
1	2	1158	C
1	2	1159	A
1	2	1162	A
1	2	1165	A
1	2	1166	G
1	2	1167	U
1	2	1168	G
1	2	1169	G
1	2	1176	C
1	2	1184	U
1	2	1186	U
1	2	1188	A
1	2	1189	C
1	2	1190	U
1	2	1192	A
1	2	1193	A
1	2	1198	G
1	2	1199	G
1	2	1201	A
1	2	1202	A
1	2	1204	C
1	2	1206	C
1	2	1207	A

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Mol	Chain	Res	Type
1	2	1211	G
1	2	1215	C
1	2	1216	A
1	2	1217	G
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	1236	G
1	2	1240	G
1	2	1241	A
1	2	1242	G
1	2	1243	A
1	2	1244	G
1	2	1246	U
1	2	1247	C
1	2	1254	G
1	2	1255	A
1	2	1256	U
1	2	1258	U
1	2	1259	U
1	2	1264	G
1	2	1266	G
1	2	1268	U
1	2	1269	G
1	2	1272	G
1	2	1273	C
1	2	1274	A
1	2	1281	U
1	2	1282	U
1	2	1283	C
1	2	1284	U
1	2	1285	U
1	2	1292	U
1	2	1294	G
1	2	1295	A
1	2	1306	U
1	2	1309	U
1	2	1313	U

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Mol	Chain	Res	Type
1	2	1314	U
1	2	1315	G
1	2	1317	G
1	2	1318	A
1	2	1320	A
1	2	1321	A
1	2	1323	G
1	2	1324	A
1	2	1332	C
1	2	1333	U
1	2	1336	A
1	2	1338	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	1353	G
1	2	1362	U
1	2	1366	G
1	2	1369	U
1	2	1370	G
1	2	1371	A
1	2	1376	U
1	2	1380	A
1	2	1381	G
1	2	1383	G
1	2	1386	A
1	2	1388	U
1	2	1389	A
1	2	1393	G
1	2	1396	U
1	2	1397	C
1	2	1398	A
1	2	1400	G
1	2	1408	A
1	2	1410	G
1	2	1411	U
1	2	1412	U
1	2	1413	U

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Mol	Chain	Res	Type
1	2	1417	G
1	2	1420	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	1435	U
1	2	1442	A
1	2	1444	A
1	2	1445	C
1	2	1449	C
1	2	1450	U
1	2	1455	C
1	2	1456	G
1	2	1457	C
1	2	1463	C
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	1479	C
1	2	1481	A
1	2	1484	G
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	1499	C
1	2	1501	A
1	2	1502	G
1	2	1503	A
1	2	1509	G
1	2	1512	U

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Mol	Chain	Res	Type
1	2	1513	A
1	2	1514	A
1	2	1515	U
1	2	1516	C
1	2	1519	G
1	2	1521	G
1	2	1522	A
1	2	1523	A
1	2	1533	U
1	2	1534	G
1	2	1535	C
1	2	1536	U
1	2	1537	G
1	2	1538	G
1	2	1540	G
1	2	1543	A
1	2	1544	G
1	2	1548	A
1	2	1552	U
1	2	1554	A
1	2	1555	U
1	2	1556	U
1	2	1557	A
1	2	1566	C
1	2	1570	G
1	2	1571	A
1	2	1572	G
1	2	1573	G
1	2	1574	A
1	2	1580	U
1	2	1581	A
1	2	1583	U
1	2	1584	A
1	2	1588	G
1	2	1594	C
1	2	1595	A
1	2	1597	C
1	2	1598	A
1	2	1599	G
1	2	1601	U
1	2	1604	C
1	2	1606	U

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Mol	Chain	Res	Type
1	2	1608	G
1	2	1612	A
1	2	1613	C
1	2	1614	G
1	2	1616	C
1	2	1617	C
1	2	1620	G
1	2	1628	U
1	2	1629	A
1	2	1631	A
1	2	1632	C
1	2	1633	A
1	2	1640	G
1	2	1646	A
1	2	1647	G
1	2	1649	A
1	2	1654	U
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	1663	U
1	2	1664	U
1	2	1666	G
1	2	1669	A
1	2	1675	C
1	2	1676	A
1	2	1678	G
1	2	1679	A
1	2	1680	U
1	2	1681	U
1	2	1682	U
1	2	1685	U
1	2	1686	U
1	2	1687	A
1	2	1691	A
1	2	1692	A
1	2	1693	G
1	2	1694	G
1	2	1695	G

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Mol	Chain	Res	Type
1	2	1696	G
1	2	1697	G
1	2	1701	C
1	2	1703	C
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	1714	C
1	2	1715	G
1	2	1722	C
1	2	1725	G
1	2	1729	A
1	2	1732	U
1	2	1734	G
1	2	1735	G
1	2	1736	U
1	2	1737	C
1	2	1738	A
1	2	1739	U
1	2	1742	A
1	2	1743	G
1	2	1744	A
1	2	1745	G
1	2	1748	A
1	2	1753	A
1	2	1754	A
1	2	1755	G
1	2	1758	G
1	2	1760	A
1	2	1763	A
1	2	1764	A
1	2	1766	G
1	2	1767	U
1	2	1769	U
1	2	1778	G
1	2	1780	A
1	2	1781	C
1	2	1786	G
1	2	1787	G

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Mol	Chain	Res	Type
1	2	1790	G
1	2	1791	G
1	2	1792	A
1	2	1793	U
1	2	1794	C
1	2	1795	A
1	2	1796	U
1	2	1798	A
36	1	4	G
36	1	7	G
36	1	8	U
36	1	9	G
36	1	10	G
36	1	15	G
36	1	16	U
36	1	18	G
36	1	19	G
36	1	20	A
36	1	21	A
36	1	22	G
36	1	24	G
36	1	28	A
36	1	40	C
36	1	41	C
36	1	44	A
36	1	45	U
36	1	46	G
36	1	48	C
36	1	49	C
36	1	50	U
36	1	52	G
36	1	56	C
36	1	57	G
36	1	59	A
36	1	61	C
36	1	63	G
36	1	68	G
36	1	69	C
36	1	70	G
36	1	73	A
36	1	74	C
36	1	76	A

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Mol	Chain	Res	Type
37	3	4	U
37	3	5	C
37	3	6	U
37	3	8	U
37	3	9	C
37	3	10	U
37	3	11	C
37	3	12	U
37	3	13	A
37	3	16	C
37	3	17	U
37	3	18	C
37	3	19	U
37	3	20	C
37	3	21	U
37	3	22	C
37	3	23	U
37	3	24	C

All (151) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	3	U
1	2	25	C
1	2	39	A
1	2	44	U
1	2	61	A
1	2	65	A
1	2	66	U
1	2	68	A
1	2	73	U
1	2	74	U
1	2	104	A
1	2	114	C
1	2	115	G
1	2	129	U
1	2	130	C
1	2	131	C
1	2	133	U
1	2	135	A
1	2	139	C
1	2	141	U

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Mol	Chain	Res	Type
1	2	144	A
1	2	145	U
1	2	157	U
1	2	158	U
1	2	168	A
1	2	176	U
1	2	186	G
1	2	190	C
1	2	216	A
1	2	217	A
1	2	226	U
1	2	230	U
1	2	239	C
1	2	277	U
1	2	279	U
1	2	318	U
1	2	320	C
1	2	321	G
1	2	351	A
1	2	379	U
1	2	386	A
1	2	416	A
1	2	422	G
1	2	424	A
1	2	451	A
1	2	453	U
1	2	458	G
1	2	473	A
1	2	497	G
1	2	524	A
1	2	538	G
1	2	540	A
1	2	542	C
1	2	543	A
1	2	564	C
1	2	685	A
1	2	693	U
1	2	695	U
1	2	700	C
1	2	704	C
1	2	720	G
1	2	721	U

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Mol	Chain	Res	Type
1	2	737	A
1	2	742	U
1	2	765	G
1	2	772	G
1	2	779	A
1	2	802	A
1	2	810	A
1	2	811	A
1	2	822	G
1	2	828	A
1	2	854	A
1	2	875	G
1	2	896	C
1	2	907	U
1	2	912	G
1	2	918	A
1	2	943	A
1	2	945	U
1	2	956	G
1	2	1030	U
1	2	1056	U
1	2	1080	A
1	2	1081	C
1	2	1099	G
1	2	1107	G
1	2	1158	C
1	2	1164	G
1	2	1188	A
1	2	1192	A
1	2	1198	G
1	2	1206	C
1	2	1215	C
1	2	1226	A
1	2	1243	A
1	2	1273	C
1	2	1284	U
1	2	1313	U
1	2	1320	A
1	2	1343	A
1	2	1380	A
1	2	1389	A
1	2	1409	A

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Mol	Chain	Res	Type
1	2	1412	U
1	2	1419	A
1	2	1429	C
1	2	1430	U
1	2	1431	G
1	2	1478	G
1	2	1487	U
1	2	1488	A
1	2	1491	A
1	2	1501	A
1	2	1502	G
1	2	1514	A
1	2	1515	U
1	2	1534	G
1	2	1556	U
1	2	1566	C
1	2	1571	A
1	2	1573	G
1	2	1580	U
1	2	1598	A
1	2	1613	C
1	2	1655	U
1	2	1663	U
1	2	1668	G
1	2	1678	G
1	2	1681	U
1	2	1711	G
1	2	1714	C
1	2	1725	G
1	2	1743	G
1	2	1759	U
1	2	1765	G
1	2	1792	A
1	2	1795	A
1	2	1796	U
36	1	14	A
36	1	16	U
36	1	43	G
36	1	44	A
36	1	47	U
36	1	74	C
37	3	7	C

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Mol	Chain	Res	Type
37	3	10	U
37	3	11	C
37	3	16	C
37	3	19	U
37	3	22	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 85 ligands modelled in this entry, 84 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
45	MET	k	601	-	6,7,8	0.48	0	2,7,9	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	MET	k	601	-	-	2/5/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	k	601	MET	N-CA-CB-CG
45	k	601	MET	C-CA-CB-CG

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.

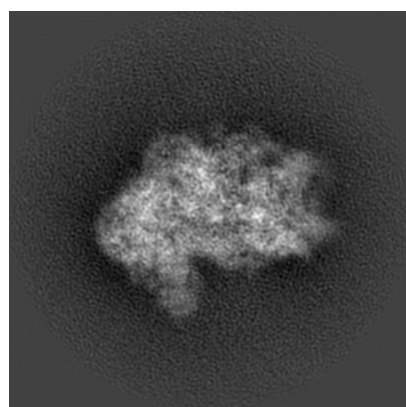
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2763. These allow visual inspection of the internal detail of the map and identification of artifacts.

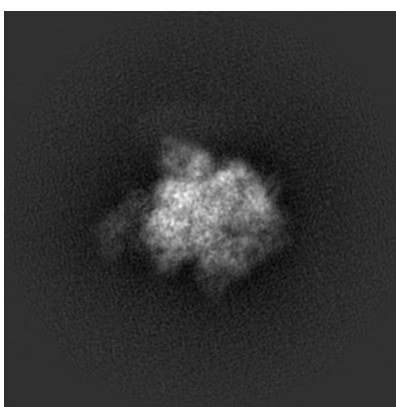
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

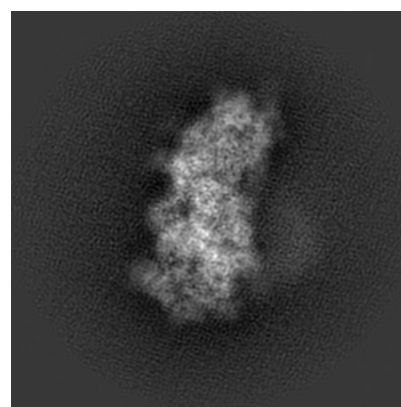
6.1.1 Primary map



X



Y

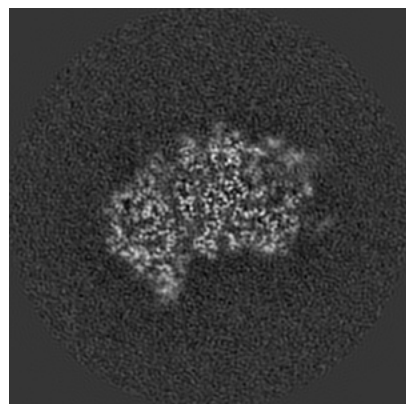


Z

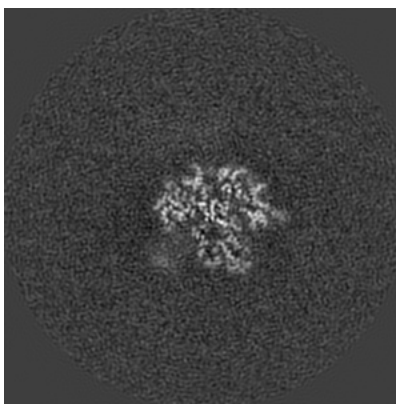
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

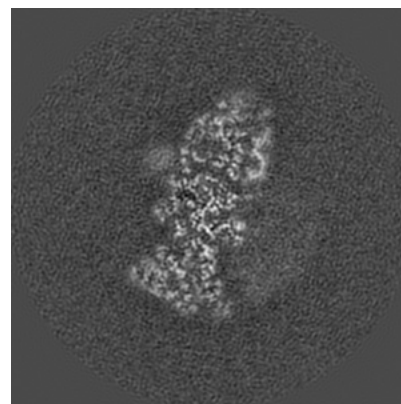
6.2.1 Primary map



X Index: 150



Y Index: 150

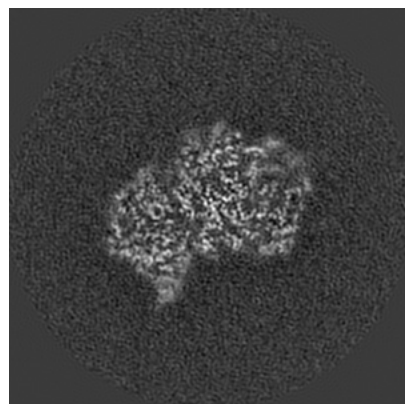


Z Index: 150

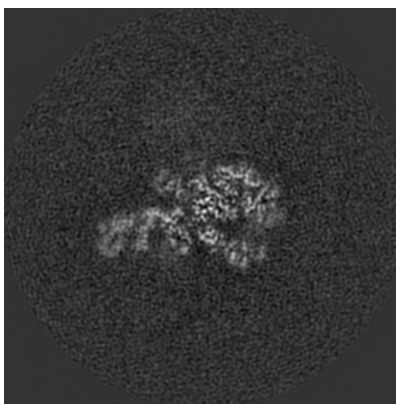
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

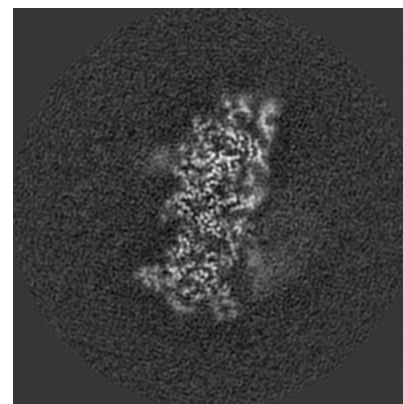
6.3.1 Primary map



X Index: 148



Y Index: 133

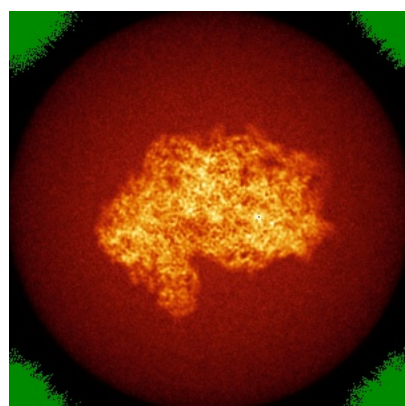


Z Index: 145

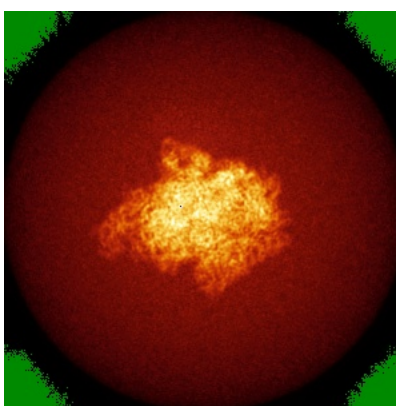
The images above show the largest variance slices of the map in three orthogonal directions.

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

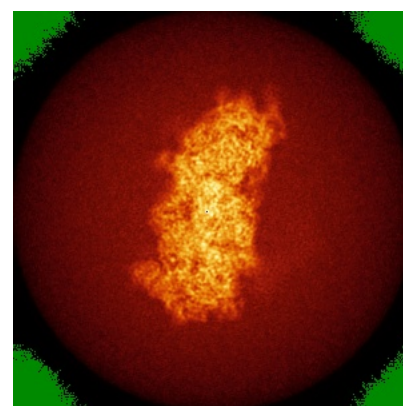
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

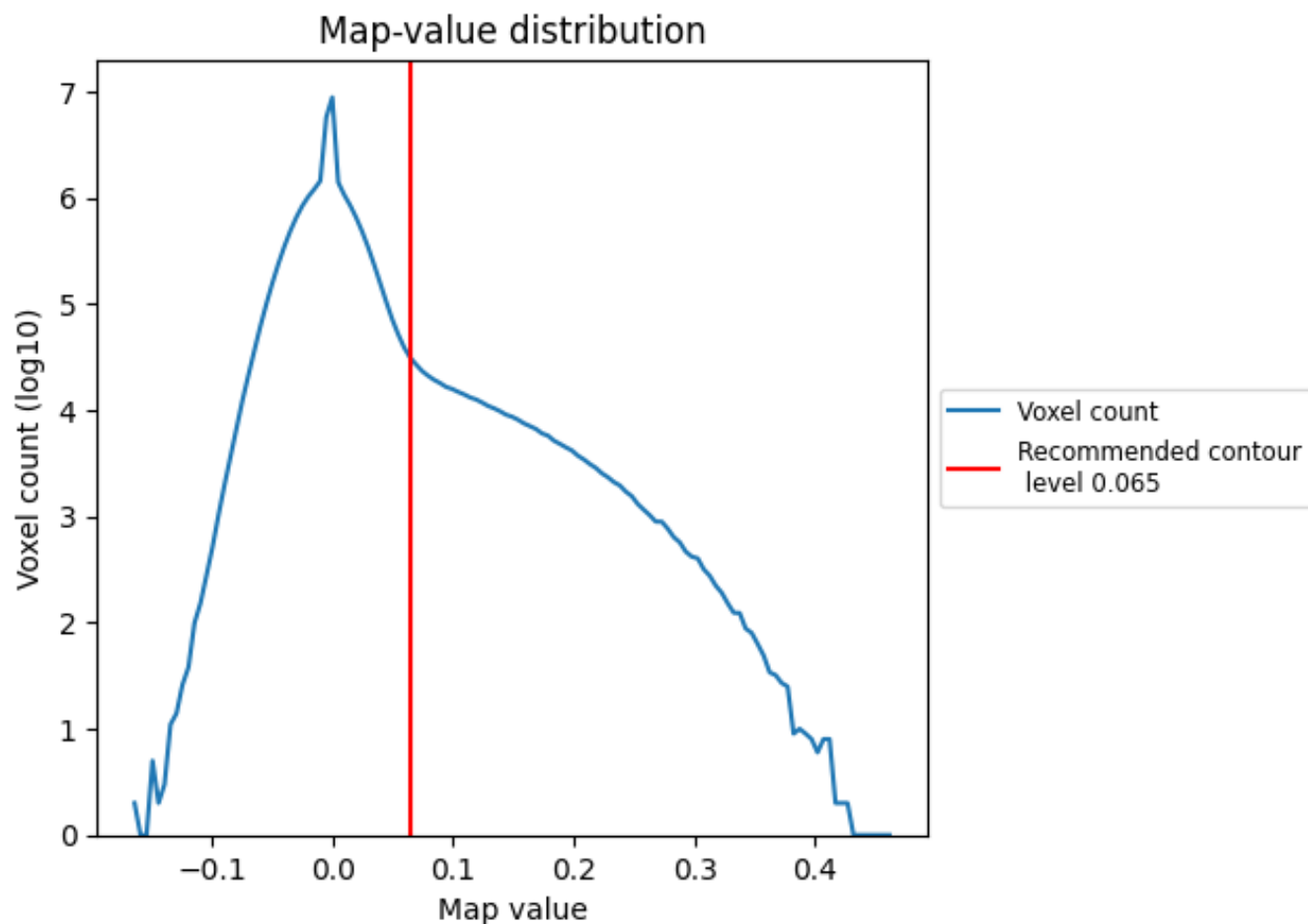
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

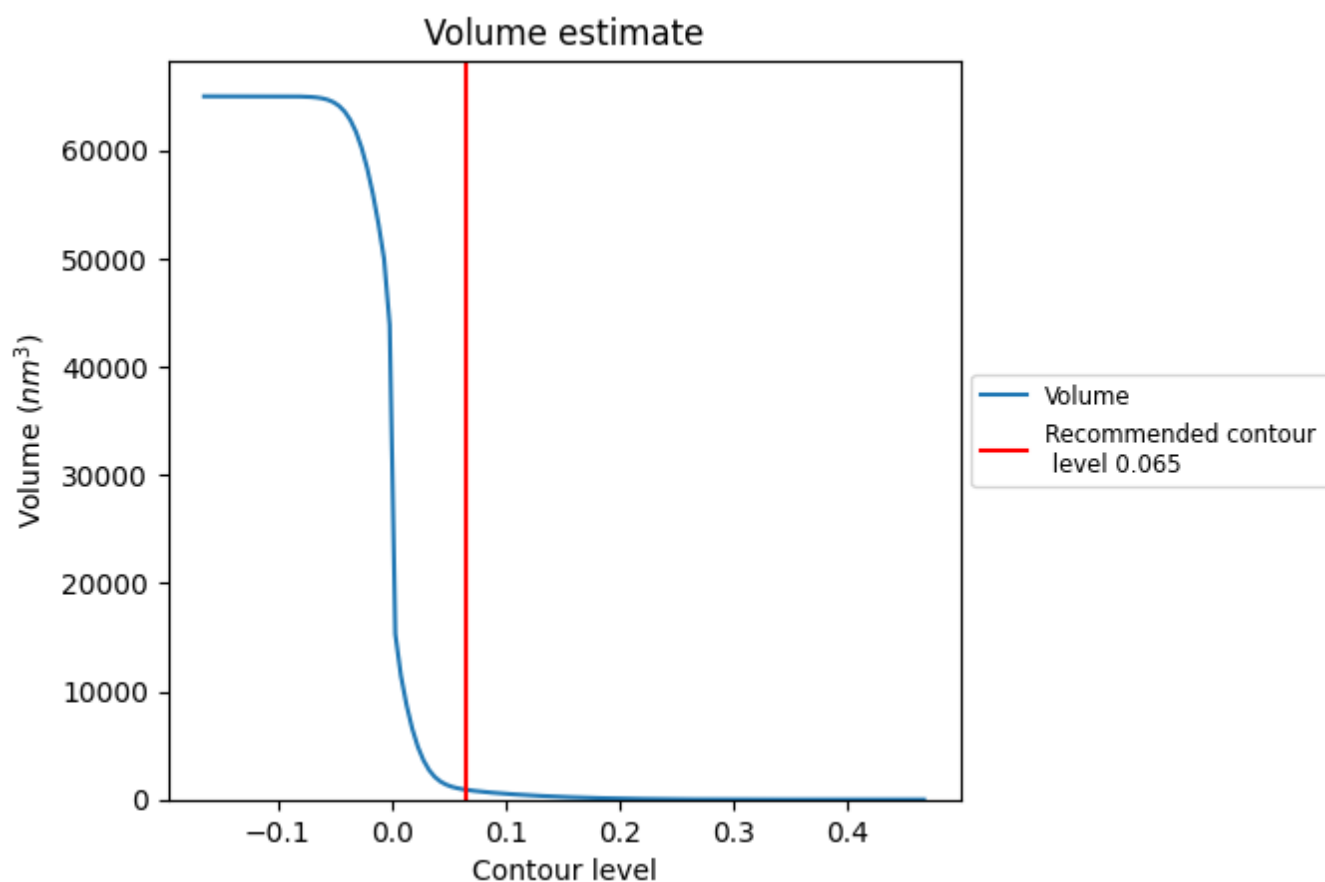
This section contains the results of statistical analysis of the map.

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.

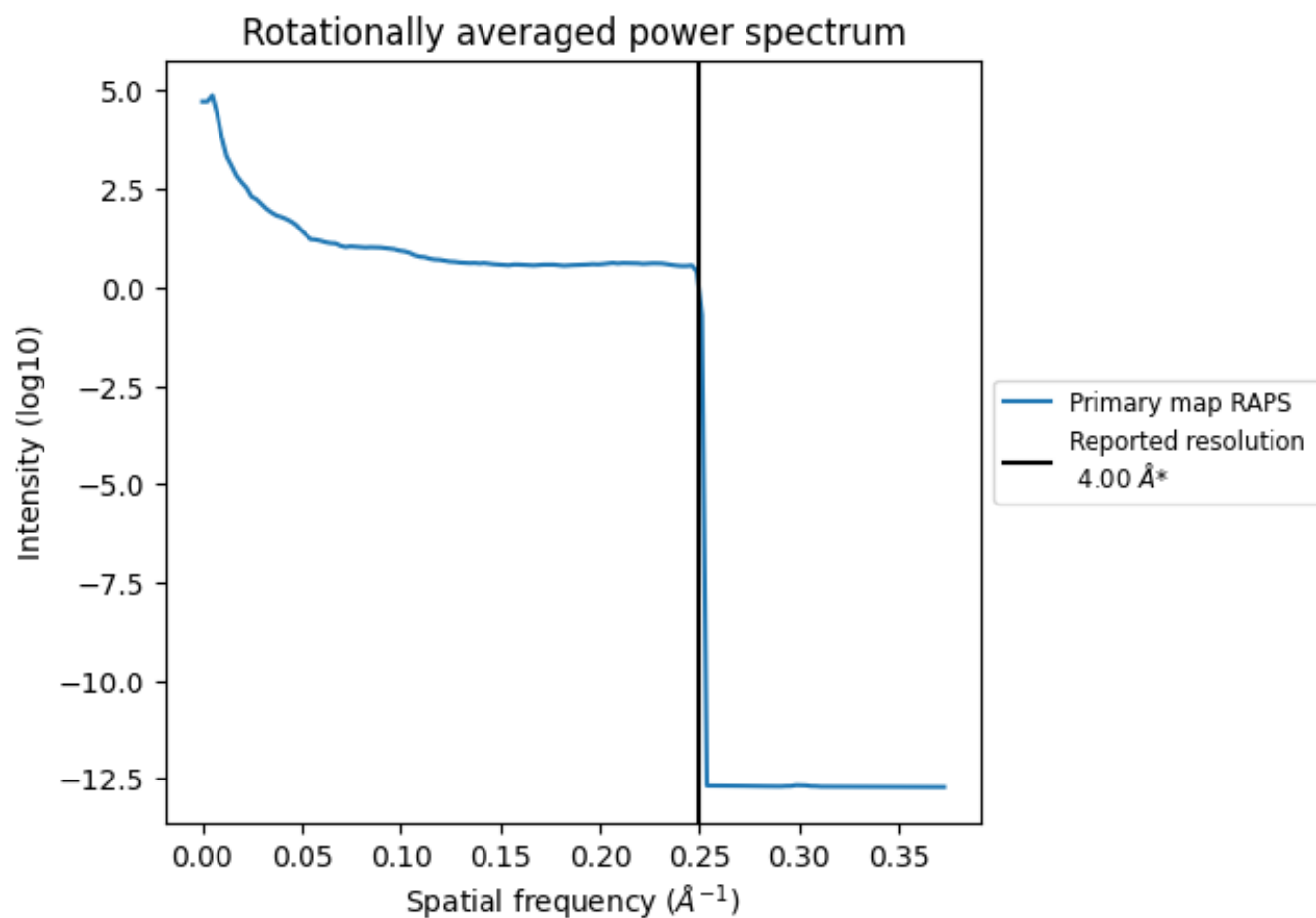
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 912 nm³; this corresponds to an approximate mass of 824 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 ⓘ

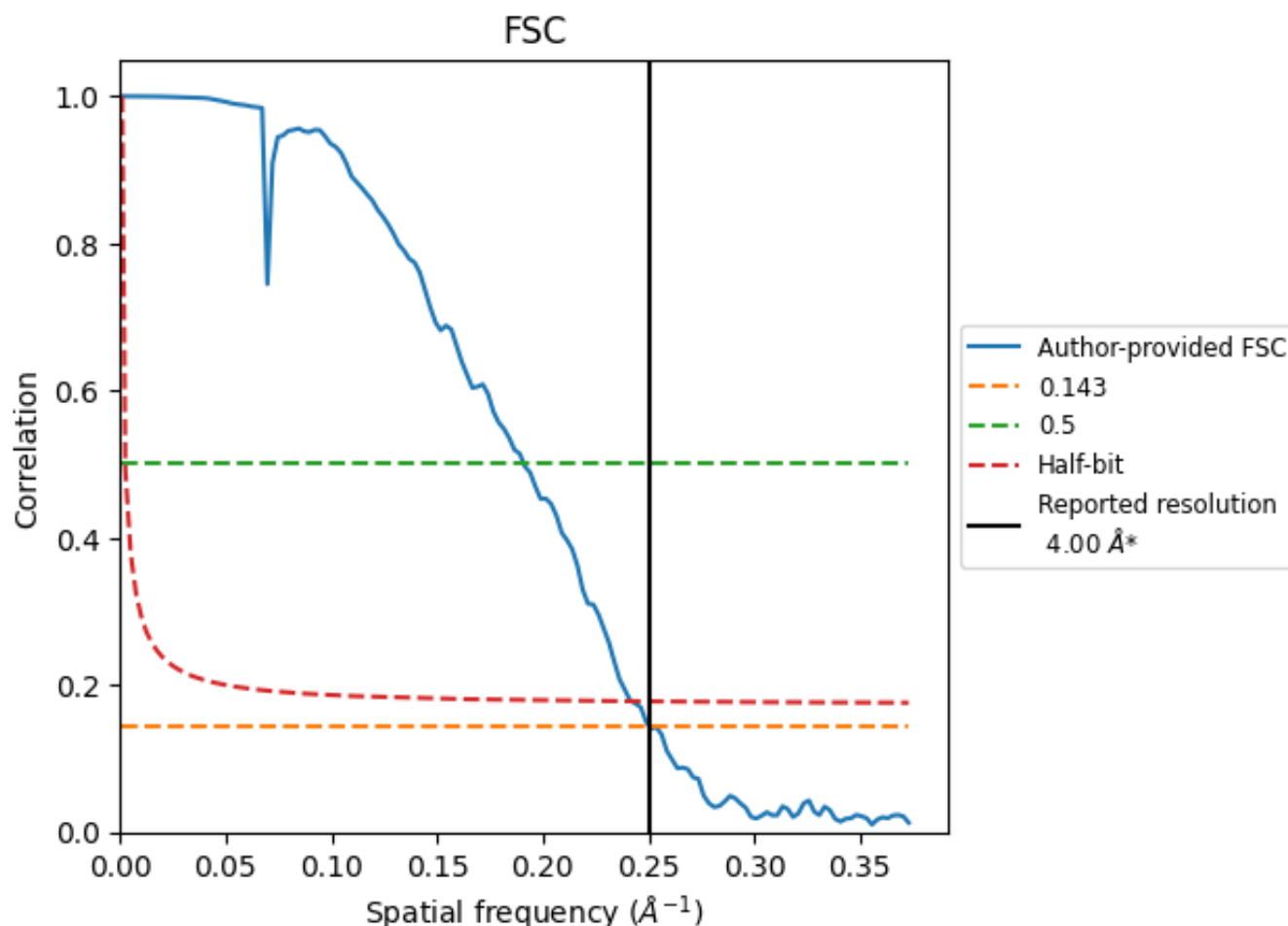


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.250 \AA^{-1}

8.2 Resolution estimates [i](#)

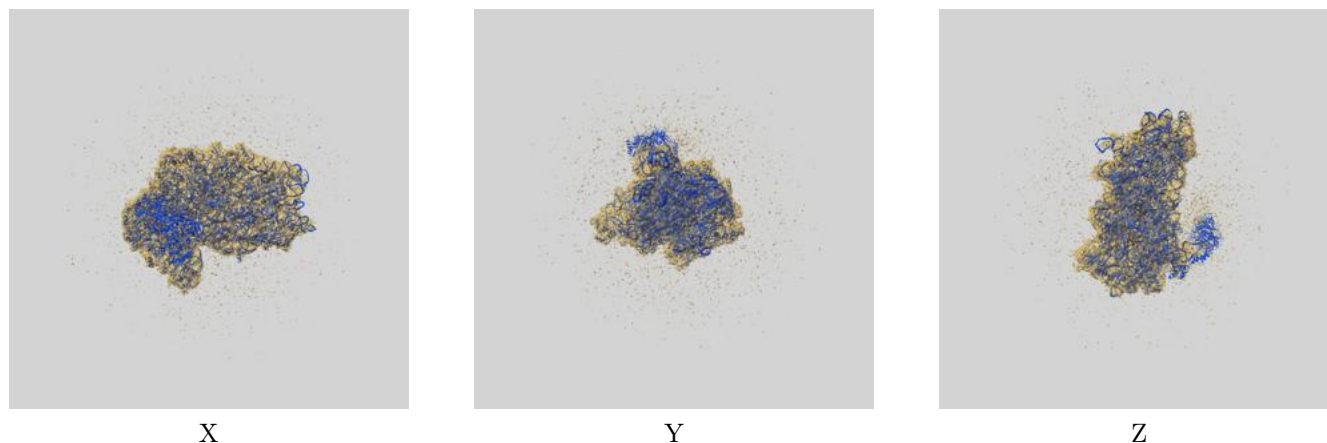
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.99	5.23	4.13
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

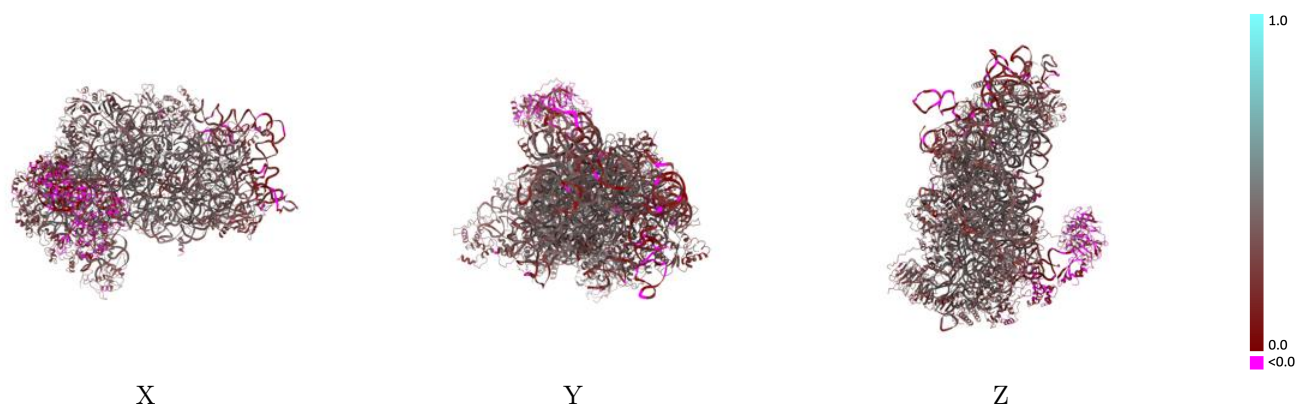
This section contains information regarding the fit between EMDB map EMD-2763 and PDB model 3J81. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



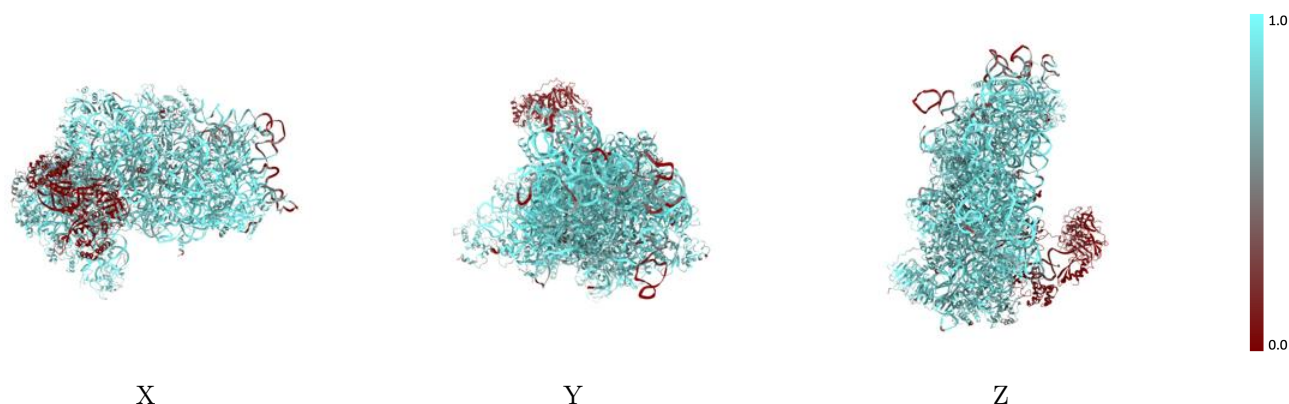
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



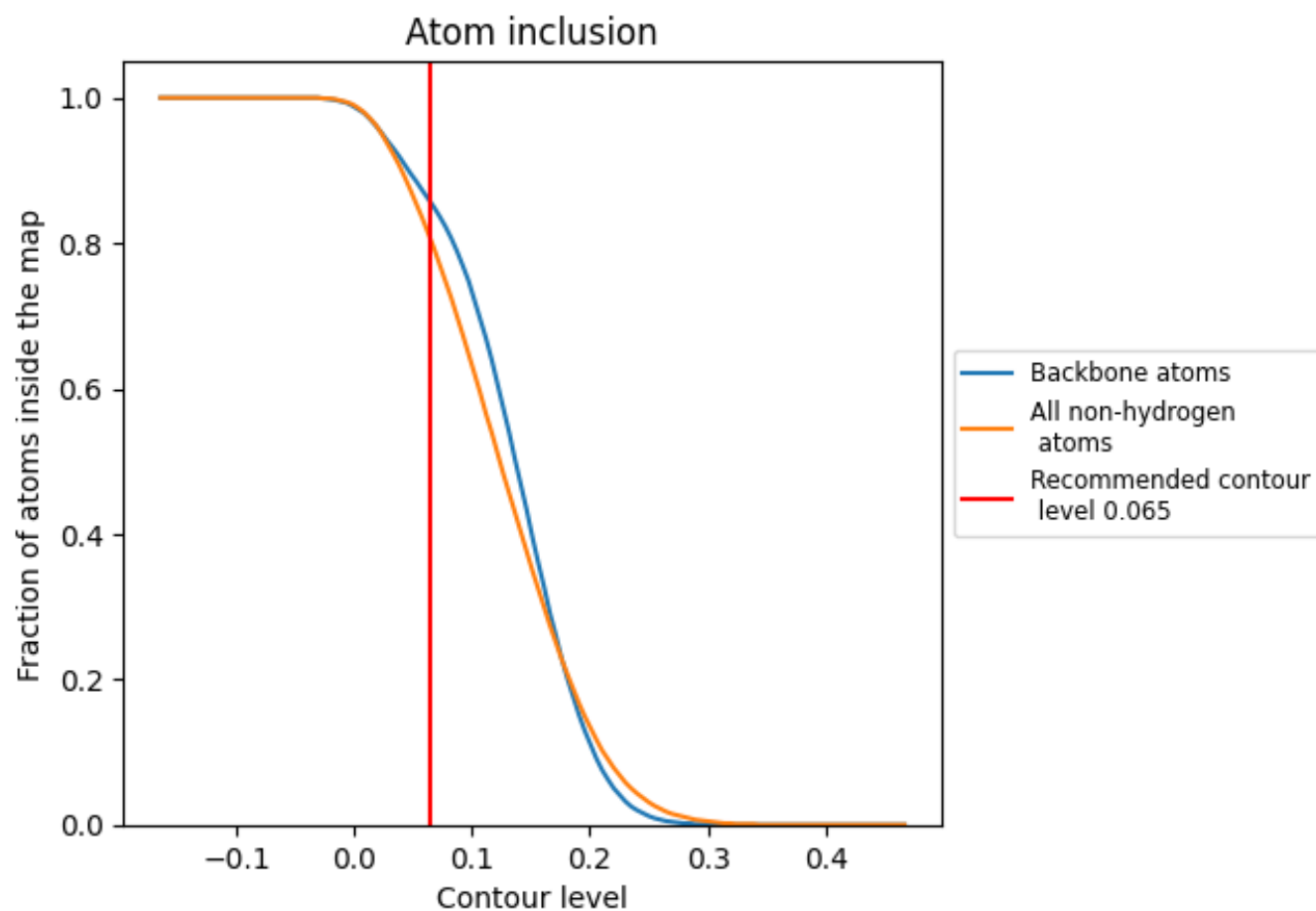
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 86% of all backbone atoms, 80% 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	 0.8040	 0.3260
1	 0.4250	 0.1400
2	 0.9160	 0.3460
3	 0.4340	 0.2930
A	 0.8470	 0.3670
B	 0.8410	 0.3410
C	 0.8070	 0.3760
D	 0.7970	 0.3470
E	 0.8050	 0.3770
F	 0.7870	 0.3340
G	 0.8300	 0.3140
H	 0.7870	 0.3140
I	 0.8070	 0.3450
J	 0.8150	 0.3620
K	 0.8040	 0.3260
L	 0.7650	 0.3730
M	 0.7230	 0.2410
N	 0.8000	 0.3400
O	 0.8340	 0.3590
P	 0.8090	 0.3190
Q	 0.8020	 0.3540
R	 0.8130	 0.3400
S	 0.7660	 0.3040
T	 0.8230	 0.3260
U	 0.7770	 0.3530
V	 0.8310	 0.3750
W	 0.8120	 0.3880
X	 0.8480	 0.4070
Y	 0.8380	 0.3520
Z	 0.6080	 0.2240
a	 0.8330	 0.3810
b	 0.8140	 0.3500
c	 0.8090	 0.3950
d	 0.8430	 0.3840
e	 0.7850	 0.3640



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Chain	Atom inclusion	Q-score
f	 0.8010	 0.2860
g	 0.8270	 0.3350
h	 0.4720	 0.2570
i	 0.6910	 0.3310
j	 0.0690	 0.0950
k	 0.0140	 0.0250
l	 0.0000	 0.0230
m	 0.1360	 0.1940