



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 03:01 PM EST

PDB ID : 3JAM
EMDB ID : EMD-3047
Title : CryoEM structure of 40S-eIF1A-eIF1 complex from yeast
Authors : Llacer, J.L.; Hussain, T.; Ramakrishnan, V.
Deposited on : 2015-06-17
Resolution : 3.46 Å(reported)
Based on initial model : 3J80

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:

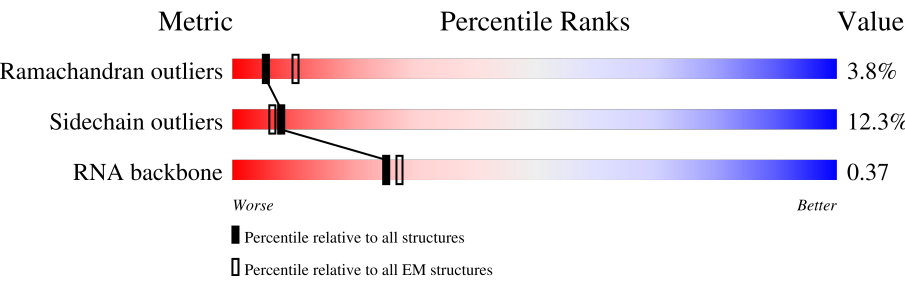
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.46 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div><div>8%</div><div>60%</div><div>38%</div><div>.</div></div>
2	A	254	<div><div>67%</div><div>14%</div><div>18%</div></div>
3	B	255	<div><div>73%</div><div>13%</div><div>13%</div><div>.</div></div>
4	C	259	<div><div>75%</div><div>9%</div><div>16%</div></div>
5	D	237	<div><div>9%</div><div>78%</div><div>15%</div><div>6%</div><div>.</div></div>
6	E	261	<div><div>83%</div><div>16%</div></div>
7	F	227	<div><div>15%</div><div>78%</div><div>13%</div><div>9%</div></div>
8	G	236	<div><div>86%</div><div>9%</div><div>.</div></div>

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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	142	
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	d	56	
32	e	63	
33	f	150	

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Mol	Chain	Length	Quality of chain
34	g	326	<div><div></div><div>19%</div><div>86%</div><div>11%</div><div>..</div></div>
35	h	25	<div><div></div><div>44%</div><div>92%</div><div>8%</div></div>
36	i	153	<div><div></div><div>39%</div><div>57%</div><div>6%</div><div>37%</div></div>
37	j	108	<div><div></div><div>44%</div><div>69%</div><div>10%</div><div>20%</div></div>

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 77850 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	208	Total	C	N	O	S	0	0
			1626	1040	286	298	2		

- Molecule 3 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	223	Total	C	N	O	S	0	0
			1774	1120	325	326	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		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
			1489	923	300	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	122	Total	C	N	O	0	0
			922	575	167	180		

- 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	123	Total	C	N	O	S	0
			980	628	179	168	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	125	Total	C	N	O	S	0
			991	619	182	187	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	0	0
			1110	693	210	207		

- Molecule 22 is a protein called uS10.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	U	106	Total	C	N	O	S	0
			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	0
			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	0
			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	0
			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		0
			1061	665	207	189		0

- Molecule 27 is a protein called eS25.

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

- Molecule 28 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	98	Total	C	N	O	S	0	0
			779	480	165	129	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	63	Total	C	N	O	S	0	0
			494	305	98	90	1		

- Molecule 31 is a protein called uS14.

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

- Molecule 32 is a protein called eS30.

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

- Molecule 33 is a protein called eS31.

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

- Molecule 34 is a protein called RACK1.

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

- 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	78	Total	Mg	0
			78	78	
38	J	1	Total	Mg	0
			1	1	
38	f	1	Total	Mg	0
			1	1	

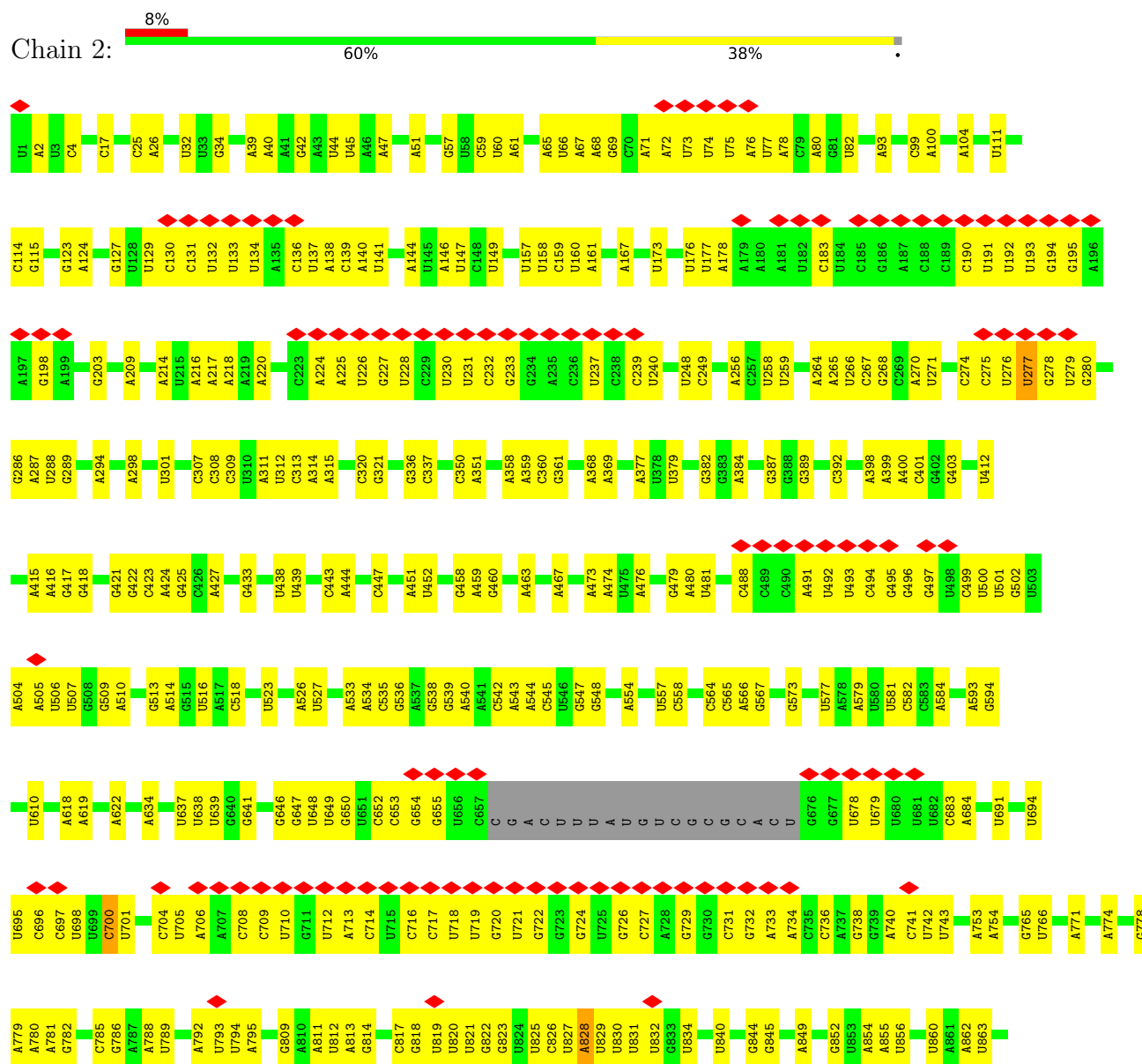
- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

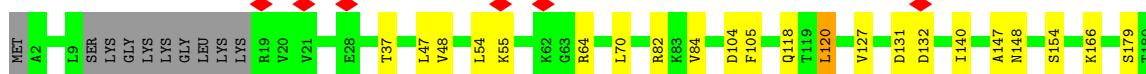
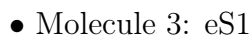
Mol	Chain	Residues	Atoms		AltConf
39	a	1	Total	Zn	0
			1	1	
39	b	1	Total	Zn	0
			1	1	
39	f	1	Total	Zn	0
			1	1	

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.

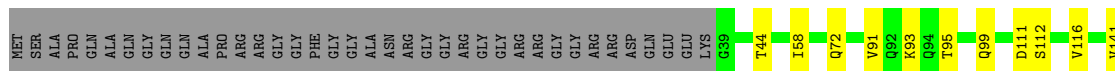
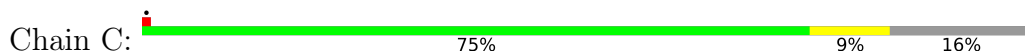
• Molecule 1: 18S rRNA



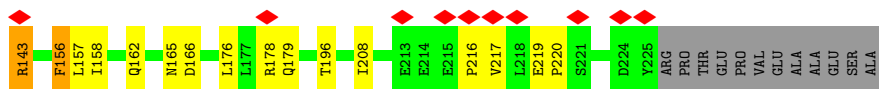
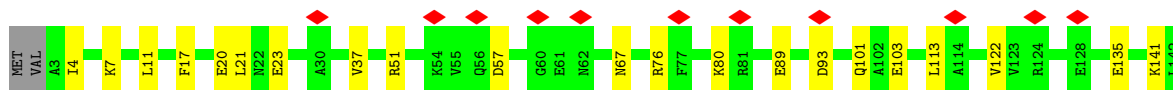
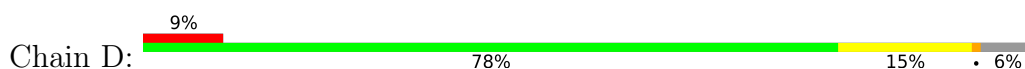




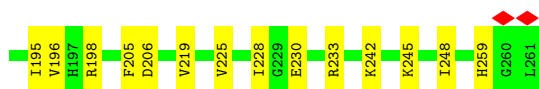
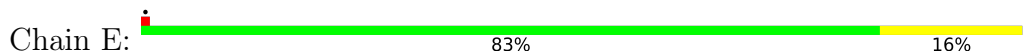
• Molecule 4: uS5



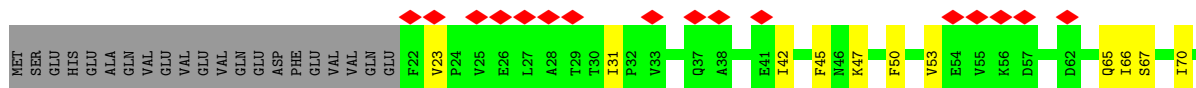
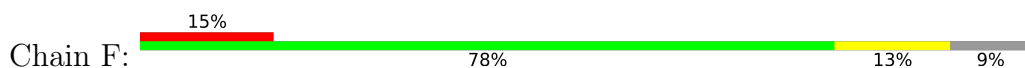
• Molecule 5: uS3



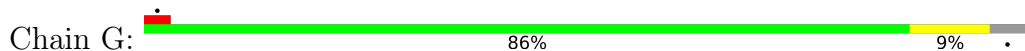
• Molecule 6: eS4

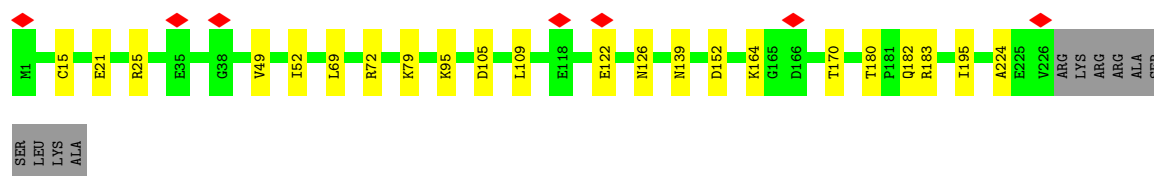


• Molecule 7: uS7

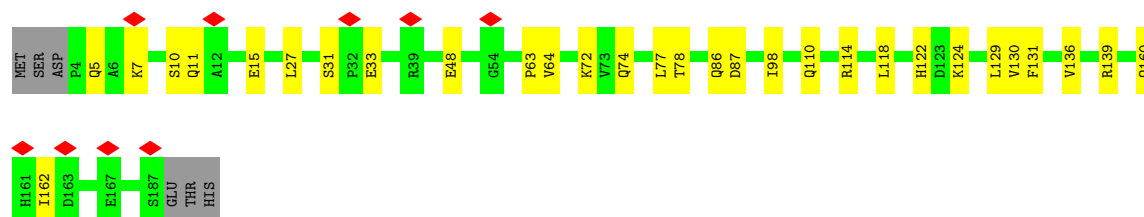
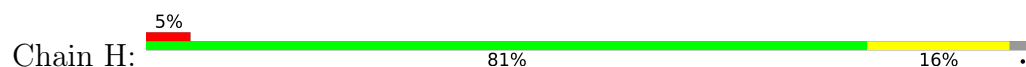


• Molecule 8: eS6

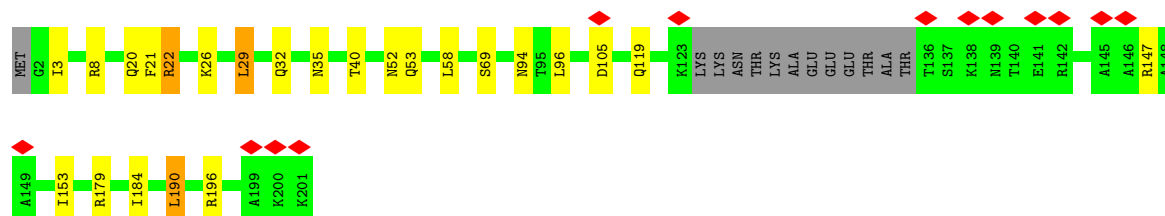
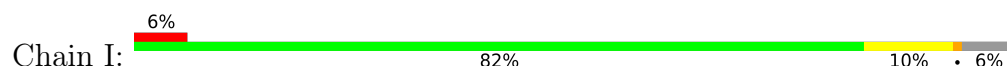




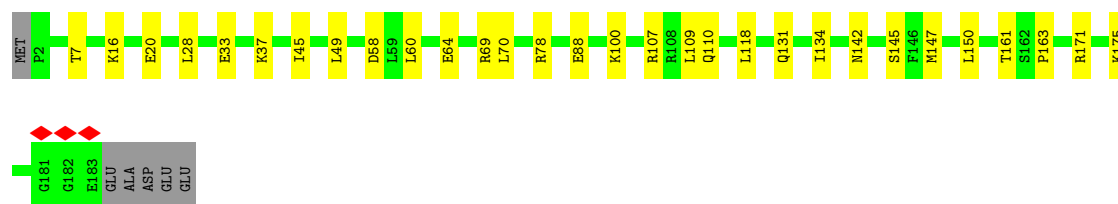
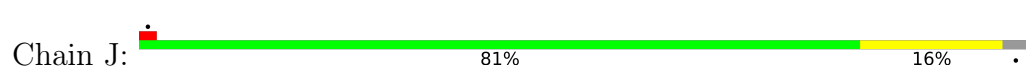
• Molecule 9: eS7



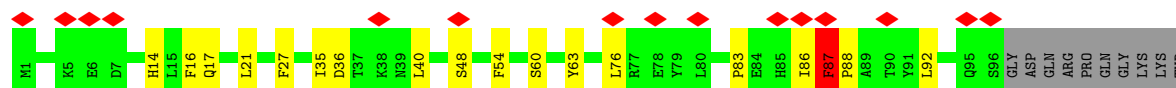
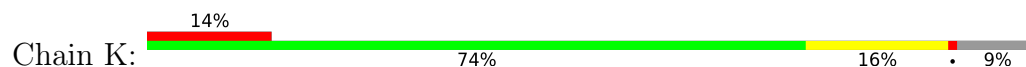
• Molecule 10: eS8



• Molecule 11: uS4

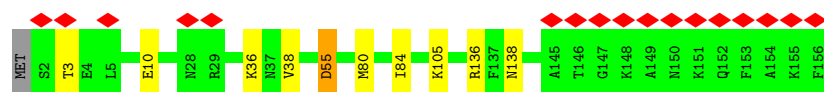


• Molecule 12: eS10

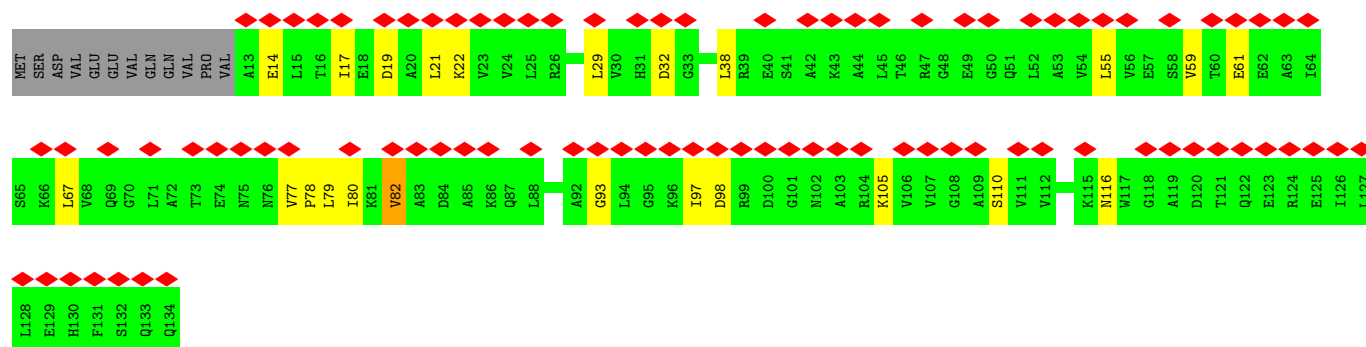
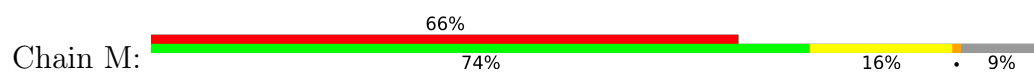


• Molecule 13: uS17

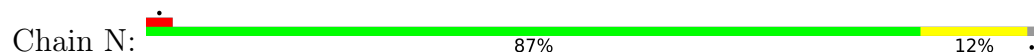




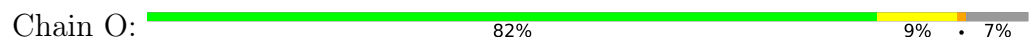
• Molecule 14: eS12



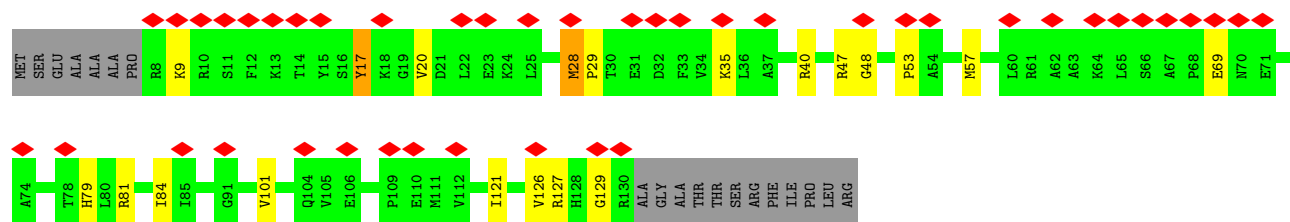
• Molecule 15: uS15



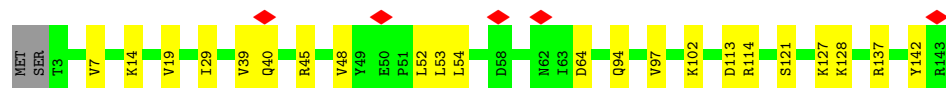
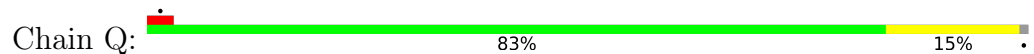
• Molecule 16: uS11




• Molecule 17: uS19

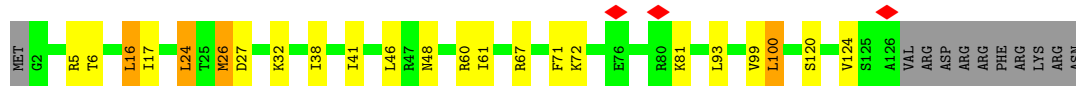


• Molecule 18: uS9




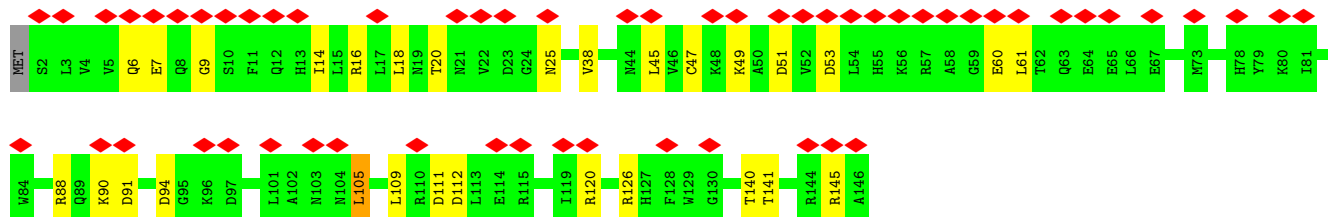
- Molecule 19: eS17

Chain R:  75% 14% 8%




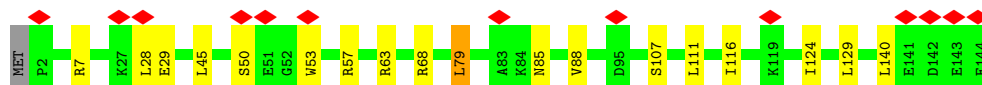
- Molecule 20: uS13

Chain S:  39% 79% 19% ..




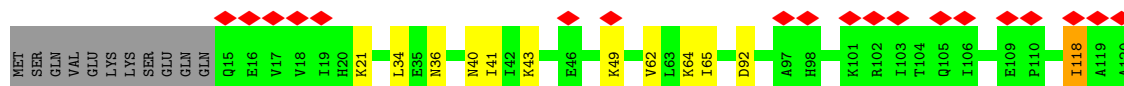
- Molecule 21: eS19

Chain T:  9% 87% 12% ..



- Molecule 22: uS10

Chain U:  16% 80% 9% 9%




- Molecule 23: eS21

Chain V:  91% 8%




- Molecule 24: uS8

Chain W:  85% 14% ..

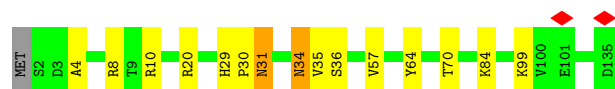
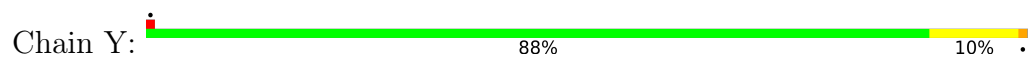


- Molecule 25: uS12

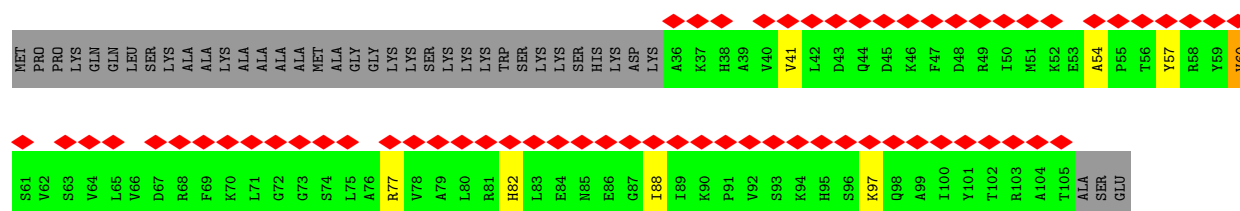
Chain X:  88% 11% ..



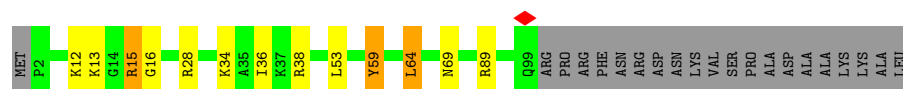
• Molecule 26: eS24



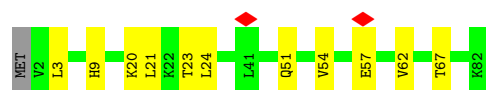
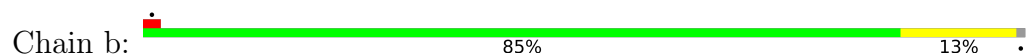
• Molecule 27: eS25



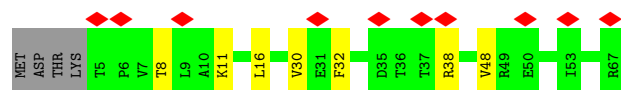
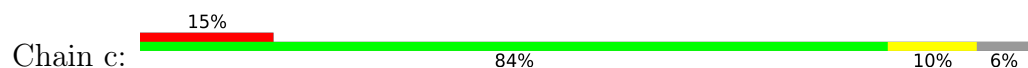
• Molecule 28: eS26



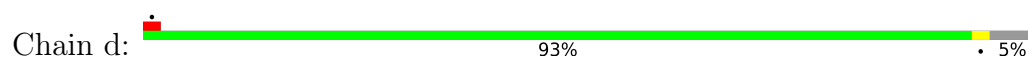
• Molecule 29: eS27

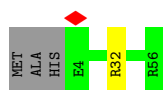


• Molecule 30: eS28

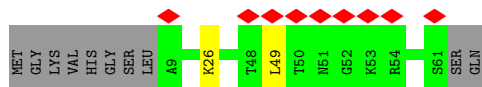
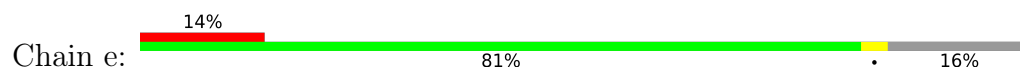


• Molecule 31: uS14

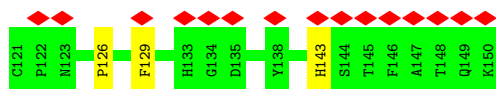
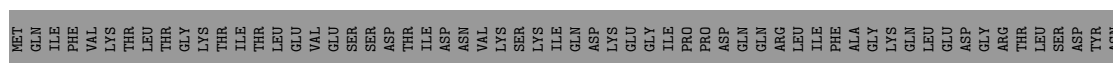
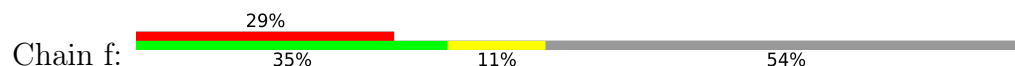




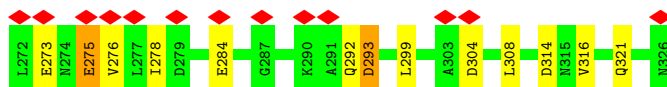
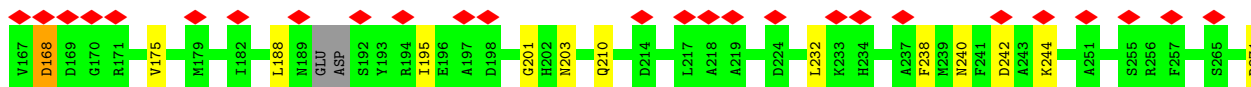
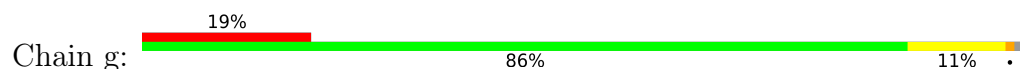
- Molecule 32: eS30



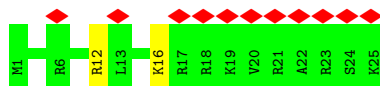
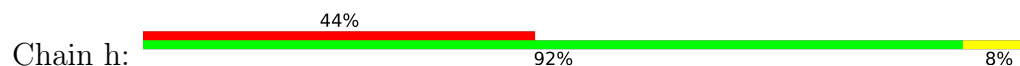
- Molecule 33: eS31



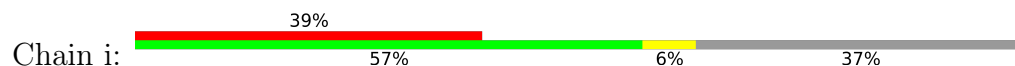
- Molecule 34: RACK1

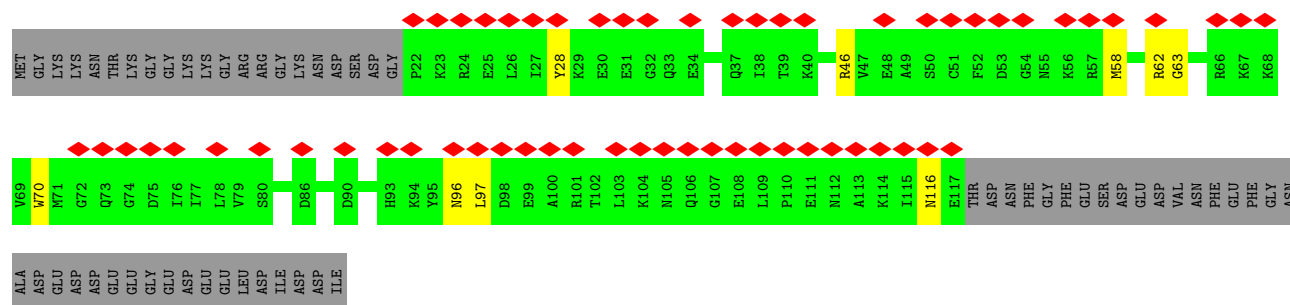


- Molecule 35: eL41

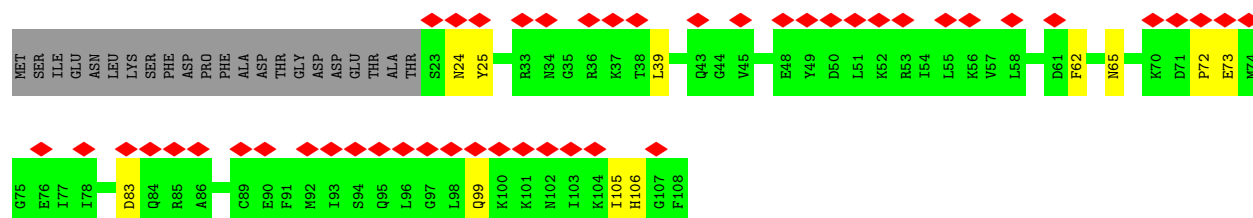
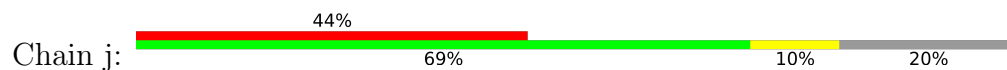


- Molecule 36: eIF1A





- Molecule 37: eIF1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	86055	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.016	Depositor
Minimum map value	-0.605	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.1	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: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.27	0/42269	0.69	8/65862 (0.0%)
2	A	0.44	0/1666	0.78	1/2279 (0.0%)
3	B	0.41	0/1798	0.73	2/2421 (0.1%)
4	C	0.42	0/1659	0.71	0/2252
5	D	0.44	0/1769	0.72	0/2378
6	E	0.39	0/2122	0.70	1/2861 (0.0%)
7	F	0.44	0/1628	0.78	0/2198
8	G	0.41	0/1835	0.71	0/2451
9	H	0.44	0/1507	0.76	2/2028 (0.1%)
10	I	0.42	0/1515	0.74	2/2029 (0.1%)
11	J	0.43	0/1495	0.82	1/2001 (0.0%)
12	K	0.49	0/831	0.74	0/1123
13	L	0.41	0/1276	0.64	0/1718
14	M	0.46	0/929	0.77	0/1255
15	N	0.44	0/1210	0.77	0/1628
16	O	0.41	0/953	0.73	0/1279
17	P	0.46	0/1000	0.72	0/1343
18	Q	0.44	0/1125	0.74	1/1510 (0.1%)
19	R	0.43	0/1002	0.82	2/1346 (0.1%)
20	S	0.42	0/1212	0.75	1/1629 (0.1%)
21	T	0.45	0/1129	0.79	1/1520 (0.1%)
22	U	0.40	0/857	0.69	0/1158
23	V	0.40	0/696	0.72	0/938
24	W	0.39	0/1039	0.77	2/1399 (0.1%)
25	X	0.41	0/1137	0.74	0/1516
26	Y	0.41	0/1075	0.72	0/1433
27	Z	0.48	0/567	0.70	0/762
28	a	0.38	0/791	0.69	0/1059
29	b	0.39	0/619	0.65	0/837
30	c	0.42	0/496	0.73	0/666
31	d	0.44	0/457	0.67	0/607
32	e	0.40	0/435	0.72	0/579

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	f	0.50	0/562	0.70	0/751
34	g	0.44	0/2521	0.63	0/3431
35	h	0.43	0/234	0.88	0/300
36	i	0.40	0/788	0.67	0/1051
37	j	0.43	0/703	0.69	0/938
All	All	0.36	0/82907	0.71	24/120536 (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
12	K	0	1
17	P	0	1
18	Q	0	1
25	X	0	1
26	Y	0	1
All	All	0	5

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1315	G	C2'-C3'-O3'	7.09	125.10	109.50
20	S	105	LEU	CA-CB-CG	7.01	131.42	115.30
10	I	29	LEU	CA-CB-CG	6.92	131.22	115.30
3	B	181	LEU	CA-CB-CG	6.79	130.92	115.30
1	2	1534	G	C2'-C3'-O3'	6.15	123.53	113.70
9	H	118	LEU	CA-CB-CG	6.12	129.37	115.30
10	I	190	LEU	CA-CB-CG	6.10	129.34	115.30
1	2	1491	A	C2'-C3'-O3'	5.79	122.96	113.70
21	T	79	LEU	CA-CB-CG	5.71	128.44	115.30
2	A	201	LEU	CA-CB-CG	5.59	128.15	115.30
6	E	38	LEU	CA-CB-CG	5.58	128.14	115.30
19	R	100	LEU	CA-CB-CG	5.57	128.11	115.30
19	R	16	LEU	CA-CB-CG	5.55	128.07	115.30
1	2	828	A	C2'-C3'-O3'	5.52	122.53	113.70
11	J	150	LEU	CA-CB-CG	5.44	127.80	115.30
1	2	1501	A	C2'-C3'-O3'	5.38	122.31	113.70
24	W	69	LEU	CA-CB-CG	5.34	127.59	115.30
9	H	77	LEU	CA-CB-CG	5.30	127.48	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1320	A	N9-C1'-C2'	5.22	120.78	114.00
1	2	277	U	C2'-C3'-O3'	5.16	121.96	113.70
3	B	120	LEU	CA-CB-CG	5.12	127.08	115.30
1	2	700	C	C2'-C3'-O3'	5.11	121.88	113.70
18	Q	52	LEU	CA-CB-CG	5.08	126.98	115.30
24	W	7	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	K	87	PHE	Peptide
17	P	28	MET	Peptide
18	Q	40	GLN	Peptide
25	X	63	GLN	Peptide
26	Y	29	HIS	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	206/254 (81%)	171 (83%)	27 (13%)	8 (4%)	3	24
3	B	219/255 (86%)	187 (85%)	20 (9%)	12 (6%)	2	16
4	C	215/259 (83%)	192 (89%)	17 (8%)	6 (3%)	5	31
5	D	221/237 (93%)	195 (88%)	17 (8%)	9 (4%)	3	23
6	E	258/261 (99%)	226 (88%)	25 (10%)	7 (3%)	5	31
7	F	204/227 (90%)	167 (82%)	28 (14%)	9 (4%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	G	224/236 (95%)	205 (92%)	15 (7%)	4 (2%)	8	39
9	H	182/190 (96%)	157 (86%)	16 (9%)	9 (5%)	2	18
10	I	184/201 (92%)	168 (91%)	9 (5%)	7 (4%)	3	24
11	J	180/188 (96%)	154 (86%)	20 (11%)	6 (3%)	4	27
12	K	94/106 (89%)	79 (84%)	9 (10%)	6 (6%)	1	13
13	L	153/156 (98%)	131 (86%)	19 (12%)	3 (2%)	7	37
14	M	120/134 (90%)	95 (79%)	18 (15%)	7 (6%)	1	15
15	N	148/151 (98%)	138 (93%)	9 (6%)	1 (1%)	22	60
16	O	125/137 (91%)	108 (86%)	11 (9%)	6 (5%)	2	19
17	P	121/142 (85%)	100 (83%)	12 (10%)	9 (7%)	1	10
18	Q	139/143 (97%)	128 (92%)	8 (6%)	3 (2%)	6	35
19	R	123/136 (90%)	104 (85%)	14 (11%)	5 (4%)	3	23
20	S	143/146 (98%)	116 (81%)	17 (12%)	10 (7%)	1	11
21	T	141/144 (98%)	125 (89%)	12 (8%)	4 (3%)	5	31
22	U	104/117 (89%)	93 (89%)	9 (9%)	2 (2%)	8	38
23	V	85/87 (98%)	70 (82%)	10 (12%)	5 (6%)	1	14
24	W	127/130 (98%)	115 (91%)	7 (6%)	5 (4%)	3	24
25	X	142/145 (98%)	121 (85%)	15 (11%)	6 (4%)	3	22
26	Y	132/135 (98%)	119 (90%)	7 (5%)	6 (4%)	2	20
27	Z	68/108 (63%)	51 (75%)	13 (19%)	4 (6%)	1	14
28	a	96/119 (81%)	82 (85%)	8 (8%)	6 (6%)	1	13
29	b	79/82 (96%)	68 (86%)	8 (10%)	3 (4%)	3	24
30	c	61/67 (91%)	55 (90%)	6 (10%)	0	100	100
31	d	51/56 (91%)	47 (92%)	4 (8%)	0	100	100
32	e	51/63 (81%)	45 (88%)	5 (10%)	1 (2%)	7	37
33	f	67/150 (45%)	40 (60%)	20 (30%)	7 (10%)	0	6
34	g	312/326 (96%)	253 (81%)	51 (16%)	8 (3%)	5	32
35	h	23/25 (92%)	23 (100%)	0	0	100	100
36	i	94/153 (61%)	83 (88%)	9 (10%)	2 (2%)	7	36
37	j	84/108 (78%)	70 (83%)	11 (13%)	3 (4%)	3	25
All	All	4976/5574 (89%)	4281 (86%)	506 (10%)	189 (4%)	5	24

All (189) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	95	ALA
3	B	55	LYS
3	B	148	ASN
4	C	141	VAL
5	D	217	VAL
5	D	220	PRO
7	F	67	SER
8	G	69	LEU
8	G	122	GLU
9	H	31	SER
9	H	64	VAL
9	H	74	GLN
9	H	136	VAL
10	I	22	ARG
10	I	147	ARG
10	I	153	ILE
12	K	60	SER
12	K	83	PRO
12	K	88	PRO
13	L	55	ASP
14	M	97	ILE
15	N	138	ASN
16	O	124	ASP
17	P	29	PRO
18	Q	39	VAL
19	R	71	PHE
24	W	78	ARG
24	W	83	ILE
25	X	12	ALA
25	X	64	PRO
26	Y	30	PRO
28	a	13	LYS
36	i	63	GLY
37	j	72	PRO
2	A	166	GLY
3	B	147	ALA
3	B	179	SER
3	B	221	PRO
6	E	3	ARG
6	E	242	LYS
6	E	245	LYS
7	F	45	PHE

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Mol	Chain	Res	Type
7	F	66	ILE
7	F	206	GLY
8	G	224	ALA
9	H	110	GLN
12	K	54	PHE
12	K	87	PHE
16	O	40	ALA
17	P	101	VAL
19	R	24	LEU
20	S	7	GLU
20	S	141	THR
22	U	49	LYS
22	U	118	ILE
23	V	9	VAL
23	V	30	SER
23	V	45	ALA
24	W	30	SER
25	X	3	LYS
26	Y	31	ASN
26	Y	34	ASN
27	Z	88	ILE
29	b	21	LEU
34	g	4	SER
36	i	96	ASN
2	A	202	TYR
3	B	54	LEU
3	B	154	SER
3	B	222	LYS
4	C	151	THR
4	C	155	GLN
4	C	253	THR
5	D	143	ARG
5	D	156	PHE
5	D	216	PRO
7	F	100	MET
7	F	102	ASN
10	I	35	ASN
10	I	40	THR
10	I	52	ASN
11	J	118	LEU
14	M	93	GLY
14	M	98	ASP

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Mol	Chain	Res	Type
14	M	110	SER
16	O	91	SER
18	Q	14	LYS
19	R	26	MET
19	R	124	VAL
20	S	6	GLN
20	S	9	GLY
20	S	60	GLU
20	S	61	LEU
21	T	28	LEU
21	T	50	SER
23	V	10	GLU
23	V	12	TYR
25	X	41	SER
25	X	63	GLN
26	Y	4	ALA
27	Z	54	ALA
28	a	59	TYR
29	b	51	GLN
33	f	87	THR
33	f	111	GLU
33	f	143	HIS
34	g	16	GLY
34	g	201	GLY
34	g	275	GLU
34	g	293	ASP
2	A	103	THR
2	A	158	VAL
2	A	195	TRP
3	B	214	LYS
4	C	44	THR
5	D	93	ASP
5	D	219	GLU
6	E	67	GLN
6	E	205	PHE
7	F	53	VAL
7	F	155	GLY
9	H	63	PRO
9	H	98	ILE
11	J	134	ILE
11	J	171	ARG
12	K	92	LEU

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Mol	Chain	Res	Type
13	L	105	LYS
14	M	78	PRO
14	M	82	VAL
16	O	25	ASP
16	O	114	ARG
17	P	28	MET
17	P	129	GLY
20	S	51	ASP
20	S	120	ARG
24	W	29	PRO
24	W	58	SER
25	X	144	ARG
26	Y	36	SER
28	a	36	ILE
37	j	24	ASN
37	j	106	HIS
3	B	207	LEU
3	B	224	ASP
4	C	112	SER
5	D	157	LEU
5	D	196	THR
6	E	195	ILE
7	F	23	VAL
8	G	152	ASP
9	H	10	SER
10	I	94	ASN
11	J	147	MET
14	M	32	ASP
16	O	42	VAL
17	P	17	TYR
17	P	69	GLU
17	P	121	ILE
18	Q	97	VAL
19	R	99	VAL
21	T	29	GLU
21	T	88	VAL
27	Z	41	VAL
28	a	15	ARG
28	a	64	LEU
29	b	62	VAL
32	e	49	LEU
33	f	118	ARG

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Mol	Chain	Res	Type
34	g	168	ASP
2	A	5	SER
2	A	21	ARG
3	B	206	PRO
6	E	105	VAL
9	H	131	PHE
11	J	110	GLN
11	J	163	PRO
13	L	3	THR
20	S	25	ASN
26	Y	64	TYR
33	f	98	VAL
34	g	64	GLY
17	P	48	GLY
17	P	53	PRO
20	S	14	ILE
33	f	126	PRO
27	Z	60	VAL
33	f	102	VAL
34	g	278	ILE
28	a	16	GLY

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%)	145 (83%)	29 (17%)	2	11
3	B	198/228 (87%)	173 (87%)	25 (13%)	4	21
4	C	176/203 (87%)	157 (89%)	19 (11%)	6	27
5	D	185/196 (94%)	155 (84%)	30 (16%)	2	12
6	E	223/224 (100%)	186 (83%)	37 (17%)	2	11
7	F	174/194 (90%)	154 (88%)	20 (12%)	5	24
8	G	192/200 (96%)	174 (91%)	18 (9%)	8	33
9	H	164/170 (96%)	145 (88%)	19 (12%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	I	147/159 (92%)	129 (88%)	18 (12%)	5	22
11	J	153/158 (97%)	130 (85%)	23 (15%)	3	15
12	K	88/96 (92%)	75 (85%)	13 (15%)	3	16
13	L	136/137 (99%)	128 (94%)	8 (6%)	19	52
14	M	97/109 (89%)	80 (82%)	17 (18%)	2	9
15	N	127/128 (99%)	110 (87%)	17 (13%)	4	19
16	O	96/104 (92%)	85 (88%)	11 (12%)	5	24
17	P	105/119 (88%)	93 (89%)	12 (11%)	5	24
18	Q	117/119 (98%)	100 (86%)	17 (14%)	3	16
19	R	112/124 (90%)	92 (82%)	20 (18%)	2	8
20	S	128/129 (99%)	109 (85%)	19 (15%)	3	16
21	T	117/118 (99%)	103 (88%)	14 (12%)	5	23
22	U	96/107 (90%)	85 (88%)	11 (12%)	5	24
23	V	73/73 (100%)	69 (94%)	4 (6%)	21	53
24	W	110/111 (99%)	97 (88%)	13 (12%)	5	23
25	X	119/120 (99%)	108 (91%)	11 (9%)	9	34
26	Y	108/109 (99%)	98 (91%)	10 (9%)	9	34
27	Z	60/88 (68%)	55 (92%)	5 (8%)	11	38
28	a	83/100 (83%)	73 (88%)	10 (12%)	5	23
29	b	71/72 (99%)	63 (89%)	8 (11%)	6	25
30	c	55/59 (93%)	48 (87%)	7 (13%)	4	20
31	d	46/48 (96%)	45 (98%)	1 (2%)	52	77
32	e	47/55 (86%)	46 (98%)	1 (2%)	53	78
33	f	58/133 (44%)	48 (83%)	10 (17%)	2	10
34	g	265/272 (97%)	231 (87%)	34 (13%)	4	20
35	h	23/23 (100%)	21 (91%)	2 (9%)	10	37
36	i	83/130 (64%)	76 (92%)	7 (8%)	11	38
37	j	77/96 (80%)	69 (90%)	8 (10%)	7	29
All	All	4283/4722 (91%)	3755 (88%)	528 (12%)	8	22

All (528) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	9	LEU
2	A	15	GLN
2	A	28	ASN
2	A	32	HIS
2	A	33	GLN
2	A	37	VAL
2	A	50	VAL
2	A	53	THR
2	A	58	VAL
2	A	59	LEU
2	A	62	ARG
2	A	88	LYS
2	A	93	THR
2	A	108	THR
2	A	109	ASN
2	A	111	ILE
2	A	112	THR
2	A	123	VAL
2	A	133	ILE
2	A	134	LYS
2	A	157	ASP
2	A	165	ARG
2	A	167	LYS
2	A	170	ILE
2	A	177	LEU
2	A	193	GLN
2	A	198	MET
2	A	201	LEU
2	A	205	ARG
3	B	37	THR
3	B	47	LEU
3	B	48	VAL
3	B	64	ARG
3	B	70	LEU
3	B	82	ARG
3	B	84	VAL
3	B	104	ASP
3	B	105	PHE
3	B	118	GLN
3	B	120	LEU
3	B	127	VAL
3	B	131	ASP
3	B	132	ASP

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Mol	Chain	Res	Type
3	B	140	ILE
3	B	166	LYS
3	B	181	LEU
3	B	183	GLN
3	B	189	ILE
3	B	191	GLU
3	B	196	GLU
3	B	207	LEU
3	B	208	GLN
3	B	213	ARG
3	B	228	LEU
4	C	58	ILE
4	C	72	GLN
4	C	91	VAL
4	C	93	LYS
4	C	95	THR
4	C	99	GLN
4	C	111	ASP
4	C	116	VAL
4	C	145	ARG
4	C	146	ARG
4	C	155	GLN
4	C	199	GLU
4	C	212	LEU
4	C	213	GLU
4	C	223	ILE
4	C	230	LEU
4	C	234	LEU
4	C	235	TRP
4	C	241	THR
5	D	4	ILE
5	D	7	LYS
5	D	11	LEU
5	D	17	PHE
5	D	20	GLU
5	D	21	LEU
5	D	23	GLU
5	D	37	VAL
5	D	51	ARG
5	D	57	ASP
5	D	67	ASN
5	D	76	ARG

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Mol	Chain	Res	Type
5	D	80	LYS
5	D	89	GLU
5	D	101	GLN
5	D	103	GLU
5	D	113	LEU
5	D	122	VAL
5	D	135	GLU
5	D	141	LYS
5	D	143	ARG
5	D	156	PHE
5	D	158	ILE
5	D	162	GLN
5	D	165	ASN
5	D	166	ASP
5	D	176	LEU
5	D	178	ARG
5	D	179	GLN
5	D	208	ILE
6	E	7	LYS
6	E	9	LEU
6	E	18	TRP
6	E	22	LYS
6	E	38	LEU
6	E	45	ILE
6	E	51	ARG
6	E	60	GLU
6	E	69	HIS
6	E	75	LYS
6	E	77	ARG
6	E	79	ASP
6	E	91	THR
6	E	102	VAL
6	E	108	ARG
6	E	113	ARG
6	E	116	ASP
6	E	123	LEU
6	E	139	VAL
6	E	142	HIS
6	E	155	LYS
6	E	163	ASP
6	E	168	THR
6	E	180	LEU

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Mol	Chain	Res	Type
6	E	181	VAL
6	E	189	LEU
6	E	192	VAL
6	E	196	VAL
6	E	198	ARG
6	E	206	ASP
6	E	219	VAL
6	E	225	VAL
6	E	228	ILE
6	E	230	GLU
6	E	233	ARG
6	E	248	ILE
6	E	259	HIS
7	F	31	ILE
7	F	42	ILE
7	F	47	LYS
7	F	50	PHE
7	F	65	GLN
7	F	70	ILE
7	F	91	ILE
7	F	99	LEU
7	F	116	VAL
7	F	150	ARG
7	F	158	ARG
7	F	162	VAL
7	F	167	LEU
7	F	186	PHE
7	F	187	ARG
7	F	188	ASN
7	F	192	ILE
7	F	196	LEU
7	F	201	ILE
7	F	220	GLU
8	G	15	CYS
8	G	21	GLU
8	G	25	ARG
8	G	49	VAL
8	G	52	ILE
8	G	72	ARG
8	G	79	LYS
8	G	95	LYS
8	G	105	ASP

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Mol	Chain	Res	Type
8	G	109	LEU
8	G	126	ASN
8	G	139	ASN
8	G	164	LYS
8	G	170	THR
8	G	180	THR
8	G	182	GLN
8	G	183	ARG
8	G	195	ILE
9	H	5	GLN
9	H	7	LYS
9	H	11	GLN
9	H	15	GLU
9	H	27	LEU
9	H	33	GLU
9	H	48	GLU
9	H	72	LYS
9	H	78	THR
9	H	86	GLN
9	H	87	ASP
9	H	114	ARG
9	H	122	HIS
9	H	124	LYS
9	H	129	LEU
9	H	130	VAL
9	H	139	ARG
9	H	160	GLN
9	H	162	ILE
10	I	3	ILE
10	I	8	ARG
10	I	20	GLN
10	I	21	PHE
10	I	22	ARG
10	I	26	LYS
10	I	29	LEU
10	I	32	GLN
10	I	53	GLN
10	I	58	LEU
10	I	69	SER
10	I	96	LEU
10	I	105	ASP
10	I	119	GLN

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Mol	Chain	Res	Type
10	I	179	ARG
10	I	184	ILE
10	I	190	LEU
10	I	196	ARG
11	J	7	THR
11	J	16	LYS
11	J	20	GLU
11	J	28	LEU
11	J	33	GLU
11	J	37	LYS
11	J	45	ILE
11	J	49	LEU
11	J	58	ASP
11	J	60	LEU
11	J	64	GLU
11	J	69	ARG
11	J	70	LEU
11	J	78	ARG
11	J	88	GLU
11	J	100	LYS
11	J	107	ARG
11	J	109	LEU
11	J	131	GLN
11	J	142	ASN
11	J	145	SER
11	J	161	THR
11	J	175	LYS
12	K	14	HIS
12	K	16	PHE
12	K	17	GLN
12	K	21	LEU
12	K	27	PHE
12	K	35	ILE
12	K	36	ASP
12	K	40	LEU
12	K	48	SER
12	K	63	TYR
12	K	76	LEU
12	K	86	ILE
12	K	87	PHE
13	L	10	GLU
13	L	36	LYS

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Mol	Chain	Res	Type
13	L	38	VAL
13	L	55	ASP
13	L	80	MET
13	L	84	ILE
13	L	136	ARG
13	L	138	ASN
14	M	14	GLU
14	M	17	ILE
14	M	19	ASP
14	M	21	LEU
14	M	22	LYS
14	M	29	LEU
14	M	38	LEU
14	M	55	LEU
14	M	59	VAL
14	M	61	GLU
14	M	67	LEU
14	M	77	VAL
14	M	79	LEU
14	M	80	ILE
14	M	82	VAL
14	M	105	LYS
14	M	116	ASN
15	N	3	ARG
15	N	9	LYS
15	N	27	LYS
15	N	42	ARG
15	N	53	LEU
15	N	64	LYS
15	N	73	ARG
15	N	88	LEU
15	N	96	VAL
15	N	99	ARG
15	N	100	LYS
15	N	102	LEU
15	N	104	ARG
15	N	106	ARG
15	N	107	LYS
15	N	112	LYS
15	N	121	ARG
16	O	24	ASN
16	O	37	GLU

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Mol	Chain	Res	Type
16	O	49	LYS
16	O	65	GLN
16	O	86	THR
16	O	102	LEU
16	O	110	LEU
16	O	112	ILE
16	O	114	ARG
16	O	116	GLU
16	O	124	ASP
17	P	9	LYS
17	P	17	TYR
17	P	20	VAL
17	P	35	LYS
17	P	40	ARG
17	P	47	ARG
17	P	57	MET
17	P	79	HIS
17	P	81	ARG
17	P	84	ILE
17	P	126	VAL
17	P	127	ARG
18	Q	7	VAL
18	Q	19	VAL
18	Q	29	ILE
18	Q	45	ARG
18	Q	48	VAL
18	Q	53	LEU
18	Q	54	LEU
18	Q	64	ASP
18	Q	94	GLN
18	Q	102	LYS
18	Q	113	ASP
18	Q	114	ARG
18	Q	121	SER
18	Q	127	LYS
18	Q	128	LYS
18	Q	137	ARG
18	Q	142	TYR
19	R	5	ARG
19	R	6	THR
19	R	16	LEU
19	R	17	ILE

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Mol	Chain	Res	Type
19	R	24	LEU
19	R	26	MET
19	R	27	ASP
19	R	32	LYS
19	R	38	ILE
19	R	41	ILE
19	R	46	LEU
19	R	48	ASN
19	R	60	ARG
19	R	61	ILE
19	R	67	ARG
19	R	72	LYS
19	R	81	LYS
19	R	93	LEU
19	R	100	LEU
19	R	120	SER
20	S	16	ARG
20	S	18	LEU
20	S	20	THR
20	S	38	VAL
20	S	45	LEU
20	S	47	CYS
20	S	49	LYS
20	S	53	ASP
20	S	88	ARG
20	S	90	LYS
20	S	91	ASP
20	S	94	ASP
20	S	105	LEU
20	S	109	LEU
20	S	111	ASP
20	S	112	ASP
20	S	126	ARG
20	S	140	THR
20	S	145	ARG
21	T	7	ARG
21	T	45	LEU
21	T	53	TRP
21	T	57	ARG
21	T	63	ARG
21	T	68	ARG
21	T	79	LEU

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Mol	Chain	Res	Type
21	T	85	ASN
21	T	107	SER
21	T	111	LEU
21	T	116	ILE
21	T	124	ILE
21	T	129	LEU
21	T	140	LEU
22	U	21	LYS
22	U	34	LEU
22	U	36	ASN
22	U	40	ASN
22	U	41	ILE
22	U	43	LYS
22	U	62	VAL
22	U	64	LYS
22	U	65	ILE
22	U	92	ASP
22	U	118	ILE
23	V	1	MET
23	V	8	LEU
23	V	12	TYR
23	V	44	ARG
24	W	3	ARG
24	W	7	LEU
24	W	24	GLN
24	W	25	VAL
24	W	28	ARG
24	W	47	ILE
24	W	55	ASP
24	W	75	ILE
24	W	80	ASN
24	W	104	LEU
24	W	111	MET
24	W	124	LYS
24	W	129	VAL
25	X	5	LYS
25	X	9	LEU
25	X	19	ARG
25	X	30	LYS
25	X	56	LYS
25	X	73	ARG
25	X	79	ASN

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Mol	Chain	Res	Type
25	X	84	THR
25	X	94	ASN
25	X	100	ASP
25	X	107	PHE
26	Y	8	ARG
26	Y	10	ARG
26	Y	20	ARG
26	Y	31	ASN
26	Y	34	ASN
26	Y	35	VAL
26	Y	57	VAL
26	Y	70	THR
26	Y	84	LYS
26	Y	99	LYS
27	Z	57	TYR
27	Z	60	VAL
27	Z	77	ARG
27	Z	82	HIS
27	Z	97	LYS
28	a	12	LYS
28	a	15	ARG
28	a	28	ARG
28	a	34	LYS
28	a	38	ARG
28	a	53	LEU
28	a	59	TYR
28	a	64	LEU
28	a	69	ASN
28	a	89	ARG
29	b	3	LEU
29	b	9	HIS
29	b	20	LYS
29	b	23	THR
29	b	24	LEU
29	b	54	VAL
29	b	57	GLU
29	b	67	THR
30	c	8	THR
30	c	11	LYS
30	c	16	LEU
30	c	30	VAL
30	c	32	PHE

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Mol	Chain	Res	Type
30	c	38	ARG
30	c	48	VAL
31	d	32	ARG
32	e	26	LYS
33	f	82	LYS
33	f	85	TYR
33	f	90	LYS
33	f	93	HIS
33	f	94	LYS
33	f	96	LYS
33	f	105	TYR
33	f	109	ASP
33	f	116	LYS
33	f	129	PHE
34	g	43	LEU
34	g	49	THR
34	g	55	PHE
34	g	60	ARG
34	g	67	HIS
34	g	70	GLN
34	g	74	VAL
34	g	97	THR
34	g	124	ILE
34	g	137	THR
34	g	168	ASP
34	g	175	VAL
34	g	188	LEU
34	g	195	ILE
34	g	203	ASN
34	g	210	GLN
34	g	232	LEU
34	g	238	PHE
34	g	240	ASN
34	g	242	ASP
34	g	244	LYS
34	g	271	ASP
34	g	273	GLU
34	g	275	GLU
34	g	276	VAL
34	g	284	GLU
34	g	292	GLN
34	g	293	ASP

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Mol	Chain	Res	Type
34	g	299	LEU
34	g	304	ASP
34	g	308	LEU
34	g	314	ASP
34	g	316	VAL
34	g	321	GLN
35	h	12	ARG
35	h	16	LYS
36	i	28	TYR
36	i	46	ARG
36	i	58	MET
36	i	62	ARG
36	i	70	TRP
36	i	97	LEU
36	i	116	ASN
37	j	25	TYR
37	j	39	LEU
37	j	62	PHE
37	j	65	ASN
37	j	73	GLU
37	j	83	ASP
37	j	99	GLN
37	j	105	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	109	ASN
2	A	131	GLN
3	B	101	HIS
3	B	220	GLN
4	C	99	GLN
5	D	67	ASN
5	D	159	HIS
5	D	162	GLN
5	D	165	ASN
5	D	179	GLN
6	E	50	ASN
6	E	112	HIS
6	E	130	GLN
6	E	224	ASN
7	F	36	GLN

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Mol	Chain	Res	Type
7	F	39	GLN
7	F	40	GLN
7	F	46	ASN
7	F	188	ASN
7	F	226	ASN
8	G	10	ASN
8	G	13	GLN
8	G	139	ASN
9	H	42	GLN
9	H	155	ASN
10	I	116	HIS
12	K	17	GLN
12	K	58	GLN
13	L	8	GLN
13	L	22	ASN
15	N	62	GLN
16	O	12	GLN
16	O	29	HIS
16	O	80	HIS
16	O	99	GLN
17	P	79	HIS
18	Q	83	GLN
19	R	48	ASN
19	R	62	GLN
19	R	83	GLN
19	R	105	GLN
20	S	25	ASN
20	S	78	HIS
20	S	99	HIS
20	S	122	HIS
21	T	25	GLN
21	T	64	HIS
21	T	85	ASN
21	T	91	HIS
21	T	93	HIS
21	T	101	ASN
21	T	106	GLN
22	U	40	ASN
22	U	44	ASN
22	U	105	GLN
23	V	7	GLN
24	W	24	GLN

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Mol	Chain	Res	Type
25	X	18	HIS
25	X	22	ASN
25	X	79	ASN
27	Z	44	GLN
27	Z	82	HIS
28	a	17	HIS
29	b	42	ASN
31	d	10	HIS
36	i	44	ASN
36	i	55	ASN
36	i	85	GLN
37	j	84	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1778/1799 (98%)	675 (37%)	113 (6%)

All (675) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A
1	2	32	U
1	2	34	G
1	2	39	A
1	2	40	A
1	2	42	G
1	2	45	U
1	2	47	A
1	2	51	A
1	2	57	G
1	2	59	C
1	2	60	U
1	2	61	A
1	2	65	A
1	2	67	A
1	2	68	A

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Mol	Chain	Res	Type
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
1	2	80	A
1	2	82	U
1	2	93	A
1	2	100	A
1	2	104	A
1	2	111	U
1	2	114	C
1	2	115	G
1	2	123	G
1	2	124	A
1	2	127	G
1	2	129	U
1	2	130	C
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	136	C
1	2	137	U
1	2	138	A
1	2	139	C
1	2	140	A
1	2	141	U
1	2	144	A
1	2	146	A
1	2	147	U
1	2	149	U
1	2	157	U
1	2	158	U
1	2	159	C
1	2	160	U
1	2	161	A
1	2	167	A

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Mol	Chain	Res	Type
1	2	173	U
1	2	176	U
1	2	178	A
1	2	183	C
1	2	190	C
1	2	191	U
1	2	192	U
1	2	194	G
1	2	195	G
1	2	198	G
1	2	203	G
1	2	209	A
1	2	214	A
1	2	217	A
1	2	218	A
1	2	220	A
1	2	224	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	233	G
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	259	U
1	2	264	A
1	2	265	A
1	2	266	U
1	2	267	C
1	2	268	G
1	2	270	A
1	2	271	U
1	2	274	C
1	2	275	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	286	G
1	2	287	A
1	2	288	U
1	2	289	G
1	2	294	A
1	2	298	A
1	2	301	U
1	2	307	C
1	2	308	C
1	2	309	C
1	2	311	A
1	2	312	U
1	2	313	C
1	2	314	A
1	2	315	A
1	2	320	C
1	2	321	G
1	2	336	G
1	2	337	C
1	2	350	C
1	2	351	A
1	2	358	A
1	2	359	A
1	2	360	C
1	2	361	G
1	2	368	A
1	2	369	A
1	2	377	A
1	2	379	U
1	2	382	G
1	2	384	A
1	2	387	G
1	2	389	G
1	2	392	C
1	2	399	A
1	2	400	A
1	2	401	C
1	2	403	G

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Mol	Chain	Res	Type
1	2	412	U
1	2	415	A
1	2	416	A
1	2	417	G
1	2	418	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	438	U
1	2	439	U
1	2	443	C
1	2	444	A
1	2	447	C
1	2	452	U
1	2	458	G
1	2	459	A
1	2	460	G
1	2	463	A
1	2	467	A
1	2	473	A
1	2	474	A
1	2	476	A
1	2	479	G
1	2	480	A
1	2	481	U
1	2	488	C
1	2	491	A
1	2	492	U
1	2	493	U
1	2	494	C
1	2	495	G
1	2	496	G
1	2	497	G
1	2	499	C
1	2	500	U
1	2	501	U
1	2	502	G
1	2	504	A

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Mol	Chain	Res	Type
1	2	505	A
1	2	506	U
1	2	507	U
1	2	509	G
1	2	510	A
1	2	513	G
1	2	514	A
1	2	516	U
1	2	518	C
1	2	523	U
1	2	526	A
1	2	527	U
1	2	533	A
1	2	534	A
1	2	535	C
1	2	536	G
1	2	539	G
1	2	540	A
1	2	542	C
1	2	543	A
1	2	544	A
1	2	545	C
1	2	547	G
1	2	548	G
1	2	554	A
1	2	557	U
1	2	558	C
1	2	564	C
1	2	565	C
1	2	566	A
1	2	567	G
1	2	573	G
1	2	577	U
1	2	579	A
1	2	581	U
1	2	582	C
1	2	584	A
1	2	593	A
1	2	594	G
1	2	610	U
1	2	618	A
1	2	619	A

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Mol	Chain	Res	Type
1	2	622	A
1	2	634	A
1	2	637	U
1	2	638	U
1	2	639	U
1	2	641	G
1	2	646	G
1	2	647	G
1	2	648	U
1	2	649	U
1	2	650	G
1	2	652	C
1	2	653	C
1	2	654	G
1	2	655	G
1	2	678	U
1	2	679	U
1	2	683	C
1	2	684	A
1	2	691	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	704	C
1	2	705	U
1	2	706	A
1	2	708	C
1	2	709	C
1	2	710	U
1	2	712	U
1	2	713	A
1	2	714	C
1	2	716	C
1	2	717	C
1	2	718	U
1	2	719	U
1	2	721	U
1	2	722	G

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Mol	Chain	Res	Type
1	2	724	G
1	2	726	G
1	2	727	C
1	2	729	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	736	C
1	2	738	G
1	2	740	A
1	2	741	C
1	2	742	U
1	2	743	U
1	2	753	A
1	2	754	A
1	2	765	G
1	2	766	U
1	2	771	A
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	785	C
1	2	786	G
1	2	788	A
1	2	789	U
1	2	792	A
1	2	793	U
1	2	794	U
1	2	795	A
1	2	811	A
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

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Mol	Chain	Res	Type
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	831	U
1	2	832	U
1	2	834	U
1	2	840	U
1	2	844	G
1	2	845	G
1	2	849	A
1	2	852	G
1	2	855	A
1	2	856	U
1	2	860	U
1	2	862	A
1	2	863	U
1	2	872	U
1	2	875	G
1	2	876	G
1	2	877	G
1	2	895	U
1	2	896	C
1	2	897	A
1	2	898	G
1	2	904	A
1	2	905	A
1	2	911	U
1	2	913	G
1	2	914	A
1	2	915	U
1	2	919	U
1	2	920	U
1	2	927	U
1	2	932	A
1	2	933	C
1	2	934	U
1	2	941	G

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Mol	Chain	Res	Type
1	2	943	A
1	2	950	A
1	2	958	U
1	2	959	U
1	2	965	A
1	2	969	A
1	2	972	A
1	2	978	A
1	2	981	U
1	2	983	G
1	2	987	A
1	2	991	A
1	2	993	G
1	2	994	A
1	2	1003	U
1	2	1011	U
1	2	1020	C
1	2	1024	A
1	2	1025	A
1	2	1026	A
1	2	1027	C
1	2	1028	U
1	2	1030	U
1	2	1031	G
1	2	1038	A
1	2	1039	G
1	2	1041	G
1	2	1042	A
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	1075	A
1	2	1080	A
1	2	1081	C
1	2	1082	G

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Mol	Chain	Res	Type
1	2	1083	A
1	2	1091	A
1	2	1095	C
1	2	1096	U
1	2	1097	U
1	2	1098	U
1	2	1099	G
1	2	1107	G
1	2	1108	G
1	2	1110	G
1	2	1113	G
1	2	1118	G
1	2	1121	G
1	2	1130	A
1	2	1137	A
1	2	1142	A
1	2	1149	G
1	2	1150	A
1	2	1157	C
1	2	1158	C
1	2	1166	G
1	2	1167	U
1	2	1173	C
1	2	1175	G
1	2	1184	U
1	2	1189	C
1	2	1190	U
1	2	1193	A
1	2	1194	C
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	1211	G
1	2	1212	G
1	2	1215	C
1	2	1216	A
1	2	1217	G

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Mol	Chain	Res	Type
1	2	1218	A
1	2	1222	A
1	2	1224	U
1	2	1225	A
1	2	1226	A
1	2	1227	G
1	2	1228	G
1	2	1234	C
1	2	1236	G
1	2	1238	U
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	1250	U
1	2	1254	G
1	2	1258	U
1	2	1259	U
1	2	1265	U
1	2	1268	U
1	2	1269	G
1	2	1272	G
1	2	1274	A
1	2	1282	U
1	2	1283	C
1	2	1284	U
1	2	1296	G
1	2	1298	G
1	2	1305	C
1	2	1306	U
1	2	1307	G
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	1323	G
1	2	1324	A

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Mol	Chain	Res	Type
1	2	1336	A
1	2	1339	U
1	2	1340	A
1	2	1343	A
1	2	1344	A
1	2	1347	A
1	2	1349	G
1	2	1350	G
1	2	1351	U
1	2	1353	G
1	2	1356	G
1	2	1358	C
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	1368	U
1	2	1369	U
1	2	1370	G
1	2	1371	A
1	2	1380	A
1	2	1384	G
1	2	1388	U
1	2	1389	A
1	2	1396	U
1	2	1397	C
1	2	1398	A
1	2	1400	G
1	2	1404	A
1	2	1410	G
1	2	1411	U
1	2	1412	U
1	2	1413	U
1	2	1416	G
1	2	1425	A
1	2	1426	G
1	2	1429	C
1	2	1430	U
1	2	1433	G

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Mol	Chain	Res	Type
1	2	1434	A
1	2	1442	A
1	2	1443	G
1	2	1444	A
1	2	1445	C
1	2	1446	G
1	2	1449	C
1	2	1450	U
1	2	1454	C
1	2	1456	G
1	2	1457	C
1	2	1458	A
1	2	1460	G
1	2	1461	C
1	2	1463	C
1	2	1464	G
1	2	1467	A
1	2	1468	C
1	2	1469	A
1	2	1471	U
1	2	1475	G
1	2	1476	G
1	2	1481	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	1501	A
1	2	1502	G
1	2	1504	G
1	2	1505	G
1	2	1506	U
1	2	1507	C
1	2	1508	U
1	2	1509	G

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Mol	Chain	Res	Type
1	2	1512	U
1	2	1514	A
1	2	1519	G
1	2	1520	U
1	2	1521	G
1	2	1522	A
1	2	1531	C
1	2	1532	G
1	2	1533	U
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	1546	G
1	2	1552	U
1	2	1553	A
1	2	1554	A
1	2	1555	U
1	2	1557	A
1	2	1563	C
1	2	1566	C
1	2	1569	C
1	2	1570	G
1	2	1571	A
1	2	1573	G
1	2	1580	U
1	2	1581	A
1	2	1583	U
1	2	1588	G
1	2	1591	A
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	1603	G
1	2	1605	G
1	2	1606	U
1	2	1613	C

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Mol	Chain	Res	Type
1	2	1614	G
1	2	1616	C
1	2	1617	C
1	2	1632	C
1	2	1633	A
1	2	1634	C
1	2	1643	G
1	2	1647	G
1	2	1655	U
1	2	1656	G
1	2	1678	G
1	2	1679	A
1	2	1682	U
1	2	1685	U
1	2	1686	U
1	2	1687	A
1	2	1688	G
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	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	1725	G
1	2	1729	A
1	2	1730	A
1	2	1742	A
1	2	1743	G
1	2	1748	A

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Mol	Chain	Res	Type
1	2	1750	U
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	1770	C
1	2	1777	U
1	2	1778	G
1	2	1779	A
1	2	1780	A
1	2	1781	C
1	2	1784	G
1	2	1790	G
1	2	1791	G
1	2	1792	A
1	2	1794	C
1	2	1795	A
1	2	1796	U
1	2	1797	U
1	2	1798	A

All (113) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	44	U
1	2	66	U
1	2	71	A
1	2	72	A
1	2	73	U
1	2	80	A
1	2	99	C
1	2	129	U
1	2	130	C
1	2	131	C
1	2	133	U
1	2	134	U
1	2	137	U

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Mol	Chain	Res	Type
1	2	140	A
1	2	157	U
1	2	177	U
1	2	190	C
1	2	193	U
1	2	216	A
1	2	217	A
1	2	226	U
1	2	227	G
1	2	239	C
1	2	240	U
1	2	258	U
1	2	271	U
1	2	277	U
1	2	279	U
1	2	368	A
1	2	398	A
1	2	399	A
1	2	416	A
1	2	422	G
1	2	424	A
1	2	427	A
1	2	451	A
1	2	467	A
1	2	497	G
1	2	504	A
1	2	538	G
1	2	542	C
1	2	557	U
1	2	564	C
1	2	577	U
1	2	619	A
1	2	638	U
1	2	694	U
1	2	695	U
1	2	697	C
1	2	700	C
1	2	704	C
1	2	708	C
1	2	710	U
1	2	720	G
1	2	721	U

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Mol	Chain	Res	Type
1	2	742	U
1	2	765	G
1	2	779	A
1	2	792	A
1	2	794	U
1	2	809	G
1	2	818	G
1	2	828	A
1	2	854	A
1	2	911	U
1	2	912	G
1	2	914	A
1	2	1051	U
1	2	1056	U
1	2	1080	A
1	2	1095	C
1	2	1098	U
1	2	1107	G
1	2	1189	C
1	2	1195	A
1	2	1216	A
1	2	1226	A
1	2	1241	A
1	2	1242	G
1	2	1243	A
1	2	1283	C
1	2	1313	U
1	2	1315	G
1	2	1320	A
1	2	1343	A
1	2	1397	C
1	2	1412	U
1	2	1429	C
1	2	1433	G
1	2	1443	G
1	2	1455	C
1	2	1491	A
1	2	1501	A
1	2	1505	G
1	2	1515	U
1	2	1534	G
1	2	1535	C

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Mol	Chain	Res	Type
1	2	1554	A
1	2	1555	U
1	2	1580	U
1	2	1598	A
1	2	1613	C
1	2	1631	A
1	2	1632	C
1	2	1655	U
1	2	1678	G
1	2	1754	A
1	2	1759	U
1	2	1765	G
1	2	1766	G
1	2	1778	G
1	2	1791	G
1	2	1795	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 83 ligands modelled in this entry, 83 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.

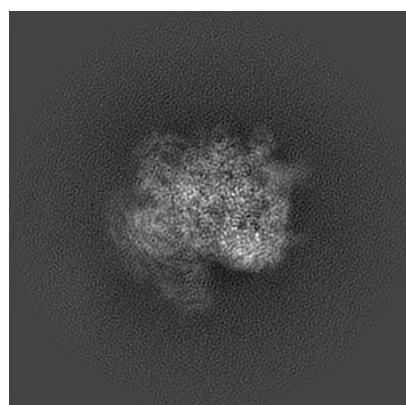
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3047. These allow visual inspection of the internal detail of the map and identification of artifacts.

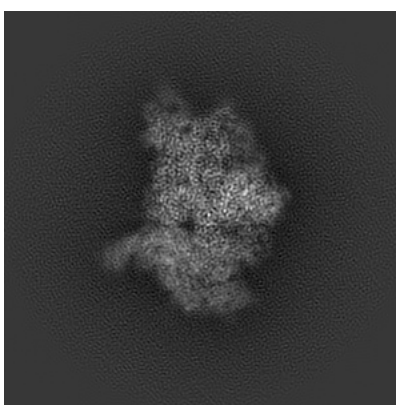
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

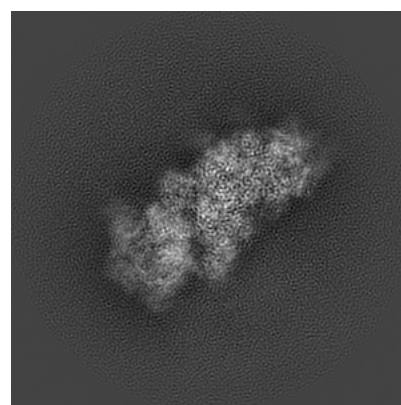
6.1.1 Primary map



X



Y

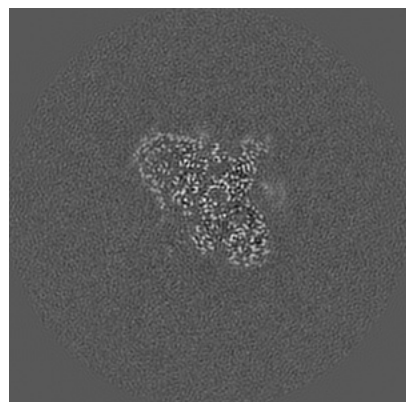


Z

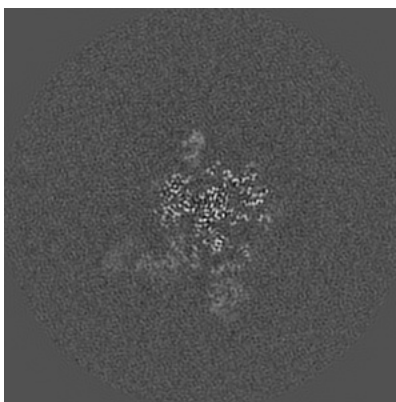
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

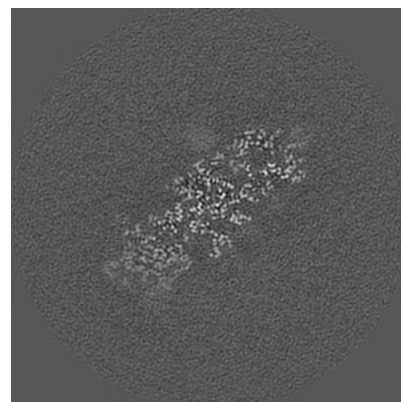
6.2.1 Primary map



X Index: 150



Y Index: 150

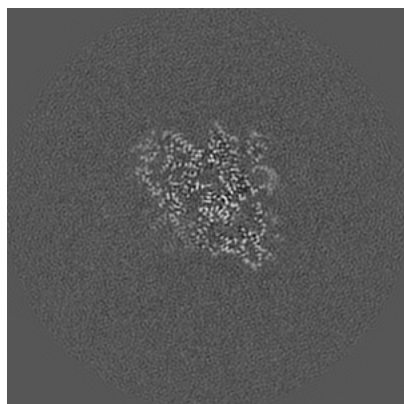


Z Index: 150

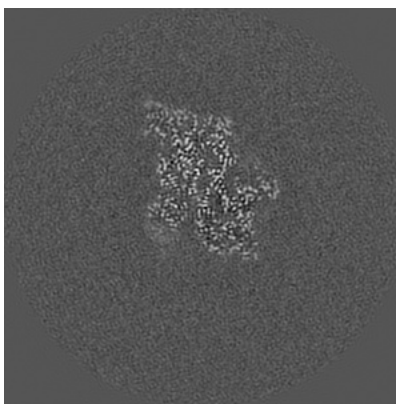
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

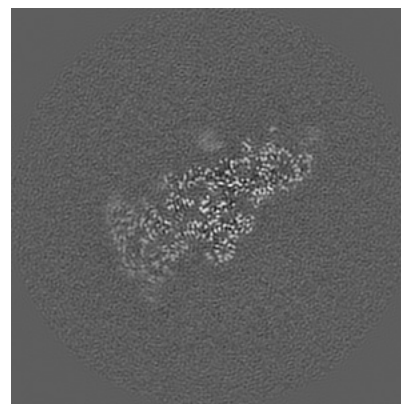
6.3.1 Primary map



X Index: 157



Y Index: 170

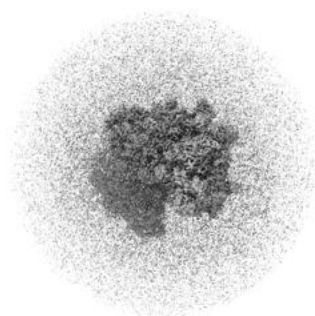


Z Index: 161

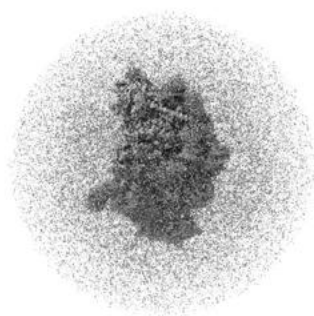
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

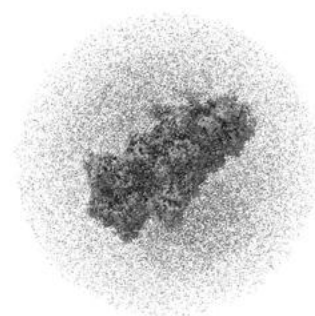
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

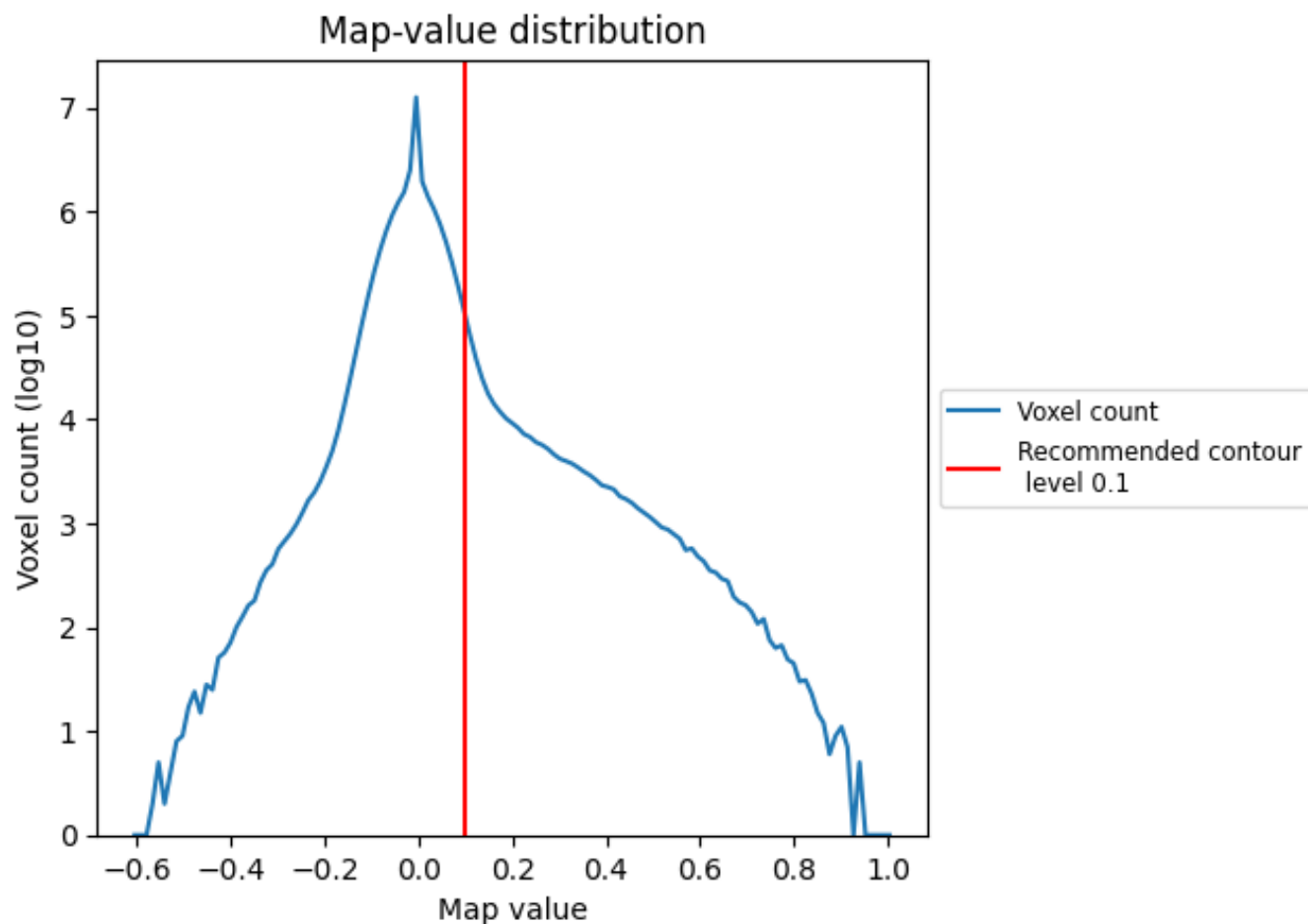
6.5 Mask visualisation

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

7 Map analysis [i](#)

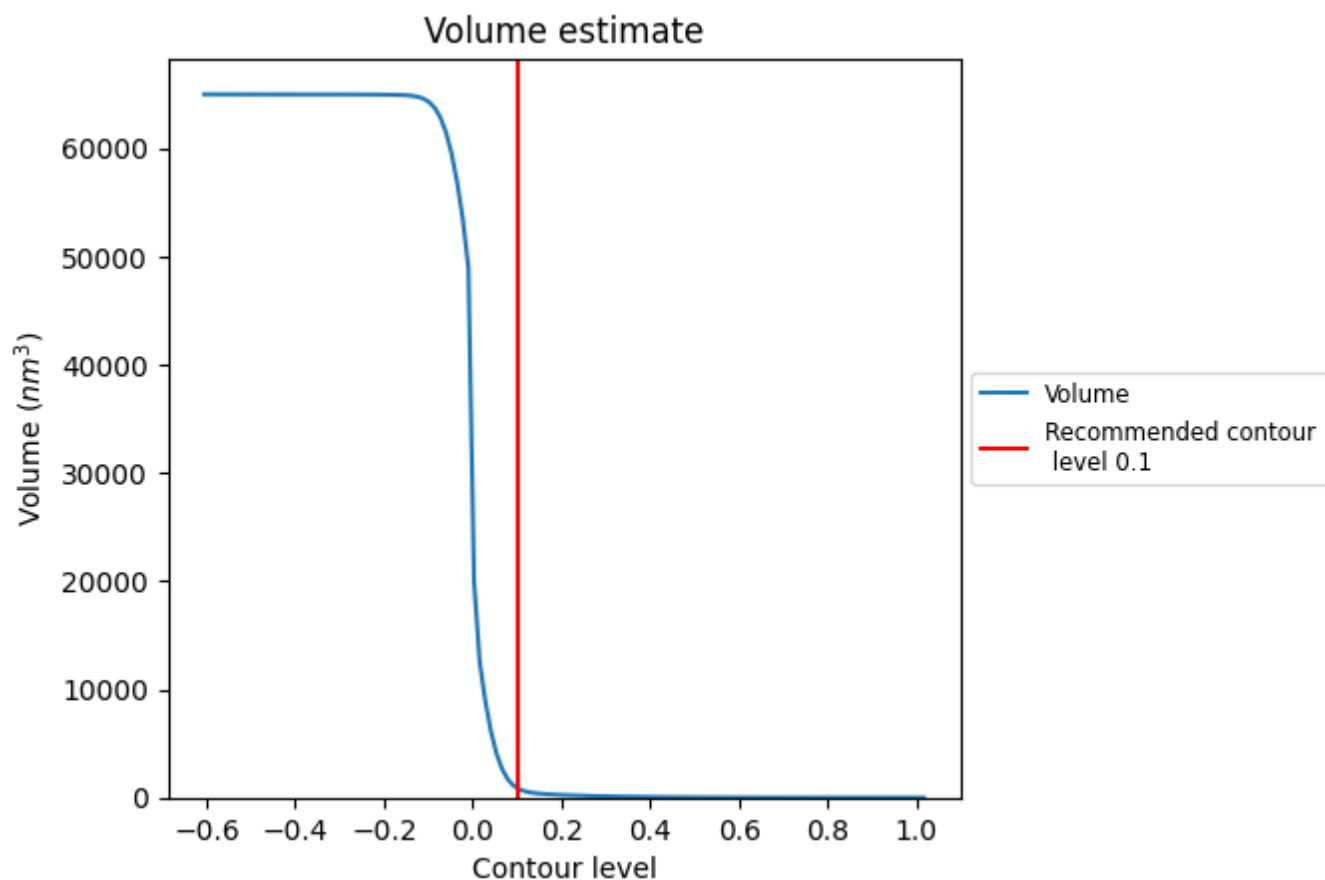
This section contains the results of statistical analysis of the map.

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.

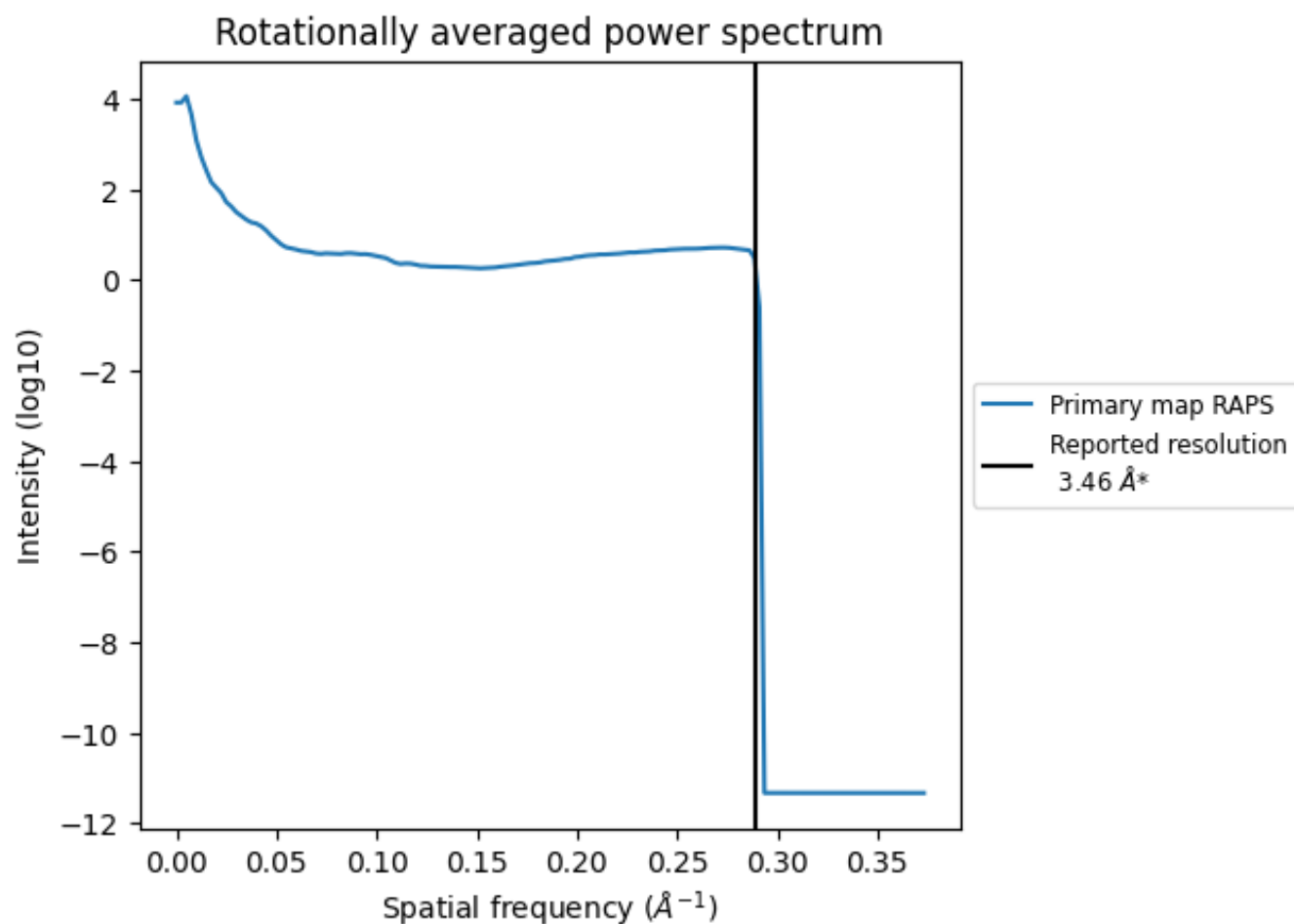
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 894 nm^3 ; this corresponds to an approximate mass of 808 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 ⓘ

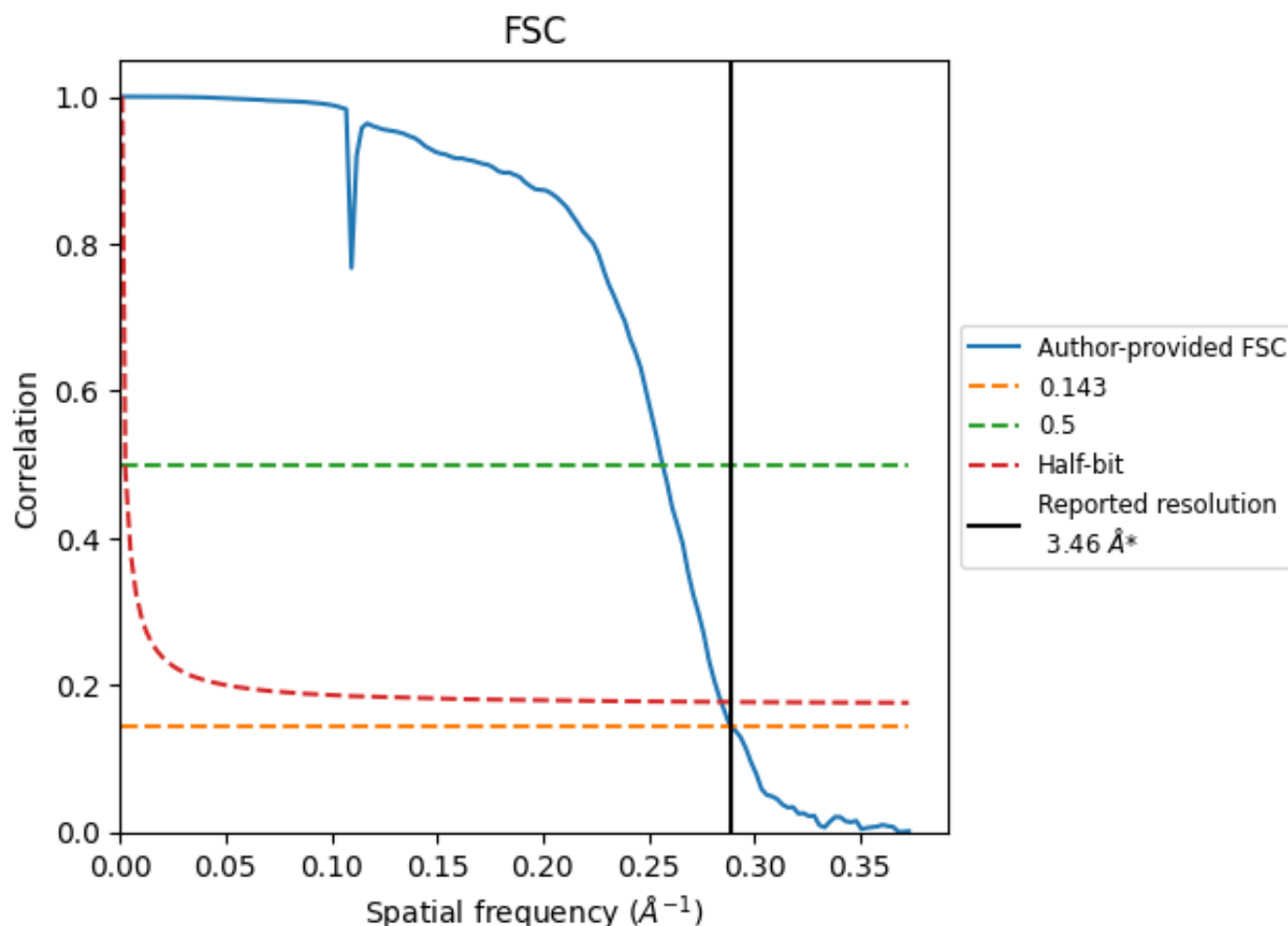


*Reported resolution corresponds to spatial frequency of 0.289 \AA^{-1}

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 0.289 Å⁻¹

8.2 Resolution estimates [i](#)

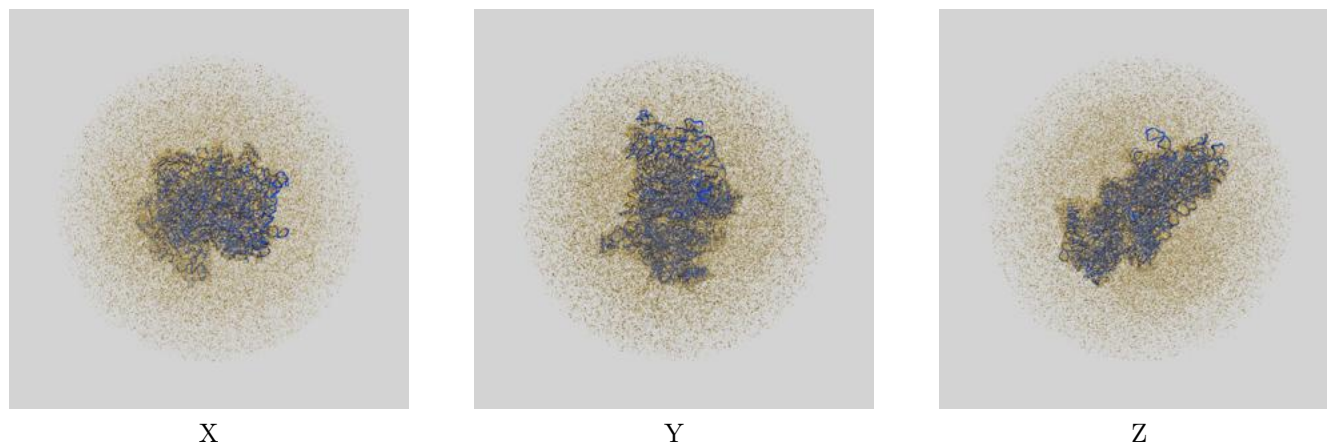
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	3.46	3.90	3.52
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

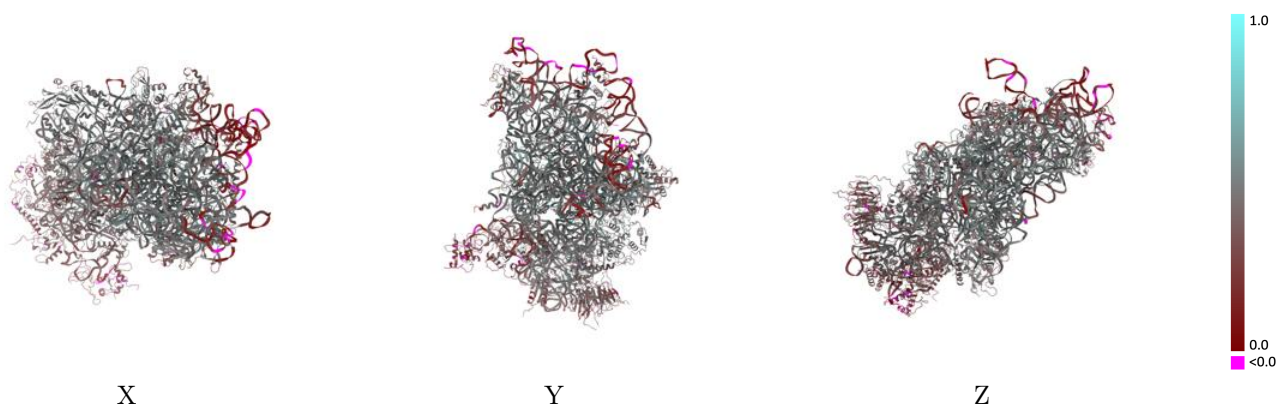
This section contains information regarding the fit between EMDB map EMD-3047 and PDB model 3JAM. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



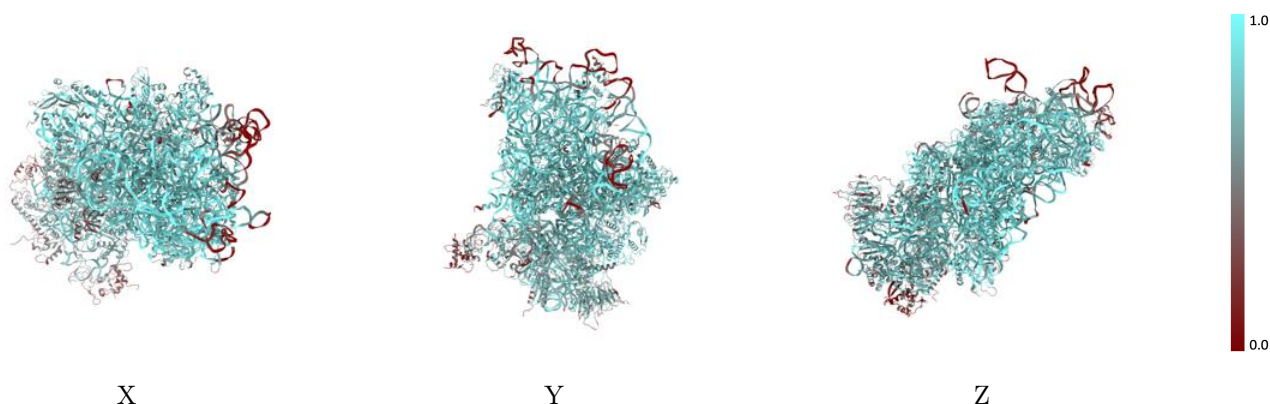
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



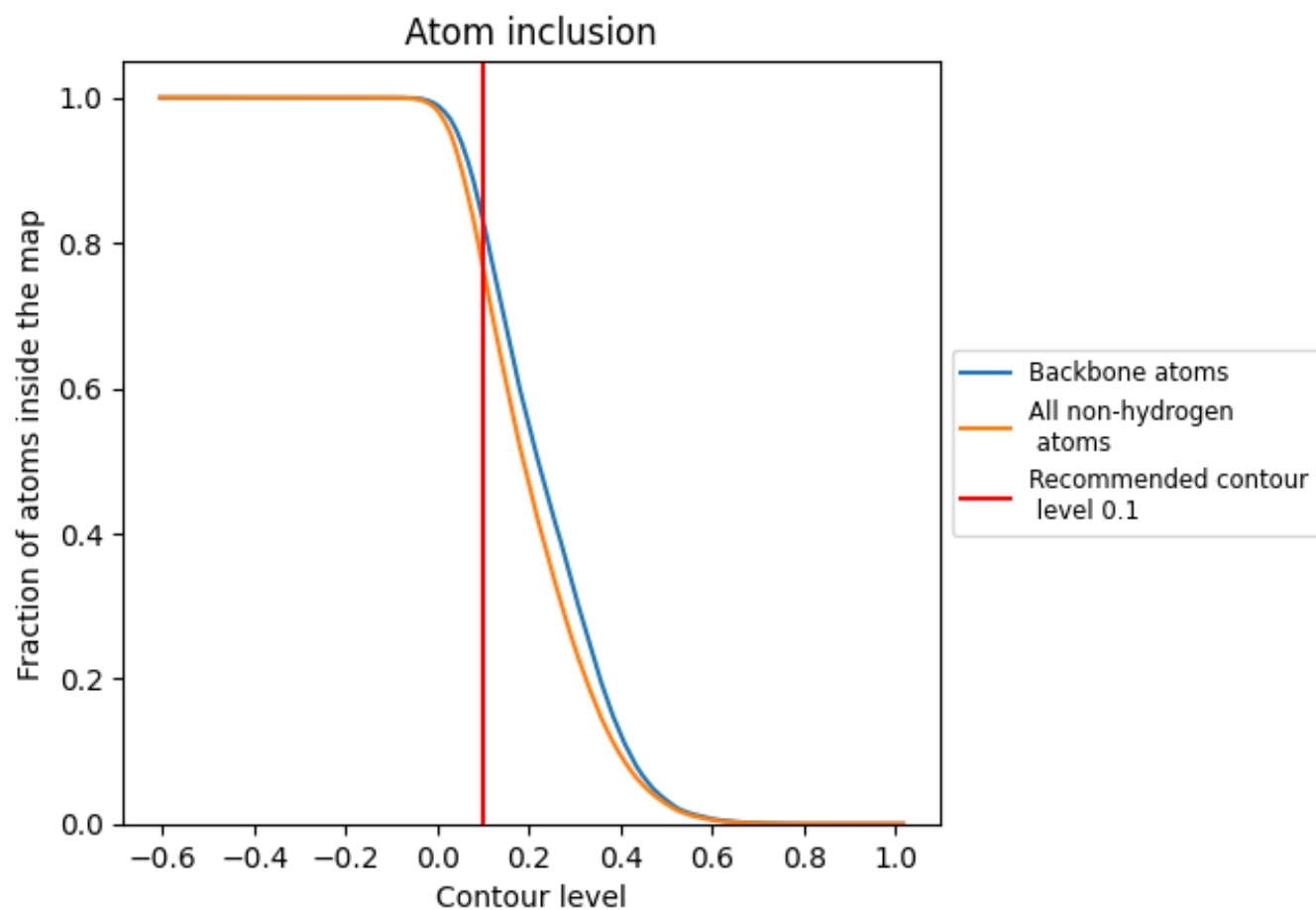
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 76% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7646	 0.4180
2	 0.8311	 0.4190
A	 0.8383	 0.4840
B	 0.7803	 0.4680
C	 0.8126	 0.4990
D	 0.6631	 0.3870
E	 0.8268	 0.4990
F	 0.6190	 0.3510
G	 0.7544	 0.4320
H	 0.7483	 0.4370
I	 0.7943	 0.4730
J	 0.8186	 0.4900
K	 0.6357	 0.3370
L	 0.7630	 0.4730
M	 0.2561	 0.1520
N	 0.8161	 0.4800
O	 0.8266	 0.4730
P	 0.4827	 0.2740
Q	 0.7463	 0.4350
R	 0.7497	 0.4360
S	 0.4805	 0.2520
T	 0.6870	 0.3690
U	 0.6373	 0.3810
V	 0.8321	 0.4880
W	 0.8560	 0.5210
X	 0.8526	 0.5200
Y	 0.8239	 0.4810
Z	 0.1160	 0.1420
a	 0.8525	 0.5060
b	 0.8156	 0.4720
c	 0.5949	 0.3680
d	 0.7963	 0.4530
e	 0.7101	 0.4570
f	 0.3346	 0.2010
g	 0.6199	 0.3420



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Chain	Atom inclusion	Q-score
h	 0.4623	 0.3630
i	 0.3579	 0.3720
j	 0.3807	 0.3470