



## Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 06:30 PM EST

PDB ID : 3JAQ  
EMDB ID : EMD-3049  
Title : Structure of a partial yeast 48S preinitiation complex in open conformation  
Authors : Llacer, J.L.; Hussain, T.; Ramakrishnan, V.  
Deposited on : 2015-06-18  
Resolution : 6.00 Å (reported)  
Based on initial models : 3CW2, 1YFG, 3J81, 4U1E, 2D74

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

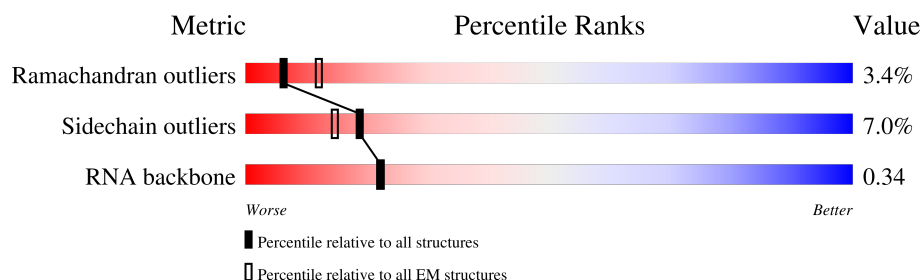
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance

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

The reported resolution of this entry is 6.00 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	75	
2	2	1781	
3	3	25	
4	A	254	
5	B	255	
6	C	259	
7	D	237	
8	E	261	

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Mol	Chain	Length	Quality of chain
9	F	227	
10	G	236	
11	H	190	
12	I	201	
13	J	188	
14	K	106	
15	L	156	
16	M	134	
17	N	151	
18	O	137	
19	P	142	
20	Q	143	
21	R	136	
22	S	146	
23	T	144	
24	U	117	
25	V	87	
26	W	130	
27	X	145	
28	Y	135	
29	Z	108	
30	a	119	
31	b	82	
32	c	67	
33	d	56	

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Mol	Chain	Length	Quality of chain
34	e	63	
35	f	150	
36	g	326	
37	h	25	
38	i	153	
39	j	304	
40	k	527	
41	l	285	
42	m	108	
43	o	92	
44	p	88	
45	q	347	
46	r	34	
47	s	52	

## 2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 89768 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 Met-tRNAi.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	75	Total	C	N	O	P	0	0
			1639	734	298	531	76		

- Molecule 2 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1780	Total	C	N	O	P	0	0
			37797	16892	6658	12467	1780		

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	2	Total	C	N	O	P	0	0
			42	19	7	14	2		

- Molecule 4 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	208	Total	C	N	O	S	0	0
			1626	1040	286	298	2		

- Molecule 5 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	222	Total	C	N	O	S	0	0
			1769	1117	324	325	3		

- Molecule 6 is a protein called uS5.

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

- Molecule 7 is a protein called uS3.

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

- Molecule 8 is a protein called eS4.

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

- Molecule 9 is a protein called uS7.

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

- Molecule 10 is a protein called eS6.

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

- Molecule 11 is a protein called eS7.

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

- Molecule 12 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	188	Total	C	N	O	S	0	0
			1489	923	300	265	1		

- Molecule 13 is a protein called uS4.

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

- Molecule 14 is a protein called eS10.

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

- Molecule 15 is a protein called uS17.

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

- Molecule 16 is a protein called eS12.

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

- Molecule 17 is a protein called uS15.

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

- Molecule 18 is a protein called uS11.

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

- Molecule 19 is a protein called uS19.

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

- Molecule 20 is a protein called uS9.

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

- Molecule 21 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	111	Total	C	N	O	S	0	0
			892	554	165	170	3		

- Molecule 22 is a protein called uS13.

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

- Molecule 23 is a protein called eS19.

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

- Molecule 24 is a protein called uS10.

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

- Molecule 25 is a protein called eS21.

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

- Molecule 26 is a protein called uS8.

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

- Molecule 27 is a protein called uS12.

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

- Molecule 28 is a protein called eS24.



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

- Molecule 29 is a protein called eS25.

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

- Molecule 30 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	98	Total	C	N	O	S		
			779	480	165	129	5	0	0

- Molecule 31 is a protein called eS27.

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

- Molecule 32 is a protein called eS28.

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

- Molecule 33 is a protein called uS14.

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

- Molecule 34 is a protein called eS30.

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

- Molecule 35 is a protein called eS31.

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

- Molecule 36 is a protein called RACK1.

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

- Molecule 37 is a protein called eL41.

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

- Molecule 38 is a protein called eIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	95	Total	C	N	O	S	0	0
			765	475	142	143	5		

- Molecule 39 is a protein called eIF2 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	249	Total	C	N	O	S	0	0
			2006	1283	333	382	8		

- Molecule 40 is a protein called eIF2 gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	396	Total	C	N	O	S	0	0
			3034	1932	542	544	16		

- Molecule 41 is a protein called eIF2 beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	128	Total	C	N	O	S	0	0
			1036	661	186	182	7		

- Molecule 42 is a protein called eIF1.

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

- Molecule 43 is a protein called eIF3a.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	o	92	Total	C	N	O	0	0
			460	276	92	92		

- Molecule 44 is a protein called eIF3c.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	p	88	Total	C	N	O	0	0
			440	264	88	88		

- Molecule 45 is a protein called eIF3i.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	342	Total	C	N	O	S	0	0
			2693	1711	443	530	9		

- Molecule 46 is a protein called eIF3b.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	34	Total	C	N	O	S	0	0
			300	192	52	54	2		

- Molecule 47 is a protein called eIF3g.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	s	52	Total	C	N	O	0	0
			418	257	82	79		

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	2	79	Total	Mg	0
			79	79	
48	C	1	Total	Mg	0
			1	1	
48	Q	1	Total	Mg	0
			1	1	

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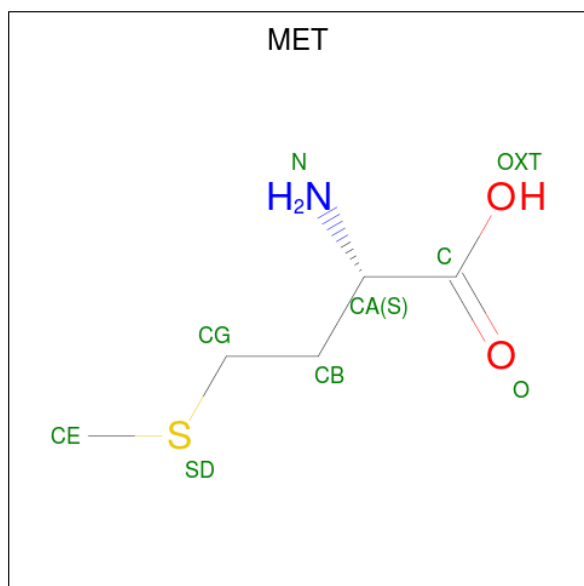
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Mol	Chain	Residues	Atoms		AltConf
48	k	1	Total	Mg	0
			1	1	

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

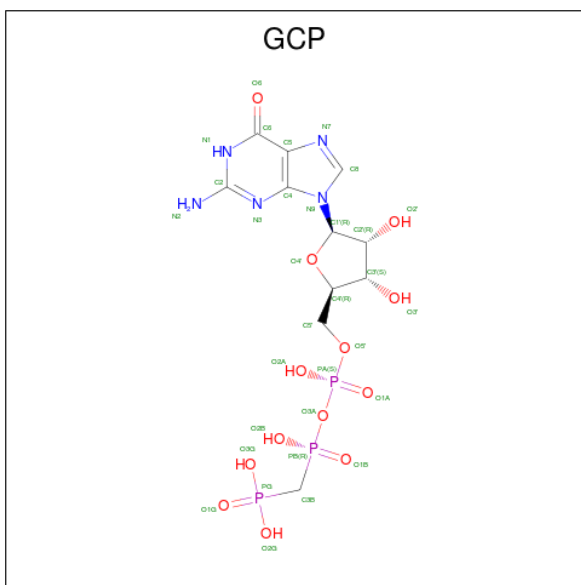
Mol	Chain	Residues	Atoms		AltConf
49	a	1	Total	Zn	0
			1	1	
49	b	1	Total	Zn	0
			1	1	
49	f	1	Total	Zn	0
			1	1	
49	l	1	Total	Zn	0
			1	1	

- Molecule 50 is METHIONINE (three-letter code: MET) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>S).



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

- Molecule 51 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



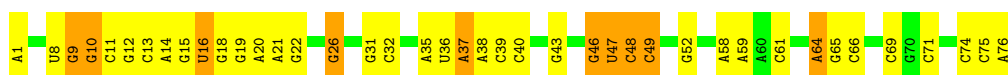
Mol	Chain	Residues	Atoms					AltConf
51	k	1	Total	C	N	O	P	0
			32	11	5	13	3	

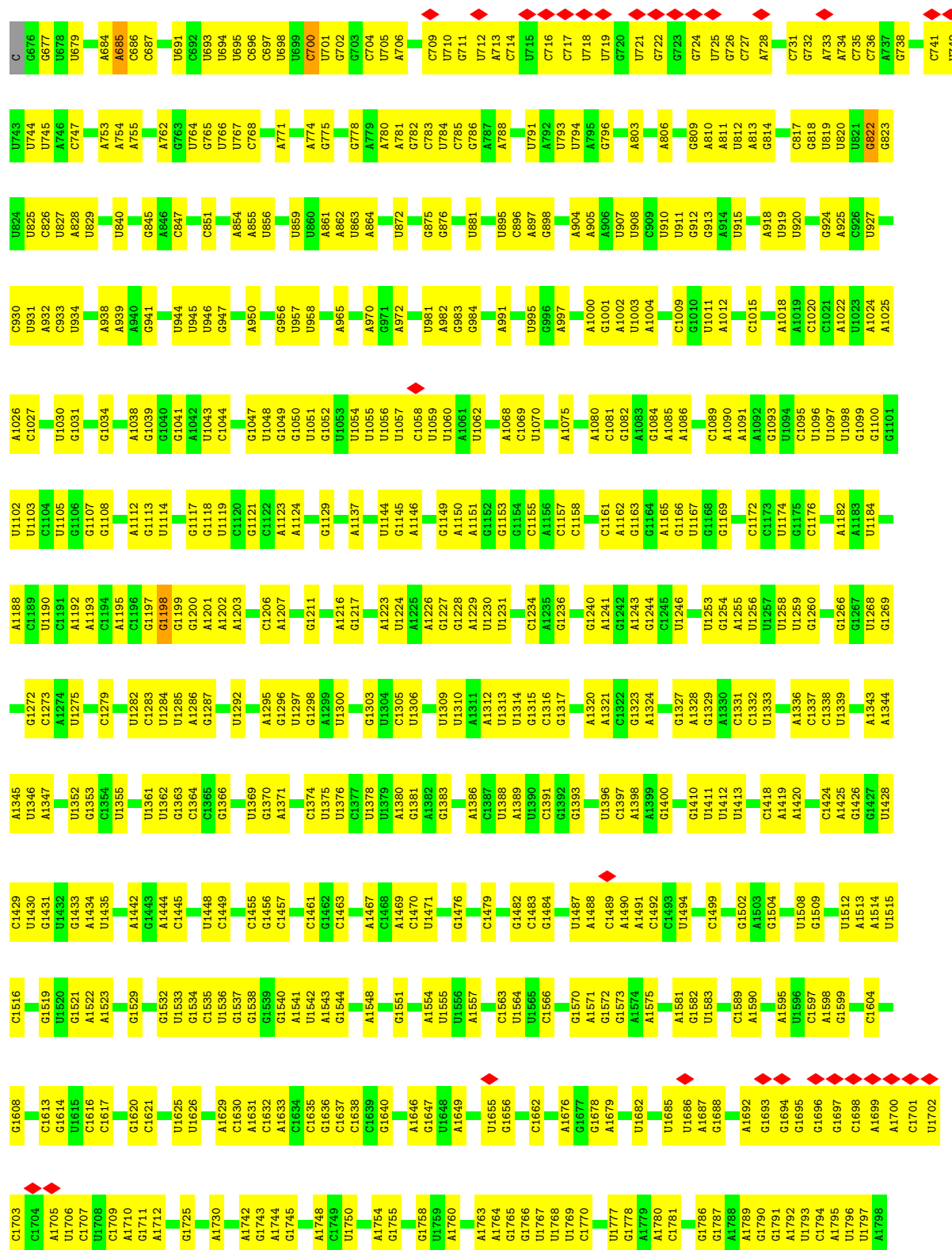
### 3 Residue-property plots

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: Met-tRNAi

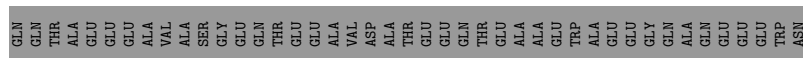
Chain 1: 



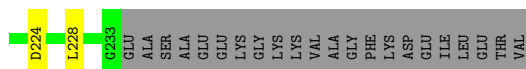
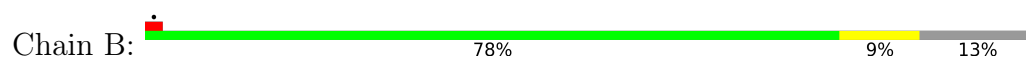




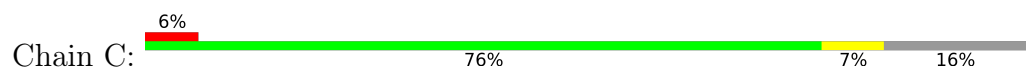
• Molecule 4: uS2



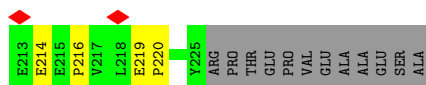
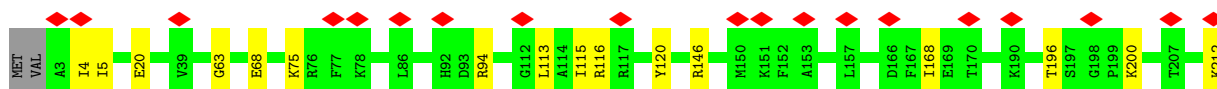
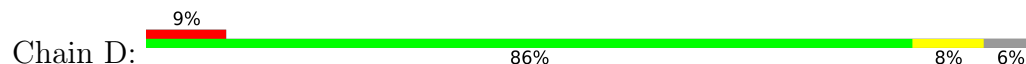
• Molecule 5: eS1



• Molecule 6: uS5



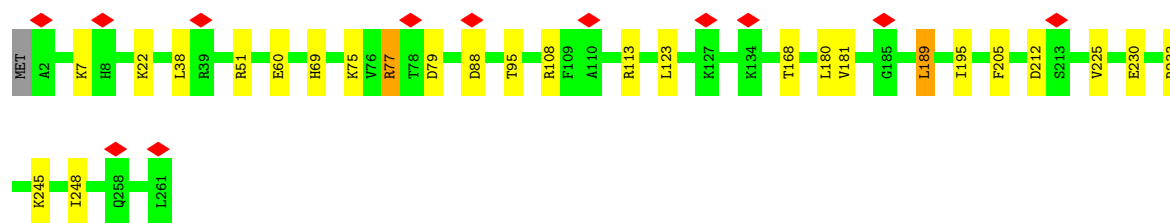
• Molecule 7: uS3



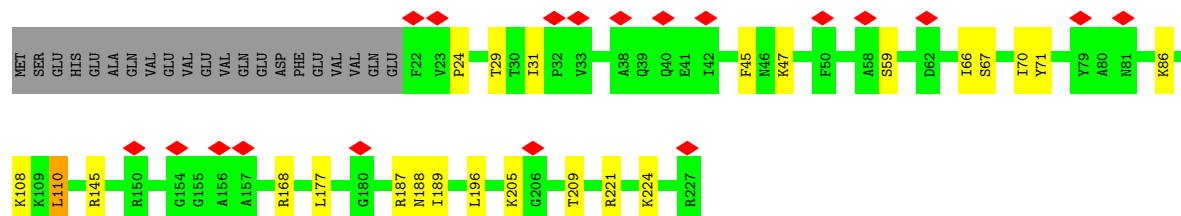
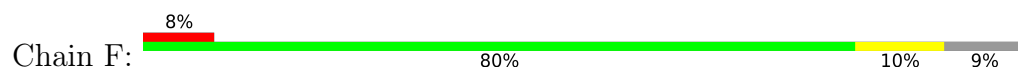
• Molecule 8: eS4



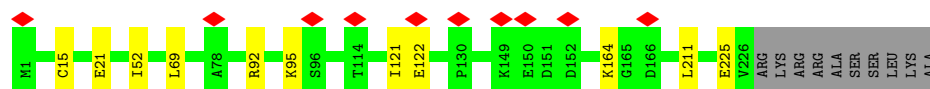




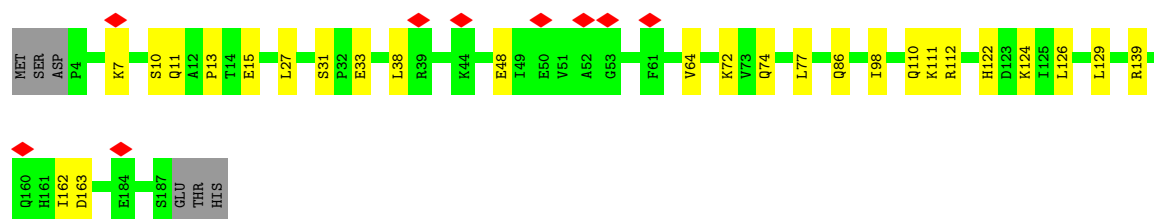
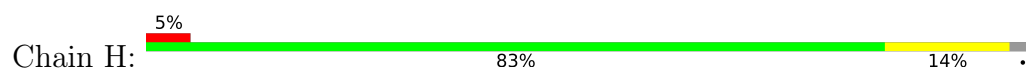
• Molecule 9: uS7



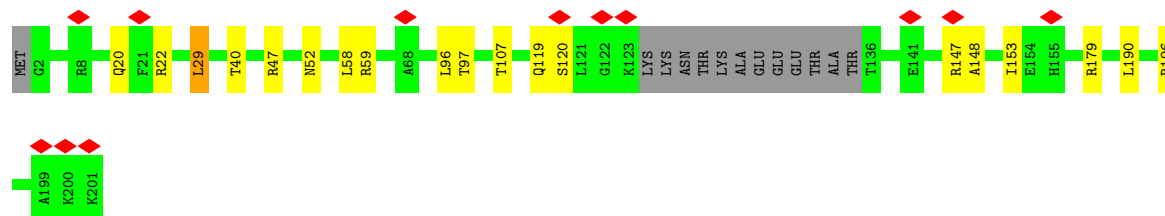
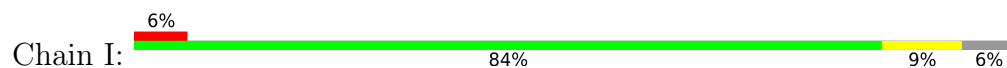
• Molecule 10: eS6




• Molecule 11: eS7



• Molecule 12: eS8




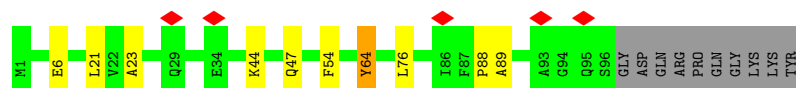
• Molecule 13: uS4

Chain J:  87% 10%



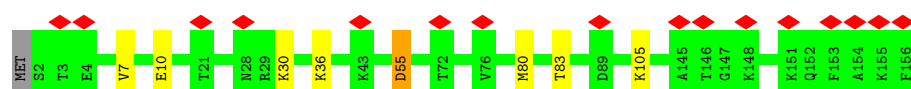
- Molecule 14: eS10

Chain K:  5% 81% 8% 9%




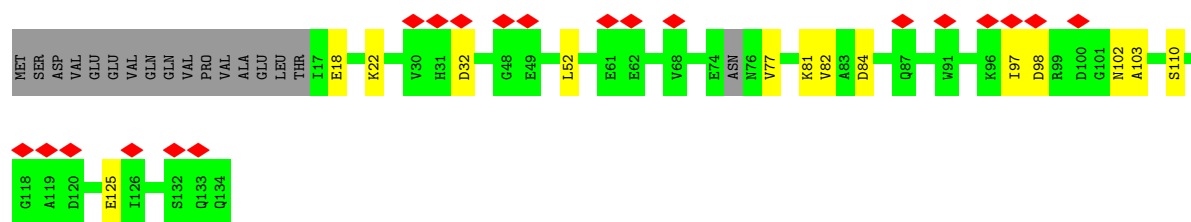
- Molecule 15: uS17

Chain L:  10% 94%



- Molecule 16: eS12

Chain M:  15% 77% 10% 13%




- Molecule 17: uS15

Chain N:  93% 5%



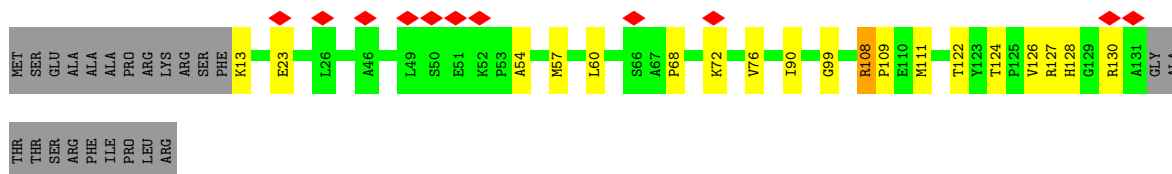
- Molecule 18: uS11

Chain O:  83% 9% 7%

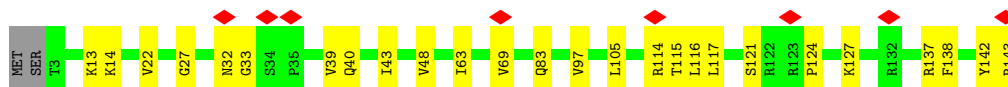
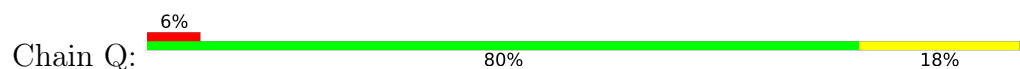


- Molecule 19: uS19

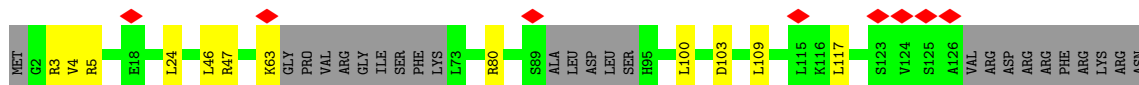
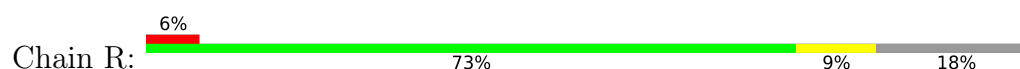
Chain P:  8% 70% 13% 16%



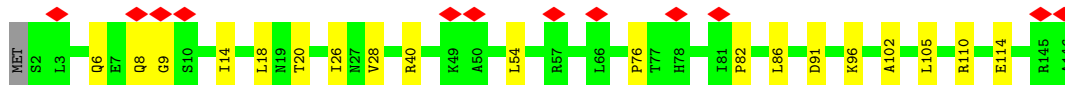
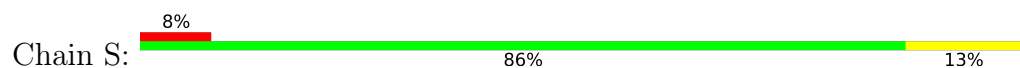
- Molecule 20: uS9



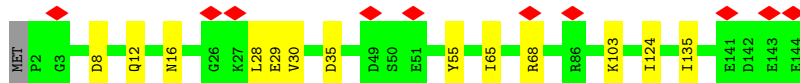
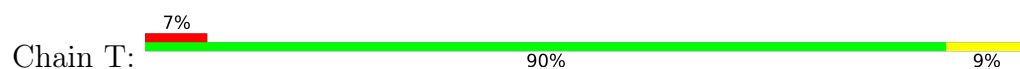
- Molecule 21: eS17



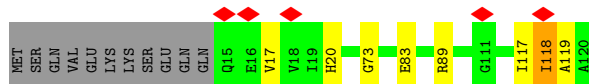
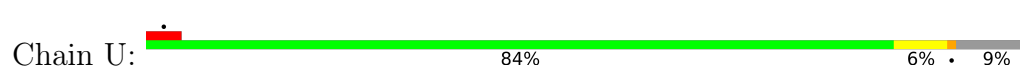
- Molecule 22: uS13



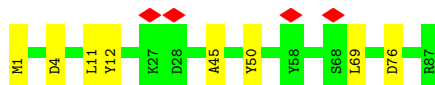
- Molecule 23: eS19



- Molecule 24: uS10



- Molecule 25: eS21




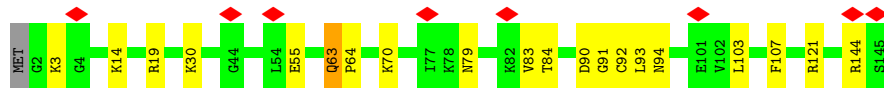
- Molecule 26: uS8

Chain W:  92% 7%




- Molecule 27: uS12

Chain X:  6% 86% 13%



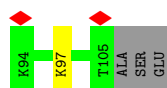
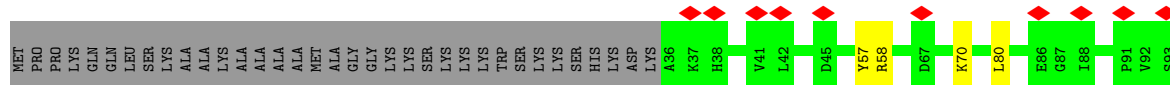
- Molecule 28: eS24

Chain Y:  90% 9%



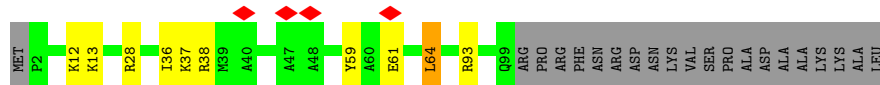
- Molecule 29: eS25

Chain Z:  11% 60% 5% 35%



- Molecule 30: eS26

Chain a:  74% 8% 18%



- Molecule 31: eS27

Chain b:  93% 6%

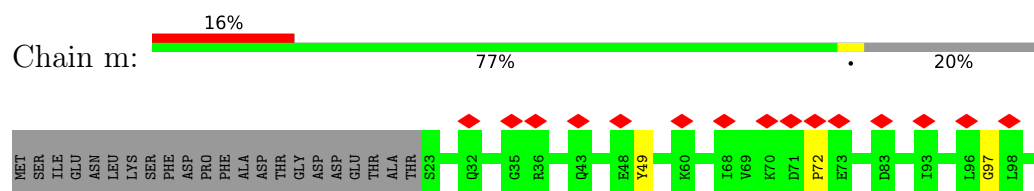


- Molecule 32: eS28

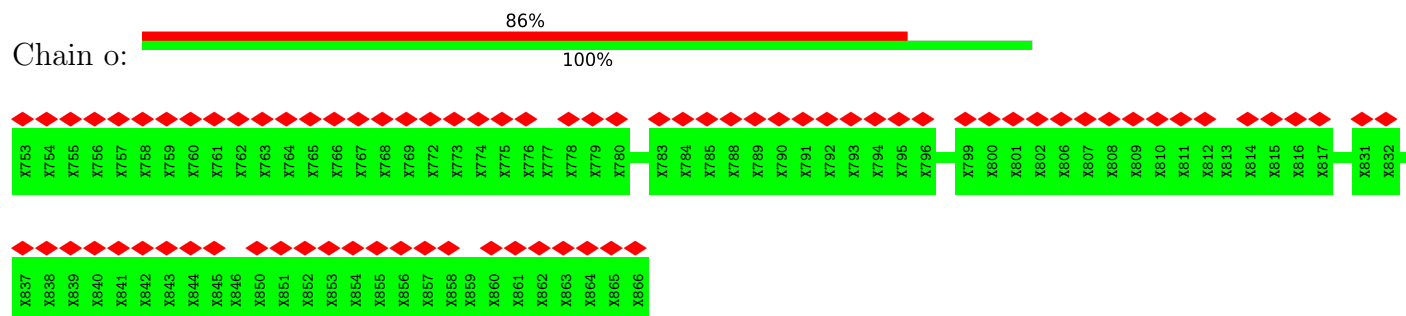




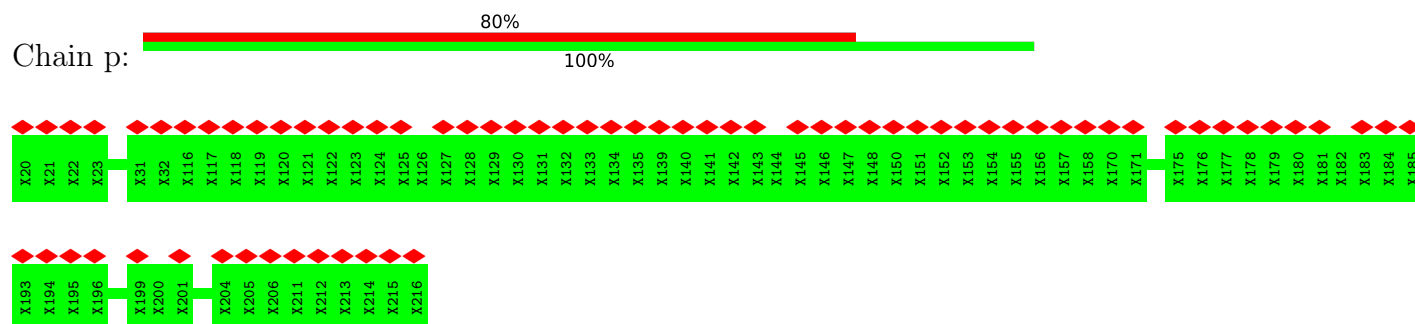
- Molecule 42: eIF1



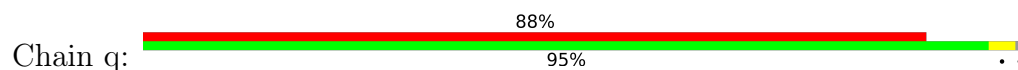
- Molecule 43: eIF3a

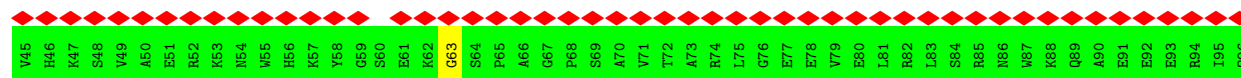


- Molecule 44: eIF3c



- Molecule 45: eIF3i







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	4547	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	27	Depositor
Minimum defocus (nm)	4000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.207	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.04	Depositor
Map size ( $\text{\AA}$ )	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.34, 1.34, 1.34	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7MG, H2U, MG, T6A, 5MC, RIA, 1MA, 2MG, 1MG, ZN, GCP, M2G

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	1	0.45	2/1530 (0.1%)	0.76	4/2380 (0.2%)
2	2	0.24	0/42269	0.65	5/65862 (0.0%)
3	3	0.22	0/46	0.64	0/69
4	A	0.42	0/1666	0.63	1/2279 (0.0%)
5	B	0.40	0/1793	0.61	0/2414
6	C	0.40	0/1659	0.59	0/2252
7	D	0.41	0/1769	0.61	0/2378
8	E	0.40	0/2122	0.62	1/2861 (0.0%)
9	F	0.40	0/1628	0.63	1/2198 (0.0%)
10	G	0.38	0/1835	0.60	0/2451
11	H	0.41	0/1507	0.62	0/2028
12	I	0.41	0/1515	0.63	2/2029 (0.1%)
13	J	0.40	0/1495	0.67	2/2001 (0.1%)
14	K	0.46	0/831	0.61	0/1123
15	L	0.42	0/1276	0.58	0/1718
16	M	0.40	0/891	0.65	0/1201
17	N	0.39	0/1210	0.60	0/1628
18	O	0.39	0/953	0.61	0/1279
19	P	0.41	0/962	0.62	0/1294
20	Q	0.41	0/1125	0.62	0/1510
21	R	0.39	0/899	0.60	0/1204
22	S	0.40	0/1212	0.66	0/1629
23	T	0.40	0/1129	0.58	0/1520
24	U	0.39	0/857	0.61	0/1158
25	V	0.38	0/696	0.61	0/938
26	W	0.40	0/1039	0.64	1/1399 (0.1%)
27	X	0.42	0/1137	0.66	2/1516 (0.1%)
28	Y	0.40	0/1075	0.59	0/1433
29	Z	0.41	0/567	0.60	0/762
30	a	0.38	0/791	0.64	0/1059
31	b	0.39	0/619	0.62	0/837
32	c	0.37	0/489	0.65	0/655

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	d	0.43	0/457	0.58	0/607
34	e	0.40	0/440	0.61	0/586
35	f	0.45	0/562	0.72	1/751 (0.1%)
36	g	0.41	0/2521	0.58	0/3431
37	h	0.35	0/234	0.61	0/300
38	i	0.38	0/775	0.60	0/1034
39	j	0.41	0/2034	0.63	0/2737
40	k	0.39	0/3079	0.60	0/4157
41	l	0.41	0/1051	0.57	0/1402
42	m	0.39	0/703	0.58	0/938
45	q	0.42	0/2757	0.57	0/3733
46	r	0.42	0/306	0.52	0/407
47	s	0.39	0/426	0.54	0/571
All	All	0.34	2/93937 (0.0%)	0.64	20/135719 (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
27	X	0	1
28	Y	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1	A	OP3-P	-9.98	1.49	1.61
1	1	65	G	P-O5'	-6.66	1.53	1.59

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	f	126	PRO	CA-N-CD	-8.85	99.11	111.50
1	1	65	G	OP1-P-OP2	-8.39	107.01	119.60
2	2	685	A	C2'-C3'-O3'	6.95	124.81	113.70
12	I	29	LEU	CA-CB-CG	6.73	130.78	115.30
1	1	65	G	O5'-P-OP2	6.33	118.29	110.70
1	1	65	G	O5'-P-OP1	6.14	118.06	110.70
2	2	1198	G	C2'-C3'-O3'	5.85	123.07	113.70
13	J	49	LEU	CA-CB-CG	5.83	128.70	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	700	C	C2'-C3'-O3'	5.61	122.68	113.70
1	1	65	G	O5'-C5'-C4'	-5.54	101.17	111.70
12	I	190	LEU	CA-CB-CG	5.47	127.89	115.30
2	2	822	G	C2'-C3'-O3'	5.34	122.25	113.70
9	F	110	LEU	CA-CB-CG	5.32	127.52	115.30
4	A	201	LEU	CA-CB-CG	5.29	127.47	115.30
27	X	103	LEU	CA-CB-CG	5.18	127.22	115.30
2	2	279	U	C2'-C3'-O3'	5.13	121.91	113.70
27	X	93	LEU	CA-CB-CG	5.11	127.05	115.30
26	W	69	LEU	CA-CB-CG	5.10	127.03	115.30
8	E	189	LEU	CA-CB-CG	5.08	127.00	115.30
13	J	93	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	X	63	GLN	Peptide
28	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	
4	A	206/254 (81%)	177 (86%)	23 (11%)	6 (3%)	4	29
5	B	218/255 (86%)	191 (88%)	18 (8%)	9 (4%)	3	22
6	C	215/259 (83%)	193 (90%)	17 (8%)	5 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	D	221/237 (93%)	198 (90%)	17 (8%)	6 (3%)	5	31
8	E	258/261 (99%)	230 (89%)	23 (9%)	5 (2%)	8	38
9	F	204/227 (90%)	170 (83%)	28 (14%)	6 (3%)	4	29
10	G	224/236 (95%)	204 (91%)	17 (8%)	3 (1%)	12	48
11	H	182/190 (96%)	166 (91%)	8 (4%)	8 (4%)	2	22
12	I	184/201 (92%)	163 (89%)	12 (6%)	9 (5%)	2	20
13	J	180/188 (96%)	153 (85%)	19 (11%)	8 (4%)	2	22
14	K	94/106 (89%)	80 (85%)	9 (10%)	5 (5%)	2	19
15	L	153/156 (98%)	133 (87%)	16 (10%)	4 (3%)	5	31
16	M	113/134 (84%)	86 (76%)	16 (14%)	11 (10%)	0	9
17	N	148/151 (98%)	141 (95%)	5 (3%)	2 (1%)	11	46
18	O	125/137 (91%)	101 (81%)	16 (13%)	8 (6%)	1	16
19	P	117/142 (82%)	91 (78%)	18 (15%)	8 (7%)	1	15
20	Q	139/143 (97%)	114 (82%)	13 (9%)	12 (9%)	1	11
21	R	105/136 (77%)	92 (88%)	10 (10%)	3 (3%)	4	29
22	S	143/146 (98%)	115 (80%)	20 (14%)	8 (6%)	2	18
23	T	141/144 (98%)	128 (91%)	13 (9%)	0	100	100
24	U	104/117 (89%)	88 (85%)	11 (11%)	5 (5%)	2	20
25	V	85/87 (98%)	79 (93%)	4 (5%)	2 (2%)	6	33
26	W	127/130 (98%)	114 (90%)	9 (7%)	4 (3%)	4	27
27	X	142/145 (98%)	121 (85%)	13 (9%)	8 (6%)	2	18
28	Y	132/135 (98%)	120 (91%)	8 (6%)	4 (3%)	4	28
29	Z	68/108 (63%)	55 (81%)	12 (18%)	1 (2%)	10	45
30	a	96/119 (81%)	83 (86%)	8 (8%)	5 (5%)	2	19
31	b	79/82 (96%)	69 (87%)	8 (10%)	2 (2%)	5	32
32	c	60/67 (90%)	56 (93%)	3 (5%)	1 (2%)	9	42
33	d	51/56 (91%)	37 (72%)	12 (24%)	2 (4%)	3	23
34	e	52/63 (82%)	41 (79%)	9 (17%)	2 (4%)	3	24
35	f	67/150 (45%)	50 (75%)	12 (18%)	5 (8%)	1	13
36	g	312/326 (96%)	267 (86%)	39 (12%)	6 (2%)	8	38
37	h	23/25 (92%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	i	93/153 (61%)	82 (88%)	8 (9%)	3 (3%)	4	26
39	j	243/304 (80%)	212 (87%)	24 (10%)	7 (3%)	4	29
40	k	388/527 (74%)	335 (86%)	39 (10%)	14 (4%)	3	25
41	l	120/285 (42%)	106 (88%)	13 (11%)	1 (1%)	19	60
42	m	84/108 (78%)	74 (88%)	8 (10%)	2 (2%)	6	33
45	q	340/347 (98%)	307 (90%)	29 (8%)	4 (1%)	13	50
46	r	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
47	s	50/52 (96%)	44 (88%)	5 (10%)	1 (2%)	7	38
All	All	6118/7123 (86%)	5319 (87%)	594 (10%)	205 (3%)	6	26

All (205) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	H	31	SER
11	H	64	VAL
11	H	74	GLN
14	K	88	PRO
19	P	126	VAL
20	Q	138	PHE
22	S	40	ARG
24	U	118	ILE
26	W	83	ILE
27	X	64	PRO
27	X	92	CYS
28	Y	30	PRO
30	a	59	TYR
31	b	21	LEU
34	e	47	VAL
42	m	72	PRO
4	A	202	TYR
5	B	221	PRO
7	D	4	ILE
7	D	216	PRO
7	D	220	PRO
9	F	66	ILE
10	G	122	GLU
10	G	225	GLU
11	H	110	GLN
11	H	163	ASP

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Mol	Chain	Res	Type
12	I	40	THR
12	I	148	ALA
12	I	153	ILE
13	J	150	LEU
15	L	55	ASP
16	M	98	ASP
17	N	3	ARG
18	O	40	ALA
18	O	124	ASP
20	Q	27	GLY
20	Q	39	VAL
20	Q	115	THR
20	Q	116	LEU
20	Q	121	SER
21	R	103	ASP
24	U	119	ALA
25	V	12	TYR
27	X	90	ASP
33	d	23	ILE
33	d	25	GLY
35	f	102	VAL
38	i	64	LYS
39	j	49	SER
39	j	196	GLU
41	l	129	LEU
5	B	8	ARG
5	B	131	ASP
5	B	207	LEU
6	C	111	ASP
6	C	253	THR
8	E	95	THR
8	E	195	ILE
8	E	205	PHE
9	F	67	SER
9	F	205	LYS
11	H	10	SER
12	I	22	ARG
12	I	52	ASN
12	I	120	SER
13	J	171	ARG
14	K	23	ALA
15	L	30	LYS

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Mol	Chain	Res	Type
15	L	105	LYS
16	M	82	VAL
16	M	102	ASN
18	O	25	ASP
19	P	54	ALA
20	Q	14	LYS
20	Q	40	GLN
20	Q	124	PRO
20	Q	142	TYR
22	S	102	ALA
25	V	45	ALA
26	W	58	SER
27	X	3	LYS
28	Y	36	SER
30	a	13	LYS
32	c	35	ASP
36	g	4	SER
36	g	146	LEU
39	j	57	ARG
39	j	64	ARG
40	k	127	ARG
40	k	255	ARG
40	k	383	GLU
45	q	164	LYS
47	s	63	GLY
4	A	39	LYS
4	A	103	THR
4	A	109	ASN
4	A	207	PRO
5	B	54	LEU
5	B	224	ASP
6	C	151	THR
6	C	155	GLN
7	D	219	GLU
8	E	77	ARG
9	F	71	TYR
13	J	118	LEU
13	J	136	VAL
14	K	89	ALA
16	M	18	GLU
16	M	84	ASP
17	N	12	SER

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Mol	Chain	Res	Type
18	O	18	ARG
18	O	42	VAL
18	O	114	ARG
19	P	90	ILE
19	P	108	ARG
19	P	128	HIS
20	Q	32	ASN
21	R	24	LEU
24	U	17	VAL
24	U	89	ARG
26	W	29	PRO
27	X	144	ARG
28	Y	64	TYR
29	Z	97	LYS
35	f	85	TYR
36	g	129	ASP
38	i	44	ASN
39	j	6	CYS
40	k	126	VAL
40	k	273	THR
45	q	116	MET
45	q	261	LYS
4	A	158	VAL
5	B	22	ASP
5	B	177	GLN
6	C	96	ARG
7	D	196	THR
8	E	245	LYS
9	F	24	PRO
9	F	59	SER
11	H	13	PRO
11	H	98	ILE
12	I	59	ARG
12	I	107	THR
13	J	120	LYS
13	J	134	ILE
13	J	147	MET
14	K	54	PHE
16	M	32	ASP
16	M	77	VAL
16	M	81	LYS
16	M	110	SER

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Mol	Chain	Res	Type
21	R	5	ARG
22	S	14	ILE
22	S	28	VAL
22	S	76	PRO
22	S	91	ASP
26	W	30	SER
27	X	63	GLN
28	Y	4	ALA
30	a	36	ILE
30	a	61	GLU
31	b	62	VAL
35	f	90	LYS
36	g	201	GLY
39	j	120	GLN
40	k	321	PHE
40	k	408	ARG
40	k	497	GLU
45	q	165	GLY
5	B	148	ASN
12	I	147	ARG
13	J	35	GLY
14	K	64	TYR
15	L	7	VAL
16	M	103	ALA
19	P	109	PRO
27	X	70	LYS
30	a	64	LEU
35	f	98	VAL
36	g	64	GLY
39	j	5	HIS
40	k	225	PRO
40	k	324	ASN
7	D	63	GLY
16	M	97	ILE
27	X	91	GLY
34	e	12	GLY
38	i	45	GLY
18	O	120	PRO
20	Q	33	GLY
22	S	82	PRO
24	U	73	GLY
40	k	270	ILE

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Mol	Chain	Res	Type
18	O	88	GLY
19	P	68	PRO
19	P	99	GLY
22	S	9	GLY
42	m	97	GLY
10	G	69	LEU
35	f	122	PRO
40	k	176	ARG
40	k	392	PRO
36	g	106	GLY
40	k	335	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	
4	A	174/211 (82%)	159 (91%)	15 (9%)	10	33
5	B	198/228 (87%)	182 (92%)	16 (8%)	11	35
6	C	176/203 (87%)	161 (92%)	15 (8%)	10	33
7	D	185/196 (94%)	171 (92%)	14 (8%)	13	37
8	E	223/224 (100%)	201 (90%)	22 (10%)	8	26
9	F	174/194 (90%)	156 (90%)	18 (10%)	7	25
10	G	192/200 (96%)	184 (96%)	8 (4%)	30	54
11	H	164/170 (96%)	146 (89%)	18 (11%)	6	23
12	I	147/159 (92%)	138 (94%)	9 (6%)	18	44
13	J	153/158 (97%)	144 (94%)	9 (6%)	19	45
14	K	88/96 (92%)	82 (93%)	6 (7%)	16	41
15	L	136/137 (99%)	131 (96%)	5 (4%)	34	58
16	M	93/109 (85%)	90 (97%)	3 (3%)	39	62
17	N	127/128 (99%)	119 (94%)	8 (6%)	18	43
18	O	96/104 (92%)	90 (94%)	6 (6%)	18	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	P	101/119 (85%)	89 (88%)	12 (12%)	5	20
20	Q	117/119 (98%)	103 (88%)	14 (12%)	5	20
21	R	102/124 (82%)	93 (91%)	9 (9%)	10	31
22	S	128/129 (99%)	117 (91%)	11 (9%)	10	33
23	T	117/118 (99%)	104 (89%)	13 (11%)	6	22
24	U	96/107 (90%)	92 (96%)	4 (4%)	30	54
25	V	73/73 (100%)	67 (92%)	6 (8%)	11	34
26	W	110/111 (99%)	106 (96%)	4 (4%)	35	59
27	X	119/120 (99%)	109 (92%)	10 (8%)	11	34
28	Y	108/109 (99%)	101 (94%)	7 (6%)	17	42
29	Z	60/88 (68%)	56 (93%)	4 (7%)	16	41
30	a	83/100 (83%)	77 (93%)	6 (7%)	14	39
31	b	71/72 (99%)	68 (96%)	3 (4%)	30	54
32	c	54/59 (92%)	51 (94%)	3 (6%)	21	46
33	d	46/48 (96%)	43 (94%)	3 (6%)	17	42
34	e	47/55 (86%)	42 (89%)	5 (11%)	6	24
35	f	58/133 (44%)	51 (88%)	7 (12%)	5	20
36	g	265/272 (97%)	244 (92%)	21 (8%)	12	36
37	h	23/23 (100%)	22 (96%)	1 (4%)	29	54
38	i	81/130 (62%)	75 (93%)	6 (7%)	13	38
39	j	224/274 (82%)	193 (86%)	31 (14%)	3	17
40	k	332/449 (74%)	324 (98%)	8 (2%)	49	69
41	l	119/246 (48%)	114 (96%)	5 (4%)	30	54
42	m	77/96 (80%)	76 (99%)	1 (1%)	69	82
45	q	297/301 (99%)	290 (98%)	7 (2%)	49	69
46	r	33/33 (100%)	33 (100%)	0	100	100
47	s	43/43 (100%)	43 (100%)	0	100	100
All	All	5310/6068 (88%)	4937 (93%)	373 (7%)	19	40

All (373) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	LEU

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Mol	Chain	Res	Type
4	A	37	VAL
4	A	59	LEU
4	A	72	ASP
4	A	88	LYS
4	A	93	THR
4	A	101	ARG
4	A	112	THR
4	A	134	LYS
4	A	165	ARG
4	A	167	LYS
4	A	170	ILE
4	A	177	LEU
4	A	193	GLN
4	A	198	MET
5	B	29	TRP
5	B	54	LEU
5	B	70	LEU
5	B	82	ARG
5	B	104	ASP
5	B	118	GLN
5	B	124	ASN
5	B	127	VAL
5	B	140	ILE
5	B	155	TYR
5	B	171	ILE
5	B	181	LEU
5	B	184	LEU
5	B	196	GLU
5	B	208	GLN
5	B	228	LEU
6	C	83	ASP
6	C	84	GLU
6	C	91	VAL
6	C	96	ARG
6	C	101	THR
6	C	116	VAL
6	C	145	ARG
6	C	146	ARG
6	C	166	LYS
6	C	212	LEU
6	C	230	LEU
6	C	233	ASN

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Mol	Chain	Res	Type
6	C	234	LEU
6	C	235	TRP
6	C	236	GLU
7	D	5	ILE
7	D	20	GLU
7	D	68	GLU
7	D	75	LYS
7	D	94	ARG
7	D	113	LEU
7	D	115	ILE
7	D	116	ARG
7	D	120	TYR
7	D	146	ARG
7	D	168	ILE
7	D	200	LYS
7	D	212	LYS
7	D	214	GLU
8	E	7	LYS
8	E	22	LYS
8	E	38	LEU
8	E	51	ARG
8	E	60	GLU
8	E	69	HIS
8	E	75	LYS
8	E	77	ARG
8	E	79	ASP
8	E	88	ASP
8	E	108	ARG
8	E	113	ARG
8	E	123	LEU
8	E	168	THR
8	E	180	LEU
8	E	181	VAL
8	E	189	LEU
8	E	212	ASP
8	E	225	VAL
8	E	230	GLU
8	E	233	ARG
8	E	248	ILE
9	F	29	THR
9	F	31	ILE
9	F	45	PHE

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Mol	Chain	Res	Type
9	F	47	LYS
9	F	70	ILE
9	F	86	LYS
9	F	108	LYS
9	F	110	LEU
9	F	145	ARG
9	F	168	ARG
9	F	177	LEU
9	F	187	ARG
9	F	188	ASN
9	F	189	ILE
9	F	196	LEU
9	F	209	THR
9	F	221	ARG
9	F	224	LYS
10	G	15	CYS
10	G	21	GLU
10	G	52	ILE
10	G	92	ARG
10	G	95	LYS
10	G	121	ILE
10	G	164	LYS
10	G	211	LEU
11	H	7	LYS
11	H	11	GLN
11	H	15	GLU
11	H	27	LEU
11	H	33	GLU
11	H	38	LEU
11	H	48	GLU
11	H	72	LYS
11	H	77	LEU
11	H	86	GLN
11	H	111	LYS
11	H	112	ARG
11	H	122	HIS
11	H	124	LYS
11	H	126	LEU
11	H	129	LEU
11	H	139	ARG
11	H	162	ILE
12	I	20	GLN

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Mol	Chain	Res	Type
12	I	29	LEU
12	I	47	ARG
12	I	58	LEU
12	I	96	LEU
12	I	97	THR
12	I	119	GLN
12	I	179	ARG
12	I	196	ARG
13	J	8	TYR
13	J	28	LEU
13	J	33	GLU
13	J	37	LYS
13	J	45	ILE
13	J	100	LYS
13	J	103	ASP
13	J	107	ARG
13	J	161	THR
14	K	6	GLU
14	K	21	LEU
14	K	44	LYS
14	K	47	GLN
14	K	64	TYR
14	K	76	LEU
15	L	10	GLU
15	L	36	LYS
15	L	55	ASP
15	L	80	MET
15	L	83	THR
16	M	22	LYS
16	M	52	LEU
16	M	125	GLU
17	N	3	ARG
17	N	20	ARG
17	N	27	LYS
17	N	64	LYS
17	N	70	LYS
17	N	88	LEU
17	N	100	LYS
17	N	107	LYS
18	O	29	HIS
18	O	49	LYS
18	O	65	GLN

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Mol	Chain	Res	Type
18	O	92	LYS
18	O	110	LEU
18	O	114	ARG
19	P	13	LYS
19	P	23	GLU
19	P	57	MET
19	P	60	LEU
19	P	72	LYS
19	P	76	VAL
19	P	108	ARG
19	P	111	MET
19	P	122	THR
19	P	124	THR
19	P	127	ARG
19	P	130	ARG
20	Q	13	LYS
20	Q	22	VAL
20	Q	43	ILE
20	Q	48	VAL
20	Q	63	ILE
20	Q	69	VAL
20	Q	83	GLN
20	Q	97	VAL
20	Q	105	LEU
20	Q	114	ARG
20	Q	117	LEU
20	Q	127	LYS
20	Q	137	ARG
20	Q	143	ARG
21	R	3	ARG
21	R	4	VAL
21	R	46	LEU
21	R	47	ARG
21	R	63	LYS
21	R	80	ARG
21	R	100	LEU
21	R	109	LEU
21	R	117	LEU
22	S	6	GLN
22	S	8	GLN
22	S	18	LEU
22	S	20	THR

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Mol	Chain	Res	Type
22	S	26	ILE
22	S	54	LEU
22	S	86	LEU
22	S	96	LYS
22	S	105	LEU
22	S	110	ARG
22	S	114	GLU
23	T	8	ASP
23	T	12	GLN
23	T	16	ASN
23	T	28	LEU
23	T	29	GLU
23	T	30	VAL
23	T	35	ASP
23	T	55	TYR
23	T	65	ILE
23	T	68	ARG
23	T	103	LYS
23	T	124	ILE
23	T	135	ILE
24	U	20	HIS
24	U	83	GLU
24	U	117	ILE
24	U	118	ILE
25	V	1	MET
25	V	4	ASP
25	V	11	LEU
25	V	50	TYR
25	V	69	LEU
25	V	76	ASP
26	W	7	LEU
26	W	24	GLN
26	W	47	ILE
26	W	111	MET
27	X	14	LYS
27	X	19	ARG
27	X	30	LYS
27	X	55	GLU
27	X	79	ASN
27	X	83	VAL
27	X	84	THR
27	X	94	ASN

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Mol	Chain	Res	Type
27	X	107	PHE
27	X	121	ARG
28	Y	5	ILE
28	Y	8	ARG
28	Y	35	VAL
28	Y	72	PHE
28	Y	84	LYS
28	Y	99	LYS
28	Y	105	ARG
29	Z	57	TYR
29	Z	58	ARG
29	Z	70	LYS
29	Z	80	LEU
30	a	12	LYS
30	a	28	ARG
30	a	37	LYS
30	a	38	ARG
30	a	64	LEU
30	a	93	ARG
31	b	3	LEU
31	b	57	GLU
31	b	67	THR
32	c	9	LEU
32	c	33	LEU
32	c	50	GLU
33	d	20	GLN
33	d	39	ASP
33	d	44	ARG
34	e	15	LYS
34	e	20	LYS
34	e	39	LEU
34	e	49	LEU
34	e	54	ARG
35	f	97	LYS
35	f	103	LEU
35	f	111	GLU
35	f	119	LYS
35	f	120	GLU
35	f	138	TYR
35	f	143	HIS
36	g	6	ILE
36	g	8	LEU

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Mol	Chain	Res	Type
36	g	10	LEU
36	g	50	GLU
36	g	70	GLN
36	g	77	ASP
36	g	103	ARG
36	g	124	ILE
36	g	146	LEU
36	g	151	TRP
36	g	172	ILE
36	g	175	VAL
36	g	188	LEU
36	g	198	ASP
36	g	206	ILE
36	g	210	GLN
36	g	238	PHE
36	g	281	LEU
36	g	297	VAL
36	g	314	ASP
36	g	321	GLN
37	h	21	ARG
38	i	23	LYS
38	i	24	ARG
38	i	62	ARG
38	i	70	TRP
38	i	89	CYS
38	i	114	LYS
39	j	7	ARG
39	j	11	ASN
39	j	13	TYR
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	47	LEU
39	j	57	ARG
39	j	59	ILE
39	j	64	ARG
39	j	87	LYS
39	j	103	GLN
39	j	113	ARG

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Mol	Chain	Res	Type
39	j	121	ILE
39	j	123	LEU
39	j	126	LEU
39	j	127	TYR
39	j	137	LYS
39	j	152	GLU
39	j	154	VAL
39	j	159	GLU
39	j	166	LEU
39	j	172	TYR
39	j	185	ARG
39	j	230	LEU
39	j	235	LEU
39	j	244	LEU
39	j	251	ILE
40	k	228	GLN
40	k	291	ILE
40	k	337	VAL
40	k	395	LEU
40	k	402	VAL
40	k	403	ASP
40	k	410	ASP
40	k	432	ILE
41	l	129	LEU
41	l	141	ILE
41	l	180	ILE
41	l	206	ASP
41	l	211	LEU
42	m	49	TYR
45	q	94	VAL
45	q	244	VAL
45	q	253	ILE
45	q	272	LYS
45	q	276	ARG
45	q	317	ILE
45	q	328	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	69	ASN
4	A	109	ASN

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Mol	Chain	Res	Type
5	B	49	ASN
5	B	118	GLN
5	B	124	ASN
5	B	160	HIS
5	B	220	GLN
6	C	76	GLN
6	C	233	ASN
7	D	165	ASN
8	E	69	HIS
8	E	98	ASN
8	E	112	HIS
9	F	188	ASN
10	G	10	ASN
11	H	155	ASN
12	I	84	HIS
15	L	8	GLN
15	L	22	ASN
18	O	65	GLN
19	P	98	ASN
19	P	103	ASN
19	P	128	HIS
20	Q	77	GLN
20	Q	83	GLN
20	Q	94	GLN
20	Q	100	GLN
20	Q	139	GLN
21	R	29	GLN
22	S	89	GLN
22	S	136	GLN
23	T	16	ASN
23	T	17	ASN
23	T	23	GLN
24	U	105	GLN
25	V	33	GLN
26	W	80	ASN
27	X	22	ASN
27	X	79	ASN
28	Y	22	GLN
32	c	27	GLN
34	e	17	GLN
35	f	133	HIS
36	g	18	ASN

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Mol	Chain	Res	Type
36	g	292	GLN
39	j	26	GLN
39	j	238	GLN
40	k	102	ASN
40	k	221	ASN
40	k	248	GLN
40	k	286	GLN
40	k	376	ASN
40	k	465	ASN
42	m	43	GLN
42	m	67	ASN
42	m	79	GLN
42	m	99	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	73/75 (97%)	38 (52%)	12 (16%)
2	2	1778/1781 (99%)	814 (45%)	118 (6%)
3	3	1/25 (4%)	0	0
All	All	1852/1881 (98%)	852 (46%)	130 (7%)

All (852) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	8	U
1	1	9	1MG
1	1	10	2MG
1	1	11	C
1	1	12	G
1	1	13	C
1	1	14	A
1	1	15	G
1	1	16	H2U
1	1	18	G
1	1	19	G
1	1	20	A
1	1	21	A
1	1	22	G
1	1	26	M2G
1	1	31	G

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Mol	Chain	Res	Type
1	1	32	C
1	1	35	A
1	1	36	U
1	1	37	T6A
1	1	38	A
1	1	39	C
1	1	40	C
1	1	43	G
1	1	46	7MG
1	1	47	H2U
1	1	48	5MC
1	1	49	5MC
1	1	52	G
1	1	59	A
1	1	61	C
1	1	64	RIA
1	1	66	C
1	1	69	C
1	1	71	C
1	1	74	C
1	1	75	C
1	1	76	A
2	2	2	A
2	2	4	C
2	2	5	U
2	2	8	U
2	2	9	U
2	2	11	A
2	2	13	C
2	2	19	A
2	2	24	U
2	2	25	C
2	2	26	A
2	2	27	U
2	2	31	C
2	2	34	G
2	2	35	U
2	2	36	C
2	2	37	U
2	2	42	G
2	2	45	U
2	2	46	A

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Mol	Chain	Res	Type
2	2	47	A
2	2	50	C
2	2	51	A
2	2	54	C
2	2	55	A
2	2	56	U
2	2	57	G
2	2	59	C
2	2	60	U
2	2	61	A
2	2	62	A
2	2	63	G
2	2	64	U
2	2	65	A
2	2	67	A
2	2	68	A
2	2	69	G
2	2	70	C
2	2	72	A
2	2	73	U
2	2	74	U
2	2	75	U
2	2	76	A
2	2	77	U
2	2	79	C
2	2	80	A
2	2	82	U
2	2	90	C
2	2	95	G
2	2	104	A
2	2	111	U
2	2	114	C
2	2	116	U
2	2	123	G
2	2	124	A
2	2	127	G
2	2	129	U
2	2	130	C
2	2	131	C
2	2	132	U
2	2	133	U
2	2	134	U

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Mol	Chain	Res	Type
2	2	136	C
2	2	137	U
2	2	138	A
2	2	139	C
2	2	140	A
2	2	141	U
2	2	144	A
2	2	146	A
2	2	147	U
2	2	157	U
2	2	158	U
2	2	159	C
2	2	160	U
2	2	161	A
2	2	167	A
2	2	172	A
2	2	173	U
2	2	175	C
2	2	176	U
2	2	177	U
2	2	178	A
2	2	183	C
2	2	185	C
2	2	190	C
2	2	191	U
2	2	192	U
2	2	194	G
2	2	195	G
2	2	198	G
2	2	208	U
2	2	209	A
2	2	217	A
2	2	218	A
2	2	220	A
2	2	225	A
2	2	226	U
2	2	227	G
2	2	228	U
2	2	230	U
2	2	231	U
2	2	232	C
2	2	233	G

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Mol	Chain	Res	Type
2	2	237	U
2	2	239	C
2	2	240	U
2	2	249	C
2	2	256	A
2	2	259	U
2	2	264	A
2	2	265	A
2	2	266	U
2	2	270	A
2	2	271	U
2	2	274	C
2	2	275	C
2	2	276	U
2	2	277	U
2	2	278	G
2	2	279	U
2	2	280	G
2	2	286	G
2	2	287	A
2	2	288	U
2	2	294	A
2	2	298	A
2	2	300	A
2	2	301	U
2	2	307	C
2	2	308	C
2	2	311	A
2	2	312	U
2	2	313	C
2	2	314	A
2	2	315	A
2	2	319	U
2	2	320	C
2	2	321	G
2	2	322	A
2	2	332	A
2	2	336	G
2	2	337	C
2	2	345	G
2	2	349	U
2	2	351	A

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Mol	Chain	Res	Type
2	2	358	A
2	2	359	A
2	2	360	C
2	2	369	A
2	2	377	A
2	2	379	U
2	2	380	C
2	2	382	G
2	2	384	A
2	2	386	A
2	2	387	G
2	2	389	G
2	2	397	G
2	2	398	A
2	2	399	A
2	2	400	A
2	2	401	C
2	2	402	G
2	2	403	G
2	2	413	C
2	2	415	A
2	2	416	A
2	2	421	G
2	2	422	G
2	2	423	C
2	2	424	A
2	2	425	G
2	2	426	C
2	2	433	G
2	2	434	C
2	2	438	U
2	2	439	U
2	2	440	A
2	2	443	C
2	2	444	A
2	2	447	C
2	2	448	C
2	2	452	U
2	2	455	A
2	2	458	G
2	2	459	A
2	2	463	A

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Mol	Chain	Res	Type
2	2	469	A
2	2	473	A
2	2	476	A
2	2	478	C
2	2	479	G
2	2	480	A
2	2	481	U
2	2	482	A
2	2	483	C
2	2	488	C
2	2	489	C
2	2	490	C
2	2	491	A
2	2	492	U
2	2	493	U
2	2	495	G
2	2	496	G
2	2	497	G
2	2	499	C
2	2	501	U
2	2	502	G
2	2	504	A
2	2	505	A
2	2	506	U
2	2	507	U
2	2	509	G
2	2	516	U
2	2	517	A
2	2	518	C
2	2	519	A
2	2	522	G
2	2	523	U
2	2	524	A
2	2	525	A
2	2	527	U
2	2	530	C
2	2	531	U
2	2	532	U
2	2	533	A
2	2	534	A
2	2	535	C
2	2	537	A

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Mol	Chain	Res	Type
2	2	538	G
2	2	539	G
2	2	540	A
2	2	541	A
2	2	542	C
2	2	543	A
2	2	544	A
2	2	547	G
2	2	548	G
2	2	553	C
2	2	554	A
2	2	556	G
2	2	557	U
2	2	558	C
2	2	563	G
2	2	564	C
2	2	565	C
2	2	567	G
2	2	568	C
2	2	570	G
2	2	571	C
2	2	573	G
2	2	577	U
2	2	578	A
2	2	579	A
2	2	580	U
2	2	581	U
2	2	584	A
2	2	586	C
2	2	587	U
2	2	593	A
2	2	594	G
2	2	605	A
2	2	610	U
2	2	612	G
2	2	614	A
2	2	618	A
2	2	619	A
2	2	620	A
2	2	622	A
2	2	634	A
2	2	637	U

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Mol	Chain	Res	Type
2	2	638	U
2	2	640	G
2	2	641	G
2	2	647	G
2	2	649	U
2	2	650	G
2	2	651	U
2	2	652	C
2	2	653	C
2	2	654	G
2	2	655	G
2	2	656	U
2	2	657	C
2	2	677	G
2	2	679	U
2	2	684	A
2	2	686	C
2	2	687	C
2	2	691	U
2	2	693	U
2	2	694	U
2	2	696	C
2	2	697	C
2	2	698	U
2	2	700	C
2	2	701	U
2	2	702	G
2	2	704	C
2	2	705	U
2	2	706	A
2	2	709	C
2	2	710	U
2	2	711	G
2	2	712	U
2	2	713	A
2	2	714	C
2	2	716	C
2	2	717	C
2	2	718	U
2	2	719	U
2	2	721	U
2	2	722	G

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Mol	Chain	Res	Type
2	2	725	U
2	2	726	G
2	2	727	C
2	2	728	A
2	2	731	C
2	2	732	G
2	2	733	A
2	2	734	A
2	2	735	C
2	2	736	C
2	2	738	G
2	2	741	C
2	2	742	U
2	2	744	U
2	2	745	U
2	2	747	C
2	2	753	A
2	2	754	A
2	2	755	A
2	2	762	A
2	2	764	U
2	2	765	G
2	2	766	U
2	2	767	U
2	2	768	C
2	2	771	A
2	2	774	A
2	2	775	G
2	2	778	G
2	2	780	A
2	2	781	A
2	2	782	G
2	2	783	C
2	2	784	U
2	2	785	C
2	2	786	G
2	2	788	A
2	2	791	U
2	2	793	U
2	2	794	U
2	2	796	G
2	2	803	A

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Mol	Chain	Res	Type
2	2	806	A
2	2	809	G
2	2	810	A
2	2	811	A
2	2	813	A
2	2	814	G
2	2	817	C
2	2	818	G
2	2	819	U
2	2	820	U
2	2	822	G
2	2	823	G
2	2	825	U
2	2	826	C
2	2	827	U
2	2	828	A
2	2	829	U
2	2	840	U
2	2	845	G
2	2	847	C
2	2	851	C
2	2	854	A
2	2	855	A
2	2	856	U
2	2	859	U
2	2	861	A
2	2	862	A
2	2	863	U
2	2	864	A
2	2	872	U
2	2	875	G
2	2	876	G
2	2	881	U
2	2	895	U
2	2	897	A
2	2	898	G
2	2	904	A
2	2	905	A
2	2	907	U
2	2	908	U
2	2	910	U
2	2	912	G

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Mol	Chain	Res	Type
2	2	913	G
2	2	915	U
2	2	918	A
2	2	919	U
2	2	920	U
2	2	924	G
2	2	925	A
2	2	927	U
2	2	930	C
2	2	931	U
2	2	932	A
2	2	933	C
2	2	934	U
2	2	938	A
2	2	939	A
2	2	941	G
2	2	944	U
2	2	946	U
2	2	947	G
2	2	950	A
2	2	956	G
2	2	957	U
2	2	958	U
2	2	965	A
2	2	970	A
2	2	972	A
2	2	981	U
2	2	982	A
2	2	983	G
2	2	984	G
2	2	991	A
2	2	995	U
2	2	997	A
2	2	1000	A
2	2	1001	G
2	2	1002	A
2	2	1003	U
2	2	1004	A
2	2	1009	C
2	2	1011	U
2	2	1012	A
2	2	1015	C

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Mol	Chain	Res	Type
2	2	1018	A
2	2	1020	C
2	2	1022	A
2	2	1024	A
2	2	1025	A
2	2	1026	A
2	2	1027	C
2	2	1030	U
2	2	1031	G
2	2	1034	G
2	2	1038	A
2	2	1039	G
2	2	1041	G
2	2	1043	U
2	2	1044	C
2	2	1047	G
2	2	1048	U
2	2	1049	G
2	2	1050	G
2	2	1051	U
2	2	1052	G
2	2	1054	U
2	2	1055	U
2	2	1056	U
2	2	1057	U
2	2	1058	C
2	2	1059	U
2	2	1060	U
2	2	1062	U
2	2	1068	A
2	2	1069	C
2	2	1070	U
2	2	1075	A
2	2	1080	A
2	2	1081	C
2	2	1082	G
2	2	1084	G
2	2	1085	A
2	2	1086	A
2	2	1089	C
2	2	1090	A
2	2	1091	A

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Mol	Chain	Res	Type
2	2	1093	G
2	2	1095	C
2	2	1096	U
2	2	1097	U
2	2	1098	U
2	2	1099	G
2	2	1100	G
2	2	1102	U
2	2	1103	U
2	2	1105	U
2	2	1108	G
2	2	1112	A
2	2	1113	G
2	2	1114	U
2	2	1117	G
2	2	1118	G
2	2	1119	U
2	2	1121	G
2	2	1123	A
2	2	1124	A
2	2	1129	G
2	2	1137	A
2	2	1144	U
2	2	1145	G
2	2	1146	A
2	2	1149	G
2	2	1150	A
2	2	1151	A
2	2	1153	G
2	2	1155	C
2	2	1157	C
2	2	1158	C
2	2	1161	C
2	2	1162	A
2	2	1163	G
2	2	1165	A
2	2	1166	G
2	2	1167	U
2	2	1169	G
2	2	1172	C
2	2	1174	U
2	2	1176	C

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Mol	Chain	Res	Type
2	2	1182	A
2	2	1184	U
2	2	1188	A
2	2	1190	U
2	2	1192	A
2	2	1193	A
2	2	1197	G
2	2	1198	G
2	2	1199	G
2	2	1200	G
2	2	1201	A
2	2	1202	A
2	2	1203	A
2	2	1207	A
2	2	1211	G
2	2	1216	A
2	2	1217	G
2	2	1223	A
2	2	1224	U
2	2	1226	A
2	2	1227	G
2	2	1228	G
2	2	1229	A
2	2	1230	U
2	2	1231	U
2	2	1234	C
2	2	1236	G
2	2	1240	G
2	2	1241	A
2	2	1243	A
2	2	1244	G
2	2	1246	U
2	2	1253	U
2	2	1254	G
2	2	1255	A
2	2	1256	U
2	2	1258	U
2	2	1259	U
2	2	1260	G
2	2	1266	G
2	2	1268	U
2	2	1269	G

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Mol	Chain	Res	Type
2	2	1272	G
2	2	1273	C
2	2	1275	U
2	2	1279	C
2	2	1282	U
2	2	1283	C
2	2	1284	U
2	2	1285	U
2	2	1286	A
2	2	1287	G
2	2	1292	U
2	2	1295	A
2	2	1296	G
2	2	1297	U
2	2	1298	G
2	2	1300	U
2	2	1303	G
2	2	1305	C
2	2	1306	U
2	2	1309	U
2	2	1310	U
2	2	1312	A
2	2	1313	U
2	2	1314	U
2	2	1315	G
2	2	1316	C
2	2	1317	G
2	2	1320	A
2	2	1321	A
2	2	1323	G
2	2	1324	A
2	2	1327	G
2	2	1328	A
2	2	1329	G
2	2	1331	C
2	2	1332	C
2	2	1333	U
2	2	1336	A
2	2	1337	C
2	2	1338	C
2	2	1339	U
2	2	1343	A

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Mol	Chain	Res	Type
2	2	1344	A
2	2	1345	A
2	2	1346	U
2	2	1347	A
2	2	1352	U
2	2	1353	G
2	2	1355	U
2	2	1361	U
2	2	1362	U
2	2	1364	C
2	2	1366	G
2	2	1369	U
2	2	1370	G
2	2	1371	A
2	2	1374	C
2	2	1375	U
2	2	1376	U
2	2	1378	U
2	2	1380	A
2	2	1381	G
2	2	1383	G
2	2	1386	A
2	2	1388	U
2	2	1389	A
2	2	1391	C
2	2	1393	G
2	2	1396	U
2	2	1397	C
2	2	1398	A
2	2	1400	G
2	2	1410	G
2	2	1411	U
2	2	1412	U
2	2	1413	U
2	2	1418	C
2	2	1419	A
2	2	1420	A
2	2	1425	A
2	2	1426	G
2	2	1428	U
2	2	1429	C
2	2	1430	U

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Mol	Chain	Res	Type
2	2	1431	G
2	2	1433	G
2	2	1434	A
2	2	1435	U
2	2	1442	A
2	2	1444	A
2	2	1445	C
2	2	1448	U
2	2	1449	C
2	2	1455	C
2	2	1456	G
2	2	1457	C
2	2	1461	C
2	2	1463	C
2	2	1467	A
2	2	1469	A
2	2	1470	C
2	2	1471	U
2	2	1476	G
2	2	1479	C
2	2	1482	G
2	2	1483	C
2	2	1484	G
2	2	1488	A
2	2	1489	C
2	2	1490	A
2	2	1491	A
2	2	1492	C
2	2	1494	U
2	2	1499	C
2	2	1502	G
2	2	1504	G
2	2	1508	U
2	2	1509	G
2	2	1512	U
2	2	1513	A
2	2	1514	A
2	2	1515	U
2	2	1516	C
2	2	1519	G
2	2	1521	G
2	2	1522	A

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Mol	Chain	Res	Type
2	2	1523	A
2	2	1529	G
2	2	1532	G
2	2	1533	U
2	2	1534	G
2	2	1535	C
2	2	1536	U
2	2	1538	G
2	2	1540	G
2	2	1541	A
2	2	1542	U
2	2	1543	A
2	2	1544	G
2	2	1548	A
2	2	1551	G
2	2	1554	A
2	2	1555	U
2	2	1557	A
2	2	1563	C
2	2	1564	U
2	2	1566	C
2	2	1570	G
2	2	1571	A
2	2	1572	G
2	2	1573	G
2	2	1575	A
2	2	1581	A
2	2	1582	G
2	2	1583	U
2	2	1589	C
2	2	1590	A
2	2	1595	A
2	2	1597	C
2	2	1598	A
2	2	1599	G
2	2	1604	C
2	2	1608	G
2	2	1613	C
2	2	1614	G
2	2	1616	C
2	2	1617	C
2	2	1620	G

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Mol	Chain	Res	Type
2	2	1621	C
2	2	1625	U
2	2	1626	U
2	2	1629	A
2	2	1630	C
2	2	1631	A
2	2	1632	C
2	2	1633	A
2	2	1635	C
2	2	1636	G
2	2	1637	C
2	2	1638	C
2	2	1640	G
2	2	1646	A
2	2	1647	G
2	2	1649	A
2	2	1655	U
2	2	1656	G
2	2	1662	C
2	2	1676	A
2	2	1678	G
2	2	1679	A
2	2	1682	U
2	2	1685	U
2	2	1686	U
2	2	1687	A
2	2	1688	G
2	2	1692	A
2	2	1693	G
2	2	1694	G
2	2	1695	G
2	2	1696	G
2	2	1697	G
2	2	1698	C
2	2	1699	A
2	2	1700	A
2	2	1701	C
2	2	1702	U
2	2	1703	C
2	2	1705	A
2	2	1706	U
2	2	1707	C

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Mol	Chain	Res	Type
2	2	1709	C
2	2	1710	A
2	2	1711	G
2	2	1712	A
2	2	1725	G
2	2	1730	A
2	2	1742	A
2	2	1743	G
2	2	1744	A
2	2	1745	G
2	2	1748	A
2	2	1750	U
2	2	1754	A
2	2	1755	G
2	2	1758	G
2	2	1760	A
2	2	1763	A
2	2	1764	A
2	2	1766	G
2	2	1767	U
2	2	1768	U
2	2	1769	U
2	2	1770	C
2	2	1777	U
2	2	1778	G
2	2	1780	A
2	2	1781	C
2	2	1786	G
2	2	1787	G
2	2	1789	A
2	2	1790	G
2	2	1791	G
2	2	1792	A
2	2	1793	U
2	2	1794	C
2	2	1795	A
2	2	1796	U
2	2	1797	U

All (130) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	1	9	1MG
1	1	10	2MG
1	1	16	H2U
1	1	19	G
1	1	20	A
1	1	36	U
1	1	37	T6A
1	1	38	A
1	1	46	7MG
1	1	47	H2U
1	1	48	5MC
1	1	74	C
2	2	25	C
2	2	44	U
2	2	45	U
2	2	46	A
2	2	55	A
2	2	58	U
2	2	61	A
2	2	66	U
2	2	68	A
2	2	74	U
2	2	103	A
2	2	115	G
2	2	130	C
2	2	131	C
2	2	133	U
2	2	134	U
2	2	157	U
2	2	177	U
2	2	189	C
2	2	190	C
2	2	193	U
2	2	216	A
2	2	217	A
2	2	239	C
2	2	258	U
2	2	265	A
2	2	270	A
2	2	271	U
2	2	275	C

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Mol	Chain	Res	Type
2	2	277	U
2	2	279	U
2	2	321	G
2	2	349	U
2	2	379	U
2	2	399	A
2	2	451	A
2	2	454	C
2	2	497	G
2	2	524	A
2	2	538	G
2	2	542	C
2	2	543	A
2	2	564	C
2	2	580	U
2	2	593	A
2	2	608	U
2	2	619	A
2	2	637	U
2	2	654	G
2	2	685	A
2	2	693	U
2	2	695	U
2	2	700	C
2	2	721	U
2	2	724	G
2	2	784	U
2	2	793	U
2	2	810	A
2	2	812	U
2	2	813	A
2	2	822	G
2	2	826	C
2	2	827	U
2	2	828	A
2	2	854	A
2	2	855	A
2	2	896	C
2	2	907	U
2	2	911	U
2	2	912	G
2	2	918	A

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Mol	Chain	Res	Type
2	2	945	U
2	2	946	U
2	2	956	G
2	2	1000	A
2	2	1001	G
2	2	1002	A
2	2	1015	C
2	2	1022	A
2	2	1030	U
2	2	1051	U
2	2	1056	U
2	2	1080	A
2	2	1096	U
2	2	1097	U
2	2	1099	G
2	2	1107	G
2	2	1123	A
2	2	1195	A
2	2	1198	G
2	2	1206	C
2	2	1226	A
2	2	1284	U
2	2	1314	U
2	2	1343	A
2	2	1363	G
2	2	1380	A
2	2	1411	U
2	2	1412	U
2	2	1424	C
2	2	1430	U
2	2	1455	C
2	2	1487	U
2	2	1488	A
2	2	1491	A
2	2	1514	A
2	2	1534	G
2	2	1537	G
2	2	1571	A
2	2	1613	C
2	2	1631	A
2	2	1655	U
2	2	1678	G

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Mol	Chain	Res	Type
2	2	1706	U
2	2	1765	G
2	2	1789	A
2	2	1790	G
2	2	1792	A

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

11 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	5MC	1	48	1	18,22,23	1.09	1 (5%)	26,32,35	1.45	4 (15%)
1	H2U	1	16	1	18,21,22	0.86	1 (5%)	21,30,33	1.23	2 (9%)
1	1MA	1	58	1	16,25,26	1.80	4 (25%)	18,37,40	1.25	3 (16%)
1	H2U	1	47	1	18,21,22	0.78	1 (5%)	21,30,33	1.36	3 (14%)
1	1MG	1	9	1	18,26,27	1.05	1 (5%)	19,39,42	1.58	4 (21%)
1	2MG	1	10	1	18,26,27	0.98	0	16,38,41	1.48	3 (18%)
1	5MC	1	49	1	18,22,23	1.08	1 (5%)	26,32,35	1.38	5 (19%)
1	RIA	1	64	1	31,38,39	1.21	3 (9%)	39,57,60	2.50	11 (28%)
1	M2G	1	26	1	20,27,28	1.69	2 (10%)	22,40,43	1.27	5 (22%)
1	7MG	1	46	1	22,26,27	1.49	4 (18%)	29,39,42	2.52	6 (20%)
1	T6A	1	37	1	27,34,35	1.10	2 (7%)	29,49,52	2.41	9 (31%)

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
1	5MC	1	48	1	-	1/7/25/26	0/2/2/2
1	H2U	1	16	1	-	3/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	1MA	1	58	1	-	1/3/25/26	0/3/3/3
1	H2U	1	47	1	-	5/7/38/39	0/2/2/2
1	1MG	1	9	1	-	0/3/25/26	0/3/3/3
1	2MG	1	10	1	-	2/5/27/28	0/3/3/3
1	5MC	1	49	1	-	3/7/25/26	0/2/2/2
1	RIA	1	64	1	-	4/13/51/52	0/4/4/4
1	M2G	1	26	1	-	6/7/29/30	0/3/3/3
1	7MG	1	46	1	-	0/7/37/38	0/3/3/3
1	T6A	1	37	1	-	13/19/41/42	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	58	1MA	C2-N3	5.47	1.35	1.29
1	1	26	M2G	C2-N3	5.41	1.37	1.30
1	1	64	RIA	P'-O3X	-3.69	1.40	1.54
1	1	26	M2G	C2-N2	3.66	1.42	1.35
1	1	58	1MA	C6-N6	3.41	1.36	1.27
1	1	49	5MC	C6-C5	3.28	1.40	1.34
1	1	48	5MC	C6-C5	3.23	1.39	1.34
1	1	46	7MG	C5-C4	3.22	1.48	1.38
1	1	37	T6A	C5-C4	2.90	1.48	1.40
1	1	46	7MG	C4-N9	-2.90	1.34	1.37
1	1	46	7MG	C8-N9	2.76	1.47	1.46
1	1	46	7MG	C5-C6	2.21	1.49	1.43
1	1	9	1MG	C5-C4	2.13	1.48	1.43
1	1	16	H2U	C2-N3	-2.12	1.34	1.38
1	1	64	RIA	C2-N1	2.11	1.37	1.33
1	1	64	RIA	O4'-C1A	2.10	1.44	1.41
1	1	58	1MA	C5-C4	2.02	1.48	1.43
1	1	37	T6A	O4'-C1'	2.01	1.43	1.41
1	1	47	H2U	C2-N3	-2.01	1.34	1.38
1	1	58	1MA	O4'-C1'	2.00	1.43	1.41

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	64	RIA	O2A-C1'-O1'	-8.59	102.13	111.43
1	1	46	7MG	N9-C4-N3	8.43	138.07	125.47
1	1	37	T6A	C2-N1-C6	7.40	122.94	116.59
1	1	64	RIA	O2A-C1'-C2'	-6.66	94.14	107.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	37	T6A	N6-C10-N11	5.98	122.12	113.76
1	1	64	RIA	O5'-P'-O1X	5.69	122.43	106.47
1	1	46	7MG	C5-C4-N3	-5.29	118.05	128.13
1	1	64	RIA	C1'-O2A-C2A	4.89	130.07	117.96
1	1	46	7MG	N9-C8-N7	-4.85	96.45	103.38
1	1	46	7MG	C2-N3-C4	4.48	120.28	112.30
1	1	37	T6A	O10-C10-N6	-3.83	117.14	123.62
1	1	37	T6A	N3-C2-N1	-3.66	122.95	128.68
1	1	10	2MG	C3'-C2'-C1'	3.66	106.48	100.98
1	1	9	1MG	C3'-C2'-C1'	3.52	106.28	100.98
1	1	37	T6A	C4-C5-N7	-3.31	105.95	109.40
1	1	48	5MC	O2-C2-N3	-3.22	117.10	122.33
1	1	64	RIA	O2X-P'-O5'	-3.05	98.61	106.73
1	1	48	5MC	C5-C4-N3	-2.89	118.55	121.67
1	1	16	H2U	C4-N3-C2	-2.89	123.40	125.79
1	1	46	7MG	C5-C6-N1	2.86	116.03	110.99
1	1	49	5MC	O2-C2-N3	-2.83	117.73	122.33
1	1	49	5MC	C5-C4-N3	-2.78	118.68	121.67
1	1	64	RIA	O3X-P'-O5'	2.77	114.09	106.73
1	1	64	RIA	O1'-C1'-C2'	2.76	108.54	104.98
1	1	26	M2G	N1-C2-N2	2.73	120.36	118.04
1	1	26	M2G	C3'-C2'-C1'	2.72	105.08	100.98
1	1	9	1MG	C5-C6-N1	2.70	117.97	113.90
1	1	47	H2U	C4-N3-C2	-2.69	123.56	125.79
1	1	9	1MG	O6-C6-C5	-2.68	119.44	124.19
1	1	47	H2U	C5-C4-N3	2.68	119.65	116.65
1	1	58	1MA	C3'-C2'-C1'	2.64	104.95	100.98
1	1	16	H2U	C3'-C2'-C1'	2.57	106.31	101.43
1	1	26	M2G	C5-C6-N1	2.56	118.47	113.95
1	1	64	RIA	C5-C6-N6	2.50	124.15	120.35
1	1	48	5MC	C3'-C2'-C1'	2.48	106.14	101.43
1	1	49	5MC	C3'-C2'-C1'	2.47	106.12	101.43
1	1	37	T6A	O3'-C3'-C4'	2.42	118.06	111.05
1	1	49	5MC	CM5-C5-C6	-2.42	119.62	122.85
1	1	9	1MG	C8-N7-C5	2.42	107.60	102.99
1	1	10	2MG	C5-C6-N1	2.42	118.22	113.95
1	1	58	1MA	C5-C6-N1	2.38	117.45	113.90
1	1	58	1MA	C8-N7-C5	2.37	107.51	102.99
1	1	47	H2U	C3'-C2'-C1'	2.36	105.91	101.43
1	1	48	5MC	CM5-C5-C6	-2.31	119.76	122.85
1	1	26	M2G	C8-N7-C5	2.29	107.36	102.99
1	1	64	RIA	P'-O5'-C5'	-2.29	111.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	37	T6A	C3'-C2'-C1'	2.28	104.42	100.98
1	1	10	2MG	C8-N7-C5	2.28	107.33	102.99
1	1	49	5MC	C5-C6-N1	-2.20	121.08	123.34
1	1	26	M2G	O6-C6-C5	-2.18	120.11	124.37
1	1	46	7MG	CM7-N7-C5	2.16	131.97	126.40
1	1	37	T6A	C2'-C3'-C4'	2.10	106.72	102.64
1	1	37	T6A	ODB-C13-C12	2.05	121.45	114.21
1	1	64	RIA	C4-C5-N7	2.02	111.51	109.40
1	1	64	RIA	O1'-C4'-C5'	-2.02	102.74	109.37

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	16	H2U	C3'-C4'-C5'-O5'
1	1	26	M2G	C3'-C4'-C5'-O5'
1	1	26	M2G	N1-C2-N2-CM1
1	1	26	M2G	N3-C2-N2-CM1
1	1	37	T6A	C5-C6-N6-C10
1	1	37	T6A	N11-C12-C13-ODB
1	1	37	T6A	C14-C12-C13-ODA
1	1	37	T6A	C14-C12-C13-ODB
1	1	37	T6A	C13-C12-C14-O14
1	1	37	T6A	C13-C12-C14-C15
1	1	47	H2U	O4'-C4'-C5'-O5'
1	1	47	H2U	C3'-C4'-C5'-O5'
1	1	47	H2U	O4'-C1'-N1-C2
1	1	47	H2U	O4'-C1'-N1-C6
1	1	64	RIA	C5'-O5'-P'-O1X
1	1	64	RIA	C5'-O5'-P'-O2X
1	1	64	RIA	C5'-O5'-P'-O3X
1	1	16	H2U	O4'-C4'-C5'-O5'
1	1	37	T6A	O4'-C4'-C5'-O5'
1	1	49	5MC	O4'-C4'-C5'-O5'
1	1	37	T6A	C3'-C4'-C5'-O5'
1	1	49	5MC	C3'-C4'-C5'-O5'
1	1	37	T6A	N11-C12-C14-O14
1	1	37	T6A	N11-C12-C13-ODA
1	1	26	M2G	O4'-C4'-C5'-O5'
1	1	47	H2U	C4'-C5'-O5'-P
1	1	26	M2G	N3-C2-N2-CM2
1	1	10	2MG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	1	16	H2U	C4'-C5'-O5'-P
1	1	48	5MC	C4'-C5'-O5'-P
1	1	37	T6A	N11-C12-C14-C15
1	1	10	2MG	C3'-C4'-C5'-O5'
1	1	37	T6A	N1-C6-N6-C10
1	1	49	5MC	C4'-C5'-O5'-P
1	1	37	T6A	C4'-C5'-O5'-P
1	1	26	M2G	N1-C2-N2-CM2
1	1	64	RIA	O1'-C4'-C5'-O5'
1	1	58	1MA	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 88 ligands modelled in this entry, 86 are monoatomic - leaving 2 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	$\# Z  > 2$
51	GCP	k	603	48	27,34,34	1.91	7 (25%)	34,54,54	1.97	8 (23%)
50	MET	k	601	-	6,7,8	0.45	0	2,7,9	0.38	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
51	GCP	k	603	48	-	0/15/38/38	0/3/3/3
50	MET	k	601	-	-	0/5/6/8	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	k	603	GCP	PG-O1G	5.35	1.61	1.50
51	k	603	GCP	C5-C6	4.78	1.49	1.41
51	k	603	GCP	PG-O3G	-2.83	1.48	1.54
51	k	603	GCP	PB-O3A	2.77	1.61	1.58
51	k	603	GCP	PG-O2G	2.76	1.61	1.54
51	k	603	GCP	C5-C4	2.69	1.48	1.40
51	k	603	GCP	PB-O2B	2.17	1.61	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	k	603	GCP	C2-N3-C4	5.27	121.38	115.36
51	k	603	GCP	C2-N1-C6	4.02	122.31	115.93
51	k	603	GCP	C4-C5-C6	-3.99	116.99	120.80
51	k	603	GCP	C5-C6-N1	-3.75	118.31	123.43
51	k	603	GCP	N3-C2-N1	-3.54	122.51	127.22
51	k	603	GCP	PB-O3A-PA	-3.34	121.98	132.56
51	k	603	GCP	C3'-C2'-C1'	2.90	105.34	100.98
51	k	603	GCP	C4-C5-N7	-2.82	106.46	109.40

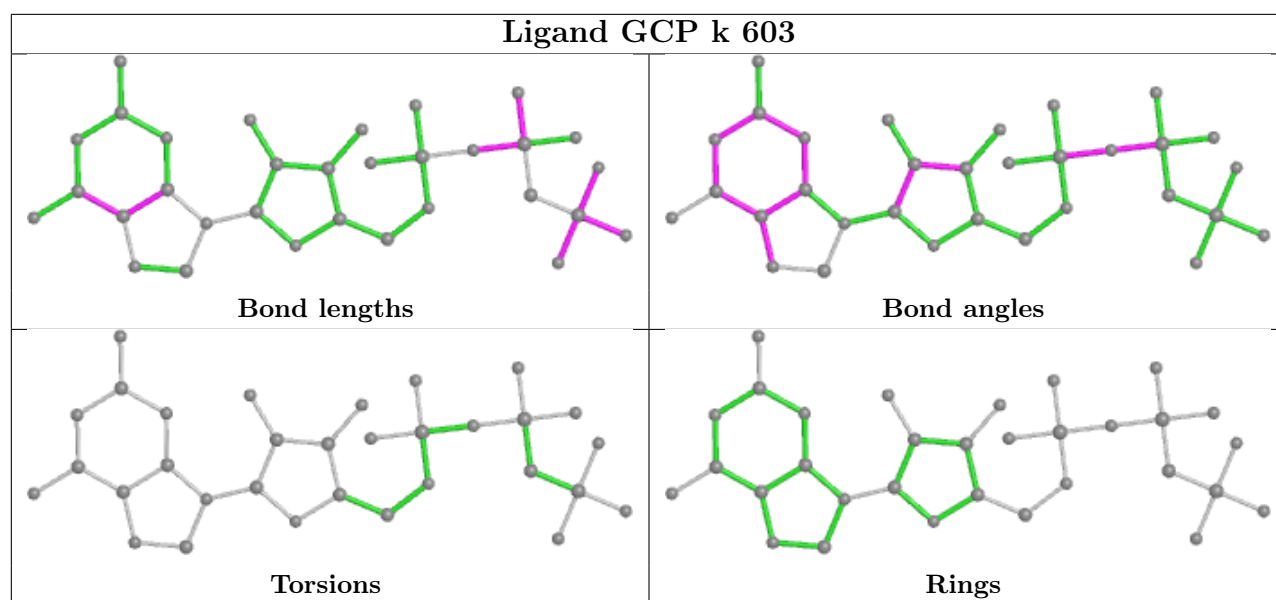
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
44	p	6
43	o	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	p	32:UNK	C	116:UNK	N	41.18
1	p	158:UNK	C	170:UNK	N	14.29
1	p	185:UNK	C	193:UNK	N	9.56
1	o	846:UNK	C	850:UNK	N	7.84
1	o	818:UNK	C	829:UNK	N	7.14
1	o	769:UNK	C	772:UNK	N	6.87
1	p	148:UNK	C	150:UNK	N	6.72
1	o	834:UNK	C	837:UNK	N	6.07
1	p	135:UNK	C	139:UNK	N	5.95
1	o	802:UNK	C	806:UNK	N	5.00
1	p	206:UNK	C	211:UNK	N	4.75
1	o	785:UNK	C	788:UNK	N	3.58

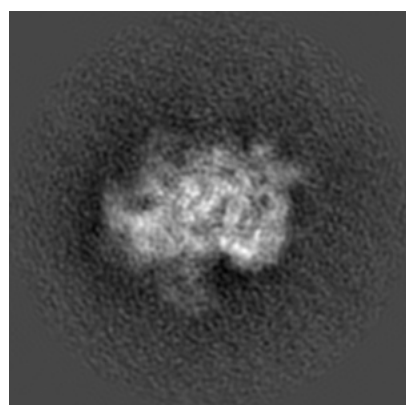
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3049. These allow visual inspection of the internal detail of the map and identification of artifacts.

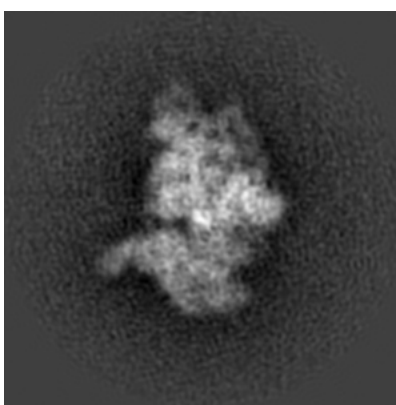
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

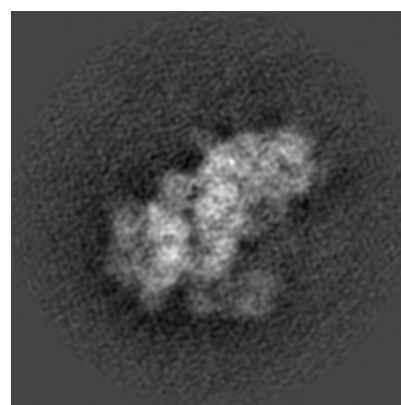
#### 6.1.1 Primary map



X



Y

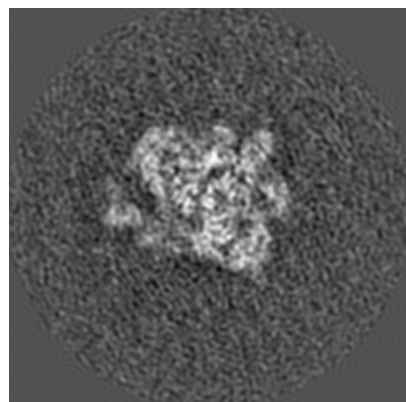


Z

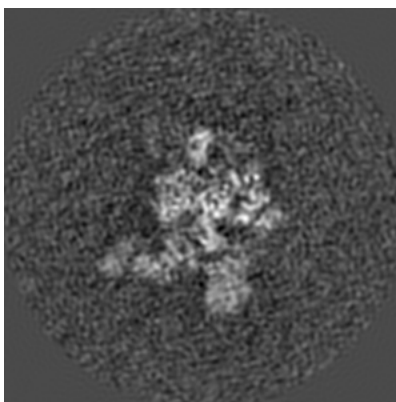
The images above show the map projected in three orthogonal directions.

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

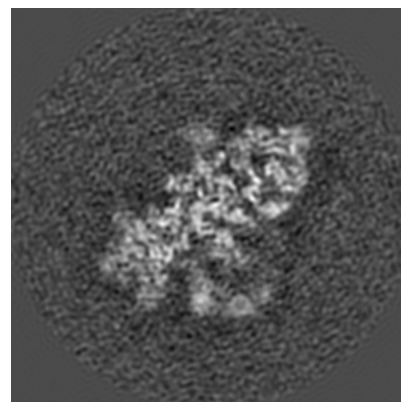
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

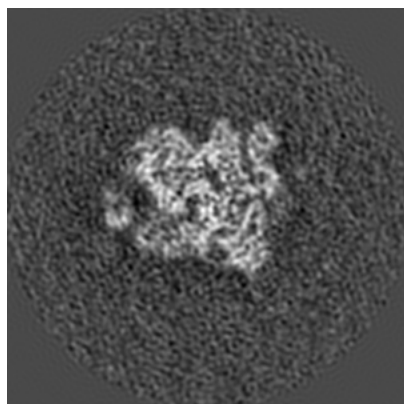


Z Index: 150

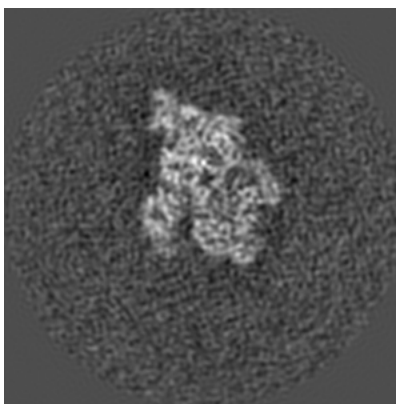
The images above show central slices of the map in three orthogonal directions.

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

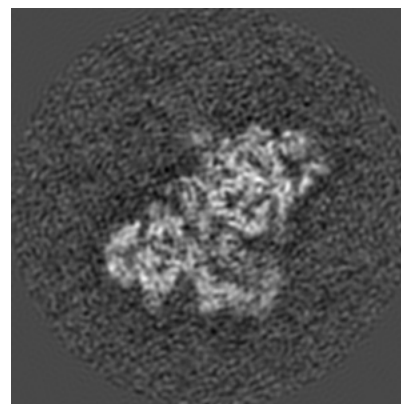
### 6.3.1 Primary map



X Index: 155



Y Index: 171



Z Index: 143

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 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

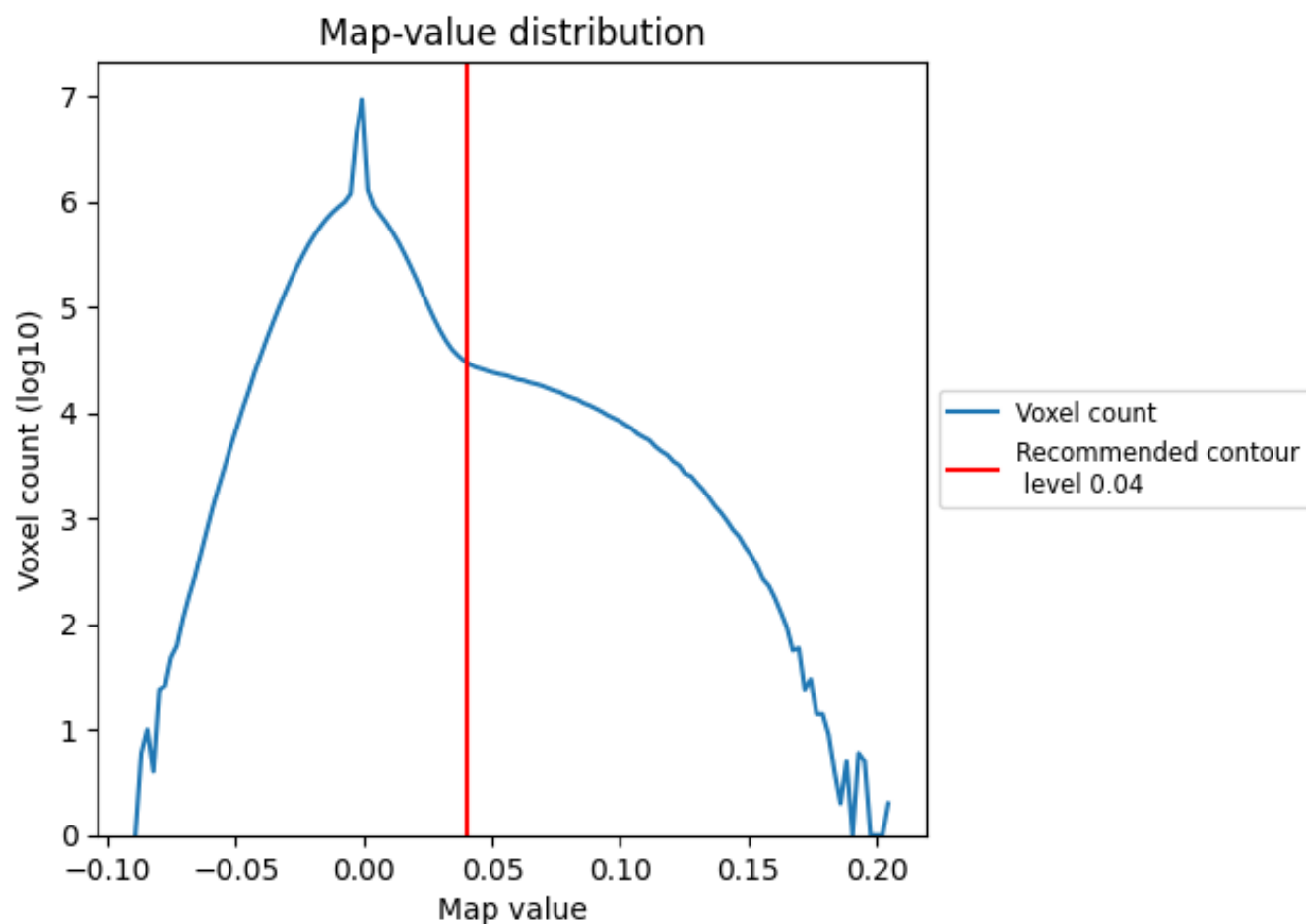
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

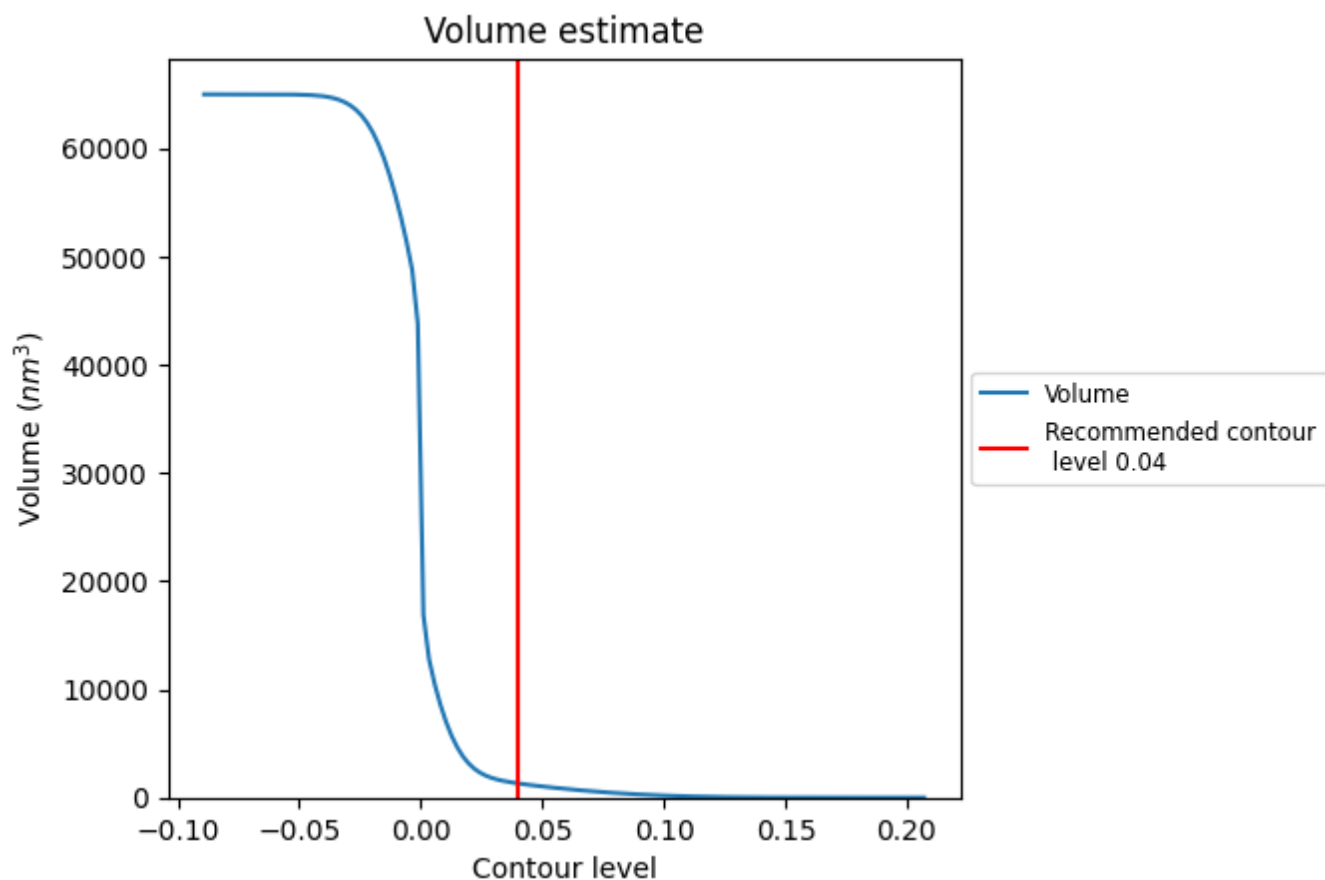
This section contains the results of statistical analysis of the map.

### 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.

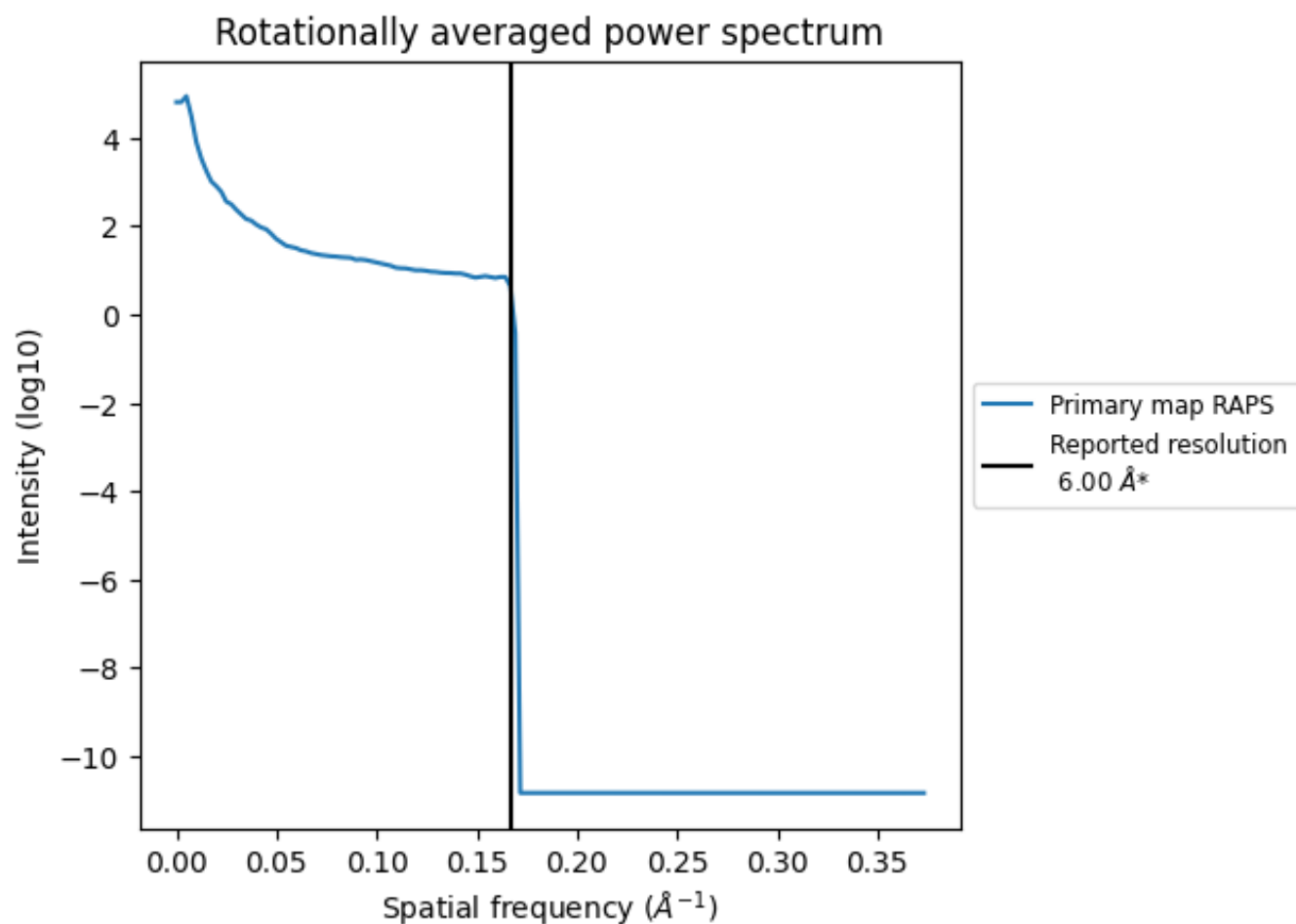
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1309  $\text{nm}^3$ ; this corresponds to an approximate mass of 1182 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 ⓘ

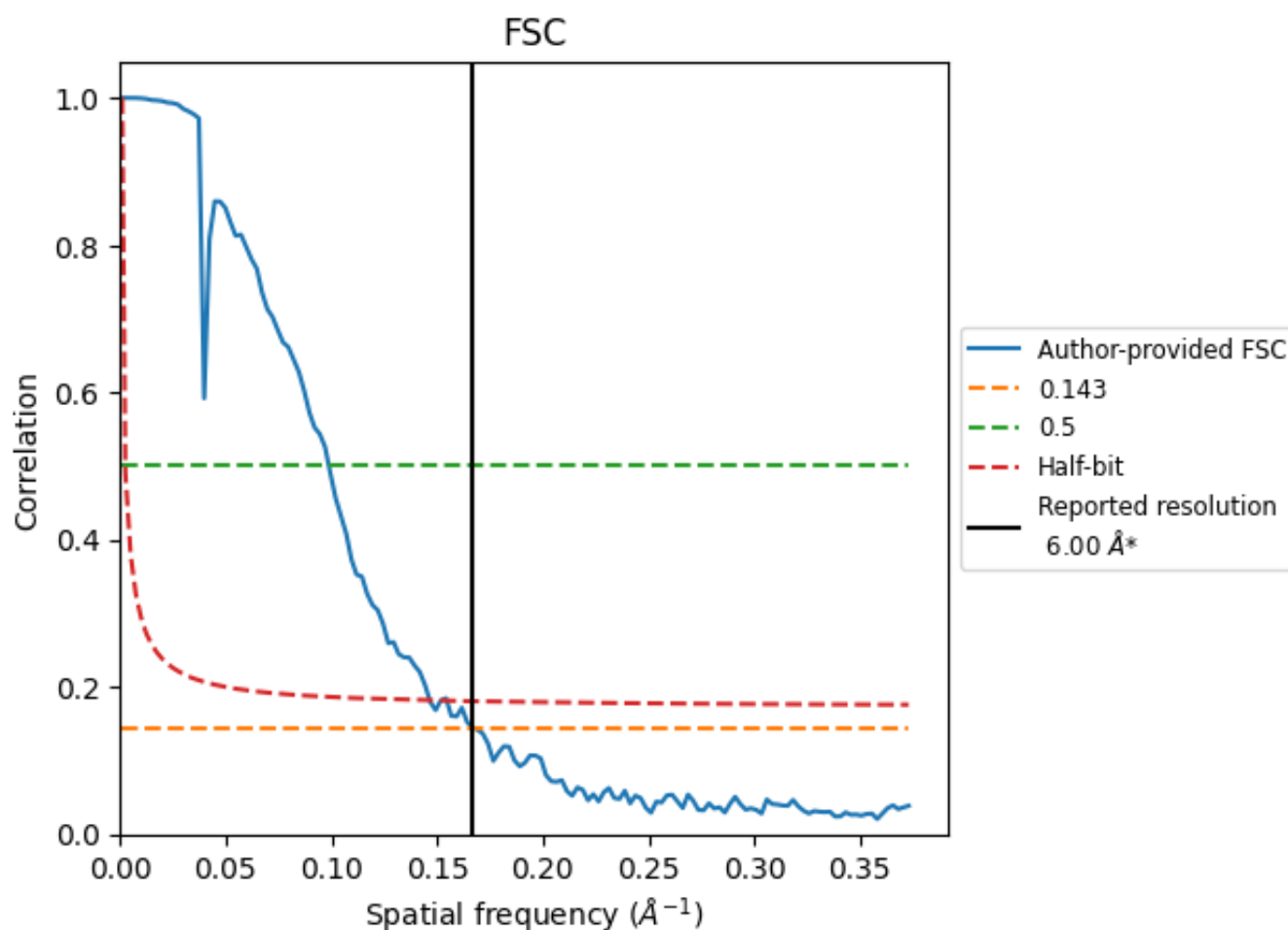


\*Reported resolution corresponds to spatial frequency of 0.167 Å<sup>-1</sup>

## 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 0.167 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

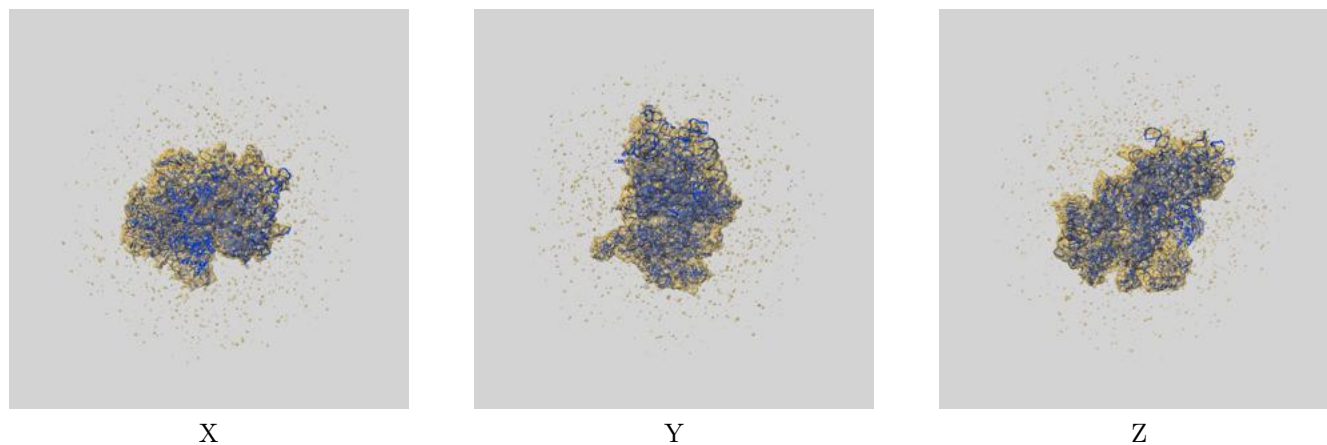
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.00	-	-
Author-provided FSC curve	5.95	10.12	6.83
Unmasked-calculated*	-	-	-

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

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

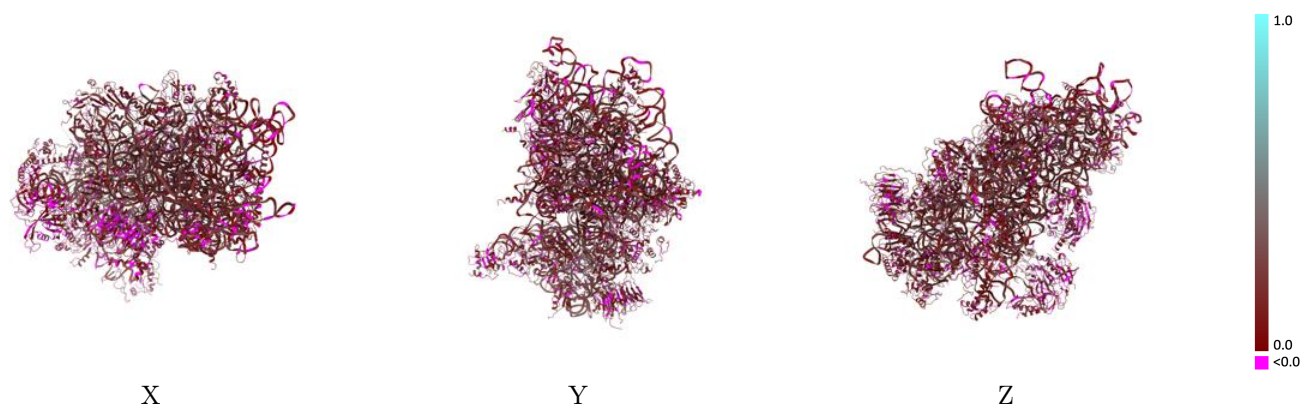
This section contains information regarding the fit between EMDB map EMD-3049 and PDB model 3JAQ. Per-residue inclusion information can be found in section [3](#) on page [14](#).

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



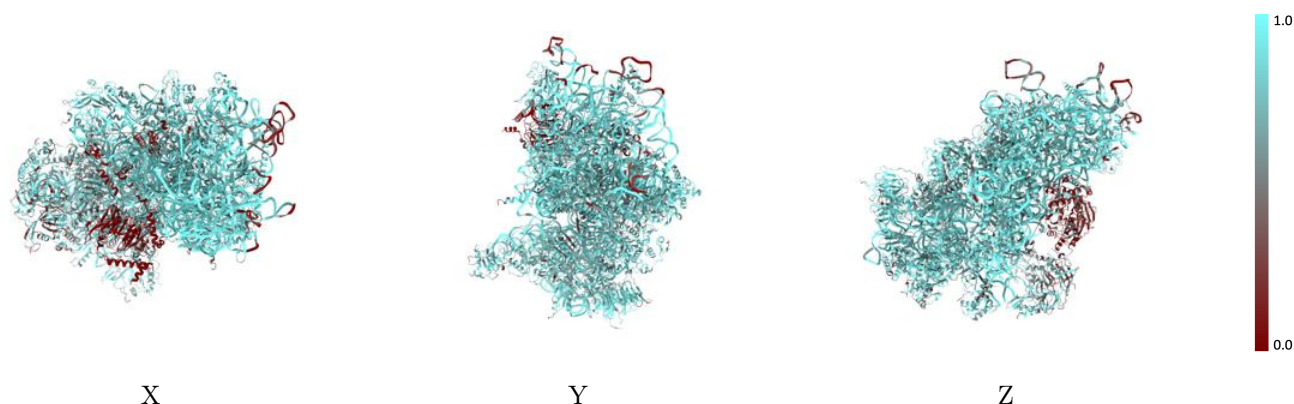
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



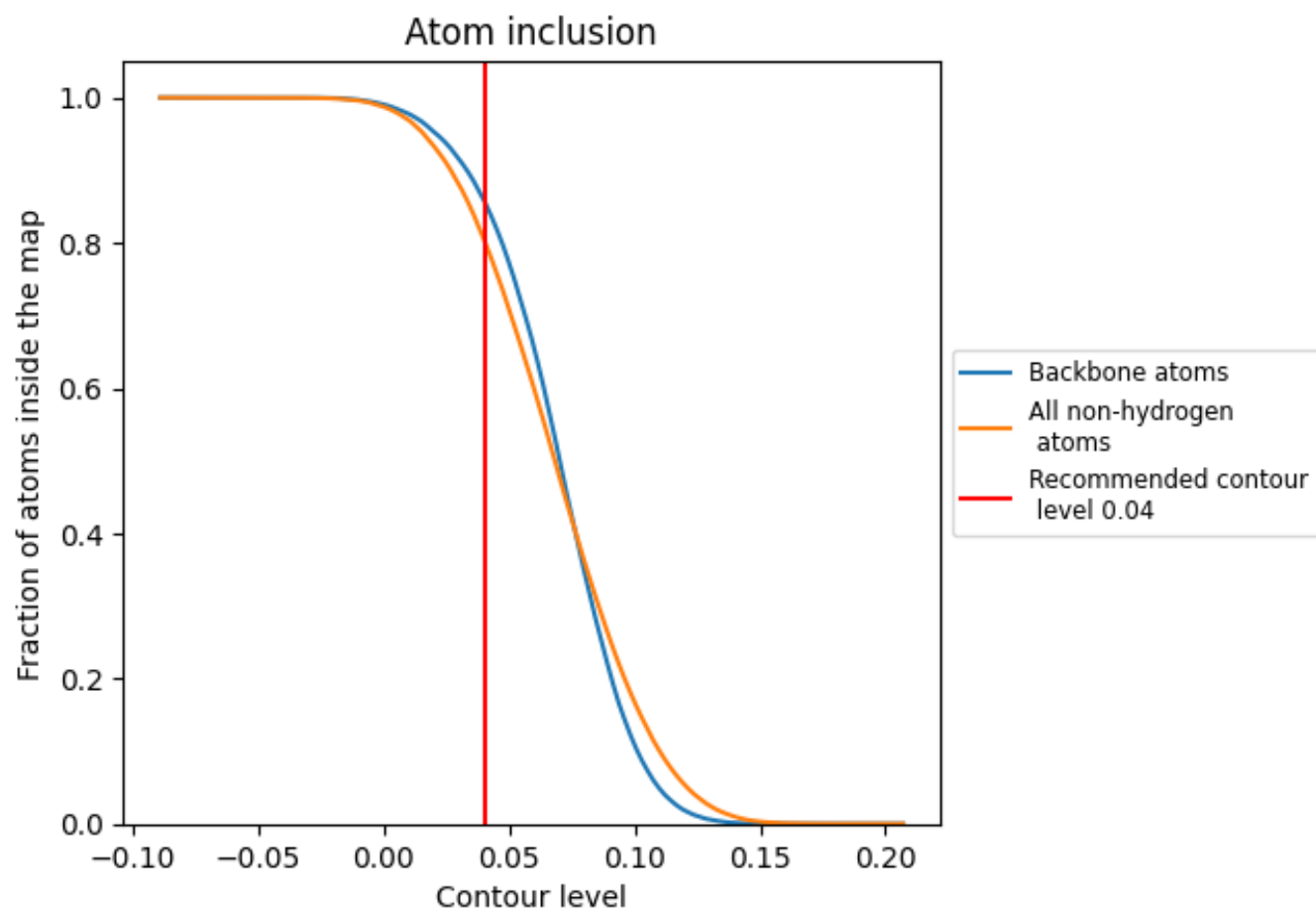
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

## 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8038	 0.1620
1	 0.9231	 0.1750
2	 0.9241	 0.1950
3	 0.3810	 0.2400
A	 0.8200	 0.1520
B	 0.8362	 0.1370
C	 0.7478	 0.1680
D	 0.7354	 0.1560
E	 0.7917	 0.1540
F	 0.7583	 0.1520
G	 0.8215	 0.1310
H	 0.8109	 0.1520
I	 0.8236	 0.1460
J	 0.7924	 0.1490
K	 0.7940	 0.1450
L	 0.7259	 0.1560
M	 0.7296	 0.1240
N	 0.8283	 0.1650
O	 0.8386	 0.1190
P	 0.7963	 0.1290
Q	 0.8030	 0.1390
R	 0.7793	 0.1580
S	 0.7849	 0.1280
T	 0.8296	 0.1290
U	 0.7892	 0.1510
V	 0.7751	 0.1670
W	 0.7600	 0.1480
X	 0.7619	 0.1660
Y	 0.8074	 0.1440
Z	 0.6796	 0.1480
a	 0.7761	 0.1550
b	 0.8505	 0.1700
c	 0.7966	 0.1710
d	 0.8150	 0.1530
e	 0.7542	 0.1830



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Chain	Atom inclusion	Q-score
f	 0.6981	 0.1200
g	 0.8362	 0.1270
h	 0.4009	 0.0700
i	 0.6506	 0.1460
j	 0.6843	 0.1390
k	 0.5691	 0.0870
l	 0.6894	 0.1340
m	 0.6061	 0.1630
o	 0.2043	 0.1540
p	 0.2477	 0.1960
q	 0.1280	 0.0570
r	 0.0000	 0.0860
s	 0.0321	 0.1180