



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:54 PM UTC

PDB ID : 8FFZ / pdb_00008ffz
EMDB ID : EMD-29071
Title : TFIIIA-TFIIC-Brf1-TBP complex bound to 5S rRNA gene
Authors : Talyzina, A.; He, Y.
Deposited on : 2022-12-11
Resolution : 3.80 Å(reported)

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:

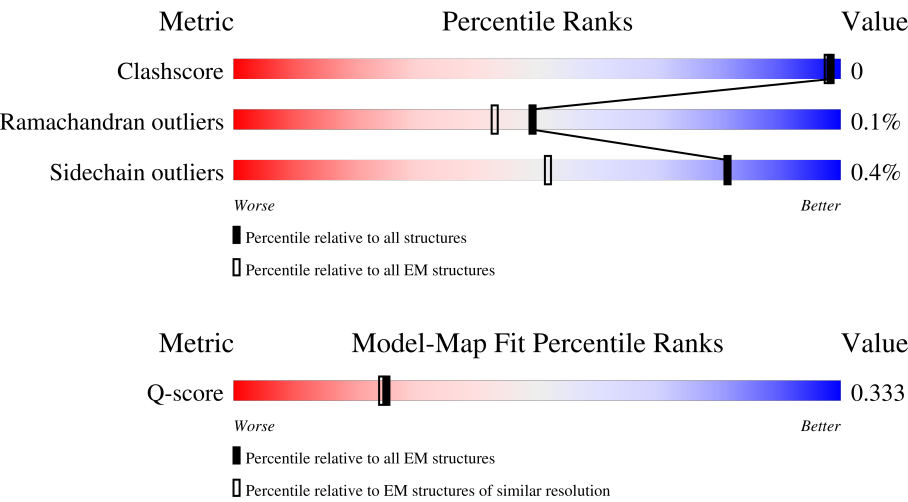
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.80 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.



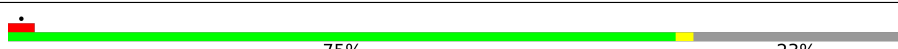
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	A	451	10% 67% 30%
2	B	1160	11% 75% 22%
3	C	1025	41% 75% 22%
4	D	649	39% 60%

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Mol	Chain	Length	Quality of chain
5	E	672	
6	F	588	
7	G	435	
8	H	736	
9	I	171	
10	J	171	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	ZN	A	505	-	-	X	-
11	ZN	A	506	-	-	X	-
11	ZN	A	507	-	-	X	-
11	ZN	A	508	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 38962 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 protein called Transcription factor IIIA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	314	2597	1631	482	461	23	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	430	ALA	-	expression tag	UNP P39933
A	431	ASP	-	expression tag	UNP P39933
A	432	PRO	-	expression tag	UNP P39933
A	433	ASN	-	expression tag	UNP P39933
A	434	SER	-	expression tag	UNP P39933
A	435	SER	-	expression tag	UNP P39933
A	436	SER	-	expression tag	UNP P39933
A	437	VAL	-	expression tag	UNP P39933
A	438	ASP	-	expression tag	UNP P39933
A	439	LYS	-	expression tag	UNP P39933
A	440	LEU	-	expression tag	UNP P39933
A	441	ALA	-	expression tag	UNP P39933
A	442	ALA	-	expression tag	UNP P39933
A	443	ALA	-	expression tag	UNP P39933
A	444	LEU	-	expression tag	UNP P39933
A	445	GLU	-	expression tag	UNP P39933
A	446	HIS	-	expression tag	UNP P39933
A	447	HIS	-	expression tag	UNP P39933
A	448	HIS	-	expression tag	UNP P39933
A	449	HIS	-	expression tag	UNP P39933
A	450	HIS	-	expression tag	UNP P39933
A	451	HIS	-	expression tag	UNP P39933

- Molecule 2 is a protein called Transcription factor tau 138 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	905	Total	C	N	O	S	0	0
			7330	4685	1255	1366	24		

- Molecule 3 is a protein called Transcription factor tau 131 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	797	Total	C	N	O	S	0	0
			6627	4242	1121	1237	27		

- Molecule 4 is a protein called Transcription factor tau 95 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	262	Total	C	N	O	S	0	0
			2070	1318	346	400	6		

- Molecule 5 is a protein called Transcription factor tau 91 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	518	Total	C	N	O	S	0	0
			4097	2623	678	779	17		

- Molecule 6 is a protein called Transcription factor tau 60 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	585	Total	C	N	O	S	0	0
			4743	3048	773	899	23		

- Molecule 7 is a protein called Transcription factor tau 55 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	336	Total	C	N	O	S	0	0
			2705	1734	448	511	12		

- Molecule 8 is a protein called Transcription factor IIIB 70 kDa subunit, TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	328	Total	C	N	O	S	0	0
			2593	1656	460	466	11		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	383	ALA	-	linker	UNP P29056
H	384	MET	-	linker	UNP P29056
H	385	PRO	-	linker	UNP P29056
H	386	TRP	-	linker	UNP P29056
H	567	GLY	-	linker	UNP P13393
H	568	SER	-	linker	UNP P13393
H	569	GLY	-	linker	UNP P13393
H	570	SER	-	linker	UNP P13393
H	571	GLY	-	linker	UNP P13393
H	572	SER	-	linker	UNP P13393
H	573	GLY	-	linker	UNP P13393
H	574	SER	-	linker	UNP P13393
H	575	GLY	-	linker	UNP P13393
H	576	SER	-	linker	UNP P13393
H	577	GLY	-	linker	UNP P13393
H	578	SER	-	linker	UNP P13393

- Molecule 9 is a DNA chain called DNA (151-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	151	Total	C	N	O	P	0	0
			3090	1471	560	908	151		

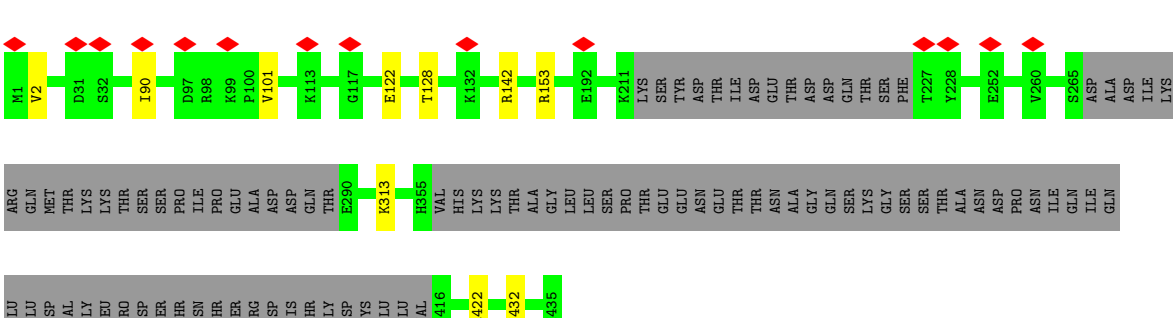
- Molecule 10 is a DNA chain called DNA (151-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	151	Total	C	N	O	P	0	0
			3101	1474	572	904	151		

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

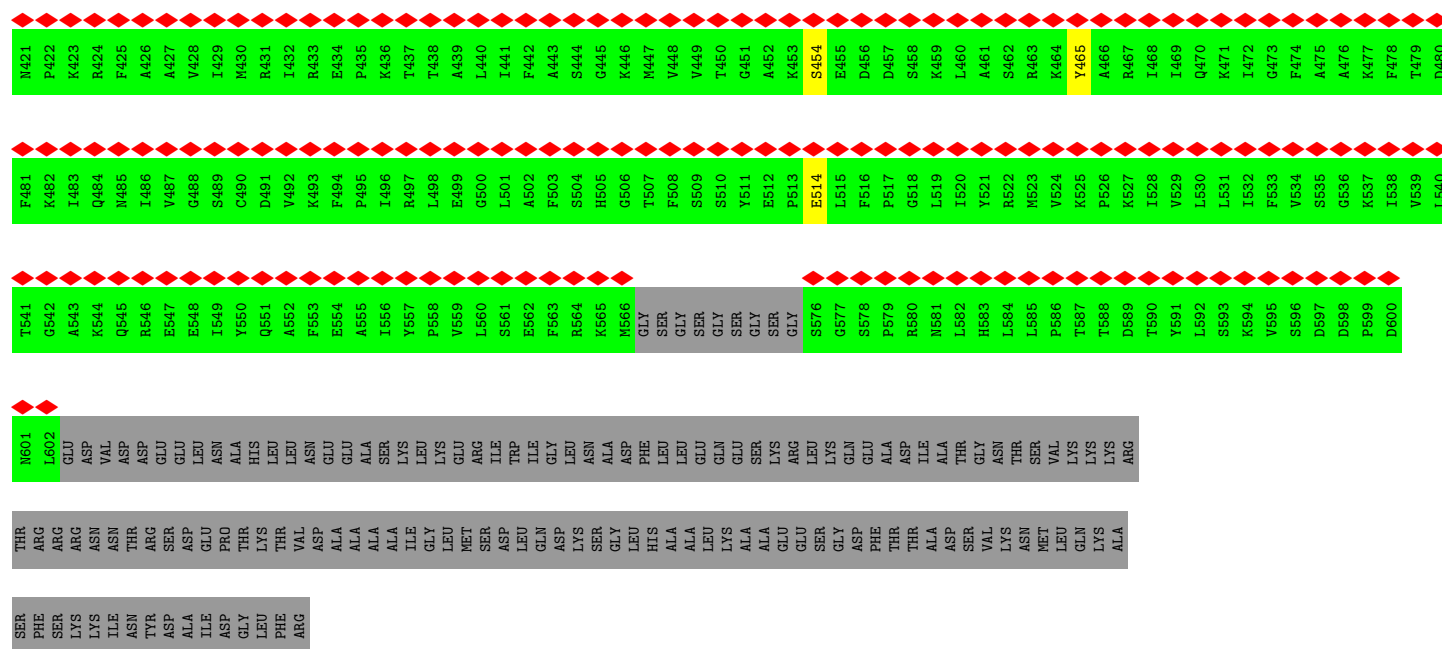
Mol	Chain	Residues	Atoms		AltConf
11	A	9	Total	Zn	0
			9	9	

- Chain F: 

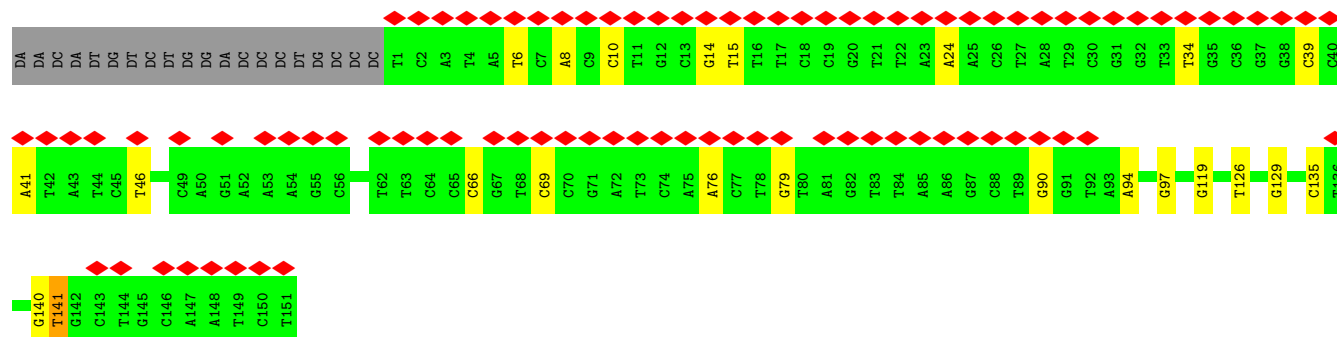
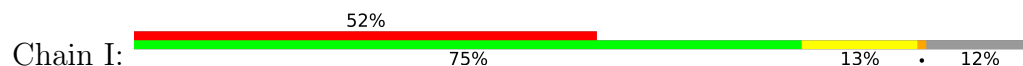
- Chain G: 
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- Chain H: 

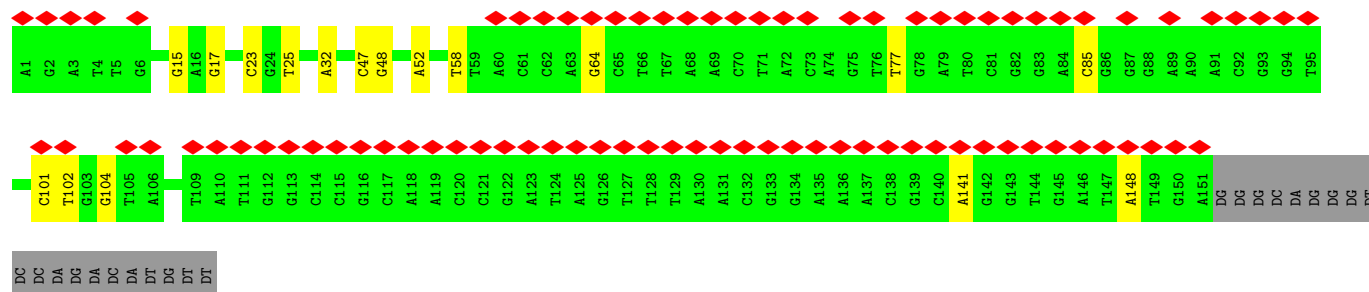
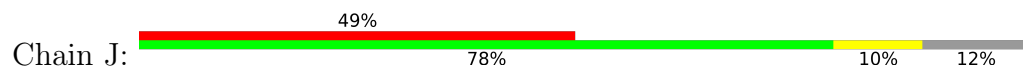
Position	Residue	Score	Label
1	ILE	1.81	
2	ASP	1.82	
3	GLY	1.83	
4	GLU	1.84	
5	ASN	1.85	
6	ILE	1.86	
7	THR	1.87	
8	GLY	1.88	
9	GLN	1.89	
10	THR	1.90	
11	ASN	1.91	
12	GLU	1.92	
13	THR	1.93	
14	ALA	1.94	
15	LYS	1.95	
16	LYS	1.96	
17	PRO	1.97	
18	SER	1.98	
19	GLU	1.99	
20	ALA	2.00	
21	THR	2.01	
22	PRO	2.02	
23	GLY	2.03	
24	GLN	2.04	
25	GLU	2.05	
26	LEU	2.06	
27	SER	2.07	
28	LYS	2.08	
29	GLU	2.09	
30	VAL	2.10	
31	PHE	2.11	
32	TYR	2.12	
33	LEU	2.13	
34	GLN	2.14	
35	PHE	2.15	
36	SER	2.16	
37	GLU	2.17	
38	ARG	2.18	
39	ALA	2.19	
40	VAL	2.20	
41	VAL	2.21	
42	GLU	2.22	
43	ARG	2.23	
44	ILE	2.24	
45	LYS	2.25	
46	ALA	2.26	
47	THR	2.27	
48	ASN	2.28	
49	GLY	2.29	
50	LYS	2.30	
51	VAL	2.31	
52	LYS	2.32	
53	THR	2.33	
54	GLY	2.34	
55	ASN	2.35	
56	GLY	2.36	
57	ARG	2.37	
58	LYS	2.38	
59	ILE	2.39	
60	ILE	2.40	



• Molecule 9: DNA (151-MER)



• Molecule 10: DNA (151-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78512	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.102	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.016	Depositor
Map size ($\text{\AA}$)	405.504, 405.504, 405.504	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.056, 1.056, 1.056	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

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	A	0.81	0/2665	1.33	4/3584 (0.1%)
2	B	0.72	0/7445	1.32	14/10016 (0.1%)
3	C	0.76	0/6761	1.35	17/9123 (0.2%)
4	D	0.69	0/2112	1.32	2/2851 (0.1%)
5	E	0.71	0/4190	1.32	13/5685 (0.2%)
6	F	0.71	0/4854	1.32	10/6585 (0.2%)
7	G	0.73	0/2773	1.30	6/3761 (0.2%)
8	H	0.86	0/2638	1.43	2/3549 (0.1%)
9	I	0.70	0/3464	1.31	7/5343 (0.1%)
10	J	0.70	0/3480	1.31	5/5370 (0.1%)
All	All	0.74	0/40382	1.33	80/55867 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	3
3	C	0	4
4	D	0	3
5	E	0	2
6	F	0	1
8	H	0	1
9	I	0	17
10	J	0	12
All	All	0	45

There are no bond length outliers.

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	724	ALA	N-CA-C	7.75	119.37	111.07
3	C	821	CYS	N-CA-C	6.98	119.73	111.71
5	E	279	GLY	N-CA-C	6.74	119.38	111.63
1	A	187	ASP	N-CA-C	6.71	119.34	110.08
6	F	423	PHE	N-CA-C	6.55	118.97	111.11
2	B	775	ASP	N-CA-C	6.48	118.92	111.02
3	C	391	ARG	NE-CZ-NH2	6.43	124.98	119.20
3	C	435	ARG	NE-CZ-NH2	6.42	124.98	119.20
5	E	479	ASP	CA-CB-CG	6.36	118.96	112.60
2	B	432	GLY	N-CA-C	6.32	121.42	114.40
7	G	101	VAL	CA-C-N	6.21	126.83	122.60
7	G	101	VAL	C-N-CA	6.21	126.83	122.60
8	H	454	SER	CA-C-N	6.20	128.88	120.38
8	H	454	SER	C-N-CA	6.20	128.88	120.38
6	F	353	ARG	NE-CZ-NH2	6.07	124.67	119.20
9	I	8	DA	C4'-C3'-O3'	6.07	119.11	110.00
1	A	252	ASN	CA-CB-CG	6.05	118.65	112.60
7	G	313	LYS	N-CA-C	5.86	117.34	111.07
3	C	196	TRP	N-CA-C	5.86	117.67	111.28
2	B	1121	LEU	N-CA-C	5.85	119.00	109.59
6	F	350	ASP	CA-CB-CG	5.81	118.41	112.60
3	C	822	ARG	N-CA-C	5.79	118.91	109.06
6	F	413	LEU	N-CA-C	5.76	118.43	111.40
5	E	328	HIS	N-CA-C	5.72	120.26	113.28
5	E	340	CYS	N-CA-C	5.68	117.81	109.24
3	C	490	PHE	CA-CB-CG	5.63	119.44	113.80
2	B	405	ARG	NE-CZ-NH2	5.61	124.25	119.20
3	C	417	ASP	CA-CB-CG	5.56	118.16	112.60
2	B	652	ASP	CA-CB-CG	5.56	118.16	112.60
10	J	102	DT	C4'-C3'-O3'	5.55	118.33	110.00
7	G	142	ARG	NE-CZ-NH2	5.52	124.17	119.20
4	D	214	LEU	N-CA-C	5.51	118.04	111.71
2	B	859	ARG	NE-CZ-NH2	5.48	124.13	119.20
3	C	335	ARG	NE-CZ-NH2	5.48	124.13	119.20
2	B	152	LEU	N-CA-C	5.47	117.89	109.07
9	I	69	DC	O5'-C5'-C4'	5.47	119.01	110.80
6	F	89	ARG	NE-CZ-NH2	5.46	124.11	119.20
2	B	465	PHE	N-CA-C	5.44	117.71	110.53
7	G	422	ARG	NE-CZ-NH2	5.42	124.08	119.20
5	E	386	PHE	N-CA-C	5.42	117.08	108.79
10	J	58	DT	C4'-C3'-O3'	5.42	118.13	110.00
7	G	153	ARG	NE-CZ-NH2	5.39	124.06	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	386	ARG	NE-CZ-NH2	5.38	124.05	119.20
10	J	32	DA	O5'-C5'-C4'	5.36	118.83	110.80
6	F	246	TYR	N-CA-C	5.36	117.53	109.23
9	I	10	DC	C4'-C3'-O3'	5.34	118.01	110.00
10	J	15	DG	O5'-C5'-C4'	5.33	118.80	110.80
9	I	126	DT	C5'-C4'-O4'	5.32	117.38	109.40
10	J	23	DC	C5'-C4'-O4'	5.30	117.35	109.40
2	B	329	ASN	OD1-CG-ND2	-5.26	117.34	122.60
5	E	648	ASN	N-CA-C	-5.24	102.53	110.28
2	B	437	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	120	ARG	NE-CZ-NH2	5.21	123.89	119.20
3	C	808	PHE	CA-CB-CG	5.21	119.01	113.80
1	A	187	ASP	CA-CB-CG	5.19	117.79	112.60
2	B	210	LYS	CA-C-N	5.17	127.21	120.28
2	B	210	LYS	C-N-CA	5.17	127.21	120.28
6	F	349	TYR	N-CA-C	5.17	116.92	109.07
3	C	298	ARG	NE-CZ-NH2	5.15	123.83	119.20
3	C	268	ARG	NE-CZ-NH2	5.14	123.83	119.20
5	E	381	VAL	CA-C-N	5.14	127.55	120.72
5	E	381	VAL	C-N-CA	5.14	127.55	120.72
5	E	591	LYS	N-CA-C	5.10	117.24	111.02
9	I	41	DA	O5'-C5'-C4'	5.08	118.41	110.80
5	E	281	ARG	NE-CZ-NH2	5.07	123.77	119.20
5	E	585	ARG	NE-CZ-NH2	5.07	123.77	119.20
3	C	141	ARG	NE-CZ-NH2	5.06	123.76	119.20
5	E	629	ASP	N-CA-C	5.06	117.64	110.50
3	C	728	ARG	NE-CZ-NH2	5.06	123.75	119.20
6	F	194	VAL	N-CA-C	5.05	115.25	108.17
2	B	204	ARG	NE-CZ-NH2	5.05	123.74	119.20
9	I	135	DC	O5'-C5'-C4'	5.05	118.37	110.80
9	I	141	DT	O5'-C5'-C4'	5.04	118.36	110.80
3	C	186	PHE	N-CA-C	5.04	116.46	111.07
6	F	518	THR	N-CA-C	5.03	117.05	109.41
5	E	219	LYS	N-CA-C	5.03	117.49	111.71
3	C	722	THR	N-CA-C	5.02	119.25	113.38
4	D	229	PRO	N-CA-C	5.02	116.83	110.70
2	B	22	LYS	N-CA-C	5.01	118.35	111.54
6	F	71	PHE	CA-CB-CG	5.00	118.80	113.80

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	45	ARG	Sidechain
1	A	62	ARG	Sidechain
2	B	1154	TYR	Sidechain
2	B	339	TYR	Sidechain
2	B	908	ARG	Sidechain
3	C	1000	TYR	Sidechain
3	C	257	TYR	Sidechain
3	C	879	TYR	Sidechain
3	C	963	TYR	Sidechain
4	D	107	ARG	Sidechain
4	D	161	ARG	Sidechain
4	D	244	TYR	Sidechain
5	E	235	TYR	Sidechain
5	E	552	ARG	Sidechain
6	F	529	ARG	Sidechain
8	H	465	TYR	Sidechain
9	I	119	DG	Sidechain
9	I	129	DG	Sidechain
9	I	14	DG	Sidechain
9	I	140	DG	Sidechain
9	I	141	DT	Sidechain
9	I	15	DT	Sidechain
9	I	24	DA	Sidechain
9	I	34	DT	Sidechain
9	I	39	DC	Sidechain
9	I	46	DT	Sidechain
9	I	6	DT	Sidechain
9	I	66	DC	Sidechain
9	I	76	DA	Sidechain
9	I	79	DG	Sidechain
9	I	90	DG	Sidechain
9	I	94	DA	Sidechain
9	I	97	DG	Sidechain
10	J	101	DC	Sidechain
10	J	104	DG	Sidechain
10	J	141	DA	Sidechain
10	J	148	DA	Sidechain
10	J	17	DG	Sidechain
10	J	25	DT	Sidechain
10	J	47	DC	Sidechain
10	J	48	DG	Sidechain
10	J	52	DA	Sidechain
10	J	64	DG	Sidechain

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Mol	Chain	Res	Type	Group
10	J	77	DT	Sidechain
10	J	85	DC	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2597	0	2549	10	0
2	B	7330	0	7550	6	0
3	C	6627	0	6547	5	0
4	D	2070	0	2097	1	0
5	E	4097	0	4072	2	0
6	F	4743	0	4705	1	0
7	G	2705	0	2653	0	0
8	H	2593	0	2692	0	0
9	I	3090	0	1701	0	0
10	J	3101	0	1699	0	0
11	A	9	0	0	10	0
All	All	38962	0	36265	24	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (24) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:CYS:HG	11:A:507:ZN:ZN	0.76	0.94
1:A:227:CYS:HG	11:A:506:ZN:ZN	0.87	0.81
1:A:367:CYS:HG	11:A:508:ZN:ZN	0.85	0.81
1:A:168:CYS:HG	11:A:505:ZN:ZN	0.96	0.76
1:A:113:CYS:SG	11:A:503:ZN:ZN	1.86	0.64
1:A:227:CYS:SG	11:A:506:ZN:ZN	1.86	0.64
1:A:168:CYS:SG	11:A:505:ZN:ZN	1.87	0.62
1:A:367:CYS:SG	11:A:508:ZN:ZN	1.88	0.62
1:A:258:CYS:SG	11:A:507:ZN:ZN	1.89	0.60
1:A:255:CYS:SG	11:A:507:ZN:ZN	1.87	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:747:ALA:CB	3:C:785:ILE:HD12	2.40	0.52
2:B:982:TYR:CD1	2:B:1009:VAL:HG21	2.47	0.49
2:B:359:ILE:HG22	2:B:360:THR:HG23	1.95	0.48
2:B:332:TYR:CD2	5:E:324:PRO:HA	2.52	0.45
6:F:235:VAL:HG22	6:F:272:PRO:HB3	1.98	0.45
2:B:824:ILE:HD12	2:B:824:ILE:H	1.82	0.45
2:B:976:PHE:CE1	2:B:1096:THR:HG23	2.54	0.43
3:C:740:MET:HE1	3:C:778:MET:HG3	2.01	0.42
4:D:35:ARG:HH22	4:D:113:GLU:CD	2.28	0.41
3:C:525:TYR:CZ	3:C:541:SER:HB3	2.56	0.41
3:C:943:TYR:CE1	3:C:965:LEU:HD21	2.56	0.41
5:E:473:ALA:HB2	5:E:526:TYR:CZ	2.56	0.41
2:B:827:LEU:HA	2:B:830:TRP:CD1	2.57	0.40
3:C:628:VAL:CG2	3:C:663:ILE:HG21	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	
1	A	310/451 (69%)	285 (92%)	25 (8%)	0	100	100
2	B	883/1160 (76%)	842 (95%)	40 (4%)	1 (0%)	48	79
3	C	787/1025 (77%)	760 (97%)	27 (3%)	0	100	100
4	D	258/649 (40%)	245 (95%)	13 (5%)	0	100	100
5	E	516/672 (77%)	484 (94%)	31 (6%)	1 (0%)	43	73
6	F	581/588 (99%)	541 (93%)	40 (7%)	0	100	100
7	G	328/435 (75%)	307 (94%)	19 (6%)	2 (1%)	21	54
8	H	322/736 (44%)	297 (92%)	24 (8%)	1 (0%)	36	67
All	All	3985/5716 (70%)	3761 (94%)	219 (6%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	653	THR
7	G	122	GLU
8	H	514	GLU
5	E	227	ILE
7	G	90	ILE

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	
1	A	297/422 (70%)	297 (100%)	0	100	100
2	B	825/1049 (79%)	820 (99%)	5 (1%)	78	79
3	C	719/925 (78%)	718 (100%)	1 (0%)	88	89
4	D	243/588 (41%)	241 (99%)	2 (1%)	73	76
5	E	460/592 (78%)	458 (100%)	2 (0%)	84	83
6	F	541/544 (99%)	540 (100%)	1 (0%)	87	87
7	G	295/384 (77%)	292 (99%)	3 (1%)	68	74
8	H	282/623 (45%)	282 (100%)	0	100	100
All	All	3662/5127 (71%)	3648 (100%)	14 (0%)	81	83

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	76	ILE
2	B	87	ILE
2	B	145	ILE
2	B	256	VAL
2	B	343	ASP
3	C	767	VAL
4	D	24	LEU
4	D	644	VAL
5	E	291	LEU

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Mol	Chain	Res	Type
5	E	420	LEU
6	F	353	ARG
7	G	2	VAL
7	G	128	THR
7	G	432	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	359	ASN
2	B	311	GLN
2	B	336	ASN
2	B	411	ASN
2	B	450	ASN
2	B	790	HIS
2	B	1093	GLN
3	C	179	ASN
3	C	245	GLN
3	C	361	ASN
3	C	444	ASN
3	C	763	GLN
3	C	912	ASN
3	C	930	GLN
3	C	934	GLN
4	D	72	HIS
4	D	131	ASN
5	E	352	HIS
5	E	361	HIS
5	E	394	ASN
6	F	49	ASN
6	F	108	ASN
6	F	364	GLN
6	F	397	GLN
6	F	525	ASN
7	G	56	ASN
8	H	184	HIS
8	H	470	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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.

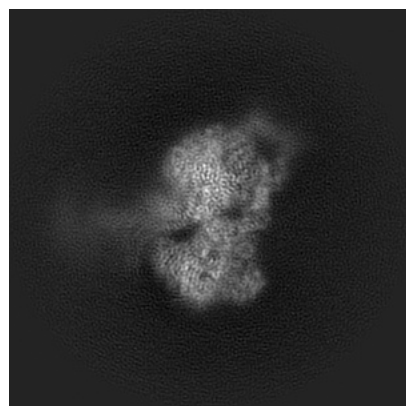
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29071. These allow visual inspection of the internal detail of the map and identification of artifacts.

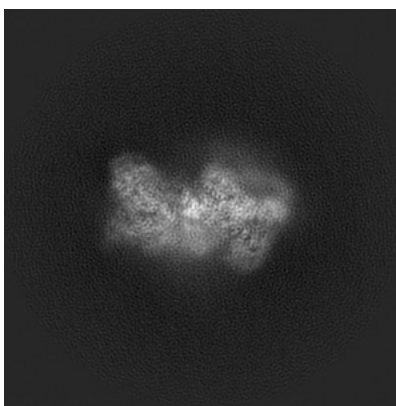
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

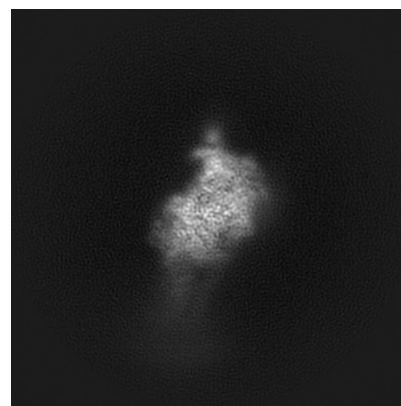
6.1.1 Primary map



X

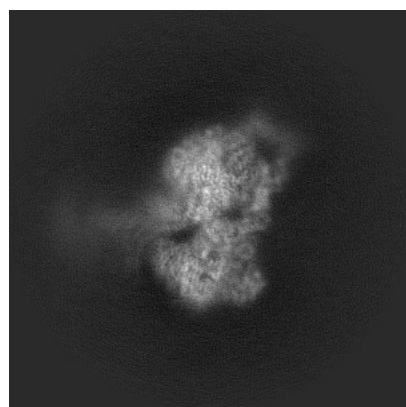


Y

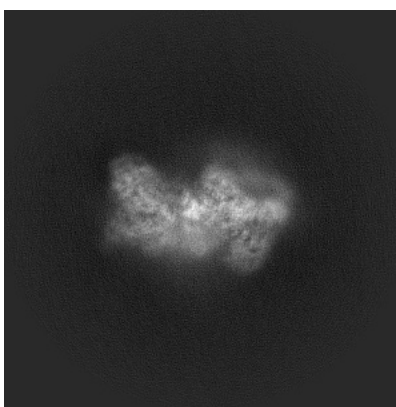


Z

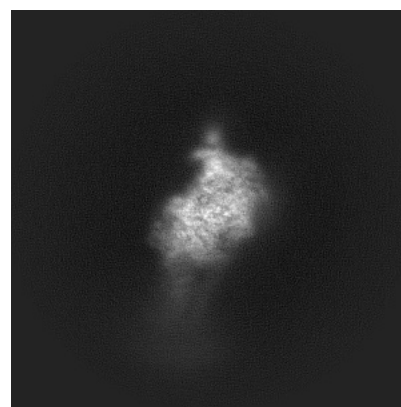
6.1.2 Raw map



X



Y

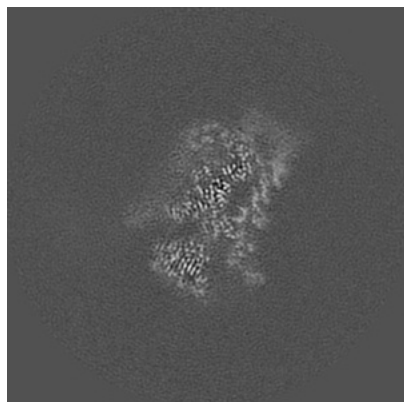


Z

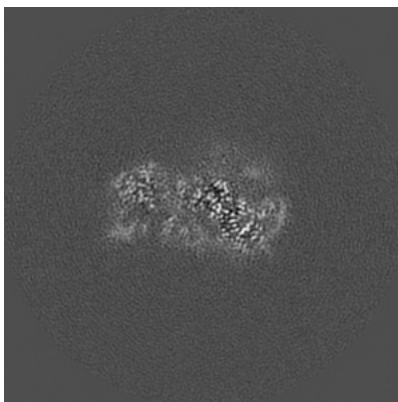
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

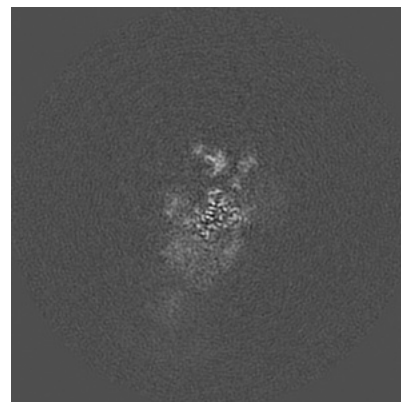
6.2.1 Primary map



X Index: 192

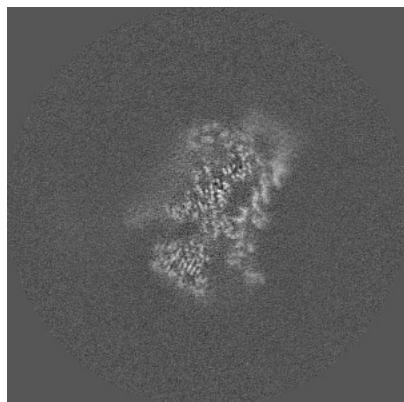


Y Index: 192

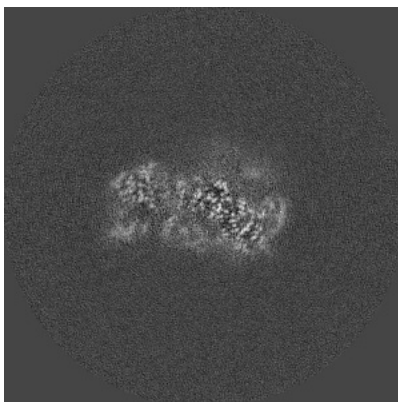


Z Index: 192

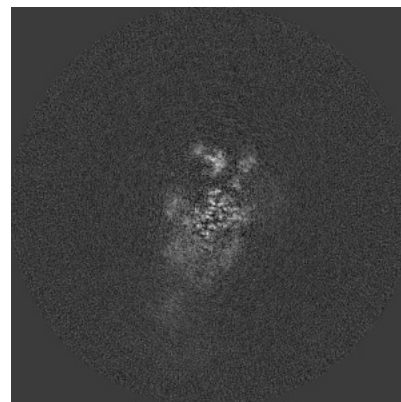
6.2.2 Raw map



X Index: 192



Y Index: 192

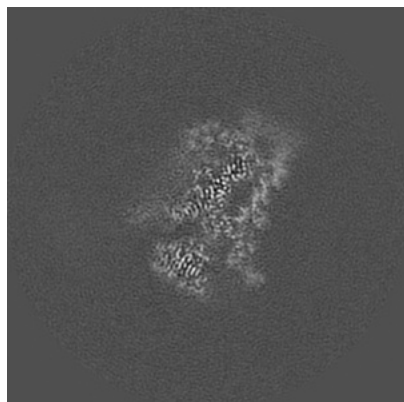


Z Index: 192

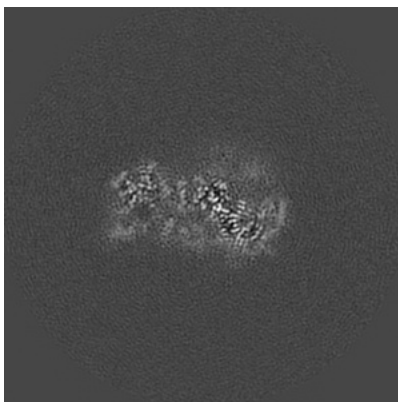
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

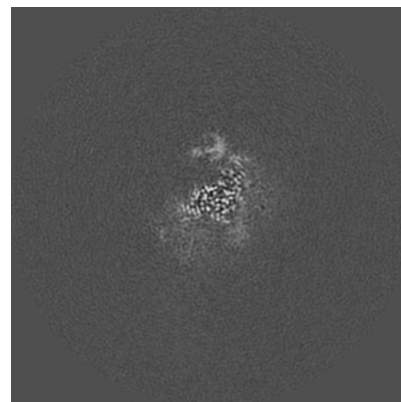
6.3.1 Primary map



X Index: 193

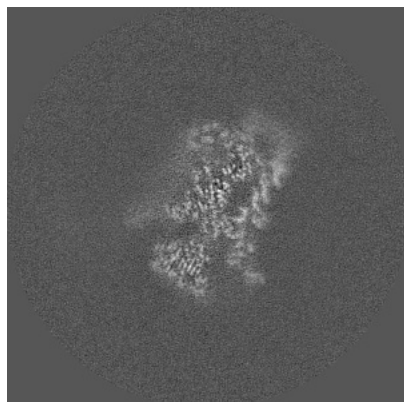


Y Index: 191

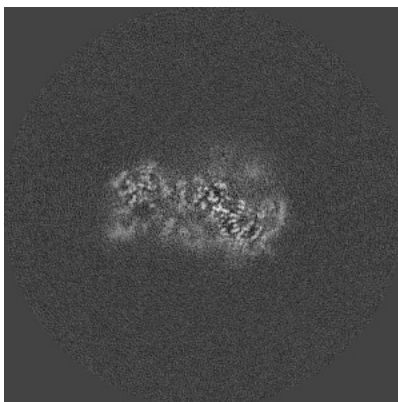


Z Index: 210

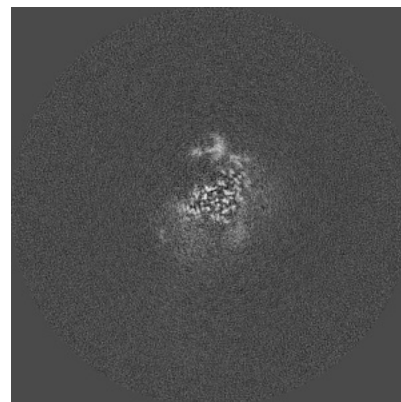
6.3.2 Raw map



X Index: 192



Y Index: 191

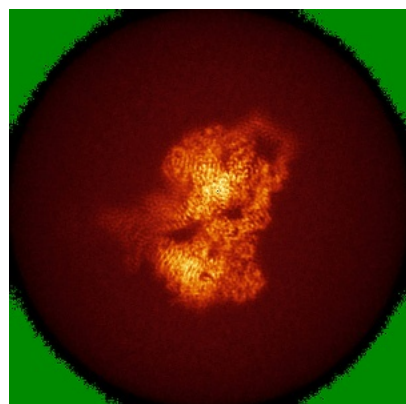


Z Index: 210

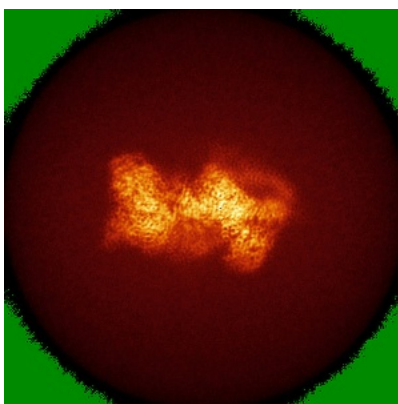
The images above show the largest variance slices of the map in three orthogonal directions.

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

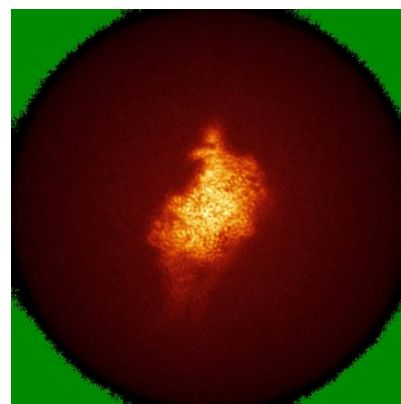
6.4.1 Primary map



X

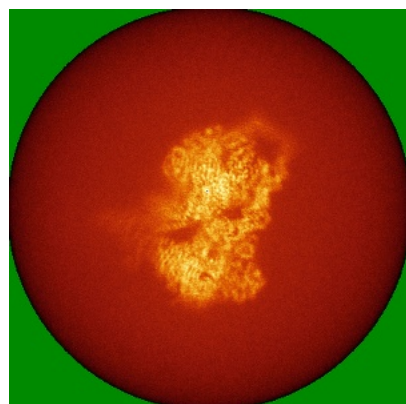


Y

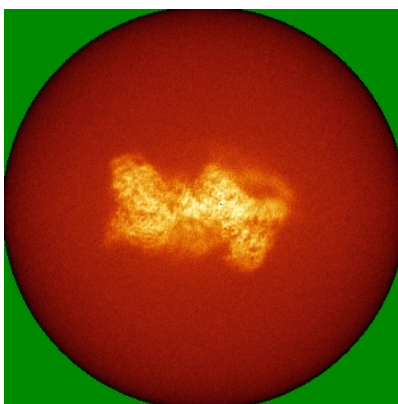


Z

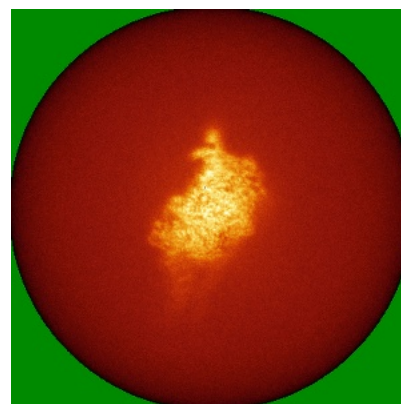
6.4.2 Raw map



X



Y

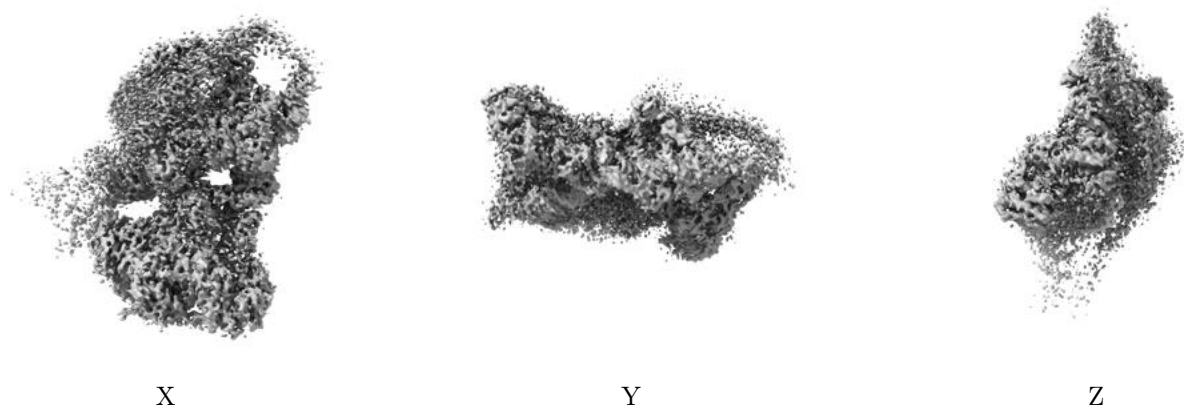


Z

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

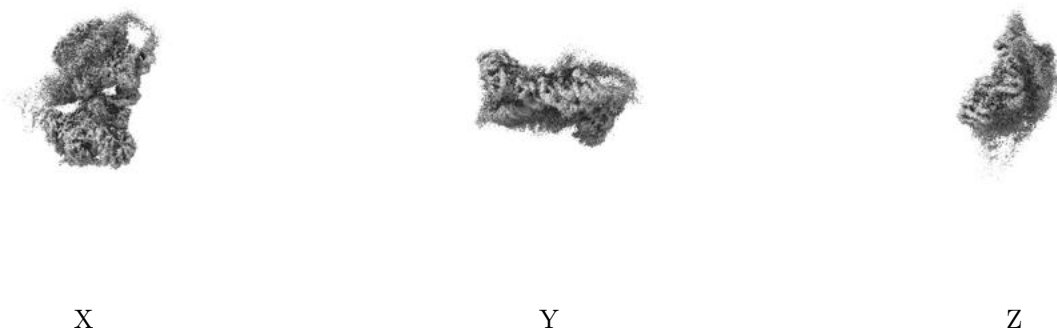
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

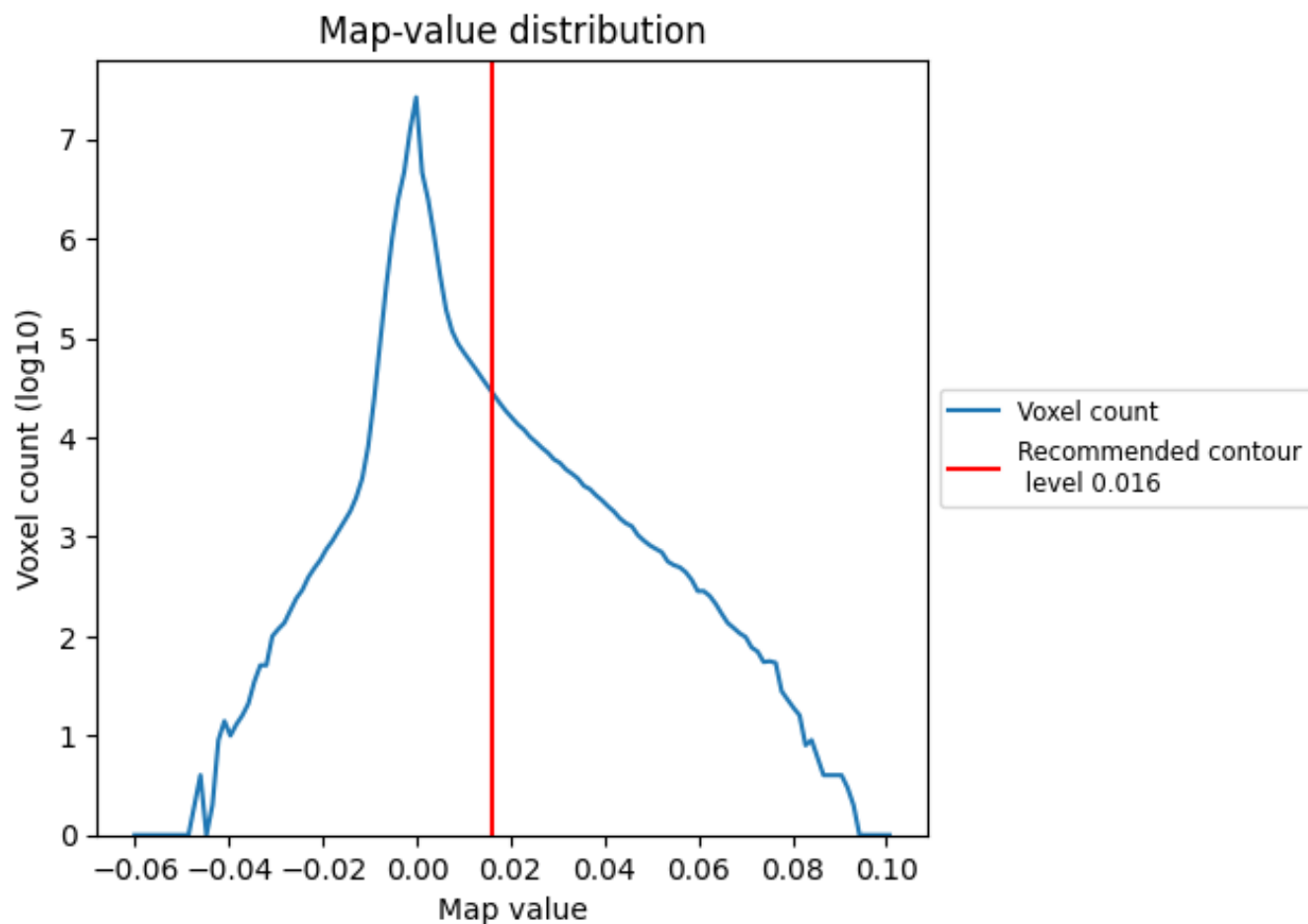
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

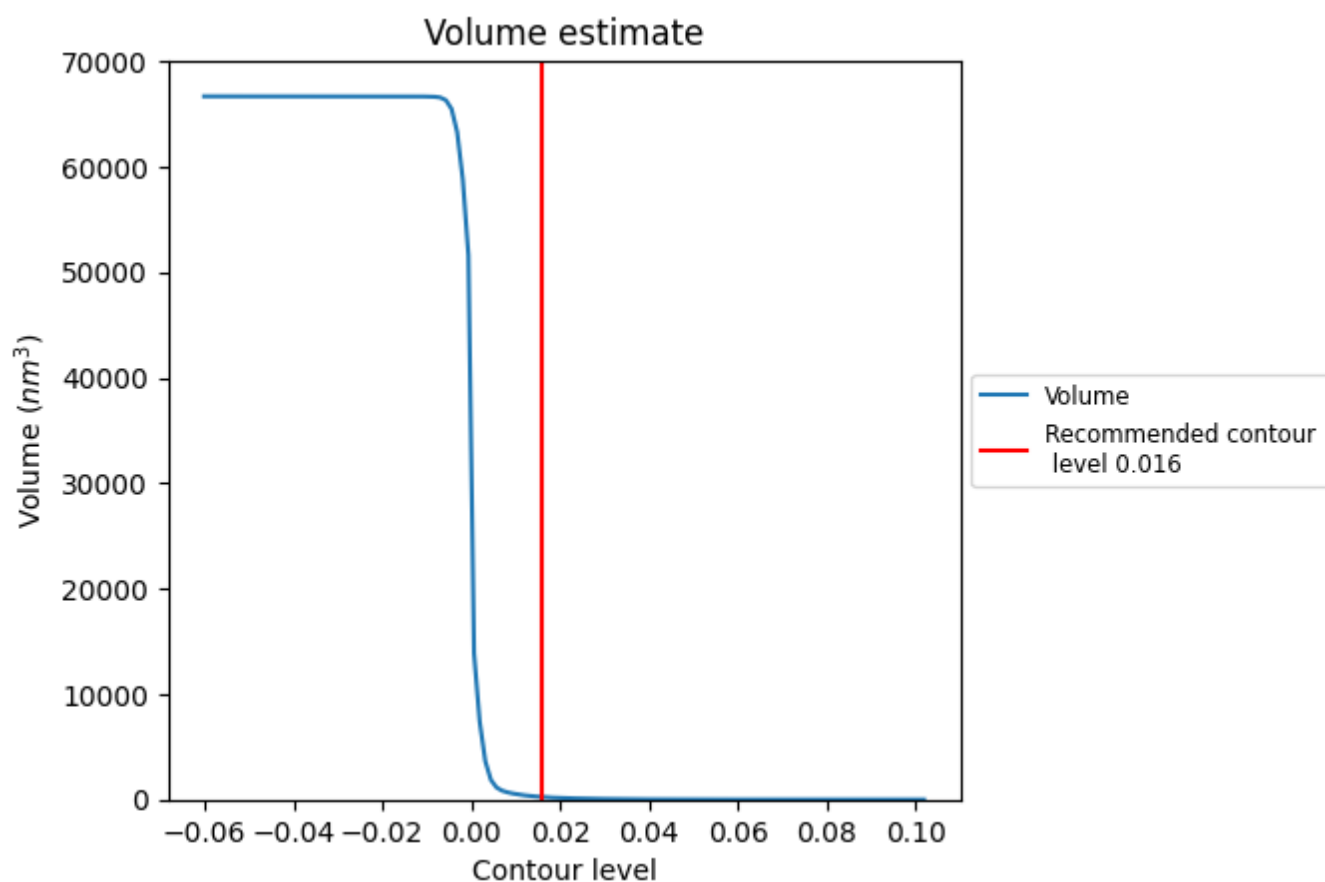
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

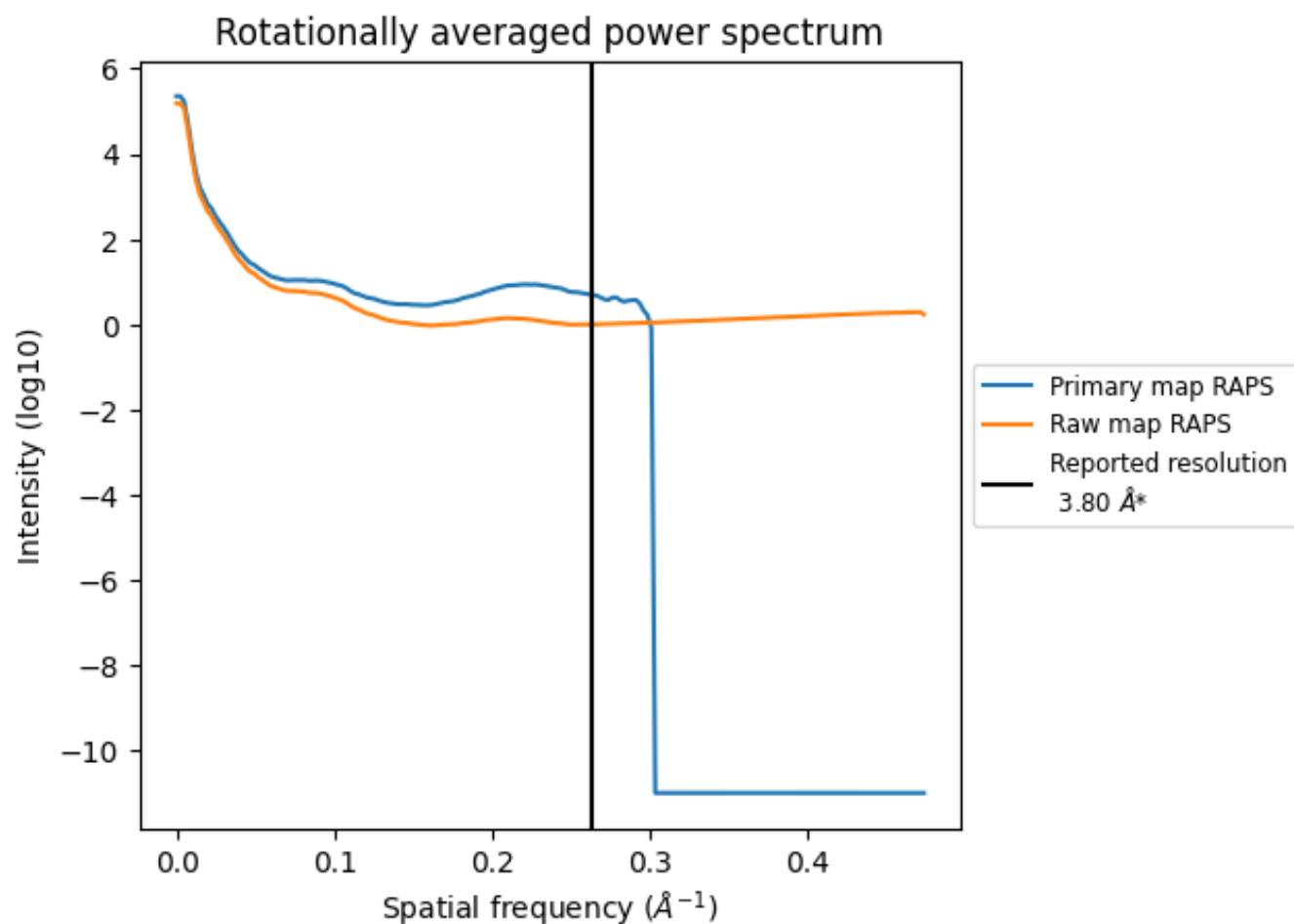
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 242 nm³; this corresponds to an approximate mass of 219 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 ⓘ

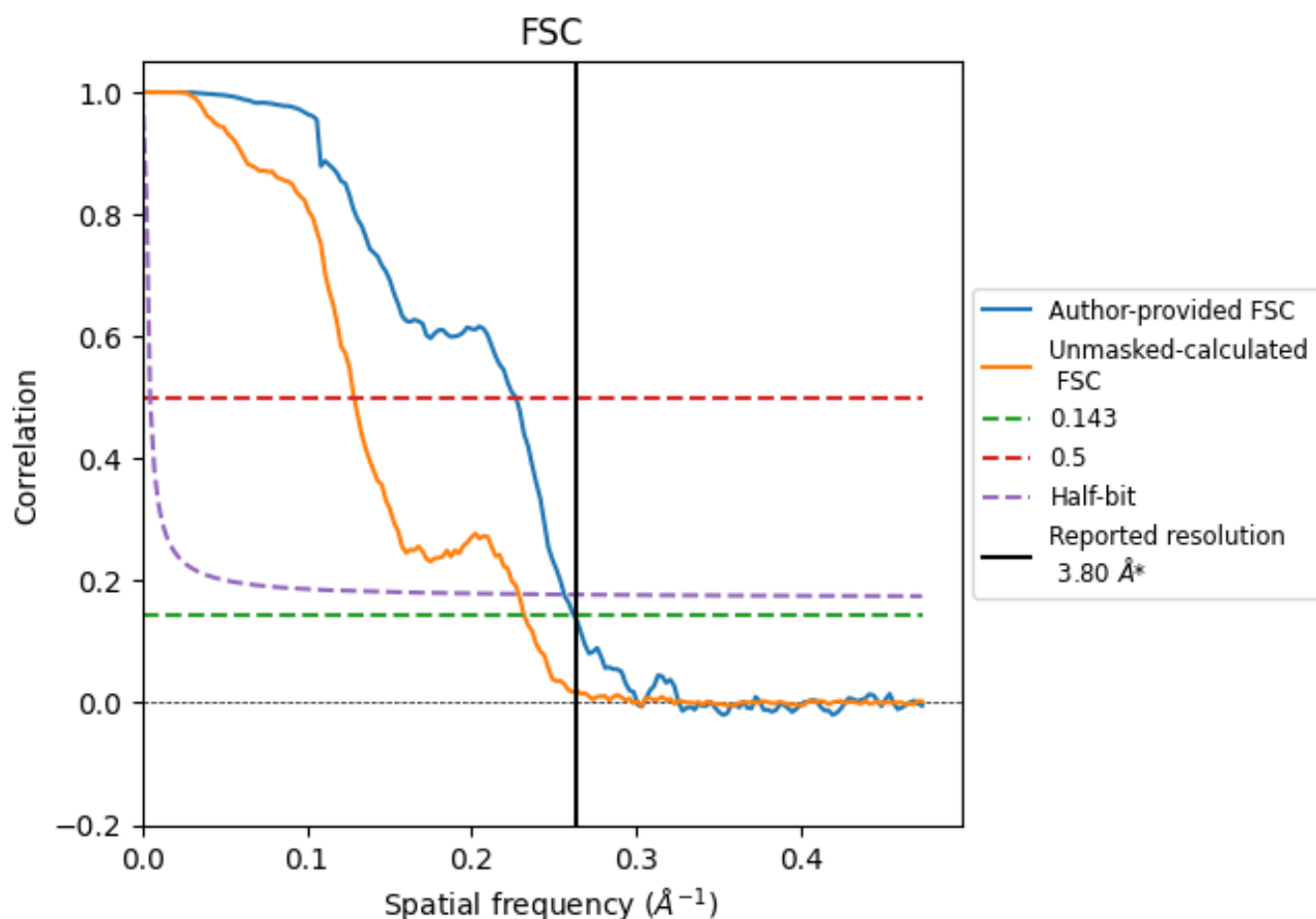


*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

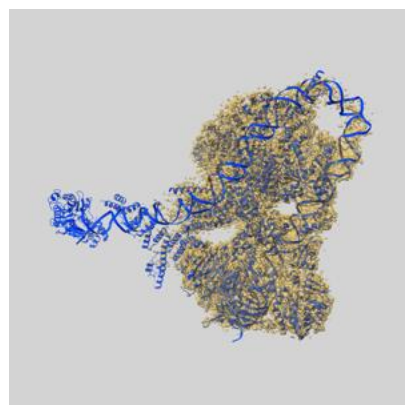
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.81	4.41	3.90
Unmasked-calculated*	4.31	7.78	4.38

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.31 differs from the reported value 3.8 by more than 10 %

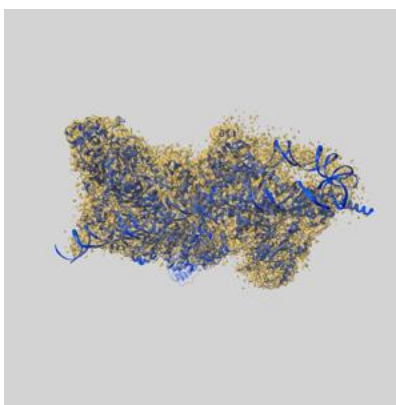
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29071 and PDB model 8FFZ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

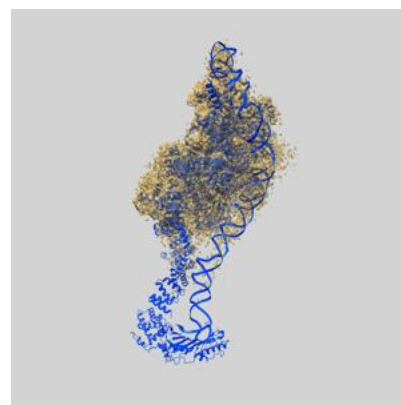
9.1 Map-model overlay [i](#)



X



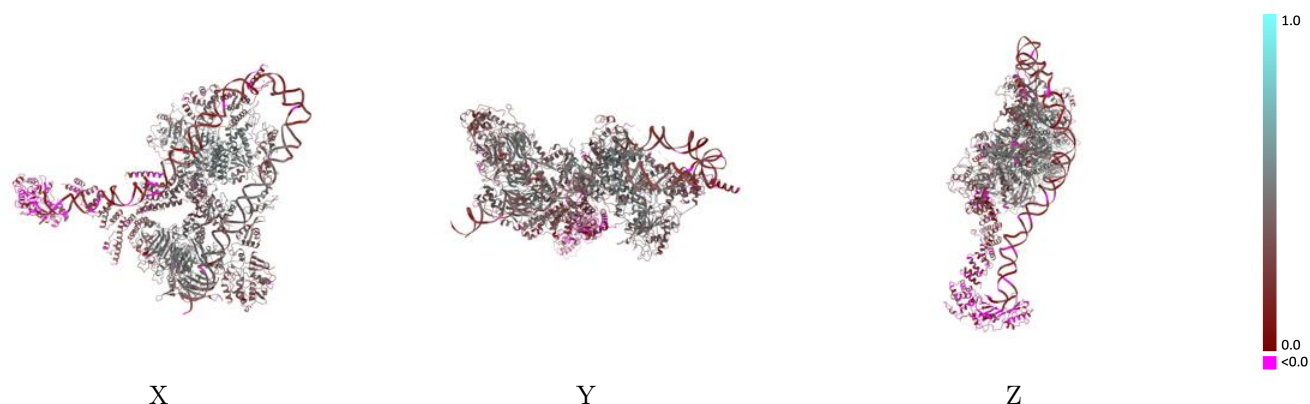
Y



Z

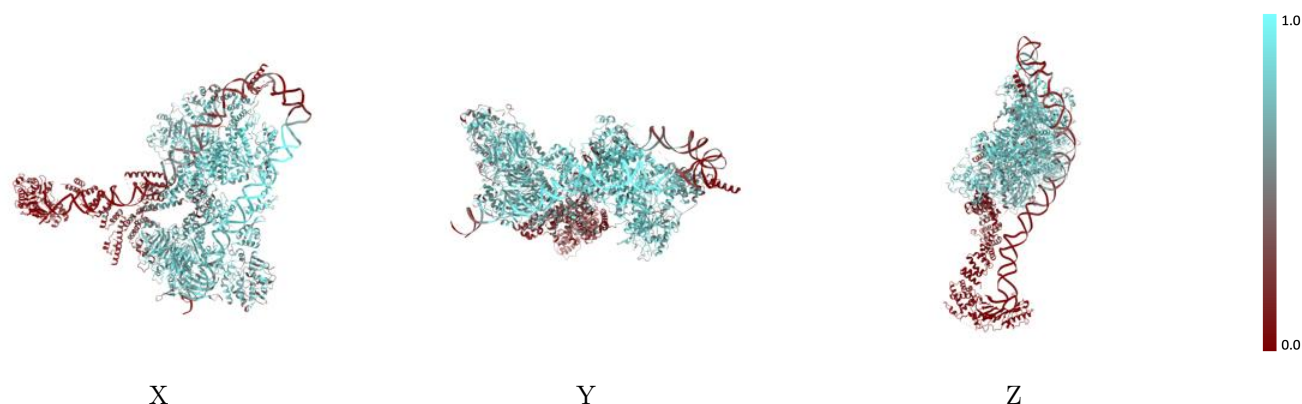
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



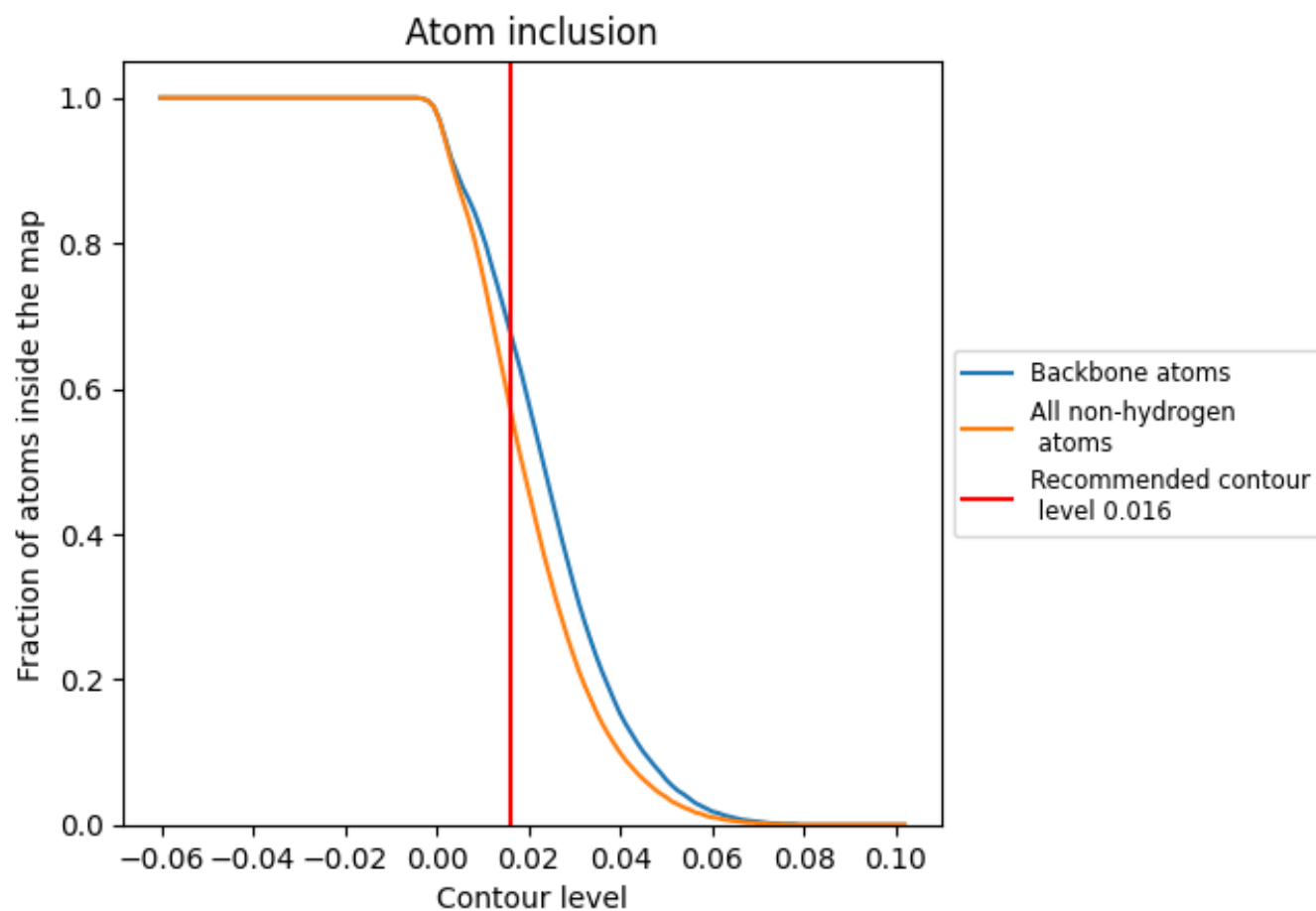
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 57% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5740	 0.3330
A	 0.6860	 0.3460
B	 0.6810	 0.3740
C	 0.4290	 0.3050
D	 0.8220	 0.4710
E	 0.7600	 0.4400
F	 0.7160	 0.4110
G	 0.7440	 0.4030
H	 0.0000	 0.0300
I	 0.4050	 0.2330
J	 0.4080	 0.2290

