



wwPDB EM Validation Summary Report ⓘ

Jun 7, 2023 – 09:05 PM EDT

PDB ID : 8EZA
EMDB ID : EMD-28732
Title : NHEJ Long-range complex with PAXX
Authors : Chen, S.; He, Y.
Deposited on : 2022-10-31
Resolution : 4.39 Å (reported)

This is a wwPDB EM Validation Summary 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.dev50
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) : 2.33

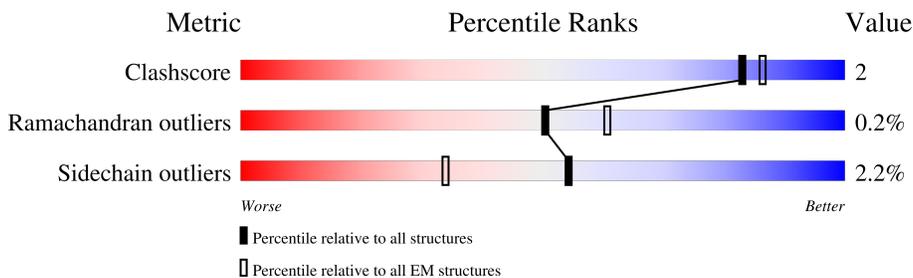
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.39 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	S	204	
1	T	204	
2	A	609	
2	J	609	
3	B	732	
3	K	732	
4	C	4128	
4	L	4128	

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Mol	Chain	Length	Quality of chain
5	Q	20	90% 10%
5	R	20	90% 10%
6	D	31	48% 48% .
6	M	31	45% 52% .
7	E	30	13% 47% 33% 7%
7	N	30	13% 47% 30% 10%
8	H	299	16% 61% 11% . 25%
8	I	299	13% 61% 10% .. 27%
9	F	336	25% 54% 7% .. 37%
9	G	336	37% 43% 14% . 42%
9	O	336	24% 52% 9% .. 37%
9	P	336	38% 41% 15% . 42%
10	X	911	25% . 72%
10	Y	911	25% . 72%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 93588 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 Protein PAXX.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	S	23	168	107	30	30	1	0	0
1	T	23	168	107	30	30	1	0	0

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	J	497	4021	2577	680	746	18	0	0
2	A	497	4021	2577	680	746	18	0	0

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	K	531	4259	2723	711	801	24	0	0
3	B	531	4259	2723	711	801	24	0	0

- Molecule 4 is a protein called DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	3720	29811	19106	5059	5451	195	0	0
4	C	3720	29811	19106	5059	5451	195	0	0

- Molecule 5 is a protein called PRKDC_HUMAN DNA-dependent protein kinase catalytic subunit – Unknown region.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	R	20	Total	C	N	O	0	0
			101	60	20	21		
5	Q	20	Total	C	N	O	0	0
			101	60	20	21		

- Molecule 6 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	31	Total	C	N	O	P	0	0
			634	304	113	186	31		
6	D	31	Total	C	N	O	P	0	0
			634	304	113	186	31		

- Molecule 7 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	30	Total	C	N	O	P	0	0
			616	295	110	181	30		
7	E	30	Total	C	N	O	P	0	0
			616	295	110	181	30		

- Molecule 8 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	223	Total	C	N	O	S	0	0
			1779	1140	298	326	15		
8	I	218	Total	C	N	O	S	0	0
			1737	1111	290	321	15		

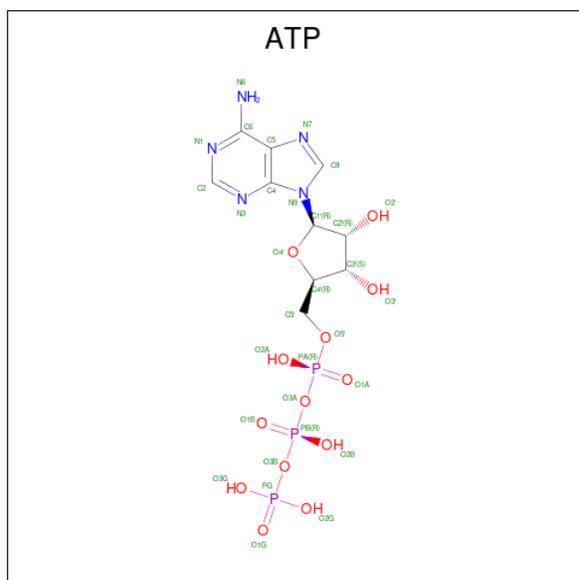
- Molecule 9 is a protein called DNA repair protein XRCC4.

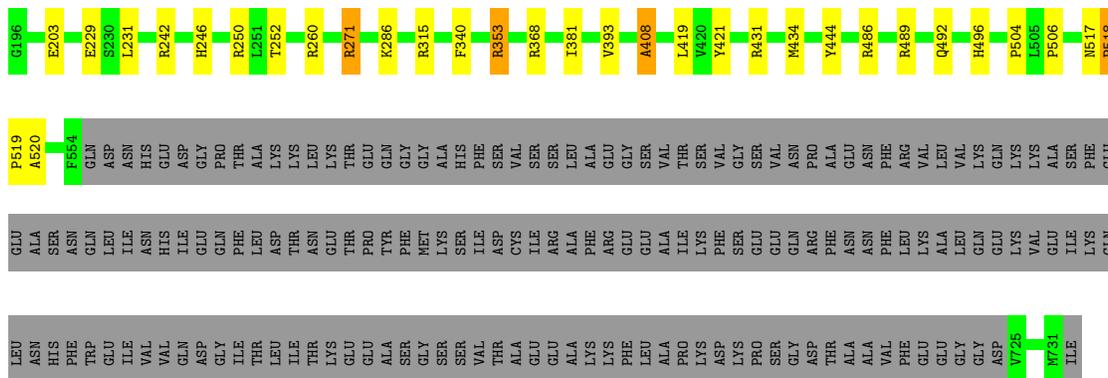
Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	213	Total	C	N	O	S	0	0
			1736	1093	308	327	8		
9	G	195	Total	C	N	O	S	0	0
			1595	1012	272	304	7		
9	O	213	Total	C	N	O	S	0	0
			1736	1093	308	327	8		
9	P	195	Total	C	N	O	S	0	0
			1595	1012	272	304	7		

- Molecule 10 is a protein called DNA ligase 4.

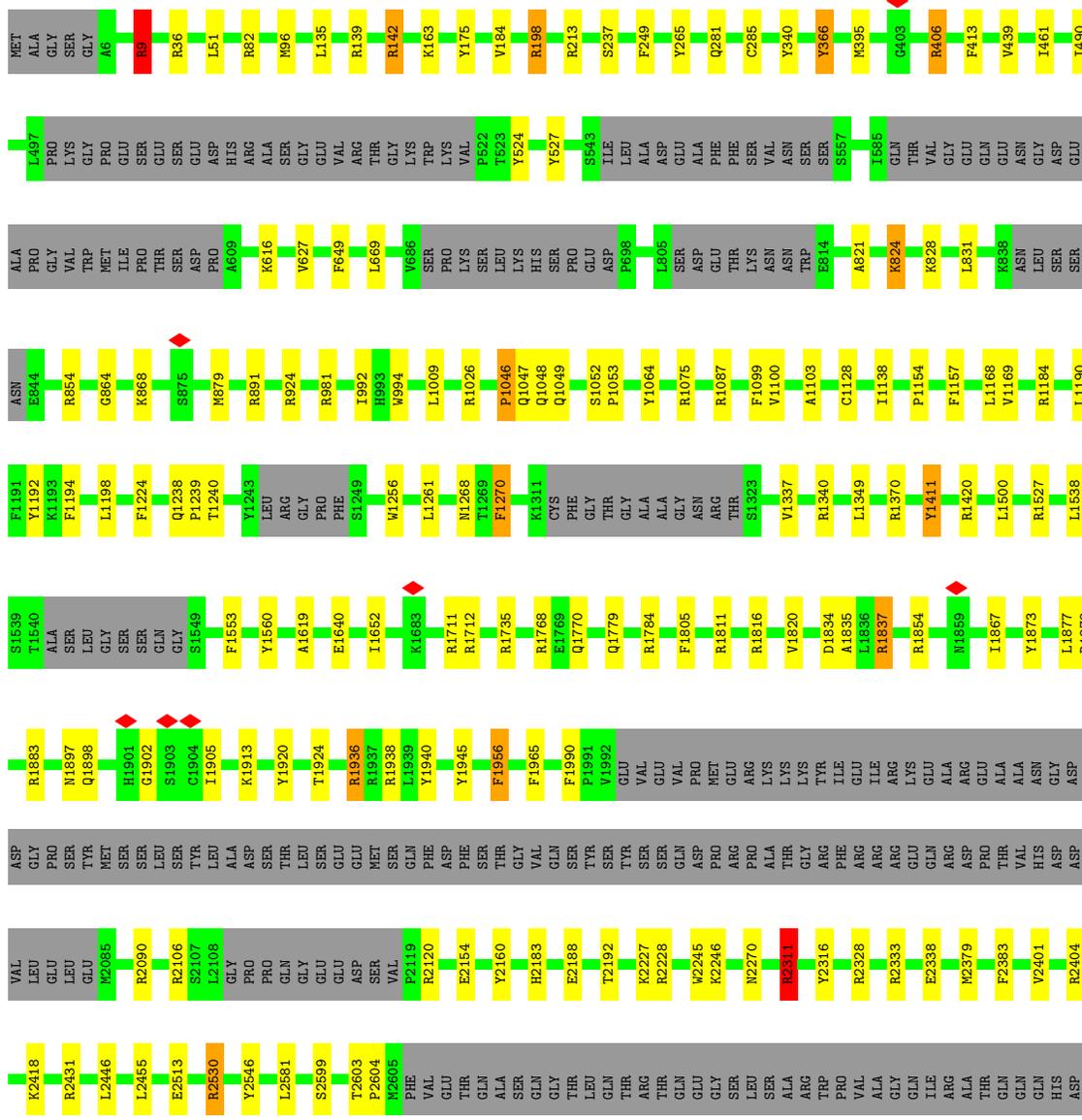
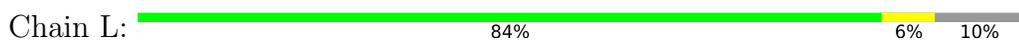
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	X	254	2064	1314	348	389	13	0	0
10	Y	254	2064	1314	348	389	13	0	0

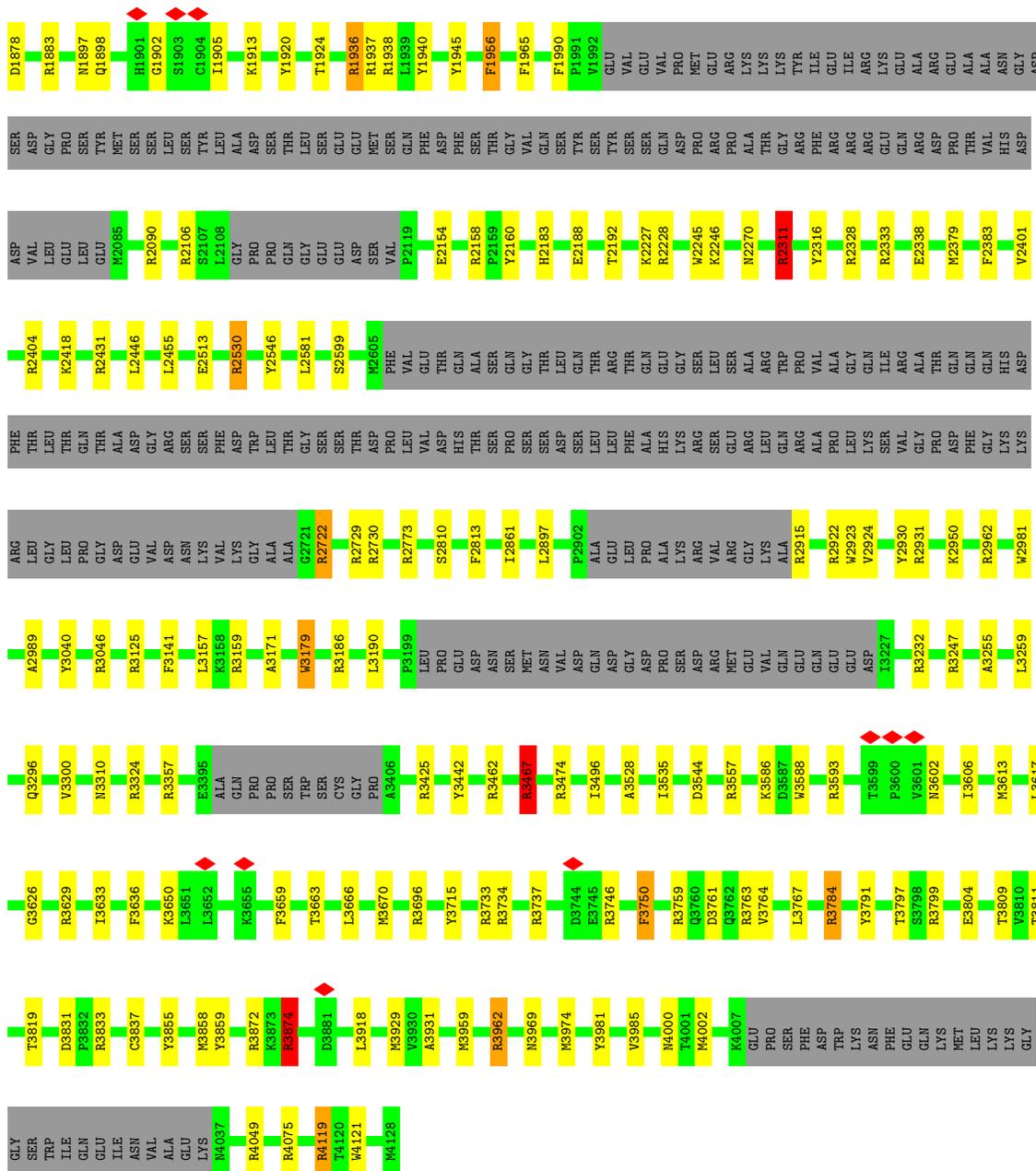
- Molecule 11 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).





● Molecule 4: DNA-dependent protein kinase catalytic subunit

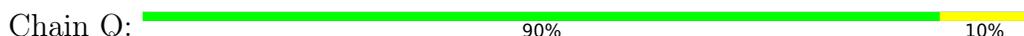




● Molecule 5: PRKDC_HUMAN DNA-dependent protein kinase catalytic subunit – Unknown region



● Molecule 5: PRKDC_HUMAN DNA-dependent protein kinase catalytic subunit – Unknown region



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	138252	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 ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.123	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (\AA)	517.92, 517.92, 517.92	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.079, 1.079, 1.079	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	S	0.66	0/172	1.01	0/229
1	T	0.67	0/172	1.04	0/229
2	A	1.23	9/4101 (0.2%)	1.20	34/5523 (0.6%)
2	J	1.23	9/4101 (0.2%)	1.20	34/5523 (0.6%)
3	B	0.66	0/4340	1.08	17/5853 (0.3%)
3	K	0.66	0/4340	1.08	17/5853 (0.3%)
4	C	0.68	8/30414 (0.0%)	1.05	91/41079 (0.2%)
4	L	0.68	8/30414 (0.0%)	1.05	85/41079 (0.2%)
6	D	1.64	7/710 (1.0%)	2.57	73/1093 (6.7%)
6	M	1.64	6/710 (0.8%)	2.57	73/1093 (6.7%)
7	E	1.69	4/690 (0.6%)	2.32	53/1063 (5.0%)
7	N	1.68	4/690 (0.6%)	2.32	55/1063 (5.2%)
8	H	0.79	7/1814 (0.4%)	1.18	14/2454 (0.6%)
8	I	0.79	6/1771 (0.3%)	1.11	6/2395 (0.3%)
9	F	0.70	2/1765 (0.1%)	1.11	8/2367 (0.3%)
9	G	0.71	0/1622	1.17	10/2178 (0.5%)
9	O	0.70	2/1765 (0.1%)	1.11	8/2367 (0.3%)
9	P	0.72	0/1622	1.19	10/2178 (0.5%)
10	X	0.73	1/2112 (0.0%)	1.11	9/2851 (0.3%)
10	Y	0.73	1/2112 (0.0%)	1.11	9/2851 (0.3%)
All	All	0.79	74/95437 (0.1%)	1.15	606/129321 (0.5%)

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
2	A	0	3
2	J	0	3
3	B	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	K	0	5
4	C	0	27
4	L	0	28
6	D	0	15
6	M	0	15
7	E	0	11
7	N	0	11
8	H	0	2
8	I	0	4
9	F	0	5
9	G	0	3
9	O	0	5
9	P	0	3
All	All	0	145

The worst 5 of 74 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	334	THR	CB-CG2	39.55	2.82	1.52
2	J	334	THR	CB-CG2	39.51	2.82	1.52
2	J	334	THR	N-CA	30.85	2.08	1.46
2	A	334	THR	N-CA	30.84	2.08	1.46
2	J	333	GLU	CB-CG	28.12	2.05	1.52

The worst 5 of 606 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	334	THR	N-CA-CB	-13.33	84.97	110.30
2	A	334	THR	N-CA-CB	-13.30	85.03	110.30
2	J	333	GLU	CA-CB-CG	-13.07	84.64	113.40
2	A	333	GLU	CA-CB-CG	-13.06	84.67	113.40
3	B	231	LEU	CB-CG-CD1	13.04	133.17	111.00

There are no chirality outliers.

5 of 145 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	71	TYR	Sidechain
2	A	88	TYR	Sidechain
2	J	137	HIS	Sidechain
2	J	71	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	J	88	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	S	168	0	169	15	0
1	T	168	0	169	16	0
2	A	4021	0	4100	52	0
2	J	4021	0	4100	53	0
3	B	4259	0	4301	8	0
3	K	4259	0	4301	8	0
4	C	29811	0	30286	98	0
4	L	29811	0	30286	97	0
5	Q	101	0	23	1	0
5	R	101	0	23	1	0
6	D	634	0	348	4	0
6	M	634	0	348	4	0
7	E	616	0	339	5	0
7	N	616	0	339	5	0
8	H	1779	0	1797	15	0
8	I	1737	0	1744	13	0
9	F	1736	0	1739	20	0
9	G	1595	0	1592	34	0
9	O	1736	0	1739	24	0
9	P	1595	0	1592	36	0
10	X	2064	0	2012	14	0
10	Y	2064	0	2012	14	0
11	C	31	0	12	0	0
11	L	31	0	12	0	0
All	All	93588	0	93383	440	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 2.

The worst 5 of 440 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)
2:A:333:GLU:CB	2:A:333:GLU:CA	1.83	1.57
2:J:333:GLU:CA	2:J:333:GLU:CB	1.83	1.56
2:A:333:GLU:CA	2:A:333:GLU:N	1.68	1.56
2:J:333:GLU:CA	2:J:333:GLU:C	1.77	1.52
2:J:333:GLU:CA	2:J:333:GLU:N	1.68	1.50

There are no symmetry-related clashes.

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	
1	S	21/204 (10%)	18 (86%)	3 (14%)	0	100	100
1	T	21/204 (10%)	17 (81%)	4 (19%)	0	100	100
2	A	493/609 (81%)	461 (94%)	32 (6%)	0	100	100
2	J	493/609 (81%)	460 (93%)	33 (7%)	0	100	100
3	B	525/732 (72%)	477 (91%)	42 (8%)	6 (1%)	14	52
3	K	525/732 (72%)	476 (91%)	43 (8%)	6 (1%)	14	52
4	C	3686/4128 (89%)	3440 (93%)	245 (7%)	1 (0%)	100	100
4	L	3686/4128 (89%)	3442 (93%)	243 (7%)	1 (0%)	100	100
8	H	217/299 (73%)	202 (93%)	13 (6%)	2 (1%)	17	56
8	I	212/299 (71%)	201 (95%)	10 (5%)	1 (0%)	29	68
9	F	209/336 (62%)	201 (96%)	7 (3%)	1 (0%)	29	68
9	G	191/336 (57%)	178 (93%)	12 (6%)	1 (0%)	29	68
9	O	209/336 (62%)	201 (96%)	7 (3%)	1 (0%)	29	68
9	P	191/336 (57%)	176 (92%)	12 (6%)	3 (2%)	9	45
10	X	250/911 (27%)	241 (96%)	9 (4%)	0	100	100
10	Y	250/911 (27%)	241 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11179/15110 (74%)	10432 (93%)	724 (6%)	23 (0%)	50 81

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	145	SER
3	K	146	GLN
3	K	518	PRO
3	K	520	ALA
3	B	145	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	S	18/160 (11%)	18 (100%)	0	100 100
1	T	18/160 (11%)	18 (100%)	0	100 100
2	A	452/548 (82%)	446 (99%)	6 (1%)	69 82
2	J	452/548 (82%)	446 (99%)	6 (1%)	69 82
3	B	481/649 (74%)	468 (97%)	13 (3%)	44 66
3	K	481/649 (74%)	468 (97%)	13 (3%)	44 66
4	C	3325/3671 (91%)	3289 (99%)	36 (1%)	73 85
4	L	3325/3671 (91%)	3289 (99%)	36 (1%)	73 85
8	H	198/262 (76%)	189 (96%)	9 (4%)	27 54
8	I	193/262 (74%)	178 (92%)	15 (8%)	12 38
9	F	191/303 (63%)	174 (91%)	17 (9%)	9 33
9	G	178/303 (59%)	158 (89%)	20 (11%)	6 25
9	O	191/303 (63%)	175 (92%)	16 (8%)	11 36
9	P	178/303 (59%)	158 (89%)	20 (11%)	6 25
10	X	230/808 (28%)	221 (96%)	9 (4%)	32 57
10	Y	230/808 (28%)	221 (96%)	9 (4%)	32 57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	10141/13408 (76%)	9916 (98%)	225 (2%)	54 71

5 of 225 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	2227	LYS
9	P	163	GLU
9	F	110	SER
9	P	115	LYS
10	Y	792	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
4	L	4068	HIS
1	T	187	ASN
3	B	246	HIS
9	O	277	GLN
4	C	4068	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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
11	ATP	C	4201	-	26,33,33	1.25	1 (3%)	31,52,52	1.49	4 (12%)
11	ATP	L	4201	-	26,33,33	1.25	2 (7%)	31,52,52	1.56	5 (16%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ATP	C	4201	-	-	4/18/38/38	0/3/3/3
11	ATP	L	4201	-	-	6/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	4201	ATP	O4'-C1'	3.75	1.46	1.41
11	L	4201	ATP	O4'-C1'	3.59	1.46	1.41
11	L	4201	ATP	C2'-C1'	2.10	1.56	1.53

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	4201	ATP	C4-C5-N7	4.18	113.76	109.40
11	C	4201	ATP	C4-C5-N7	4.15	113.72	109.40
11	L	4201	ATP	PB-O3B-PG	-3.44	121.03	132.83
11	C	4201	ATP	PB-O3B-PG	-3.27	121.62	132.83
11	L	4201	ATP	PA-O3A-PB	-2.87	122.97	132.83

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	L	4201	ATP	C5'-O5'-PA-O1A
11	L	4201	ATP	O4'-C4'-C5'-O5'
11	L	4201	ATP	C3'-C4'-C5'-O5'
11	C	4201	ATP	O4'-C4'-C5'-O5'

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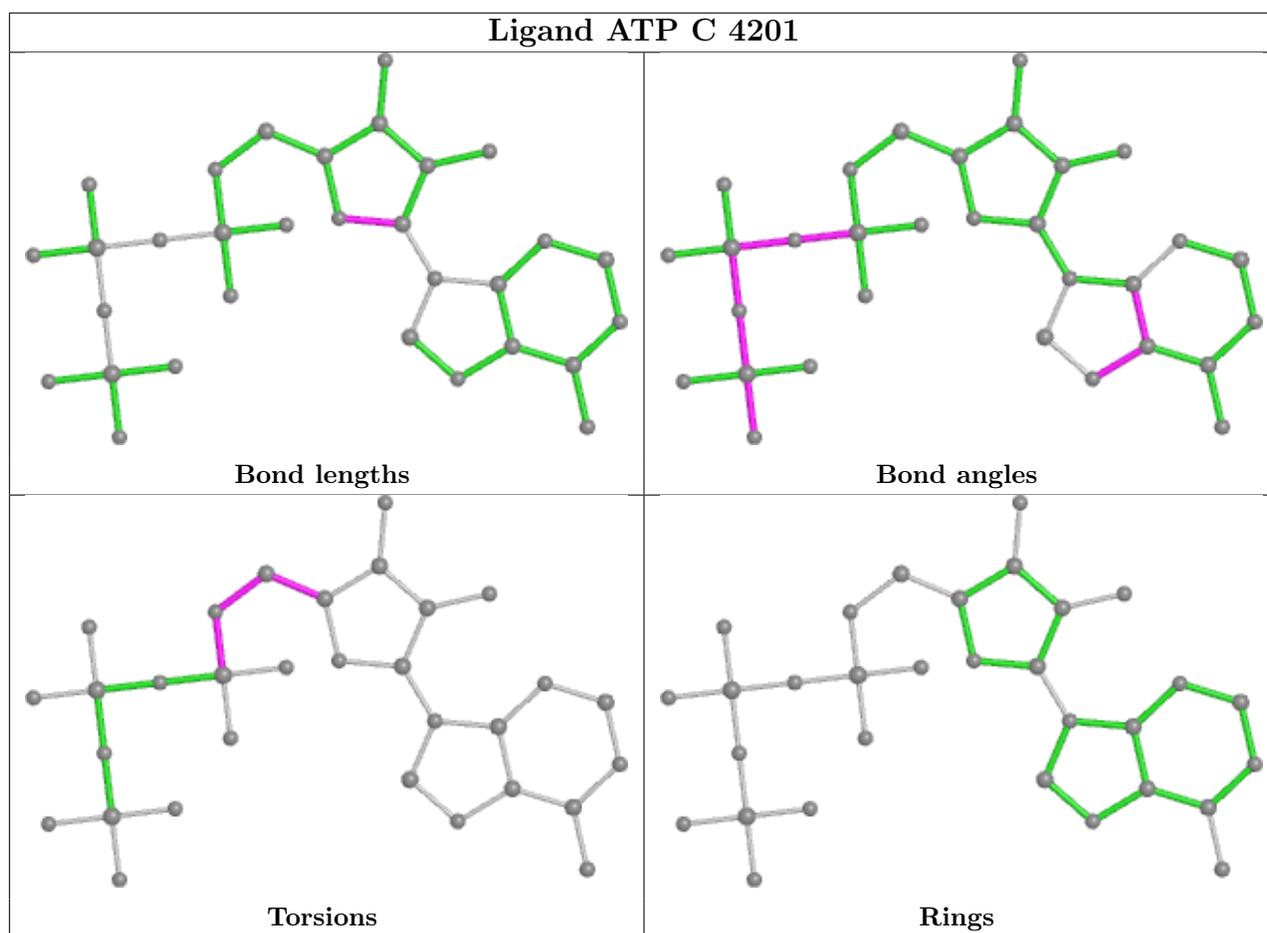
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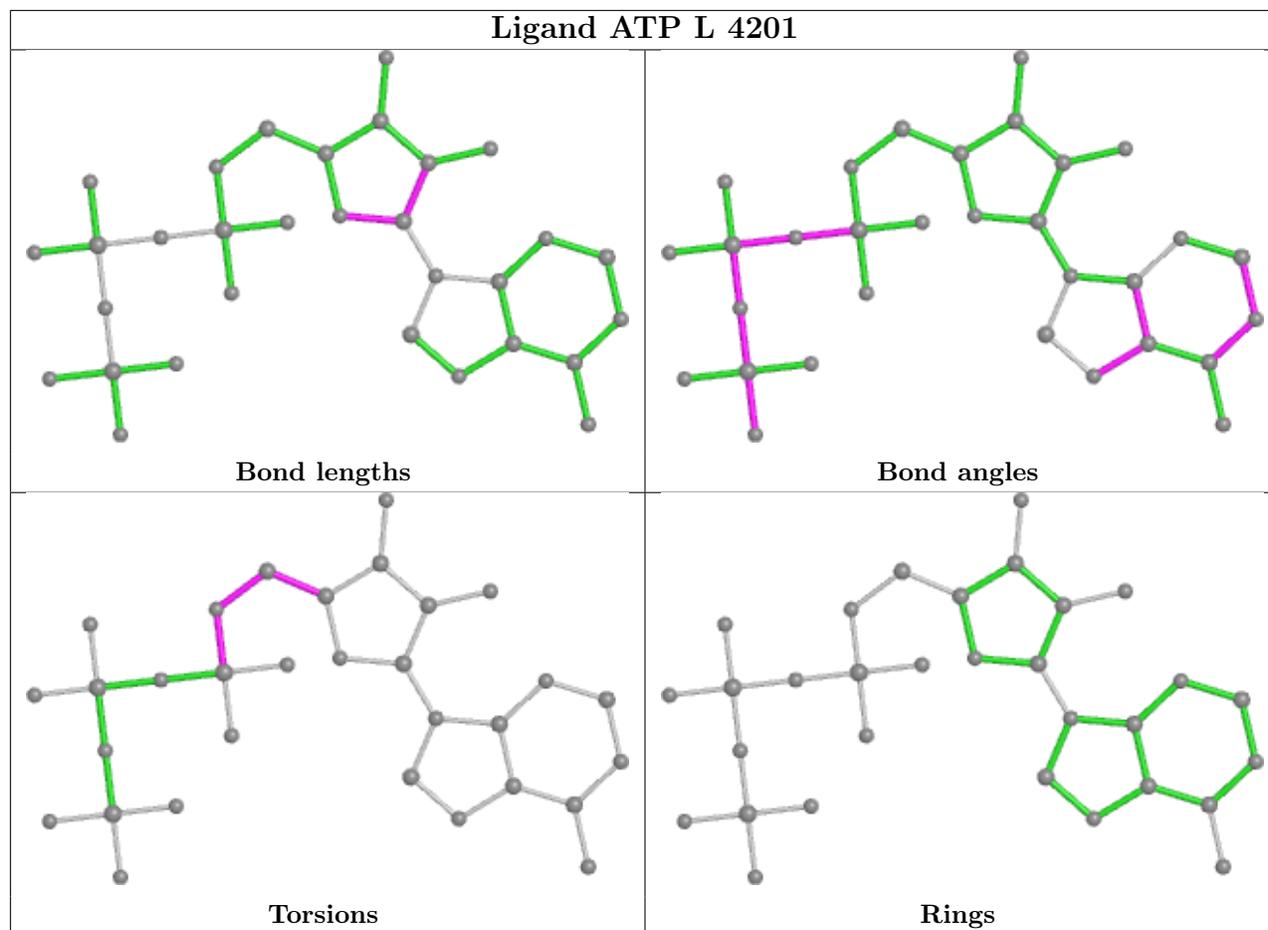
Mol	Chain	Res	Type	Atoms
11	C	4201	ATP	C3'-C4'-C5'-O5'

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](#)

There are no chain breaks in this entry.

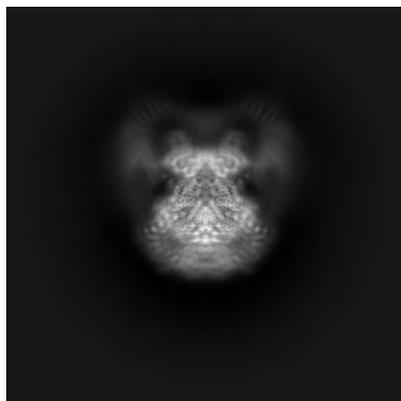
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28732. These allow visual inspection of the internal detail of the map and identification of artifacts.

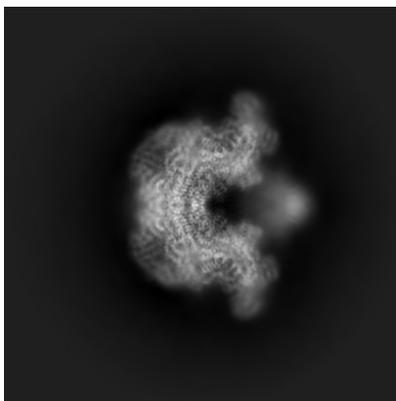
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

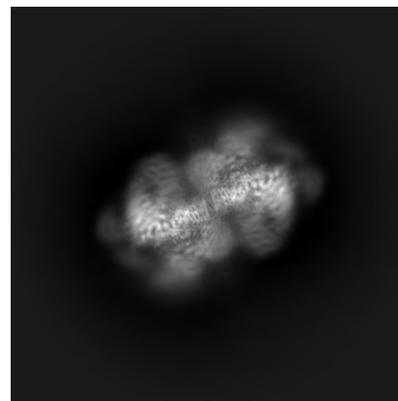
6.1.1 Primary map



X

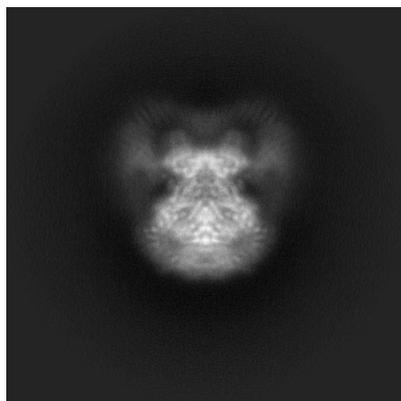


Y

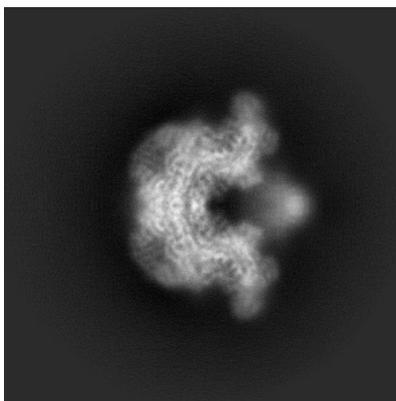


Z

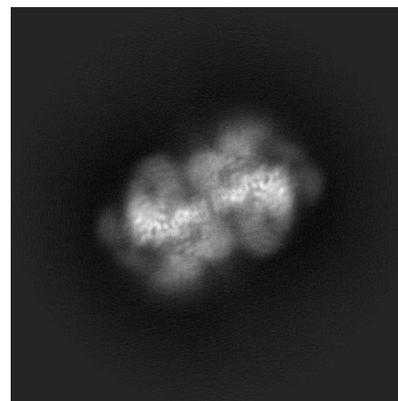
6.1.2 Raw map



X



Y

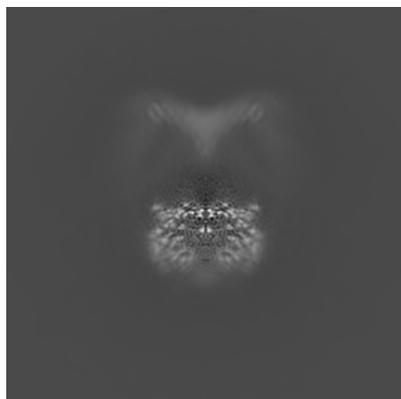


Z

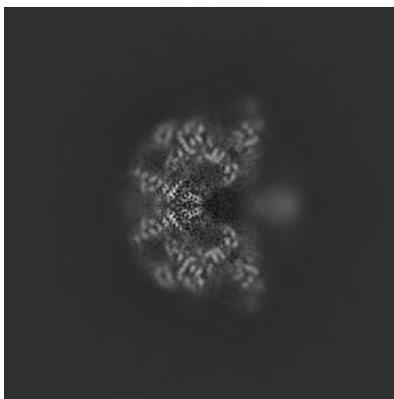
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

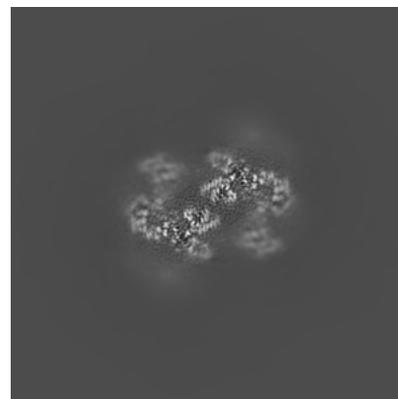
6.2.1 Primary map



X Index: 240

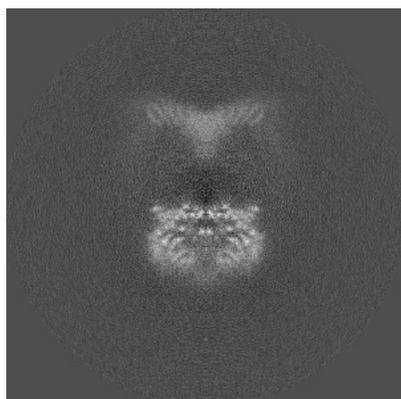


Y Index: 240

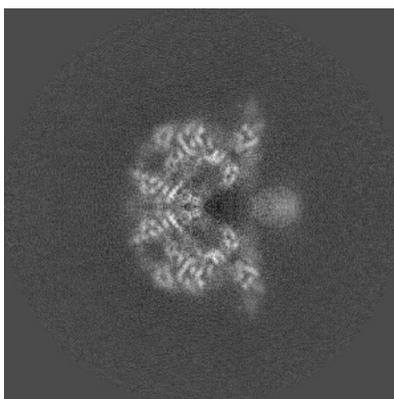


Z Index: 240

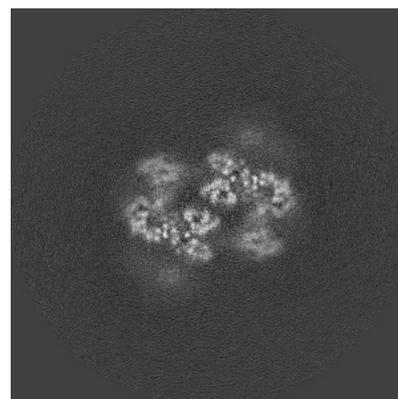
6.2.2 Raw map



X Index: 240



Y Index: 240

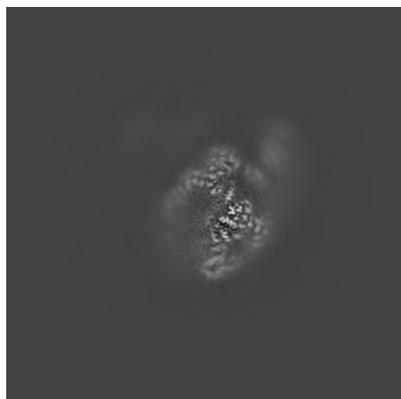


Z Index: 240

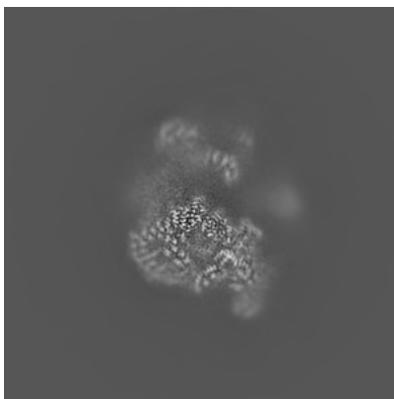
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

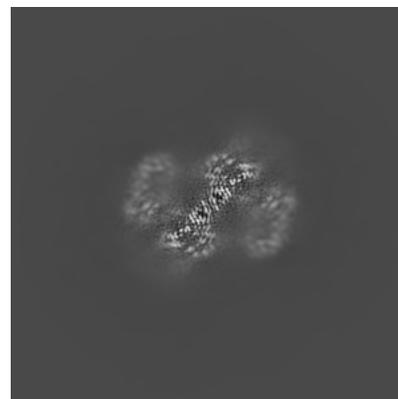
6.3.1 Primary map



X Index: 278



Y Index: 226

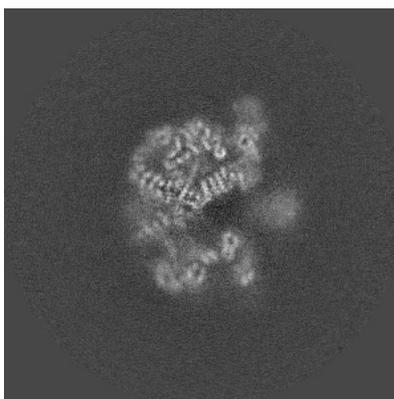


Z Index: 227

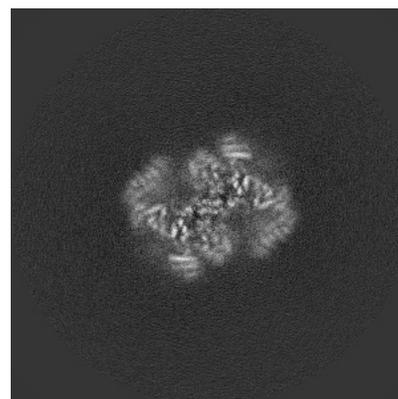
6.3.2 Raw map



X Index: 196



Y Index: 247

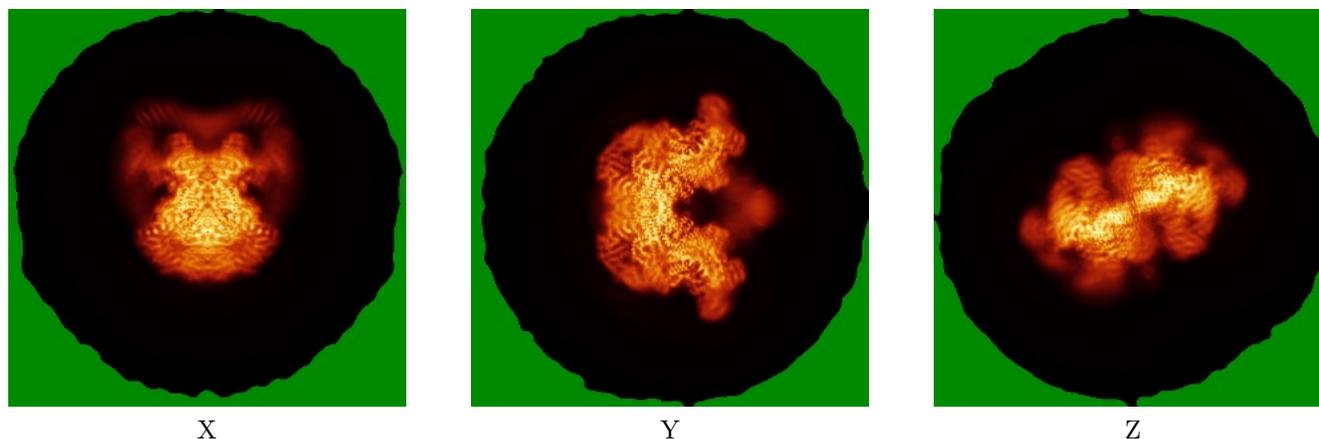


Z Index: 211

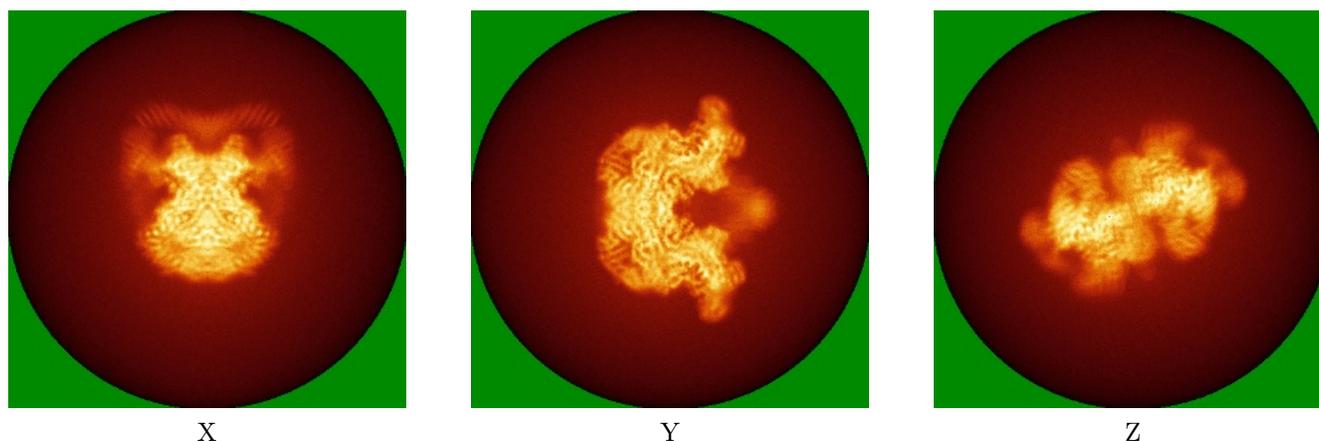
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



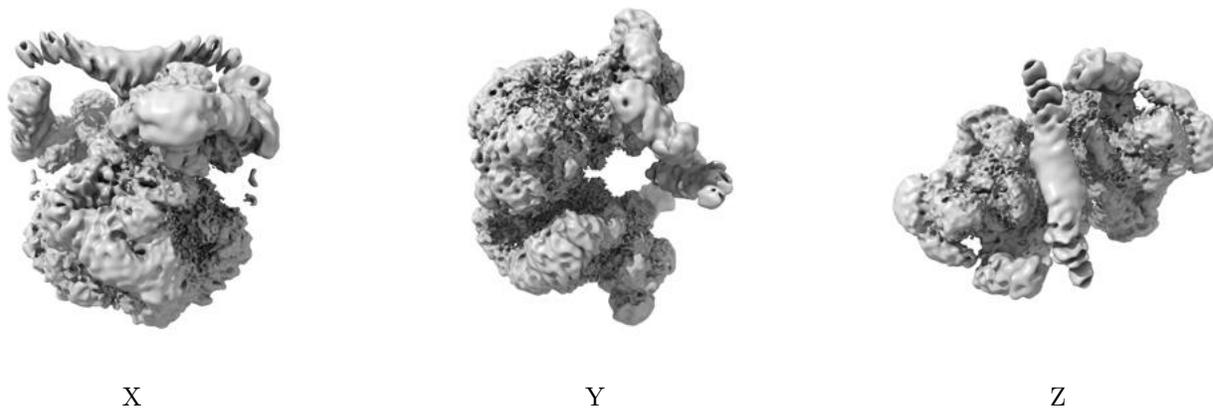
6.4.2 Raw map



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.

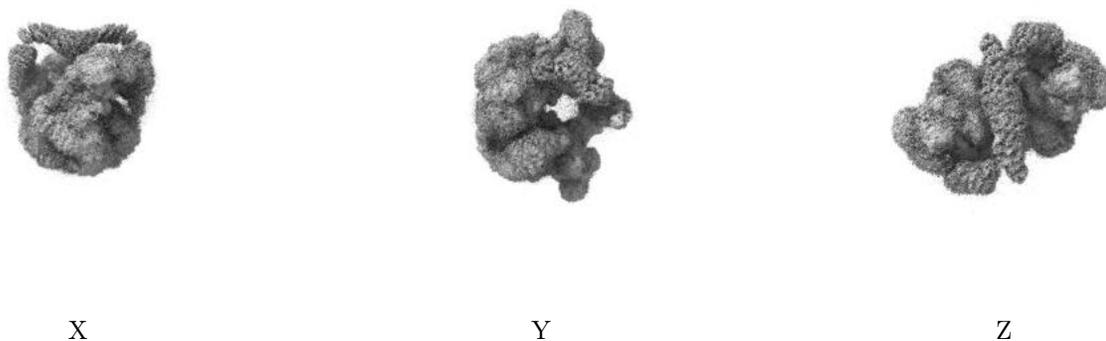
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

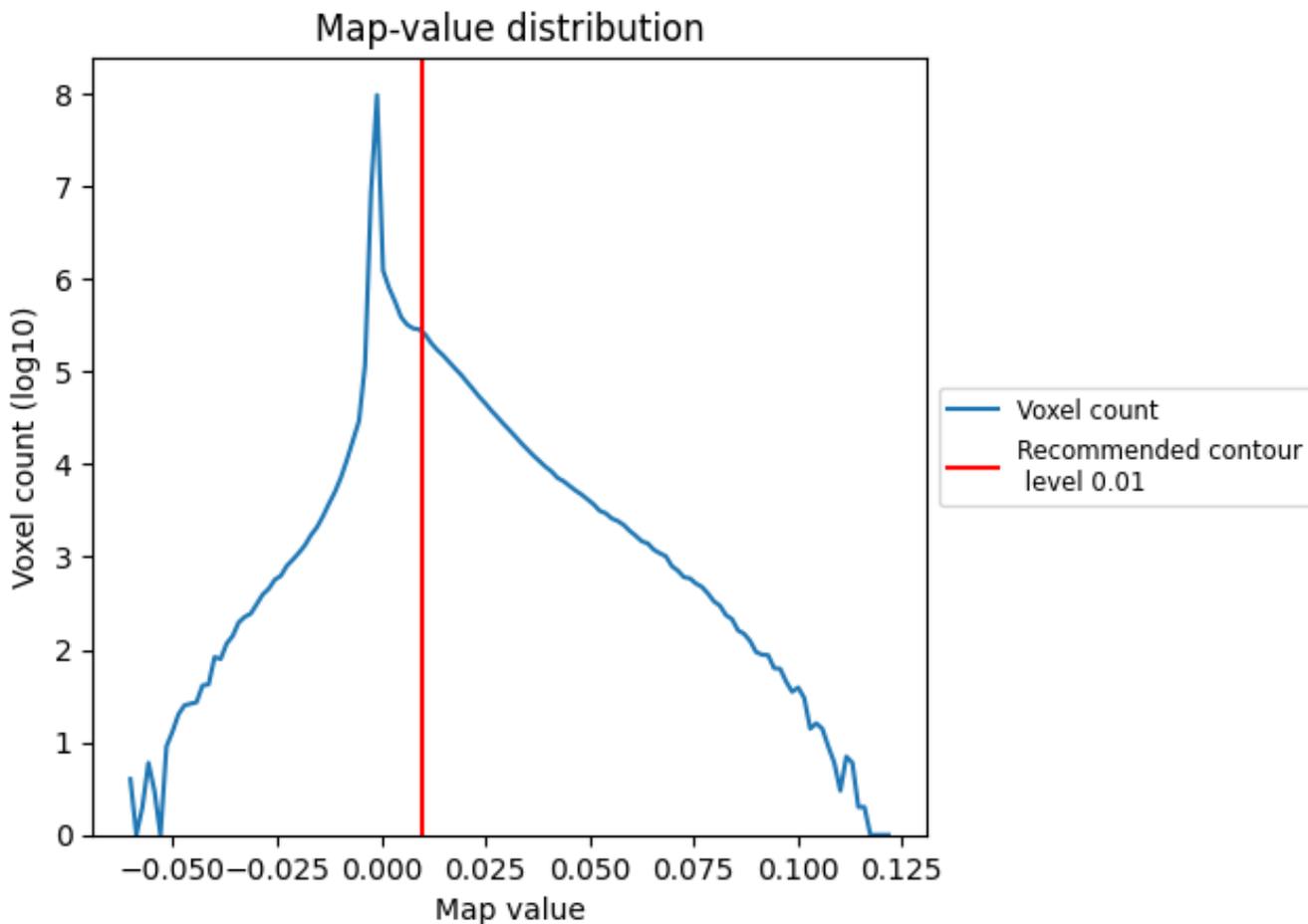
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

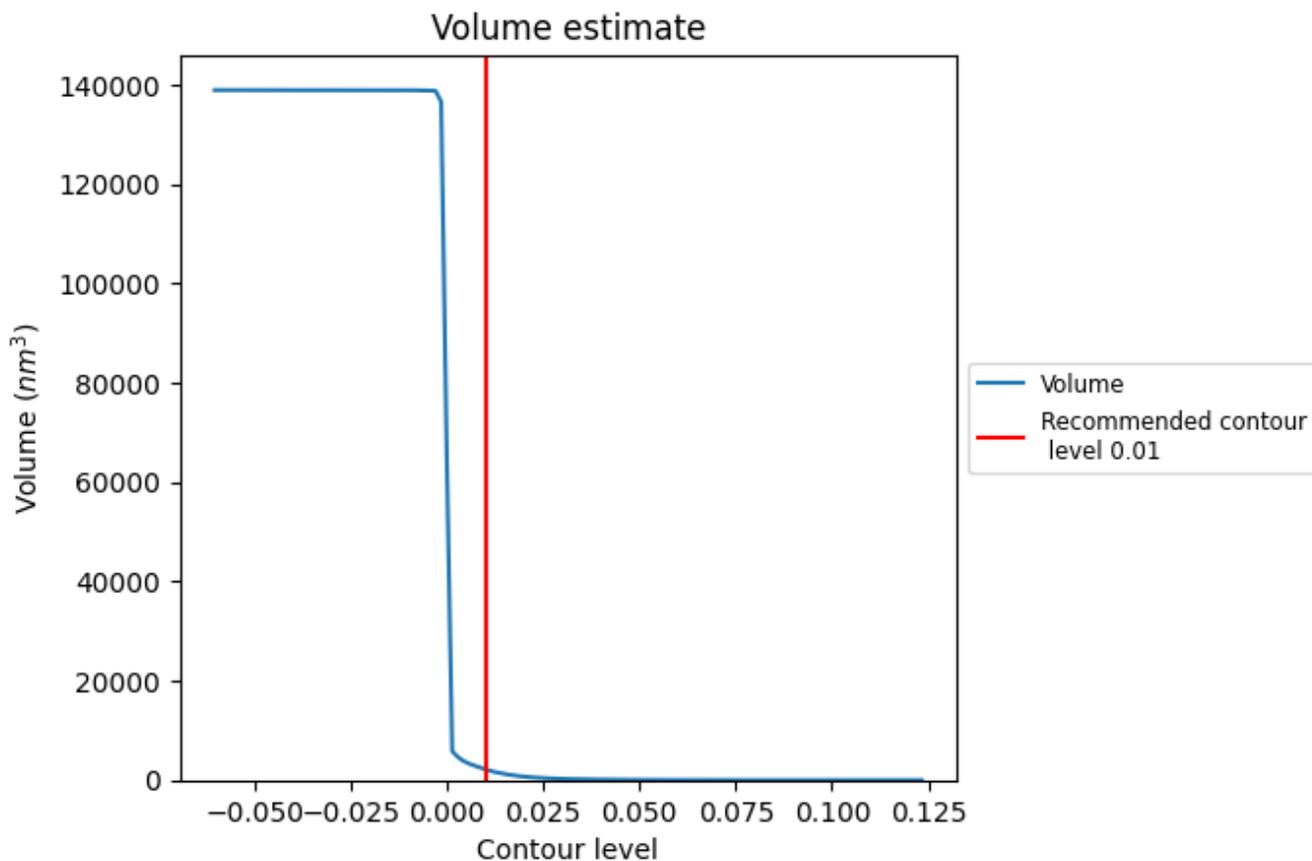
This section contains the results of statistical analysis of the map.

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.

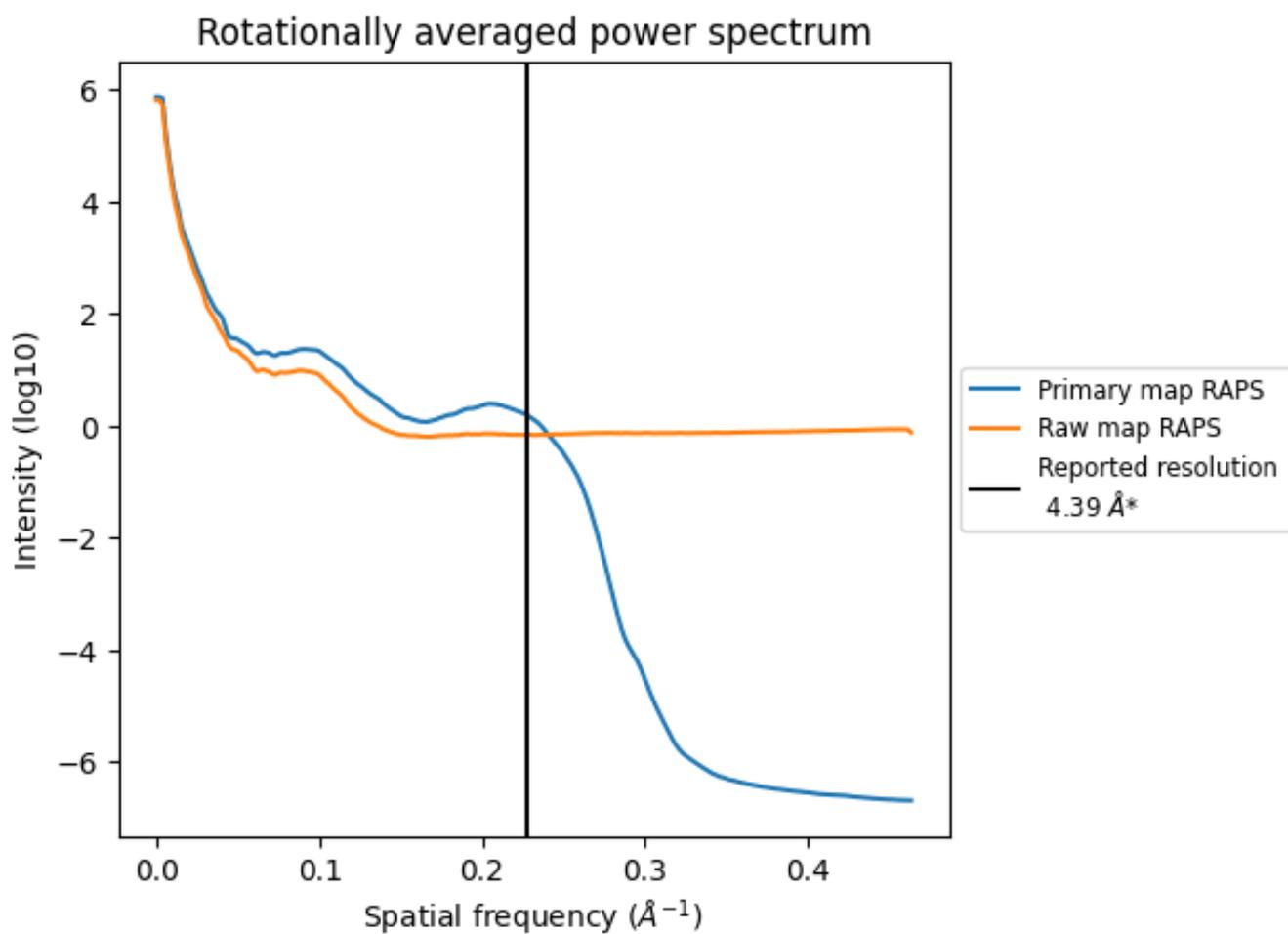
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 2174 nm³; this corresponds to an approximate mass of 1964 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 i

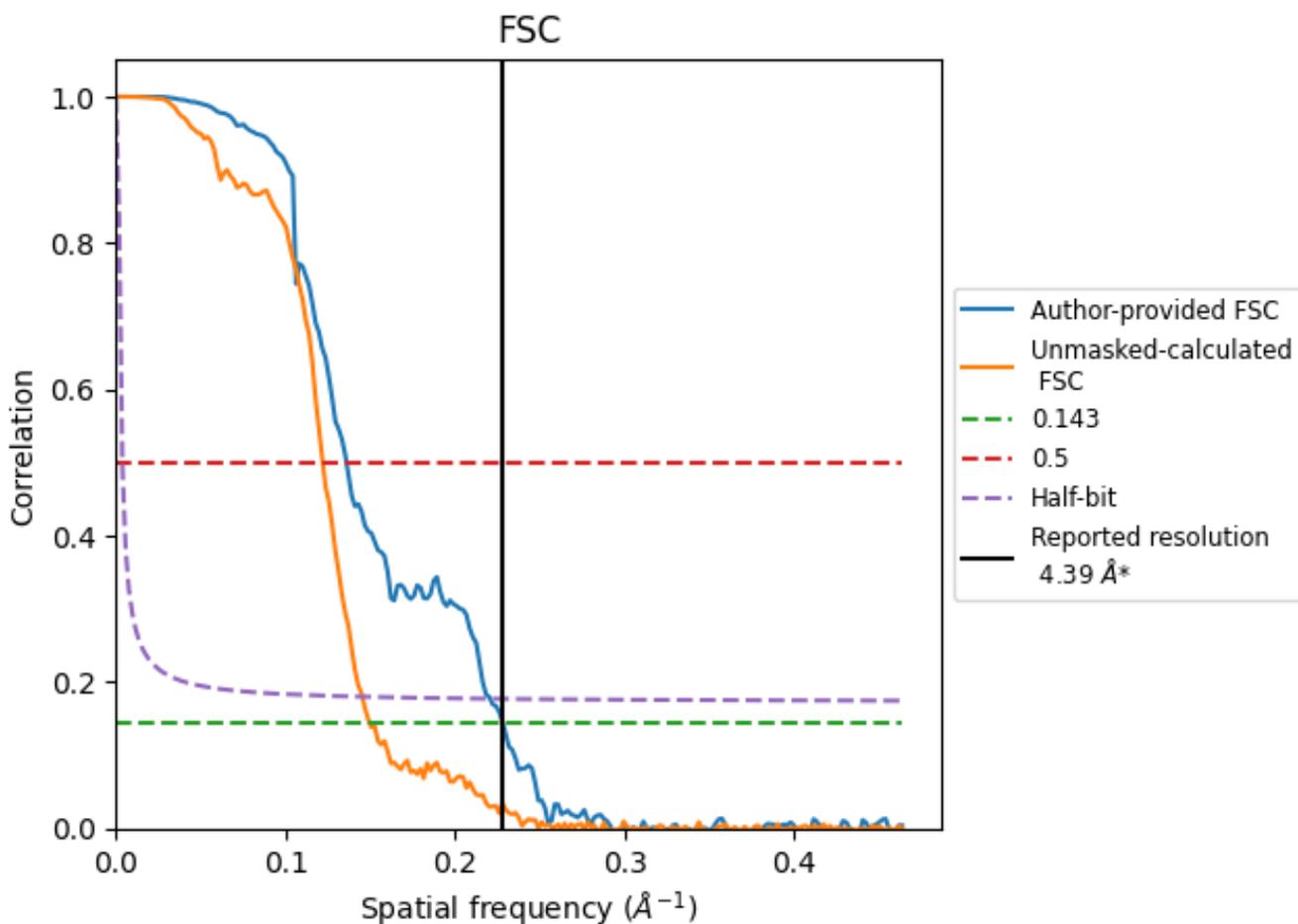


*Reported resolution corresponds to spatial frequency of 0.228 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.228 Å⁻¹

8.2 Resolution estimates

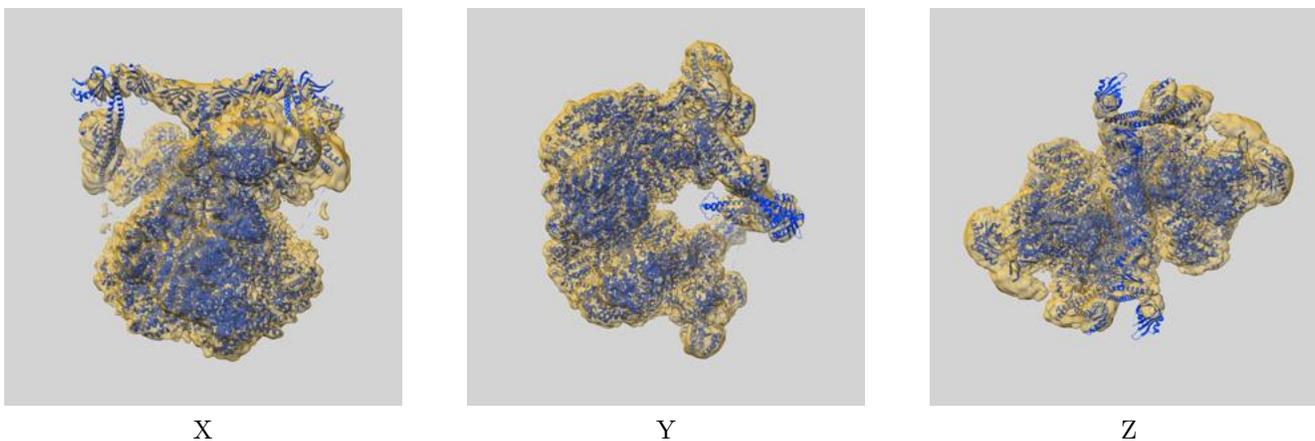
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.39	-	-
Author-provided FSC curve	4.38	7.36	4.53
Unmasked-calculated*	6.68	8.19	6.88

*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 6.68 differs from the reported value 4.39 by more than 10 %

9 Map-model fit [i](#)

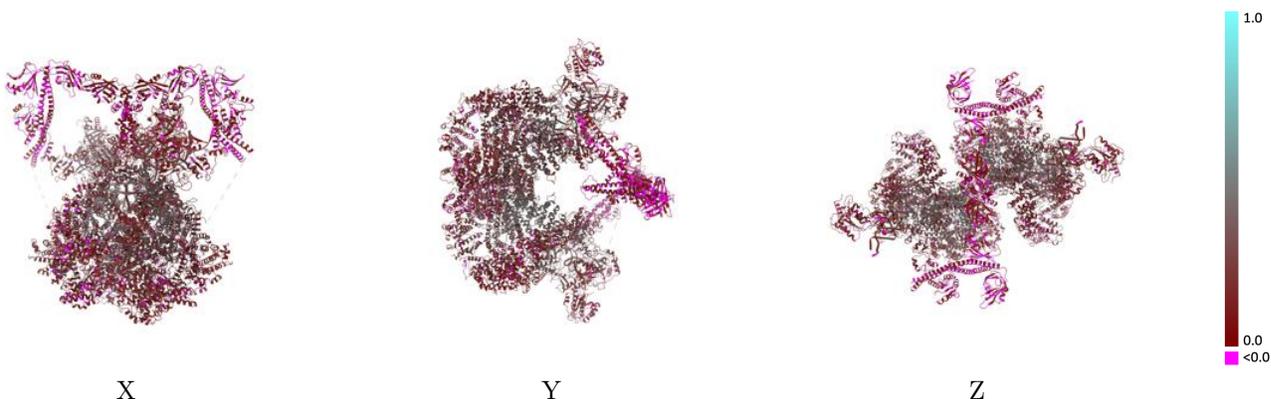
This section contains information regarding the fit between EMDB map EMD-28732 and PDB model 8EZA. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



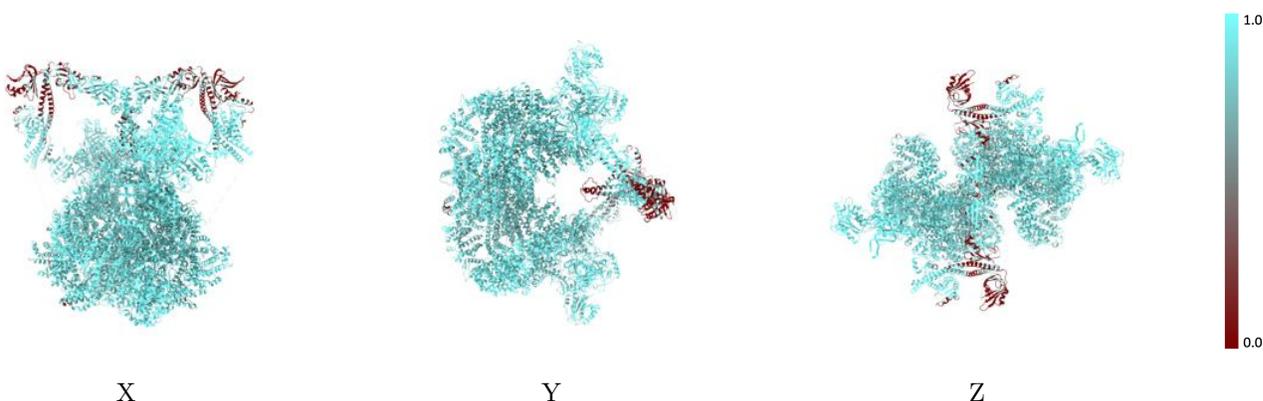
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



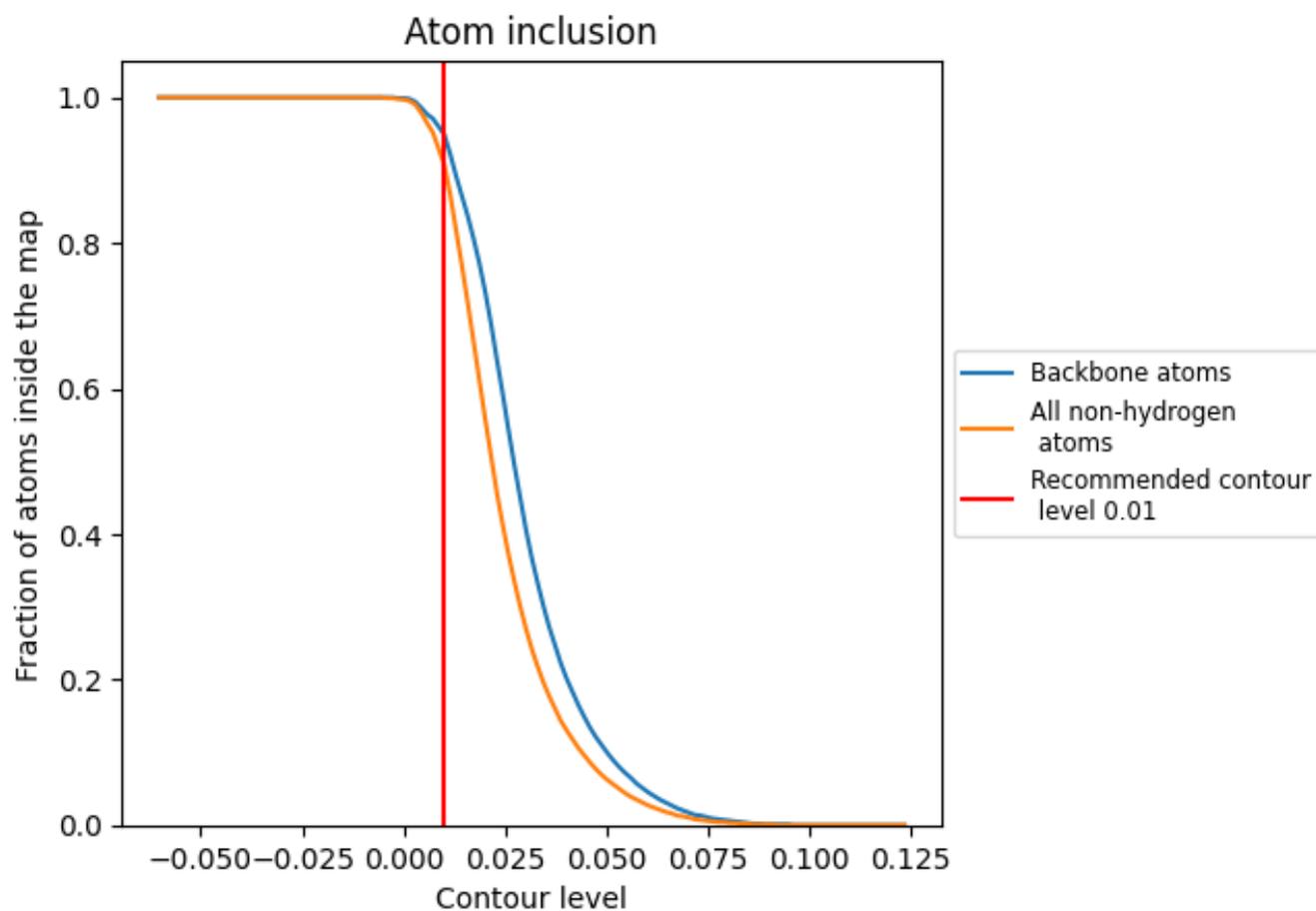
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9080	 0.2160
A	 0.9600	 0.2620
B	 0.9690	 0.2070
C	 0.9430	 0.2350
D	 0.9980	 0.3170
E	 0.9970	 0.3350
F	 0.5590	 0.0430
G	 0.3530	 0.0410
H	 0.7720	 0.0650
I	 0.7740	 0.0580
J	 0.9650	 0.2640
K	 0.9700	 0.2060
L	 0.9470	 0.2500
M	 0.9950	 0.3240
N	 0.9970	 0.3330
O	 0.5650	 0.0420
P	 0.3530	 0.0440
Q	 0.9700	 0.2200
R	 0.9700	 0.2180
S	 0.9760	 0.2800
T	 0.9760	 0.2830
X	 0.9170	 0.1090
Y	 0.9120	 0.1110

