



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 09:32 PM UTC

PDB ID : 8RHB / pdb_00008rhb
EMDB ID : EMD-19174
Title : Microtubule-associated kinesin-1 tail complex bound to AMPPNP, single-headed state
Authors : Atherton, J.; Chegkazi, M.S.; Steiner, R.A.
Deposited on : 2023-12-15
Resolution : 3.00 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:

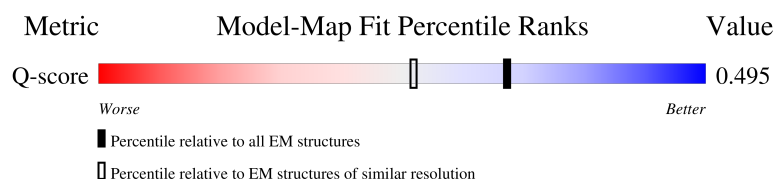
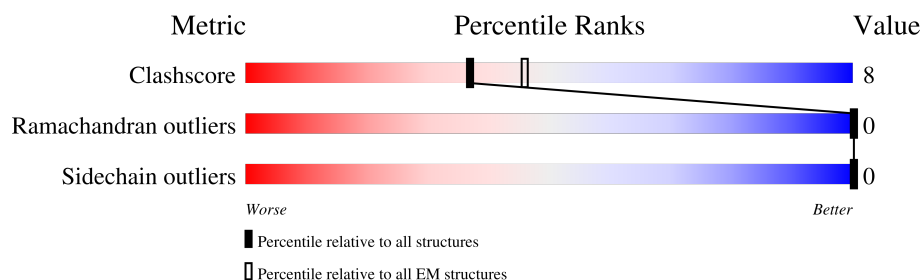
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 3.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	B	445	
2	K	963	
2	T	963	
3	A	451	

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Mol	Chain	Length	Quality of chain
4	t	6	67% 33%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 9539 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 Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	426	Total	C	N	O	S	0	0
			3351	2106	575	644	26		

- Molecule 2 is a protein called Kinesin-1 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	330	Total	C	N	O	S	0	0
			2585	1609	444	516	16		
2	T	6	Total	C	N	O		6	0
			43	28	8	7			

- Molecule 3 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	428	Total	C	N	O	S	0	0
			3358	2130	571	635	22		

- Molecule 4 is a protein called Kif5b Tail.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	t	6	Total	C	N	O	6	0
			47	31	10	6		

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



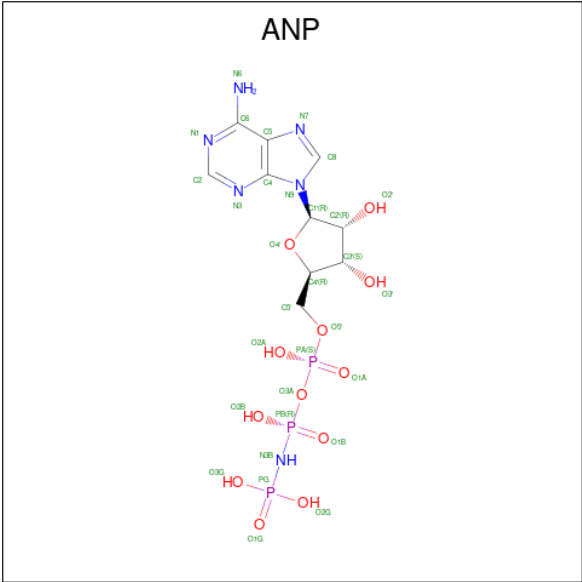
Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total 28	C 10	N 5	O 11	P 2	0

- Molecule 6 is TAXOL (CCD ID: TA1) (formula: $C_{47}H_{51}NO_{14}$).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			62	47	1	14	

- Molecule 7 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$).

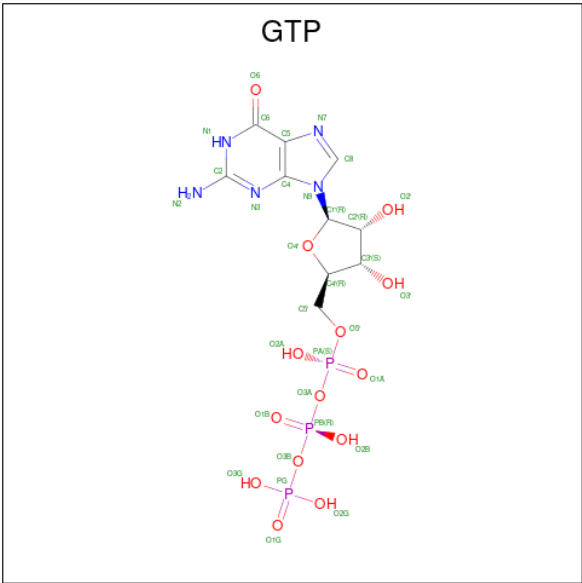


Mol	Chain	Residues	Atoms					AltConf
7	K	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	K	1	Total	Mg	0
			1	1	
8	A	1	Total	Mg	0
			1	1	

- Molecule 9 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



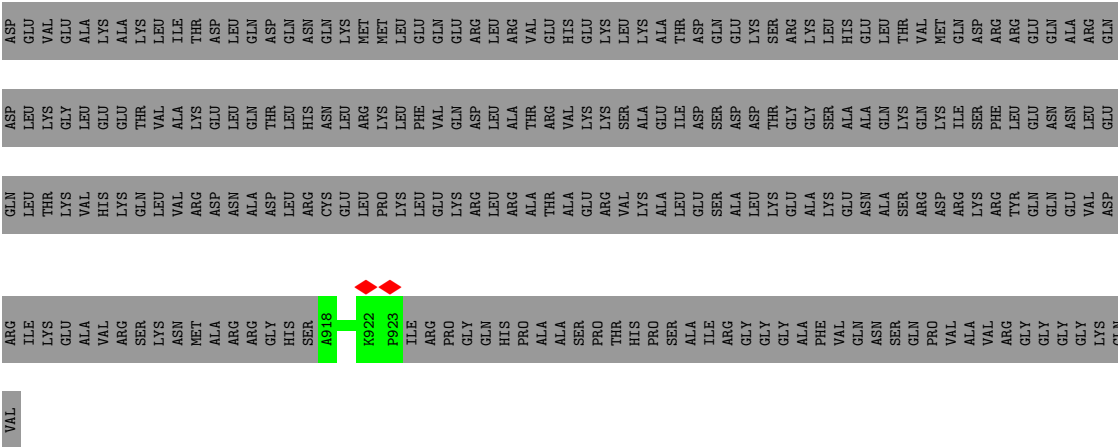
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	A	1	32	10	5	14	3	0

ASN	VAL	ALA	TLE	GLU	GLN	ARG
ASN	ARG	LYS	THR	LEU	LEU	ARG
MET	ASP	GLU	ASP	VAL	GLU	ALA
ARG	ASN	LEU	LEU	GLN	SER	ALA
ARG	ALA	GLN	GLN	LEU	THR	MET
GLY	ASP	THR	ASP	ARG	GLN	MET
HIS	LEU	LEU	GLN	ALA	THR	ALA
SER	ARG	HIS	ASN	GLN	GLU	SER
ALA	CYS	ASN	GLN	GLU	SER	LEU
GLN	GLU	LEU	LYS	LYS	ASN	LEU
ILE	LEU	ARG	MET	VAL	LYS	ASP
ALA	PRO	LYS	MET	HIS	LYS	ASP
LYS	LYS	LEU	LEU	GLU	LEU	LEU
PRO	LEU	PHE	GLU	MET	GLU	ALA
ILE	GLU	VAL	GLN	GLU	GLU	ALA
ARG	LYS	GLN	GLU	LYS	ASN	ILE
PRO	ARG	ASP	ARG	GLU	GLY	ILE
GLY	LEU	LEU	LEU	HIS	LYS	ILE
GLY	ARG	ALA	ARG	LEU	GLU	ALA
HIS	ALA	THR	VAL	ASN	LEU	VAL
PRO	THR	ARG	GLU	GLU	GLY	VAL
ALA	ALA	VAL	HIS	VAL	ALA	ASN
ALA	GLU	LYS	GLU	GLN	CYS	ASN
ALA	ARG	LYS	LYS	THR	GLN	ASP
SER	ARG	SER	LEU	ALA	LEU	VAL
PRO	VAL	SER	LEU	ALA	LEU	VAL
THR	LYS	ALA	LYS	ASN	ARG	LYS
HIS	ALA	GLU	ALA	GLU	ILE	GLN
PRO	LEU	ILE	THR	VAL	SER	PRO
PRO	GLU	ASP	ASP	LYS	GLN	GLY
ALA	SER	SER	GLN	GLN	HIS	GLY
ILE	ALA	ASP	GLU	ALA	GLU	THR
ARG	LEU	ASP	LYS	VAL	ALA	GLY
GLY	LYS	THR	ARG	GLU	LYS	MET
GLY	GLU	GLY	LYS	GLN	ILE	ILE
ALA	LYS	GLY	LYS	GLN	LYS	ASP
PHE	LYS	SER	LEU	ILE	SER	GLU
VAL	GLU	ALA	HIS	GLU	LEU	GLU
GLN	ASN	GLN	LEU	SER	THR	THR
ASN	SER	LYS	THR	ARG	TYR	VAL
SER	ARG	GLN	VAL	GLU	LEU	ALA
GLN	ASP	LYS	MET	THR	GLN	ARG
PRO	ARG	ILE	GLN	THR	ASN	ARG
VAL	LYS	SER	ASP	HIS	ASN	LEU
ALA	ARG	PHE	ARG	GLN	VAL	TYR
VAL	TYR	ALA	ARG	LYS	GLU	ILE
ARG	GLN	GLU	ARG	ILE	GLN	SER
GLY	GLN	ASN	GLN	ILE	LYS	LYS
GLY	GLU	ASN	GLN	SER	LYS	MET
GLY	GLU	ASN	ALA	SER	ARG	LYS
GLY	VAL	LEU	GLN	LEU	GLN	SER
GLY	ASP	GLU	ARG	ARG	LEU	GLU
LYS	ARG	GLN	ASP	ASP	GLU	VAL
GLN	ILE	LEU	LEU	GLU	GLU	LYS
VAL	LYS	THR	LYS	VAL	SER	THR
	GLU	GLY	GLY	GLU	VAL	MET
	ALA	VAL	LEU	ALA	ASP	VAL
	VAL	HIS	GLU	LYS	ALA	LYS
	ARG	LYS	GLU	ALA	LEU	ARG
	SER	GLN	THR	ALA	LEU	LYS
	LYS	LEU	VAL	LEU	SER	CYS

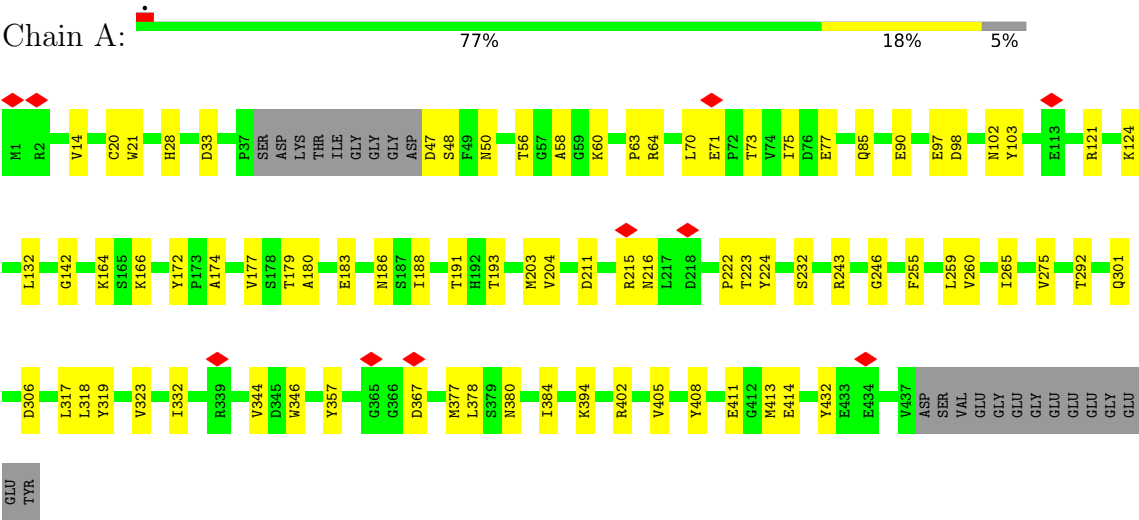
- Molecule 2: Kinesin-1 heavy chain

Chain T: 99%

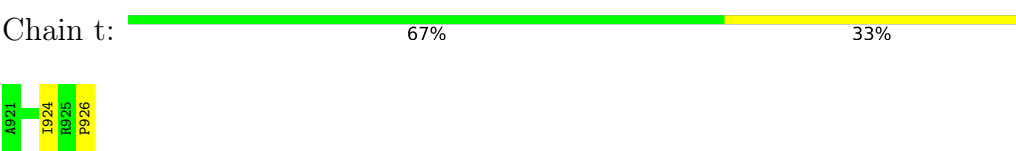
GLU	GLU	VAL	LYS	ASN	CYS	LEU	CYS	THR	ASP	SER	VAL	MET
GLU	GLU	LYS	GLU	ASP	GLU	GLU	CYS	GLY	THR	MET	TYR	ALA
SER	SER	THR	MET	ALA	GLU	ASN	CYS	ALA	ILE	ASN	ASN	ASP
VAL	VAL	MET	THR	SER	ILE	LEU	PRO	GLY	ASP	GLU	ASP	LEU
ALA	ALA	VAL	ASN	LYS	ALA	ASN	SER	ALA	GLY	LEU	ALA	GLU
LEU	LEU	ARG	GLN	GLU	LYS	ARG	TYR	VAL	LYS	GLU	LYS	CYS
SER	SER	CYS	LYS	VAL	LEU	THR	ASN	LEU	SER	PHE	LEU	ASN
GLU	GLU	LYS	LYS	LYS	TYR	ARG	GLU	ASP	ASN	HIS	ILE	LYS
LEU	LEU	ALA	ALA	VAL	GLN	GLY	THR	ALA	HIS	LYS	LYS	VAL
VAL	VAL	GLU	ALA	LEU	LEU	GLU	THR	LYS	VAL	VAL	ASP	MET
GLN	GLN	SER	GLU	GLN	ASP	THR	LYS	ASN	ALA	SER	VAL	CYS
ARG	ARG	THR	MET	ALA	ASP	VAL	SER	ILE	VAL	THR	GLU	ARG
LEU	LEU	GLN	ALA	THR	ASP	ILE	LEU	LYS	ASN	GLY	GLY	PRO
GLU	GLU	ALA	GLU	GLU	GLU	GLU	PHE	SER	MET	ILE	TYR	ASN
GLU	GLU	SER	LEU	LEU	GLU	GLU	GLY	LEU	ASN	TYR	ASN	LEU
LYS	LYS	ASN	LEU	ALA	ILE	GLN	THR	SER	GLY	LEU	GLY	ASN
VAL	VAL	LYS	LYS	VAL	ASN	PHE	GLN	ALA	HIS	ASP	THR	GLU
HIS	HIS	GLU	ILE	ASN	GLN	LEU	ARG	GLY	SER	ILE	ILE	SER
LEU	LEU	MET	LEU	TYR	GLN	LYS	ALA	GLY	SER	ILE	PHE	GLU
ASN	ASN	GLU	GLU	ASN	GLN	GLU	LYS	ASN	ARG	ALA	VAL	ASN
GLU	GLU	GLU	ALA	GLN	GLN	ALA	THR	ILE	HIS	LEU	GLY	ARG
GLU	GLU	GLU	GLY	SER	VAL	LEU	LYS	ASN	SER	LEU	GLN	GLY
HIS	HIS	LYS	ILE	GLN	GLU	LEU	ASN	ALA	ILE	ASP	THR	ASP
LEU	LEU	ALA	ALA	GLU	LYS	GLU	THR	LEU	PHE	VAL	THR	LYS
ASN	ASN	LEU	VAL	VAL	LEU	ALA	VAL	ALA	LEU	SER	SER	TYR
LYS	LYS	ALA	GLY	GLU	LYS	PHE	CYS	GLU	ILE	LYS	GLY	ILE
VAL	VAL	ALA	ASN	GLU	VAL	THR	VAL	GLY	ASN	THR	LYS	ALA
GLN	GLN	CYS	ASN	LYS	GLN	VAL	ASN	THR	LYS	LEU	THR	LYS
THR	THR	GLN	ASP	THR	MET	GLN	VAL	THR	LYS	LEU	HIS	PHE
ALA	ALA	LEU	VAL	LYS	GLU	LYS	GLU	TYR	GLN	SER	THR	GLN
ASN	ASN	ARG	LYS	GLU	ASP	ASP	LEU	VAL	GLU	VAL	MET	GLY
GLU	GLU	ILE	GLN	TYR	GLN	ILE	THR	PRO	ASN	HIS	GLU	ASP
VAL	VAL	SER	PRO	GLU	GLU	THR	ALA	TYR	THR	GLU	GLY	ASP
GLN	GLN	GLY	GLY	LEU	GLU	THR	GLU	ARG	GLN	ASN	LYS	LEU
ALA	ALA	GLU	GLY	SER	LEU	THR	GLN	SER	GLU	ASN	HIS	VAL
VAL	VAL	ALA	GLY	ASP	ALA	ASP	LYS	LYS	GLN	ARG	ASP	ILE
GLU	GLU	LYS	MET	GLU	SER	LYS	LYS	MET	LYS	VAL	PRO	ALA
GLN	GLN	ILE	ILE	ASN	THR	PRO	TYR	THR	LEU	PRO	GLU	SER
GLN	GLN	LYS	ASP	ASN	ARG	ALA	TYR	ARG	GLY	TYR	GLY	LYS
ILE	ILE	GLU	GLU	GLN	ARG	THR	GLU	ILE	GLY	VAL	MET	PRO
THR	THR	LEU	GLU	LYS	ASP	ALA	LYS	LEU	LYS	PHE	GLY	TYR
HIS	HIS	THR	PHE	SER	GLN	ILE	GLY	GLN	LEU	GLY	ILE	ALA
ARG	ARG	GLU	THR	ALA	ASN	VAL	GLY	ASP	TYR	CYS	ILE	PHE
GLU	GLU	LEU	VAL	LEU	ASN	GLY	GLU	THR	GLU	THR	PRO	ASP
GLU	GLU	ALA	ALA	LEU	ILE	ILE	GLU	VAL	VAL	GLU	ARG	ARG
HIS	HIS	ASN	LEU	ASN	ALA	ASN	ASN	GLY	ASN	PHE	VAL	PHE
GLN	GLN	VAL	TYR	ILE	ILE	PHE	ILE	ASN	GLN	VAL	GLN	GLN
LYS	LYS	GLU	ILE	ASP	LEU	THR	LEU	CYS	GLY	ASP	ASP	SER
GLN	GLN	GLN	SER	ALA	ASN	ARG	ARG	LEU	SER	ILE	ILE	SER
ILE	ILE	LYS	LYS	GLU	ASN	ALA	ASN	GLU	GLU	PRO	PHE	THR
SER	SER	ARG	MET	LEU	GLN	ARG	THR	ILE	LYS	ASN	THR	SER
SER	SER	LYS	LYS	GLN	ILE	ARG	THR	ILE	VAL	GLU	TYR	GLN
LEU	LEU	GLN	GLU	LYS	THR	THR	GLN	VAL	SER	MET	ILE	GLU
PC	PC	THR	THR	THR	GLU	ARG	THR	THR	LYS	THR	THR	GLN



• Molecule 3: Tubulin alpha-1B chain



• Molecule 4: Kif5b Tail



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	633952	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.033	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	259.91998, 259.91998, 259.91998	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.083, 1.083, 1.083	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: MG, ANP, GTP, TA1, GDP

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	B	0.19	0/3426	0.28	0/4641
2	K	0.18	0/2624	0.28	0/3538
2	T	0.16	0/43	0.16	0/57
3	A	0.19	0/3435	0.28	0/4663
4	t	0.12	0/48	0.31	0/64
All	All	0.18	0/9576	0.28	0/12963

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	B	3351	0	3237	51	0
2	K	2585	0	2557	47	0
2	T	43	0	43	0	0
3	A	3358	0	3277	51	0
4	t	47	0	51	3	0
5	B	28	0	12	1	0
6	B	62	0	51	3	0
7	K	31	0	13	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	1	0	0	0	0
8	K	1	0	0	0	0
9	A	32	0	12	0	0
All	All	9539	0	9253	142	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 8.

The worst 5 of 142 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:B:229:HIS:NE2	6:B:502:TA1:O14	2.18	0.77
2:K:123:ASP:O	4:t:926[B]:PRO:HG2	1.88	0.72
3:A:211:ASP:HB3	3:A:215:ARG:HH12	1.55	0.71
2:K:132:VAL:HG22	2:K:210:ILE:HG22	1.79	0.65
2:K:210:ILE:HD11	2:K:227:LEU:HD23	1.79	0.64

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	B	424/445 (95%)	416 (98%)	8 (2%)	0	100	100
2	K	328/963 (34%)	323 (98%)	5 (2%)	0	100	100
2	T	4/963 (0%)	4 (100%)	0	0	100	100
3	A	424/451 (94%)	402 (95%)	22 (5%)	0	100	100
4	t	4/6 (67%)	4 (100%)	0	0	100	100
All	All	1184/2828 (42%)	1149 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	B	367/381 (96%)	367 (100%)	0	100	100
2	K	295/854 (34%)	295 (100%)	0	100	100
2	T	4/854 (0%)	4 (100%)	0	100	100
3	A	362/379 (96%)	362 (100%)	0	100	100
4	t	5/5 (100%)	5 (100%)	0	100	100
All	All	1033/2473 (42%)	1033 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	31	GLN
3	A	226	ASN
3	A	380	ASN
2	K	117	ASN
1	B	133	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

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
5	GDP	B	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.83	7 (15%)
6	TA1	B	502	-	68,68,68	0.67	1 (1%)	105,105,105	1.15	9 (8%)
9	GTP	A	501	8	33,34,34	0.80	1 (3%)	50,54,54	1.56	8 (16%)
7	ANP	K	1001	8	33,33,33	1.72	4 (12%)	45,52,52	1.68	10 (22%)

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
5	GDP	B	501	-	-	3/16/32/32	0/3/3/3
6	TA1	B	502	-	-	8/41/127/127	0/7/7/7
9	GTP	A	501	8	-	8/22/38/38	0/3/3/3
7	ANP	K	1001	8	-	3/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	1001	ANP	PA-O3A	-6.93	1.52	1.59
7	K	1001	ANP	PB-O3A	-4.87	1.53	1.59
5	B	501	GDP	C5-C4	3.02	1.47	1.38
7	K	1001	ANP	O5'-C5'	-2.96	1.33	1.44
5	B	501	GDP	C6-N1	-2.62	1.33	1.38

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	GDP	C5-C4-N3	-6.76	117.64	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	501	GTP	C5-C4-N3	-5.43	119.75	128.39
5	B	501	GDP	C2-N3-C4	5.41	121.62	112.30
6	B	502	TA1	O08-C20-C21	-5.23	113.00	119.28
5	B	501	GDP	N9-C4-N3	5.15	136.25	125.95

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

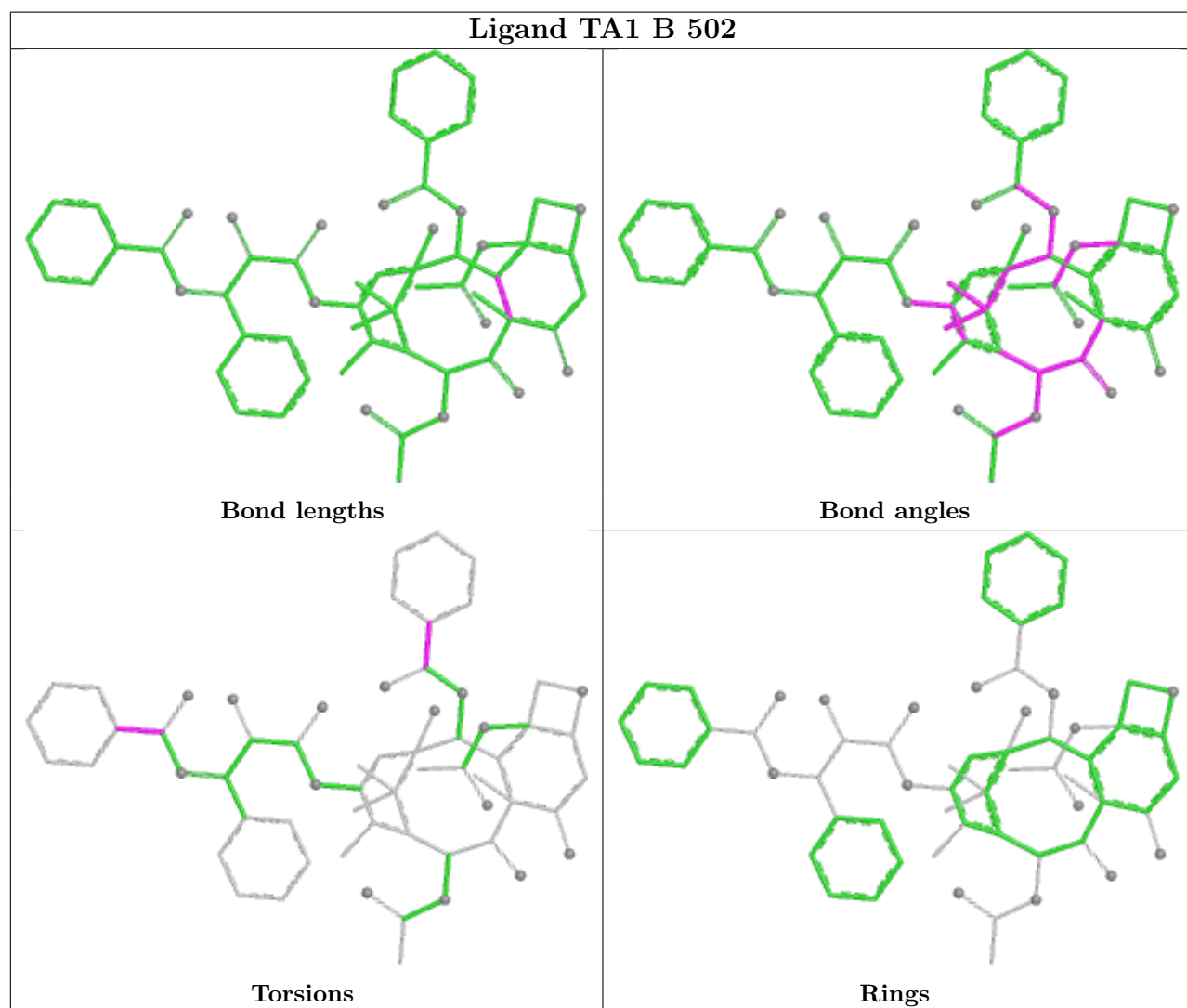
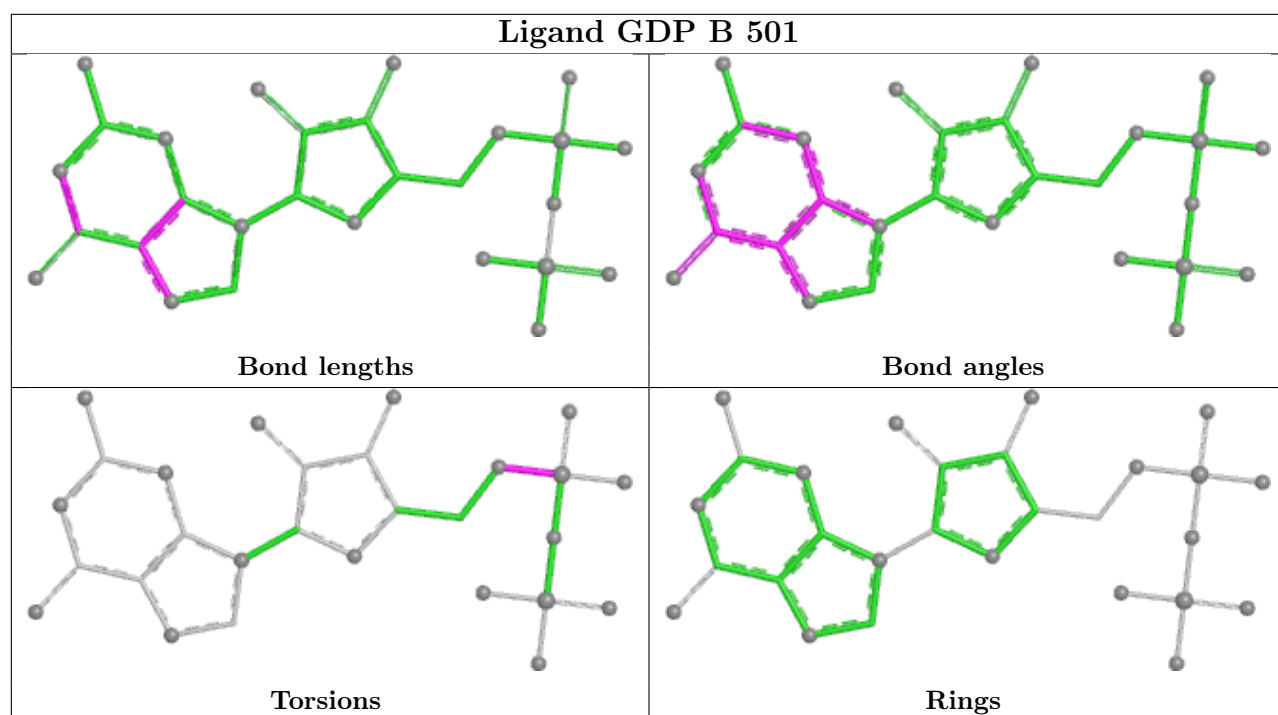
Mol	Chain	Res	Type	Atoms
5	B	501	GDP	C5'-O5'-PA-O3A
5	B	501	GDP	C5'-O5'-PA-O1A
5	B	501	GDP	C5'-O5'-PA-O2A
7	K	1001	ANP	PB-N3B-PG-O1G
7	K	1001	ANP	PG-N3B-PB-O1B

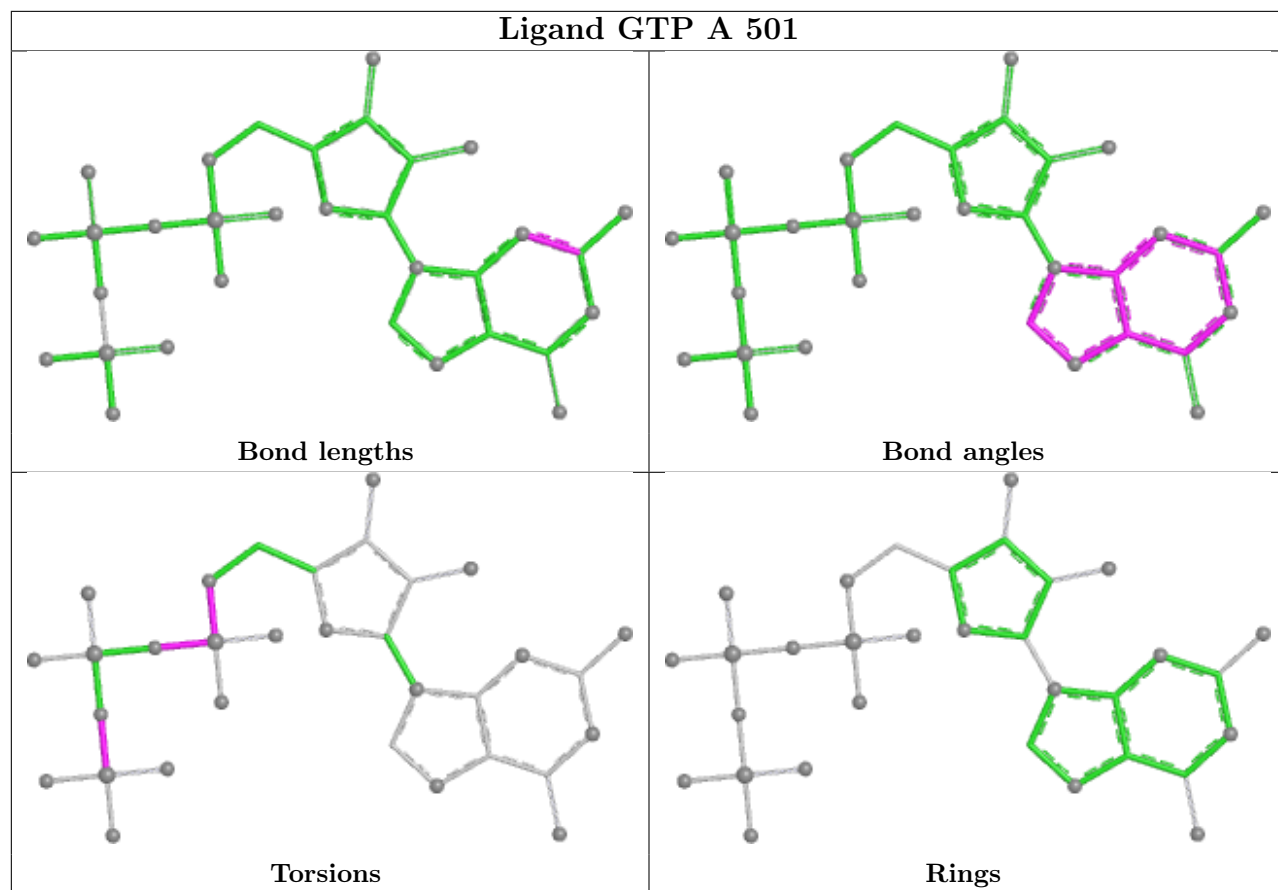
There are no ring outliers.

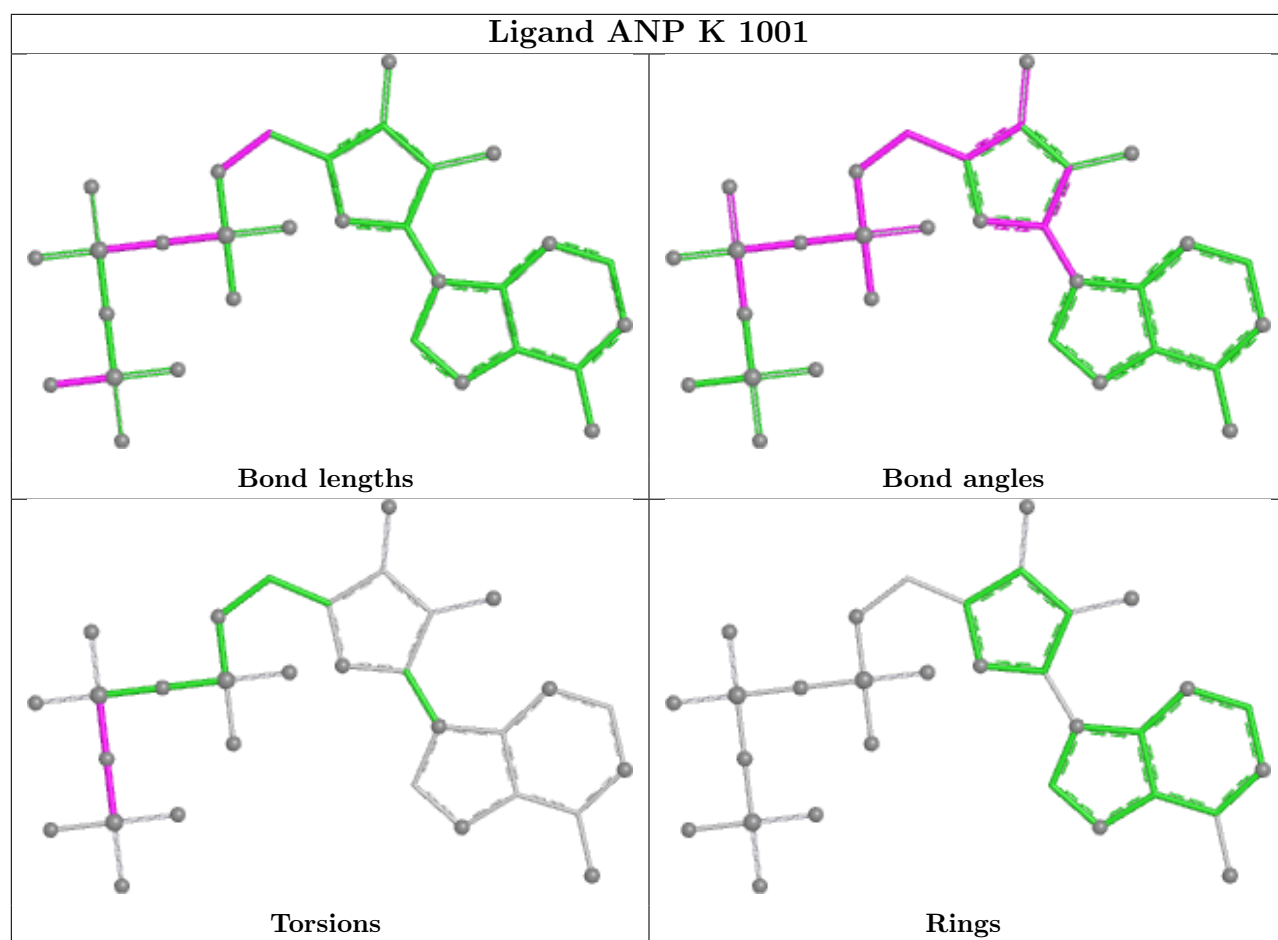
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	GDP	1	0
6	B	502	TA1	3	0
7	K	1001	ANP	3	0

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.

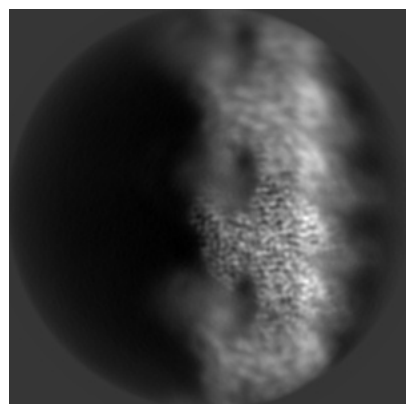
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19174. These allow visual inspection of the internal detail of the map and identification of artifacts.

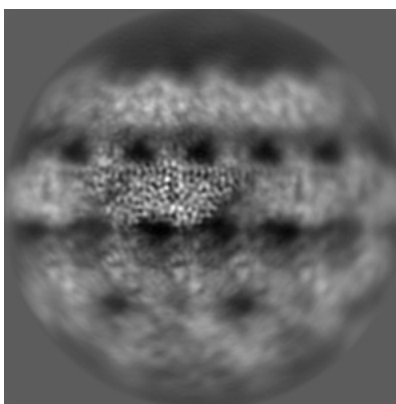
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

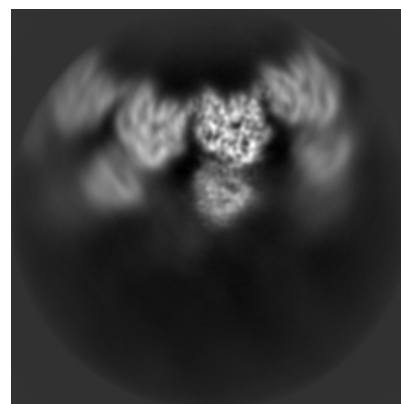
6.1.1 Primary map



X

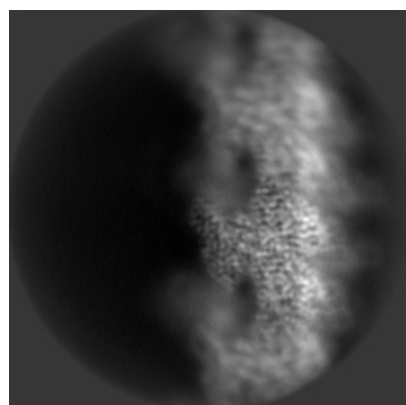


Y

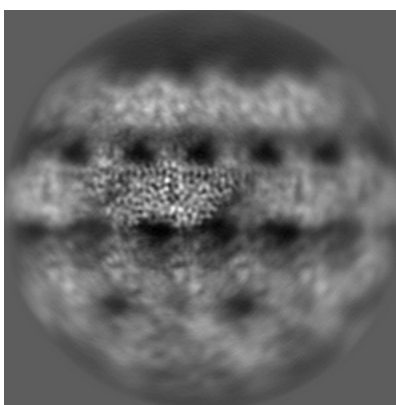


Z

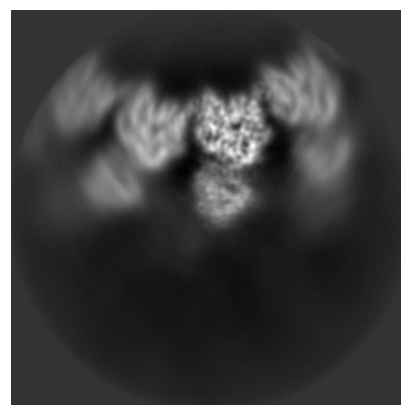
6.1.2 Raw map



X



Y

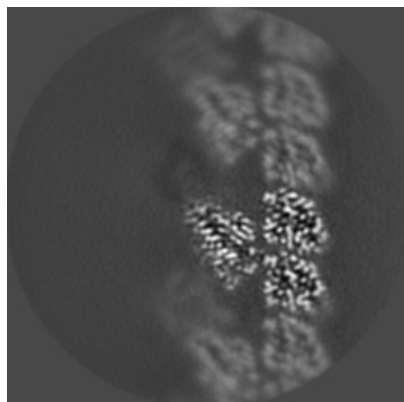


Z

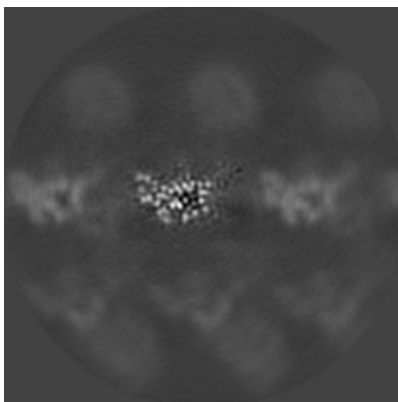
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

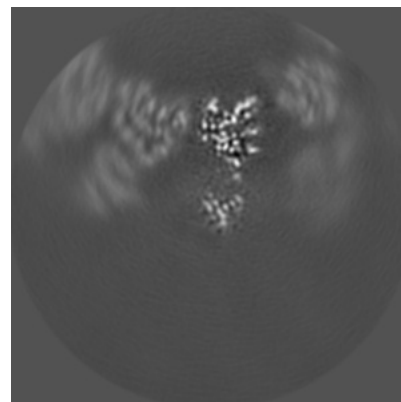
6.2.1 Primary map



X Index: 120

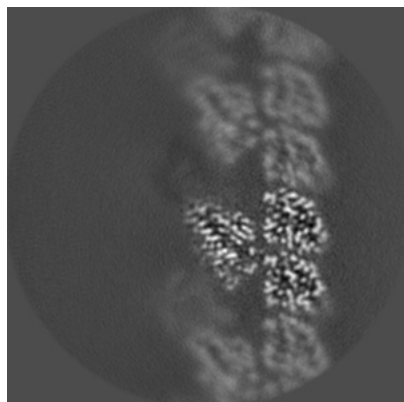


Y Index: 120

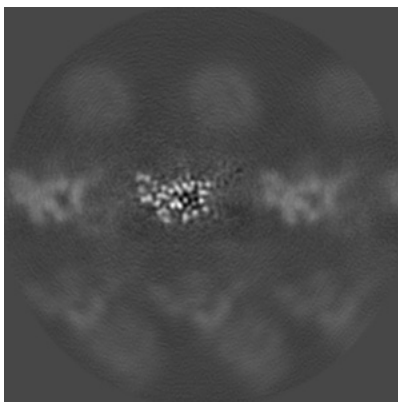


Z Index: 120

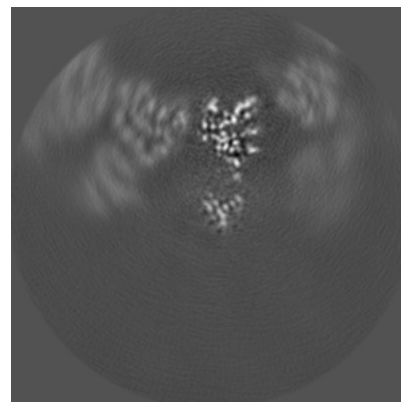
6.2.2 Raw map



X Index: 120



Y Index: 120

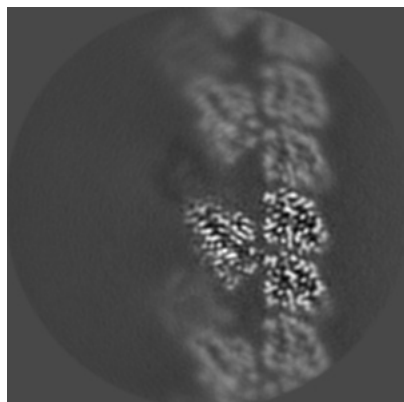


Z Index: 120

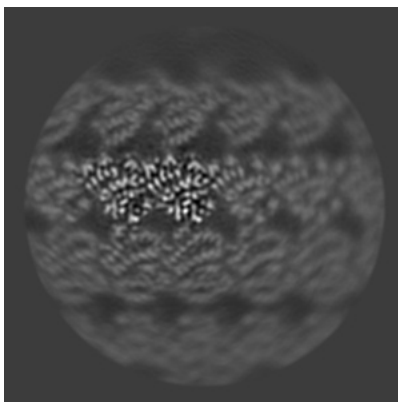
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

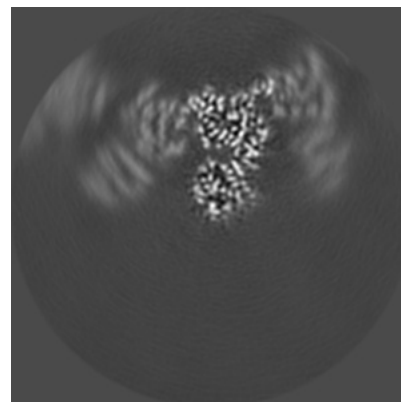
6.3.1 Primary map



X Index: 120

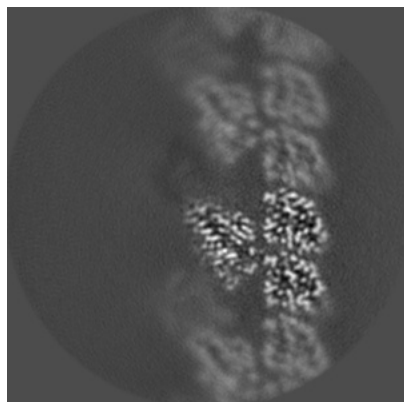


Y Index: 176

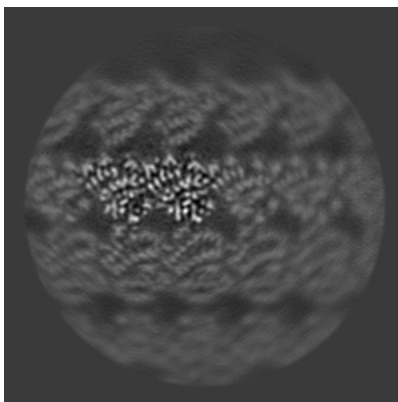


Z Index: 105

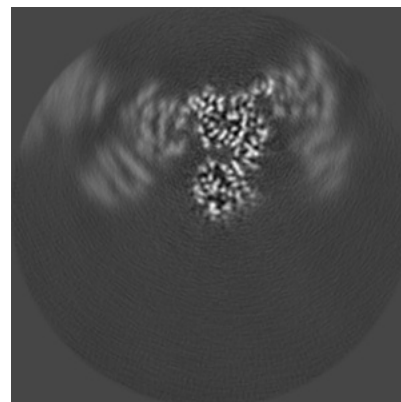
6.3.2 Raw map



X Index: 120



Y Index: 176

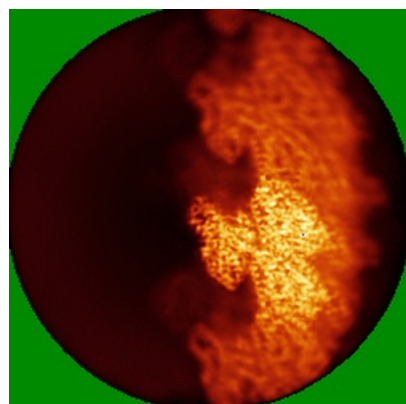


Z Index: 105

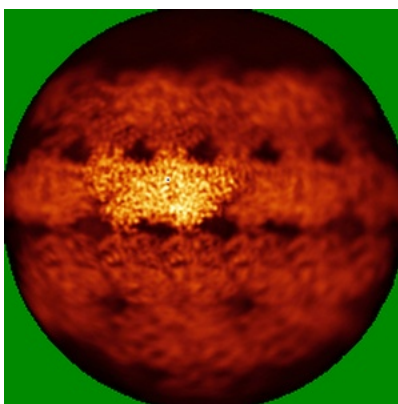
The images above show the largest variance slices of the map in three orthogonal directions.

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

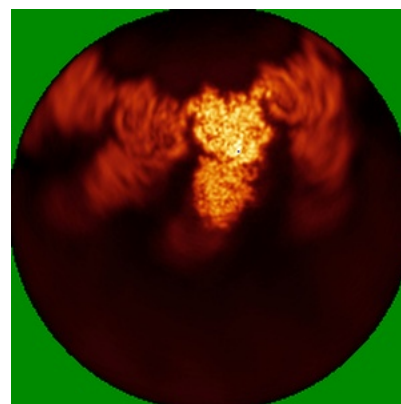
6.4.1 Primary map



X

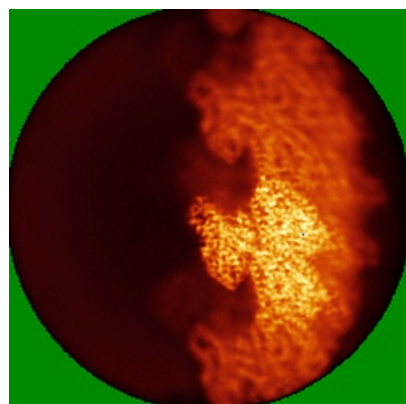


Y

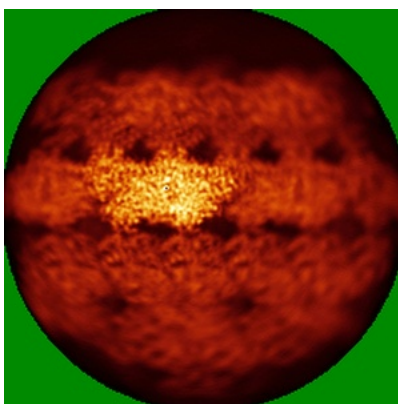


Z

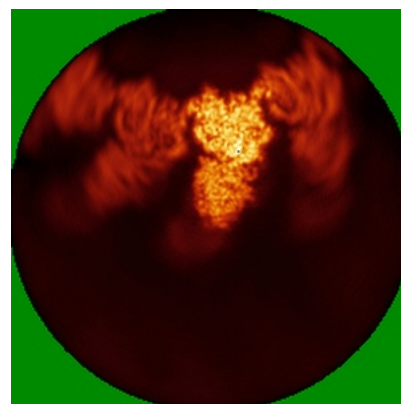
6.4.2 Raw map



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.

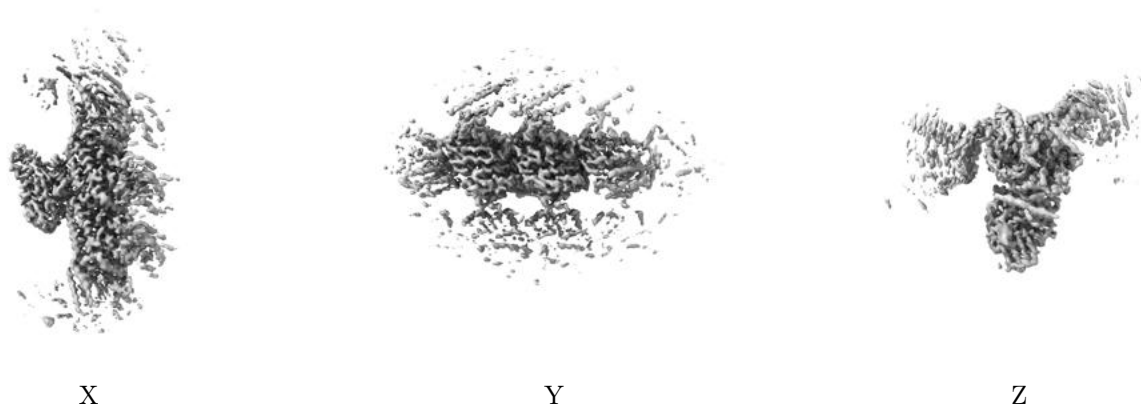
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. 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.

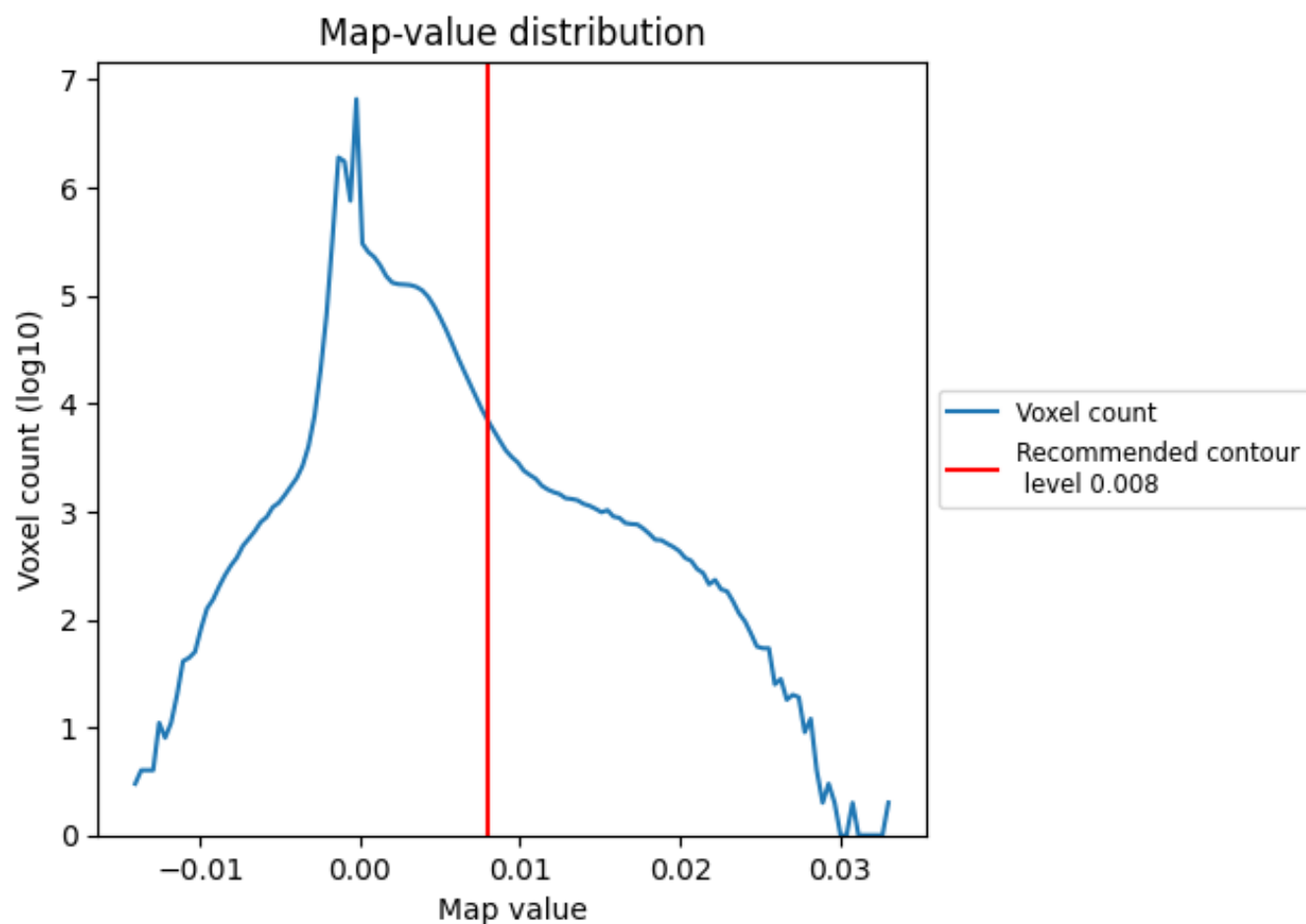
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

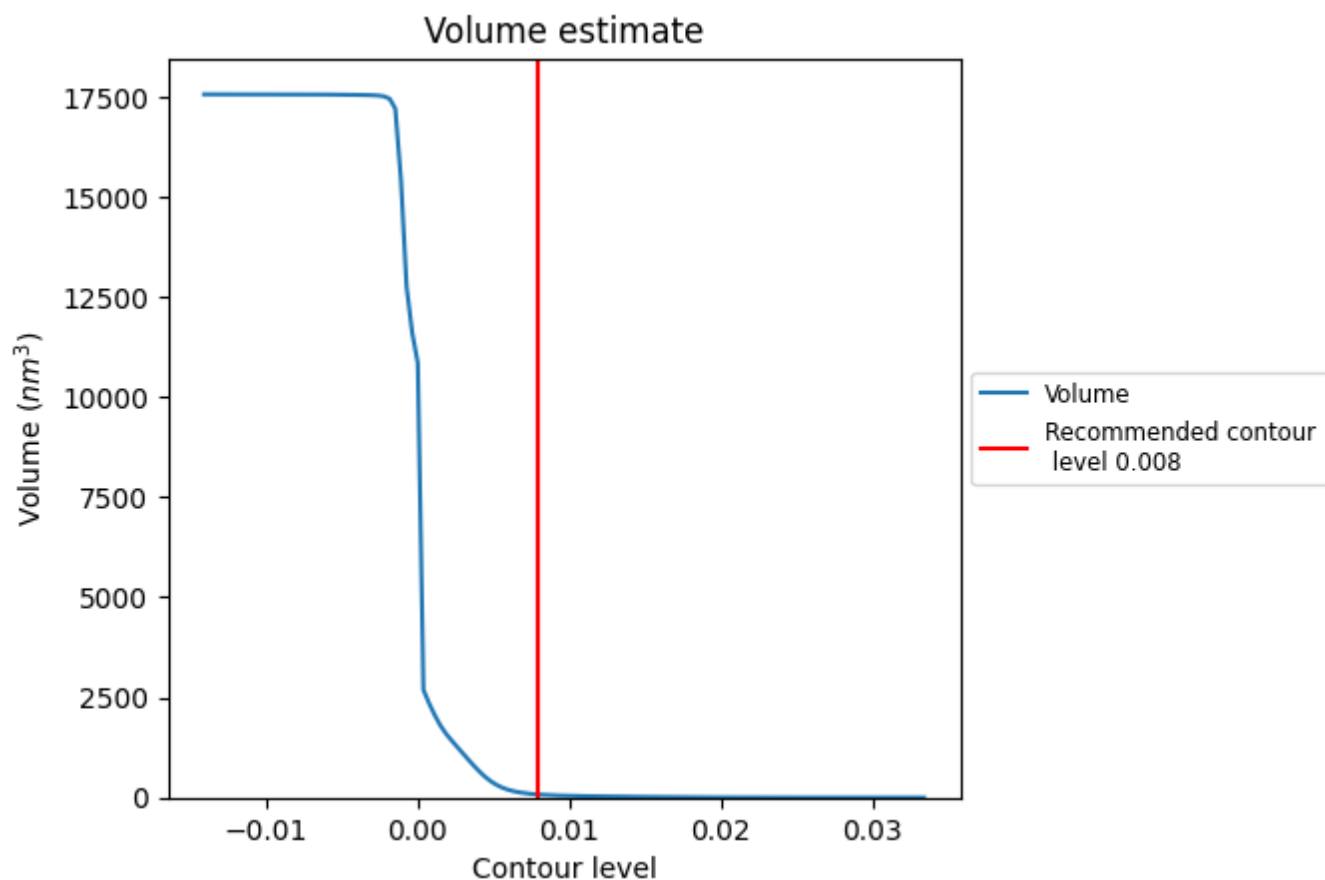
This section contains the results of statistical analysis of the map.

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.

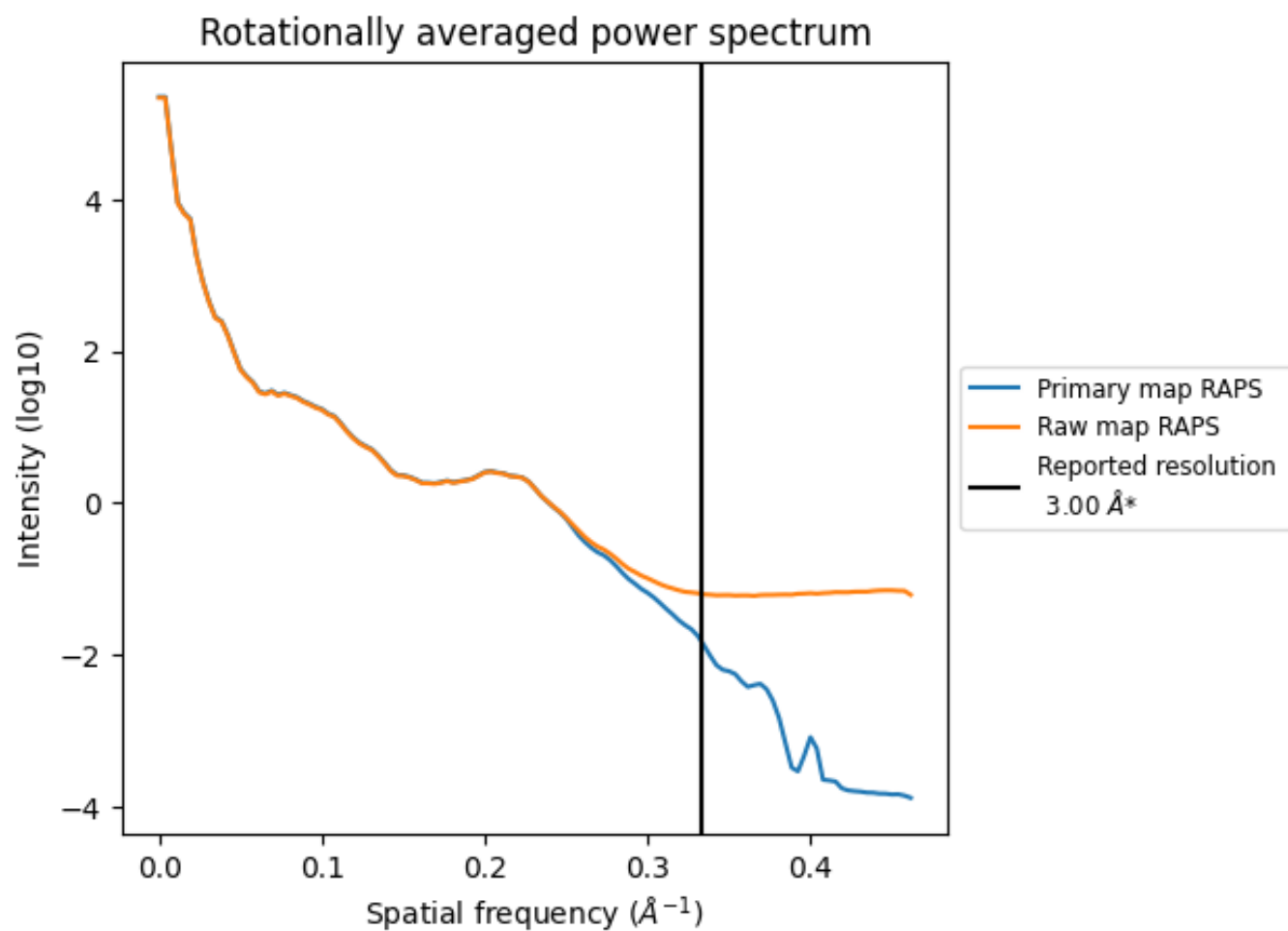
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 76 nm³; this corresponds to an approximate mass of 69 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 ⓘ

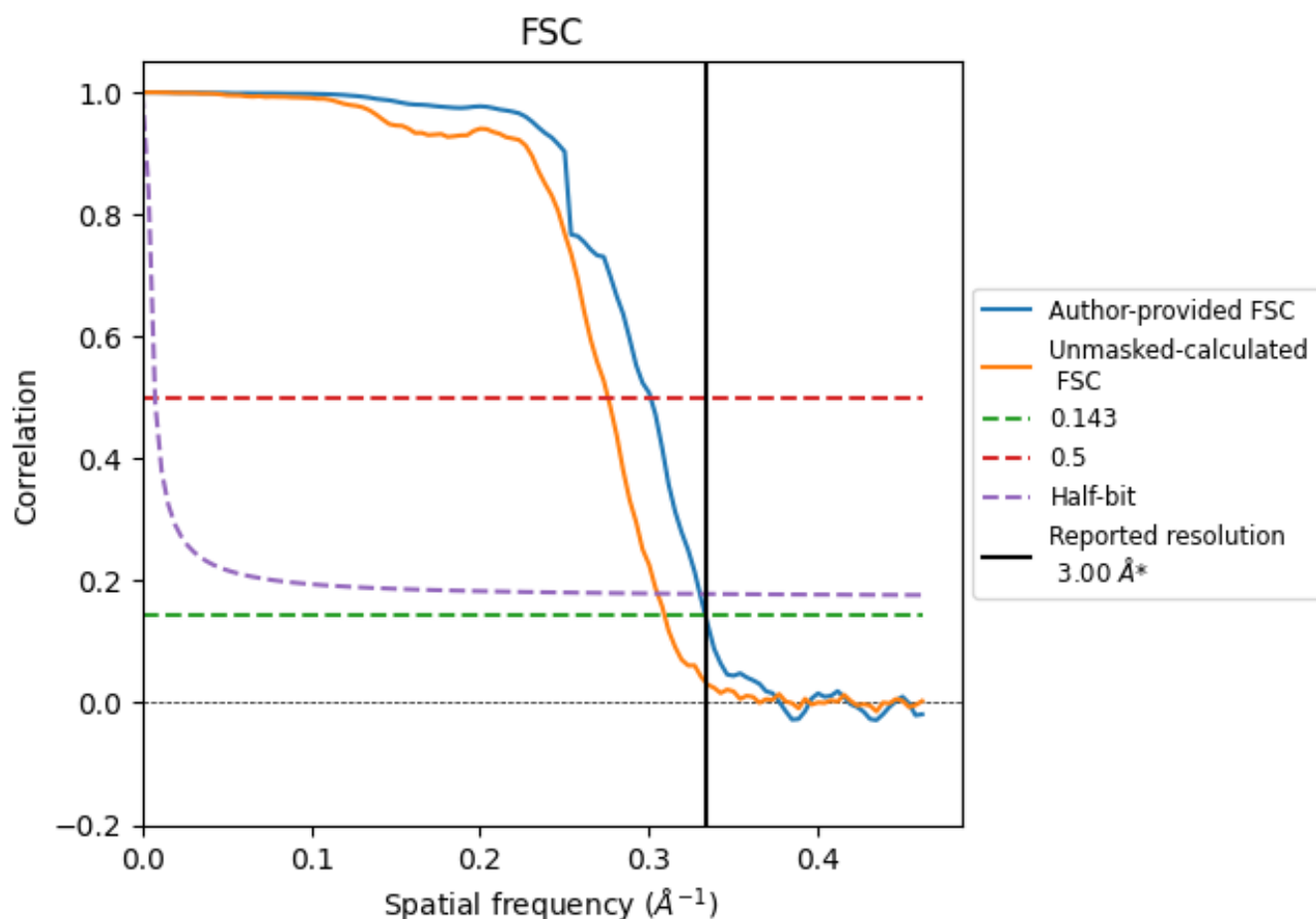


*Reported resolution corresponds to spatial frequency of $0.333 \text{ \AA}^{-1}$

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

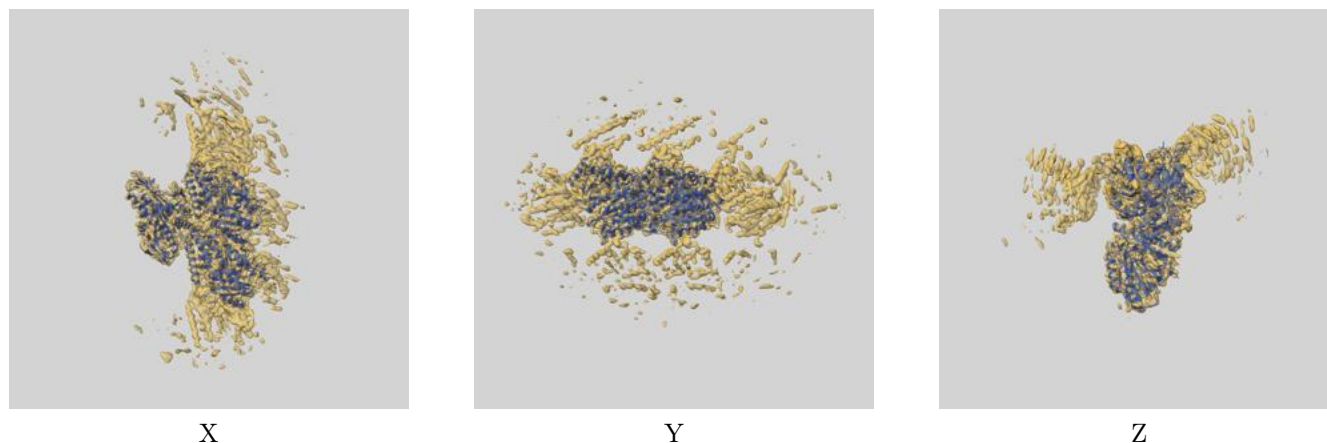
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.00	3.32	3.03
Unmasked-calculated*	3.23	3.63	3.28

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

9 Map-model fit [i](#)

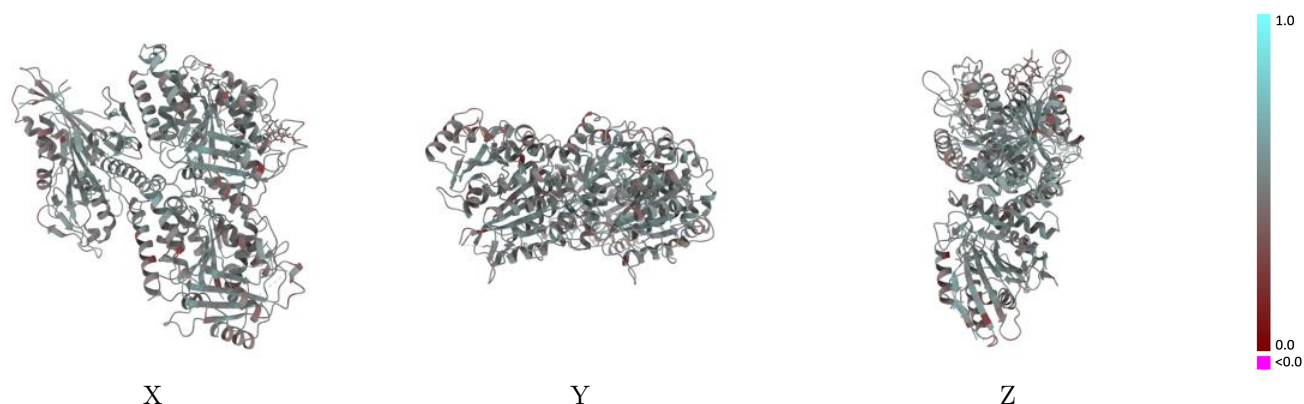
This section contains information regarding the fit between EMDB map EMD-19174 and PDB model 8RHB. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



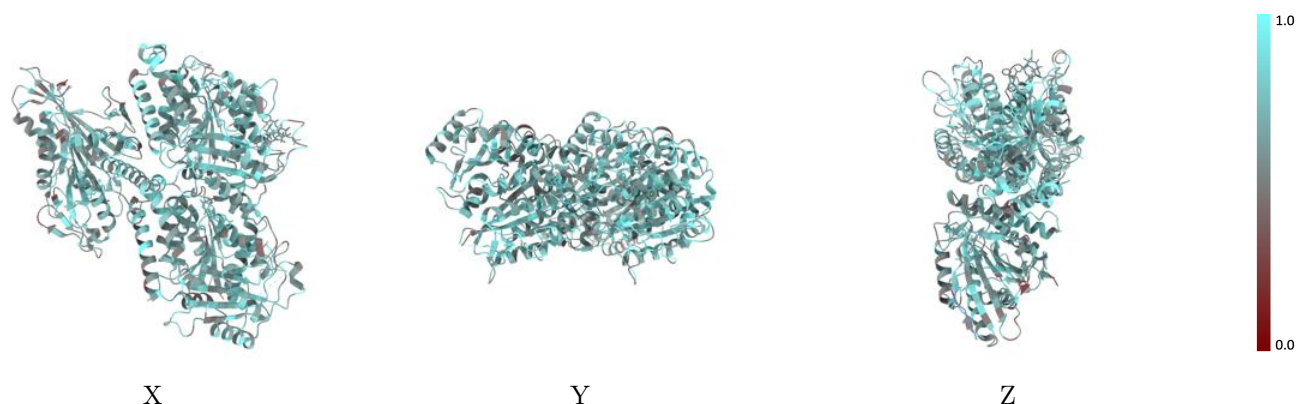
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



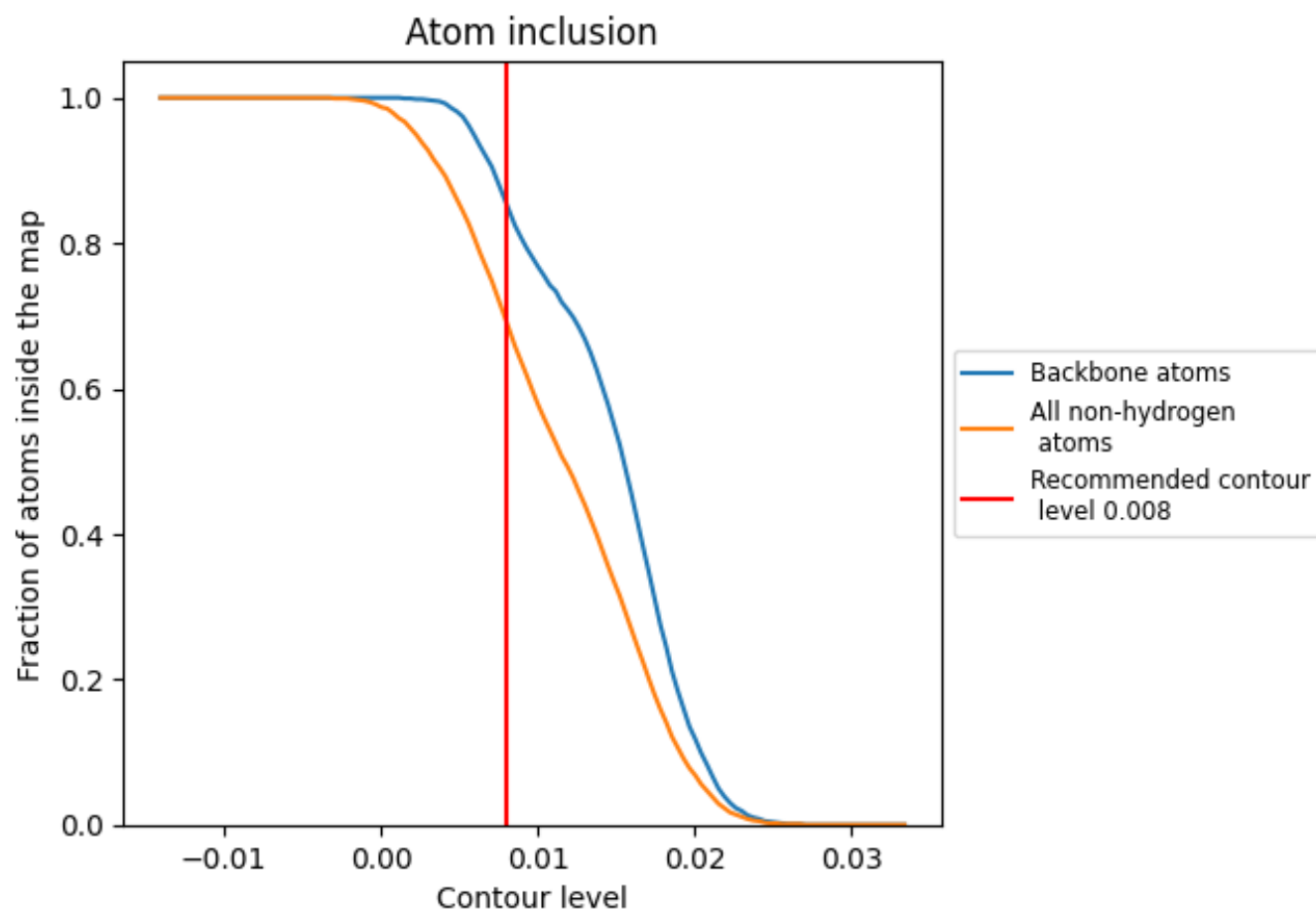
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 69% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6930	0.4950
A	0.6950	0.4910
B	0.7150	0.5020
K	0.6640	0.4920
T	0.4420	0.5090

