



## wwPDB EM Validation Summary Report ⓘ

Dec 16, 2024 – 09:34 PM EST

PDB ID : 5UCY  
EMDB ID : EMD-8539  
Title : Cryo-EM map of protofilament of microtubule doublet  
Authors : Ichikawa, M.; Liu, D.; Kastritis, P.L.; Basu, K.; Bui, K.H.  
Deposited on : 2016-12-22  
Resolution : 4.60 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

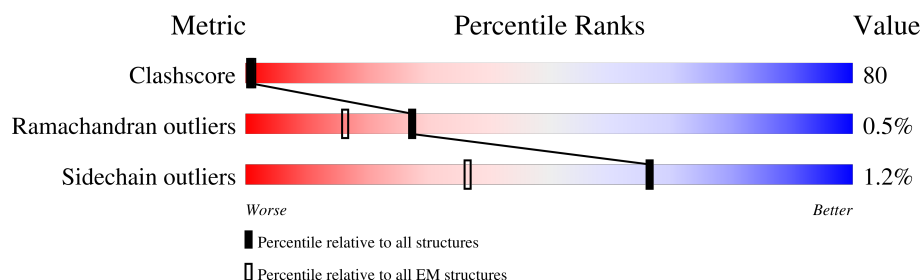
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

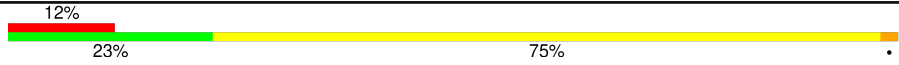

The reported resolution of this entry is 4.60 Å.

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	441	
2	B	429	

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
3	GTP	A	501	-	-	X	-
5	GDP	B	501	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8338 atoms, of which 1492 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.

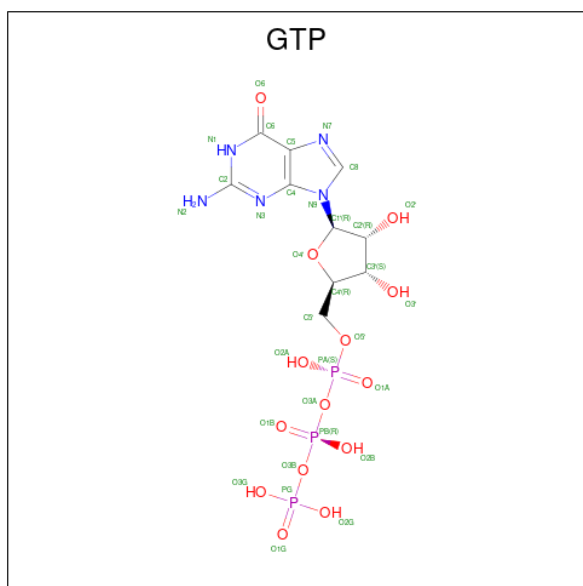
- Molecule 1 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	441	4165	2163	742	581	657	22	0	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	429	4104	2112	742	576	646	28	0	0

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

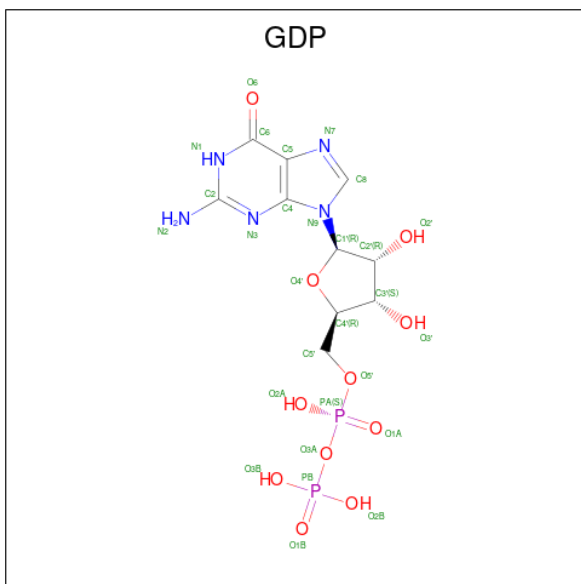


Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
3	A	1	35	10	3	5	14	3	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Mg 1 1	0

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$ ).



Mol	Chain	Residues	Atoms						AltConf
5	B	1	Total	C	H	N	O	P	0
			33	10	5	5	11	2	



Q375	E376	M377	F378	K379	R380	V381	A382			F385	T386	A387	M388	F389	R390	R391	K392	A393	F394	L395			Y398	T399	G400	E401	G402	M403	D404	E405	M406	E407	F408	T409	E410	A411	E412	S413	M414	M415			L418	V419	S420	E421	Y422			Q426	D427	A428	T429								
A315	L316	F317	R318	G319	K320	M321	S322	T323	K324	E325	V326	D327	E328	Q329	M330	L331	N332	V333	Q334	N335	K336	N337	S338	S339	Y340	F341	V342	E343	N344	I345	P346	N347	N348	I349	K350	S351	S352	I353	C354	N355	I356	P357	P358	K359	G360	L361	K362	M363	A364	V365	T366	F367	V368	G369	N370	S371	T372	A373	I374		
A254	V255	N256	L257	I258	P259	F260	P261	R262	L263	H264	F265	F266	M267	I268	G269	F270	A271	P272	L273	T274	S275	R276	G277	S278	Q279	Q280	Y281	R282	A283	L284	V285	V286	P287	E288	L289	T290	Q291	Q292	M293	F294	D295	A296	K297	N298	M299	M300	C301	A302	A303	D304	P305	R306			R309	Y310	L311	T312	A313	S314	
L192	V193	E194	N195	A196	D197	E198	C199	M200	V201	I202	D203	N204	E205	A206	L207	Y208	D209	I210	C211	F212	R213	T214	L215	K216	L217	T218	Y222	G223	D224	L225	N226	H227	L228	V229	S230	A231	A232	M233	S234	G235	V236	T237	C238	C239	L240	R241	F242	P243	G244	Q245	L246	N247	S248	D249	L250	R251	K252	L253			
C129	L130	Q131	G132	F133	Q134	I135	T136	H137	S138	V139	D140	G141	G142	E143	T143	G144	S145	G146	M147	C148	T149	L150	L151	I152	S153	K154	V155	R156	E157	E158	Y159	P160	D161	R162	I163	M164	E165	T166	F167	S168	V169	V170	P171	S172	P173	K174	V175			V180	E181	P182	Y183	N184	A185	T186	L187	S188	V189	H190	Q191
I64	L65	M66	D67	L68	E69	P70	G71	T72	M73	D74	S75	V76	R77	A78	G79	P80	S81	F81	G82	Q83	L84	F85	R86	P87	D88	N89	F90	V91	F92	G93			G96	A97	G98	N99	N100	W101	A102	K103	G104	H105	Y106	T107	E108	G109	A110	E111	L112	I113	V116	V120	E123	A124	E125	G126	C127	D128			

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23	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 ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.146	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	266.75, 266.75, 266.75	wwPDB
Map dimensions	194, 194, 194	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.375, 1.375, 1.375	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: GTP, MG, 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	A	0.58	1/3495 (0.0%)	0.61	0/4735
2	B	0.55	0/3435	0.66	3/4648 (0.1%)
All	All	0.57	1/6930 (0.0%)	0.64	3/9383 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	35	GLN	C-N	-8.21	1.15	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	252	LYS	CD-CE-NZ	8.19	130.54	111.70
2	B	150	LEU	CA-CB-CG	-5.54	102.55	115.30
2	B	58	ARG	NE-CZ-NH1	5.20	122.90	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	143	GLY	Peptide
2	B	99	ASN	Peptide

## 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	A	3423	742	3353	545	0
2	B	3362	742	3244	558	0
3	A	32	3	9	41	0
4	A	1	0	0	1	0
5	B	28	5	11	20	0
All	All	6846	1492	6617	1078	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 80.

The worst 5 of 1078 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:B:12:CYS:HB2	5:B:501:GDP:C8	1.44	1.52
2:B:12:CYS:SG	5:B:501:GDP:C6	2.05	1.49
2:B:12:CYS:HB2	5:B:501:GDP:N7	1.19	1.46
2:B:12:CYS:SG	5:B:501:GDP:C5	2.08	1.42
1:A:12:GLY:CA	3:A:501:GTP:C5	2.17	1.26

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	A	439/441 (100%)	377 (86%)	59 (13%)	3 (1%)	19	56
2	B	427/429 (100%)	388 (91%)	38 (9%)	1 (0%)	44	78
All	All	866/870 (100%)	765 (88%)	97 (11%)	4 (0%)	27	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	PHE
1	A	344	VAL
1	A	143	GLY
2	B	142	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/371 (100%)	365 (98%)	6 (2%)	58	74
2	B	365/365 (100%)	362 (99%)	3 (1%)	79	84
All	All	736/736 (100%)	727 (99%)	9 (1%)	66	79

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	281	TYR
2	B	332	ASN
1	A	268	MET
1	A	283	HIS
1	A	380	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	335	ASN
2	B	396	HIS
2	B	426	GLN
2	B	414	ASN
2	B	375	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	GTP	A	501	-	29,34,34	1.52	4 (13%)	35,54,54	1.46	7 (20%)
5	GDP	B	501	-	25,30,30	1.54	3 (12%)	30,47,47	1.54	8 (26%)

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
3	GTP	A	501	-	-	9/18/38/38	0/3/3/3
5	GDP	B	501	-	-	4/12/32/32	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	GDP	C5-C6	-4.24	1.39	1.47
3	A	501	GTP	C5-C6	-3.78	1.40	1.47
5	B	501	GDP	PB-O1B	3.51	1.61	1.50
3	A	501	GTP	PG-O1G	3.45	1.61	1.50
5	B	501	GDP	O4'-C1'	2.76	1.44	1.40

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	GDP	C2-N1-C6	-3.28	119.10	125.11
5	B	501	GDP	C8-N7-C5	3.27	108.12	102.55
3	A	501	GTP	C8-N7-C5	3.15	107.91	102.55
3	A	501	GTP	O4'-C1'-N9	3.01	112.74	108.75
3	A	501	GTP	C2-N1-C6	-2.99	119.64	125.11

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	GTP	PB-O3B-PG-O2G
3	A	501	GTP	C5'-O5'-PA-O3A
3	A	501	GTP	C5'-O5'-PA-O2A
3	A	501	GTP	C4'-C5'-O5'-PA
5	B	501	GDP	C5'-O5'-PA-O2A

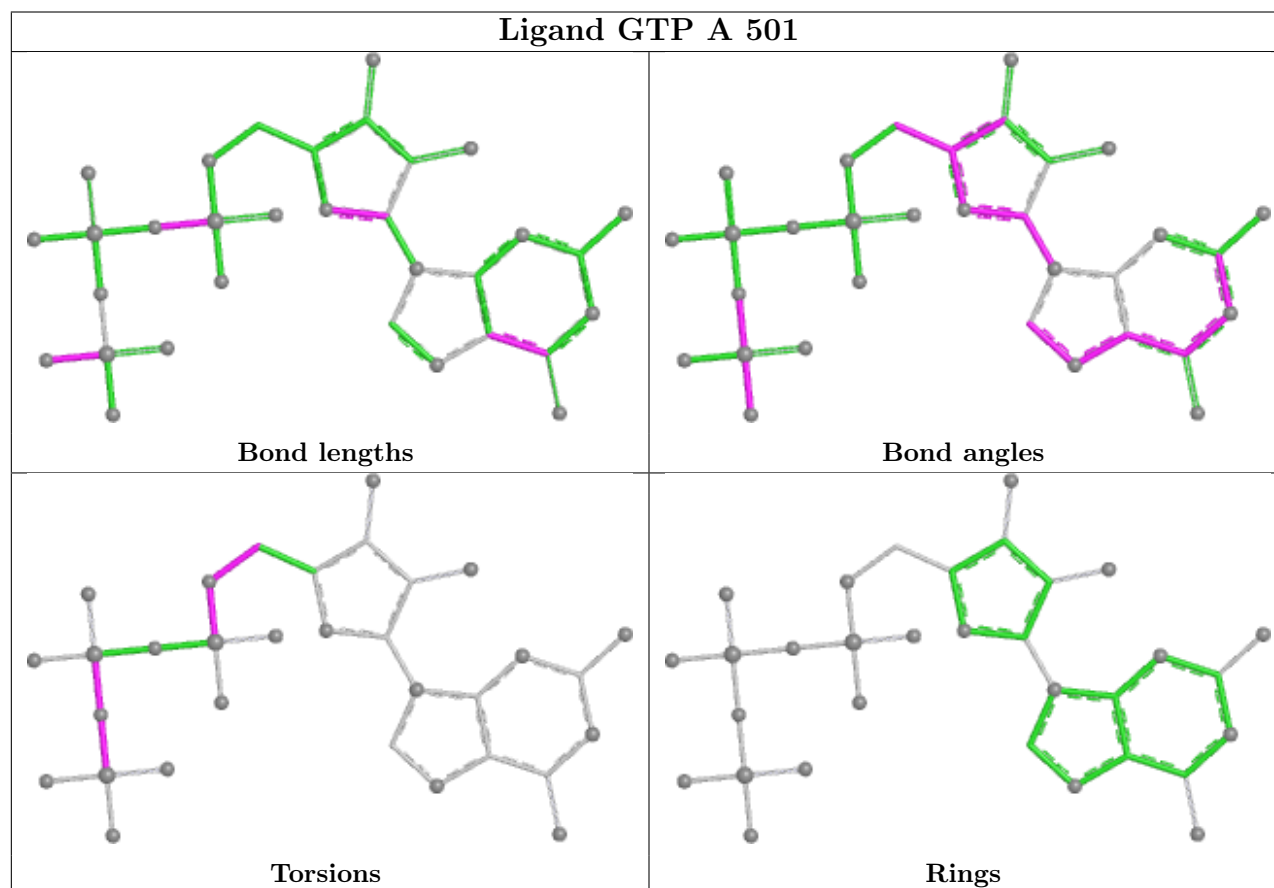
There are no ring outliers.

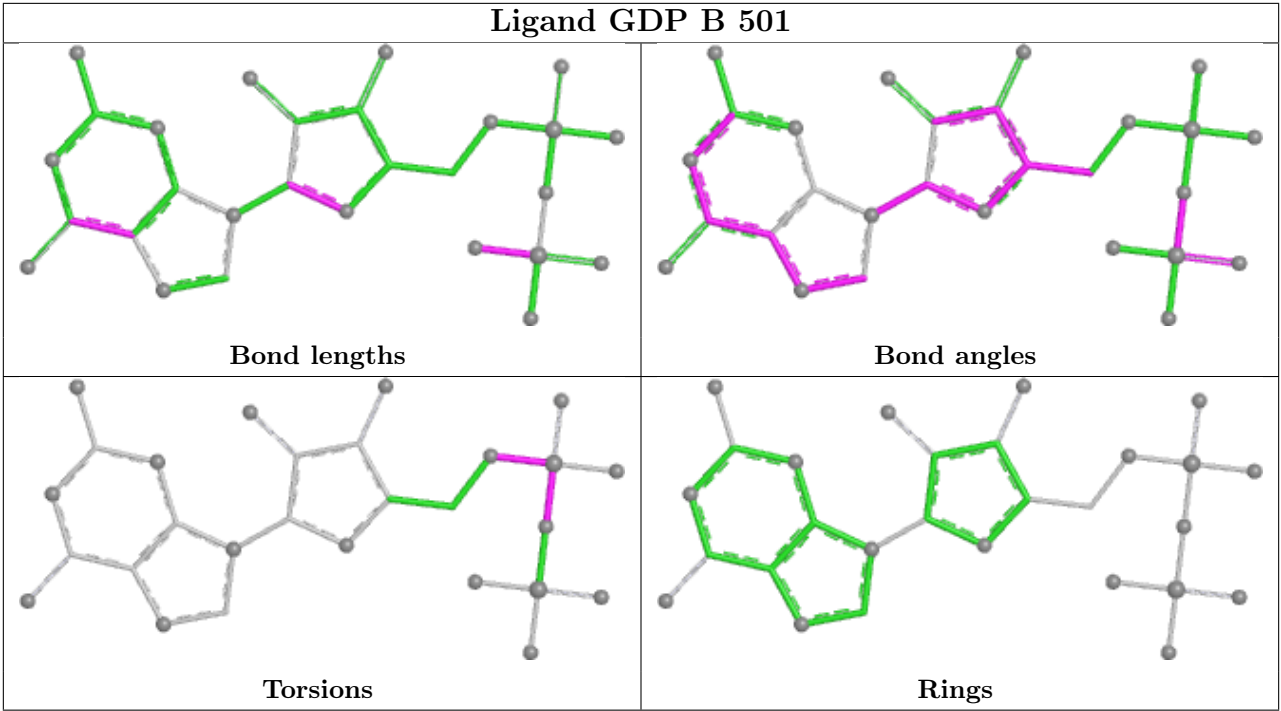
2 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GTP	41	0
5	B	501	GDP	20	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	35:GLN	C	36:MET	N	1.15

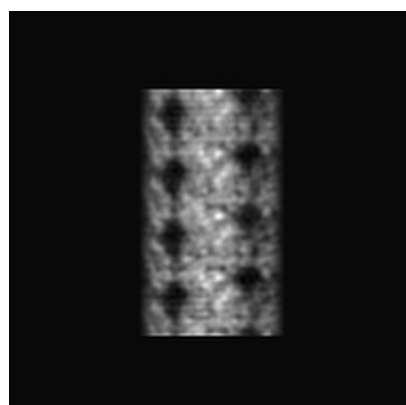
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8539. These allow visual inspection of the internal detail of the map and identification of artifacts.

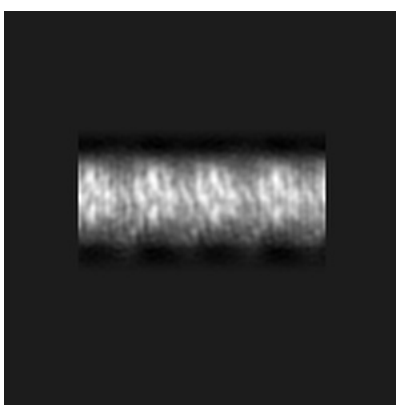
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

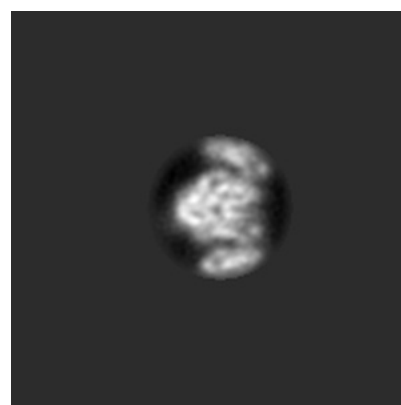
#### 6.1.1 Primary map



X



Y

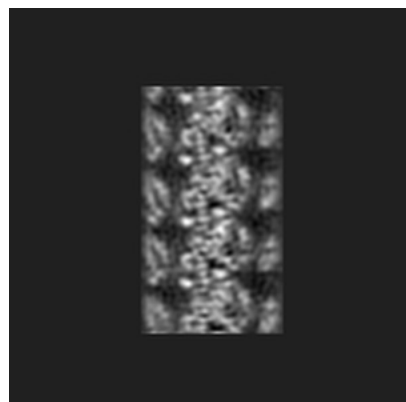


Z

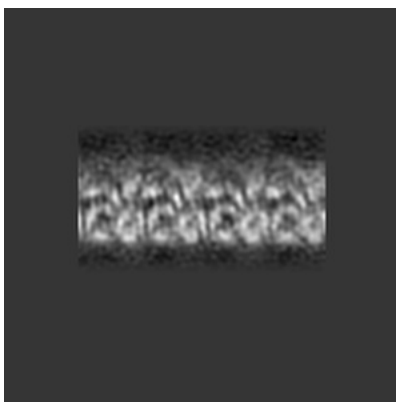
The images above show the map projected in three orthogonal directions.

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

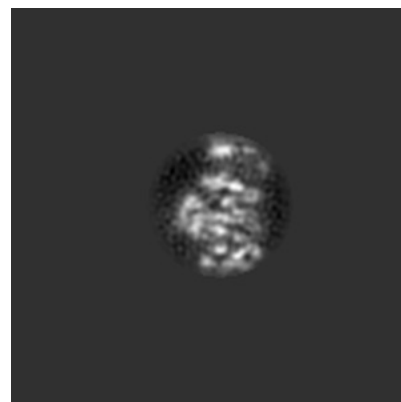
#### 6.2.1 Primary map



X Index: 97



Y Index: 97

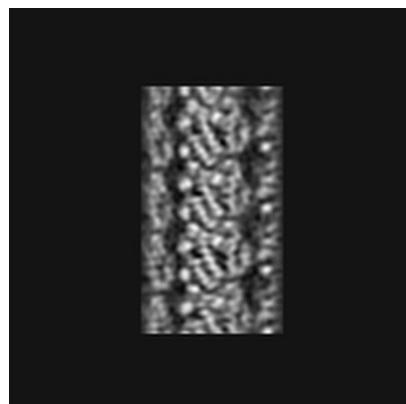


Z Index: 97

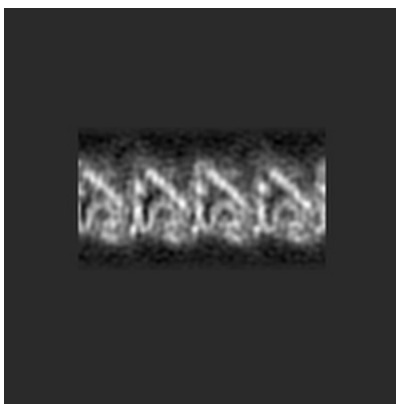
The images above show central slices of the map in three orthogonal directions.

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

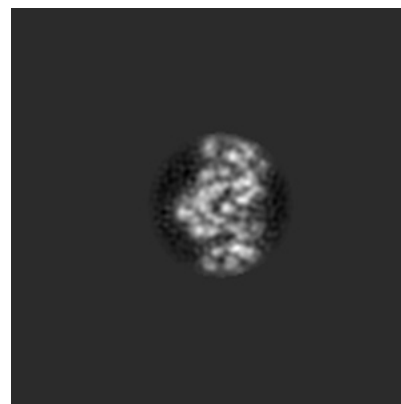
### 6.3.1 Primary map



X Index: 104



Y Index: 101

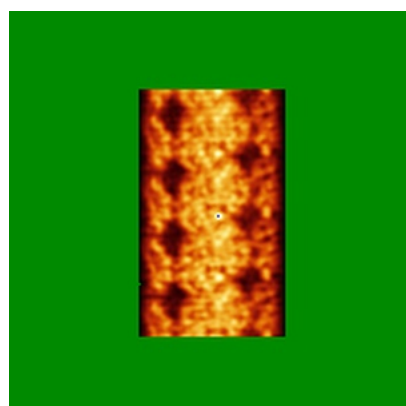


Z Index: 72

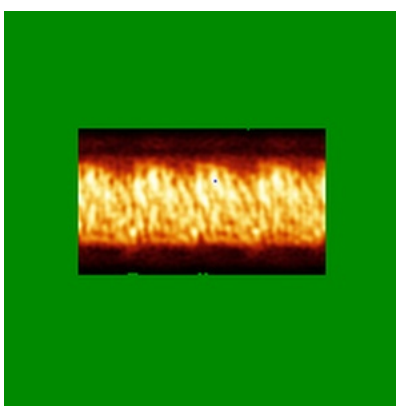
The images above show the largest variance slices of the map in three orthogonal directions.

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

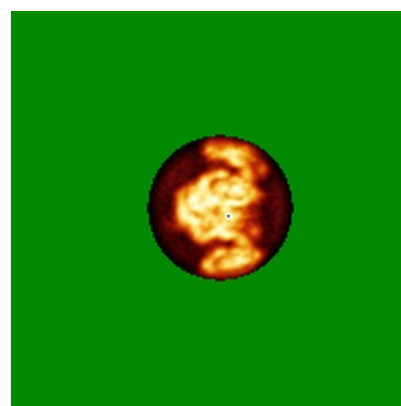
### 6.4.1 Primary map



X



Y



Z

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

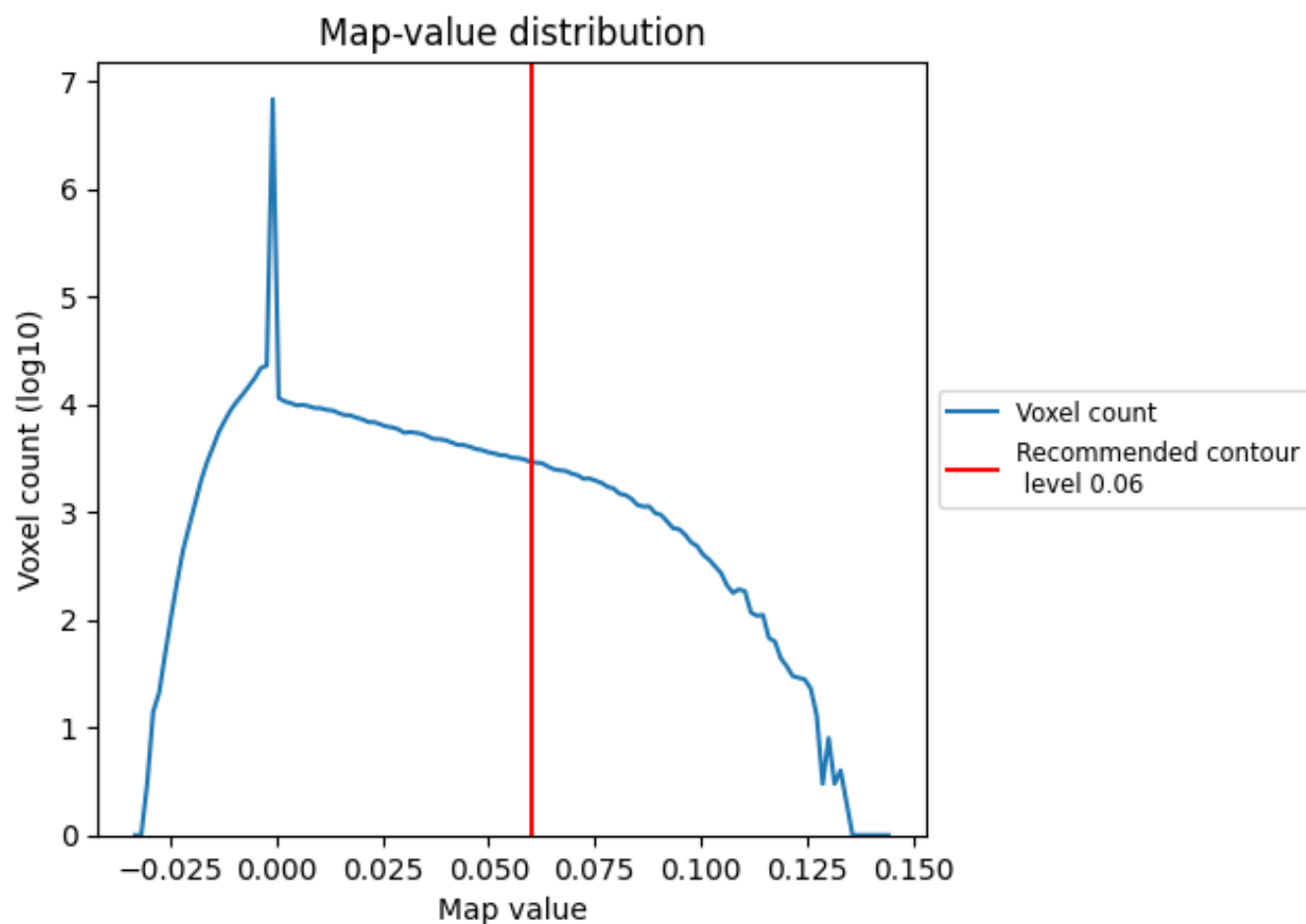
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

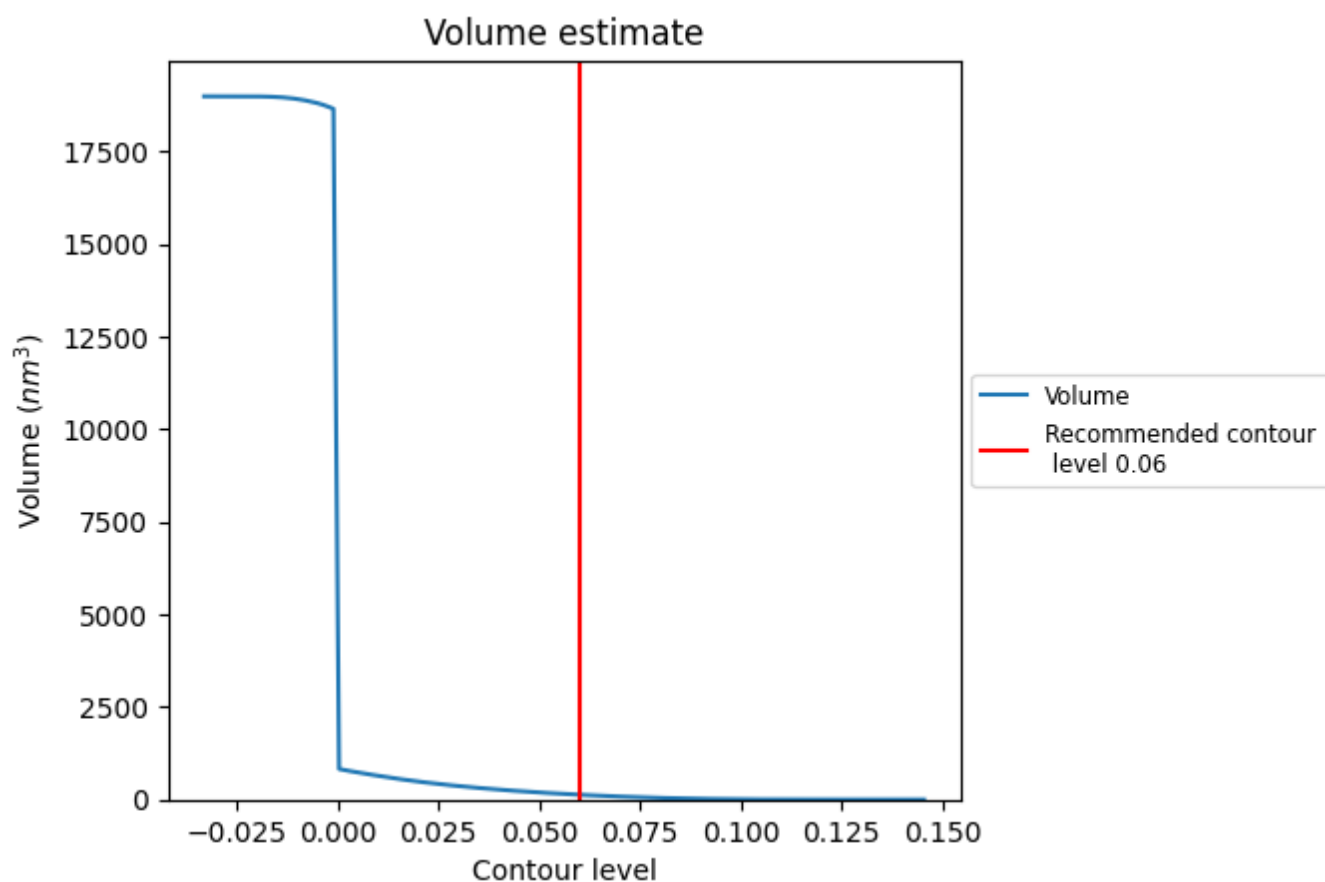
This section contains the results of statistical analysis of the map.

### 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.

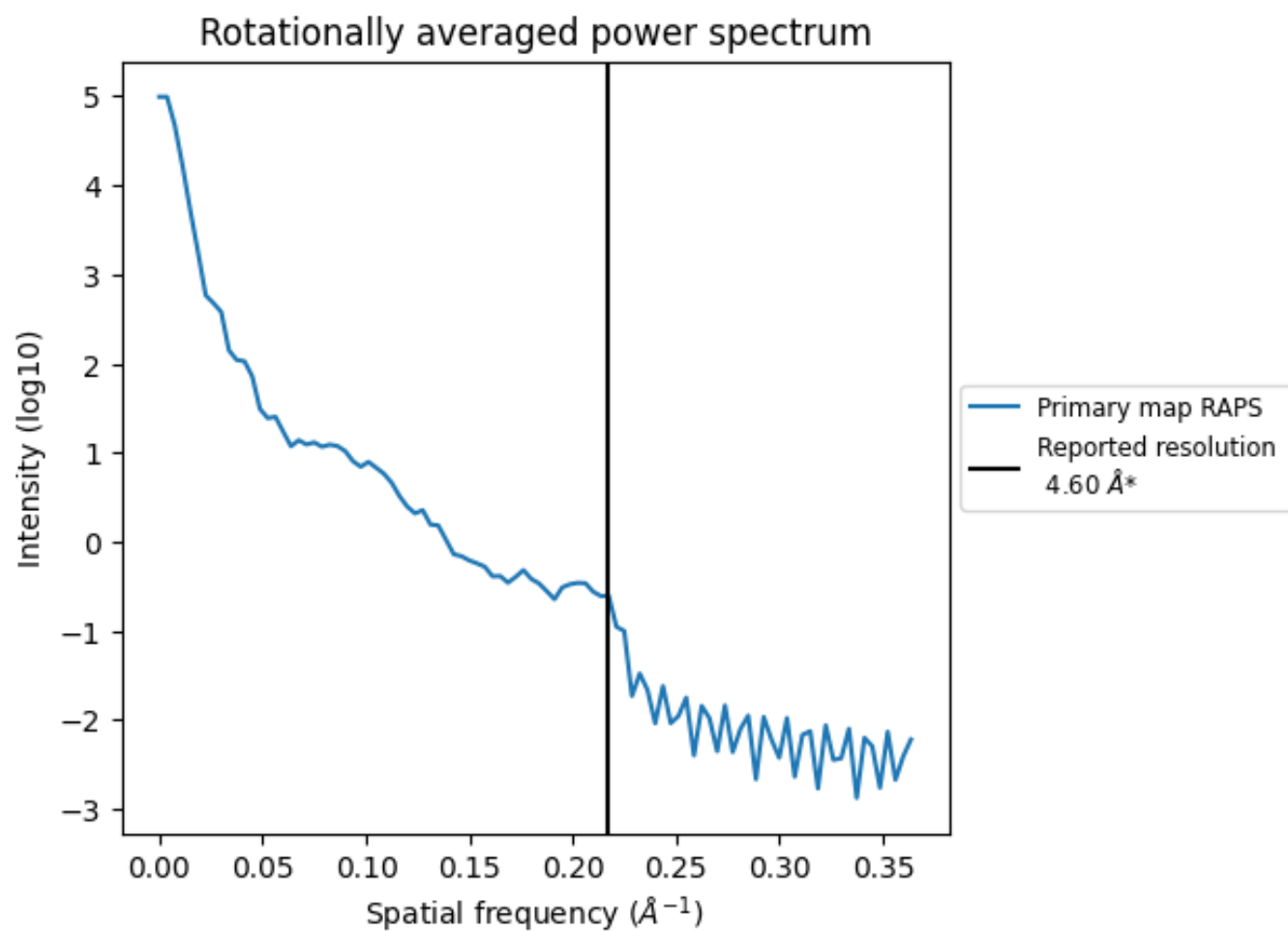
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 130 nm<sup>3</sup>; this corresponds to an approximate mass of 118 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 0.217 Å<sup>-1</sup>

## 8 Fourier-Shell correlation ⓘ

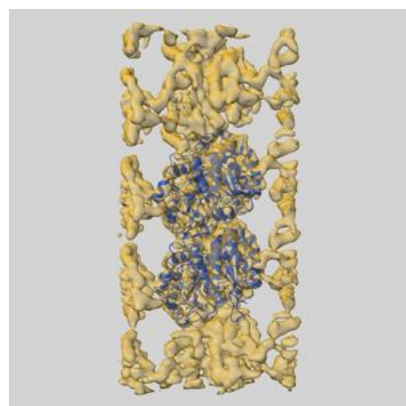
This section was not generated. No FSC curve or half-maps provided.

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

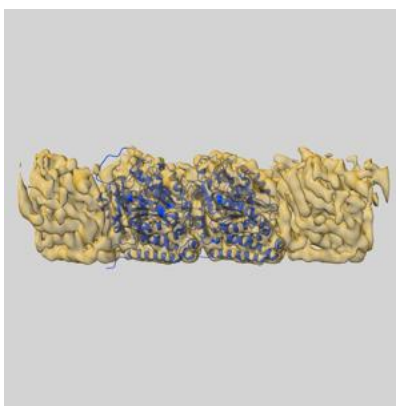
This section contains information regarding the fit between EMDB map EMD-8539 and PDB model 5UCY. Per-residue inclusion information can be found in section 3 on page 5.

### 9.1 Map-model overlays

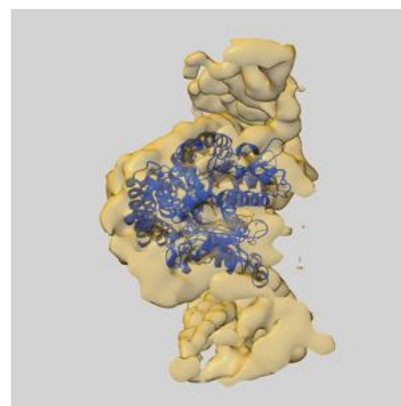
#### 9.1.1 Map-model overlay [i](#)



X

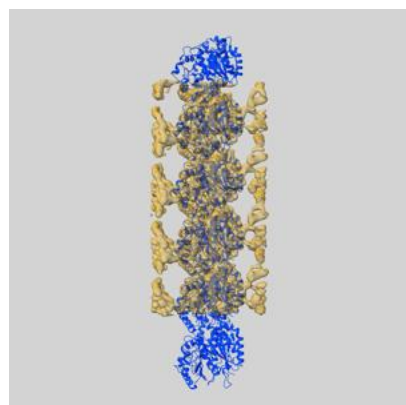


Y

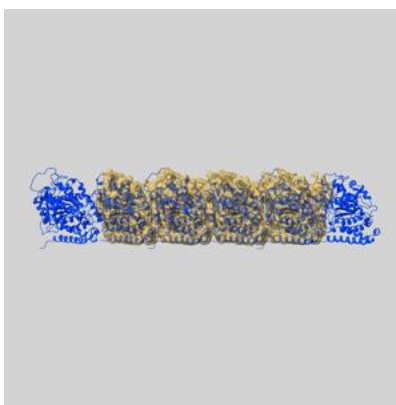


Z

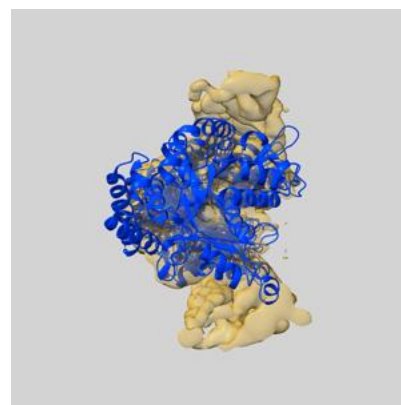
#### 9.1.2 Map-model assembly overlay [i](#)



X



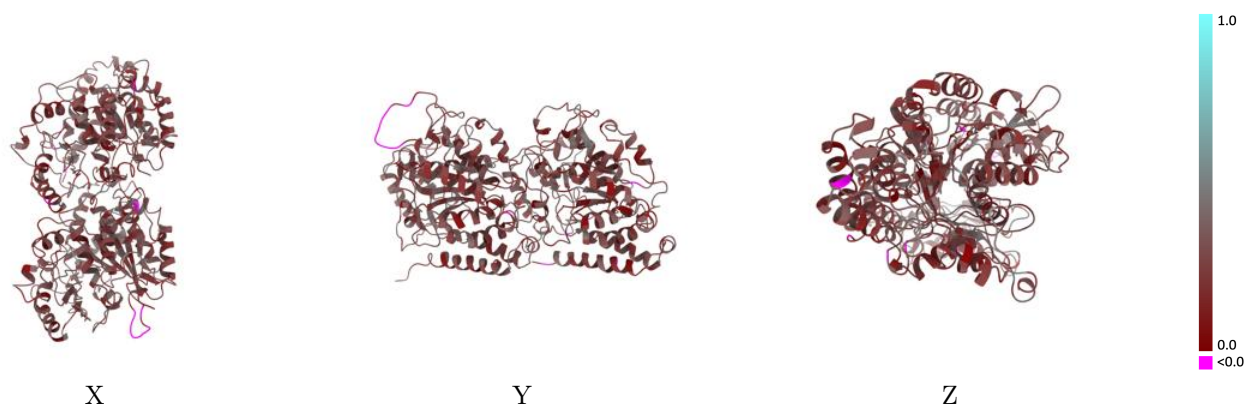
Y



Z

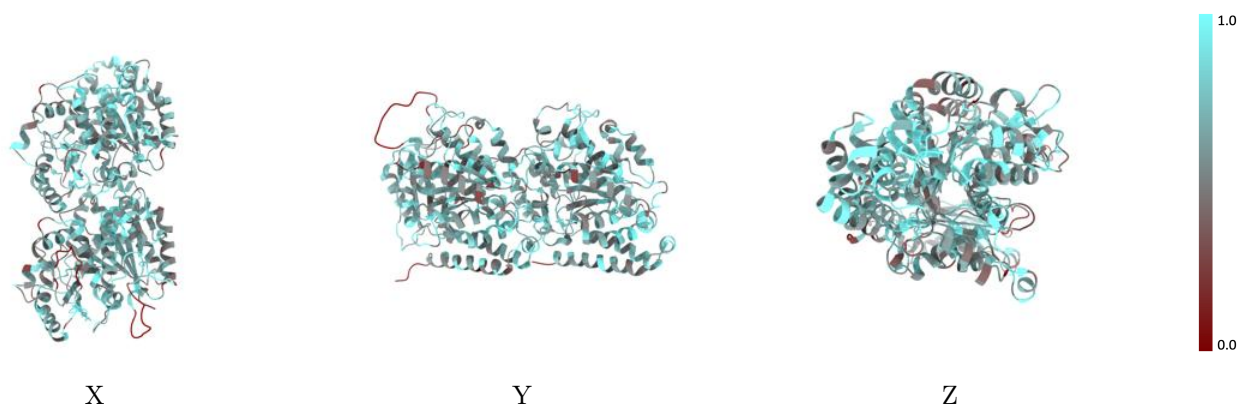
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



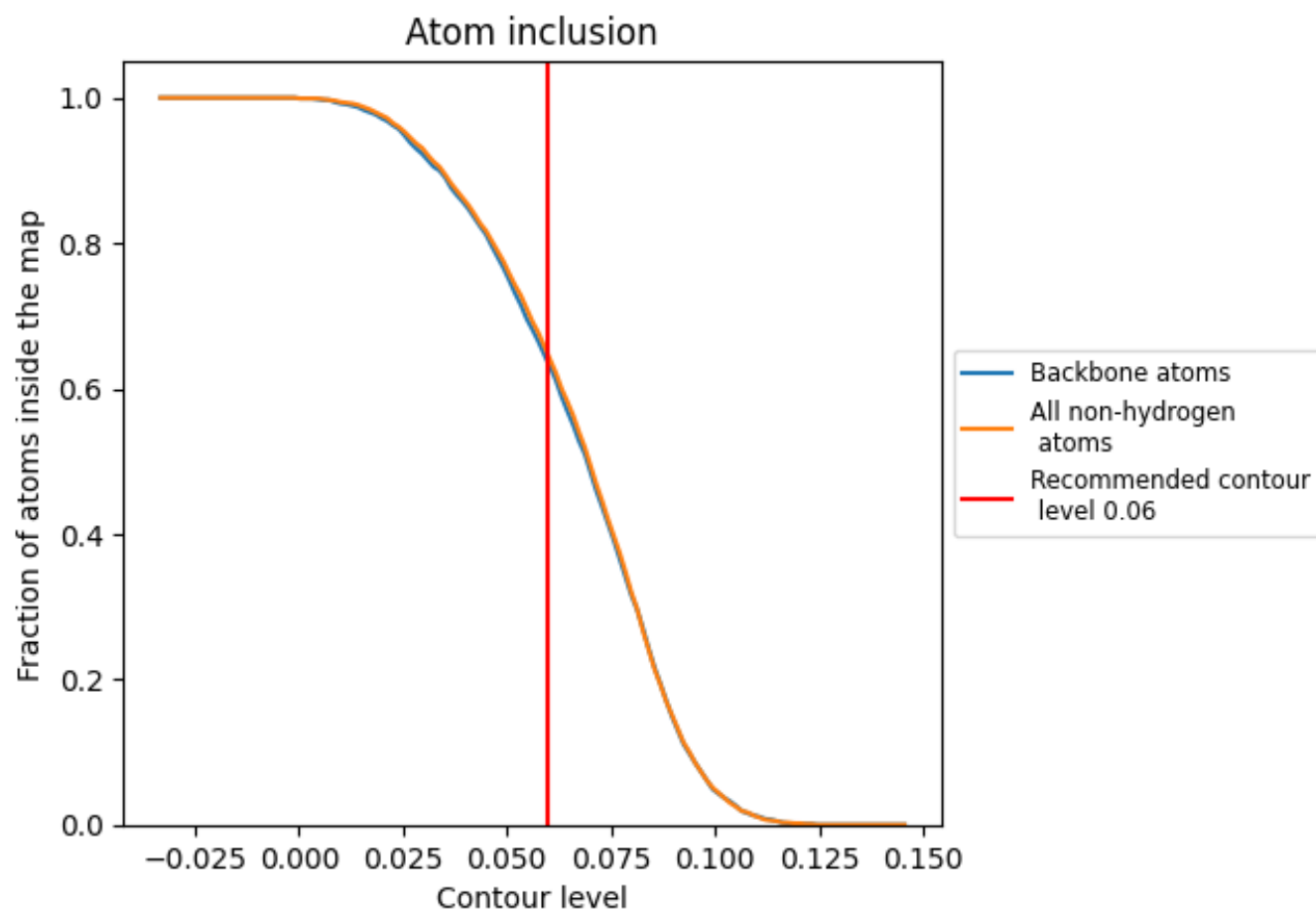
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 64% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6450	<div></div> 0.2640
A	<div></div> 0.6410	<div></div> 0.2650
B	<div></div> 0.6810	<div></div> 0.2630

