



## wwPDB EM Validation Summary Report ⓘ

Apr 22, 2025 – 12:17 PM EDT

PDB ID : 9B62 / pdb\_00009b62  
EMDB ID : EMD-44235  
Title : Human RANBP2/RAN(GTP)/RANGAP1-SUMO1/UBC9/CRM1/RAN(GT  
P) - composite map and model  
Authors : Lima, C.D.; DiMattia, M.A.  
Deposited on : 2024-03-23  
Resolution : 2.90 Å(reported)  
Based on initial models : 3gjsx, 3uin, 4l6e, 1k5d

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.dev117  
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) : 2.42

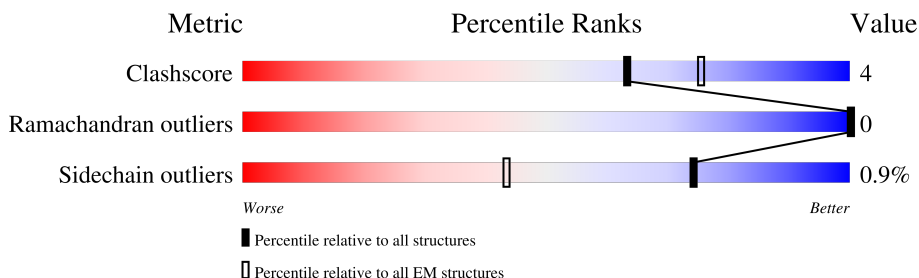
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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	1074	
2	B	222	
2	F	222	
3	C	161	
4	D	101	
5	E	619	
6	G	591	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19287 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 Exportin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1033	Total	C	N	O	S	0	0
			8380	5377	1408	1542	53		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP O14980
A	-1	HIS	-	expression tag	UNP O14980
A	0	MET	-	expression tag	UNP O14980

- Molecule 2 is a protein called GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	173	Total	C	N	O	S	0	0
			1405	914	246	240	5		
2	F	205	Total	C	N	O	S	0	0
			1643	1064	282	291	6		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP P62826
B	-4	SER	-	expression tag	UNP P62826
B	-3	HIS	-	expression tag	UNP P62826
B	-2	MET	-	expression tag	UNP P62826
B	-1	ALA	-	expression tag	UNP P62826
B	0	SER	-	expression tag	UNP P62826
B	69	LEU	GLN	engineered mutation	UNP P62826
F	-5	GLY	-	expression tag	UNP P62826
F	-4	SER	-	expression tag	UNP P62826
F	-3	HIS	-	expression tag	UNP P62826
F	-2	MET	-	expression tag	UNP P62826
F	-1	ALA	-	expression tag	UNP P62826

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	SER	-	expression tag	UNP P62826
F	69	LEU	GLN	engineered mutation	UNP P62826

- Molecule 3 is a protein called SUMO-conjugating enzyme UBC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1251	806	216	222	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P63279
C	-1	SER	-	expression tag	UNP P63279
C	0	HIS	-	expression tag	UNP P63279

- Molecule 4 is a protein called Small ubiquitin-related modifier 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	78	Total	C	N	O	S	0	0
			630	398	108	120	4		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP P63165
D	-2	SER	-	expression tag	UNP P63165
D	-1	HIS	-	expression tag	UNP P63165
D	0	MET	-	expression tag	UNP P63165
D	94	PRO	GLN	engineered mutation	UNP P63165

- Molecule 5 is a protein called E3 SUMO-protein ligase RanBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	252	Total	C	N	O	S	0	0
			2026	1298	334	386	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	2442	GLY	-	expression tag	UNP P49792

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2443	SER	-	expression tag	UNP P49792
E	2444	HIS	-	expression tag	UNP P49792
E	2445	MET	-	expression tag	UNP P49792

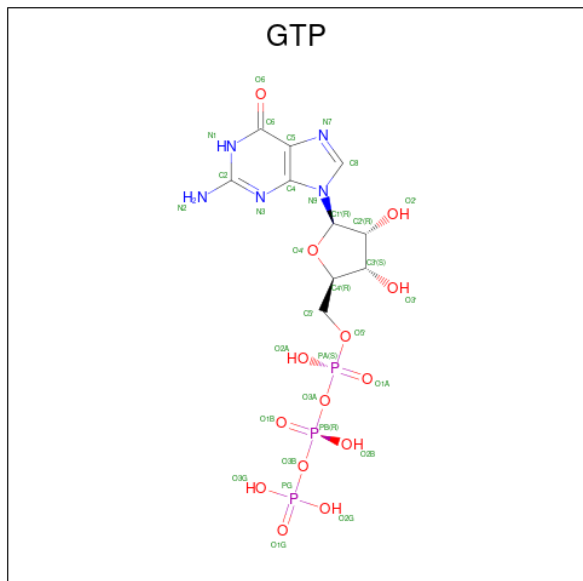
- Molecule 6 is a protein called Ran GTPase-activating protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	517	Total	C	N	O	S	0	0
			3886	2450	664	753	19		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	GLY	-	expression tag	UNP P46060
G	-2	SER	-	expression tag	UNP P46060
G	-1	HIS	-	expression tag	UNP P46060
G	0	MET	-	expression tag	UNP P46060

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

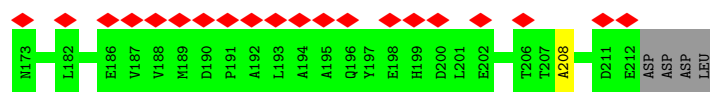


Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	F	1	Total	C	N	O	P	0
			32	10	5	14	3	

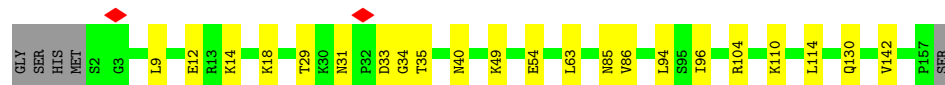
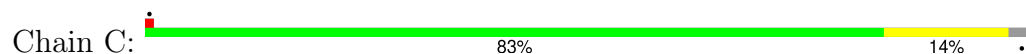
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	B	1	Total 1	Mg 1	0
8	F	1	Total 1	Mg 1	0

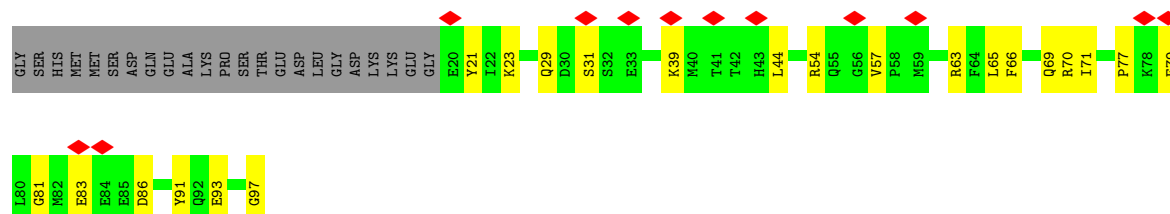




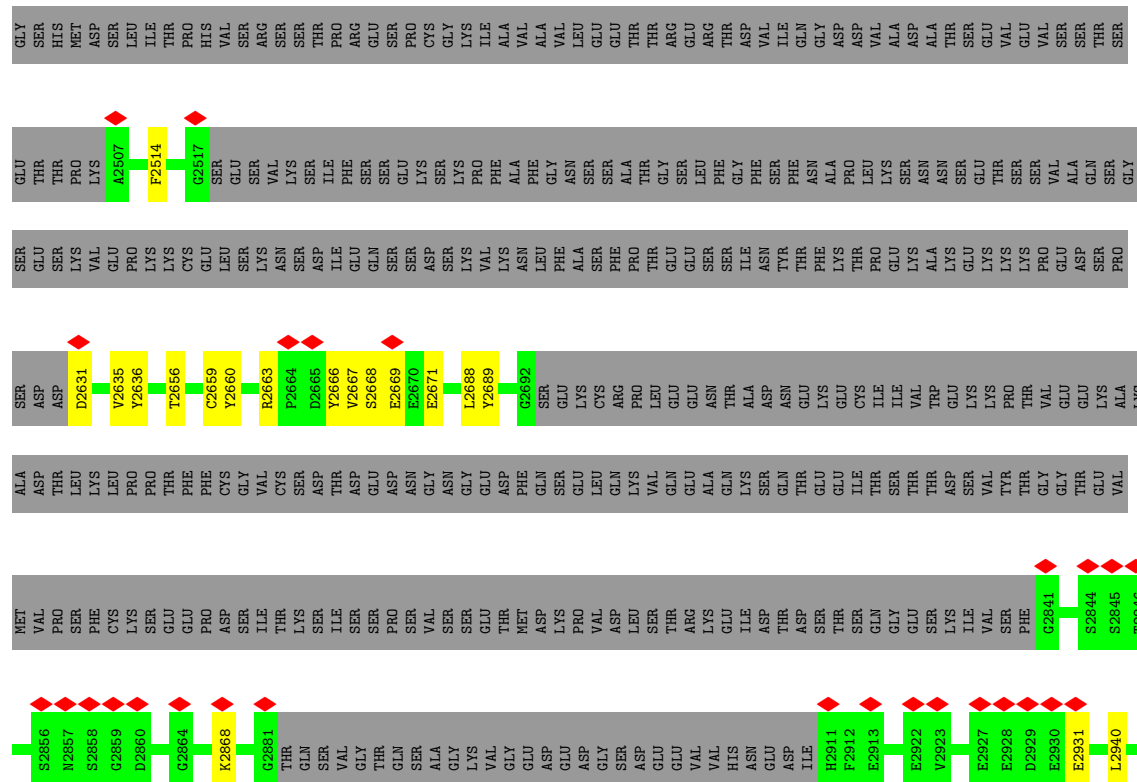
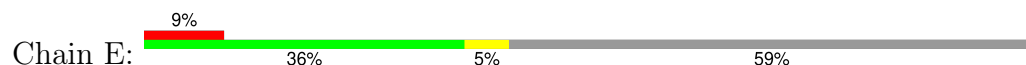
- Molecule 3: SUMO-conjugating enzyme UBC9



- Molecule 4: Small ubiquitin-related modifier 1

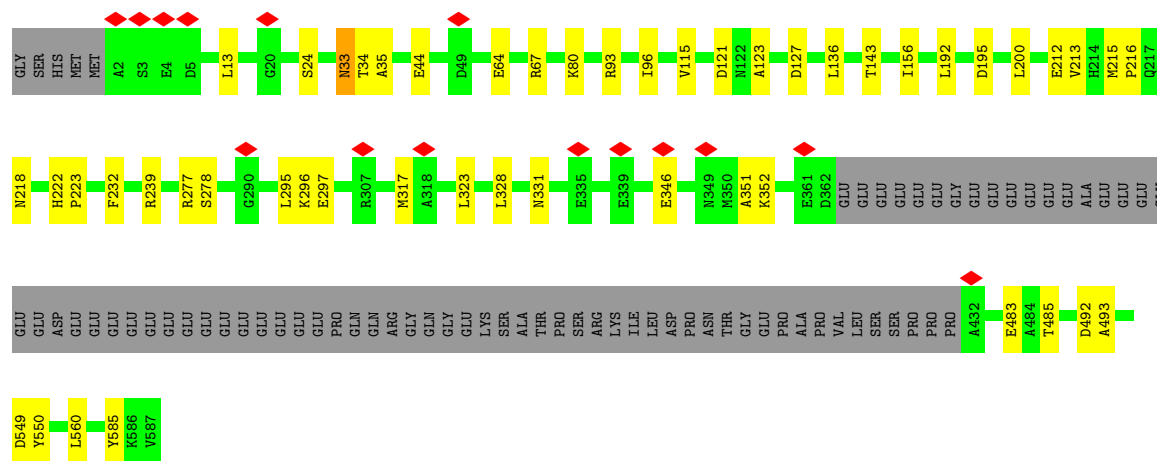
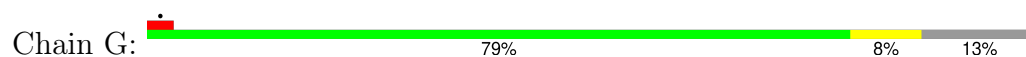


- Molecule 5: E3 SUMO-protein ligase RanBP2





- Molecule 6: Ran GTPase-activating protein 1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	534708	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	85.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	69.970	Depositor
Minimum map value	-23.626	Depositor
Average map value	0.005	Depositor
Map value standard deviation	1.201	Depositor
Recommended contour level	9	Depositor
Map size (Å)	326.40002, 326.40002, 326.40002	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7253334, 0.7253334, 0.7253334	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, GTP

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	0.25	0/8552	0.43	0/11584
2	B	0.28	0/1440	0.48	0/1944
2	F	0.28	0/1684	0.46	0/2284
3	C	0.25	0/1288	0.45	0/1747
4	D	0.24	0/641	0.46	0/858
5	E	0.25	0/2069	0.44	0/2788
6	G	0.24	0/3935	0.45	0/5312
All	All	0.25	0/19609	0.44	0/26517

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	A	8380	0	8432	53	0
2	B	1405	0	1433	16	0
2	F	1643	0	1658	18	0
3	C	1251	0	1249	20	0
4	D	630	0	627	19	0
5	E	2026	0	1984	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	3886	0	3962	33	0
7	B	32	0	12	1	0
7	F	32	0	12	0	0
8	B	1	0	0	0	0
8	F	1	0	0	0	0
All	All	19287	0	19369	156	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 4.

The worst 5 of 156 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:840:GLU:O	1:A:845:ARG:NH1	2.07	0.88
1:A:837:ASP:O	1:A:845:ARG:NH2	2.14	0.81
5:E:2656:THR:HG1	5:E:2659:CYS:HG	1.24	0.78
1:A:983:LYS:NZ	1:A:989:LEU:O	2.17	0.77
4:D:83:GLU:N	4:D:86:ASP:OD2	2.17	0.77

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	1029/1074 (96%)	1011 (98%)	18 (2%)	0	100	100
2	B	171/222 (77%)	165 (96%)	6 (4%)	0	100	100
2	F	203/222 (91%)	189 (93%)	14 (7%)	0	100	100
3	C	154/161 (96%)	151 (98%)	3 (2%)	0	100	100
4	D	76/101 (75%)	75 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	244/619 (39%)	227 (93%)	17 (7%)	0	100	100
6	G	513/591 (87%)	488 (95%)	25 (5%)	0	100	100
All	All	2390/2990 (80%)	2306 (96%)	84 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	942/979 (96%)	935 (99%)	7 (1%)	81	94
2	B	152/189 (80%)	152 (100%)	0	100	100
2	F	177/189 (94%)	174 (98%)	3 (2%)	56	83
3	C	134/139 (96%)	133 (99%)	1 (1%)	81	94
4	D	70/90 (78%)	68 (97%)	2 (3%)	37	72
5	E	219/551 (40%)	215 (98%)	4 (2%)	54	82
6	G	415/483 (86%)	412 (99%)	3 (1%)	81	94
All	All	2109/2620 (80%)	2089 (99%)	20 (1%)	74	92

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	30	HIS
6	G	33	ASN
6	G	352	LYS
6	G	136	LEU
1	A	1032	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
7	GTP	F	301	8	29,34,34	1.19	2 (6%)	35,54,54	1.36	5 (14%)
7	GTP	B	301	8	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)

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
7	GTP	F	301	8	-	2/18/38/38	0/3/3/3
7	GTP	B	301	8	-	5/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	301	GTP	C5-C6	-4.28	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	301	GTP	C5-C6	-4.25	1.39	1.47
7	B	301	GTP	C2-N3	2.04	1.38	1.33
7	F	301	GTP	C2-N3	2.01	1.38	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	301	GTP	C8-N7-C5	3.69	108.83	102.55
7	F	301	GTP	C8-N7-C5	3.67	108.80	102.55
7	F	301	GTP	C5-C6-N1	3.03	119.85	114.07
7	B	301	GTP	C5-C6-N1	3.02	119.83	114.07
7	B	301	GTP	C2-N1-C6	-3.00	119.62	125.11

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	301	GTP	PB-O3A-PA-O2A
7	B	301	GTP	C5'-O5'-PA-O1A
7	F	301	GTP	PB-O3A-PA-O2A
7	B	301	GTP	PB-O3B-PG-O2G
7	B	301	GTP	PB-O3A-PA-O1A

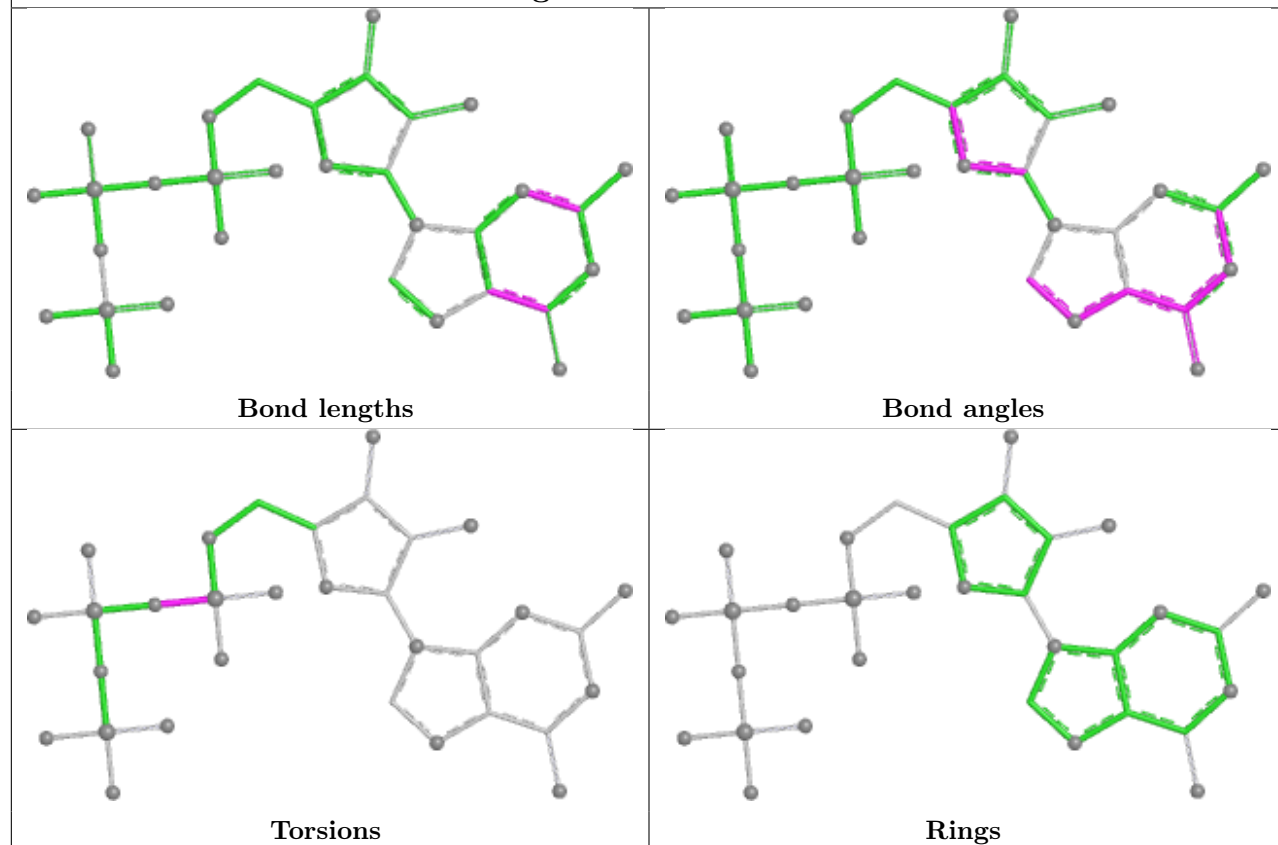
There are no ring outliers.

1 monomer is involved in 1 short contact:

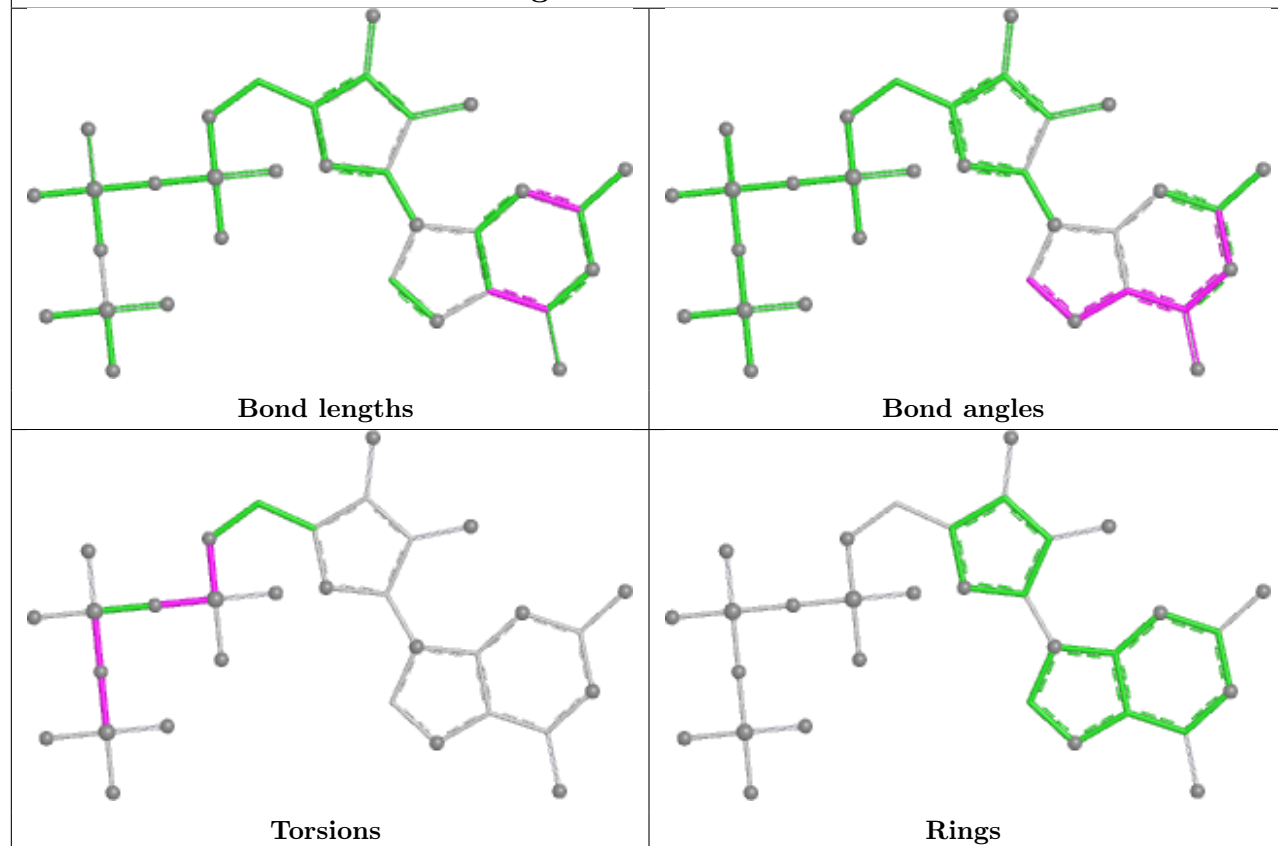
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	301	GTP	1	0

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.

## Ligand GTP F 301



## Ligand GTP B 301





## 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.

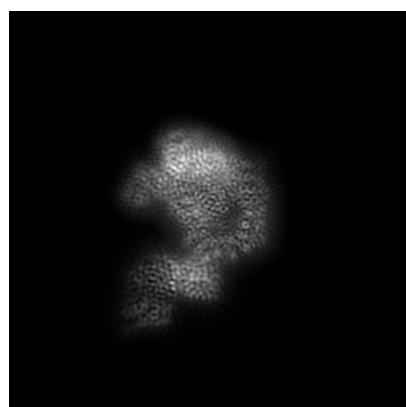
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44235. These allow visual inspection of the internal detail of the map and identification of artifacts.

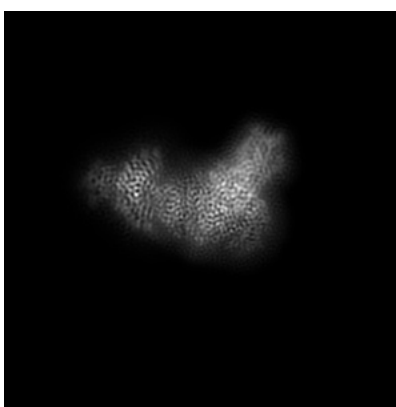
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

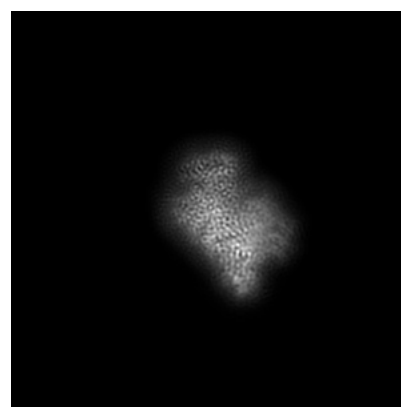
#### 6.1.1 Primary map



X



Y

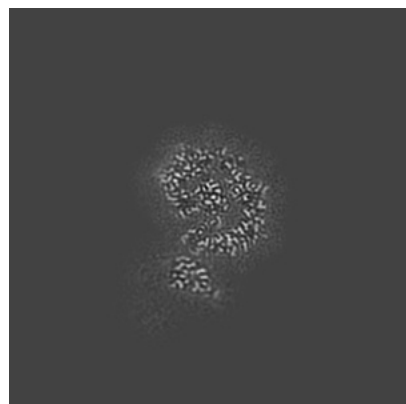


Z

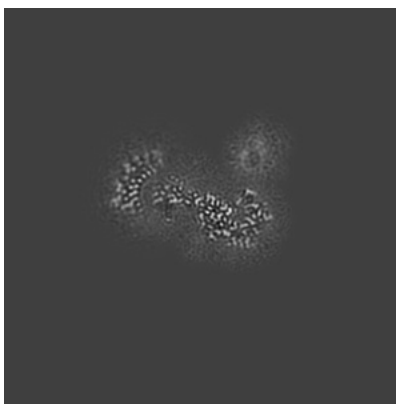
The images above show the map projected in three orthogonal directions.

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

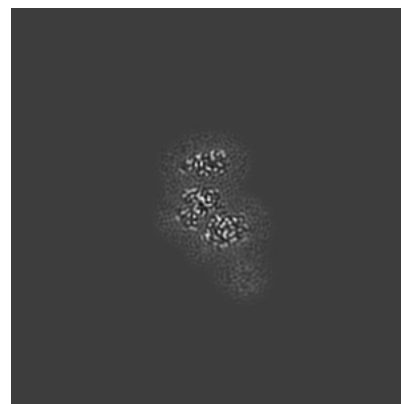
#### 6.2.1 Primary map



X Index: 225



Y Index: 225

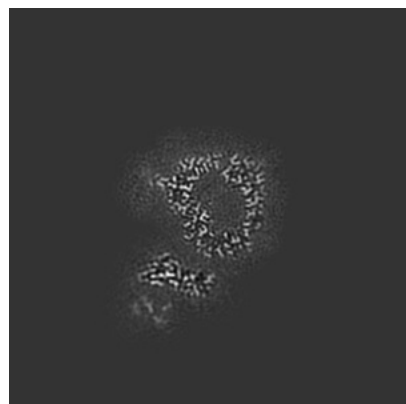


Z Index: 225

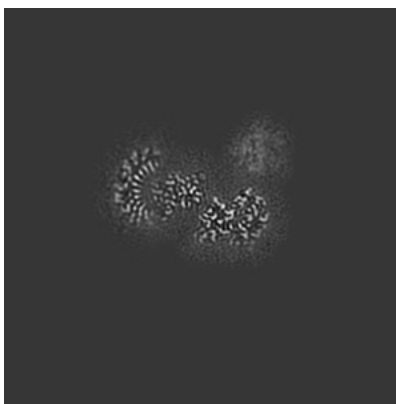
The images above show central slices of the map in three orthogonal directions.

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

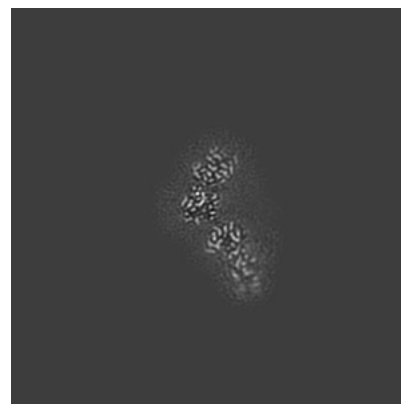
### 6.3.1 Primary map



X Index: 241



Y Index: 219

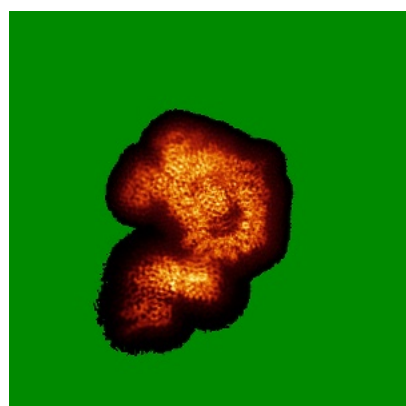


Z Index: 246

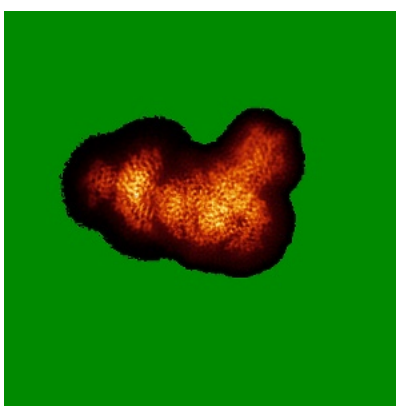
The images above show the largest variance slices of the map in three orthogonal directions.

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

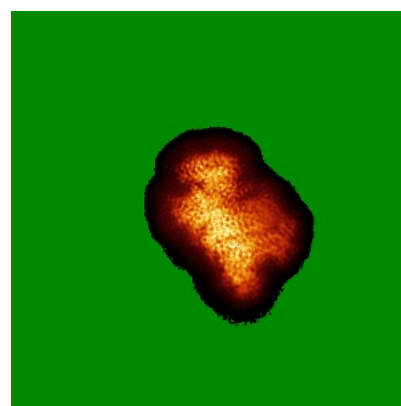
### 6.4.1 Primary map



X



Y

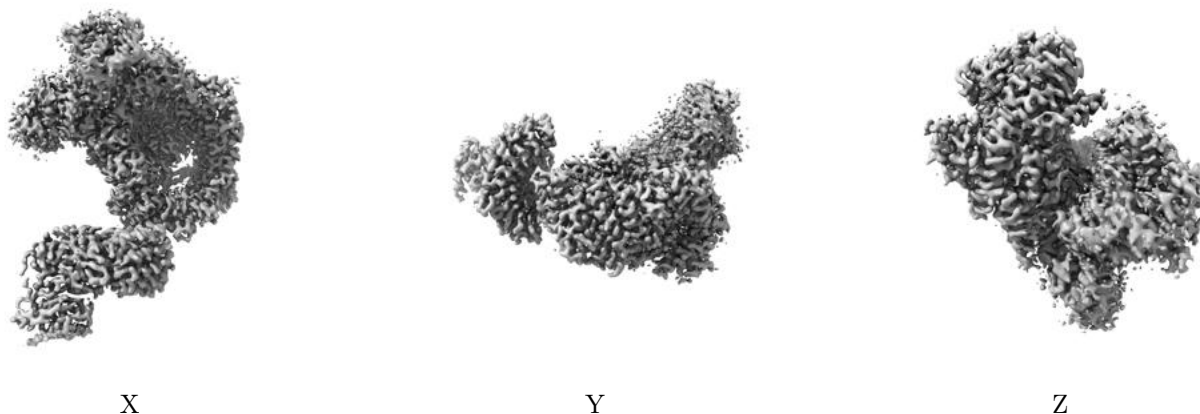


Z

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

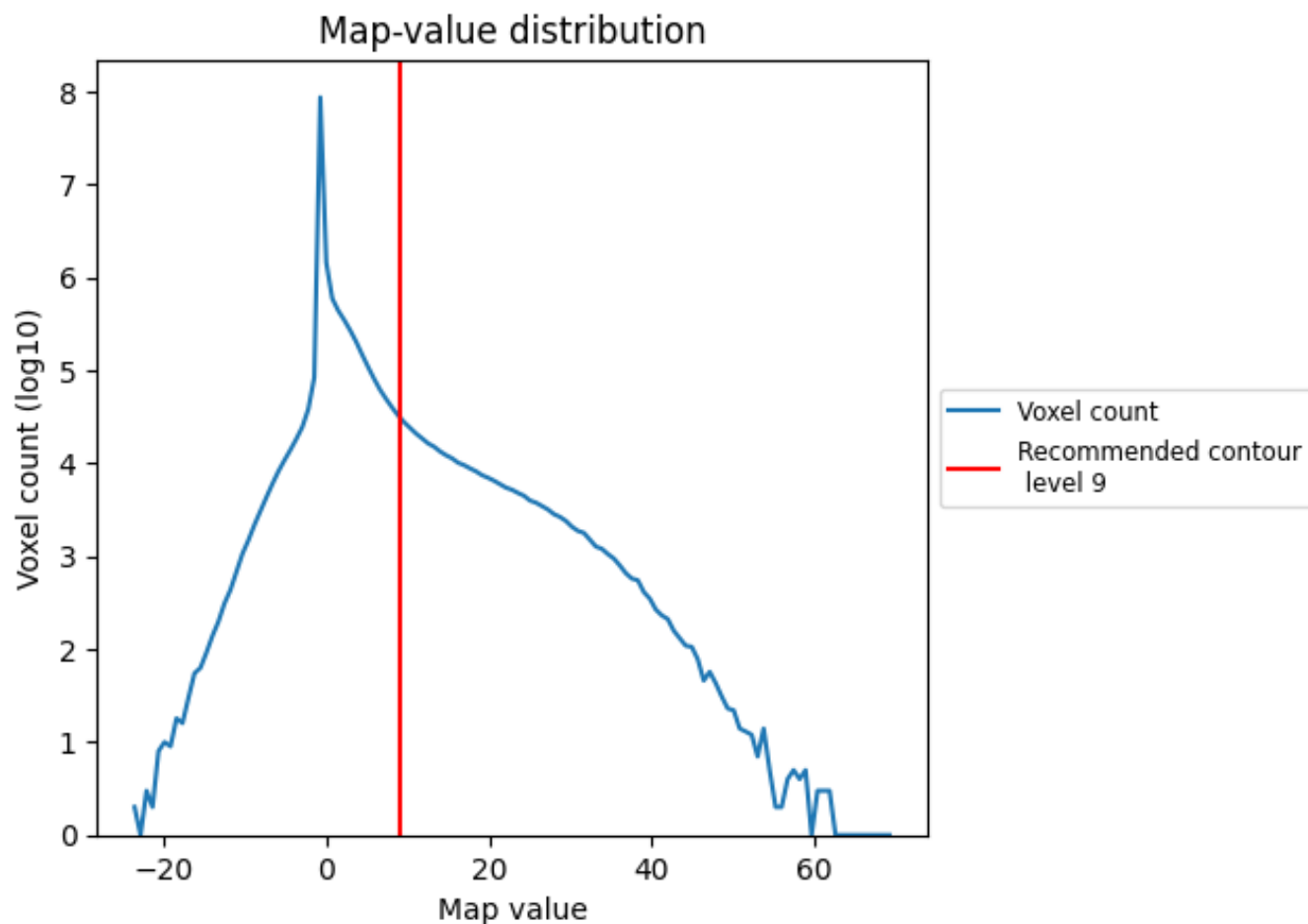
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

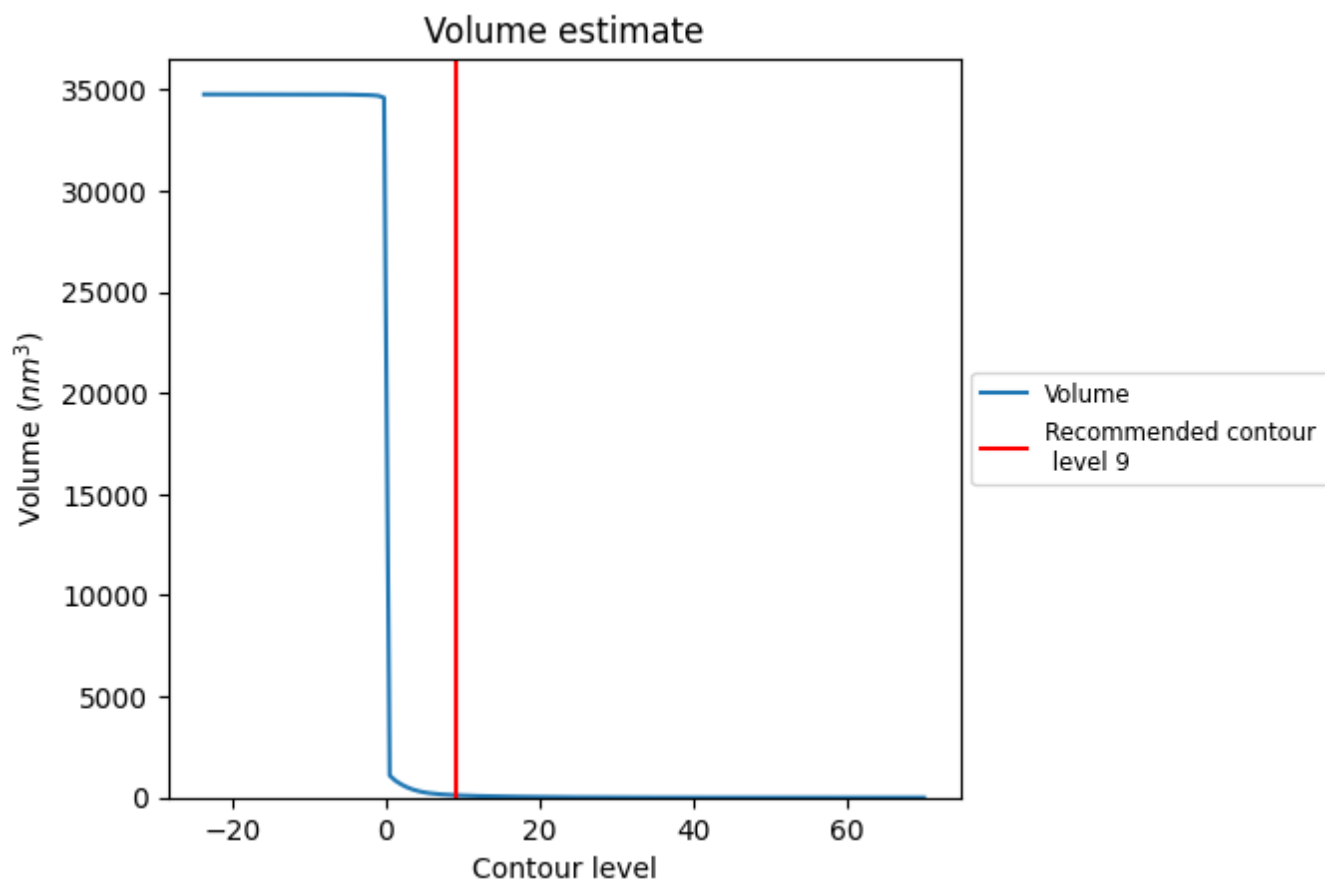
This section contains the results of statistical analysis of the map.

### 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.

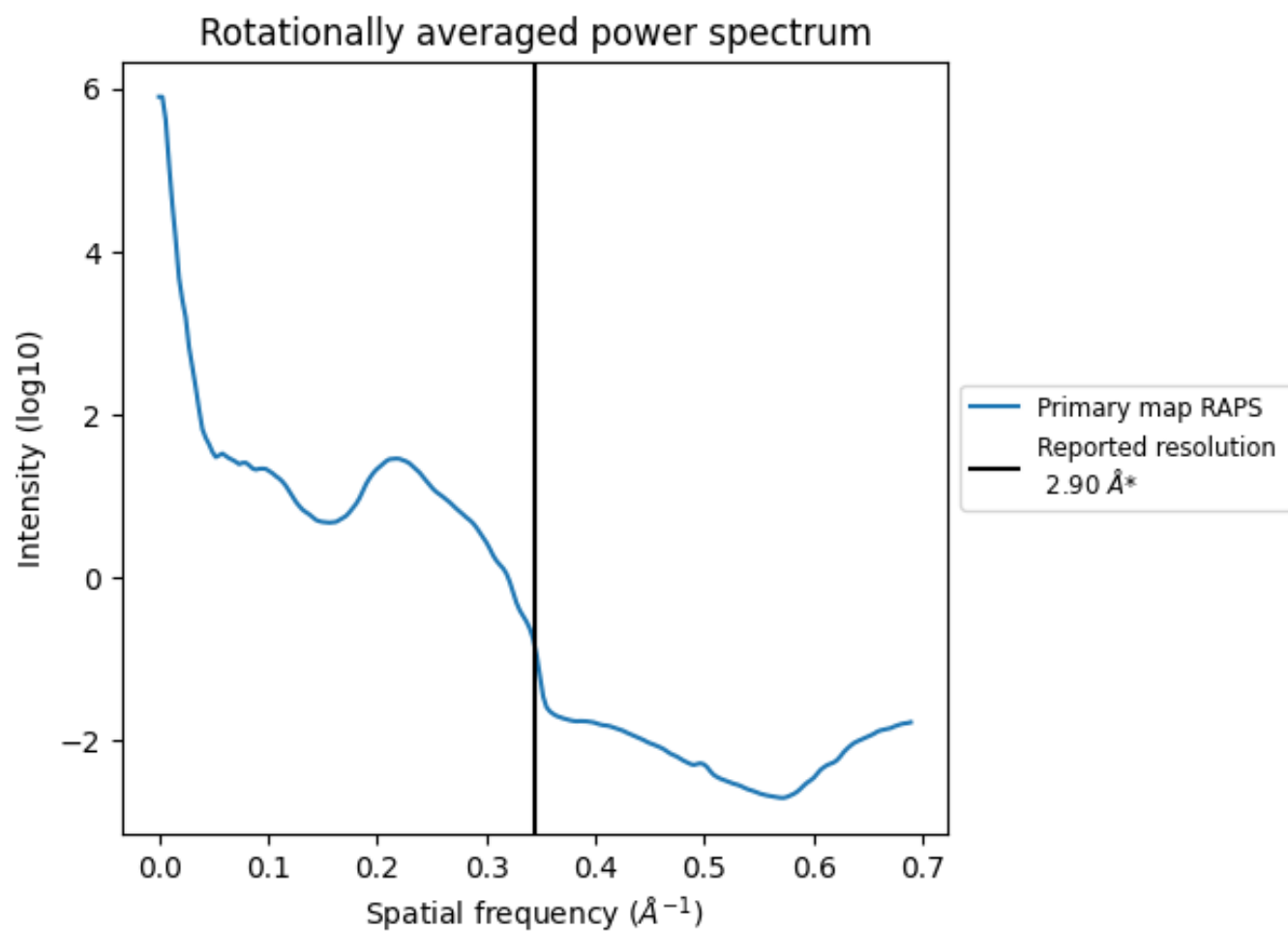
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 117  $\text{nm}^3$ ; this corresponds to an approximate mass of 105 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 0.345 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

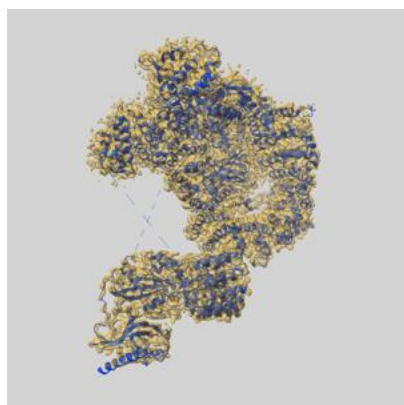
This section was not generated. No FSC curve or half-maps provided.



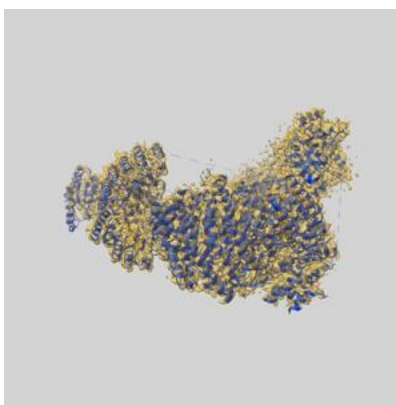
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44235 and PDB model 9B62. Per-residue inclusion information can be found in section [3](#) on page [7](#).

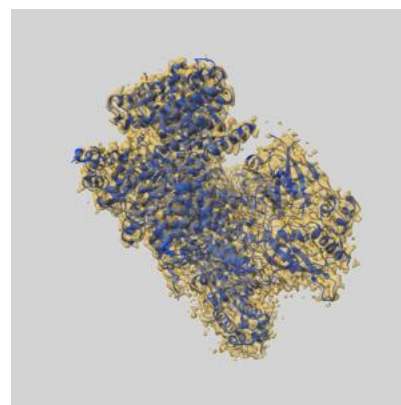
### 9.1 Map-model overlay [i](#)



X



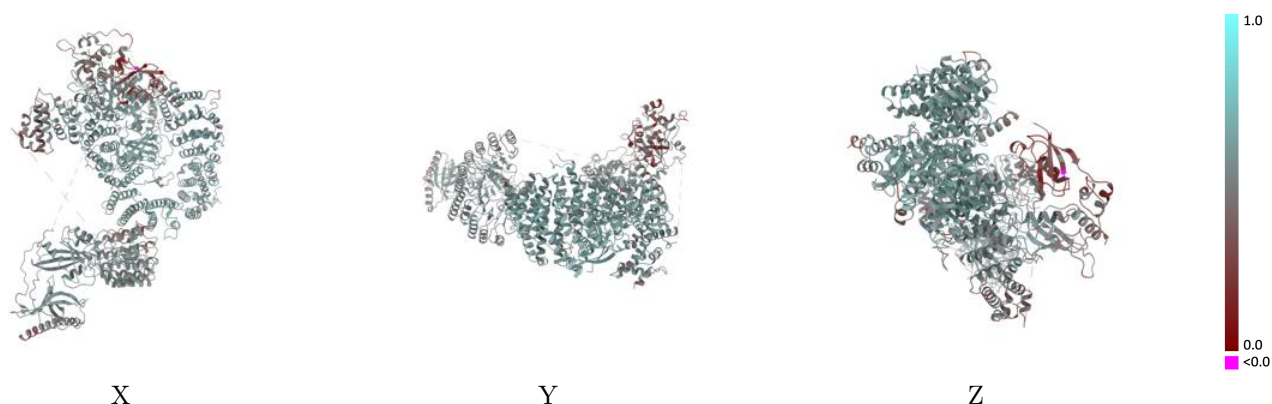
Y



Z

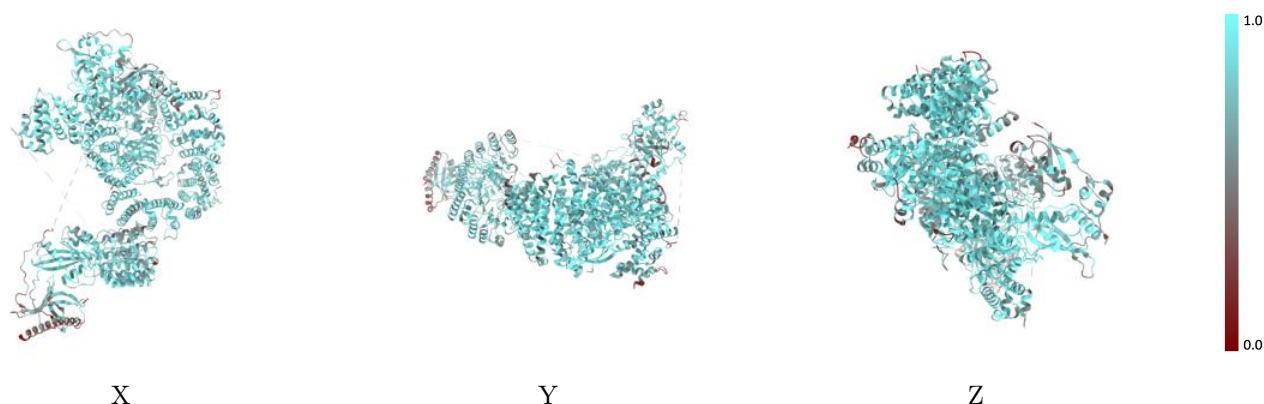
The images above show the 3D surface view of the map at the recommended contour level 9.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



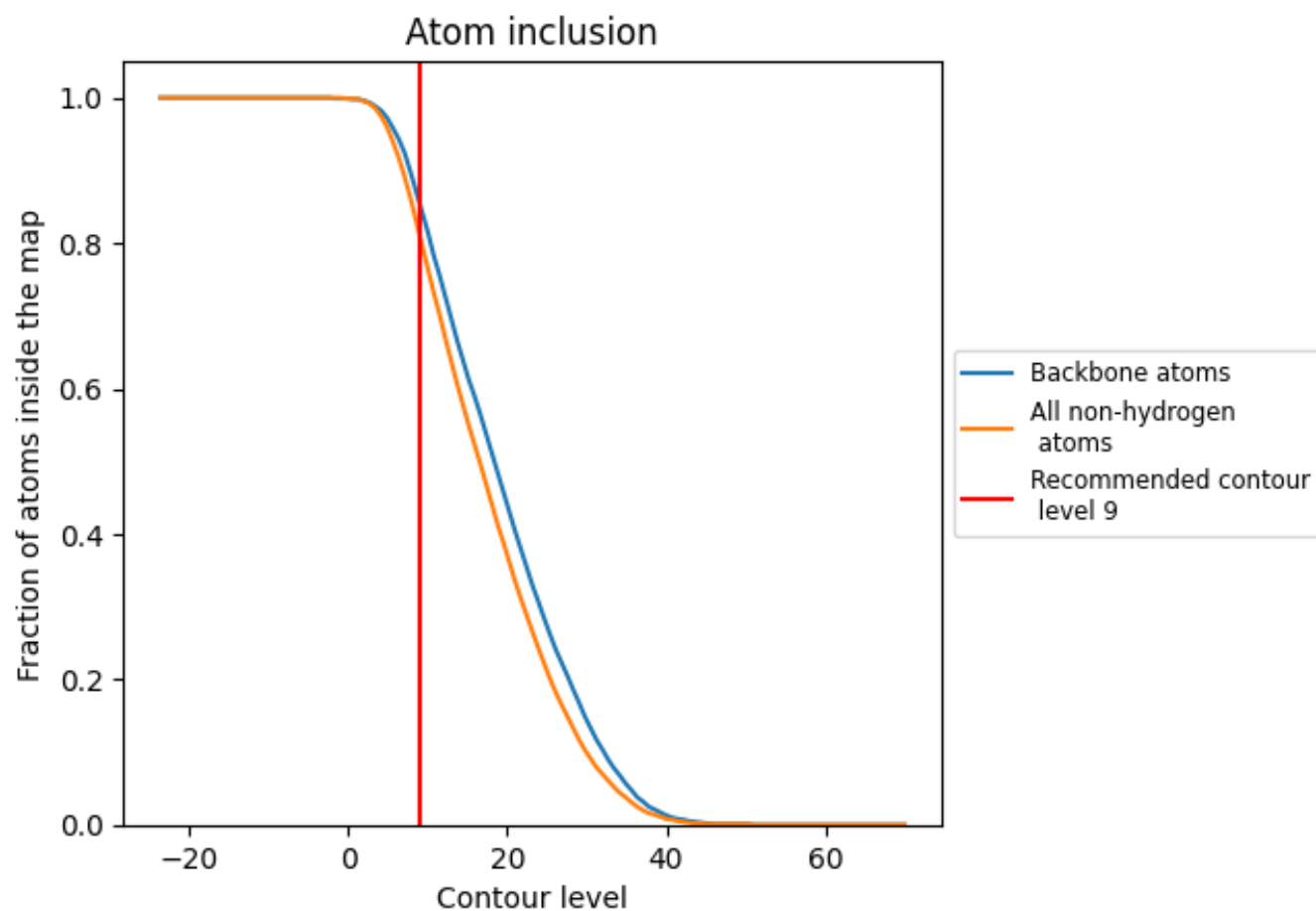
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (9).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 81% 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 (9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8090	<div><div></div></div> 0.5390
A	<div><div></div></div> 0.8540	<div><div></div></div> 0.5820
B	<div><div></div></div> 0.9240	<div><div></div></div> 0.6230
C	<div><div></div></div> 0.8820	<div><div></div></div> 0.5040
D	<div><div></div></div> 0.6200	<div><div></div></div> 0.2950
E	<div><div></div></div> 0.6150	<div><div></div></div> 0.4710
F	<div><div></div></div> 0.7730	<div><div></div></div> 0.5260
G	<div><div></div></div> 0.7940	<div><div></div></div> 0.5070

1.0

0.0

<0.0