



Full wwPDB EM Validation Report ⓘ

Feb 3, 2025 – 02:35 PM EST

PDB ID : 9MHH
EMDB ID : EMD-48278
Title : PI3KC3-C1 in complex with RAB1A. VPS34 kinase domain active conformation
Authors : Cook, A.S.I.; Hurley, J.H.; Chen, M.
Deposited on : 2024-12-11
Resolution : 4.50 Å(reported)
Based on initial model : .

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

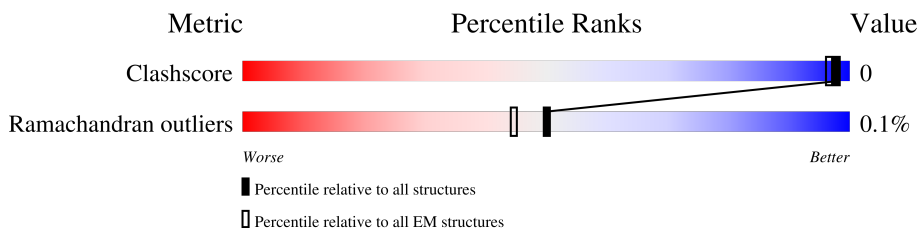
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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

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

Mol	Chain	Length	Quality of chain
1	A	1409	
2	B	887	
3	C	492	
4	D	450	
5	E	226	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11243 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 Phosphoinositide 3-kinase regulatory subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	1191	Total	C	N	O	0	0
			4764	2382	1191	1191		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q99570
A	1359	GLY	-	expression tag	UNP Q99570
A	1360	THR	-	expression tag	UNP Q99570
A	1361	GLU	-	expression tag	UNP Q99570
A	1362	ASN	-	expression tag	UNP Q99570
A	1363	LEU	-	expression tag	UNP Q99570
A	1364	TYR	-	expression tag	UNP Q99570
A	1365	PHE	-	expression tag	UNP Q99570
A	1366	GLN	-	expression tag	UNP Q99570
A	1367	SER	-	expression tag	UNP Q99570
A	1368	GLY	-	expression tag	UNP Q99570
A	1369	MET	-	expression tag	UNP Q99570
A	1370	ALA	-	expression tag	UNP Q99570
A	1371	ALA	-	expression tag	UNP Q99570
A	1372	TRP	-	expression tag	UNP Q99570
A	1373	SER	-	expression tag	UNP Q99570
A	1374	HIS	-	expression tag	UNP Q99570
A	1375	PRO	-	expression tag	UNP Q99570
A	1376	GLN	-	expression tag	UNP Q99570
A	1377	PHE	-	expression tag	UNP Q99570
A	1378	GLU	-	expression tag	UNP Q99570
A	1379	LYS	-	expression tag	UNP Q99570
A	1380	GLY	-	expression tag	UNP Q99570
A	1381	GLY	-	expression tag	UNP Q99570
A	1382	GLY	-	expression tag	UNP Q99570
A	1383	ALA	-	expression tag	UNP Q99570
A	1384	ARG	-	expression tag	UNP Q99570
A	1385	GLY	-	expression tag	UNP Q99570

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1386	GLY	-	expression tag	UNP Q99570
A	1387	SER	-	expression tag	UNP Q99570
A	1388	GLY	-	expression tag	UNP Q99570
A	1389	GLY	-	expression tag	UNP Q99570
A	1390	GLY	-	expression tag	UNP Q99570
A	1391	SER	-	expression tag	UNP Q99570
A	1392	TRP	-	expression tag	UNP Q99570
A	1393	SER	-	expression tag	UNP Q99570
A	1394	HIS	-	expression tag	UNP Q99570
A	1395	PRO	-	expression tag	UNP Q99570
A	1396	GLN	-	expression tag	UNP Q99570
A	1397	PHE	-	expression tag	UNP Q99570
A	1398	GLU	-	expression tag	UNP Q99570
A	1399	LYS	-	expression tag	UNP Q99570
A	1400	GLY	-	expression tag	UNP Q99570
A	1401	PHE	-	expression tag	UNP Q99570
A	1402	ASP	-	expression tag	UNP Q99570
A	1403	TYR	-	expression tag	UNP Q99570
A	1404	LYS	-	expression tag	UNP Q99570
A	1405	ASP	-	expression tag	UNP Q99570
A	1406	ASP	-	expression tag	UNP Q99570
A	1407	ASP	-	expression tag	UNP Q99570
A	1408	ASP	-	expression tag	UNP Q99570
A	1409	LYS	-	expression tag	UNP Q99570

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase catalytic subunit type 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	821	Total	C	N	O	0	0
			3284	1642	821	821		

- Molecule 3 is a protein called Beclin 1-associated autophagy-related key regulator.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	293	Total	C	N	O	0	0
			1172	586	293	293		

- Molecule 4 is a protein called Beclin-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	313	Total	C	N	O	0	0
			1253	626	313	314		

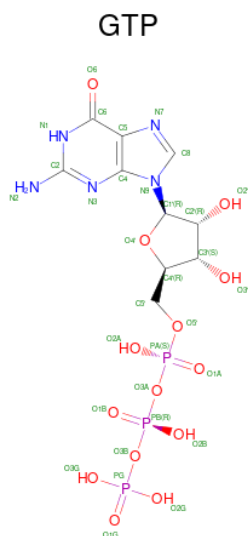
- Molecule 5 is a protein called Ras-related protein Rab-1A.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	176	Total	C	N	O	0	0
			704	352	176	176		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-20	MET	-	expression tag	UNP P62820
E	-19	LYS	-	expression tag	UNP P62820
E	-18	SER	-	expression tag	UNP P62820
E	-17	SER	-	expression tag	UNP P62820
E	-16	HIS	-	expression tag	UNP P62820
E	-15	HIS	-	expression tag	UNP P62820
E	-14	HIS	-	expression tag	UNP P62820
E	-13	HIS	-	expression tag	UNP P62820
E	-12	HIS	-	expression tag	UNP P62820
E	-11	HIS	-	expression tag	UNP P62820
E	-10	GLU	-	expression tag	UNP P62820
E	-9	ASN	-	expression tag	UNP P62820
E	-8	LEU	-	expression tag	UNP P62820
E	-7	TYR	-	expression tag	UNP P62820
E	-6	PHE	-	expression tag	UNP P62820
E	-5	GLN	-	expression tag	UNP P62820
E	-4	SER	-	expression tag	UNP P62820
E	-3	ASN	-	expression tag	UNP P62820
E	-2	ALA	-	expression tag	UNP P62820
E	-1	MET	-	expression tag	UNP P62820
E	0	GLY	-	expression tag	UNP P62820
E	70	LEU	GLN	engineered mutation	UNP P62820

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



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

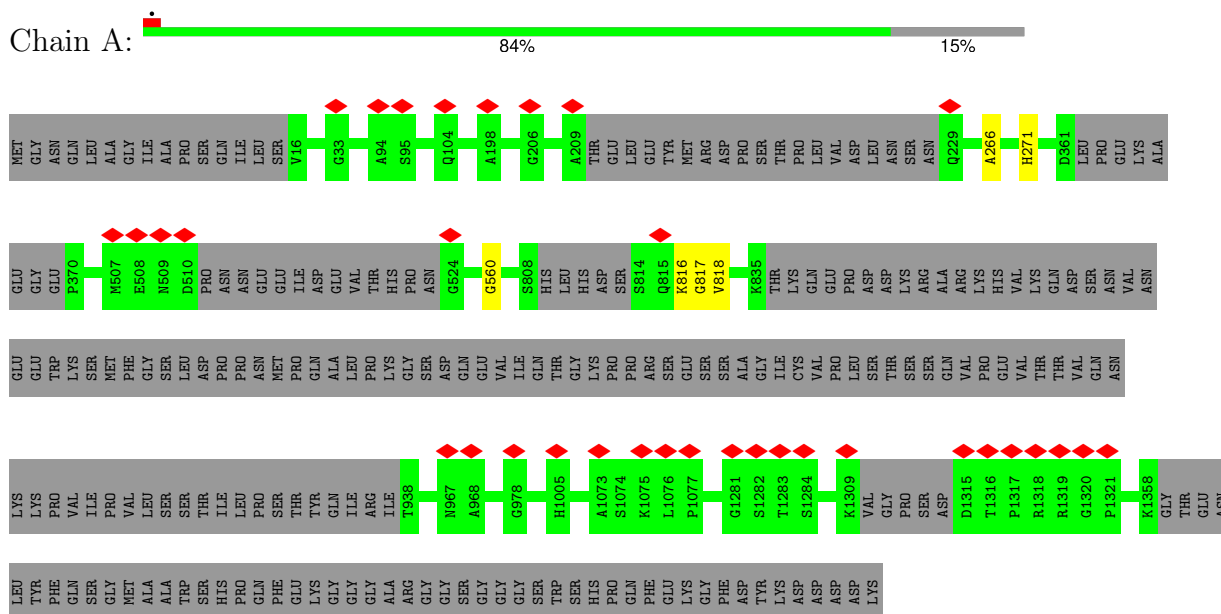
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total Mg 1 1	0
7	E	1	Total Mg 1 1	0

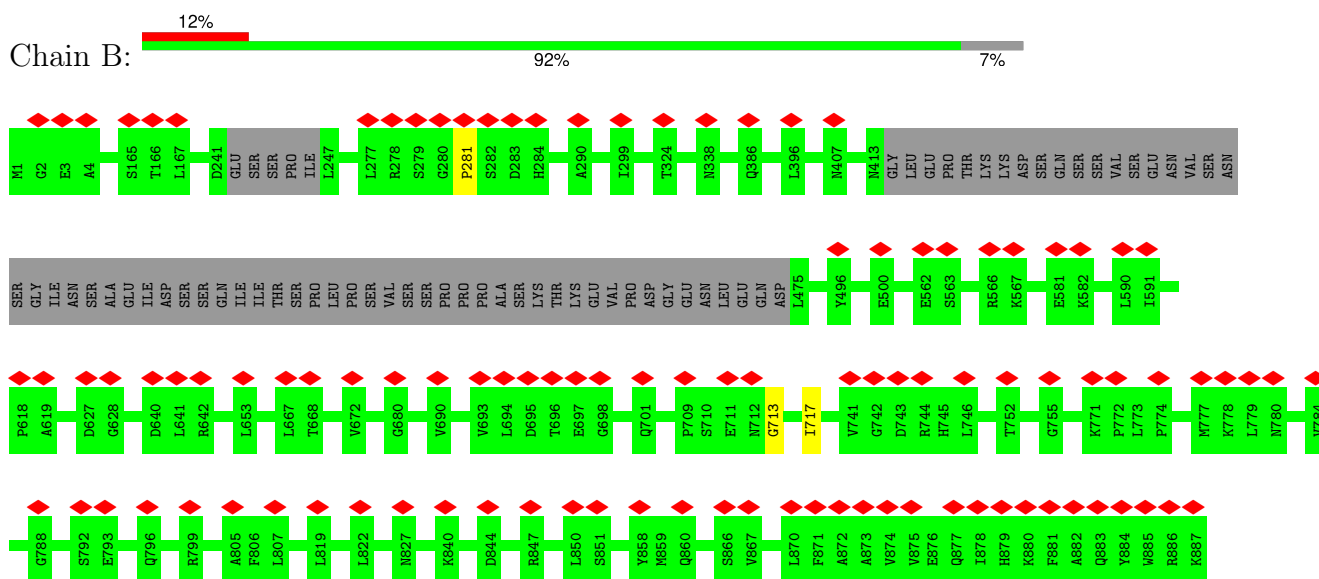
3 Residue-property plots

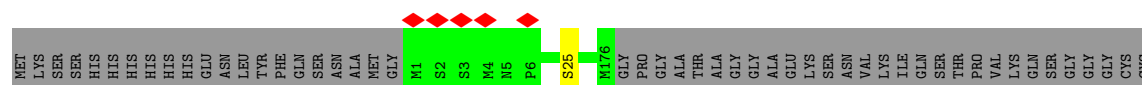
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Phosphoinositide 3-kinase regulatory subunit 4



• Molecule 2: Phosphatidylinositol 3-kinase catalytic subunit type 3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151763	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.114	Depositor
Minimum map value	-0.434	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	419.19998, 419.19998, 419.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.048, 1.048, 1.048	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

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	0.26	0/4757	0.56	0/5934
2	B	0.26	0/3281	0.54	0/4096
3	C	0.23	0/1169	0.42	0/1456
4	D	0.22	0/1252	0.43	0/1562
5	E	0.25	0/703	0.53	0/877
All	All	0.25	0/11162	0.52	0/13925

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	4764	0	1243	2	0
2	B	3284	0	861	1	0
3	C	1172	0	304	0	0
4	D	1253	0	337	0	0
5	E	704	0	195	2	0
6	A	32	0	12	0	0
6	E	32	0	12	2	0
7	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	1	0	0	0	0
All	All	11243	0	2964	5	0

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

All (5) 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)
5:E:25:SER:N	6:E:1002:GTP:O1A	1.93	1.02
5:E:25:SER:CA	6:E:1002:GTP:O1A	2.53	0.56
1:A:266:ALA:O	1:A:271:HIS:N	2.42	0.53
1:A:816:LYS:C	1:A:818:VAL:H	2.14	0.50
2:B:713:GLY:HA3	2:B:717:ILE:O	2.18	0.43

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	1177/1409 (84%)	1148 (98%)	27 (2%)	2 (0%)	44	78
2	B	815/887 (92%)	793 (97%)	21 (3%)	1 (0%)	48	83
3	C	287/492 (58%)	284 (99%)	3 (1%)	0	100	100
4	D	311/450 (69%)	305 (98%)	6 (2%)	0	100	100
5	E	174/226 (77%)	164 (94%)	10 (6%)	0	100	100
All	All	2764/3464 (80%)	2694 (98%)	67 (2%)	3 (0%)	50	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	817	GLY
2	B	281	PRO
1	A	560	GLY

5.3.2 Protein sidechains [i](#)

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

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 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	$\# Z > 2$
6	GTP	A	2001	7	29,34,34	1.29	2 (6%)	35,54,54	1.35	5 (14%)
6	GTP	E	1002	7	29,34,34	1.27	1 (3%)	35,54,54	1.40	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
6	GTP	A	2001	7	-	6/18/38/38	0/3/3/3
6	GTP	E	1002	7	-	0/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1002	GTP	C5-C6	-4.85	1.37	1.47
6	A	2001	GTP	C5-C6	-4.29	1.39	1.47
6	A	2001	GTP	PA-O3A	2.11	1.61	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2001	GTP	C8-N7-C5	3.74	108.92	102.55
6	E	1002	GTP	C8-N7-C5	3.33	108.22	102.55
6	A	2001	GTP	O4'-C1'-N9	3.28	113.09	108.75
6	E	1002	GTP	C5-C6-N1	3.24	120.25	114.07
6	E	1002	GTP	C2-N1-C6	-3.15	119.33	125.11
6	E	1002	GTP	O6-C6-C5	-2.77	118.82	124.32
6	A	2001	GTP	C5-C6-N1	2.72	119.25	114.07
6	A	2001	GTP	C2-N1-C6	-2.62	120.31	125.11
6	A	2001	GTP	O2A-PA-O3A	2.00	112.69	107.27

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2001	GTP	C5'-O5'-PA-O3A
6	A	2001	GTP	C5'-O5'-PA-O1A
6	A	2001	GTP	C5'-O5'-PA-O2A
6	A	2001	GTP	PG-O3B-PB-O1B
6	A	2001	GTP	C4'-C5'-O5'-PA
6	A	2001	GTP	PG-O3B-PB-O2B

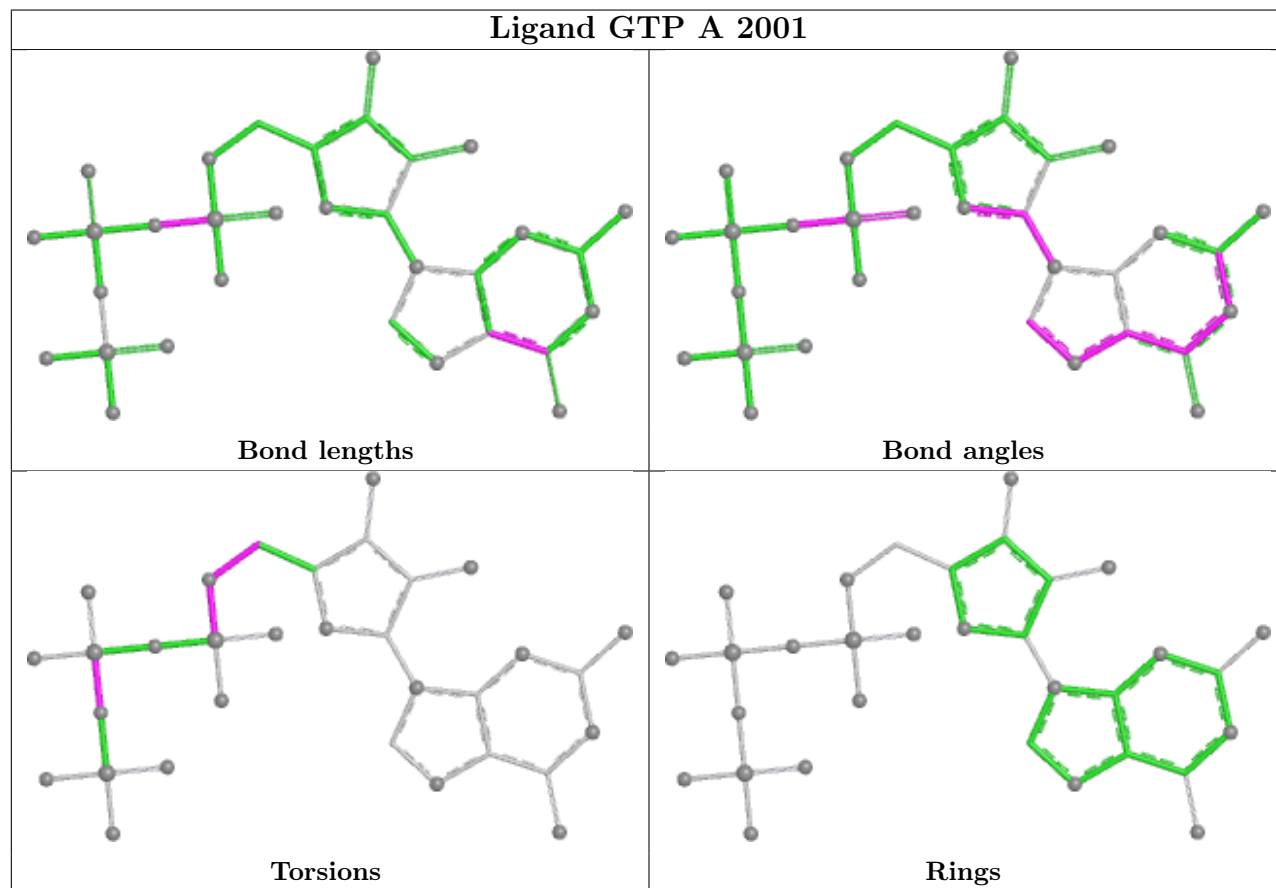
There are no ring outliers.

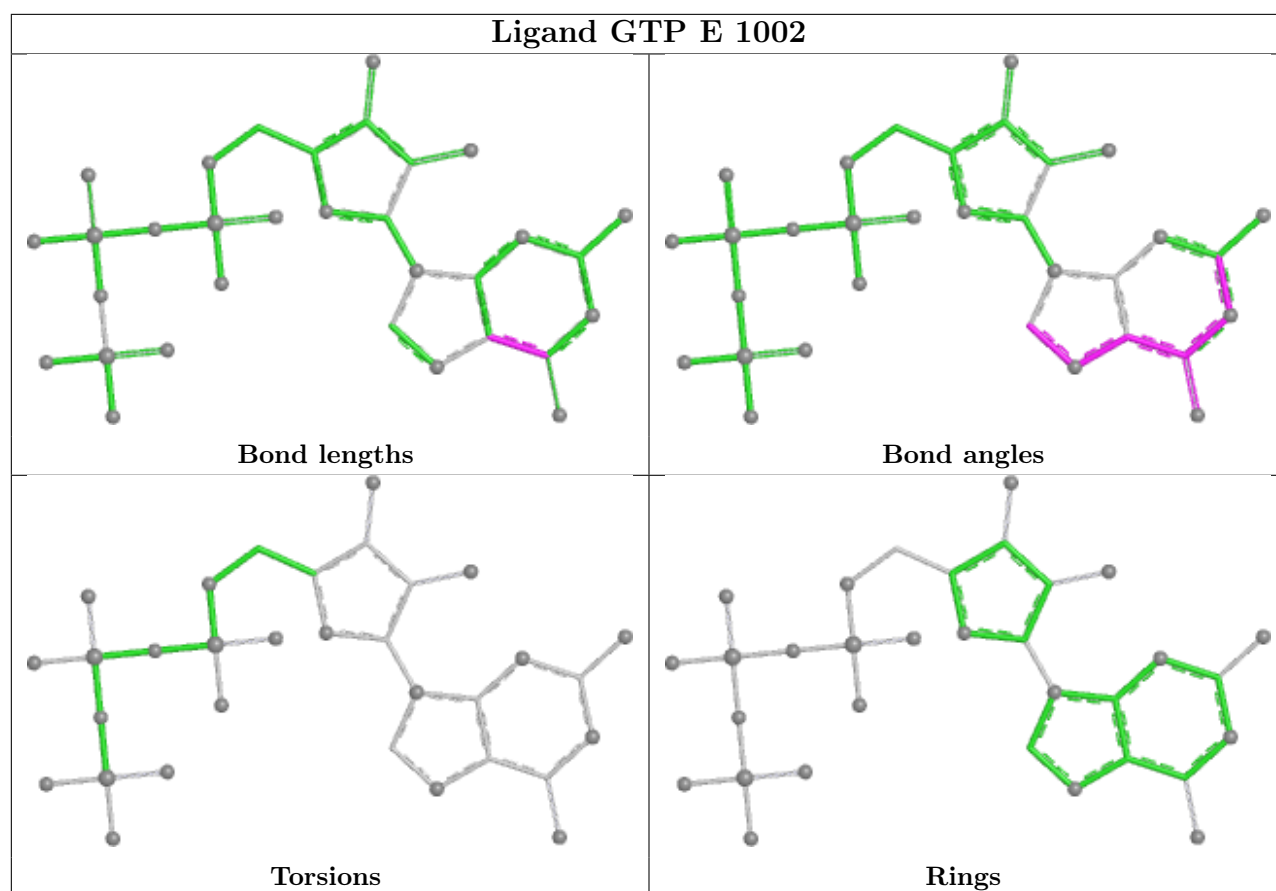
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1002	GTP	2	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.

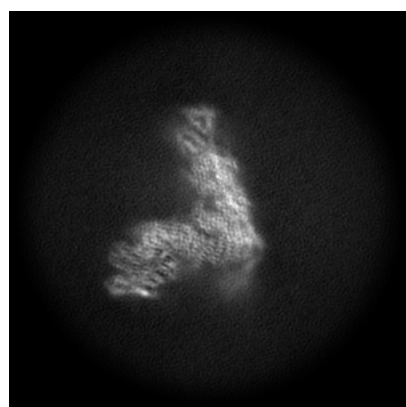
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48278. These allow visual inspection of the internal detail of the map and identification of artifacts.

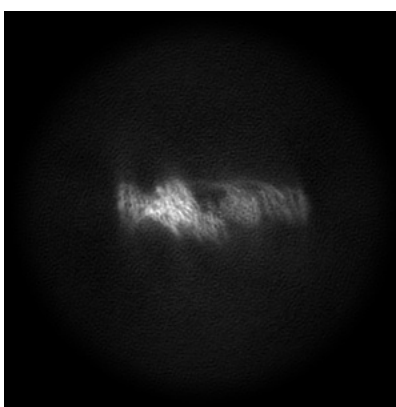
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

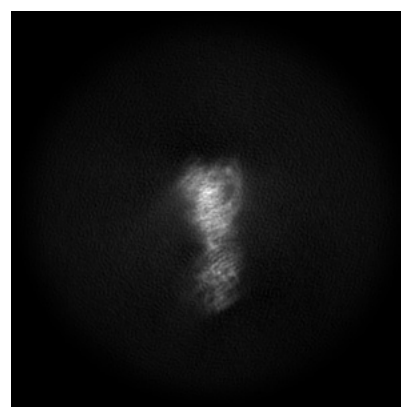
6.1.1 Primary map



X



Y

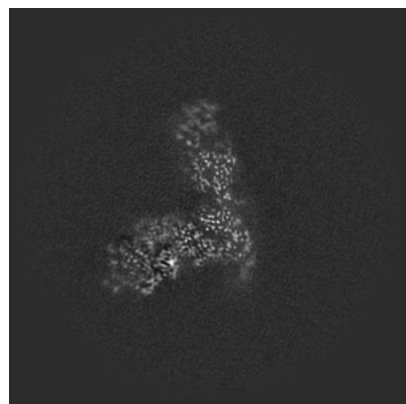


Z

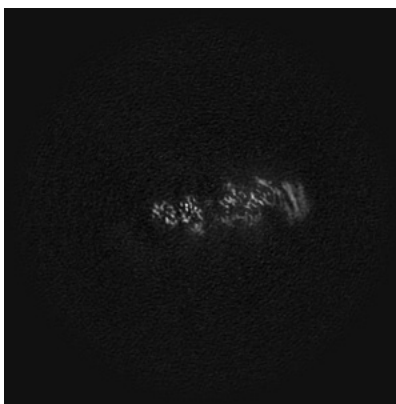
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

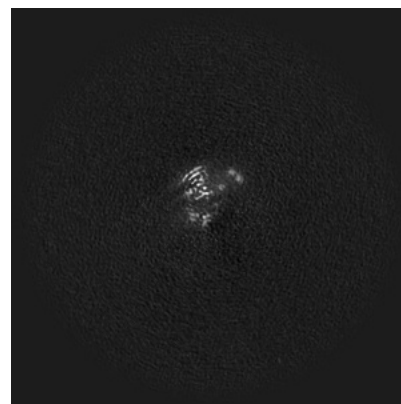
6.2.1 Primary map



X Index: 200



Y Index: 200

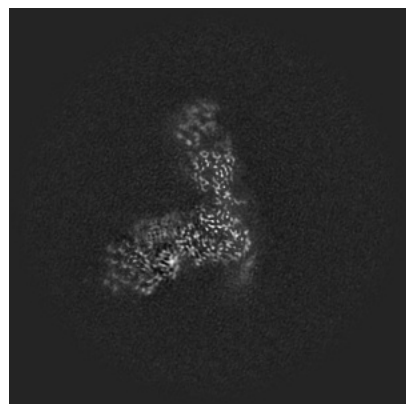


Z Index: 200

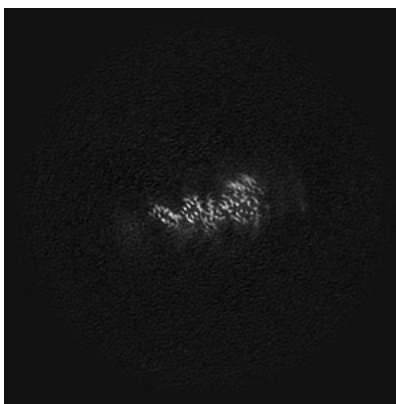
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

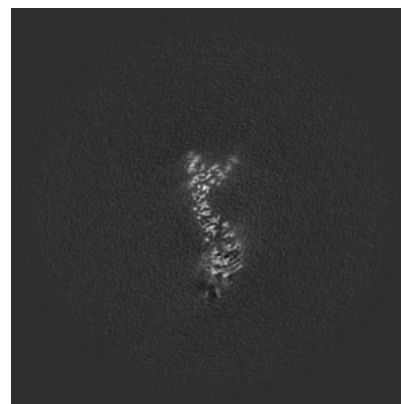
6.3.1 Primary map



X Index: 199



Y Index: 210

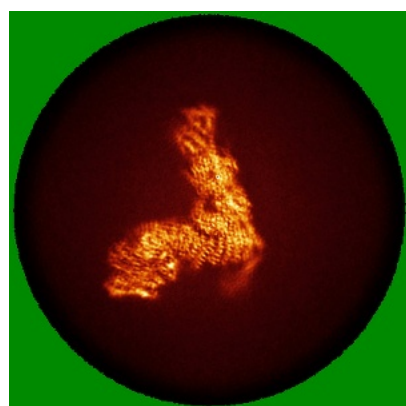


Z Index: 169

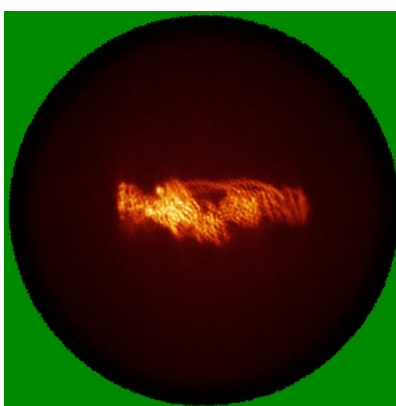
The images above show the largest variance slices of the map in three orthogonal directions.

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

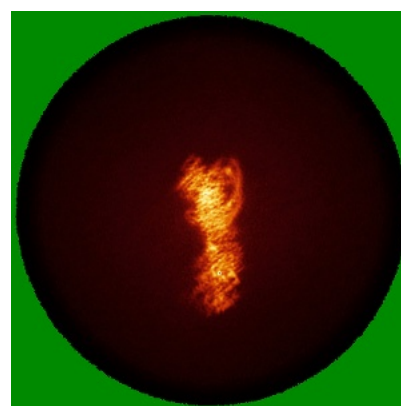
6.4.1 Primary map



X



Y

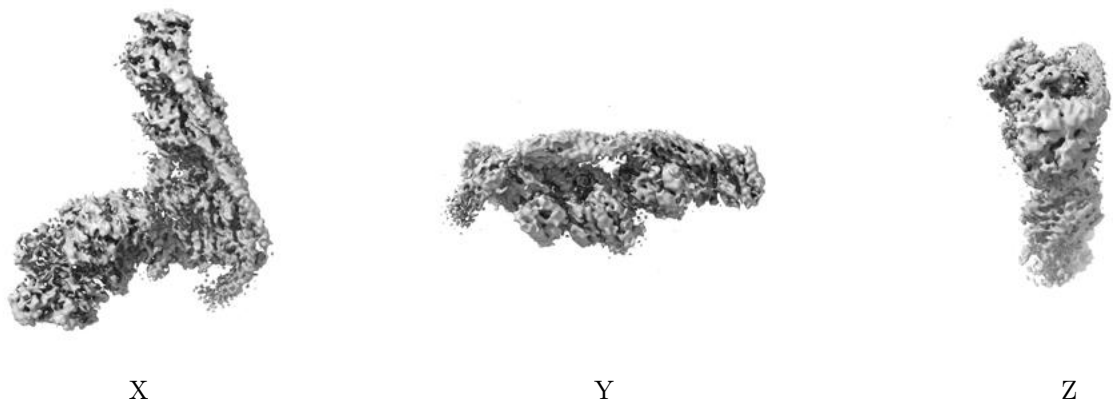


Z

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

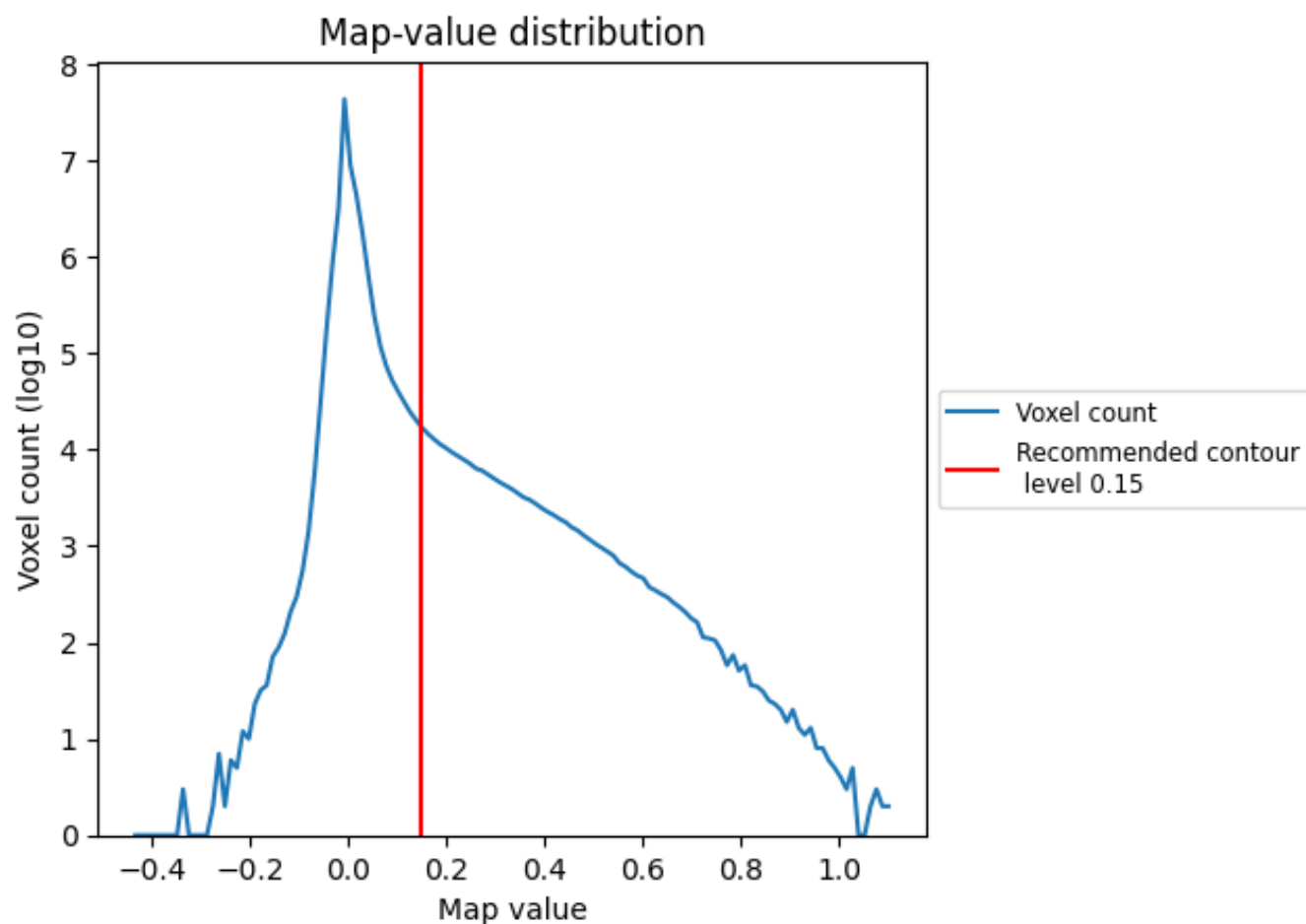
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

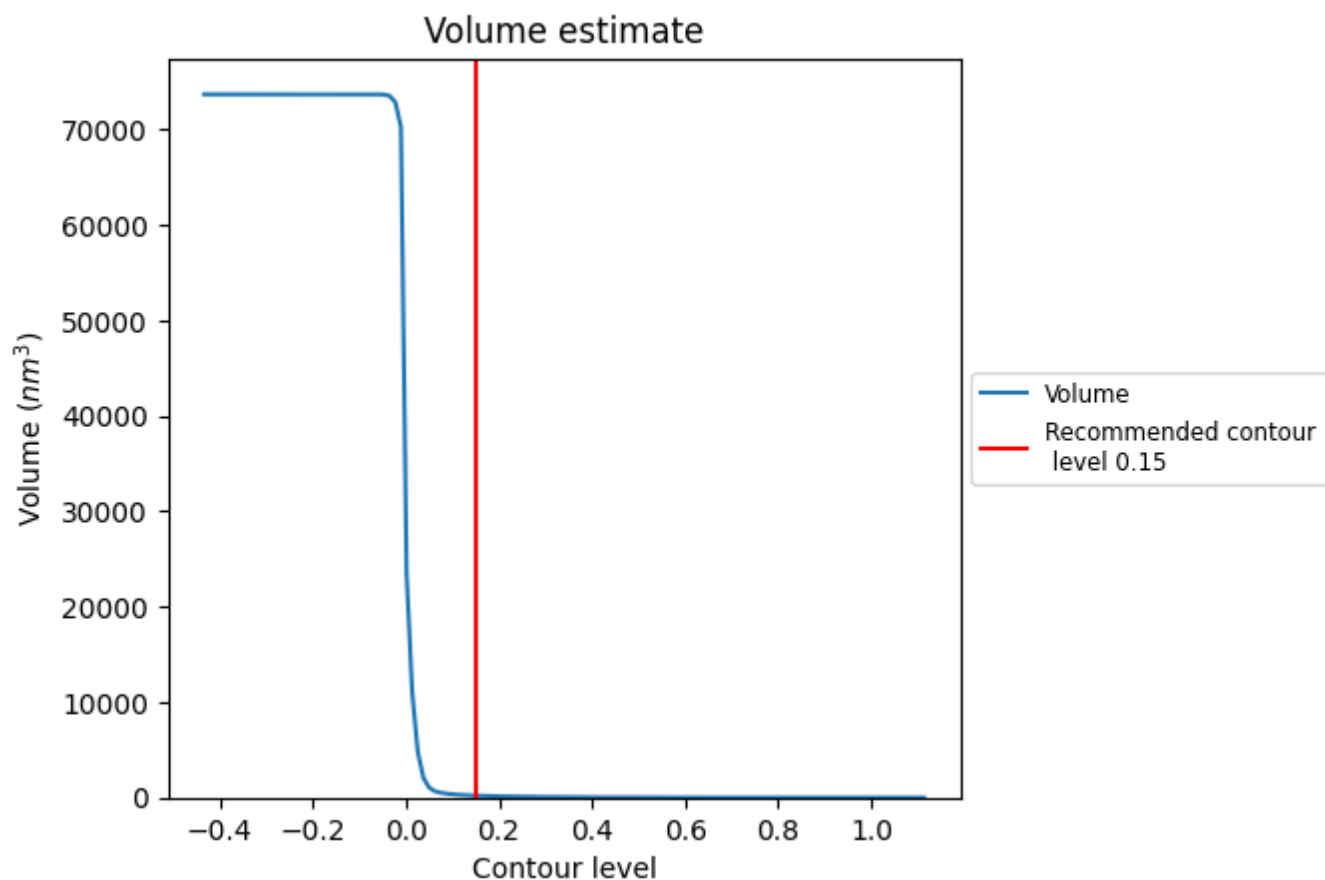
This section contains the results of statistical analysis of the map.

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.

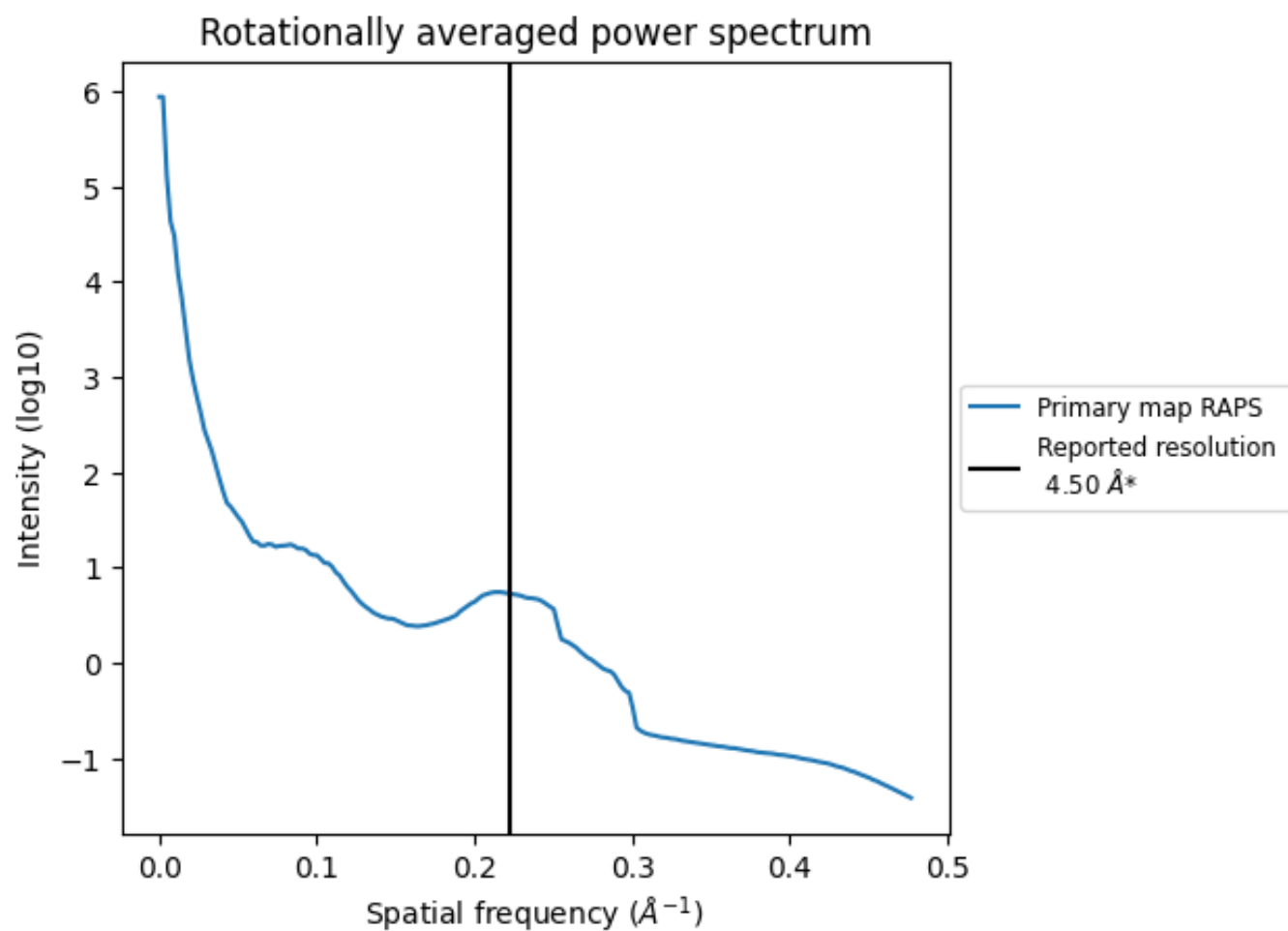
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 201 nm³; this corresponds to an approximate mass of 182 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 0.222 Å⁻¹

8 Fourier-Shell correlation

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

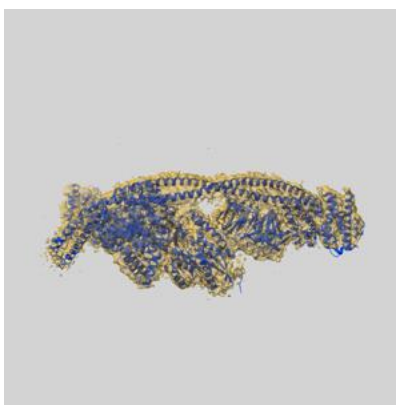
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48278 and PDB model 9MHH. Per-residue inclusion information can be found in section [3](#) on page [7](#).

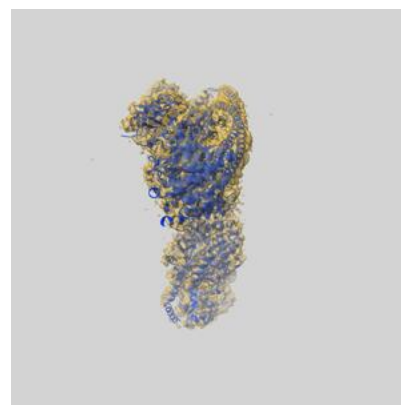
9.1 Map-model overlay [i](#)



X



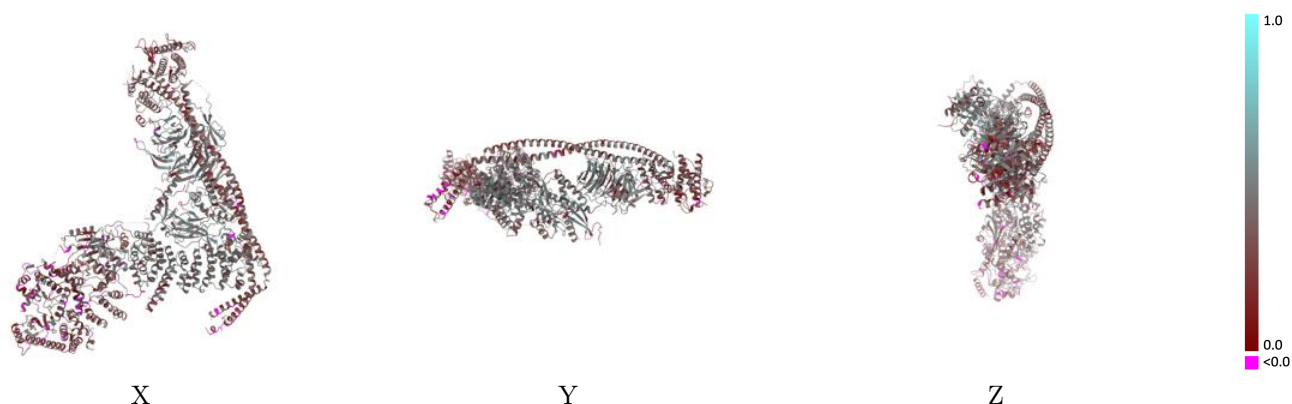
Y



Z

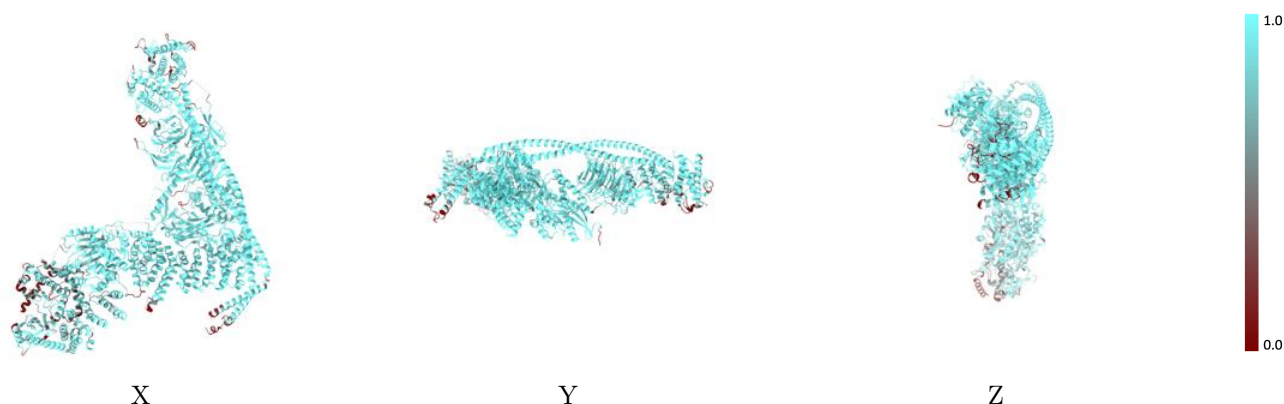
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



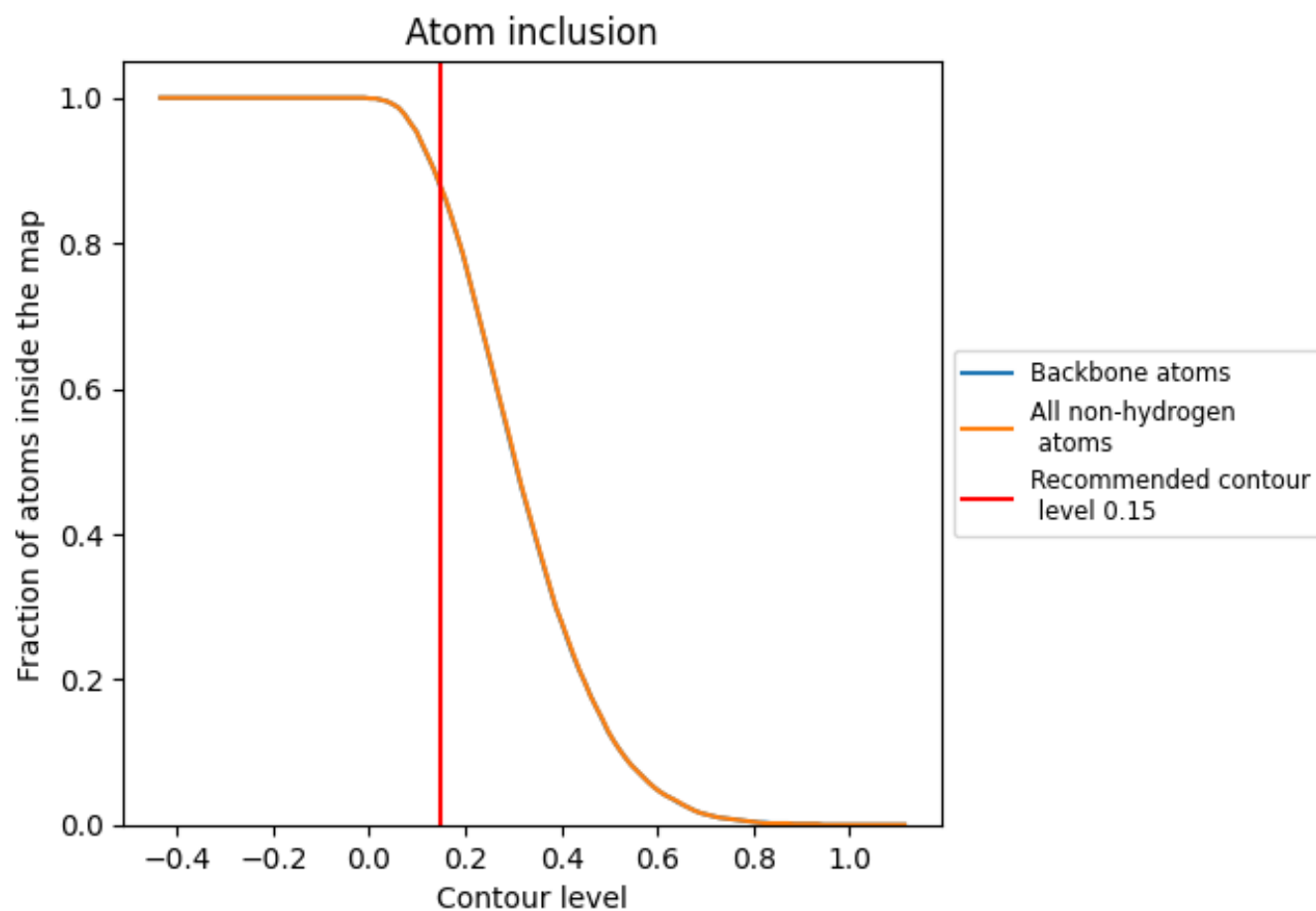
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8760	<div></div> 0.3730
A	<div></div> 0.9380	<div></div> 0.4170
B	<div></div> 0.7890	<div></div> 0.3310
C	<div></div> 0.8720	<div></div> 0.3270
D	<div></div> 0.8230	<div></div> 0.3060
E	<div></div> 0.9480	<div></div> 0.4570

