



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 01:37 PM UTC

PDB ID : 6RF2 / pdb_00006rf2
EMDB ID : EMD-4861
Title : Cryo-EM structure of the C-terminal DC repeat (CDC) of human doublecortin (DCX) bound to 13-protofilament GDP.Pi-microtubule
Authors : Manka, S.W.
Deposited on : 2019-04-12
Resolution : 4.20 Å(reported)
Based on initial model : 5IP4

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

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Mol	Chain	Length	Quality of chain
3	C	87	

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
6	PO4	a	503	-	-	X	-

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 14328 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 alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	432	3382	2144	575	642	21	0	0
1	A	432	3382	2144	575	642	21	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	?	-	SER	deletion	UNP P81947
a	?	-	ASP	deletion	UNP P81947
a	?	-	LYS	deletion	UNP P81947
a	?	-	THR	deletion	UNP P81947
a	?	-	ILE	deletion	UNP P81947
a	?	-	GLY	deletion	UNP P81947
a	?	-	GLY	deletion	UNP P81947
a	?	-	GLY	deletion	UNP P81947
a	?	-	ASP	deletion	UNP P81947
A	?	-	SER	deletion	UNP P81947
A	?	-	ASP	deletion	UNP P81947
A	?	-	LYS	deletion	UNP P81947
A	?	-	THR	deletion	UNP P81947
A	?	-	ILE	deletion	UNP P81947
A	?	-	GLY	deletion	UNP P81947
A	?	-	GLY	deletion	UNP P81947
A	?	-	GLY	deletion	UNP P81947
A	?	-	ASP	deletion	UNP P81947

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	429	3368	2115	578	650	25	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	429	3368	2115	578	650	25	0	0

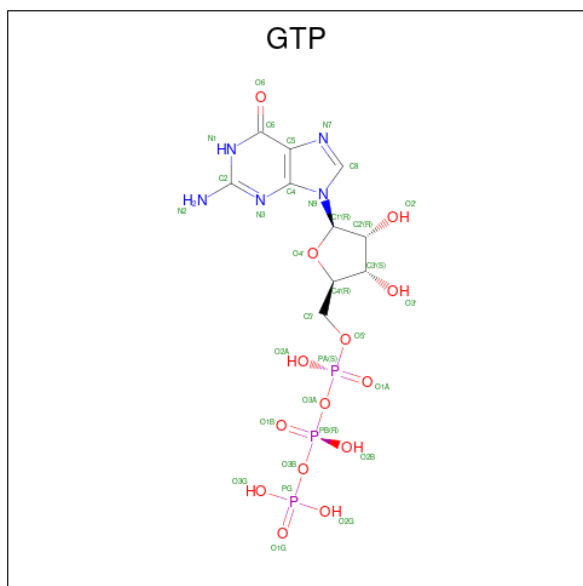
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	55	ALA	THR	conflict	UNP Q6B856
B	170	VAL	MET	conflict	UNP Q6B856
B	296	ALA	SER	conflict	UNP Q6B856
B	316	VAL	ILE	conflict	UNP Q6B856
b	55	ALA	THR	conflict	UNP Q6B856
b	170	VAL	MET	conflict	UNP Q6B856
b	296	ALA	SER	conflict	UNP Q6B856
b	316	VAL	ILE	conflict	UNP Q6B856

- Molecule 3 is a protein called Neuronal migration protein doublecortin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	87	696	448	120	126	2	0	0

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

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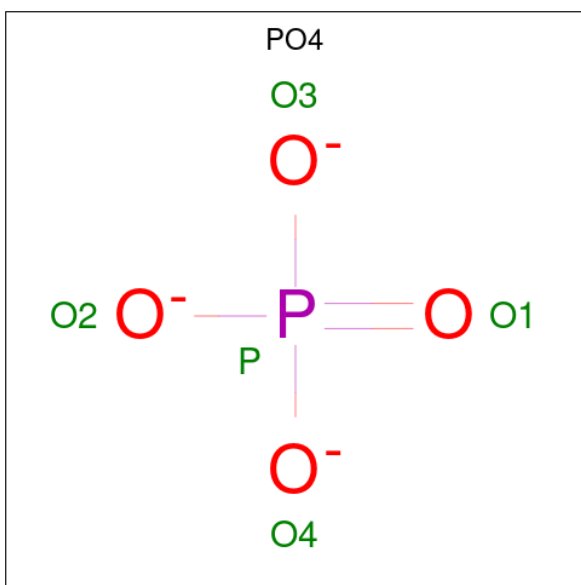
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	A	1	32	10	5	14	3	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	a	1	1	1	0
5	A	1	1	1	0

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



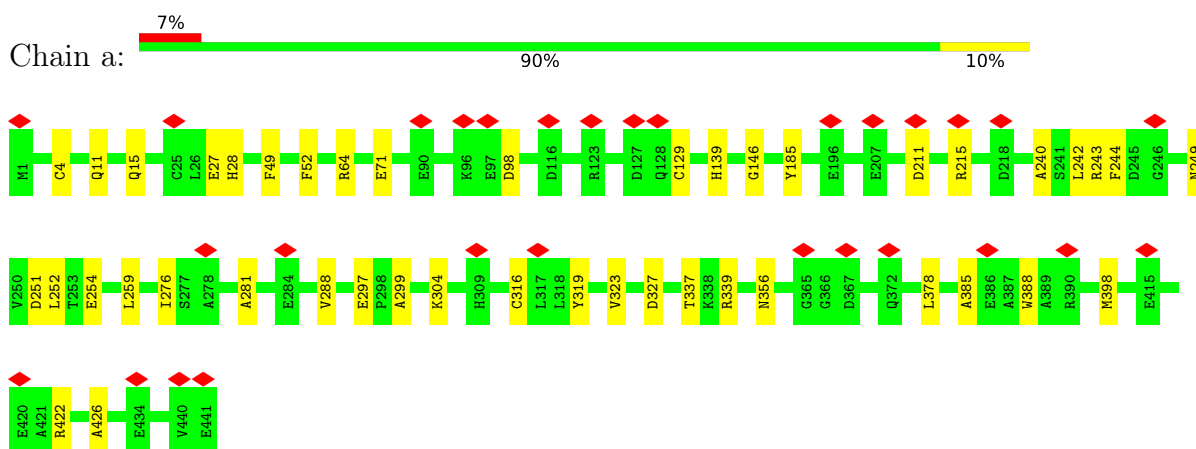
Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
6	a	1	5	4	1	0
6	A	1	5	4	1	0

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

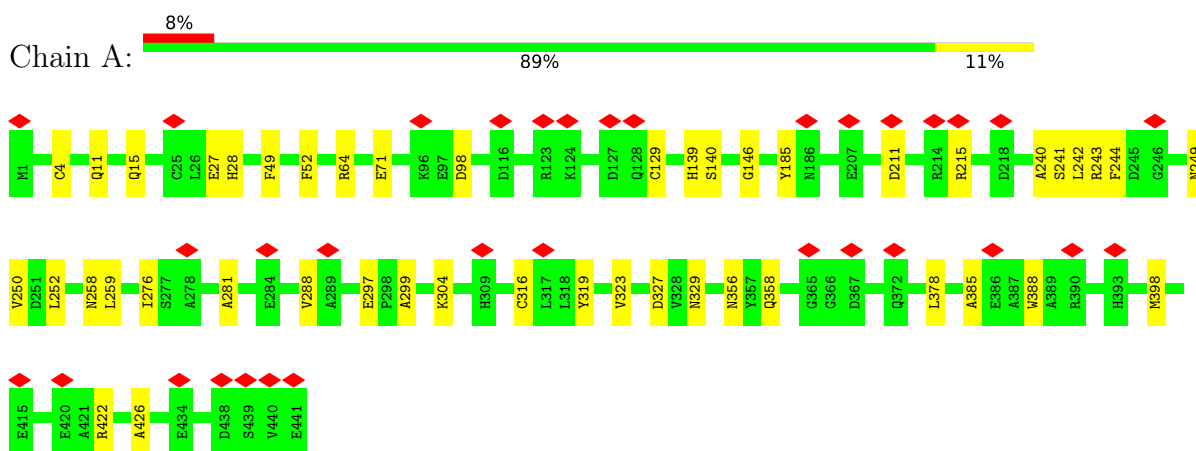
3 Residue-property plots [i](#)

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.

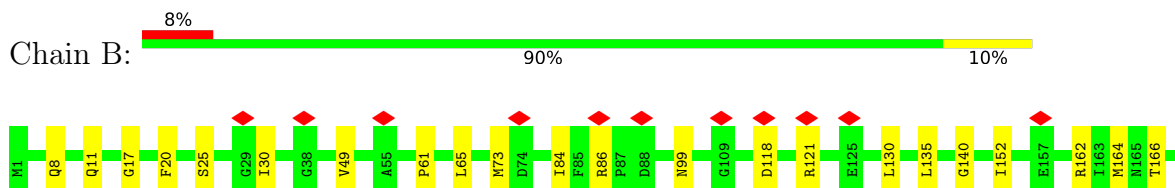
- Molecule 1: Tubulin alpha-1B chain

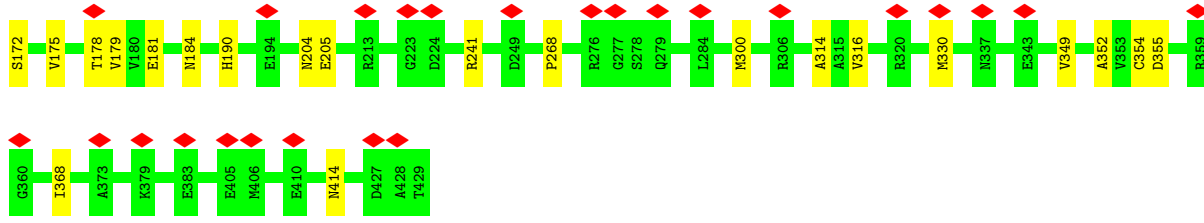


- Molecule 1: Tubulin alpha-1B chain

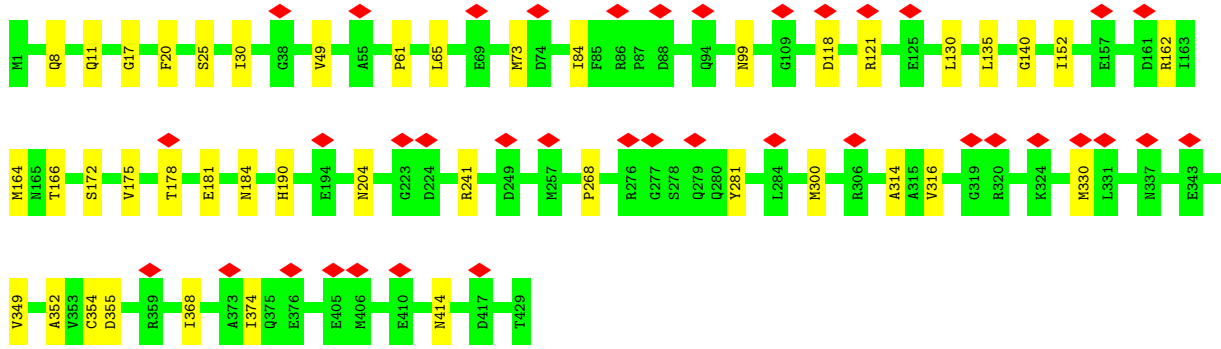
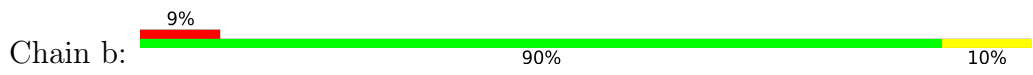


- Molecule 2: Tubulin beta-2B chain

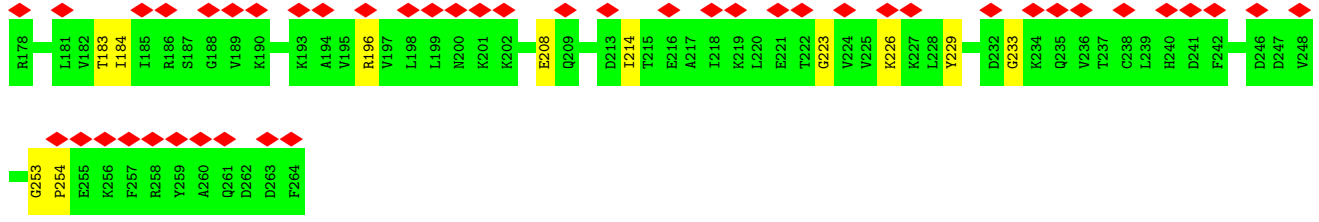
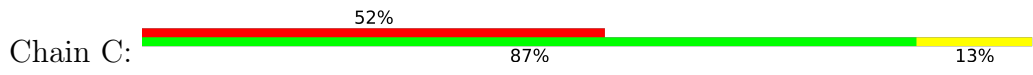




• Molecule 2: Tubulin beta-2B chain



• Molecule 3: Neuronal migration protein doublecortin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6591	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.392	Depositor
Minimum map value	-0.209	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	132.05, 83.4, 129.27	wwPDB
Map dimensions	95, 60, 93	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.3900001	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, PO4

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	0.18	0/3459	0.40	0/4697
1	a	0.18	0/3459	0.40	0/4697
2	B	0.18	0/3443	0.40	0/4666
2	b	0.18	0/3443	0.40	0/4666
3	C	0.23	0/708	0.57	0/953
All	All	0.18	0/14512	0.41	0/19679

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	3382	0	3292	29	0
1	a	3382	0	3292	27	0
2	B	3368	0	3246	25	0
2	b	3368	0	3246	24	0
3	C	696	0	720	7	0
4	A	32	0	12	1	0
4	a	32	0	12	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	a	1	0	0	0	0
6	A	5	0	0	0	0
6	a	5	0	0	2	0
7	B	28	0	12	1	0
7	b	28	0	12	3	0
All	All	14328	0	13844	107	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 107 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:339:ARG:HH22	3:C:208:GLU:HB3	1.56	0.71
1:a:71:GLU:HB3	1:a:98:ASP:HB3	1.72	0.69
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.72	0.69
1:a:249:ASN:H	2:b:11:GLN:HE22	1.44	0.65
2:B:11:GLN:HE22	1:A:249:ASN:H	1.47	0.62

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	428/432 (99%)	409 (96%)	19 (4%)	0	100	100
1	a	428/432 (99%)	409 (96%)	19 (4%)	0	100	100
2	B	427/429 (100%)	413 (97%)	14 (3%)	0	100	100
2	b	427/429 (100%)	413 (97%)	14 (3%)	0	100	100
3	C	85/87 (98%)	69 (81%)	16 (19%)	0	100	100
All	All	1795/1809 (99%)	1713 (95%)	82 (5%)	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	A	364/366 (100%)	364 (100%)	0	100	100
1	a	364/366 (100%)	364 (100%)	0	100	100
2	B	368/369 (100%)	368 (100%)	0	100	100
2	b	368/369 (100%)	368 (100%)	0	100	100
3	C	77/77 (100%)	77 (100%)	0	100	100
All	All	1541/1547 (100%)	1541 (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 39 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	375	GLN
1	A	101	ASN
2	b	384	GLN
1	A	11	GLN
1	A	258	ASN

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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	PO4	A	501	-	4,4,4	1.02	0	6,6,6	0.52	0
7	GDP	b	501	-	29,30,30	0.34	0	45,47,47	0.34	0
4	GTP	a	501	5	33,34,34	0.92	2 (6%)	50,54,54	1.61	9 (18%)
6	PO4	a	503	-	4,4,4	1.00	0	6,6,6	0.57	0
7	GDP	B	501	-	29,30,30	0.34	0	45,47,47	0.34	0
4	GTP	A	502	5	33,34,34	0.92	2 (6%)	50,54,54	1.62	9 (18%)

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	GDP	B	501	-	-	5/16/32/32	0/3/3/3
7	GDP	b	501	-	-	5/16/32/32	0/3/3/3
4	GTP	a	501	5	-	8/22/38/38	0/3/3/3
4	GTP	A	502	5	-	8/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	a	501	GTP	C2-N3	2.09	1.38	1.33
4	a	501	GTP	C5-N7	-2.06	1.34	1.39
4	A	502	GTP	C5-N7	-2.05	1.35	1.39
4	A	502	GTP	C2-N3	2.03	1.38	1.33

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	a	501	GTP	C5-C4-N3	-5.17	120.16	128.39
4	A	502	GTP	C5-C4-N3	-5.11	120.26	128.39
4	a	501	GTP	C2-N3-C4	4.69	120.38	112.30
4	A	502	GTP	C2-N3-C4	4.64	120.29	112.30
4	A	502	GTP	N9-C4-N3	3.27	132.49	125.95

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

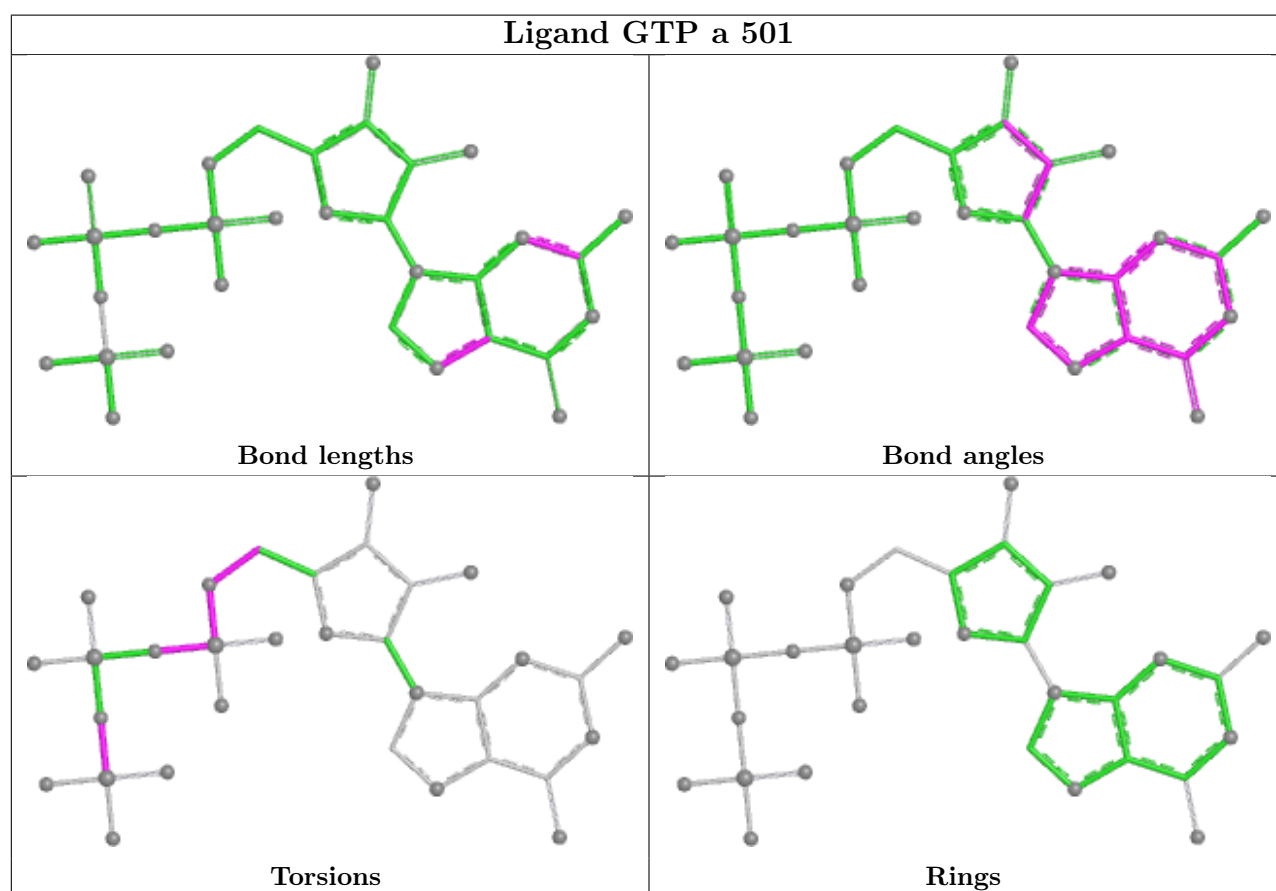
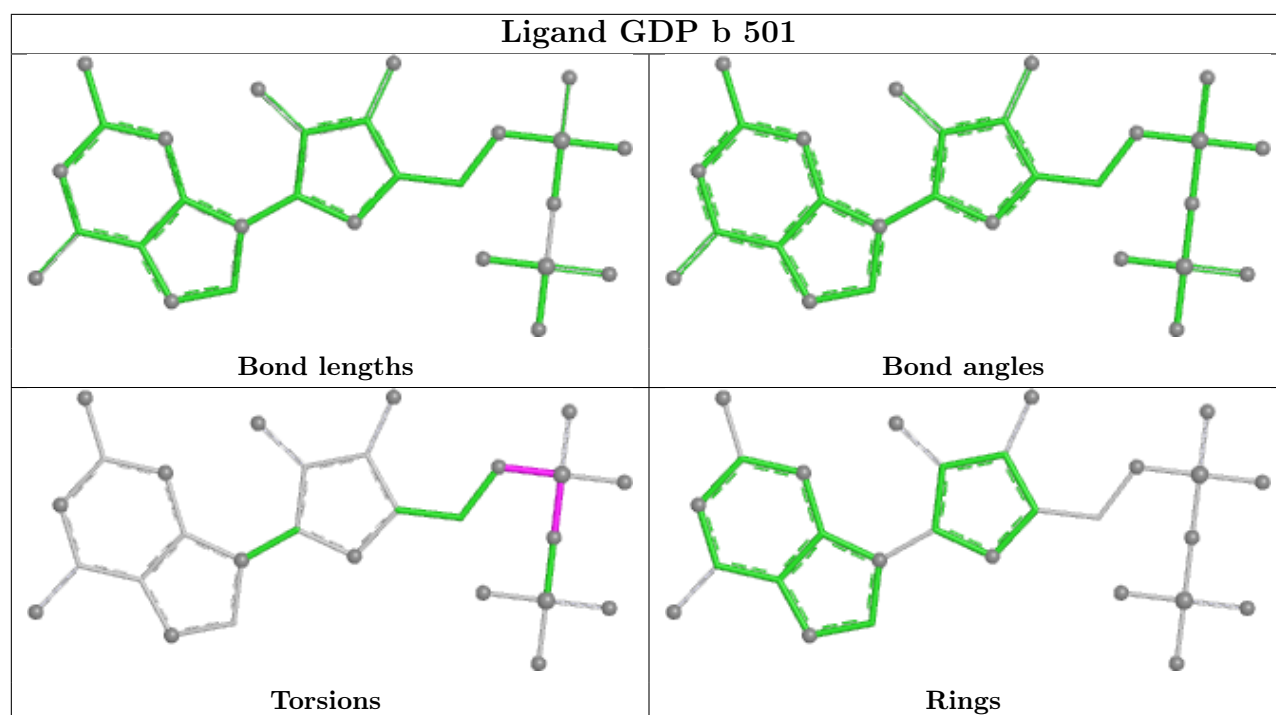
Mol	Chain	Res	Type	Atoms
4	a	501	GTP	C5'-O5'-PA-O3A
4	a	501	GTP	C5'-O5'-PA-O1A
4	a	501	GTP	C5'-O5'-PA-O2A
4	A	502	GTP	C5'-O5'-PA-O3A
7	B	501	GDP	C5'-O5'-PA-O3A

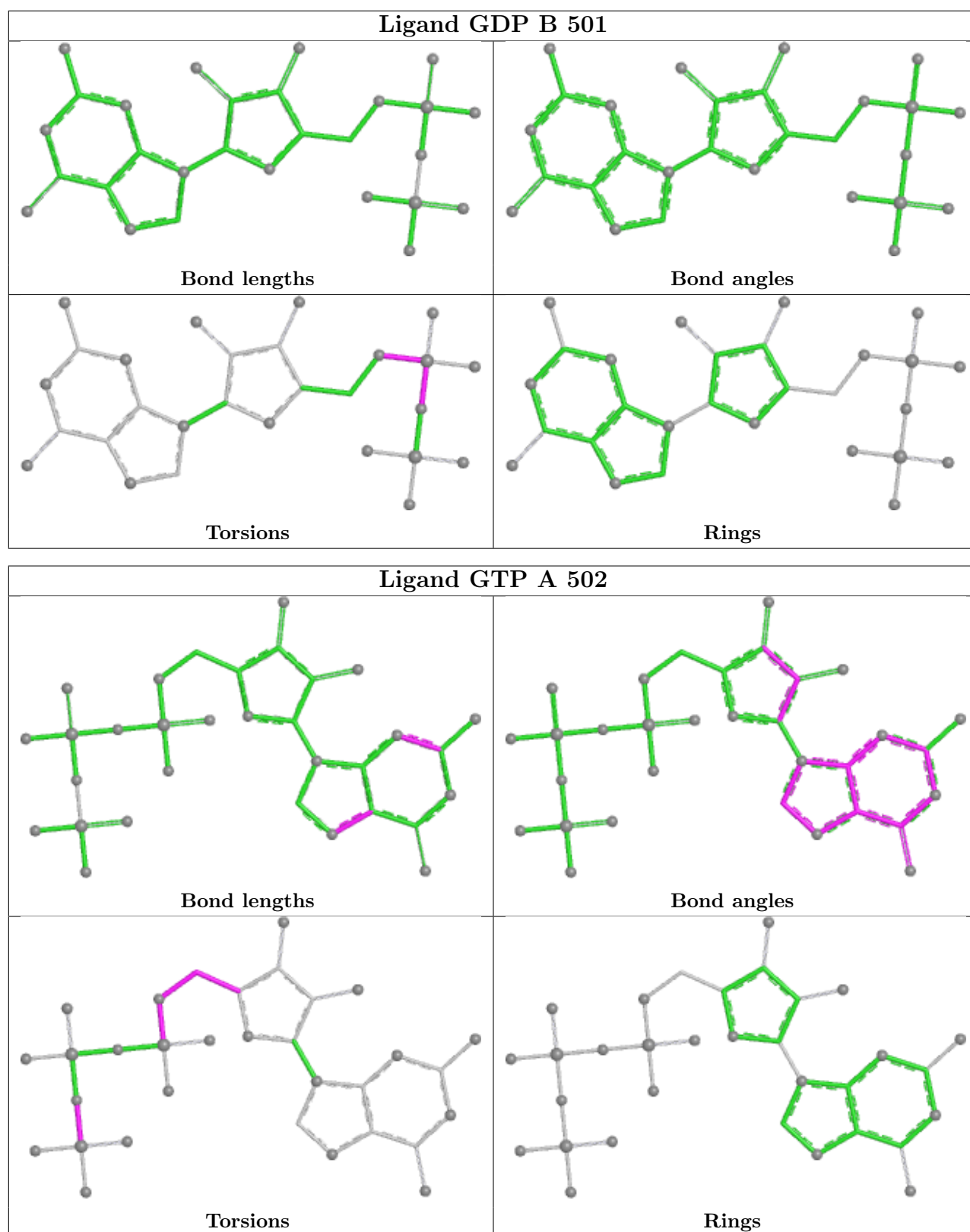
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	b	501	GDP	3	0
6	a	503	PO4	2	0
7	B	501	GDP	1	0
4	A	502	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.





5.7 Other polymers [i](#)

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
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	37:PRO	C	47:ASP	N	14.27
1	A	37:PRO	C	47:ASP	N	14.27

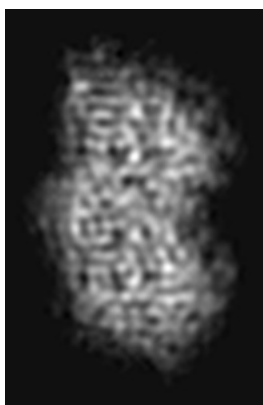
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4861. These allow visual inspection of the internal detail of the map and identification of artifacts.

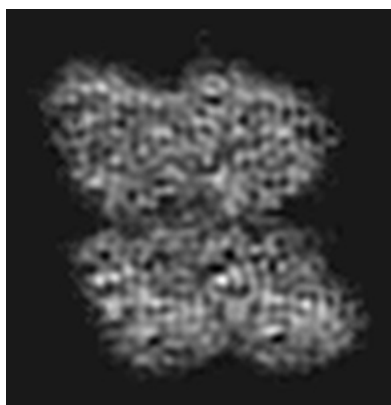
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

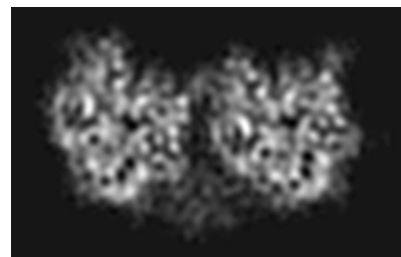
6.1.1 Primary map



X



Y

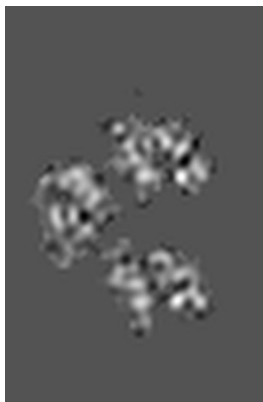


Z

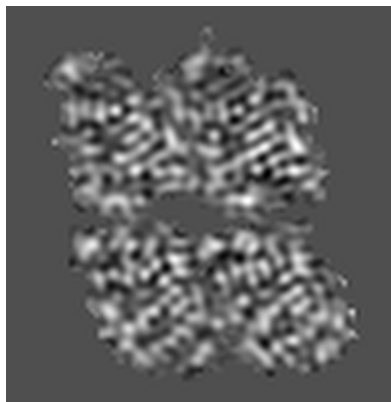
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

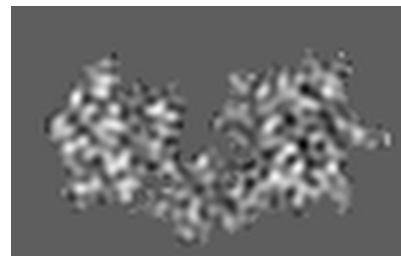
6.2.1 Primary map



X Index: 47



Y Index: 30

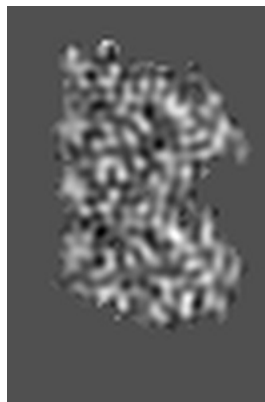


Z Index: 46

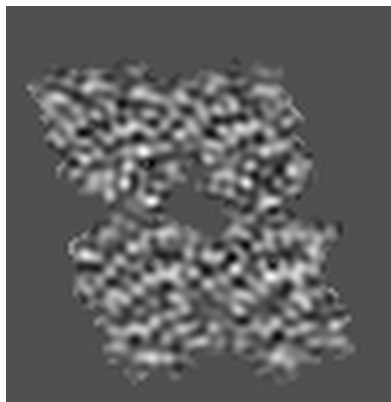
The images above show central slices of the map in three orthogonal directions.

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

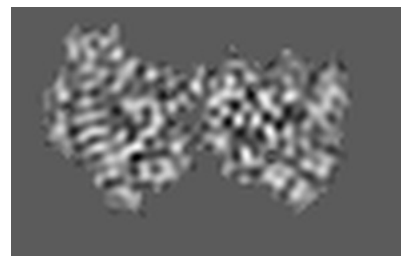
6.3.1 Primary map



X Index: 25



Y Index: 37

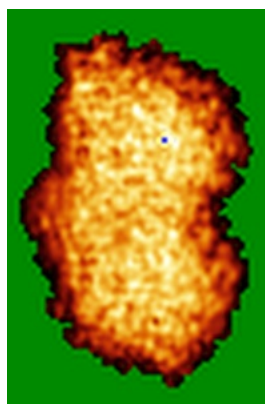


Z Index: 61

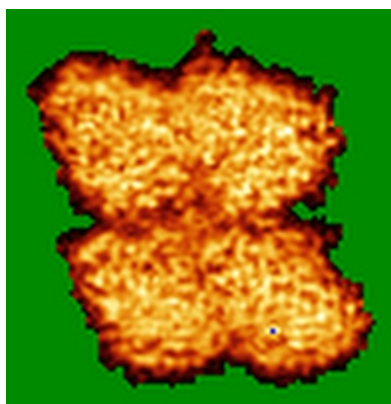
The images above show the largest variance slices of the map in three orthogonal directions.

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

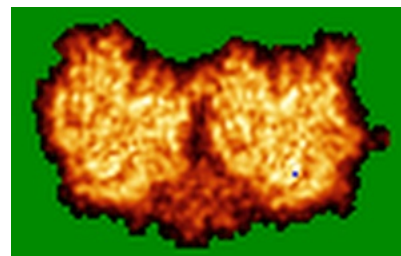
6.4.1 Primary map



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

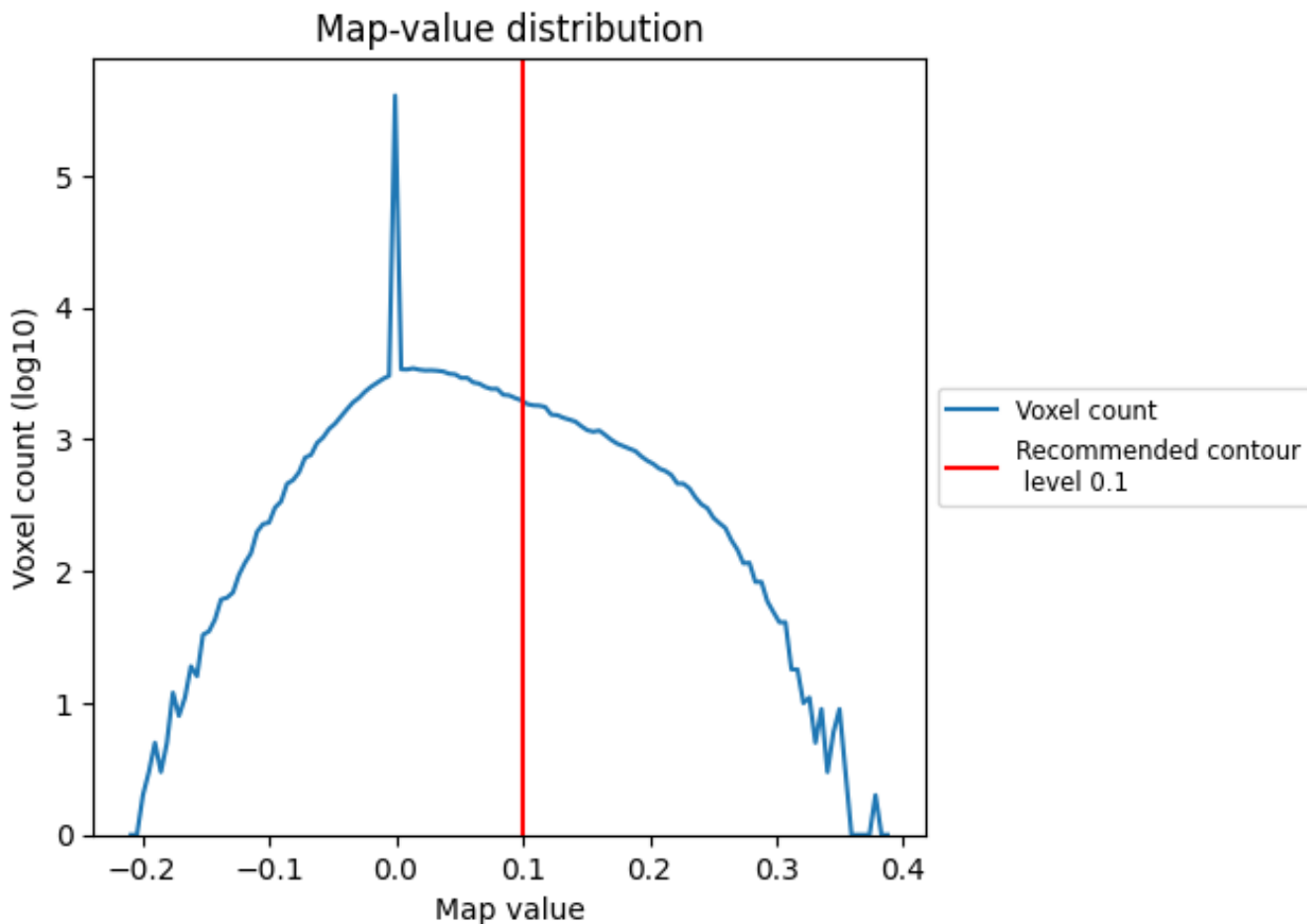
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

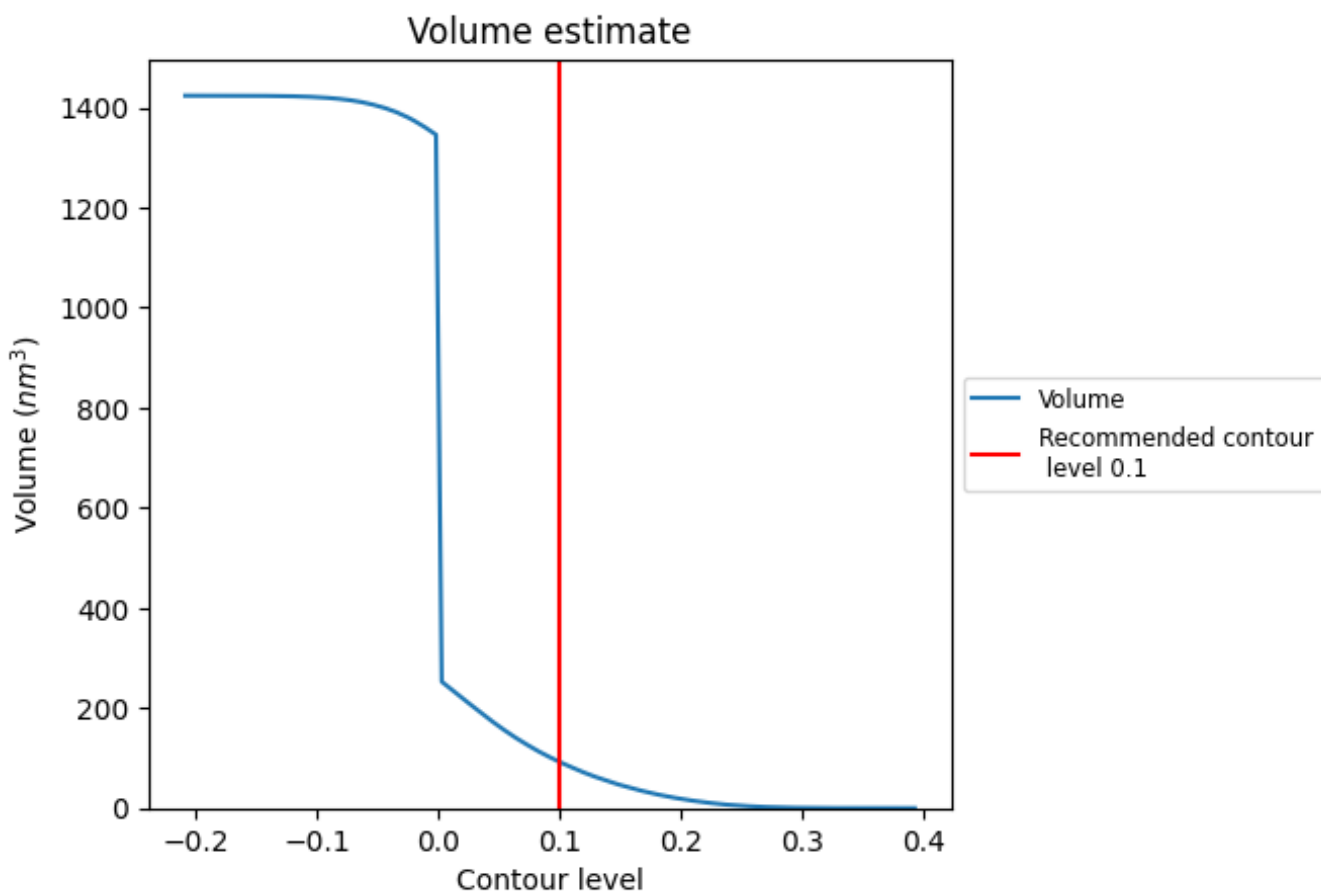
This section contains the results of statistical analysis of the map.

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 92 nm³; this corresponds to an approximate mass of 83 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

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

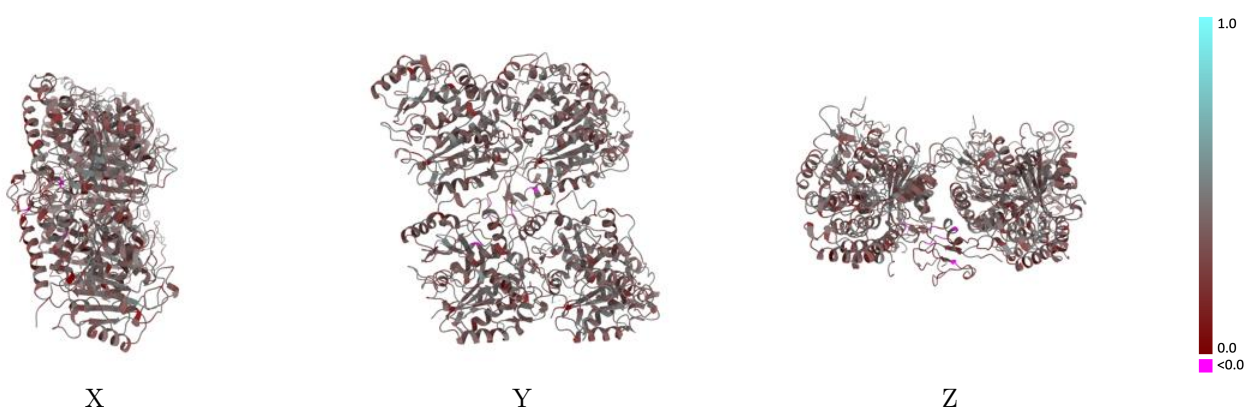
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4861 and PDB model 6RF2. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

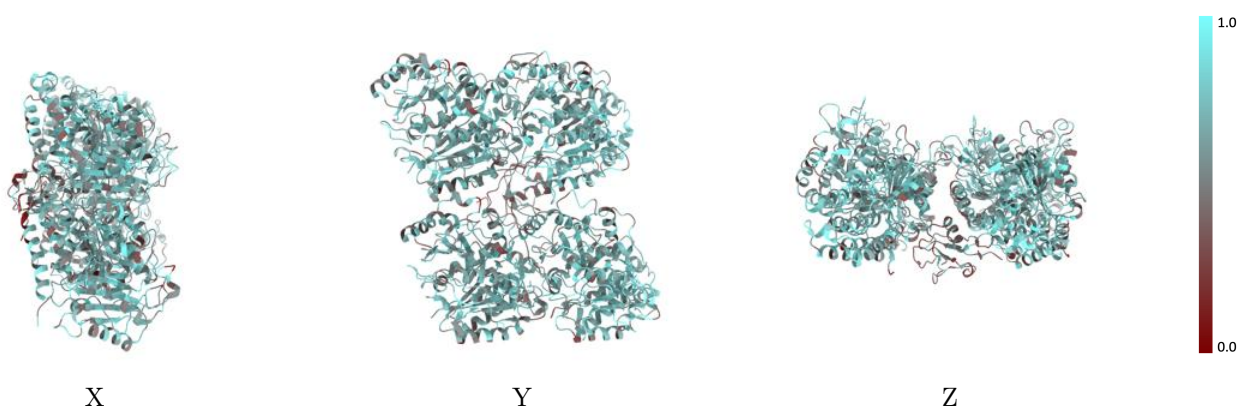
This section was not generated.

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



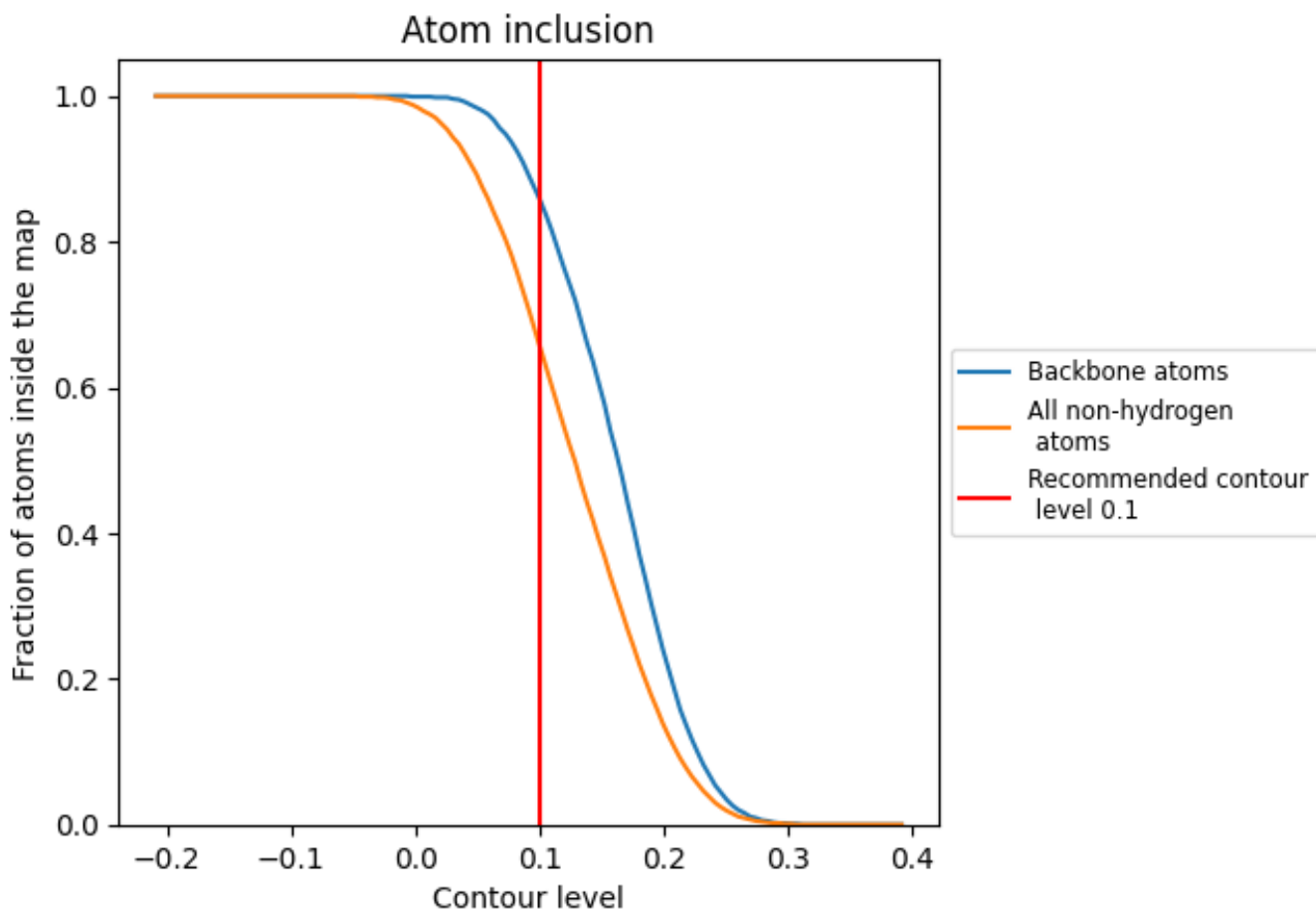
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).













9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6590	 0.3730
A	 0.6860	 0.3830
B	 0.6660	 0.3760
C	 0.4140	 0.2580
a	 0.6760	 0.3820
b	 0.6600	 0.3730

