wwPDB EM Validation Summary Report (i)

Mar 5, 2024 – 11:04 AM EST

PDB ID	:	6MLQ
EMDB ID	:	EMD-9140
Title	:	Cryo-EM structure of microtubule-bound Kif7 in the ADP state
Authors	:	Mani, N.; Jiang, S.; Wilson-Kubalek, E.M.; Ku, P.; Milligan, R.A.; Subramanian, R.
Deposited on	:	2018-09-27
Resolution	:	4.20 Å(reported)
Based on initial models	:	4A14, 3J6G

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 (i) 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 (1)) were used in the production of this report:

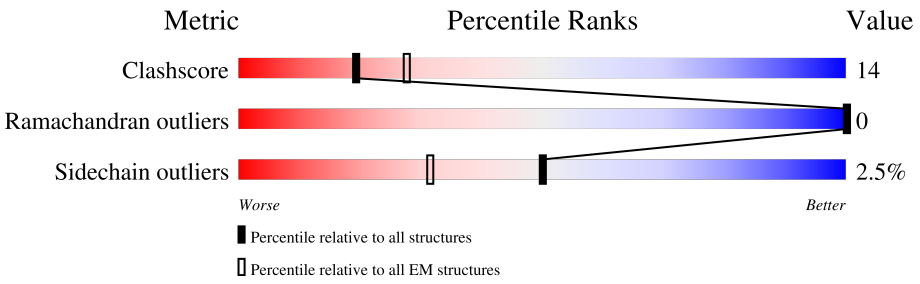
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	451	75% 16% 9%
2	B	445	73% 21% • •
3	C	399	9% 63% 18% • 18%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9197 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-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	411	3224	2042	550	612	20	0	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	426	3351	2105	575	646	25	0	0

- Molecule 3 is a protein called Kinesin-like protein KIF7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	327	2471	1547	435	480	9	0	0

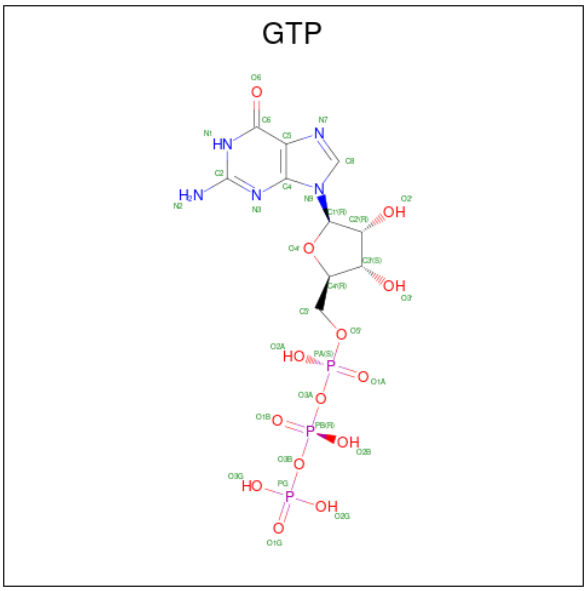
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP Q2M1P5

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

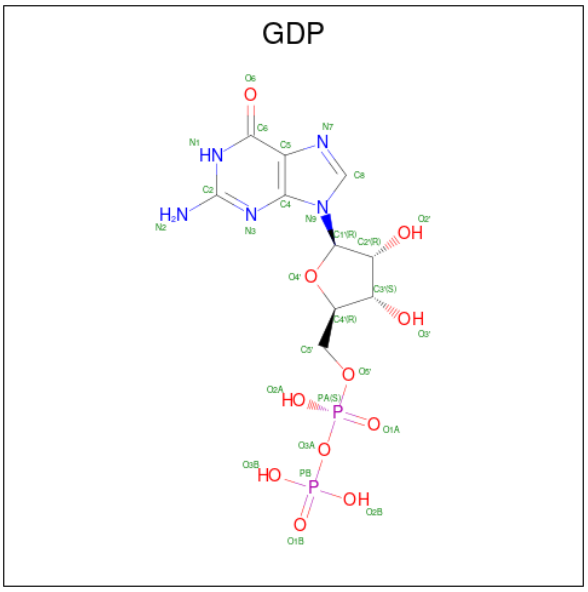
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	A	1	1	1	0
4	C	1	1	1	0

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



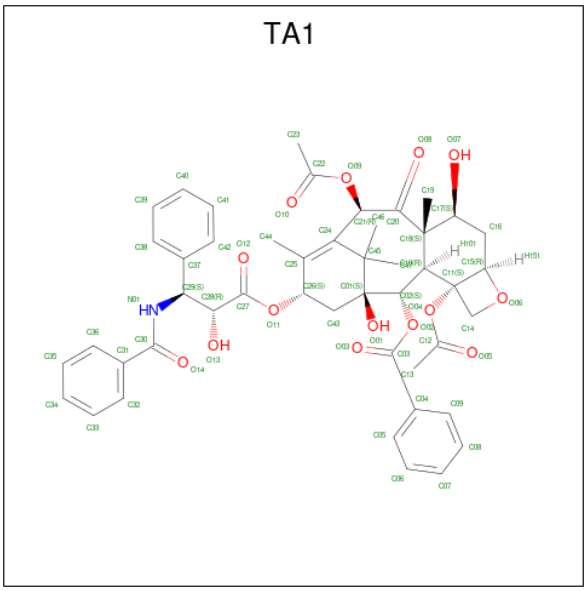
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	A	1	32	10	5	14	3	0

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



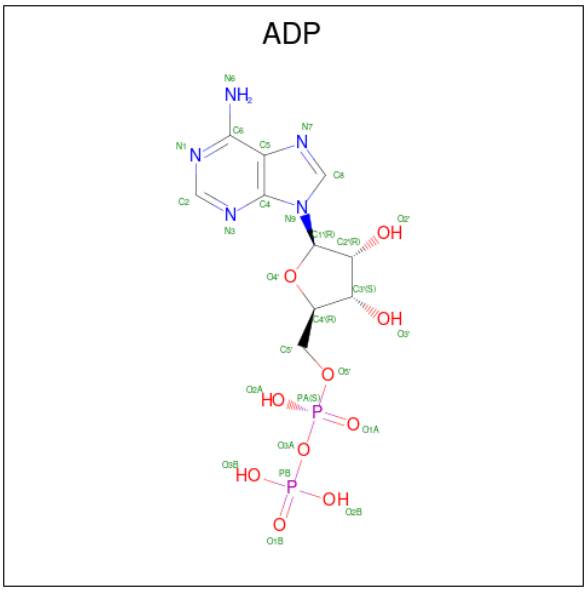
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	B	1	28	10	5	11	2	0

- Molecule 7 is TAXOL (three-letter code: TA1) (formula: $C_{47}H_{51}NO_{14}$).



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

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



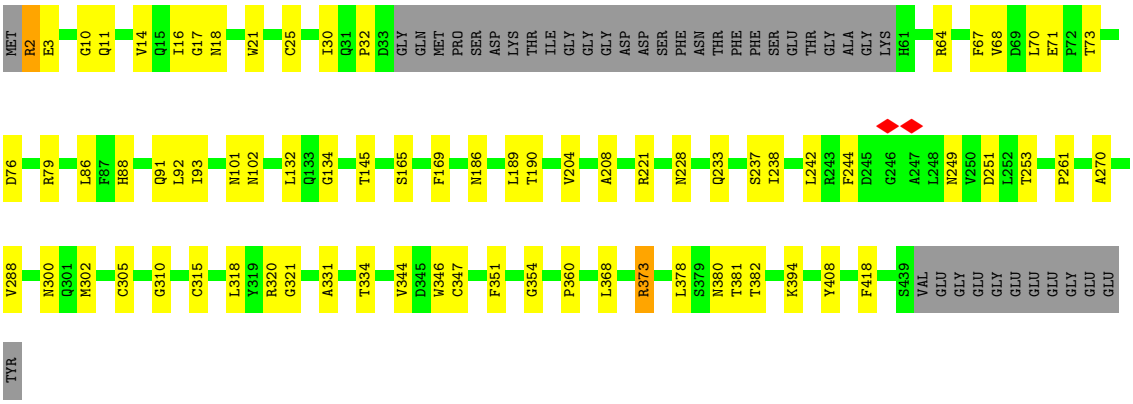
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	C	1	27	10	5	10	2	0

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.

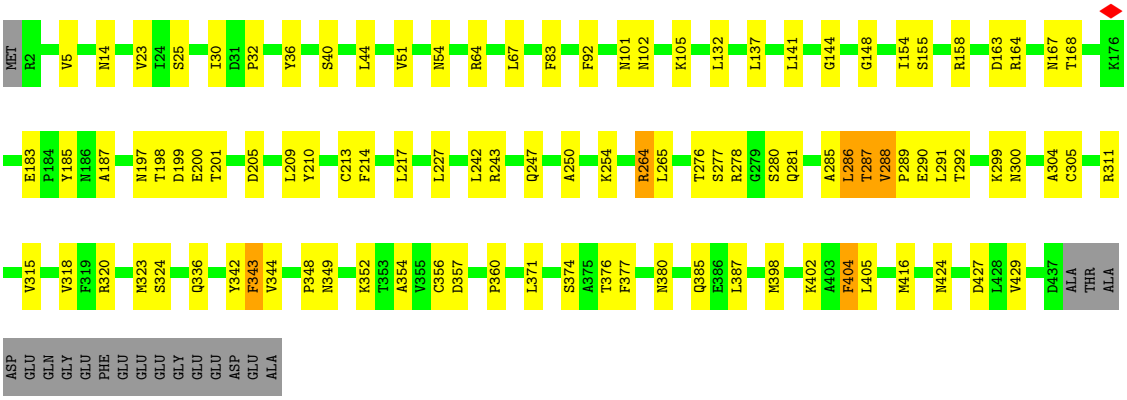
• Molecule 1: Tubulin alpha-1A chain

Chain A: 75% 16% 9%



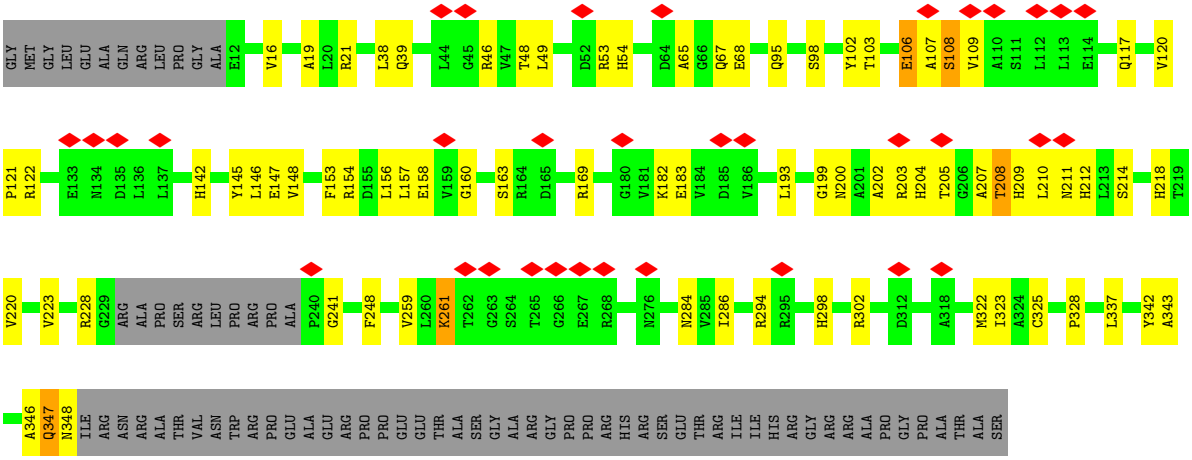
• Molecule 2: Tubulin beta chain

Chain B: 73% 21%



• Molecule 3: Kinesin-like protein KIF7

Chain C: 9% 63% 18% 18%


GLY MET GLY LEU GLU ALA GLN ARG LEU PRO GLY ALA E12 V16 A19 L20 R21 L38 Q39 L44 G45 R46 V47 T48 L49 D52 R53 H54 D64 A65 G66 Q67 E68 Q95 S98 Y102 T103 E106 A107 S108 V109 A110 S111 L112 L113 E114 Q117 V120
P121 R122 E133 N134 D135 L136 L137 H142 Y145 L146 E147 V148 F153 R154 D155 L156 L157 E158 V159 G160 S163 R164 D165 R169 G180 V181 K182 E183 V184 D185 V186 L193 G199 N200 A201 A202 R203 H204 T205 G206 A207 T208 H209 L210 N211 H212 L213 S214 H218 T219
V220 V223 R228 G229 ARG ALA PRO SER ARG LEU PRO ARG PRO ALA P240 G241 F248 V259 L260 K261 T262 G263 S264 T265 G266 E267 R268 N276 N284 V285 I286 R294 R295 H298 R302 D312 A318 M322 I323 A324 C325 P328 L337 Y342 A343
A346 Q347 N348 ILE ARG ASN ARG ALA THR VAL ASN TRP ARG PRO GLU ALA GLU ARG PRO PRO GLU GLU THR ALA SER GLY ALA ARG GLY PRO PRO ARG HIS ARG SER GLU THR ARG ILE ILE HIS ARG GLY ARG ARG ALA PRO GLY PRO ALA THR ALA SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-23.84°, rise=11.11 Å, axial sym=C1	Depositor
Number of segments used	15919	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	37	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	0.126	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	79.909996, 167.68, 112.659996	wwPDB
Map dimensions	61, 128, 86	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	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: TA1, ADP, GTP, GDP, 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	0.34	0/3297	0.60	0/4479
2	B	0.34	0/3426	0.57	0/4642
3	C	0.27	0/2509	0.54	0/3396
All	All	0.32	0/9232	0.57	0/12517

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	3
2	B	0	4
3	C	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	238	ILE	Peptide
1	A	244	PHE	Peptide
1	A	368	LEU	Peptide
2	B	183	GLU	Peptide
2	B	264	ARG	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	3224	0	3141	47	0
2	B	3351	0	3229	93	0
3	C	2471	0	2420	120	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	32	0	12	0	0
6	B	28	0	12	0	0
7	B	62	0	51	4	0
8	C	27	0	12	1	0
All	All	9197	0	8877	255	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 14.

The worst 5 of 255 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)
3:C:322:MET:CE	3:C:347:GLN:HG3	1.27	1.59
3:C:322:MET:HE1	3:C:347:GLN:CG	1.11	1.58
3:C:322:MET:HE1	3:C:347:GLN:CB	1.43	1.47
3:C:107:ALA:CB	3:C:193:LEU:CD2	1.99	1.36
3:C:107:ALA:HB2	3:C:193:LEU:CD2	1.55	1.35

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	407/451 (90%)	365 (90%)	42 (10%)	0	100	100
2	B	424/445 (95%)	380 (90%)	44 (10%)	0	100	100
3	C	323/399 (81%)	298 (92%)	25 (8%)	0	100	100
All	All	1154/1295 (89%)	1043 (90%)	111 (10%)	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	347/377 (92%)	342 (99%)	5 (1%)	67	80
2	B	367/381 (96%)	355 (97%)	12 (3%)	38	61
3	C	262/328 (80%)	255 (97%)	7 (3%)	44	66
All	All	976/1086 (90%)	952 (98%)	24 (2%)	50	68

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	380	ASN
3	C	106	GLU
2	B	424	ASN
3	C	108	SER
2	B	101	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	337	ASN
3	C	211	ASN
2	B	349	ASN
3	C	348	ASN
3	C	54	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	GDP	B	600	-	24,30,30	0.97	1 (4%)	30,47,47	1.40	4 (13%)
5	GTP	A	502	4	26,34,34	1.26	1 (3%)	32,54,54	1.50	7 (21%)
7	TA1	B	601	-	68,68,68	3.01	25 (36%)	105,105,105	2.06	25 (23%)
8	ADP	C	401	4	24,29,29	0.96	1 (4%)	29,45,45	1.46	4 (13%)

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	GDP	B	600	-	-	5/12/32/32	0/3/3/3
5	GTP	A	502	4	-	6/18/38/38	0/3/3/3
7	TA1	B	601	-	-	13/41/127/127	0/7/7/7
8	ADP	C	401	4	-	6/12/32/32	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	601	TA1	C25-C24	-10.06	1.19	1.34
7	B	601	TA1	C11-C10	7.17	1.70	1.54
7	B	601	TA1	O06-C15	-7.11	1.32	1.46
7	B	601	TA1	C43-C26	6.74	1.66	1.52
7	B	601	TA1	C14-C11	-6.05	1.36	1.53

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	601	TA1	O11-C27-C28	5.58	120.30	111.15
7	B	601	TA1	C10-C18-C17	5.39	117.03	106.54
7	B	601	TA1	C16-C15-C11	-5.11	112.43	119.61
7	B	601	TA1	O09-C22-C23	4.82	119.95	111.09
7	B	601	TA1	C21-C24-C25	-4.81	113.64	120.40

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	600	GDP	C5'-O5'-PA-O1A
6	B	600	GDP	C5'-O5'-PA-O2A
7	B	601	TA1	C28-C27-O11-C26
8	C	401	ADP	PA-O3A-PB-O3B
8	C	401	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

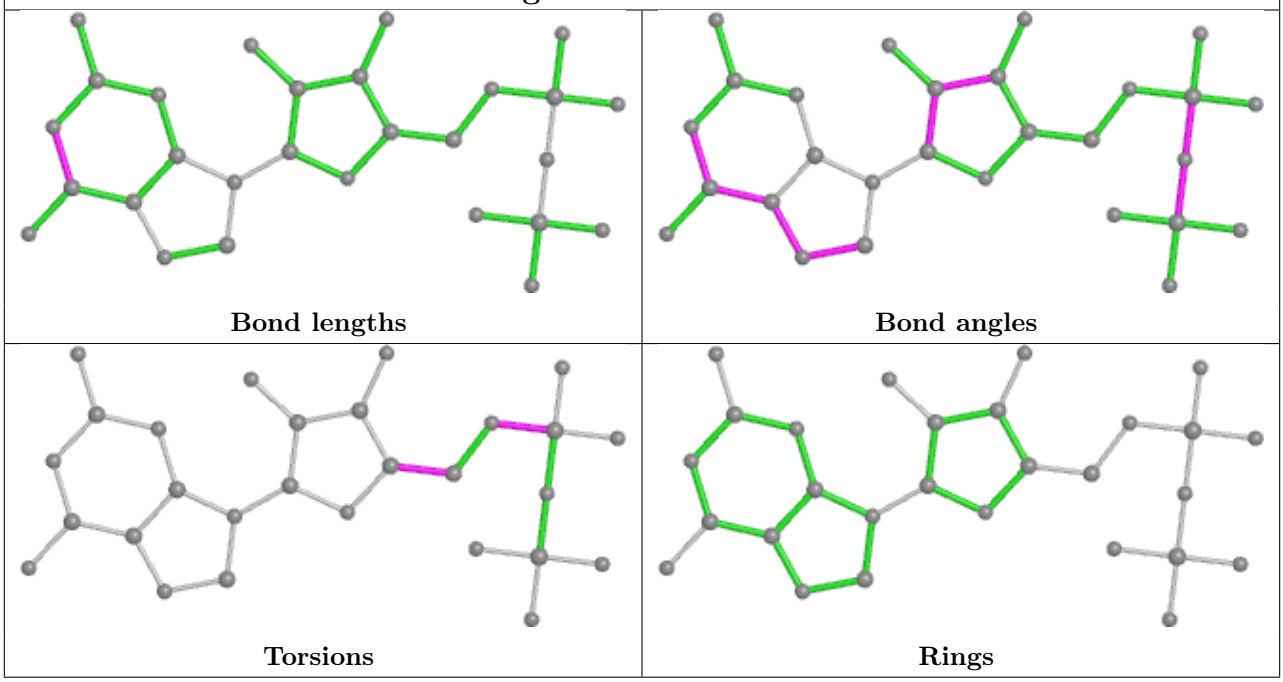
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	601	TA1	4	0
8	C	401	ADP	1	0

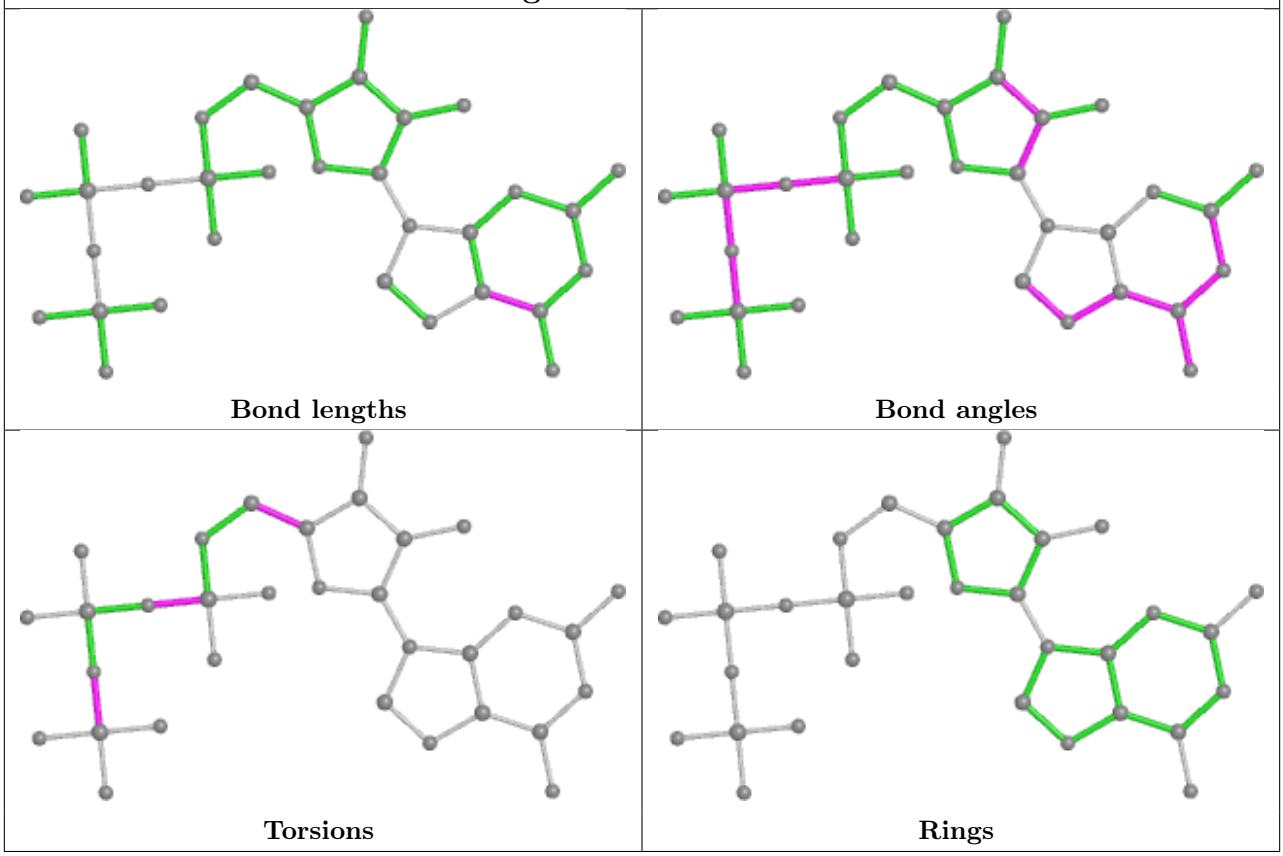
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

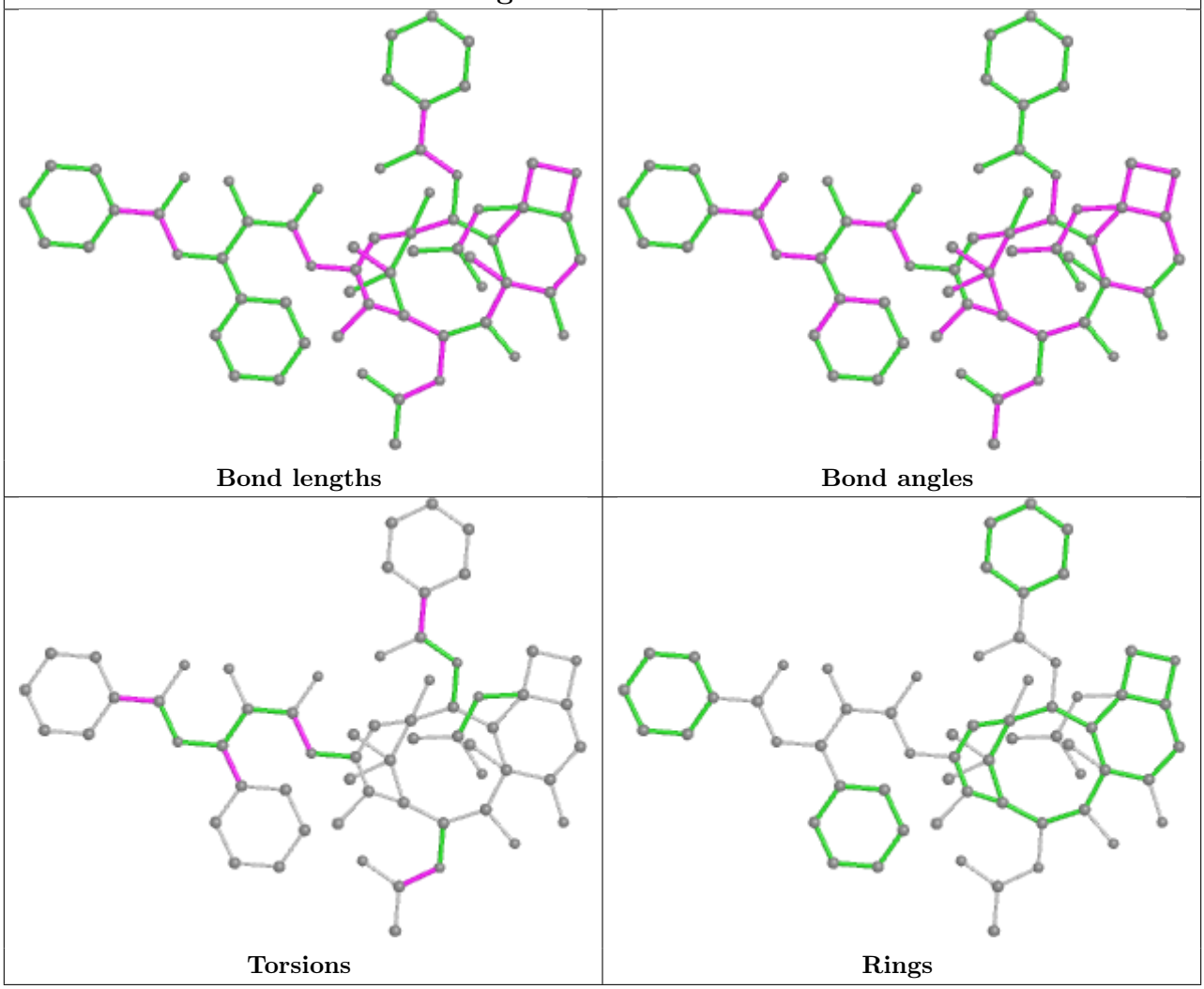
Ligand GDP B 600

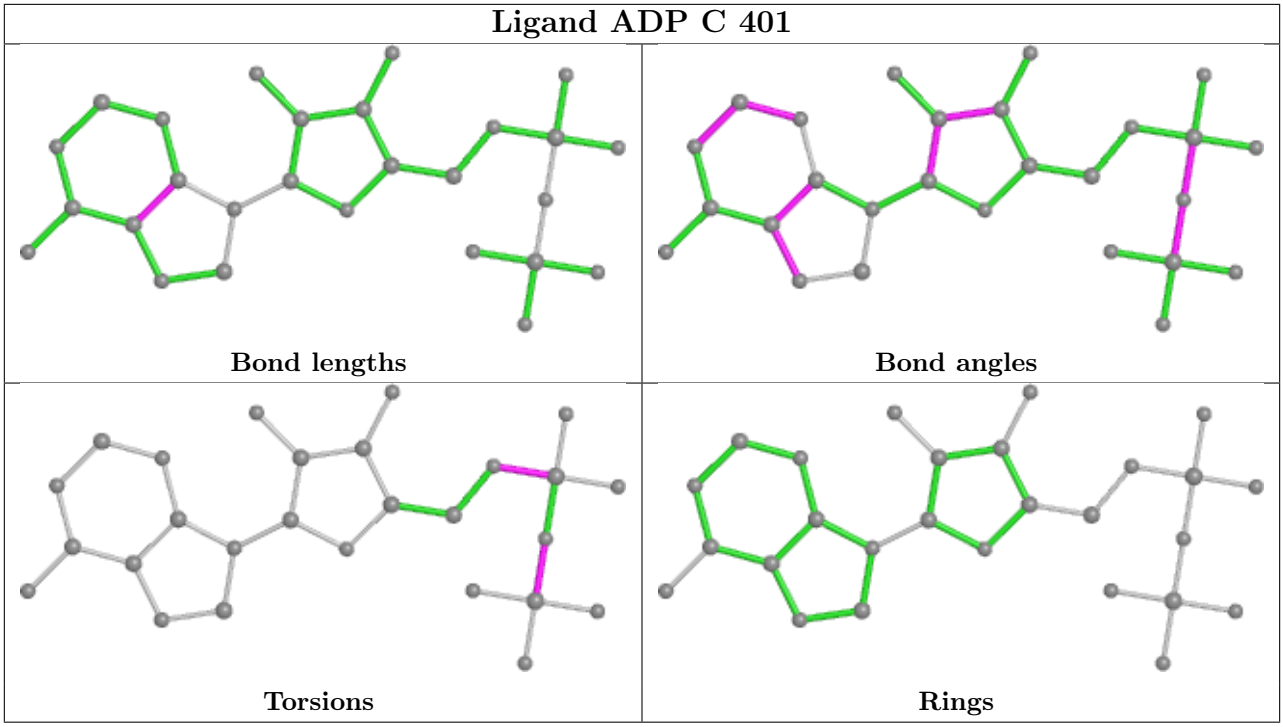


Ligand GTP A 502



Ligand TA1 B 601





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-9140. 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)

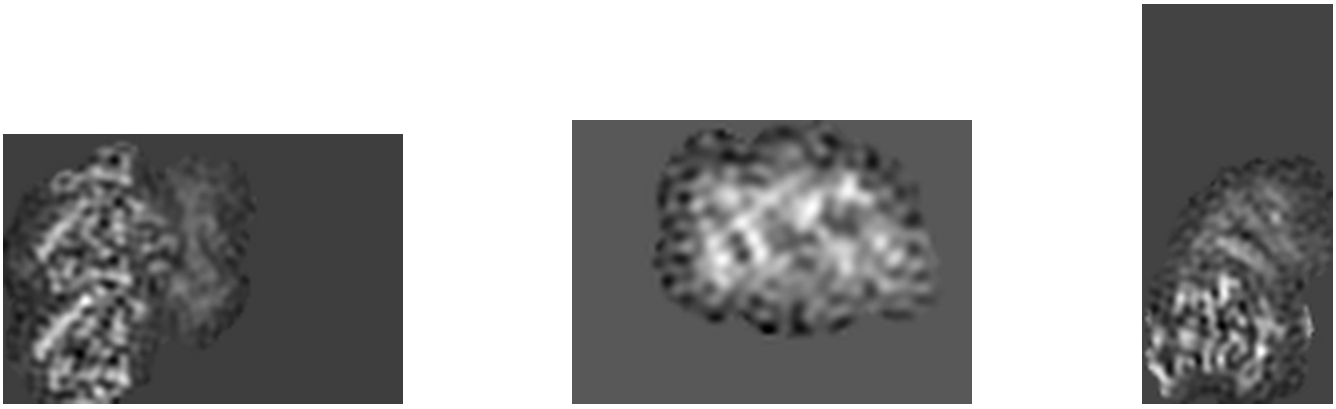
6.1.1 Primary map

X Y Z

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

6.2 Central slices (i)

6.2.1 Primary map

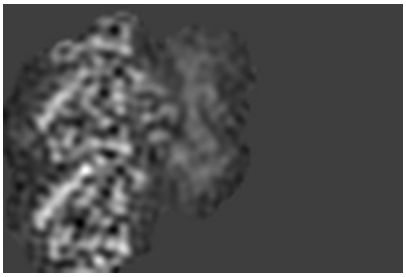


X Index: 30 Y Index: 64 Z Index: 43

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: 30

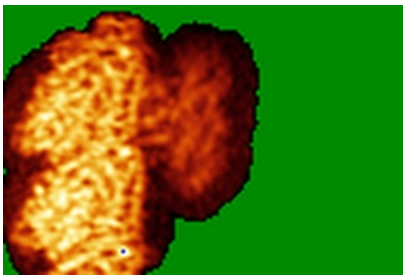
Y Index: 19

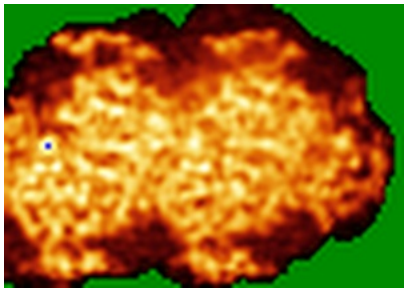
Z Index: 49

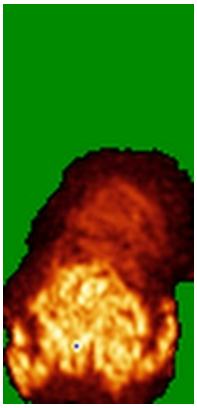
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

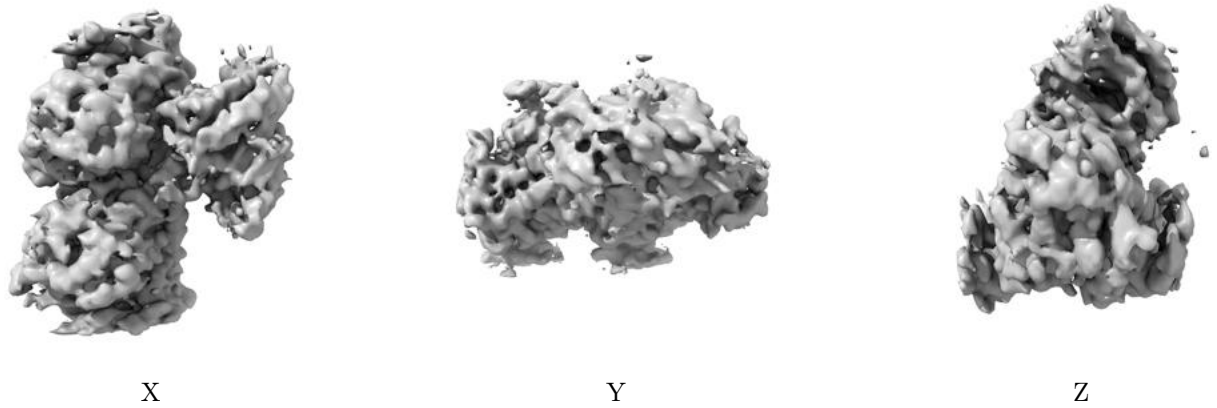

Y


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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

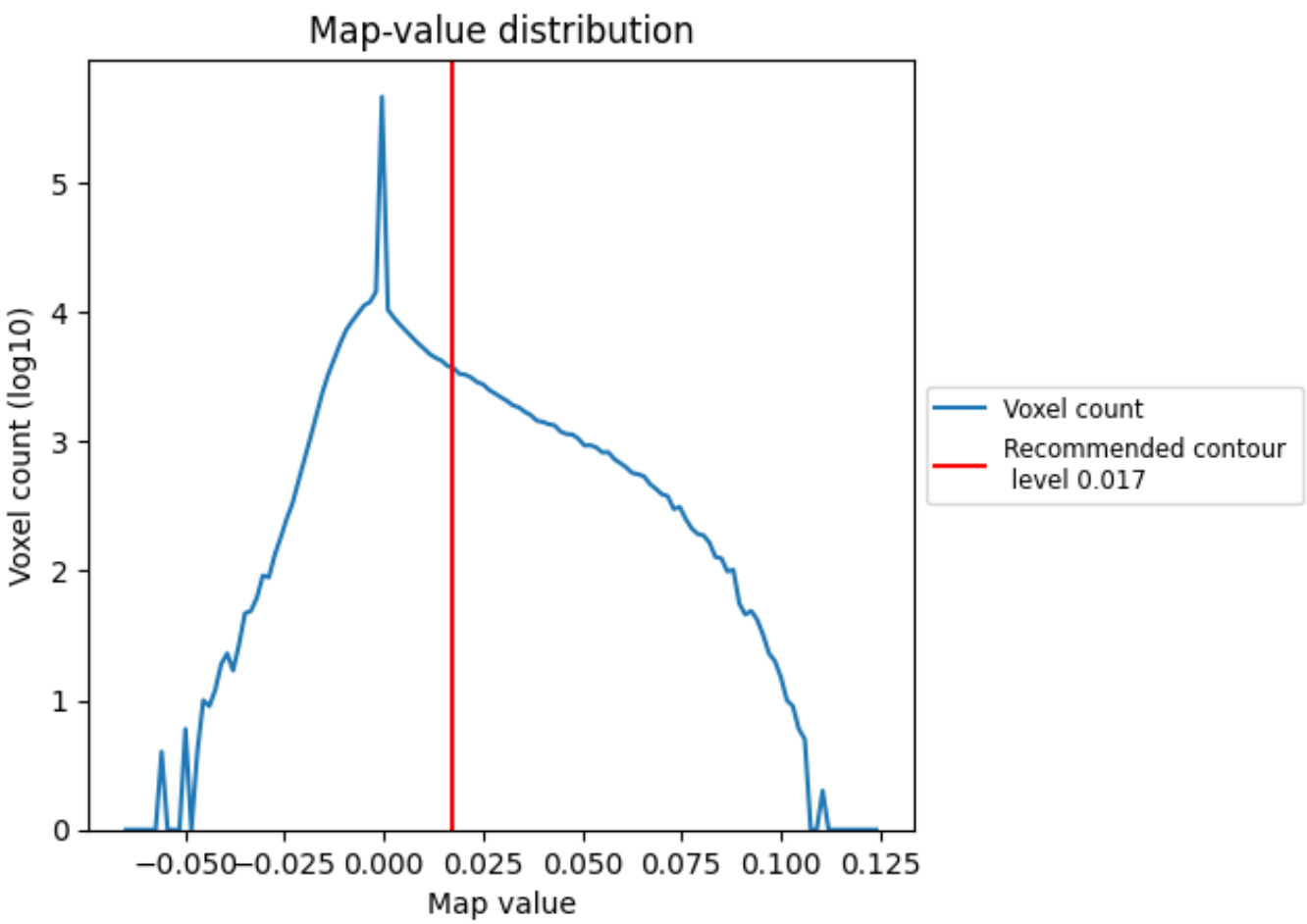
6.6 Mask visualisation (i)

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

7 Map analysis (i)

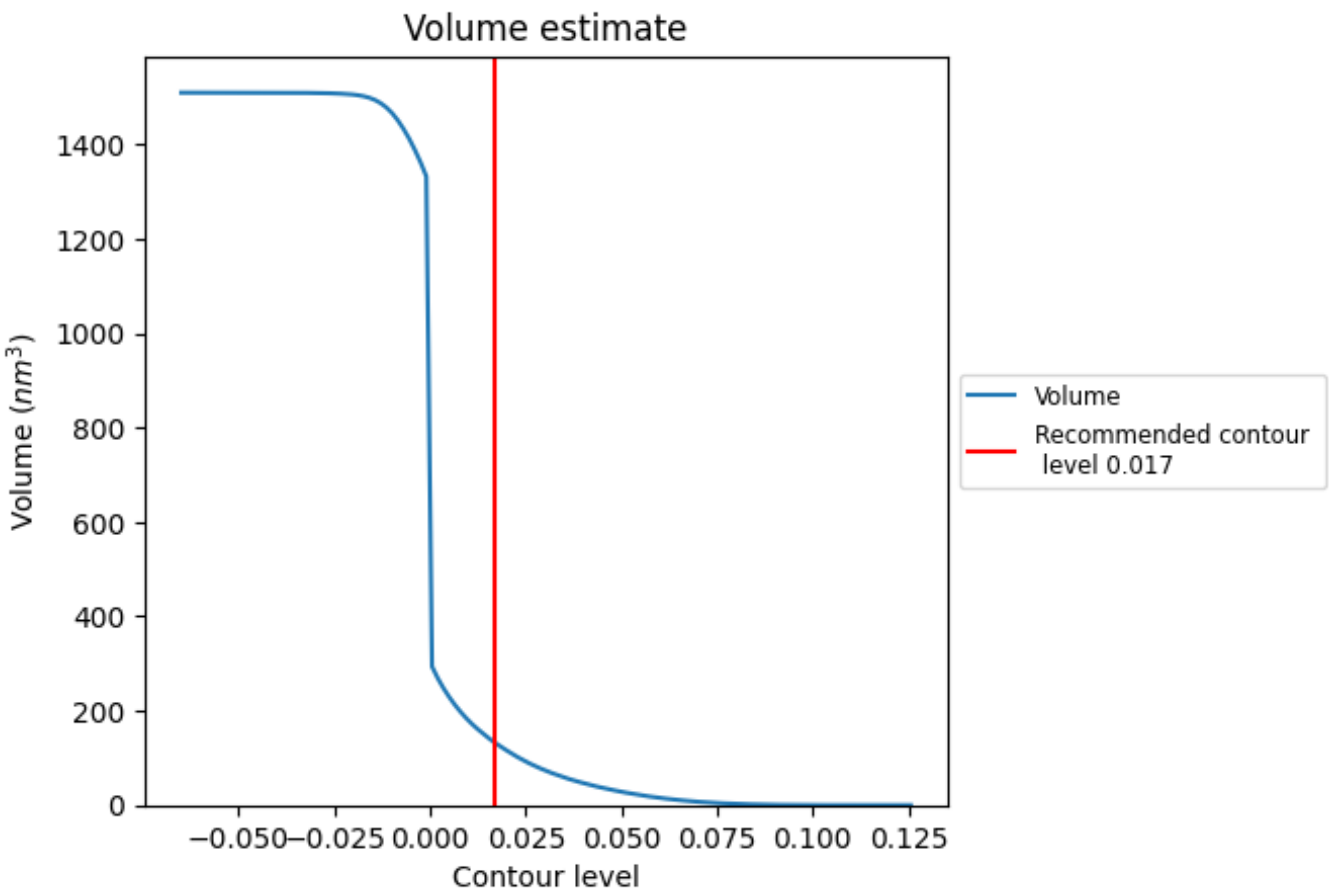
This section contains the results of statistical analysis of the map.

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 132 nm^3; this corresponds to an approximate mass of 119 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.

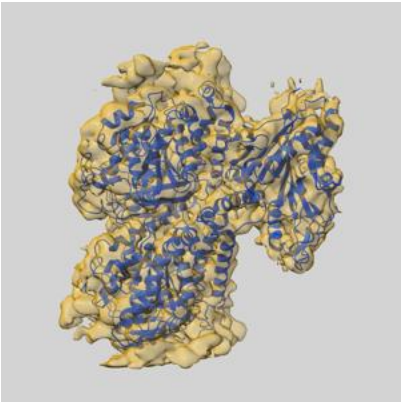
8 Fourier-Shell correlation (i)

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

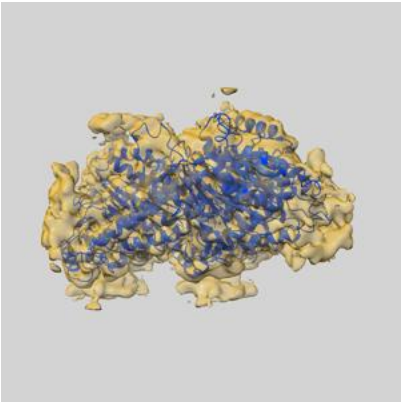
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9140 and PDB model 6MLQ. Per-residue inclusion information can be found in section 3 on page 6.

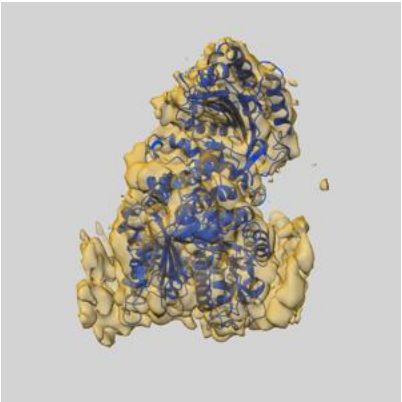
9.1 Map-model overlay (i)



X



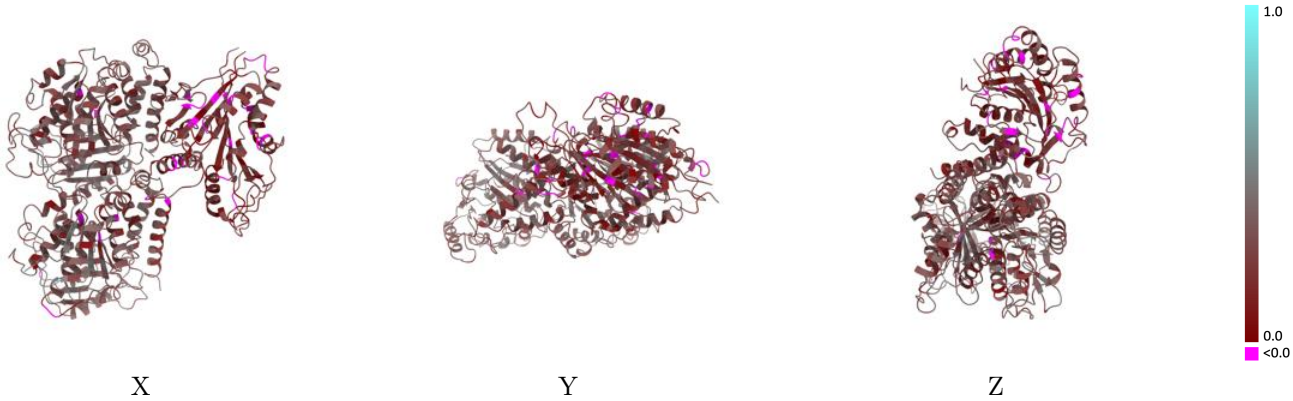
Y



Z

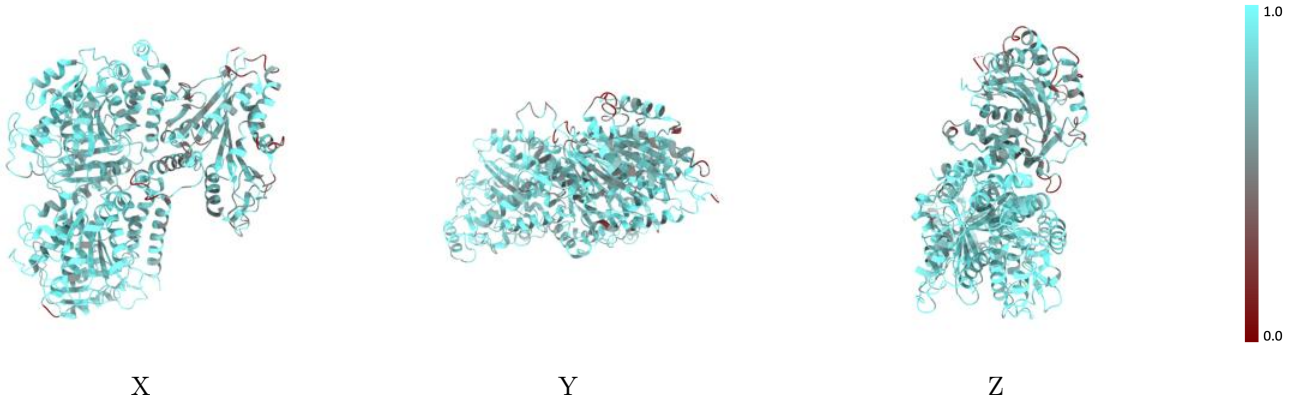
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



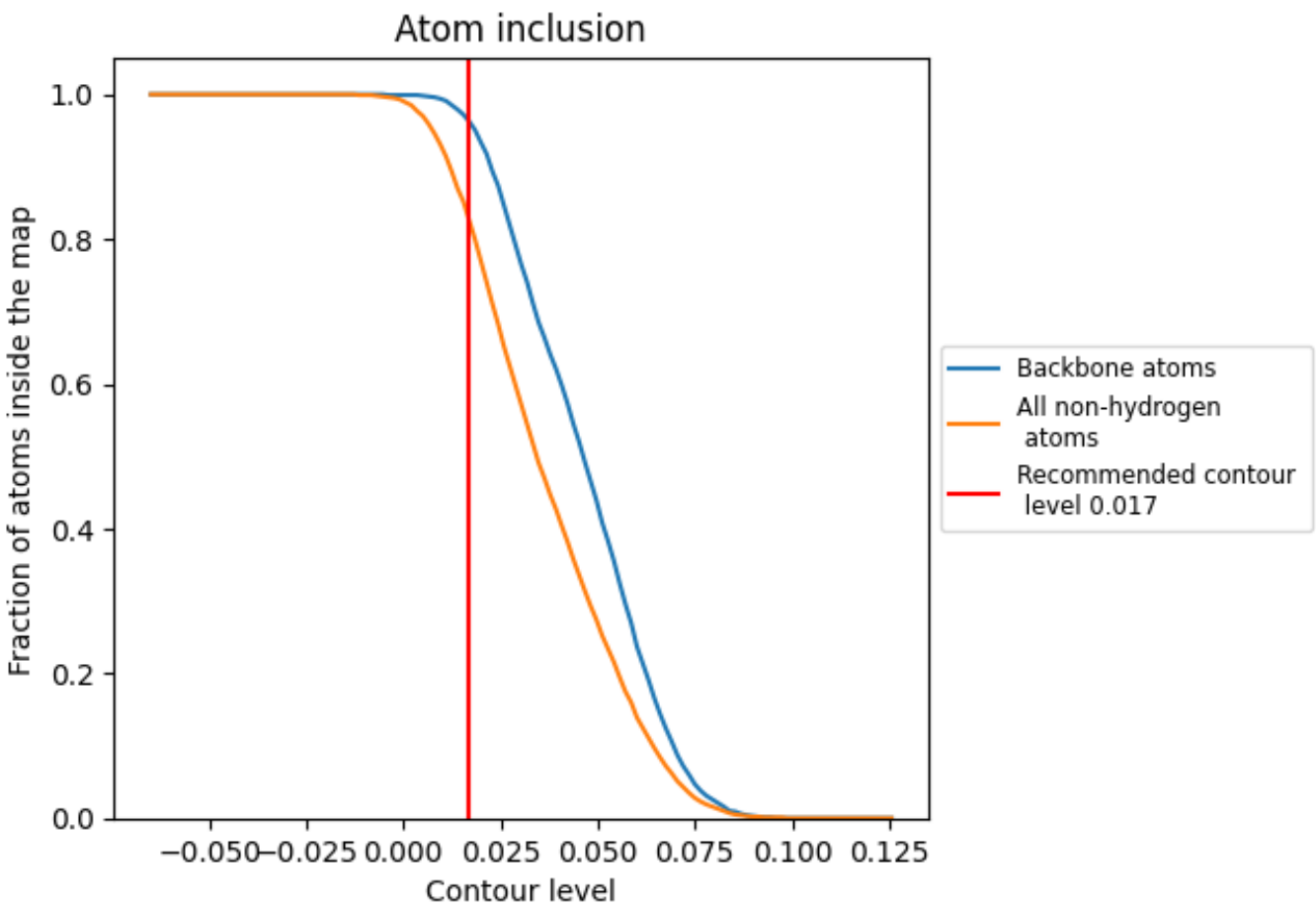
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 82% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8250	0.2830
A	0.8740	0.3160
B	0.8740	0.3090
C	0.6950	0.2050