wwPDB EM Validation Summary Report (i)

Feb 25, 2024 – 06:38 AM EST

PDB ID	:	6XLC
EMDB ID	:	EMD-22239
Title	:	Full-length Hsc82 bound to AMPPNP
Authors	:	Liu, Y.X.; Sun, M.; Myasnikov, A.G.; Elnatan, D.; Agard, D.A.
Deposited on	:	2020-06-28
Resolution	:	3.66 Å(reported)

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

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

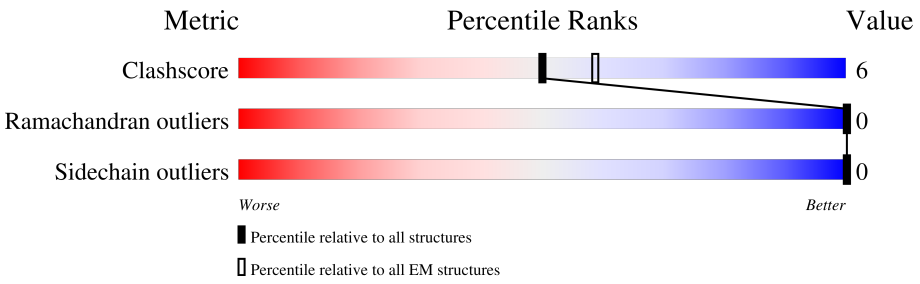
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.66 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	705	30% 72% 14% 14%
1	B	705	30% 70% 16% 14%

2 Entry composition (i)

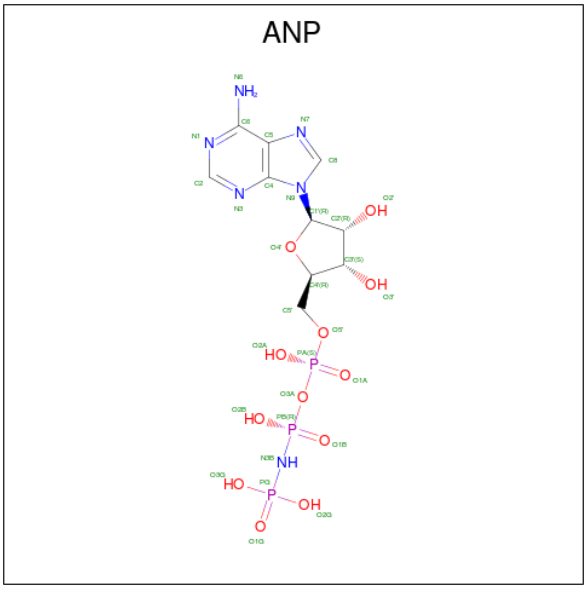
There are 3 unique types of molecules in this entry. The entry contains 9858 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-dependent molecular chaperone HSC82.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	606	4897	3133	804	951	9	0	0
1	B	606	4897	3133	804	951	9	0	0

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	31	10	6	12	3	0
2	B	1	31	10	6	12	3	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

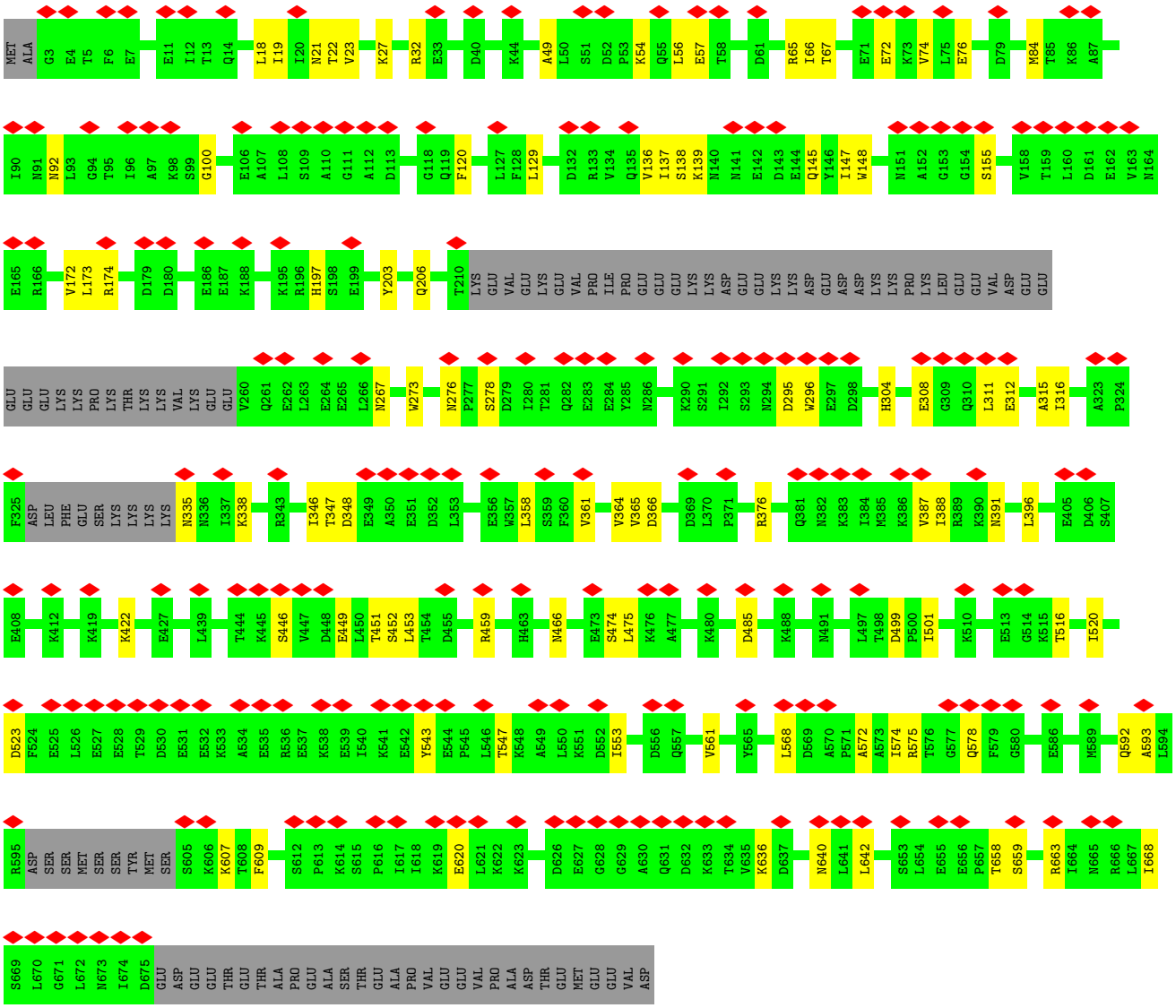
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
3	A	1	1	1	0
			Total	Mg	
3	B	1	1	1	0

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: ATP-dependent molecular chaperone HSC82

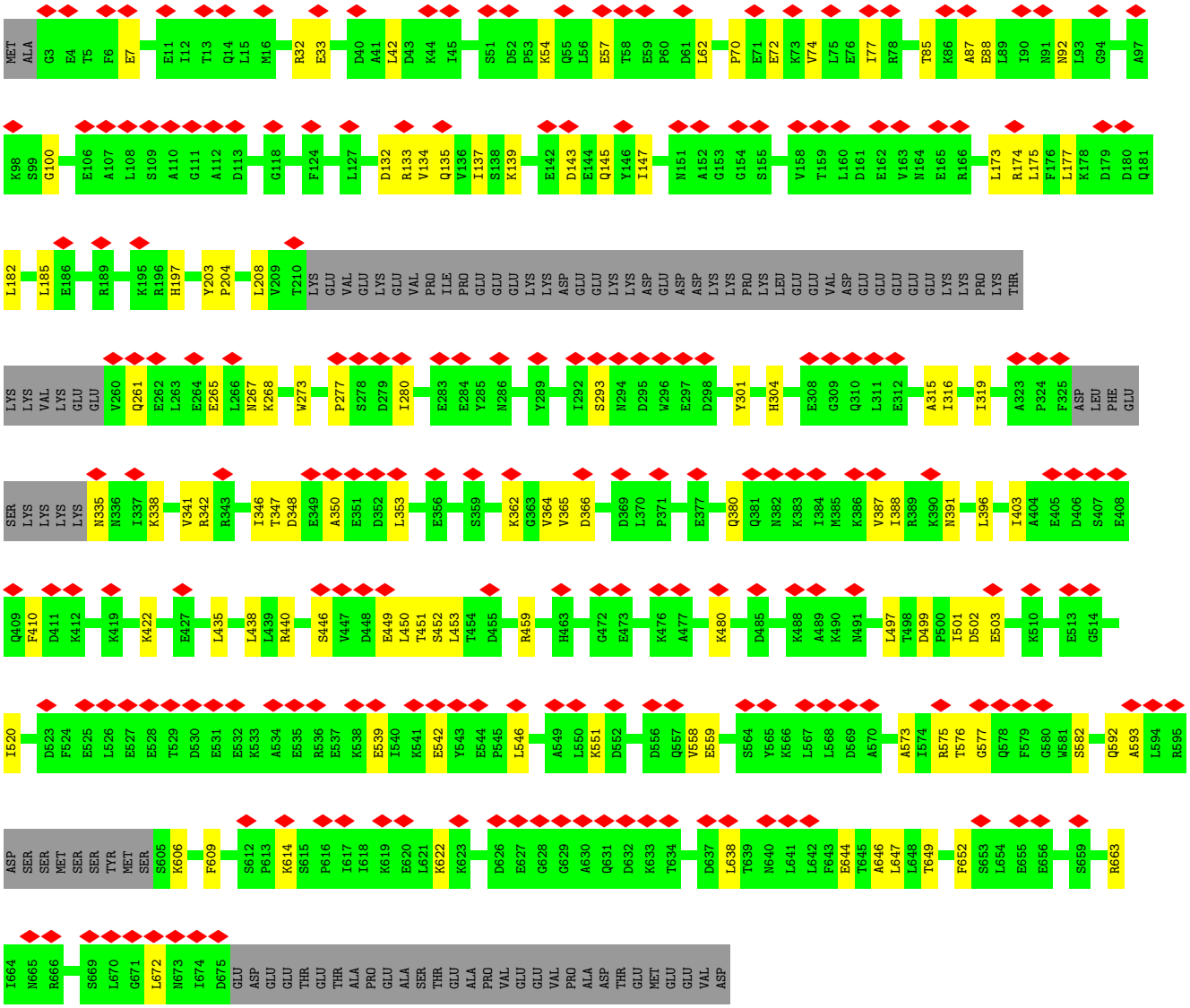
Chain A:



- Molecule 1: ATP-dependent molecular chaperone HSC82

Chain B:

30%
70%
16%
14%


MET ALA G3 E4 T5 F6 E7 E11 I12 T13 Q14 L15 M16 R32 E33 D40 A41 L42 D43 K44 I45 S51 D52 P53 K54 Q55 L56 E57 T58 E59 P60 D61 L62 P70 E71 E72 K73 V74 L75 E76 I77 R78 T85 K86 A87 E88 L89 I90 N91 N92 L93 G94 A97
K98 S99 G100 E106 A107 L108 S109 A110 G111 A112 D113 G118 F124 L127 D132 R133 V134 Q135 V136 I137 S138 K139 E142 D143 E144 Q145 Y146 I147 N151 A152 G153 G154 S155 V158 T159 L160 D161 E162 V163 N164 E165 R166 L173 R174 L175 F176 L177 K178 D179 D180 Q181
L182 L185 E186 R189 K195 R196 H197 Y203 P204 L208 V209 T210 LYS GLU VAL GLU LYS GLU VAL PRO ILE PRO GLU GLU GLU LYS LYS ASP GLU GLU LYS LYS ASP GLU ASP ASP LYS LYS PRO LYS LEU GLU GLU VAL ASP GLU GLU GLU GLU LYS LYS PRO LYS THR
LYS LYS VAL LYS GLU GLU V260 Q261 E262 L263 E264 E265 L266 N267 K268 W273 P277 S278 D279 I280 E283 E284 Y285 N286 Y289 I292 S293 N294 D295 W296 E297 D298 Y301 H304 E308 G309 Q310 L311 E312 A315 I316 I319 A323 P324 F325 ASP LEU PHE GLU
SER LYS LYS LYS LYS N335 N336 I337 K338 V341 R342 R343 I346 T347 D348 E349 A350 E351 D352 L353 E356 S359 K362 G363 V364 V365 D366 D369 L370 P371 E377 Q380 Q381 N382 K383 I384 M385 K386 V387 I388 R389 K390 N391 L396 I403 A404 E405 D406 S407 E408
Q409 F410 D411 K412 K419 K422 E427 L435 L438 L439 R440 S446 V447 D448 E449 L450 T451 S452 L453 T454 D455 R459 H463 G472 E473 K476 A477 K480 D485 K488 A489 K490 M491 L497 T498 D499 P500 I501 D502 E503 K510 E513 G514
I520 D523 F524 E525 L526 E527 E528 T529 D530 E531 E532 K533 A534 E535 R536 E537 K538 E539 I540 K541 E542 Y543 E544 P545 L546 A549 L550 K551 D552 D556 Q557 V558 E559 S564 Y565 K566 L567 L568 D569 A570 A573 I574 R575 T576 G577 Q578 F579 G580 W581 S582 Q592 A593 L594 R595
ASP SER SER MET SER SER TYR MET SER S605 K606 F609 S612 P613 K614 S615 P616 I617 I618 K619 E620 L621 K622 K623 D626 E627 G628 G629 A630 Q631 D632 K633 T634 D637 L638 T639 N640 L641 L642 F643 E644 T645 A646 L647 L648 T649 F652 S653 L654 E655 E656 S659 R663
I664 N665 R666 S669 L670 G671 L672 N673 I674 D675 GLU ASP GLU GLU THR GLU THR ALA PRO GLU ALA SER THR GLU ALA PRO VAL GLU GLU VAL PRO ALA ASP THR GLU MET GLU GLU VAL ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	48464	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 ($e^-/Å^2$)	72	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	0.164	Depositor
Minimum map value	-0.073	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0375	Depositor
Map size (Å)	271.104, 271.104, 271.104	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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: ANP, 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	0.23	0/4978	0.39	0/6711
1	B	0.24	0/4978	0.39	0/6711
All	All	0.24	0/9956	0.39	0/13422

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	4897	0	4943	60	0
1	B	4897	0	4943	66	0
2	A	31	0	13	2	0
2	B	31	0	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	9858	0	9912	118	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 6.

The worst 5 of 118 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:451:THR:HG21	1:A:459:ARG:HH22	1.52	0.74
1:B:451:THR:HG21	1:B:459:ARG:HH22	1.54	0.72
1:A:561:VAL:HG12	1:A:609:PHE:HB3	1.70	0.71
1:B:77:ILE:HB	1:B:173:LEU:HB2	1.74	0.69
1:A:136:VAL:HB	1:A:148:TRP:HB3	1.74	0.68

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	598/705 (85%)	589 (98%)	9 (2%)	0	100	100
1	B	598/705 (85%)	588 (98%)	10 (2%)	0	100	100
All	All	1196/1410 (85%)	1177 (98%)	19 (2%)	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	542/636 (85%)	542 (100%)	0	100	100
1	B	542/636 (85%)	542 (100%)	0	100	100

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1084/1272 (85%)	1084 (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 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	336	ASN
1	B	420	ASN
1	B	557	GLN
1	A	431	ASN
1	A	557	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
2	ANP	A	801	3	29,33,33	1.09	4 (13%)	31,52,52	1.09	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ANP	B	801	3	29,33,33	1.08	4 (13%)	31,52,52	1.10	2 (6%)

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
2	ANP	A	801	3	-	8/14/38/38	0/3/3/3
2	ANP	B	801	3	-	8/14/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	ANP	PG-O1G	2.46	1.50	1.46
2	A	801	ANP	PG-O1G	2.42	1.50	1.46
2	B	801	ANP	PG-N3B	2.40	1.69	1.63
2	A	801	ANP	PG-N3B	2.40	1.69	1.63
2	A	801	ANP	PB-O3A	-2.39	1.56	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	ANP	PB-O3A-PA	-3.67	119.70	132.62
2	A	801	ANP	PB-O3A-PA	-3.65	119.75	132.62
2	B	801	ANP	C5-C6-N6	2.28	123.81	120.35
2	A	801	ANP	C5-C6-N6	2.27	123.81	120.35

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ANP	PB-N3B-PG-O1G
2	A	801	ANP	PG-N3B-PB-O1B
2	A	801	ANP	C5'-O5'-PA-O1A
2	A	801	ANP	C5'-O5'-PA-O2A
2	B	801	ANP	PB-N3B-PG-O1G

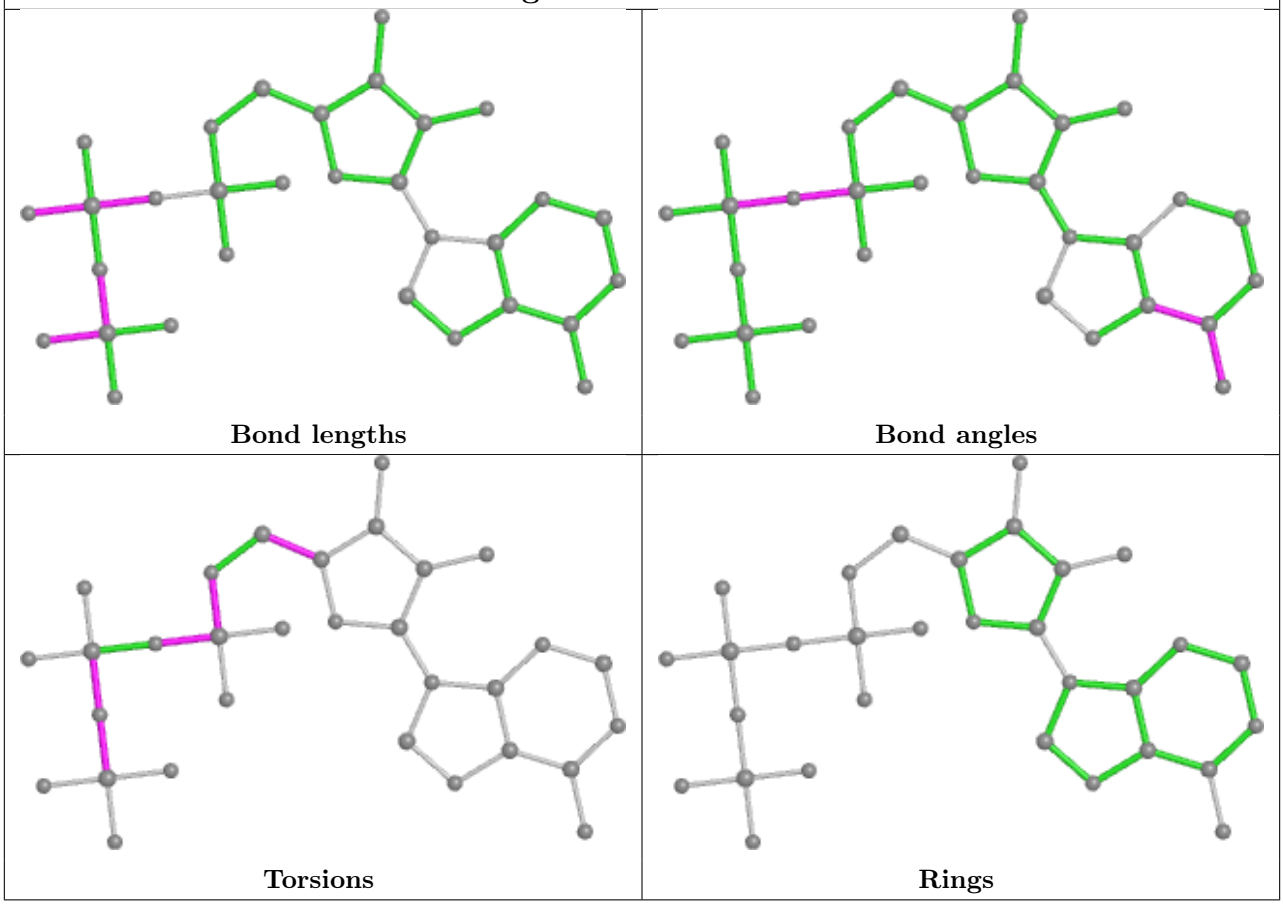
There are no ring outliers.

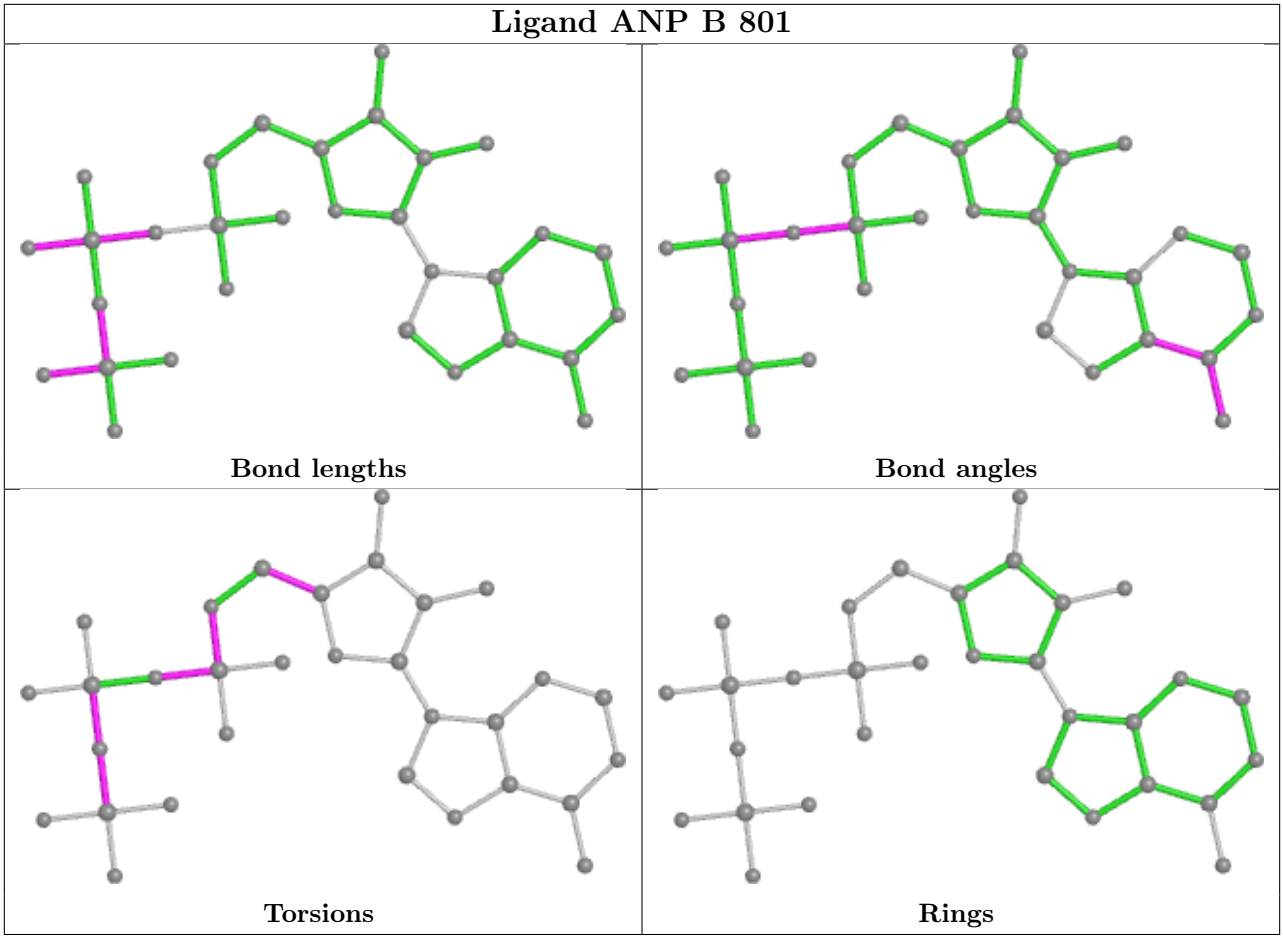
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ANP	2	0
2	B	801	ANP	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 ANP A 801





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)

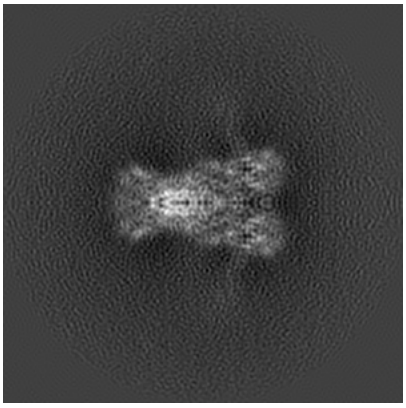
This section contains visualisations of the EMDB entry EMD-22239. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

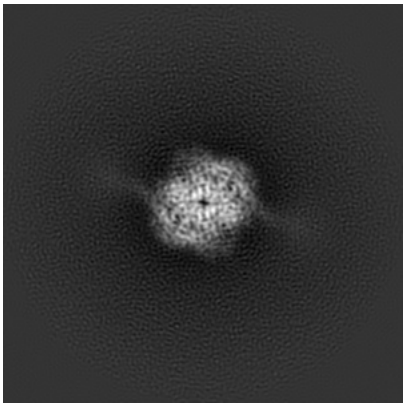
6.1 Orthogonal projections (i)

6.1.1 Primary map

X



Y



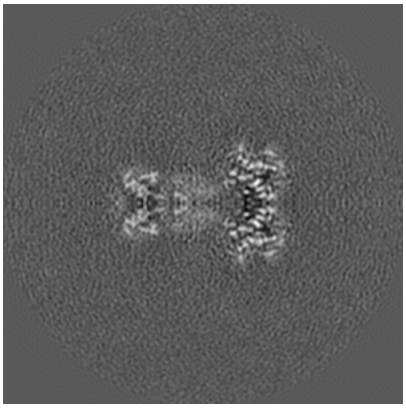
Z

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

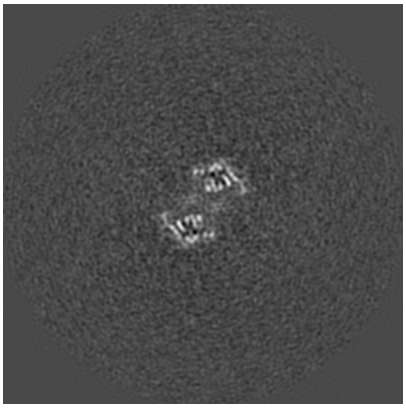
6.2 Central slices (i)

6.2.1 Primary map

X Index: 128



Y Index: 128

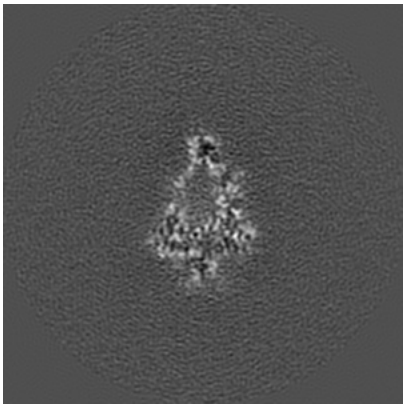


Z Index: 128

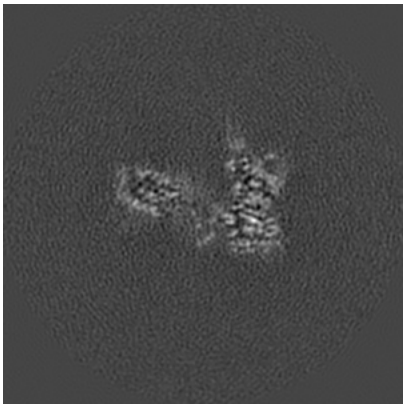
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

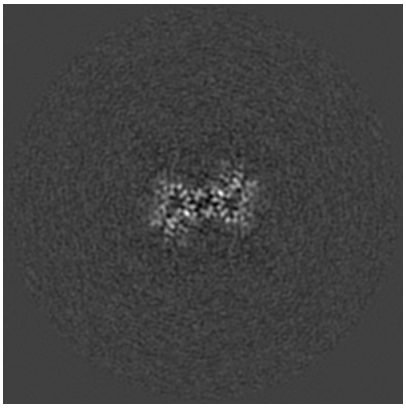
6.3.1 Primary map



X Index: 130



Y Index: 122

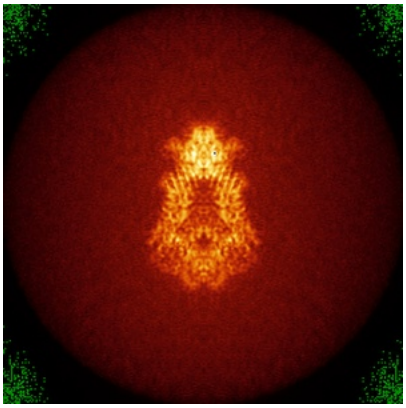


Z Index: 160

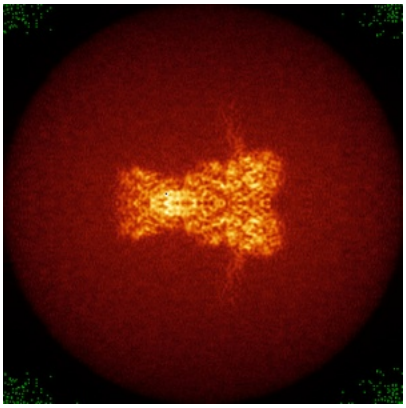
The images above show the largest variance slices of the map in three orthogonal directions.

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

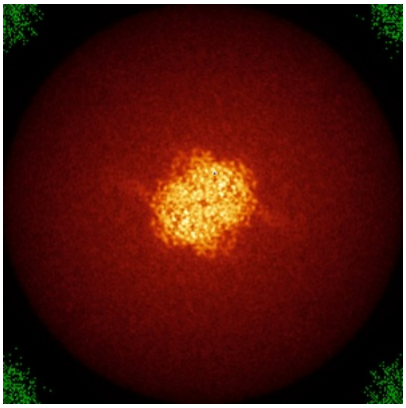
6.4.1 Primary map



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 0.0375. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

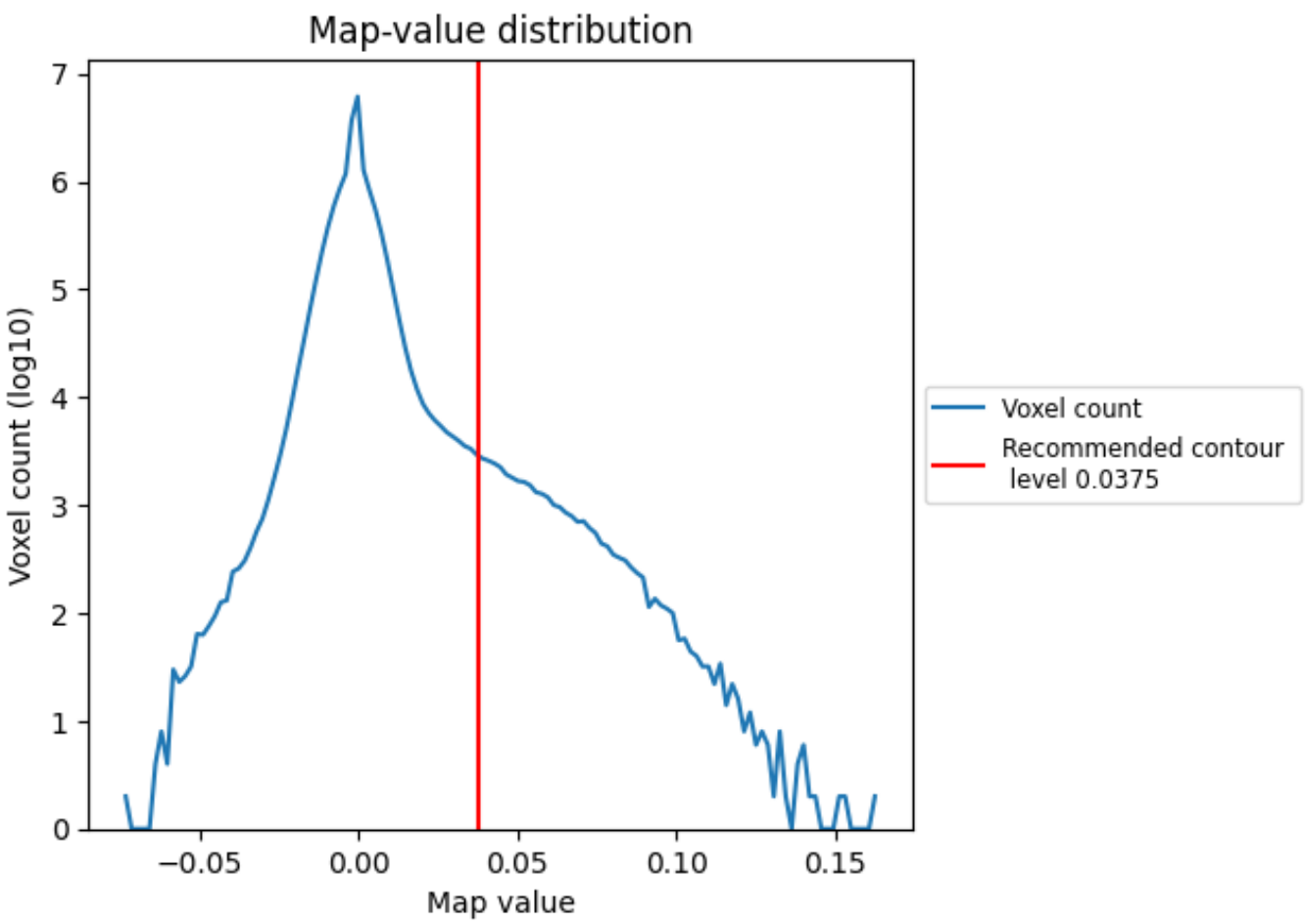
6.6 Mask visualisation (i)

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

7 Map analysis (i)

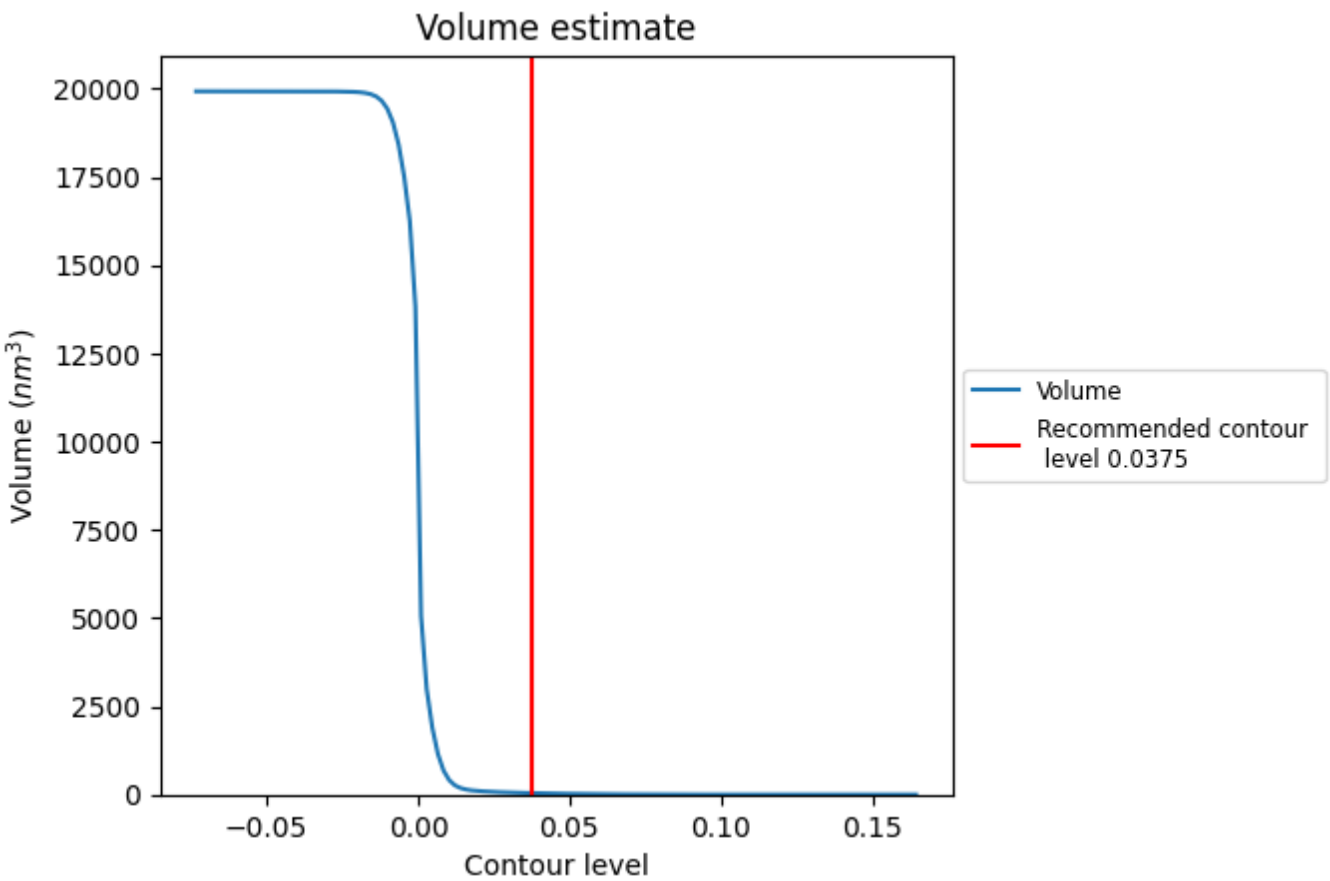
This section contains the results of statistical analysis of the map.

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.

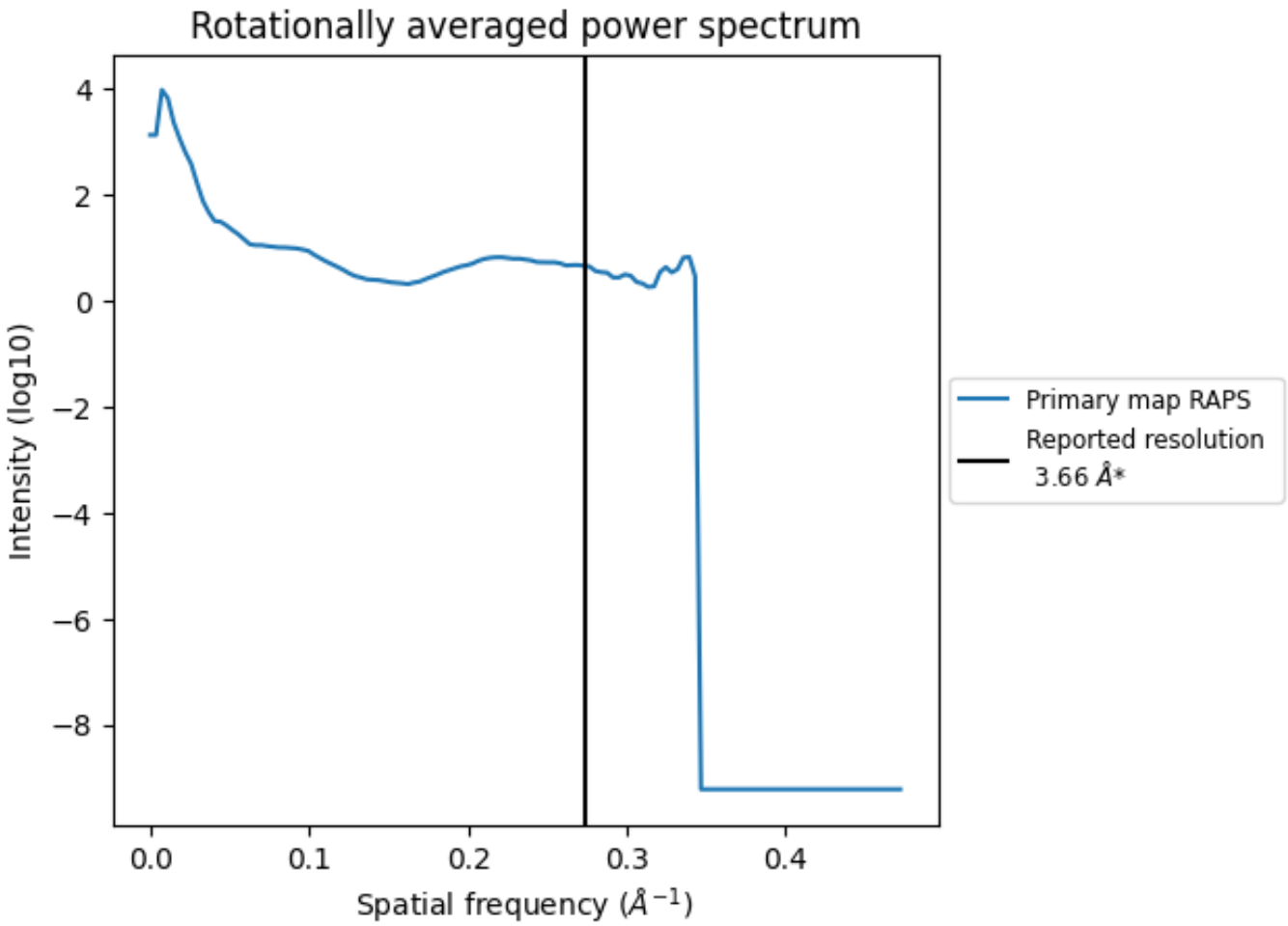
7.2 Volume estimate (i)



The volume at the recommended contour level is 41 nm^3; this corresponds to an approximate mass of 37 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)

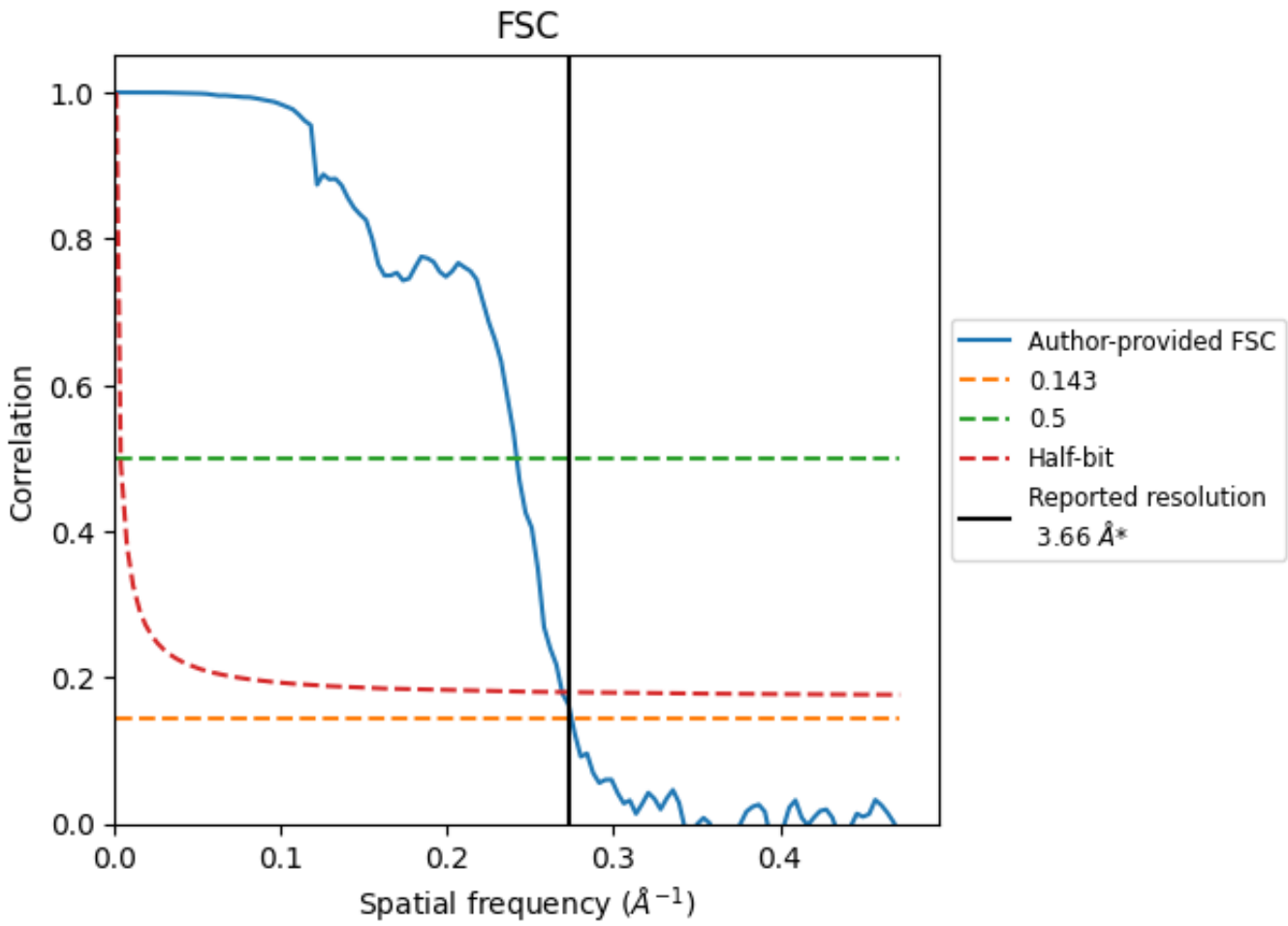


*Reported resolution corresponds to spatial frequency of 0.273 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.273 Å^{-1}

8.2 Resolution estimates (i)

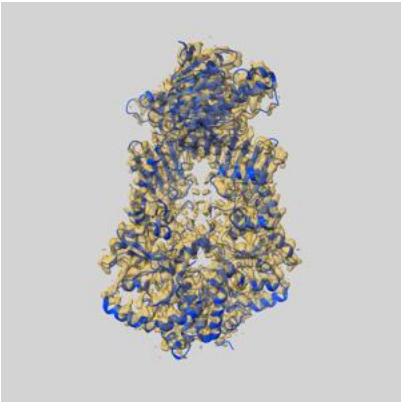
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.66	-	-
Author-provided FSC curve	3.64	4.14	3.72
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

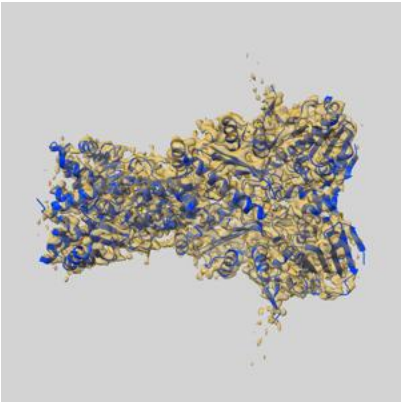
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22239 and PDB model 6XLC. Per-residue inclusion information can be found in section 3 on page 5.

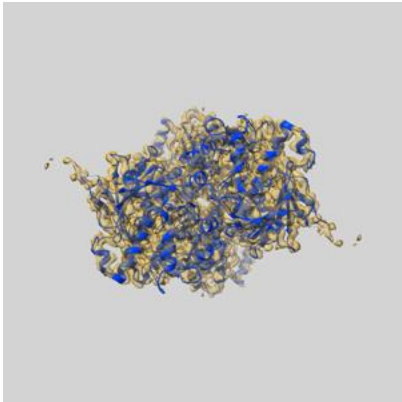
9.1 Map-model overlay (i)



X



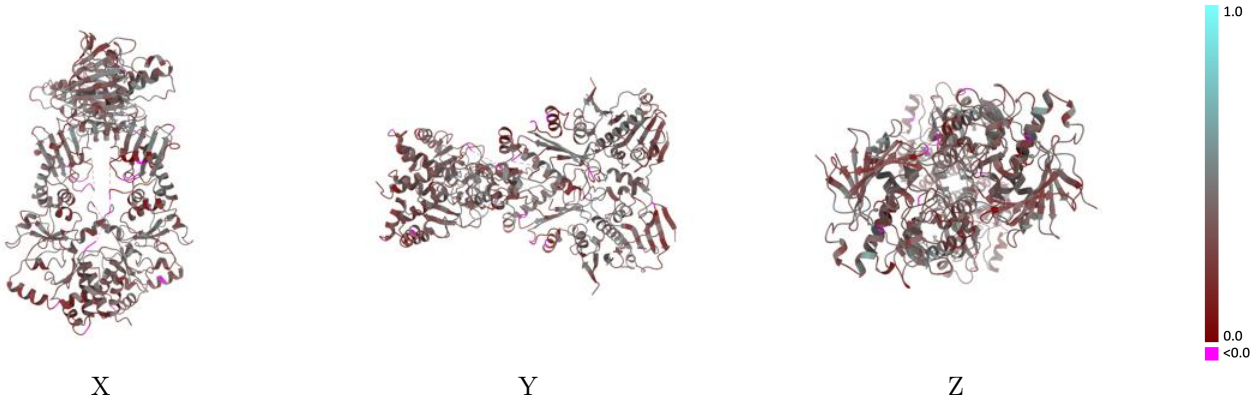
Y



Z

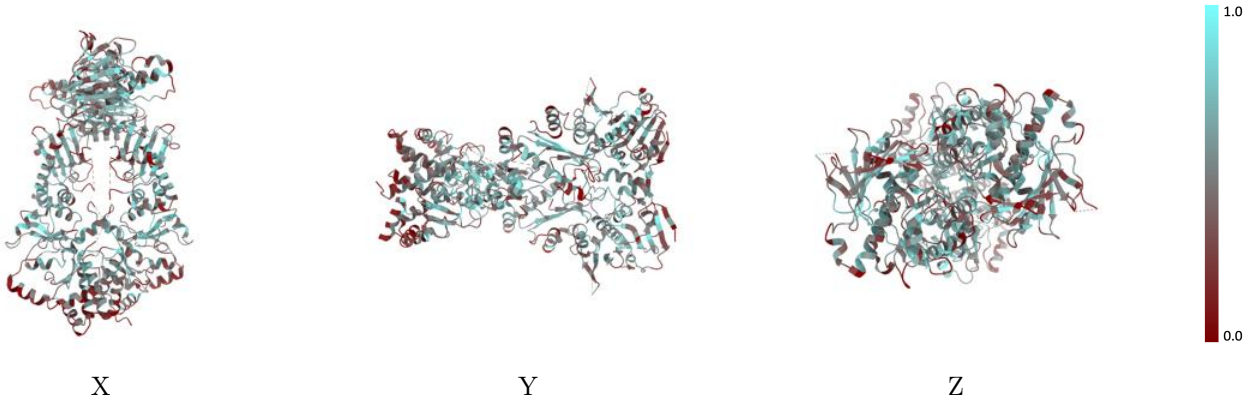
The images above show the 3D surface view of the map at the recommended contour level 0.0375 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



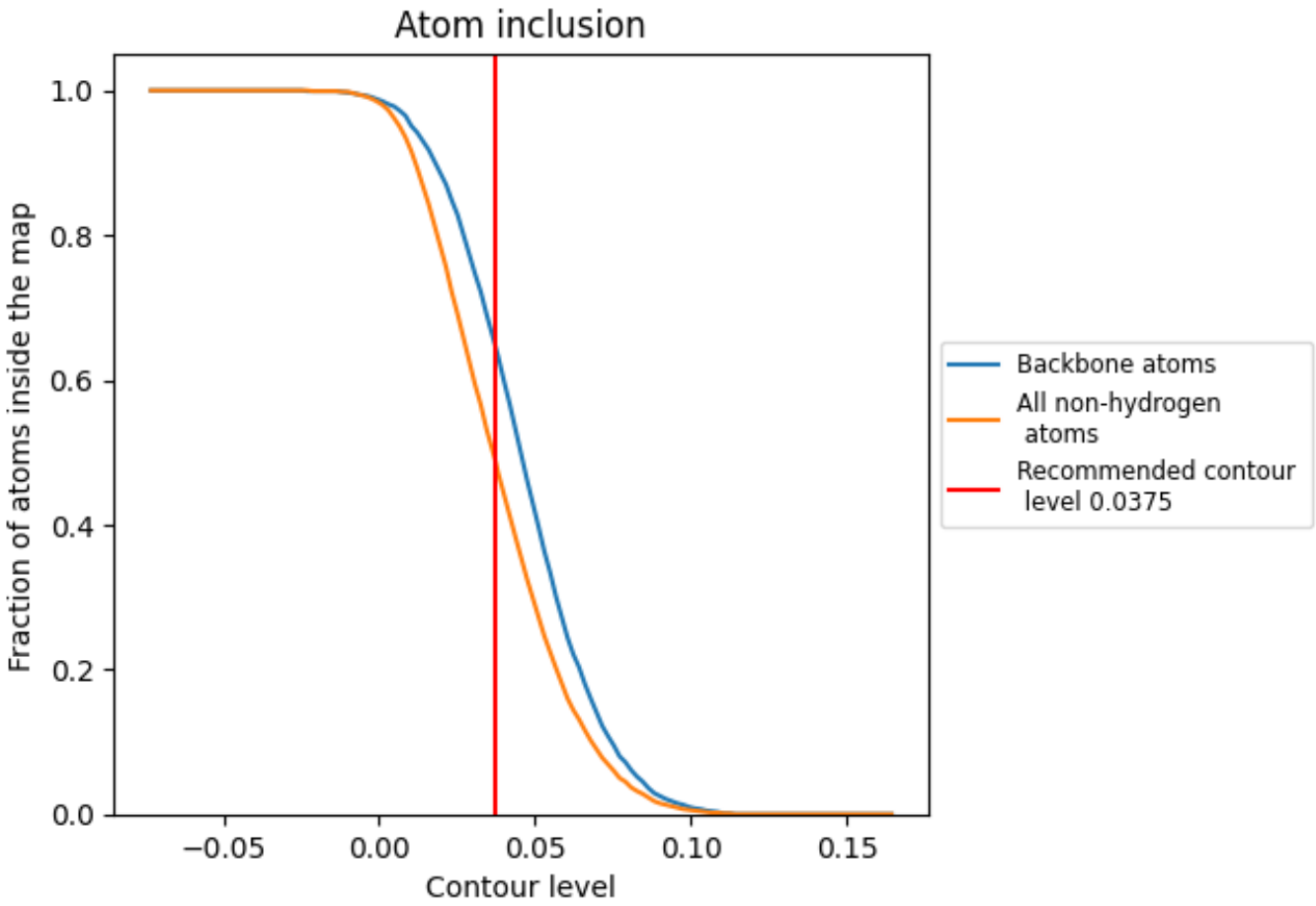
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0375).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 48% 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 (0.0375) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4850	0.3430
A	0.4860	0.3430
B	0.4840	0.3430