Full wwPDB EM Validation Report

Feb 3, 2025 – 05:01 PM EST

PDB ID	:	9DLX
EMDB ID	:	EMD-46992
Title	:	Bovine Arp2/3 complex with N-WASP CA bound to Arp3 and Arp2-ArpC1
Authors	:	Saks, A.J.; Barrie, K.R.; Dominguez, R.
Deposited on	:	2024-09-11
Resolution	:	2.91 Å(reported)

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:

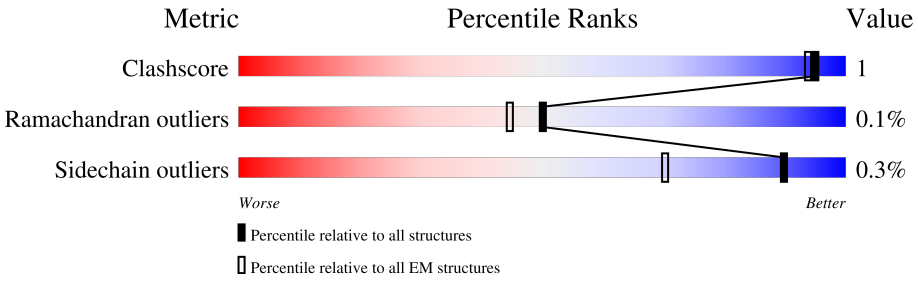
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.91 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	412	96%
2	B	390	94% 5%
3	C	370	90% 6%
4	D	285	98%
5	E	175	99%
6	F	167	98%
7	G	151	72% 28%
8	H	41	24% 71% 7% 22%

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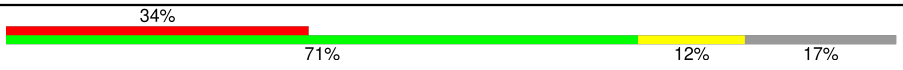
Mol	Chain	Length	Quality of chain
8	I	41	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 15551 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 Actin-related protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	405	3246	2082	547	602	15	0	0

- Molecule 2 is a protein called Actin-related protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	383	3063	1960	523	563	17	0	0

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	348	2736	1736	478	506	16	0	0

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	285	2301	1461	398	434	8	0	0

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	175	1422	913	237	263	9	0	0

- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	167	1371	875	239	248	9	0	0

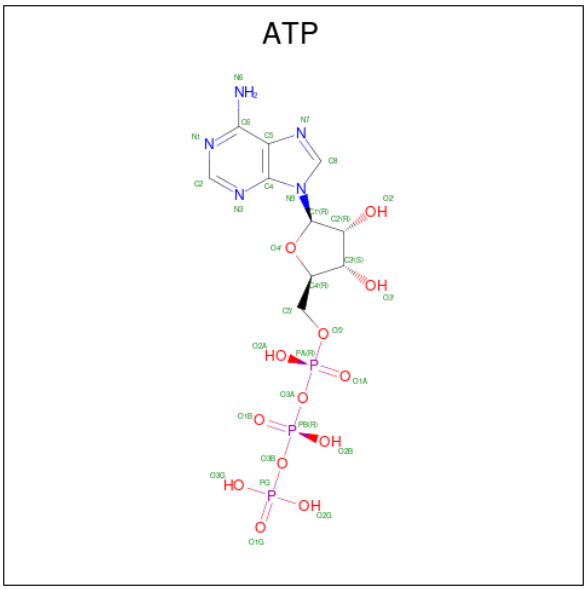
- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	109	Total	C	N	O	S	0	0
			824	522	144	156	2		

- Molecule 8 is a protein called Actin nucleation-promoting factor WASL.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	32	Total	C	N	O	S	0	0
			252	149	41	60	2		
8	I	34	Total	C	N	O	S	0	0
			272	163	43	64	2		

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	

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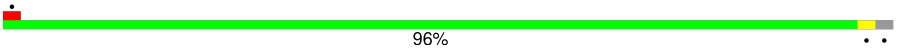
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
10	B	1	1	1	0

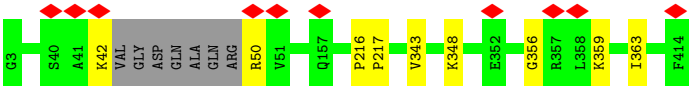
3 Residue-property plots (i)

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: Actin-related protein 3

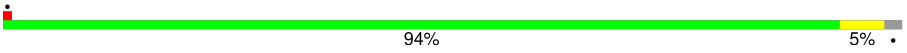
Chain A:

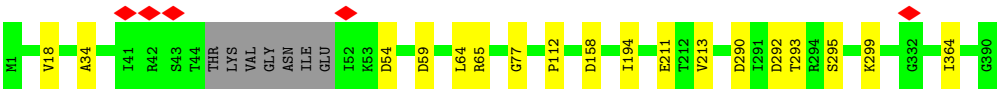




• Molecule 2: Actin-related protein 2

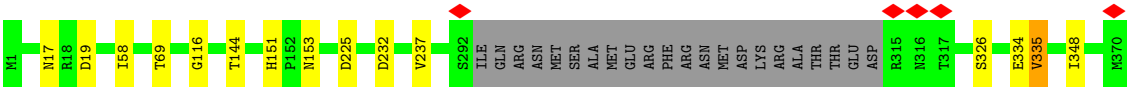
Chain B:





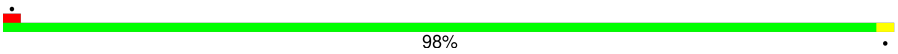
• Molecule 3: Actin-related protein 2/3 complex subunit 1A

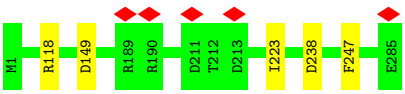
Chain C:



• Molecule 4: Actin-related protein 2/3 complex subunit 2

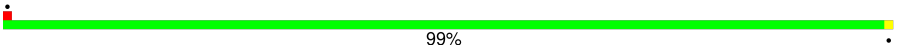
Chain D:

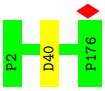




• Molecule 5: Actin-related protein 2/3 complex subunit 3

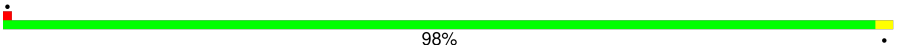
Chain E:

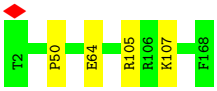




• Molecule 6: Actin-related protein 2/3 complex subunit 4

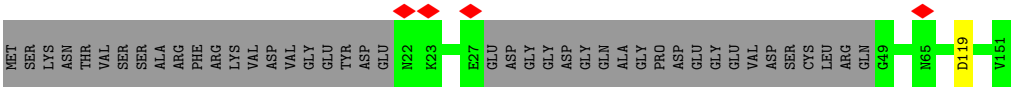
Chain F:





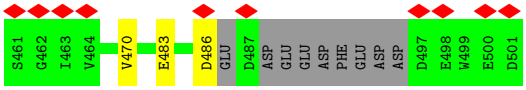
• Molecule 7: Actin-related protein 2/3 complex subunit 5

Chain G:



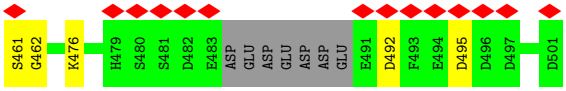
• Molecule 8: Actin nucleation-promoting factor WASL

Chain H:



• Molecule 8: Actin nucleation-promoting factor WASL

Chain I:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	292065	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	47	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	OTHER	Depositor
Maximum map value	0.237	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.042	Depositor
Map size (Å)	302.72, 302.72, 302.72	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP

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	0.30	0/3328	0.56	0/4513
2	B	0.28	0/3124	0.60	2/4219 (0.0%)
3	C	0.30	0/2807	0.61	1/3807 (0.0%)
4	D	0.30	0/2350	0.55	0/3173
5	E	0.34	0/1457	0.58	0/1966
6	F	0.32	0/1393	0.57	0/1868
7	G	0.29	0/833	0.57	0/1120
8	H	0.44	0/253	0.80	0/335
8	I	0.31	0/274	0.64	0/363
All	All	0.30	0/15819	0.58	3/21364 (0.0%)

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
8	H	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	64	LEU	CA-CB-CG	7.89	133.45	115.30
3	C	225	ASP	CB-CG-OD1	6.01	123.71	118.30
2	B	64	LEU	CB-CG-CD1	5.50	120.35	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	483	GLU	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	3246	0	3204	3	0
2	B	3063	0	3098	11	0
3	C	2736	0	2682	7	0
4	D	2301	0	2263	3	0
5	E	1422	0	1423	1	0
6	F	1371	0	1410	2	0
7	G	824	0	861	0	0
8	H	252	0	221	2	0
8	I	272	0	236	3	0
9	A	31	0	12	0	0
9	B	31	0	12	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
All	All	15551	0	15422	31	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 1.

All (31) 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:326:SER:HB2	3:C:348:ILE:HD12	1.88	0.55
6:F:105:ARG:NH1	6:F:107:LYS:O	2.43	0.51
5:E:40:ASP:N	5:E:40:ASP:OD1	2.45	0.50
3:C:232:ASP:O	3:C:237:VAL:HA	2.13	0.48
2:B:18:VAL:HG23	2:B:34:ALA:HB2	1.96	0.48
3:C:334:GLU:HG3	3:C:335:VAL:HG23	1.96	0.48
8:I:495:ASP:N	8:I:495:ASP:OD1	2.45	0.48
2:B:295:SER:OG	2:B:299:LYS:NZ	2.47	0.47
6:F:50:PRO:HB3	6:F:64:GLU:HG2	1.96	0.47
3:C:17:ASN:ND2	3:C:19:ASP:OD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:GLY:O	1:A:359:LYS:NZ	2.43	0.46
8:I:461:SER:OG	8:I:462:GLY:N	2.48	0.46
4:D:238:ASP:N	4:D:238:ASP:OD1	2.43	0.46
2:B:59:ASP:N	2:B:59:ASP:OD1	2.48	0.46
3:C:116:GLY:HA2	3:C:144:THR:HG23	1.98	0.45
2:B:292:ASP:N	2:B:292:ASP:OD1	2.50	0.45
2:B:65:ARG:NH1	2:B:211:GLU:OE2	2.50	0.45
2:B:158:ASP:OD1	2:B:158:ASP:N	2.48	0.45
3:C:58:ILE:HG12	3:C:69:THR:HG22	1.97	0.45
3:C:151:HIS:ND1	3:C:153:ASN:OD1	2.50	0.44
2:B:77:GLY:HA3	2:B:112:PRO:HG3	2.00	0.43
2:B:290:ASP:OD1	2:B:293:THR:OG1	2.37	0.43
8:H:486:ASP:OD1	8:H:486:ASP:N	2.47	0.43
2:B:364:ILE:HD11	8:H:470:VAL:HG11	2.00	0.42
1:A:343:VAL:HG11	1:A:363:ILE:HD11	2.02	0.42
4:D:149:ASP:OD1	4:D:149:ASP:N	2.48	0.41
2:B:194:ILE:HG13	2:B:213:VAL:HG11	2.01	0.41
4:D:223:ILE:HD13	4:D:247:PHE:HE2	1.86	0.40
8:I:492:ASP:OD1	8:I:492:ASP:N	2.55	0.40
1:A:216:PRO:HA	1:A:217:PRO:HD3	1.91	0.40
2:B:54:ASP:N	2:B:54:ASP:OD1	2.51	0.40

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	401/412 (97%)	382 (95%)	19 (5%)	0	100 100
2	B	379/390 (97%)	369 (97%)	10 (3%)	0	100 100
3	C	344/370 (93%)	327 (95%)	16 (5%)	1 (0%)	37 65
4	D	283/285 (99%)	272 (96%)	11 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	E	173/175 (99%)	168 (97%)	5 (3%)	0	100 100
6	F	165/167 (99%)	160 (97%)	5 (3%)	0	100 100
7	G	105/151 (70%)	100 (95%)	4 (4%)	1 (1%)	13 38
8	H	28/41 (68%)	25 (89%)	3 (11%)	0	100 100
8	I	30/41 (73%)	30 (100%)	0	0	100 100
All	All	1908/2032 (94%)	1833 (96%)	73 (4%)	2 (0%)	50 76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	119	ASP
3	C	335	VAL

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	354/359 (99%)	351 (99%)	3 (1%)	79 92
2	B	335/341 (98%)	335 (100%)	0	100 100
3	C	303/323 (94%)	303 (100%)	0	100 100
4	D	250/250 (100%)	249 (100%)	1 (0%)	89 96
5	E	157/157 (100%)	157 (100%)	0	100 100
6	F	154/154 (100%)	154 (100%)	0	100 100
7	G	89/123 (72%)	89 (100%)	0	100 100
8	H	28/37 (76%)	28 (100%)	0	100 100
8	I	30/37 (81%)	29 (97%)	1 (3%)	33 66
All	All	1700/1781 (96%)	1695 (100%)	5 (0%)	90 97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LYS
1	A	50	ARG
1	A	348	LYS
4	D	118	ARG
8	I	476	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	205	GLN
1	A	243	ASN
5	E	135	GLN
6	F	167	ASN
7	G	96	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 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	$\#\|Z\|>2$
9	ATP	A	500	10	28,33,33	0.63	0	34,52,52	0.94	2 (5%)
9	ATP	B	500	10	28,33,33	0.74	0	34,52,52	0.59	1 (2%)

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
9	ATP	A	500	10	-	0/18/38/38	0/3/3/3
9	ATP	B	500	10	-	1/18/38/38	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	500	ATP	C4'-O4'-C1'	-3.92	106.33	109.92
9	B	500	ATP	C5-C6-N6	2.28	123.79	120.31
9	A	500	ATP	C5-C6-N6	2.28	123.78	120.31

There are no chirality outliers.

All (1) torsion outliers are listed below:

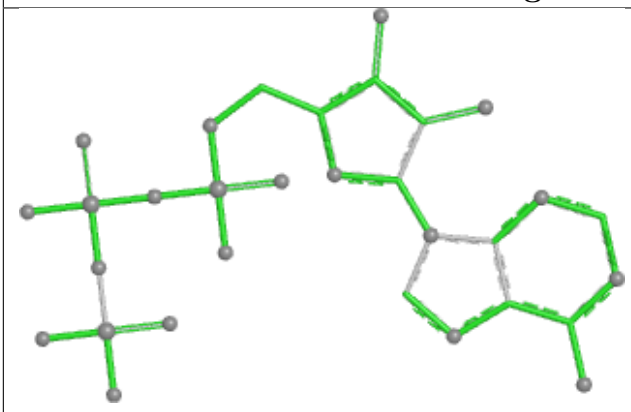
Mol	Chain	Res	Type	Atoms
9	B	500	ATP	PA-O3A-PB-O2B

There are no ring outliers.

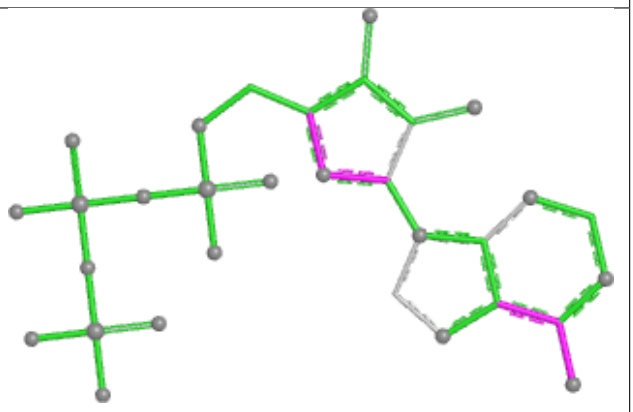
No monomer is involved in short contacts.

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.

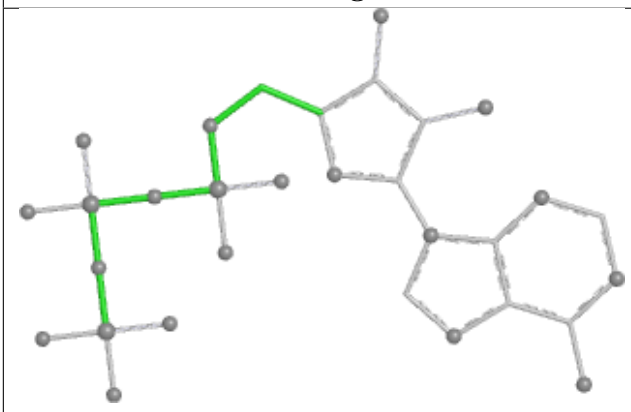
Ligand ATP A 500



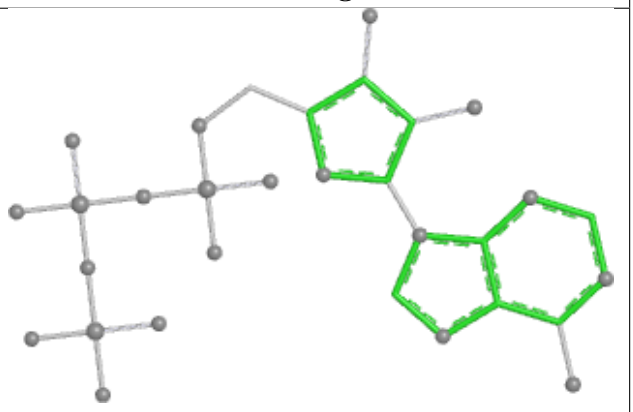
Bond lengths



Bond angles

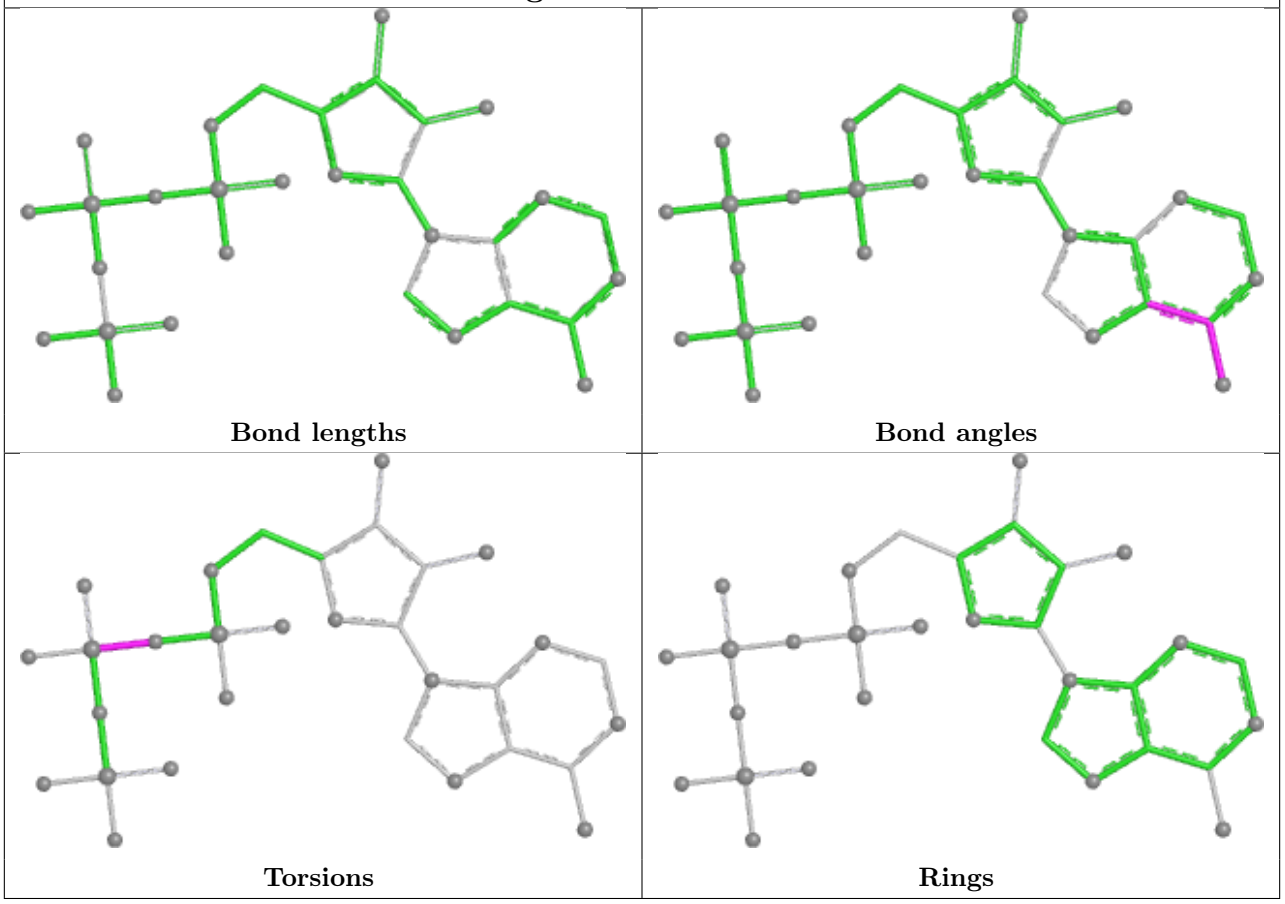


Torsions



Rings

Ligand ATP B 500



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.

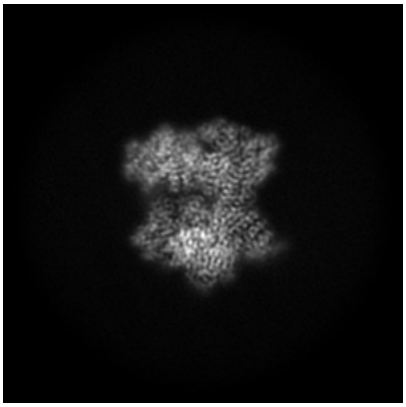
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-46992. These allow visual inspection of the internal detail of the map and identification of artifacts.

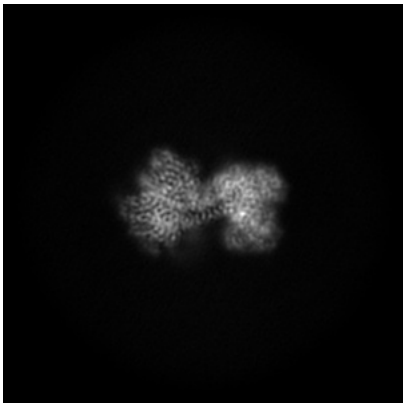
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

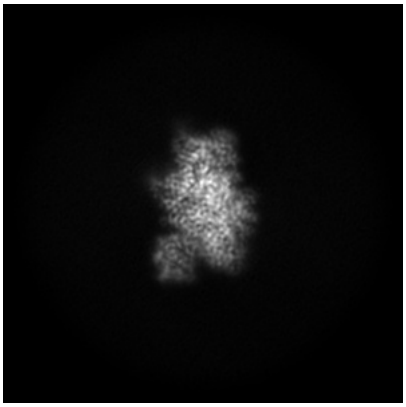
6.1.1 Primary map



X



Y

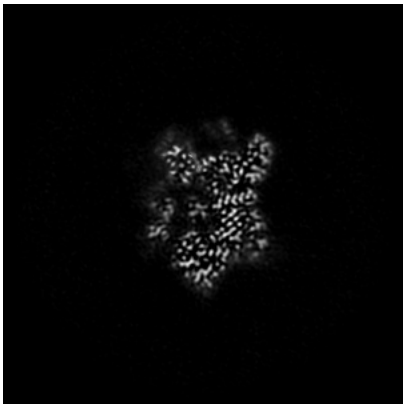


Z

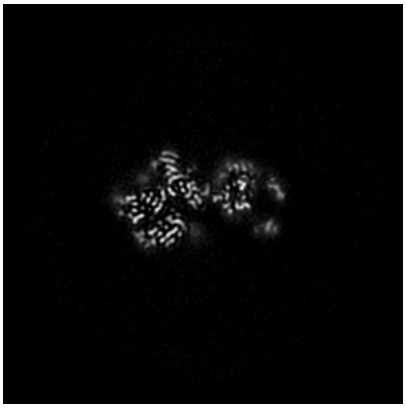
The images above show the map projected in three orthogonal directions.

6.2 Central slices

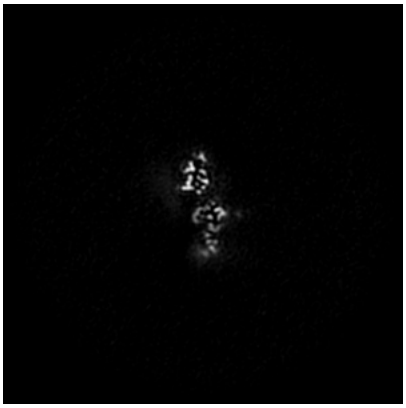
6.2.1 Primary map



X Index: 176



Y Index: 176

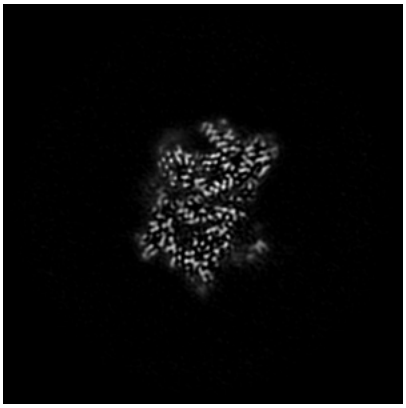


Z Index: 176

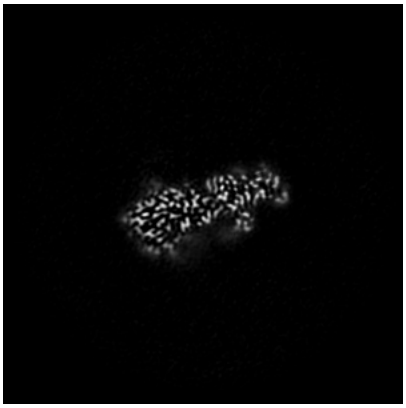
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

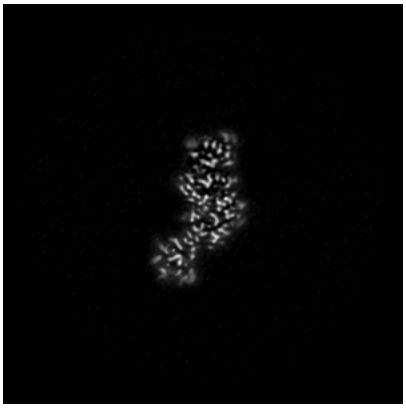
6.3.1 Primary map



X Index: 182



Y Index: 194

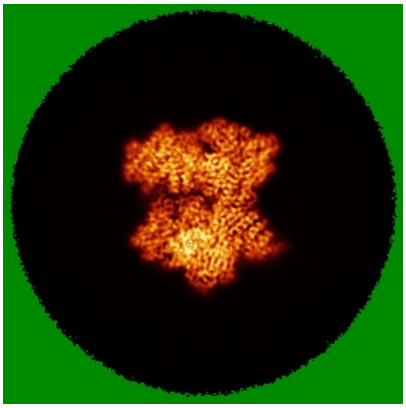


Z Index: 210

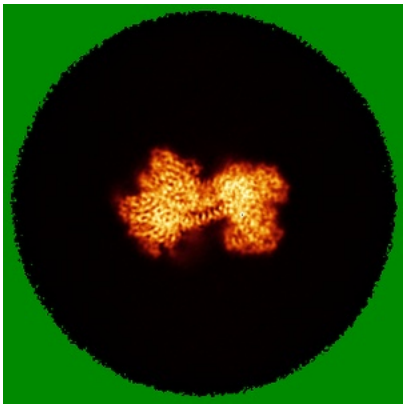
The images above show the largest variance slices of the map in three orthogonal directions.

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

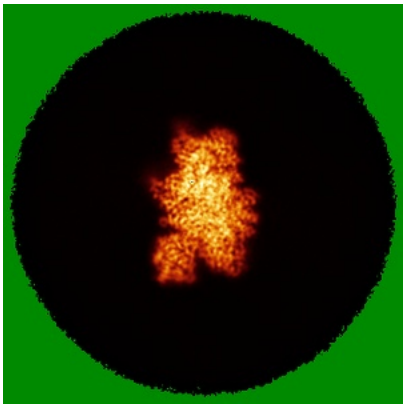
6.4.1 Primary map



X



Y

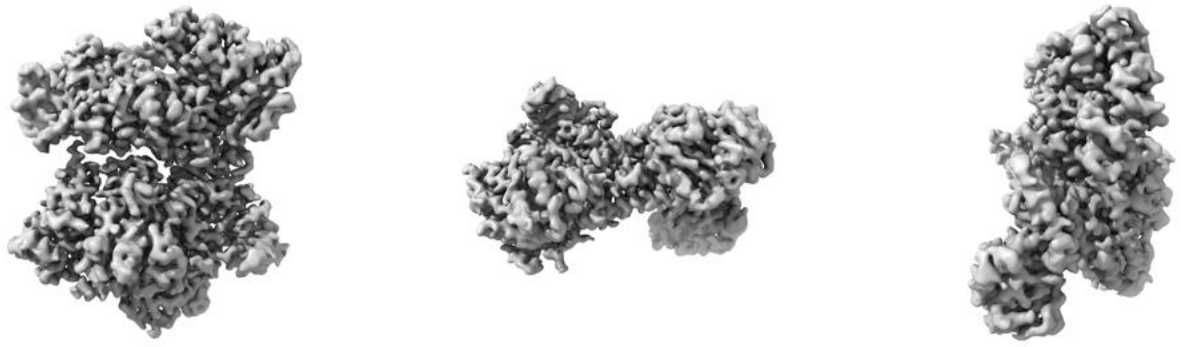


Z

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

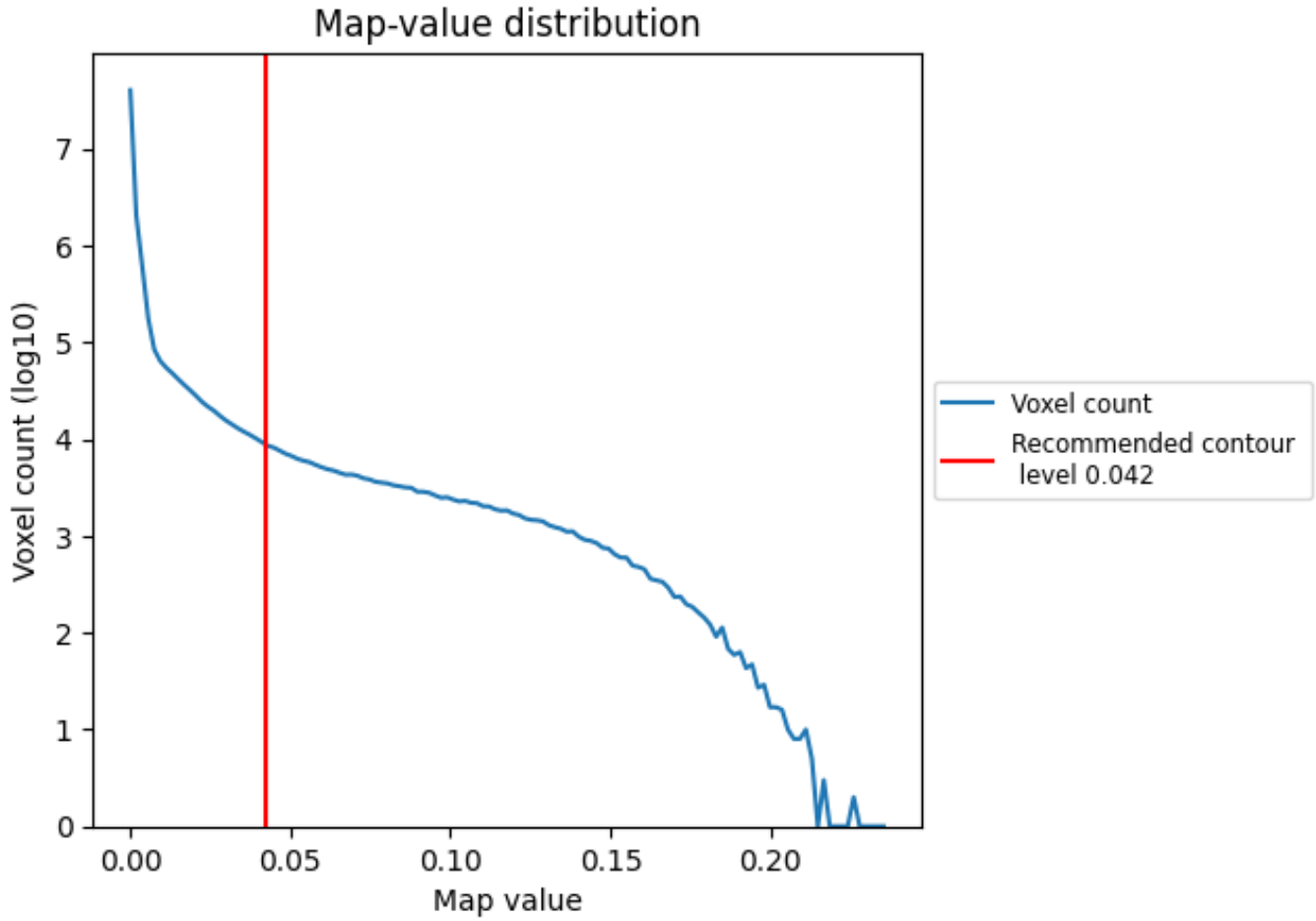
6.6 Mask visualisation (i)

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

7 Map analysis

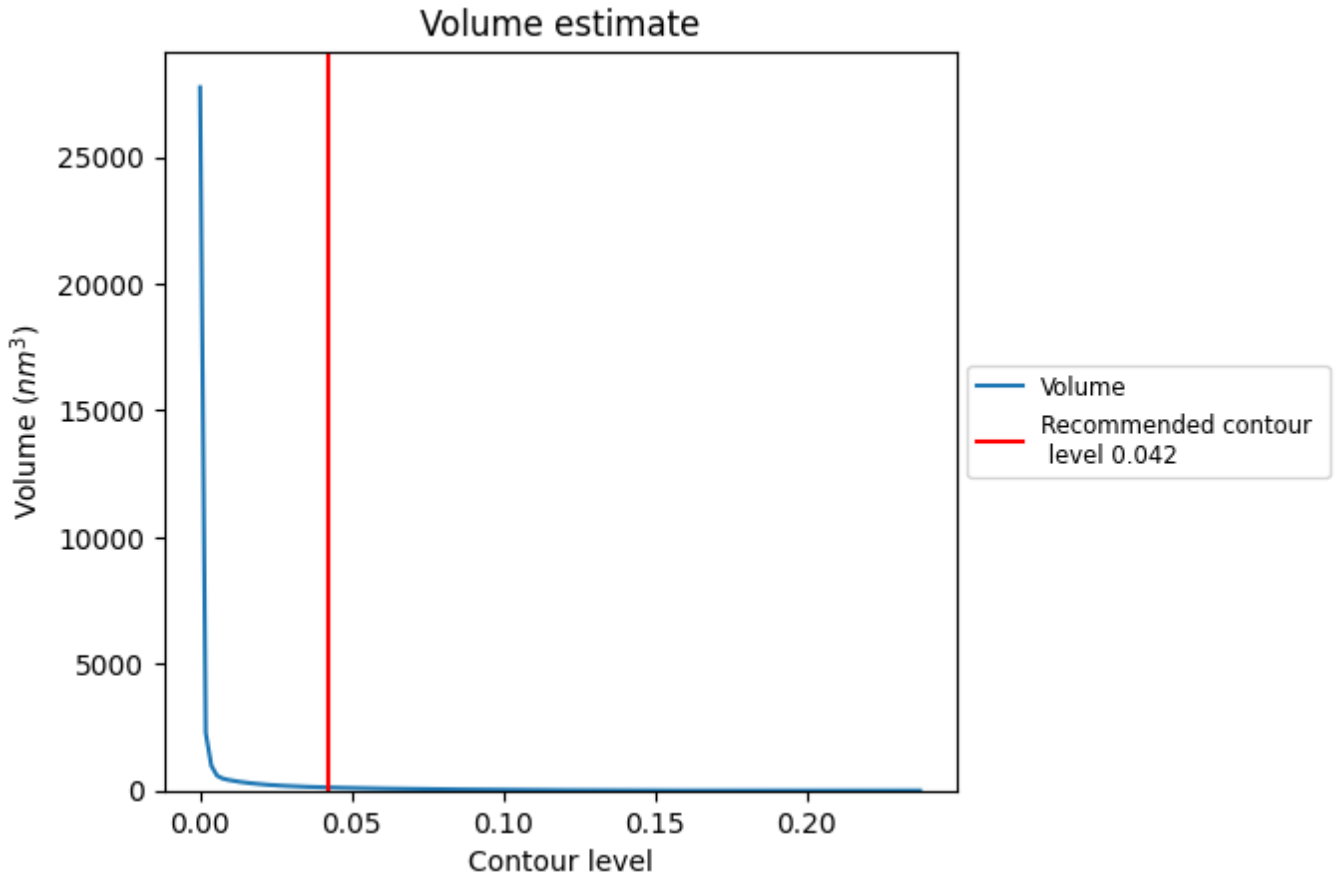
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

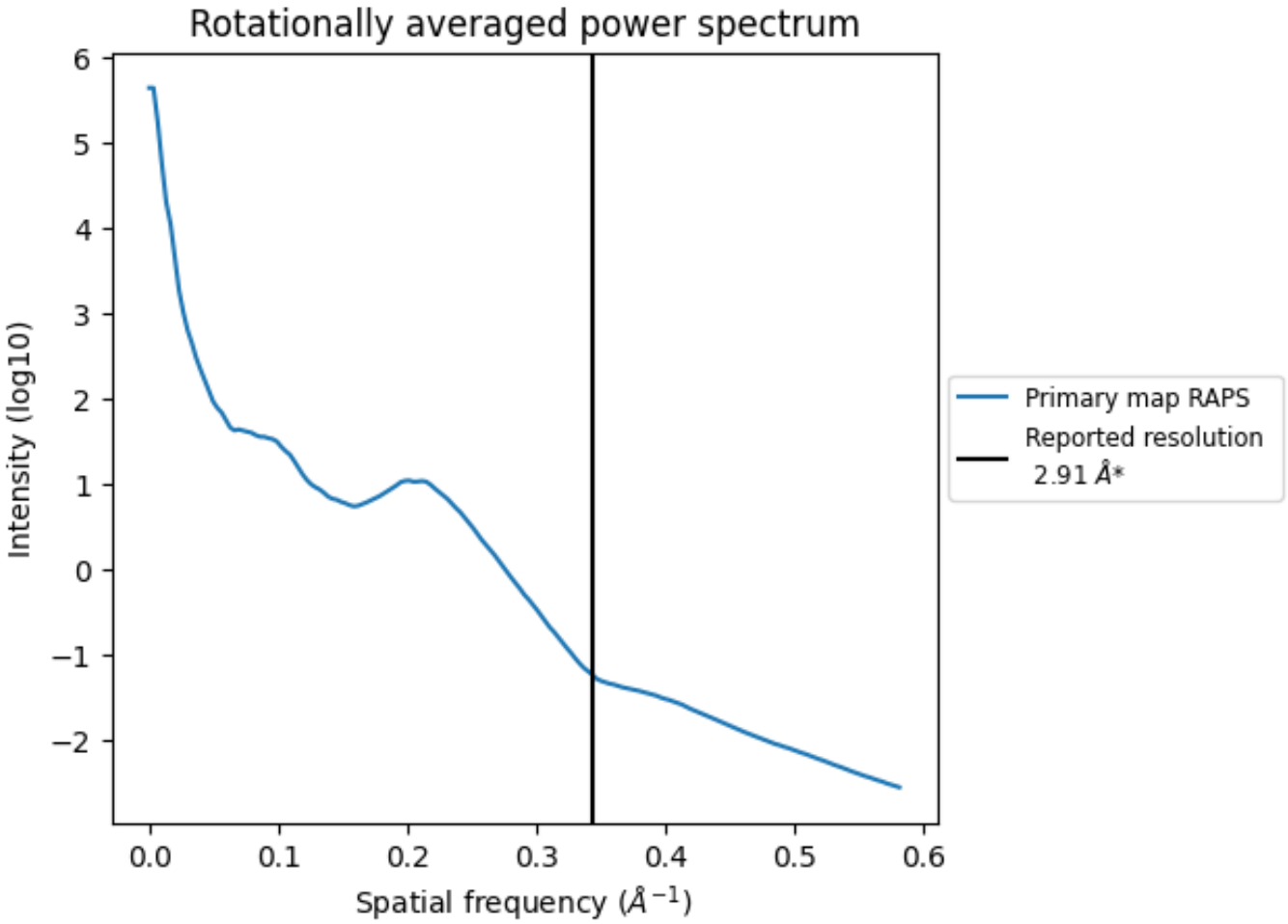
7.2 Volume estimate



The volume at the recommended contour level is 123 nm^3; this corresponds to an approximate mass of 111 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 0.344 Å^{-1}

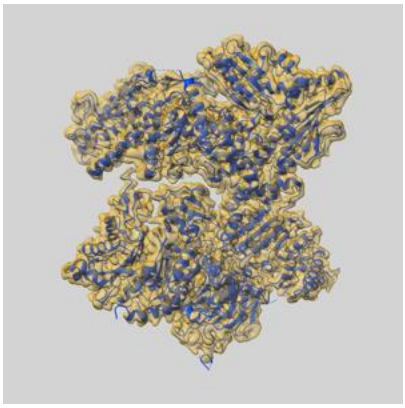
8 Fourier-Shell correlation

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

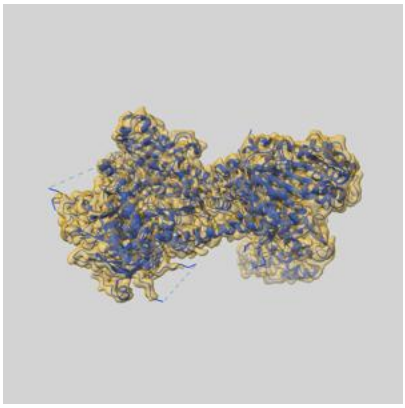
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-46992 and PDB model 9DLX. Per-residue inclusion information can be found in section 3 on page 7.

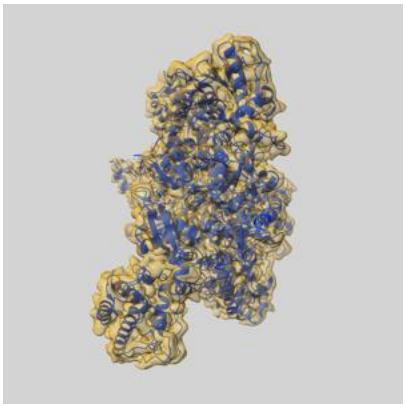
9.1 Map-model overlay



X



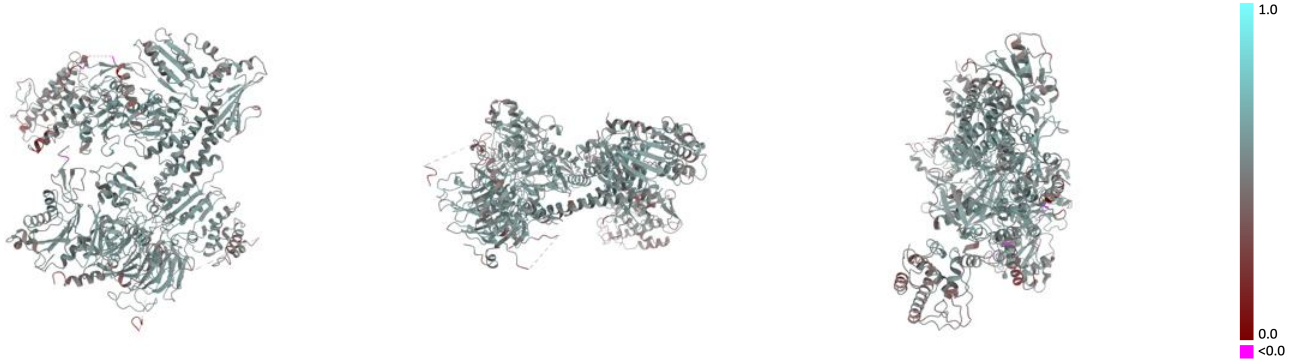
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.042 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.

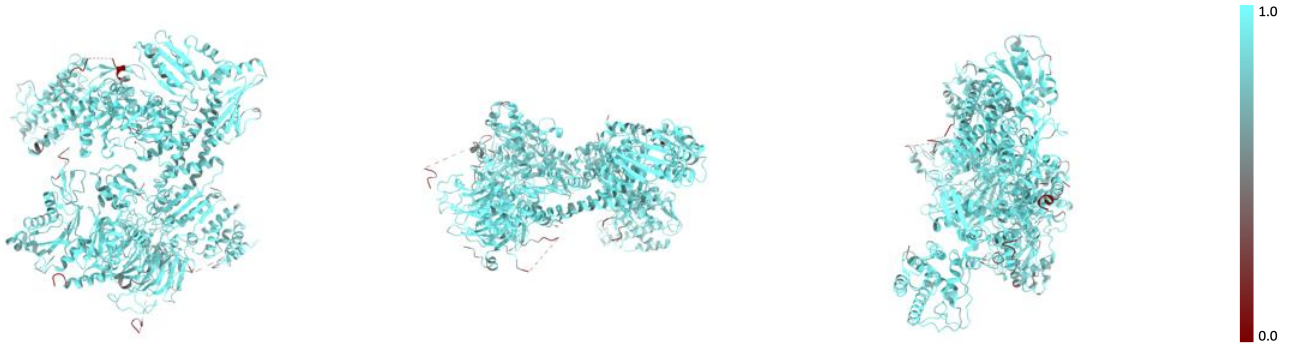
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

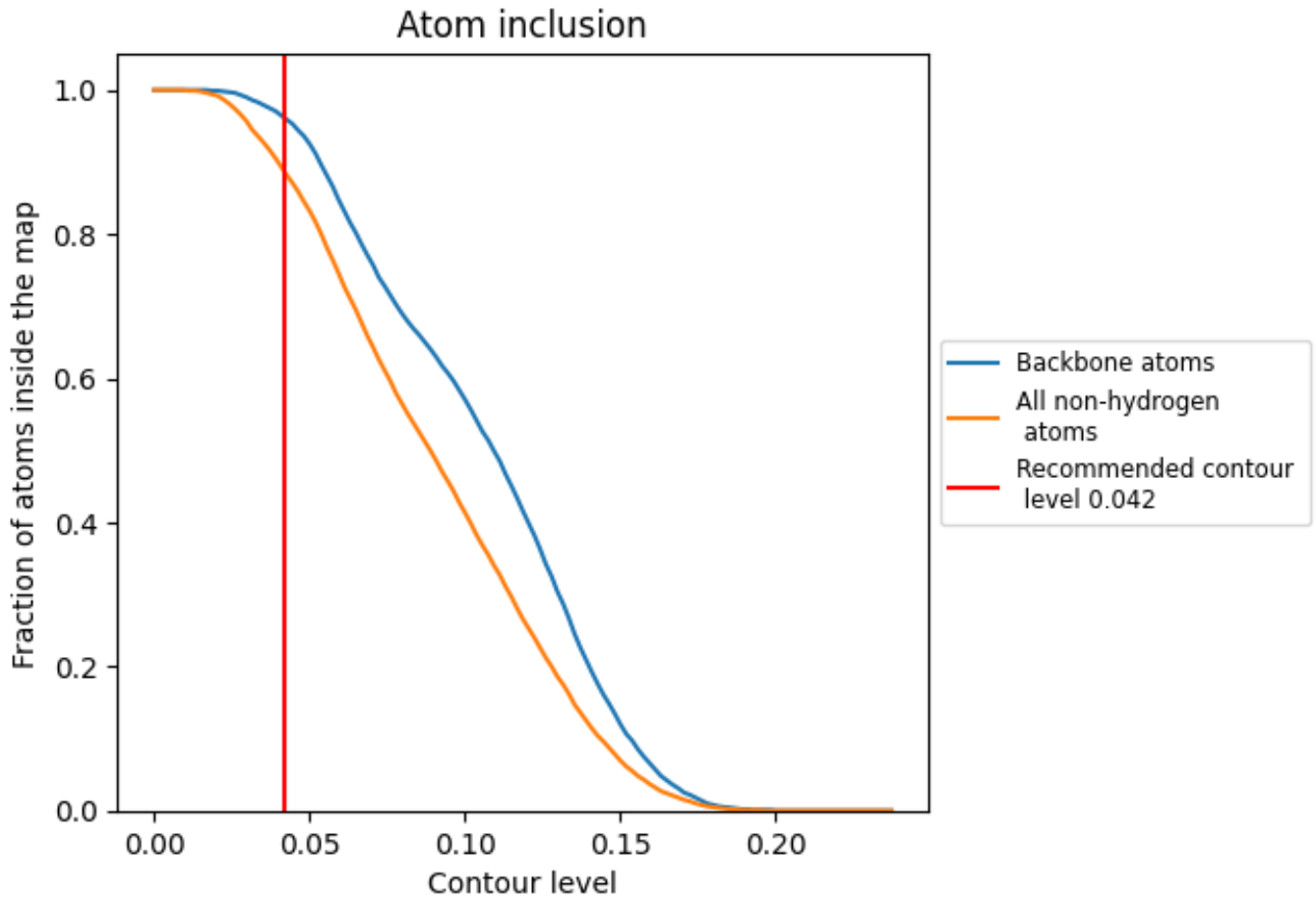
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.042).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 89% 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 (0.042) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8860	0.5270
A	0.9050	0.5380
B	0.8890	0.5390
C	0.9200	0.5570
D	0.8950	0.5240
E	0.8840	0.4700
F	0.9260	0.5590
G	0.8410	0.4980
H	0.5500	0.3710
I	0.4870	0.3400