



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 09:30 AM EST

PDB ID : 7TW6
EMDB ID : EMD-26153
Title : Cryo-EM structure of human ankyrin complex (B4P1A1) from red blood cell
Authors : Xia, X.; Liu, S.H.; Zhou, Z.H.
Deposited on : 2022-02-06
Resolution : 5.60 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 ⓘ 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

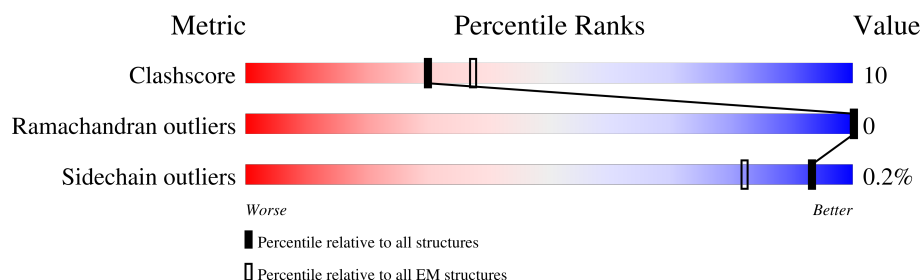
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.60 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	911	75% 17% 9%
1	B	911	71% 18% 11%
1	J	911	19% 21% 10% 68%
1	K	911	24% 7% 69%
2	E	691	72% 24% .
3	G	1881	26% 8% 66%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27184 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 Band 3 anion transport protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	830	Total	C	N	O	S	0	0
			6563	4300	1087	1151	25		
1	B	814	Total	C	N	O	S	0	0
			6435	4224	1065	1122	24		
1	K	284	Total	C	N	O	S	0	0
			2258	1439	395	418	6		
1	J	287	Total	C	N	O	S	0	0
			2285	1456	399	424	6		

- Molecule 2 is a protein called Protein 4.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	665	Total	C	N	O	S	0	0
			5236	3316	929	968	23		

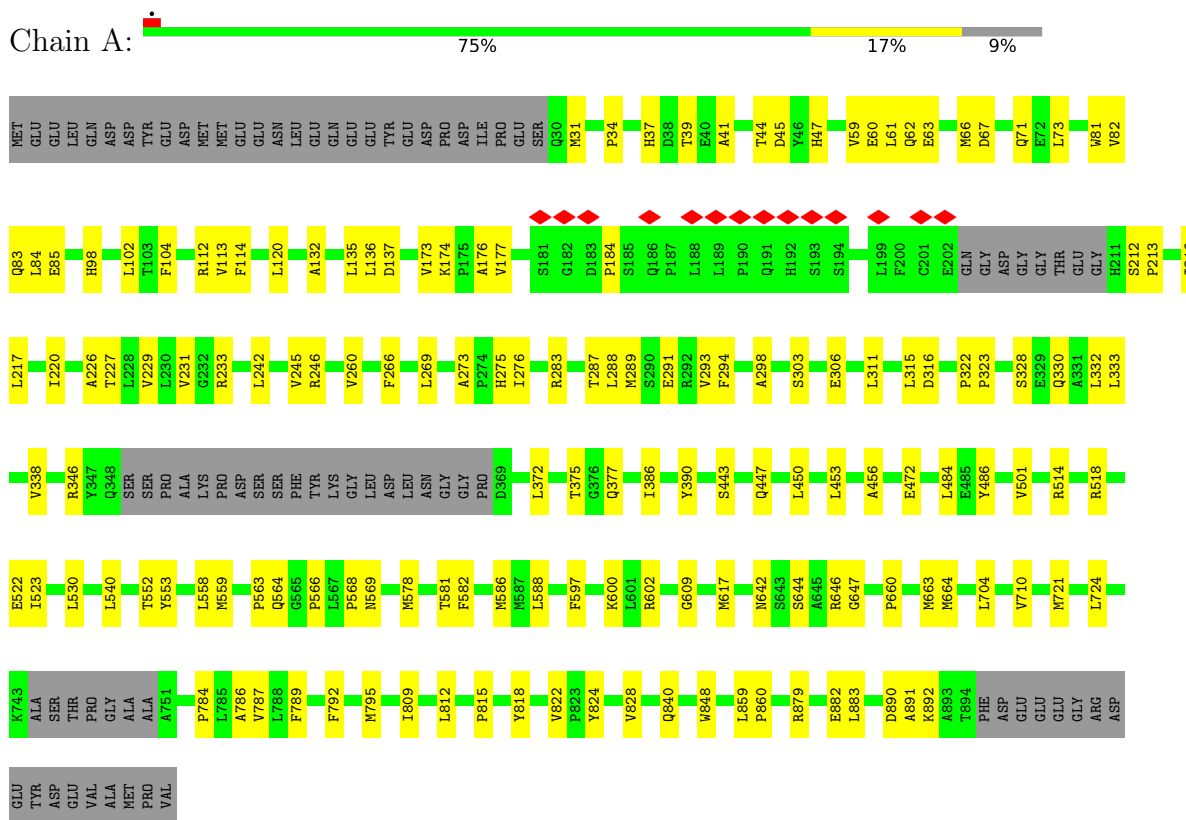
- Molecule 3 is a protein called Ankyrin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	635	Total	C	N	O	S	0	0
			4407	2736	843	814	14		

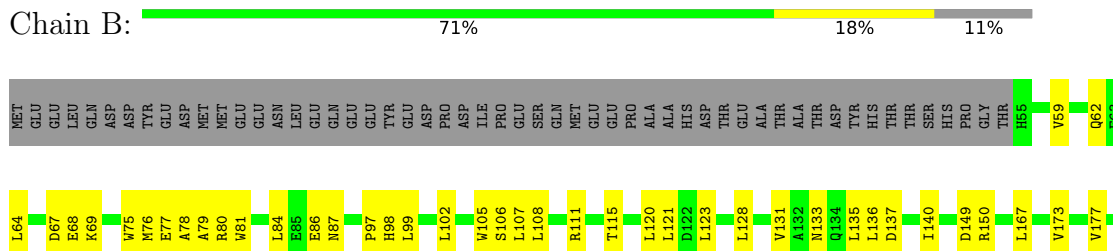
3 Residue-property plots

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

• Molecule 1: Band 3 anion transport protein



• Molecule 1: Band 3 anion transport protein





VAL
LEU
LEU
PRO
PRO
LEU
ILE
PHE
ARG
ASN
ASN
GLU
LEU
GLN
CYS
ASP
ASP
ALA
LYS
THR
PHE
ASP
GLU
GLU
GLU
GLY
ARG
ASP
GLU
TYR
ASP
GLU
VAL
ALA
MET
PRO
VAL

• Molecule 2: Protein 4.2

Chain E:  72% 24%

MET
GLY
A4
N18
E19
E20
H21
Q154
R155
T23
E157
S27
S28
R34
R35
C36
Q37
P38
L53
P54
V59
A60
L61
T62
G186
R74
A77
T81
R87
S91
V94
E95
E96
T103
T107
T108
D111
L121
Q122
V123
R126
K127
L136
N139
D145
A146
K150
N151
E152
A153
Q154
R155
M156
E157
Y158
N161
Q162
N163
Y167
L168
T170
I174
Q183
F184
E185
G186
D187
D190
L191
S197
W205
V209
L215
L219
K223
L228
P229
K244
R245
R246
T251
L252
R253
R261
V269
V270
L271
A272
R280
T291
F292
L303
I304
D305
E306
Y307
Y308
N309
E310
L313
Q327
T328
N334
L336
G342
G347
S352
A353
PRO
ASN
GLY
GLY
VAL
LEU
S362
V366
P367
V368
L376
G377
L378
S383
D384
L385
I388
V394
V395
K396
L404
V414
L418
S419
T420
K421
Q422
V423
D430
L431
T432
E444
V447
E452
M456
E457
R458
GLU
LYS
ASP
ASN
GLY
ILE
ARG
PRO
PRO
SER
LEU
GLU
THR
ALA
P473
P474
L475
Y476
L477
L478
L485
P486
L487
R488
G489
D490
T496
L497
V498
H499
H500
S501
E504
R505
A510
V516
H517
L535
L538
E539
E540
L547
L562
H567
H570
S571
E572
I583
E599
Q600
Q611
L614
E619
D620
C621
V622
I623
I625
L630
E631
H632
R633
E634
R635
F639
R640
S641
T647
K651
P652
T657
H658
V659
R663
V666
R675
N678
Y679
V684
P687
E688
L689
SER
ALA

• Molecule 3: Ankyrin-1

Chain G:  26% 8% 66%

MET
PRO
TYR
SER
VAL
GLY
PHE
ARG
GLU
ILE
ALA
ASP
ALA
ALA
THR
THR
SER
PHE
LYS
LEU
GLY
ARG
ALA
ALA
ALA
ARG
SER
GLY
ASN
LEU
ASP
LYS
ALA
VAL
VAL
GLY
ARG
VAL
GLU
ASP
VAL
ILE
ASN
THR
CYS
ASN
GLN
ASN
ASN
GLY
LEU
LEU
HIS
LEU
ALA
SER
PRO
GLU
TYR
MET
VAL
LYS
MET
GLN
VAL
LEU
HIS
PHE
THR
LYS
GLY
GLN
PHE
L174
P175
A176
I179
R182
GLU
ASN
HIS
LEU
VAL
VAL
ASN
ASN
GLY
ALA
GLN
SER
LYS
GLY
VAL
VAL
L210
Y216
E217
N218
L219
L226
A230
S231
V232
T235
A239
G239
P248
N251
V252
V255
L258
R261
C262
I265
K268
L273
T274
P275
L276
H277
A280
R281
N282
V285
I287
S288
L292
A296
P297
I298
T302
K303
L306
S307
P308
I309
M311
A312
D319
C320
L324
L325
Q326
D328
A329
E330
I331
T340
P341
H342
R343
V344
R352
K360
G361
G371
P374
H376
K380
K381
N382
V386
L390
L391
T401
A402
S403
G404
L405
T406
H409
F413
M414
H416
L417
K421
R426
H430
V432
V435
P440
L441
H442
M443
E451
Y455
A465
D469
P473
H482
M485
V486
L490
A499
T500
T505
R512
H515
T518
V519
L520
Q529
F537
T538
H541
Y546
L554
L555
L556
E557
R558
A565
Q569
N581
L582
D583
T584
V585
K586
L587
L588
R591
S594
P595
H596
S597
L606
H607
Q612
R613
Q614
V615
E616
R619
S620
L621
Y624
G625
A628
P638
L639
H640
K657
Q658
A659
L674
V675
A676
A708
L797
VAL
SER



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	111308	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.610	Depositor
Minimum map value	-1.469	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.63	Depositor
Map size (\AA)	616.0, 616.0, 616.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.2, 2.2, 2.2	Depositor

5 Model quality

5.1 Standard geometry

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	0.29	0/6720	0.52	0/9136
1	B	0.28	0/6588	0.53	0/8953
1	J	0.30	0/2333	0.57	0/3168
1	K	0.33	0/2305	0.57	0/3130
2	E	0.36	0/5345	0.59	0/7255
3	G	0.29	0/4479	0.51	0/6115
All	All	0.31	0/27770	0.54	0/37757

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

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	6563	0	6753	106	0
1	B	6435	0	6652	115	0
1	J	2285	0	2294	73	0
1	K	2258	0	2272	58	0
2	E	5236	0	5248	115	0
3	G	4407	0	4091	109	0
All	All	27184	0	27310	543	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 10.

The worst 5 of 543 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:B:76:MET:SD	1:B:173:VAL:HG11	1.68	1.32
3:G:588:LEU:HD22	3:G:591:ARG:NH2	1.57	1.17
3:G:588:LEU:CD2	3:G:591:ARG:NH2	2.15	1.08
3:G:556:LEU:HD13	3:G:591:ARG:HD2	1.49	0.93
1:B:76:MET:SD	1:B:173:VAL:CG1	2.58	0.92

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	822/911 (90%)	808 (98%)	14 (2%)	0	100	100
1	B	806/911 (88%)	791 (98%)	15 (2%)	0	100	100
1	J	283/911 (31%)	278 (98%)	5 (2%)	0	100	100
1	K	280/911 (31%)	274 (98%)	6 (2%)	0	100	100
2	E	659/691 (95%)	646 (98%)	13 (2%)	0	100	100
3	G	631/1881 (34%)	585 (93%)	46 (7%)	0	100	100
All	All	3481/6216 (56%)	3382 (97%)	99 (3%)	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	719/786 (92%)	717 (100%)	2 (0%)	92	95
1	B	707/786 (90%)	706 (100%)	1 (0%)	93	96
1	J	249/786 (32%)	249 (100%)	0	100	100
1	K	246/786 (31%)	244 (99%)	2 (1%)	81	89
2	E	568/588 (97%)	568 (100%)	0	100	100
3	G	391/1594 (24%)	391 (100%)	0	100	100
All	All	2880/5326 (54%)	2875 (100%)	5 (0%)	93	96

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

Mol	Chain	Res	Type
1	A	112	ARG
1	A	346	ARG
1	B	562	LYS
1	K	70	ASN
1	K	346	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.

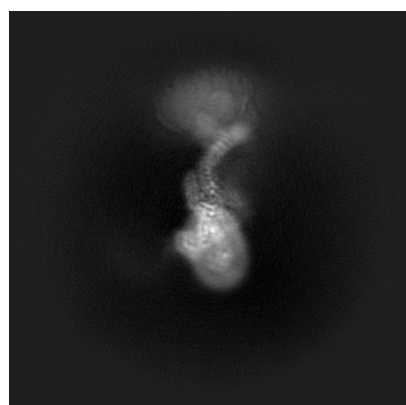
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26153. These allow visual inspection of the internal detail of the map and identification of artifacts.

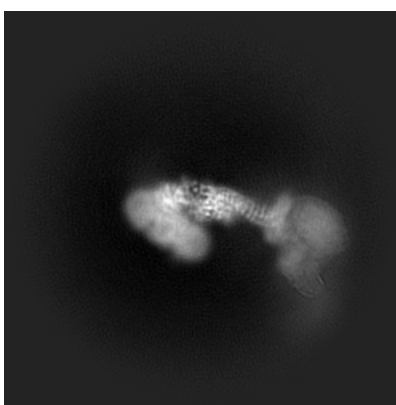
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

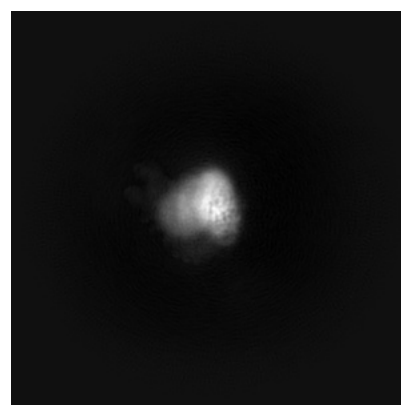
6.1.1 Primary map



X



Y

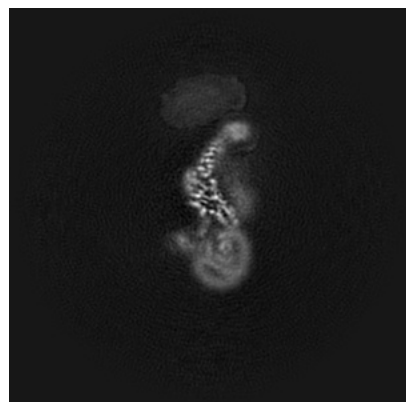


Z

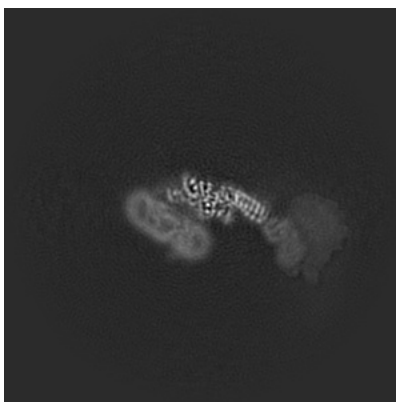
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

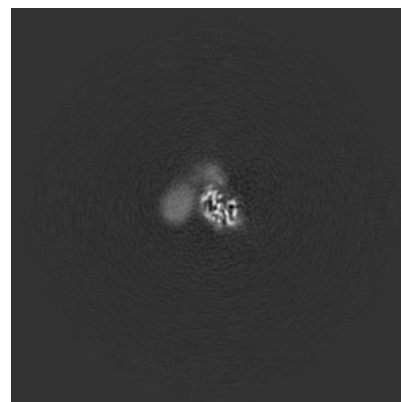
6.2.1 Primary map



X Index: 140



Y Index: 140

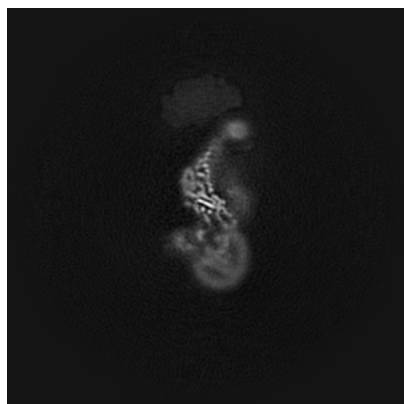


Z Index: 140

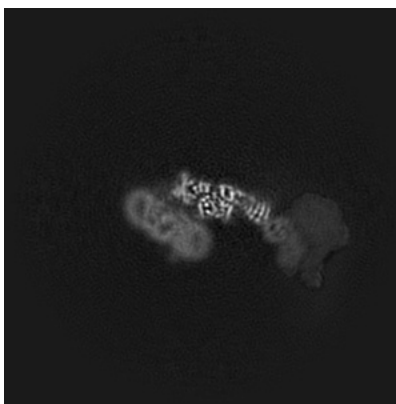
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

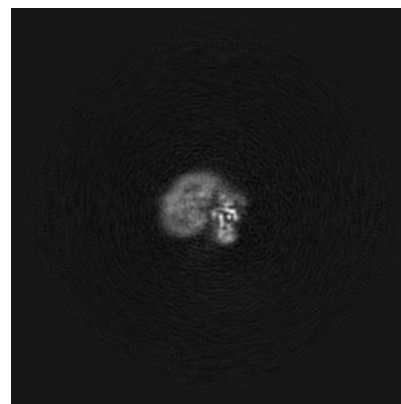
6.3.1 Primary map



X Index: 142



Y Index: 142



Z Index: 123

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.63. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

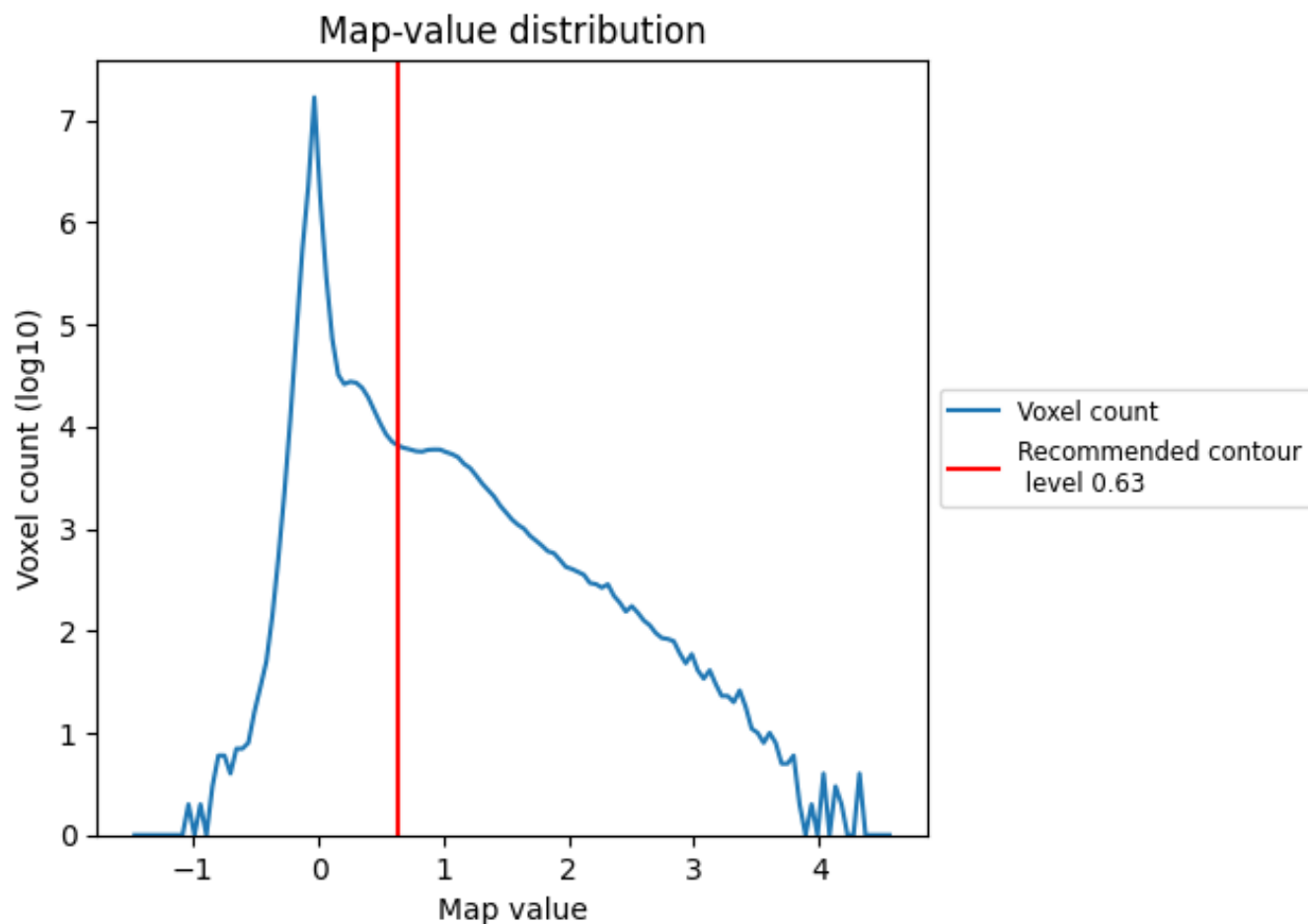
6.5 Mask visualisation

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

7 Map analysis [i](#)

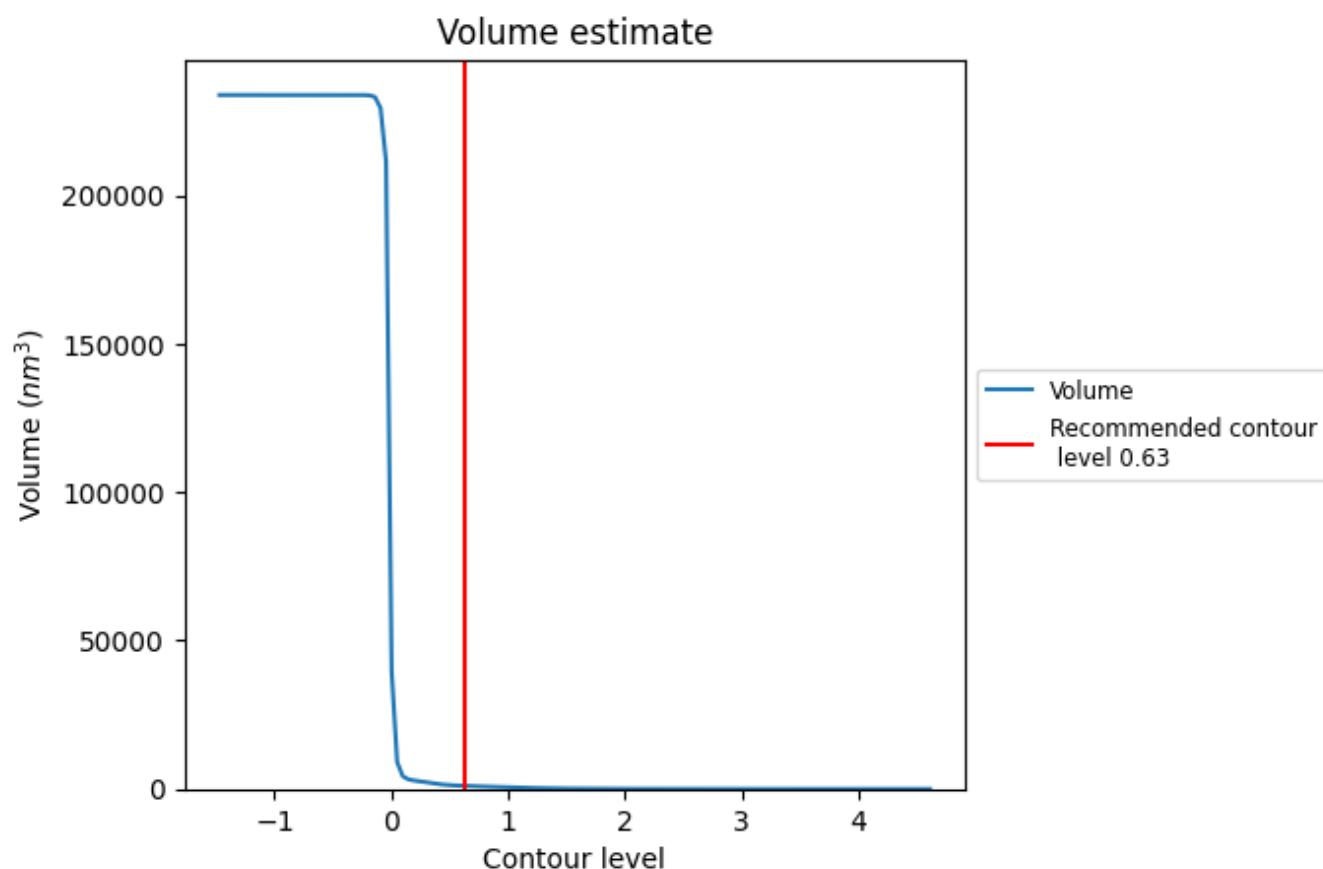
This section contains the results of statistical analysis of the map.

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.

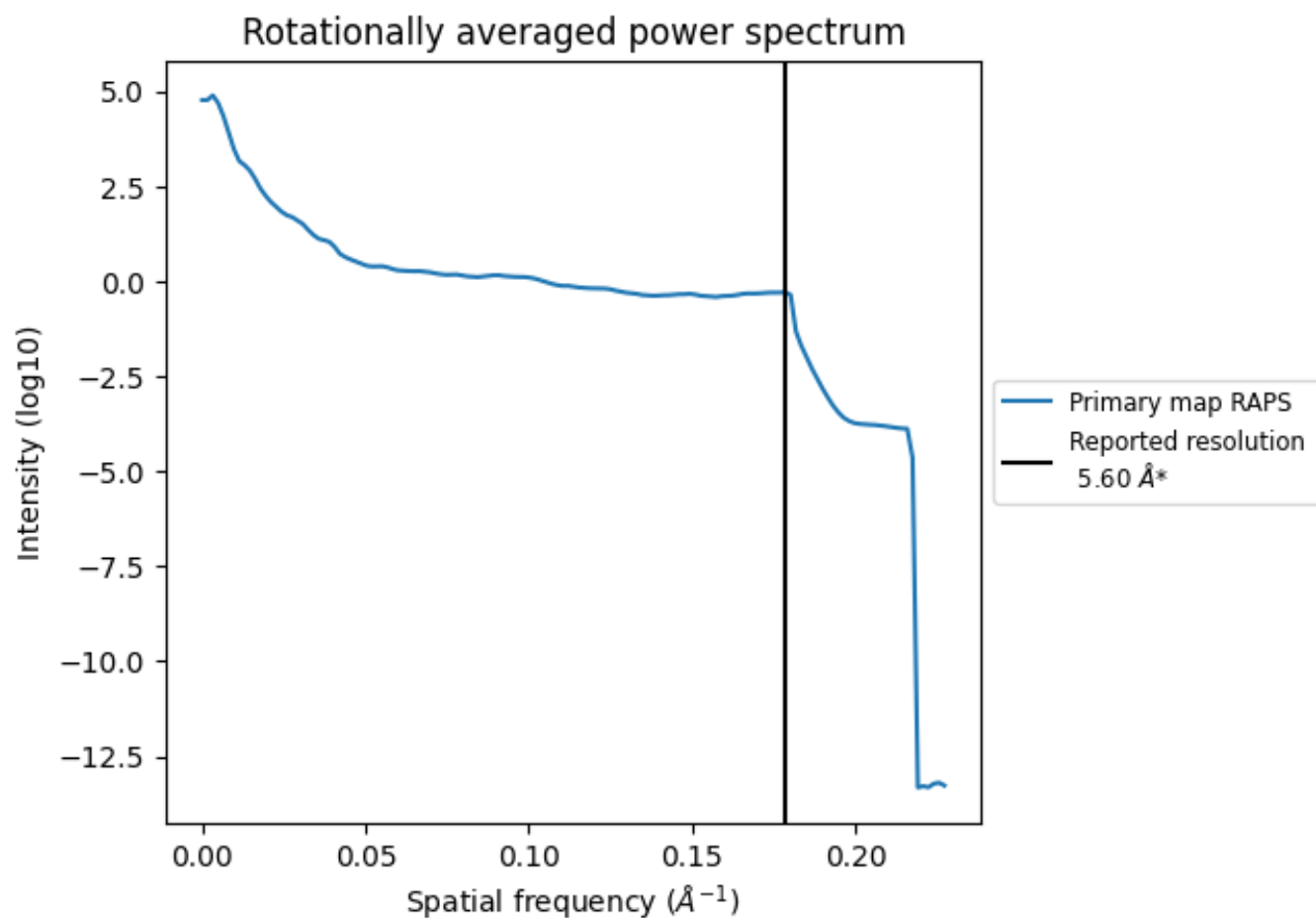
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1049 nm^3 ; this corresponds to an approximate mass of 948 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.179 Å⁻¹

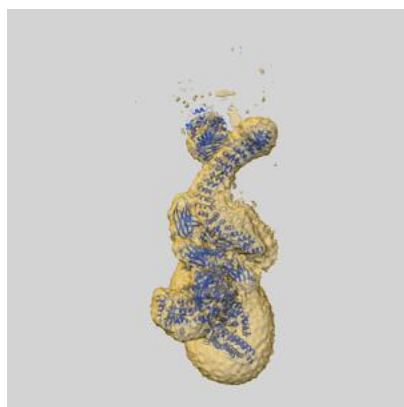
8 Fourier-Shell correlation

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

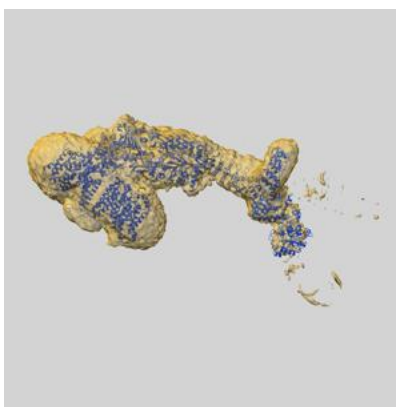
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26153 and PDB model 7TW6. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

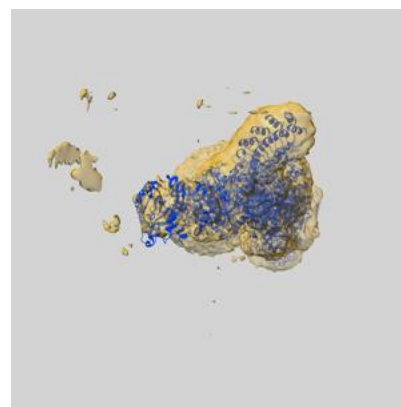
9.1 Map-model overlay [i](#)



X



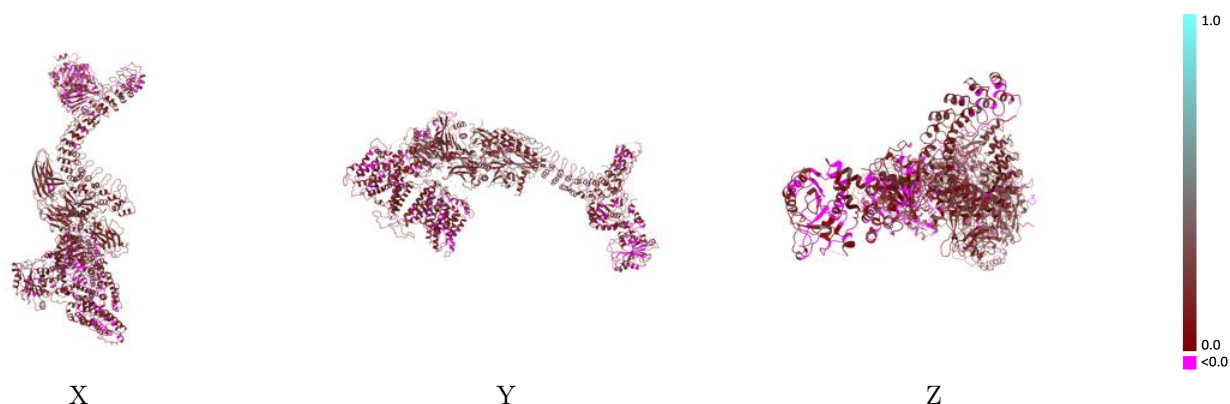
Y



Z

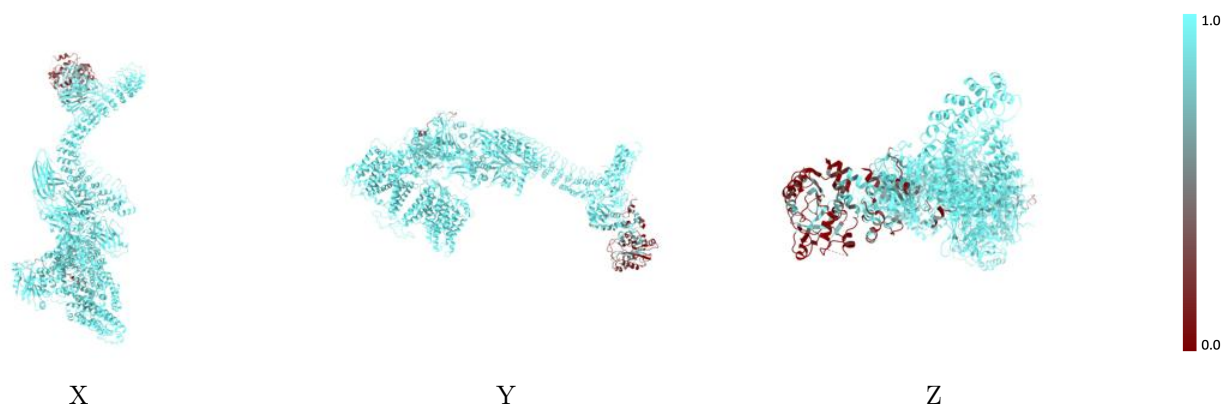
The images above show the 3D surface view of the map at the recommended contour level 0.63 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



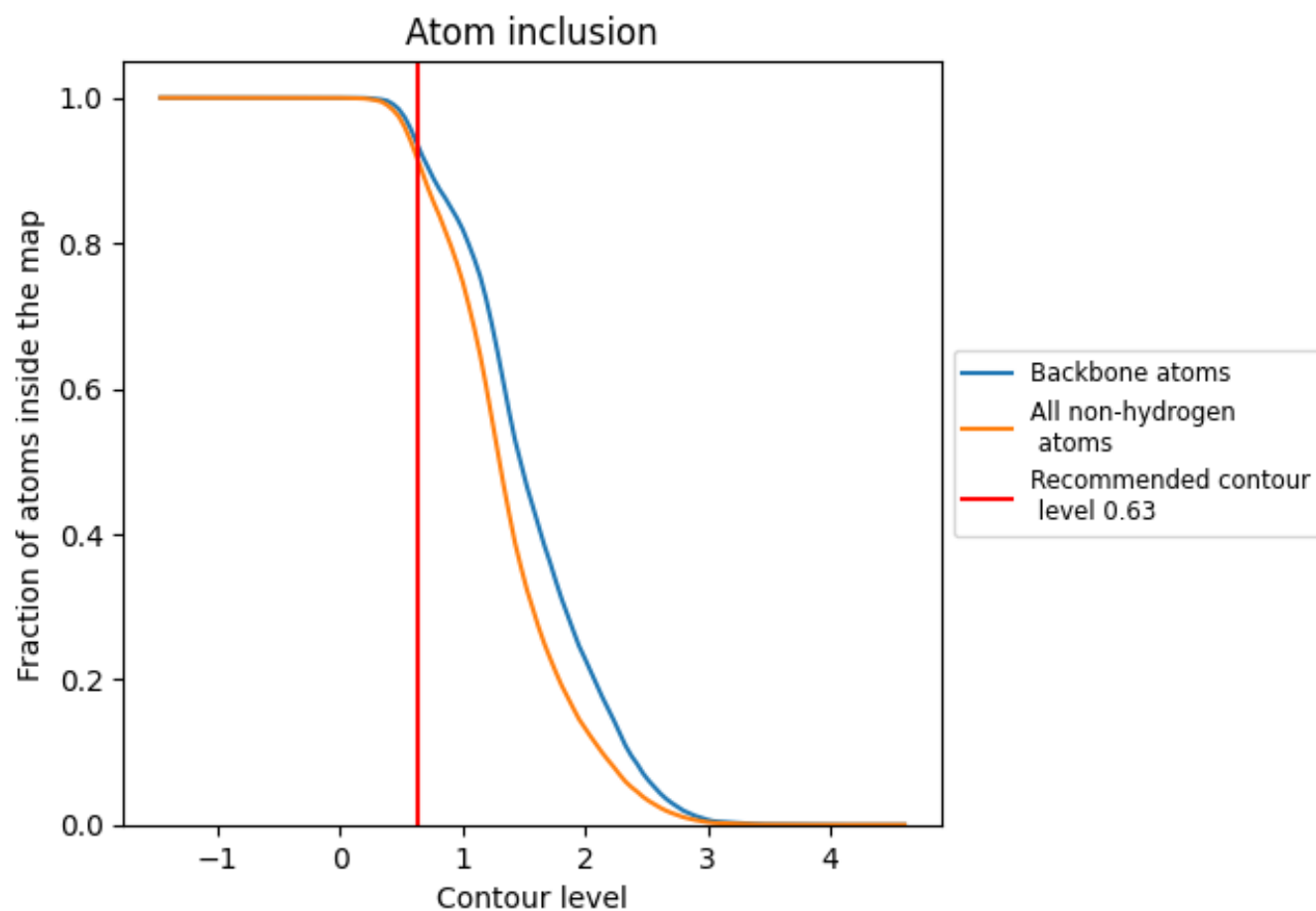
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.63).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% 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 (0.63) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9159</div>	<div><div></div>0.1430</div>
A	<div><div></div>0.9701</div>	<div><div></div>0.1240</div>
B	<div><div></div>0.9880</div>	<div><div></div>0.1260</div>
E	<div><div></div>0.9828</div>	<div><div></div>0.2090</div>
G	<div><div></div>0.9885</div>	<div><div></div>0.1820</div>
J	<div><div></div>0.3521</div>	<div><div></div>0.0520</div>
K	<div><div></div>0.8234</div>	<div><div></div>0.1070</div>

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