



wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 08:51 AM EST

PDB ID : 6X0L
EMDB ID : EMD-21978
Title : Bridging of double-strand DNA break activates PARP2/HPF1 to modify chromatin
Authors : Halic, M.; Bilokapic, S.
Deposited on : 2020-05-16
Resolution : 3.90 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) : 2.31.2

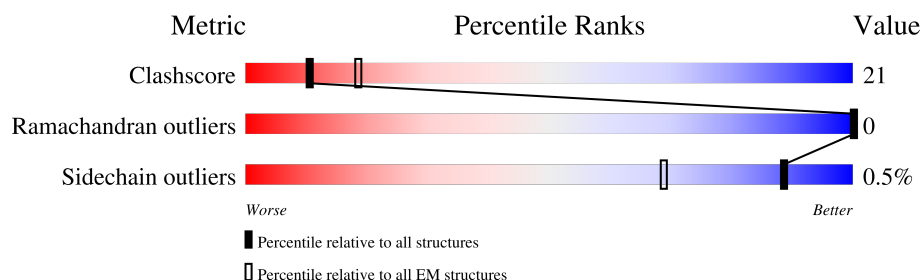
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	O	356	<div> <div>40%</div> <div>57%</div> <div>29%</div> <div>14%</div> </div>
2	P	590	<div> <div>19%</div> <div>48%</div> <div>32%</div> <div>20%</div> </div>
2	R	590	<div> <div>9%</div> <div>12%</div> <div>8%</div> <div>81%</div> </div>
3	I	167	<div> <div>94%</div> </div>
3	i	167	<div> <div>94%</div> </div>
4	J	167	<div> <div>94%</div> </div>
4	j	167	<div> <div>94%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8037 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 Histone PARylation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	306	Total	C	N	O	S	0	0
			2488	1597	415	465	11		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-9	MET	-	initiating methionine	UNP Q9NWX4
O	-8	GLY	-	expression tag	UNP Q9NWX4
O	-7	HIS	-	expression tag	UNP Q9NWX4
O	-6	HIS	-	expression tag	UNP Q9NWX4
O	-5	HIS	-	expression tag	UNP Q9NWX4
O	-4	HIS	-	expression tag	UNP Q9NWX4
O	-3	HIS	-	expression tag	UNP Q9NWX4
O	-2	HIS	-	expression tag	UNP Q9NWX4
O	-1	GLY	-	expression tag	UNP Q9NWX4
O	0	GLY	-	expression tag	UNP Q9NWX4
O	174	LYS	ARG	variant	UNP Q9NWX4

- Molecule 2 is a protein called Poly [ADP-ribose] polymerase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	474	Total	C	N	O	S	0	0
			3798	2413	654	704	27		
2	R	114	Total	C	N	O	S	0	0
			929	588	161	173	7		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	-19	MET	-	initiating methionine	UNP Q9UGN5
P	-18	GLY	-	expression tag	UNP Q9UGN5
P	-17	SER	-	expression tag	UNP Q9UGN5
P	-16	SER	-	expression tag	UNP Q9UGN5

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-15	HIS	-	expression tag	UNP Q9UGN5
P	-14	HIS	-	expression tag	UNP Q9UGN5
P	-13	HIS	-	expression tag	UNP Q9UGN5
P	-12	HIS	-	expression tag	UNP Q9UGN5
P	-11	HIS	-	expression tag	UNP Q9UGN5
P	-10	HIS	-	expression tag	UNP Q9UGN5
P	-9	SER	-	expression tag	UNP Q9UGN5
P	-8	SER	-	expression tag	UNP Q9UGN5
P	-7	GLY	-	expression tag	UNP Q9UGN5
P	-6	LEU	-	expression tag	UNP Q9UGN5
P	-5	VAL	-	expression tag	UNP Q9UGN5
P	-4	PRO	-	expression tag	UNP Q9UGN5
P	-3	ARG	-	expression tag	UNP Q9UGN5
P	-2	GLY	-	expression tag	UNP Q9UGN5
P	-1	SER	-	expression tag	UNP Q9UGN5
P	0	HIS	-	expression tag	UNP Q9UGN5
R	-19	MET	-	initiating methionine	UNP Q9UGN5
R	-18	GLY	-	expression tag	UNP Q9UGN5
R	-17	SER	-	expression tag	UNP Q9UGN5
R	-16	SER	-	expression tag	UNP Q9UGN5
R	-15	HIS	-	expression tag	UNP Q9UGN5
R	-14	HIS	-	expression tag	UNP Q9UGN5
R	-13	HIS	-	expression tag	UNP Q9UGN5
R	-12	HIS	-	expression tag	UNP Q9UGN5
R	-11	HIS	-	expression tag	UNP Q9UGN5
R	-10	HIS	-	expression tag	UNP Q9UGN5
R	-9	SER	-	expression tag	UNP Q9UGN5
R	-8	SER	-	expression tag	UNP Q9UGN5
R	-7	GLY	-	expression tag	UNP Q9UGN5
R	-6	LEU	-	expression tag	UNP Q9UGN5
R	-5	VAL	-	expression tag	UNP Q9UGN5
R	-4	PRO	-	expression tag	UNP Q9UGN5
R	-3	ARG	-	expression tag	UNP Q9UGN5
R	-2	GLY	-	expression tag	UNP Q9UGN5
R	-1	SER	-	expression tag	UNP Q9UGN5
R	0	HIS	-	expression tag	UNP Q9UGN5

- Molecule 3 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	10	Total	C	N	O	P	0	0
			204	97	38	59	10		

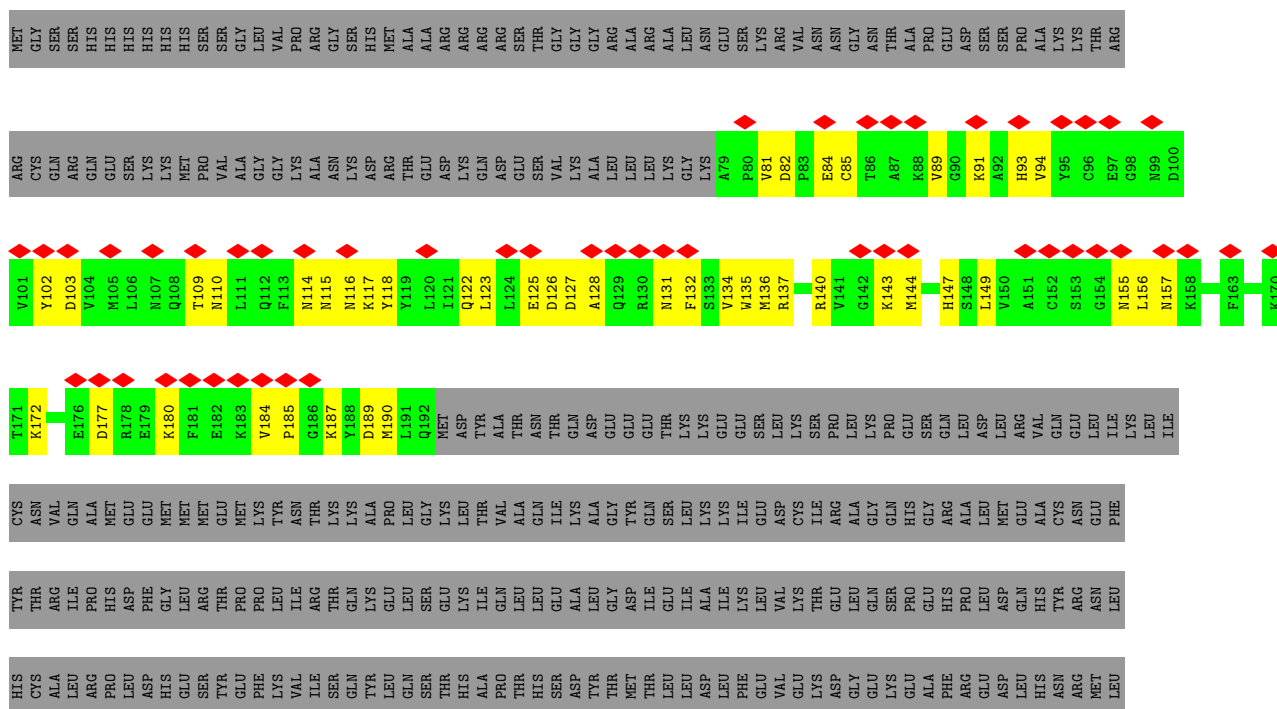
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	i	10	Total	C	N	O	P	0	0
			207	98	40	59	10		

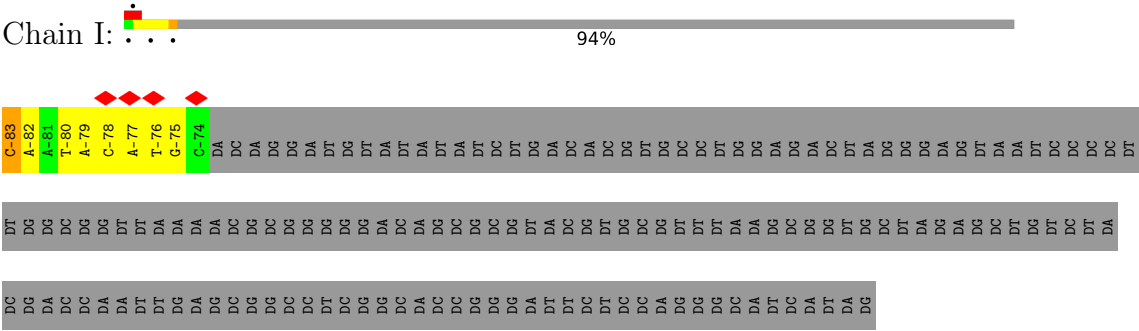
- Molecule 4 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	10	Total	C	N	O	P	0	0
			207	99	36	62	10		
4	j	10	Total	C	N	O	P	0	0
			204	97	35	62	10		

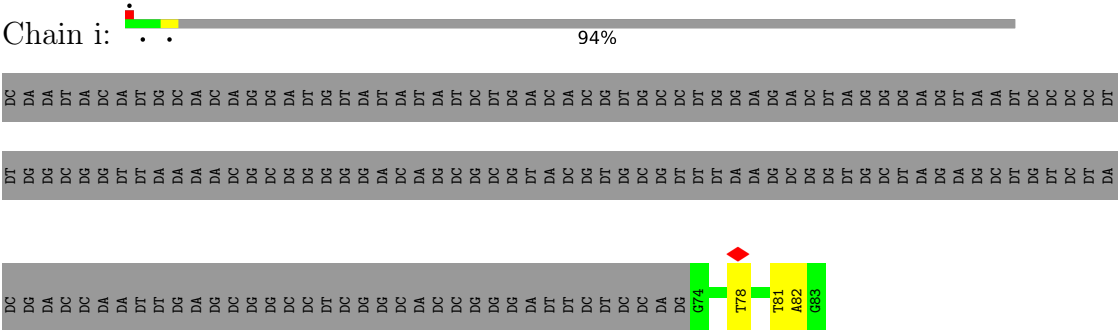


ILE	LEU	ASN	PRO	ASP	GLY	THR	THR	LEU	ASN	TRP	VAL	ASN	GLY	LEU	TYR	ILE	SER	TYR	ASN	PRO	LYS	ASN	GLN	VAL	GLY	LEU	PRO	ARG	MET	GLN	TYR	LEU	THR	LYS	GLY	ASN	PHE	GLY	LEU	ALA	PRO	SER	SER	ASP	ALA	HIS	VAL	PHE	VAL	SER	LEU	ASN	GLY	TYR	CYS	THR	THR	VAL	PRO	LEU	GLY	ARG	LEU	GLY	PRO	ALA	ASN	THR	GLY	ASP	THR	LEU	GLY
LEU	LEU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

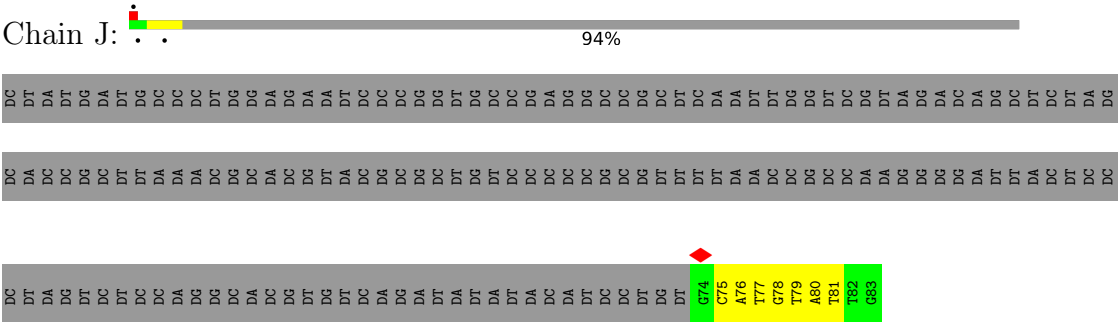
● Molecule 3: DNA (167-MER)



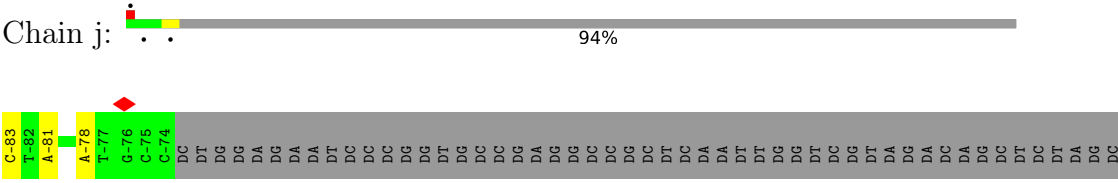
● Molecule 3: DNA (167-MER)



● Molecule 4: DNA (167-MER)



● Molecule 4: DNA (167-MER)



DT	DA	DG	DG	DC	DT	DC	DC	DA	DG	DG	DC	DA	DC	DG	DT	DG	DC	DA	DG	DA	DT	DA	DT	DA	DT	DT	DT	DT	DT
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17000	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 ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	508.8, 508.8, 508.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	O	0.31	0/2543	0.51	1/3428 (0.0%)
2	P	0.30	0/3881	0.53	1/5235 (0.0%)
2	R	0.29	0/949	0.51	0/1277
3	I	0.97	1/228 (0.4%)	0.96	0/347
3	i	1.03	2/232 (0.9%)	1.03	1/356 (0.3%)
4	J	0.65	0/231	1.11	1/355 (0.3%)
4	j	1.23	3/227 (1.3%)	0.94	0/346
All	All	0.44	6/8291 (0.1%)	0.60	4/11344 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	-83	DC	OP3-P	-10.78	1.48	1.61
4	j	-83	DC	OP3-P	-10.76	1.48	1.61
3	i	82	DA	C1'-N9	-5.86	1.39	1.47
4	j	-81	DA	C1'-N9	-5.74	1.39	1.47
4	j	-78	DA	C1'-N9	-5.05	1.40	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	i	81	DT	O4'-C1'-N1	7.21	113.05	108.00
4	J	77	DT	O4'-C1'-N1	5.49	111.84	108.00
1	O	36	ASP	CB-CG-OD2	5.19	122.97	118.30
2	P	194	ASP	CB-CG-OD2	5.15	122.93	118.30

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	O	2488	0	2466	89	0
2	P	3798	0	3775	148	0
2	R	929	0	900	27	0
3	I	204	0	113	6	0
3	i	207	0	113	0	0
4	J	207	0	115	3	0
4	j	204	0	114	0	0
All	All	8037	0	7596	271	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 21.

The worst 5 of 271 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)
2:P:80:PRO:CG	2:P:195:TYR:CD1	2.33	1.10
1:O:179:LYS:HA	1:O:182:ILE:HD12	1.38	1.03
2:P:80:PRO:HG2	2:P:195:TYR:CD1	1.96	0.98
2:P:80:PRO:HG3	2:P:195:TYR:CD1	1.98	0.98
2:P:505:LEU:HB3	2:P:533:ILE:HD12	1.61	0.81

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	O	302/356 (85%)	292 (97%)	10 (3%)	0	100	100
2	P	470/590 (80%)	442 (94%)	28 (6%)	0	100	100
2	R	112/590 (19%)	106 (95%)	6 (5%)	0	100	100
All	All	884/1536 (58%)	840 (95%)	44 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	O	271/308 (88%)	270 (100%)	1 (0%)	91	94
2	P	413/511 (81%)	411 (100%)	2 (0%)	88	93
2	R	100/511 (20%)	99 (99%)	1 (1%)	76	86
All	All	784/1330 (59%)	780 (100%)	4 (0%)	89	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	174	LYS
2	P	137	ARG
2	P	230	LYS
2	R	91	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	P	519	ASN
2	P	553	GLN
2	R	146	GLN
2	R	110	ASN
2	R	122	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](#)

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.

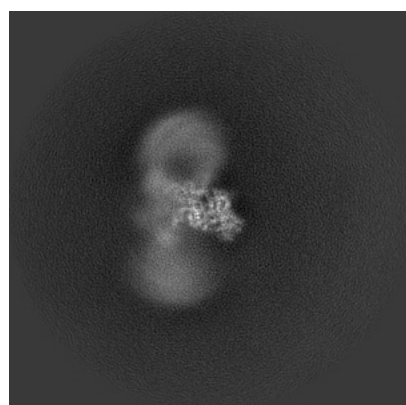
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21978. These allow visual inspection of the internal detail of the map and identification of artifacts.

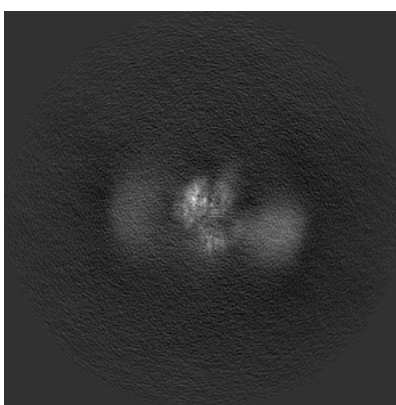
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

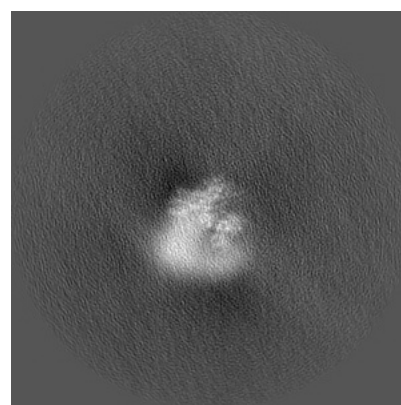
6.1.1 Primary map



X



Y

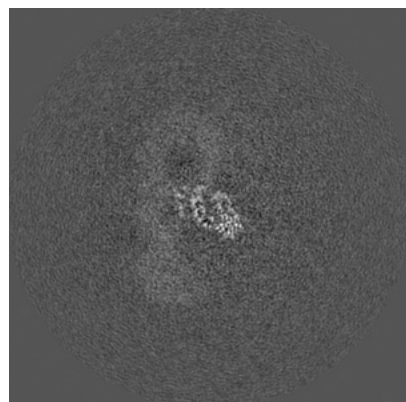


Z

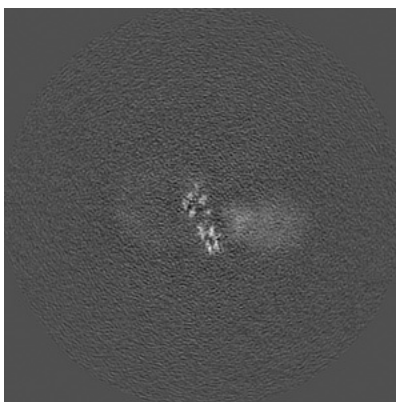
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

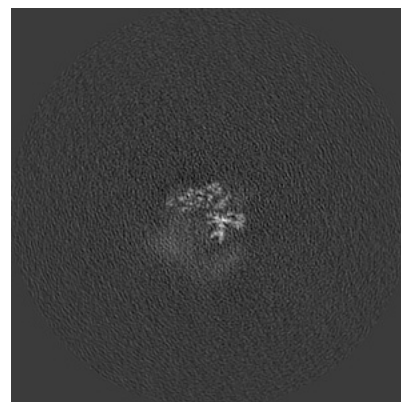
6.2.1 Primary map



X Index: 240



Y Index: 240

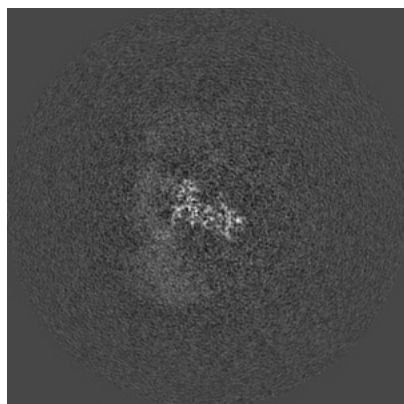


Z Index: 240

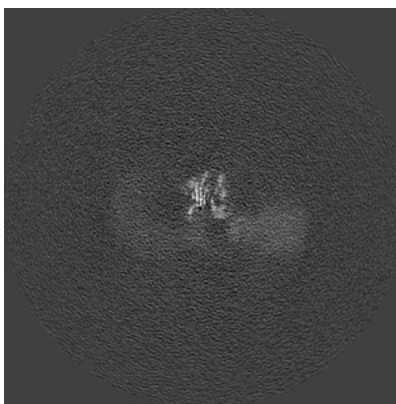
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

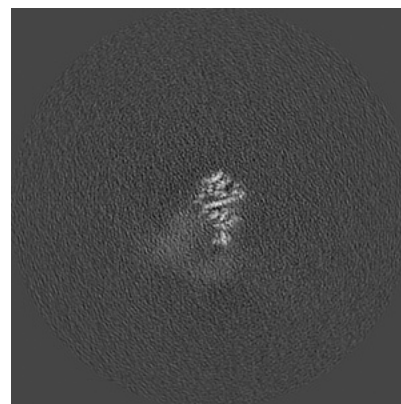
6.3.1 Primary map



X Index: 250



Y Index: 227



Z Index: 227

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

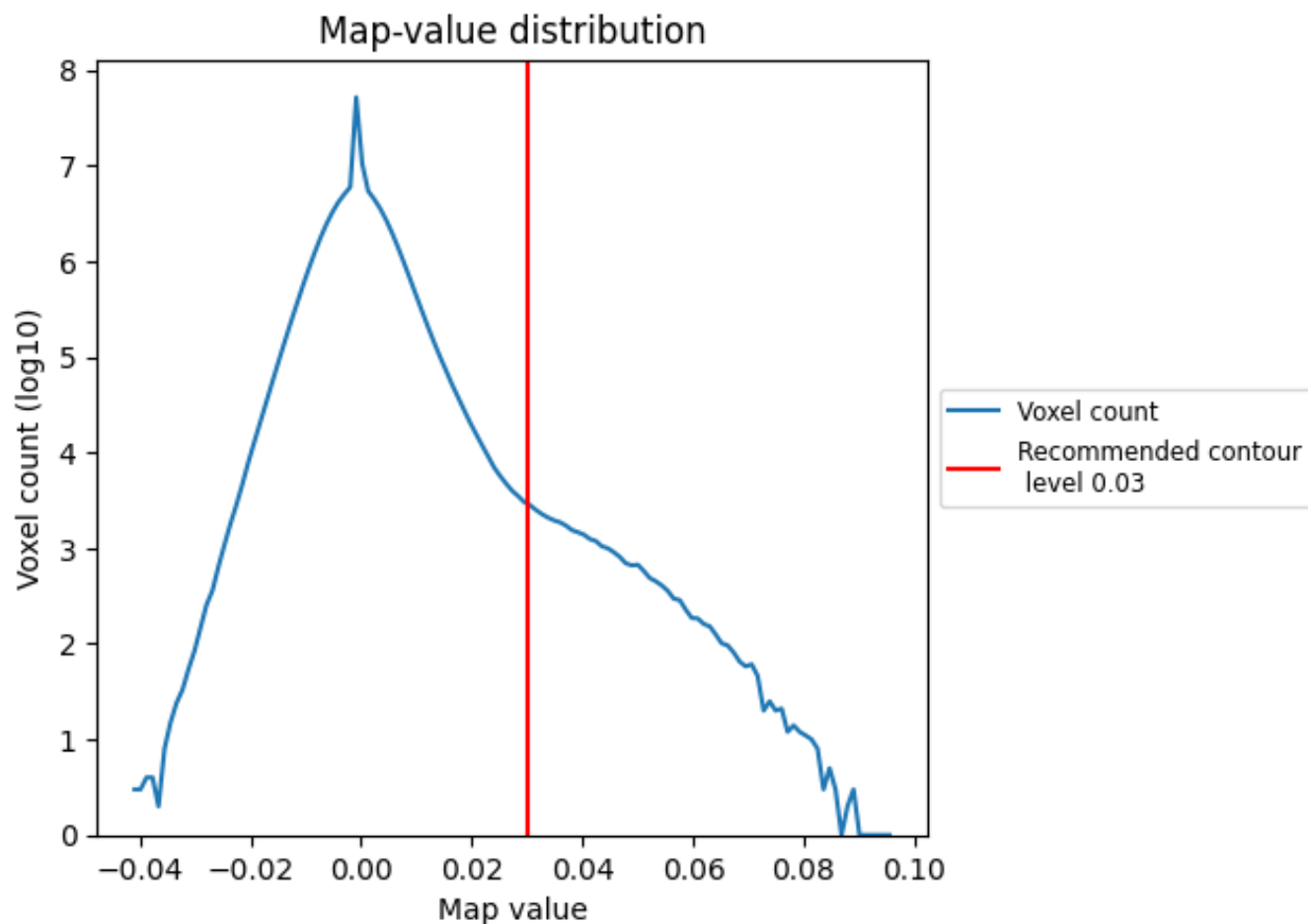
6.5 Mask visualisation

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

7 Map analysis [i](#)

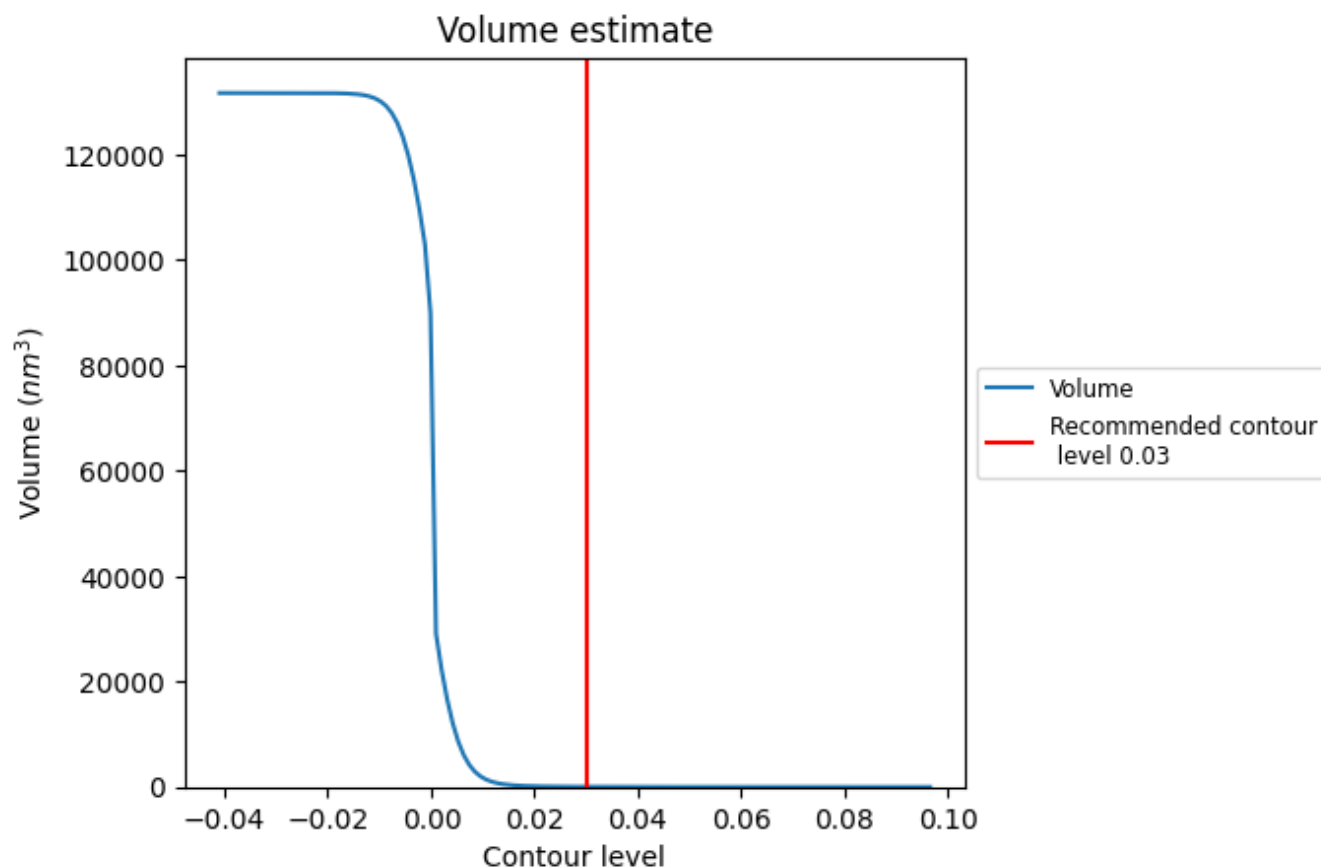
This section contains the results of statistical analysis of the map.

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.

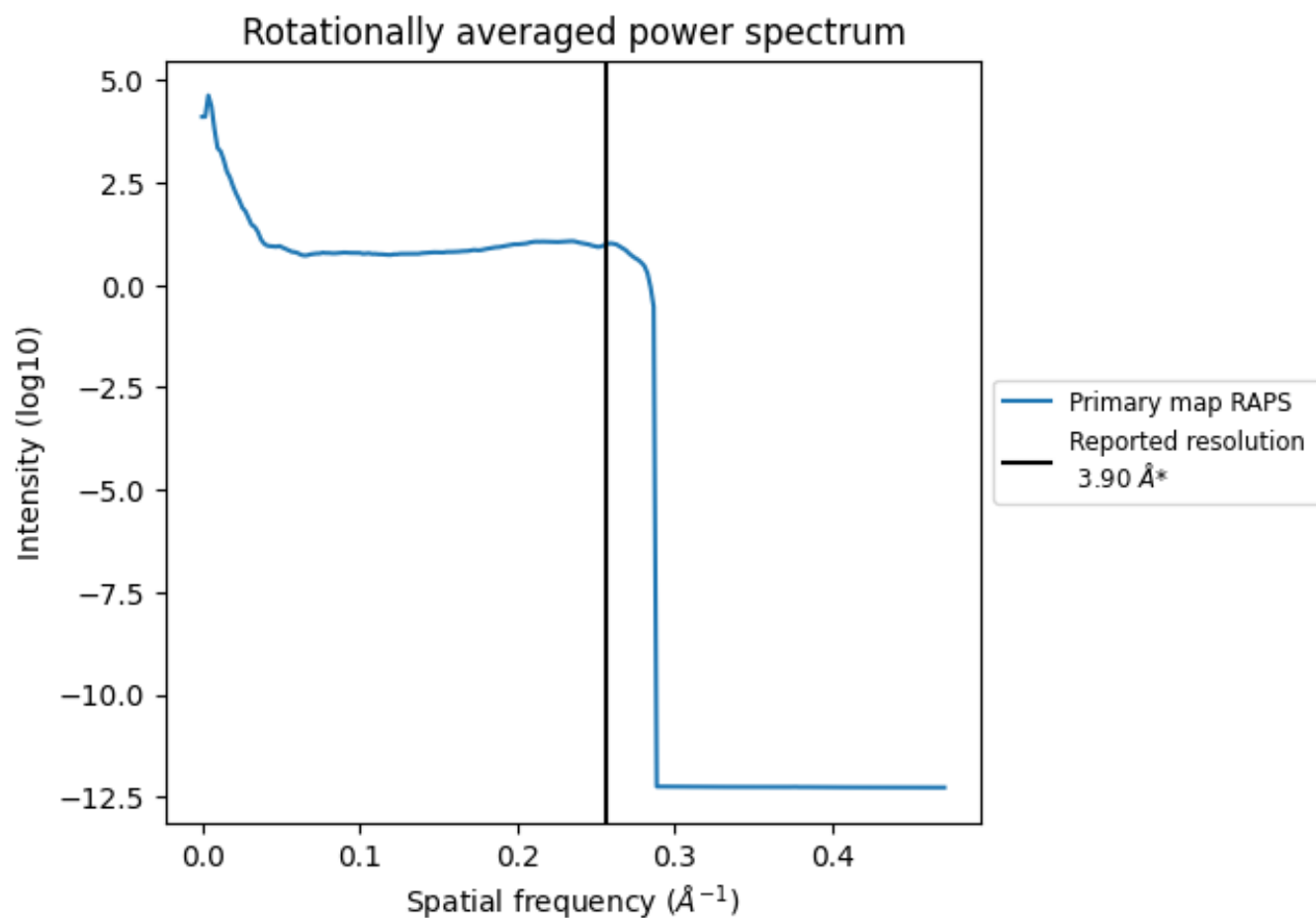
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 40 nm^3 ; this corresponds to an approximate mass of 36 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 0.256 Å⁻¹

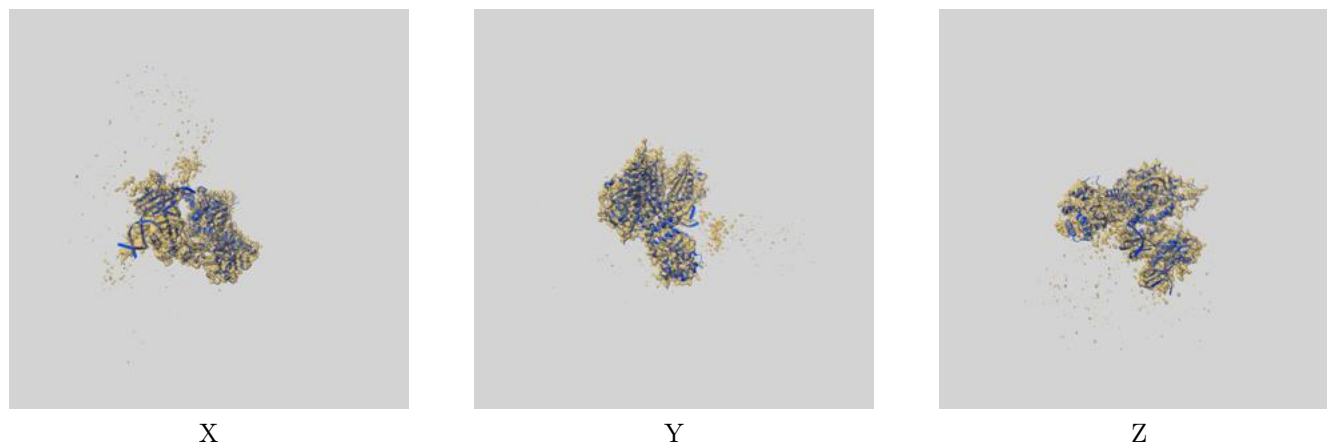
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

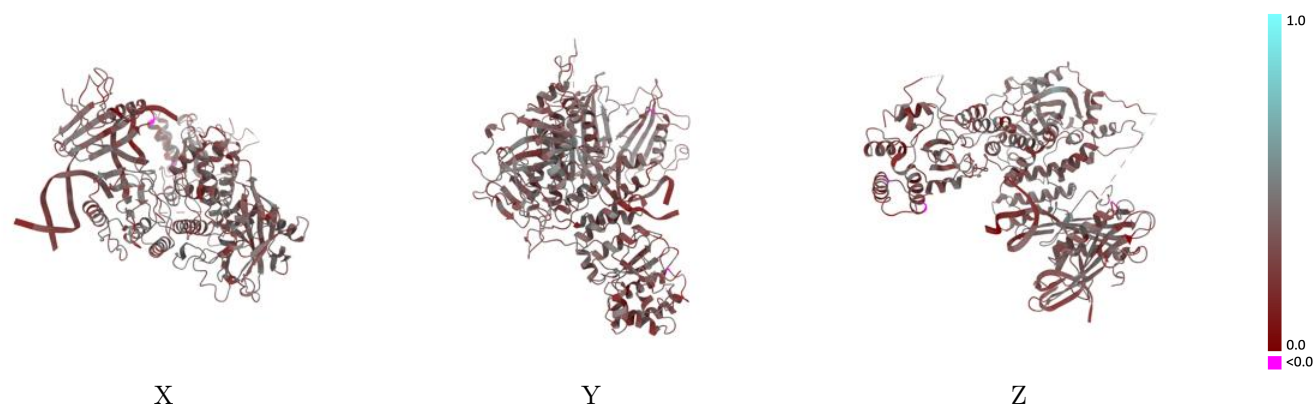
This section contains information regarding the fit between EMDB map EMD-21978 and PDB model 6X0L. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



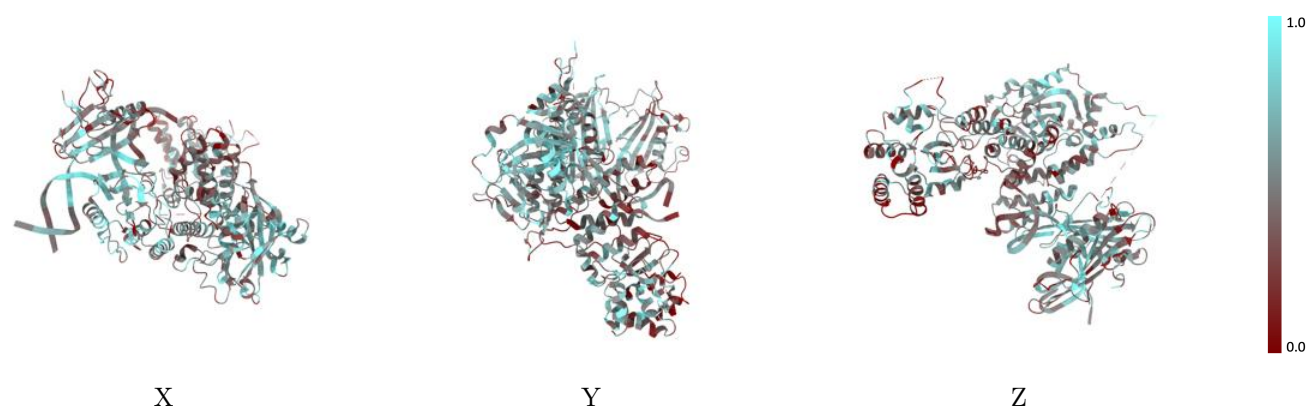
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



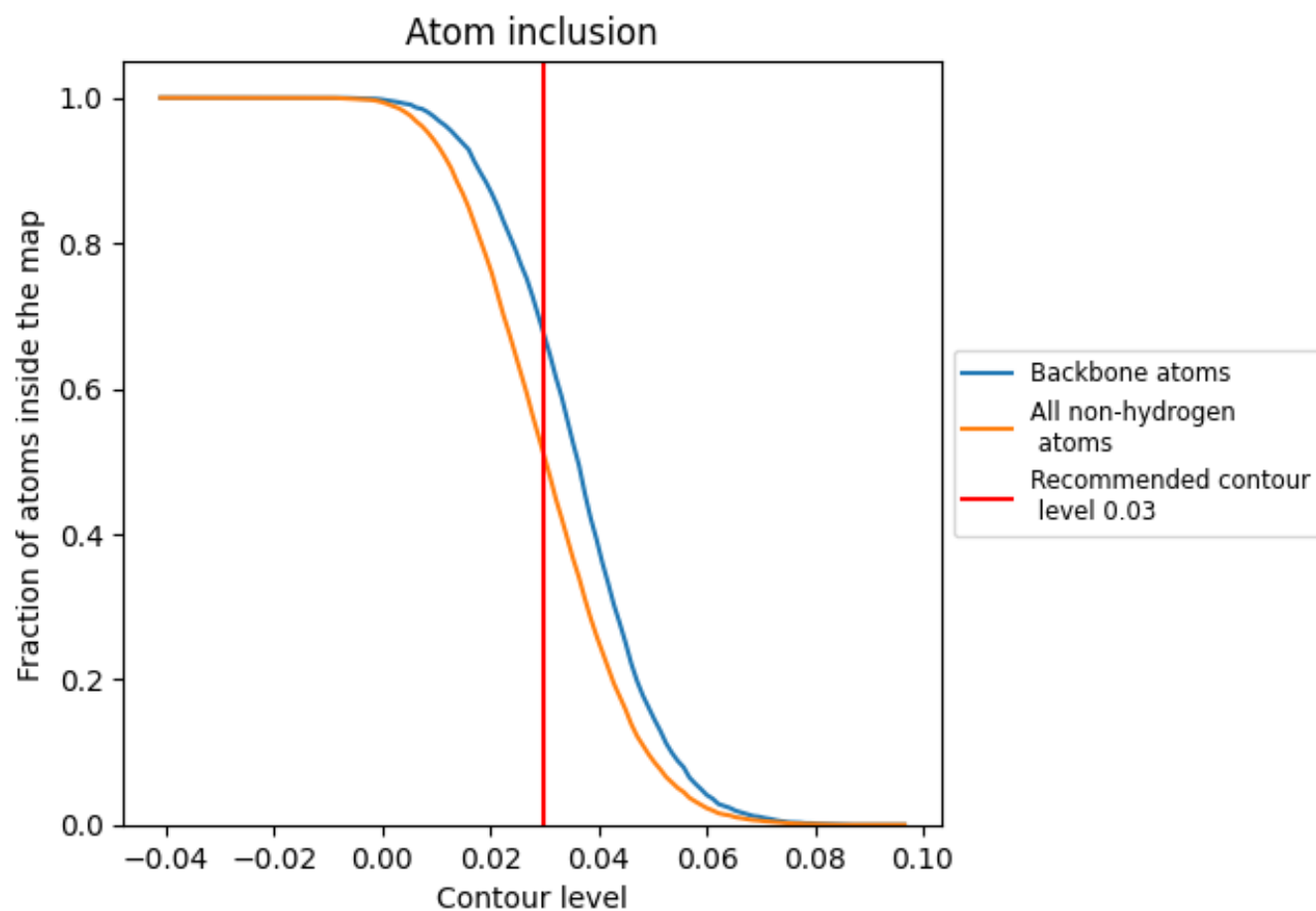
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 51% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.5063	<div><div></div></div> 0.3390
I	<div><div></div></div> 0.5343	<div><div></div></div> 0.2510
J	<div><div></div></div> 0.5845	<div><div></div></div> 0.2850
O	<div><div></div></div> 0.4237	<div><div></div></div> 0.3210
P	<div><div></div></div> 0.5596	<div><div></div></div> 0.3700
R	<div><div></div></div> 0.4393	<div><div></div></div> 0.3250
i	<div><div></div></div> 0.5942	<div><div></div></div> 0.2650
j	<div><div></div></div> 0.6275	<div><div></div></div> 0.2840

1.0

0.0

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