Full wwPDB EM Validation Report ⓘ

Jul 9, 2024 – 09:22 pm BST

PDB ID	:	9ENP
EMDB ID	:	EMD-19837
Title	:	HSV-1 DNA polymerase-processivity factor complex in exonuclease state with 1-bp DNA mismatch
Authors	:	Gustavsson, E.; Grunewald, K.; Elias, P.; Hallberg, B.M.
Deposited on	:	2024-03-13
Resolution	:	2.12 Å(reported)
Based on initial model	:	7LUF

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:

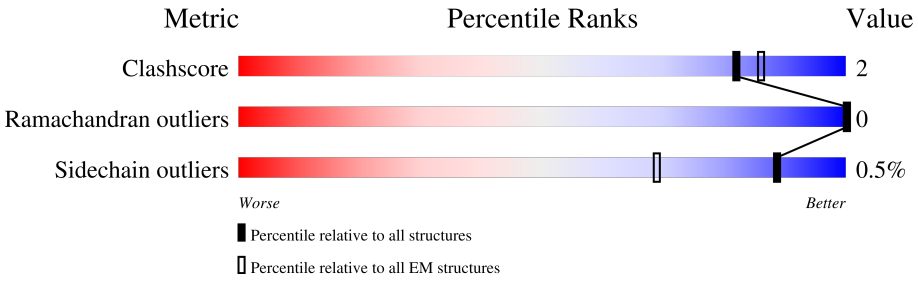
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.12 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	1235	5% 84% · 13%
2	B	488	· 54% · 45%
3	C	46	9% 50% 7% 43%
4	D	67	6% 30% 6% 64%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11552 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 DNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1072	8467	5425	1481	1521	40	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	330	ARG	ALA	variant	UNP P04293

- Molecule 2 is a protein called DNA polymerase processivity factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	266	2049	1303	360	379	7	0	0

- Molecule 3 is a DNA chain called DNA (46-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
3	C	26	523	248	97	150	26	2	0	0

- Molecule 4 is a DNA chain called DNA (67-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	D	24	503	236	97	146	24	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
5	A	2	2	2	0

- Molecule 6 is water.

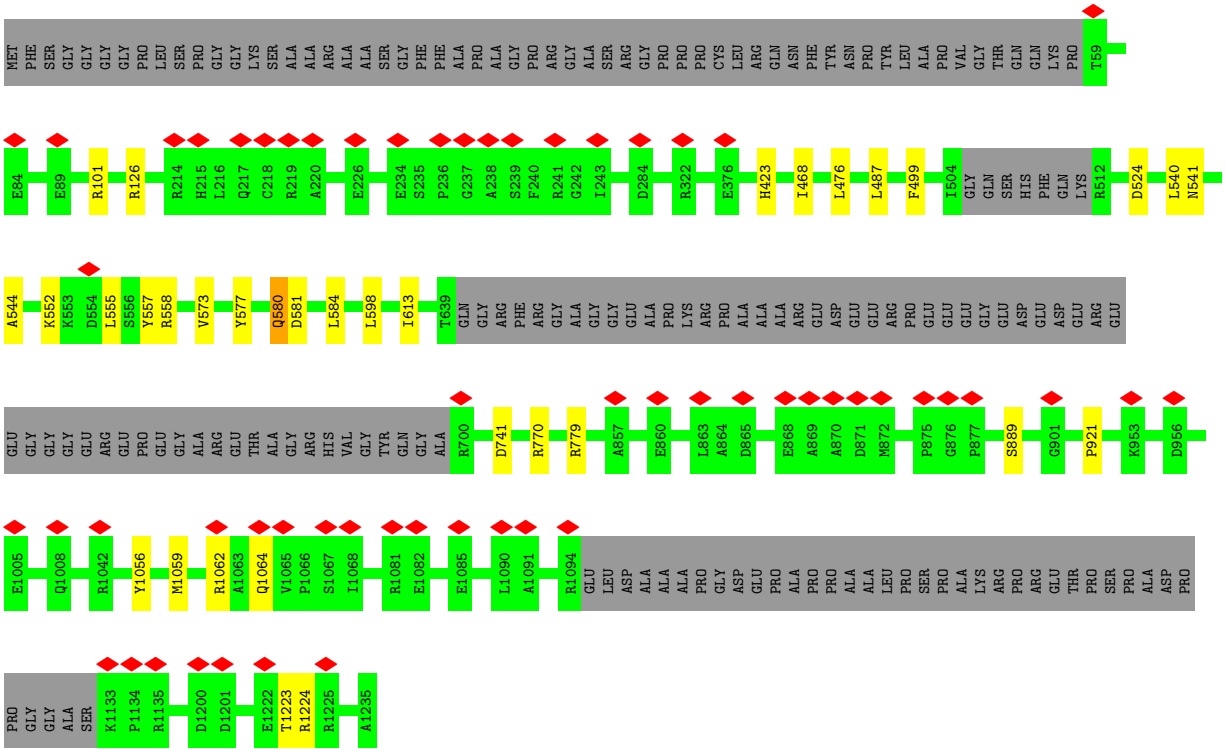
Mol	Chain	Residues	Atoms	AltConf
6	A	5	Total O 6 6	1
6	C	2	Total O 2 2	0

3 Residue-property plots (i)

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

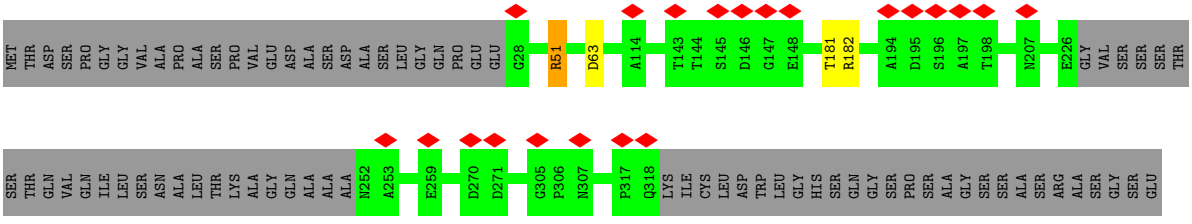
• Molecule 1: DNA polymerase catalytic subunit

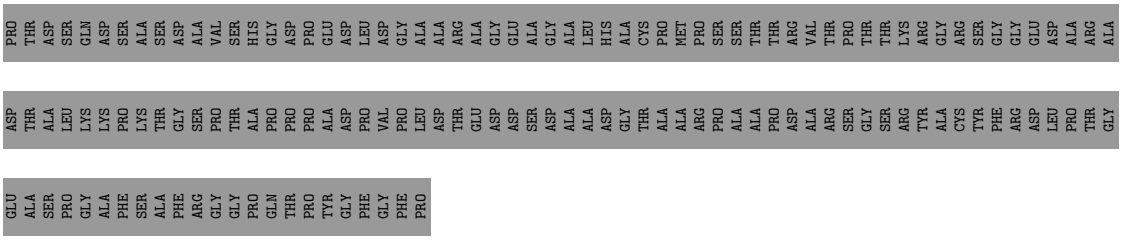
Chain A:



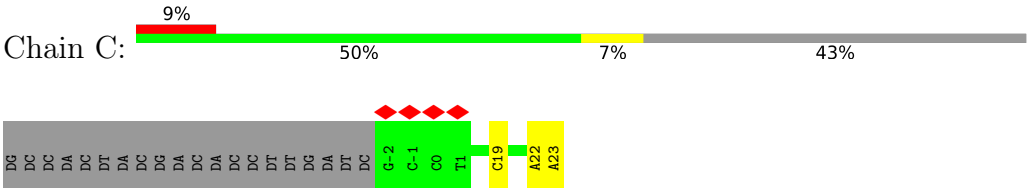
• Molecule 2: DNA polymerase processivity factor

Chain B:

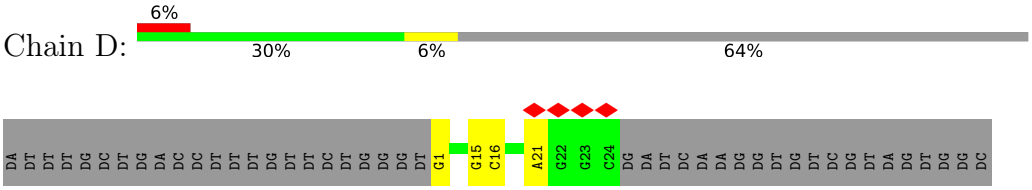




- Molecule 3: DNA (46-MER)



- Molecule 4: DNA (67-MER)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	577658	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.711	Depositor
Minimum map value	-0.289	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	384.0, 384.0, 384.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8, 0.8, 0.8	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.38	0/8665	0.74	6/11752 (0.1%)
2	B	0.34	0/2087	0.67	0/2840
3	C	0.69	0/537	1.25	1/823 (0.1%)
4	D	0.62	0/565	1.27	3/873 (0.3%)
All	All	0.41	0/11854	0.80	10/16288 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	126	ARG	NE-CZ-NH2	9.86	125.23	120.30
4	D	1	DG	O4'-C1'-N9	7.95	113.56	108.00
1	A	770	ARG	NE-CZ-NH1	-6.95	116.82	120.30
4	D	21	DA	O4'-C1'-N9	6.95	112.86	108.00
1	A	126	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	A	101	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	A	126	ARG	CD-NE-CZ	5.99	131.99	123.60
4	D	15	DG	O4'-C1'-N9	5.97	112.18	108.00
3	C	19	DC	O4'-C1'-N1	5.66	111.96	108.00
1	A	779	ARG	NE-CZ-NH1	-5.26	117.67	120.30

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	A	8467	0	8474	54	0
2	B	2049	0	2091	3	0
3	C	523	0	290	0	0
4	D	503	0	270	1	0
5	A	2	0	0	0	0
6	A	6	0	0	0	0
6	C	2	0	0	0	0
All	All	11552	0	11125	56	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 2.

All (56) 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:573:VAL:O	1:A:577[B]:TYR:HD2	1.32	1.12
1:A:540:LEU:HG	1:A:552:LYS:NZ	1.70	1.06
1:A:573:VAL:CG1	1:A:577[B]:TYR:HE2	1.68	1.06
1:A:573:VAL:O	1:A:577[B]:TYR:CD2	2.14	1.00
1:A:487:LEU:HB3	1:A:499:PHE:CD2	2.00	0.96
1:A:573:VAL:HG13	1:A:577[B]:TYR:HE2	1.29	0.94
1:A:552:LYS:HD3	1:A:584:LEU:HD13	1.50	0.94
1:A:552:LYS:HD3	1:A:584:LEU:CD1	2.00	0.92
1:A:487:LEU:HD13	1:A:499:PHE:CE2	2.07	0.90
1:A:476:LEU:HD22	1:A:499:PHE:HE2	1.40	0.87
1:A:540:LEU:HG	1:A:552:LYS:HZ1	1.39	0.87
1:A:552:LYS:CD	1:A:584:LEU:CD1	2.55	0.85
1:A:1062:ARG:HG3	1:A:1064:GLN:HG3	1.59	0.84
1:A:476:LEU:HD22	1:A:499:PHE:CE2	2.13	0.83
1:A:573:VAL:CG1	1:A:577[B]:TYR:CE2	2.60	0.81
1:A:552:LYS:CD	1:A:584:LEU:HD13	2.11	0.81
1:A:573:VAL:HG13	1:A:577[B]:TYR:CE2	2.18	0.77
1:A:423:HIS:CE1	1:A:580[B]:GLN:HE21	2.01	0.76
1:A:573:VAL:HG12	1:A:577[B]:TYR:HE2	1.47	0.76
1:A:541:ASN:HA	1:A:552:LYS:CE	2.16	0.76
1:A:573:VAL:HG12	1:A:577[B]:TYR:CE2	2.21	0.76
1:A:1224:ARG:NH1	2:B:63:ASP:OD2	2.19	0.74
1:A:487:LEU:HD13	1:A:499:PHE:CD2	2.22	0.74
1:A:487:LEU:HD13	1:A:499:PHE:HE2	1.53	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ASN:HA	1:A:552:LYS:HE2	1.75	0.69
1:A:476:LEU:HD21	1:A:499:PHE:CZ	2.29	0.67
1:A:540:LEU:CD2	1:A:581:ASP:OD1	2.43	0.67
1:A:476:LEU:HD21	1:A:499:PHE:HZ	1.61	0.66
1:A:487:LEU:HB3	1:A:499:PHE:HD2	1.56	0.66
1:A:1062:ARG:NE	1:A:1064:GLN:OE1	2.26	0.66
1:A:423:HIS:HE1	1:A:580[B]:GLN:HE21	1.42	0.64
1:A:552:LYS:HD3	1:A:584:LEU:HD11	1.79	0.63
1:A:476:LEU:CD2	1:A:499:PHE:CE2	2.80	0.63
1:A:541:ASN:HA	1:A:552:LYS:HE3	1.80	0.62
1:A:552:LYS:HD2	1:A:584:LEU:CD1	2.27	0.62
1:A:552:LYS:CD	1:A:584:LEU:HD11	2.30	0.59
1:A:540:LEU:HG	1:A:552:LYS:HZ3	1.63	0.59
1:A:476:LEU:CD2	1:A:499:PHE:CZ	2.87	0.57
1:A:552:LYS:HZ2	1:A:584:LEU:HD13	1.70	0.55
1:A:555:LEU:CD1	1:A:577[B]:TYR:CD2	2.91	0.54
1:A:487:LEU:CB	1:A:499:PHE:HD2	2.21	0.52
1:A:1062:ARG:HG3	1:A:1064:GLN:CG	2.36	0.52
2:B:51:ARG:HH22	4:D:16:DC:H3'	1.75	0.51
1:A:557:TYR:CE1	1:A:558:ARG:HG3	2.47	0.49
1:A:544:ALA:HB3	1:A:552:LYS:HE2	1.95	0.47
1:A:487:LEU:CB	1:A:499:PHE:CD2	2.84	0.46
2:B:181:THR:HG22	2:B:182:ARG:H	1.81	0.45
1:A:555:LEU:HD11	1:A:577[B]:TYR:CE2	2.52	0.44
1:A:540:LEU:CG	1:A:552:LYS:HZ1	2.21	0.44
1:A:1056:TYR:HA	1:A:1059:MET:HG2	1.99	0.43
1:A:540:LEU:HD23	1:A:581:ASP:OD1	2.19	0.43
1:A:555:LEU:HD11	1:A:577[B]:TYR:CD2	2.54	0.42
1:A:468:ILE:HG12	1:A:524:ASP:HB2	2.02	0.42
1:A:598:LEU:HD22	1:A:613:ILE:HG12	2.02	0.41
1:A:487:LEU:HD22	1:A:499:PHE:CE2	2.55	0.41
1:A:540:LEU:O	1:A:552:LYS:NZ	2.53	0.41

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	1066/1235 (86%)	1049 (98%)	17 (2%)	0	100 100
2	B	262/488 (54%)	252 (96%)	10 (4%)	0	100 100
All	All	1328/1723 (77%)	1301 (98%)	27 (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	887/996 (89%)	881 (99%)	6 (1%)	84 88
2	B	227/388 (58%)	226 (100%)	1 (0%)	91 94
All	All	1114/1384 (80%)	1107 (99%)	7 (1%)	89 90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	580[A]	GLN
1	A	580[B]	GLN
1	A	741	ASP
1	A	889	SER
1	A	921	PRO
1	A	1223	THR
2	B	51	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	423	HIS
2	B	207	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\|>2$
3	AS	C	22	3	18,23,24	0.81	1 (5%)	17,33,36	0.95	2 (11%)
3	AS	C	23	3	18,23,24	0.62	0	17,33,36	0.77	1 (5%)

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
3	AS	C	22	3	-	0/3/21/22	0/3/3/3
3	AS	C	23	3	-	0/3/21/22	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	22	AS	O5'-C5'	2.27	1.50	1.44

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	22	AS	C4'-O4'-C1'	-2.41	103.63	109.45
3	C	23	AS	C5-C6-N6	2.20	123.69	120.35
3	C	22	AS	C5-C6-N6	2.19	123.68	120.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

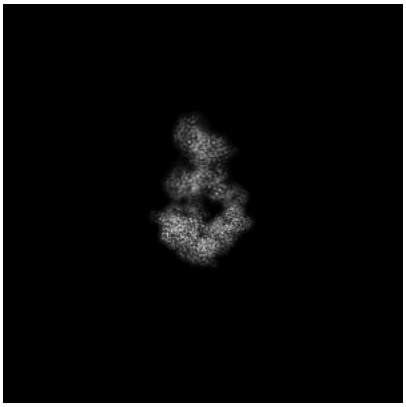
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19837. These allow visual inspection of the internal detail of the map and identification of artifacts.

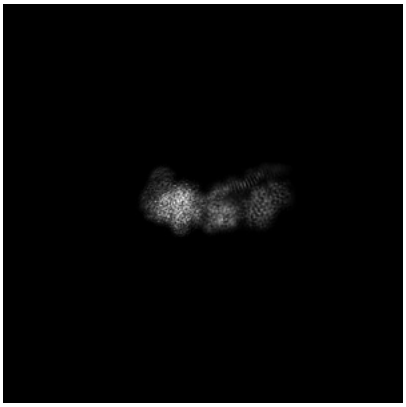
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

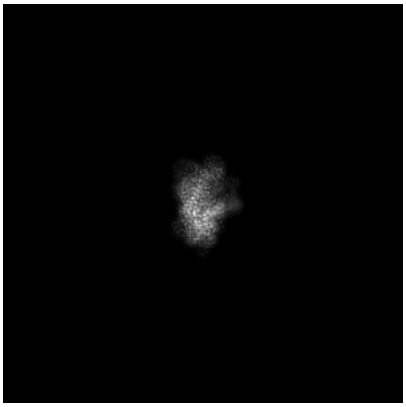
6.1.1 Primary map



X



Y

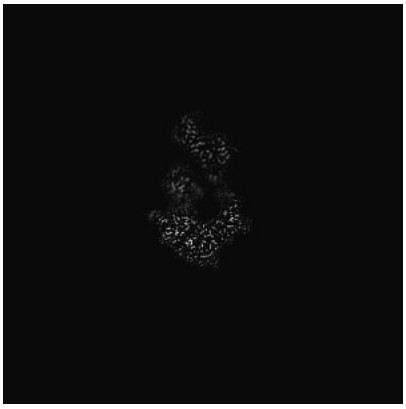


Z

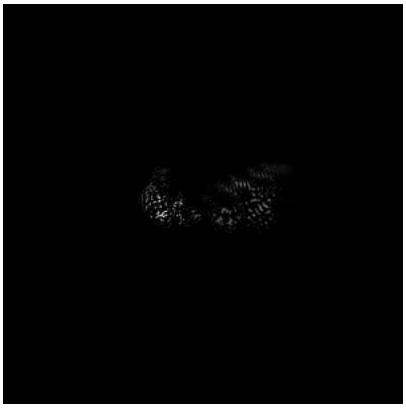
The images above show the map projected in three orthogonal directions.

6.2 Central slices

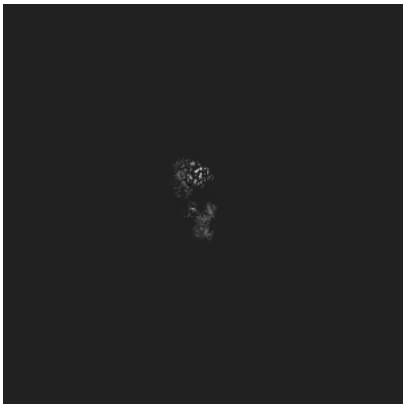
6.2.1 Primary map



X Index: 240



Y Index: 240

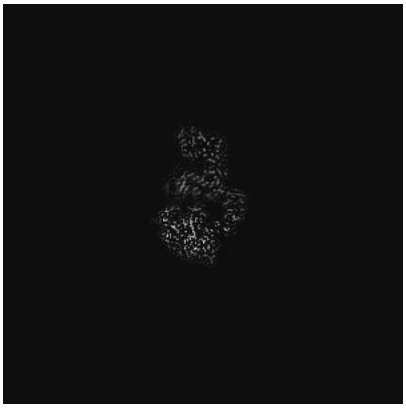


Z Index: 240

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

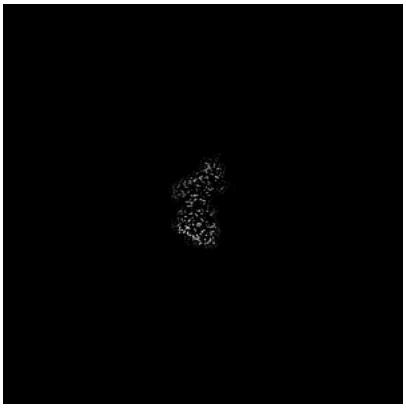
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 230

Y Index: 229

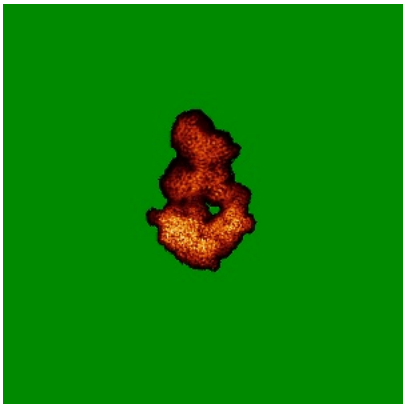


Z Index: 208

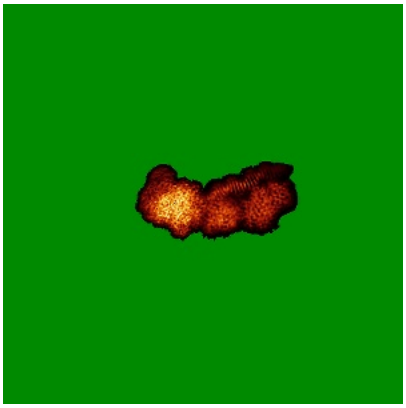
The images above show the largest variance slices of the map in three orthogonal directions.

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

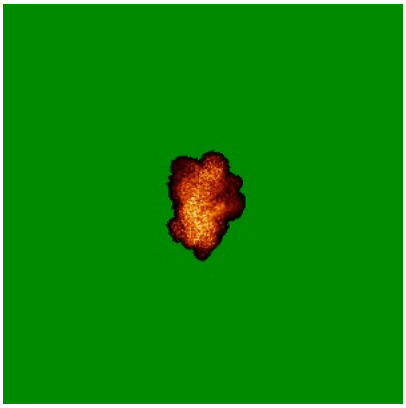
6.4.1 Primary map



X



Y

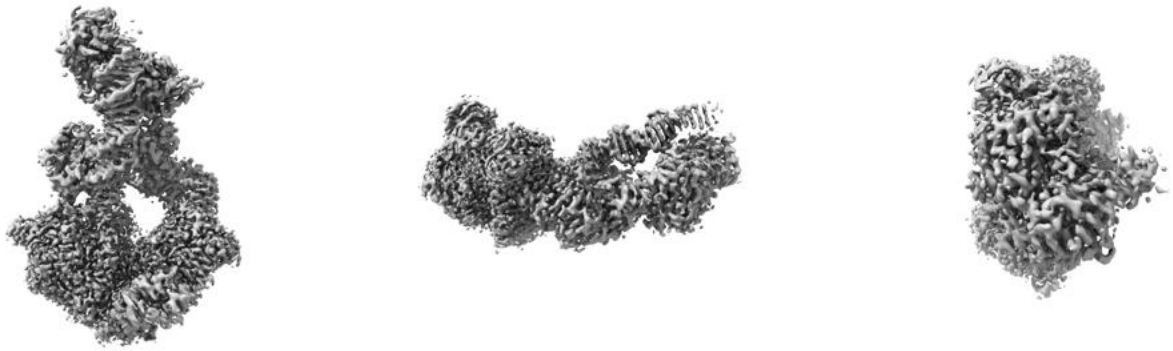


Z

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

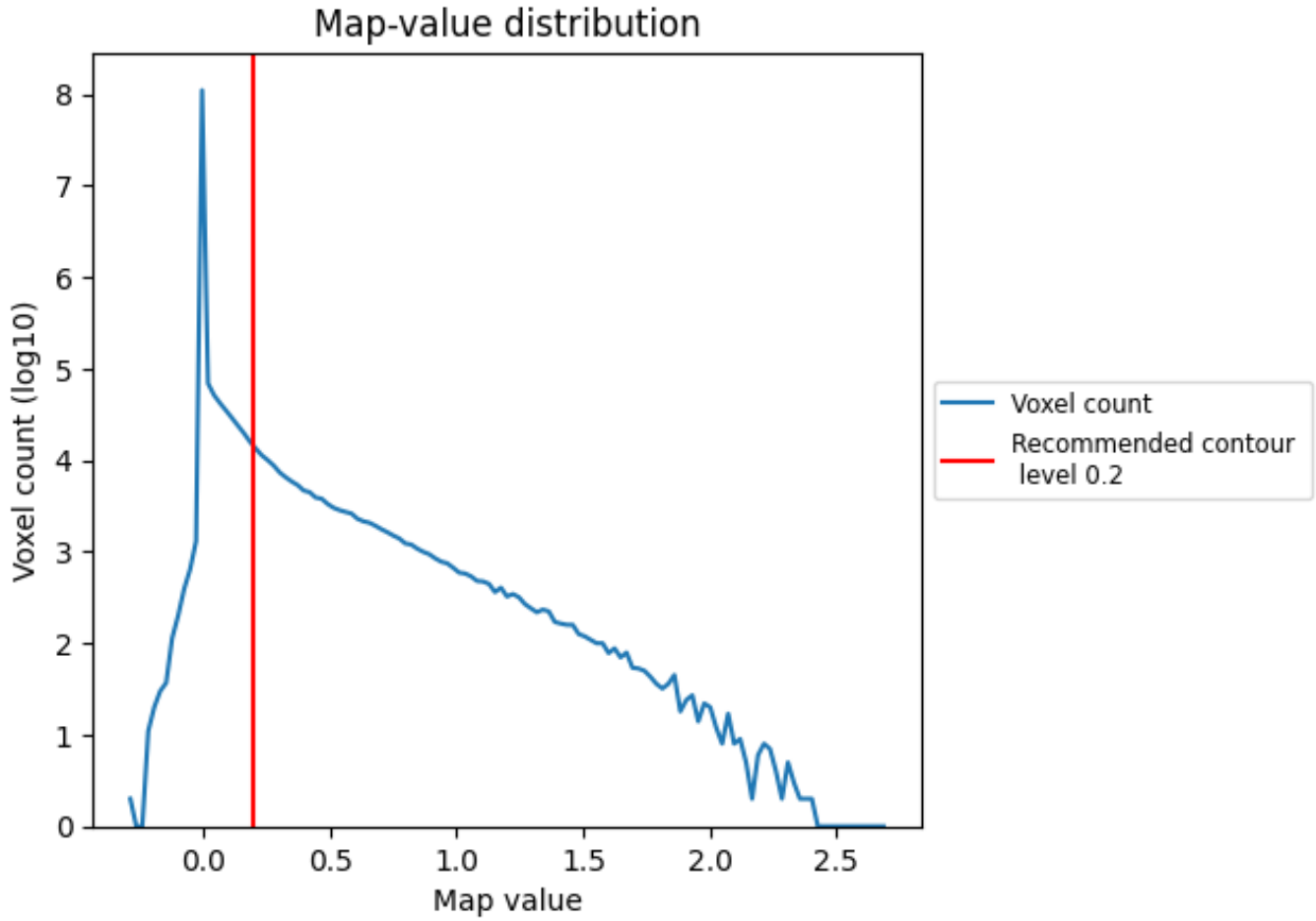
6.6 Mask visualisation (i)

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

7 Map analysis

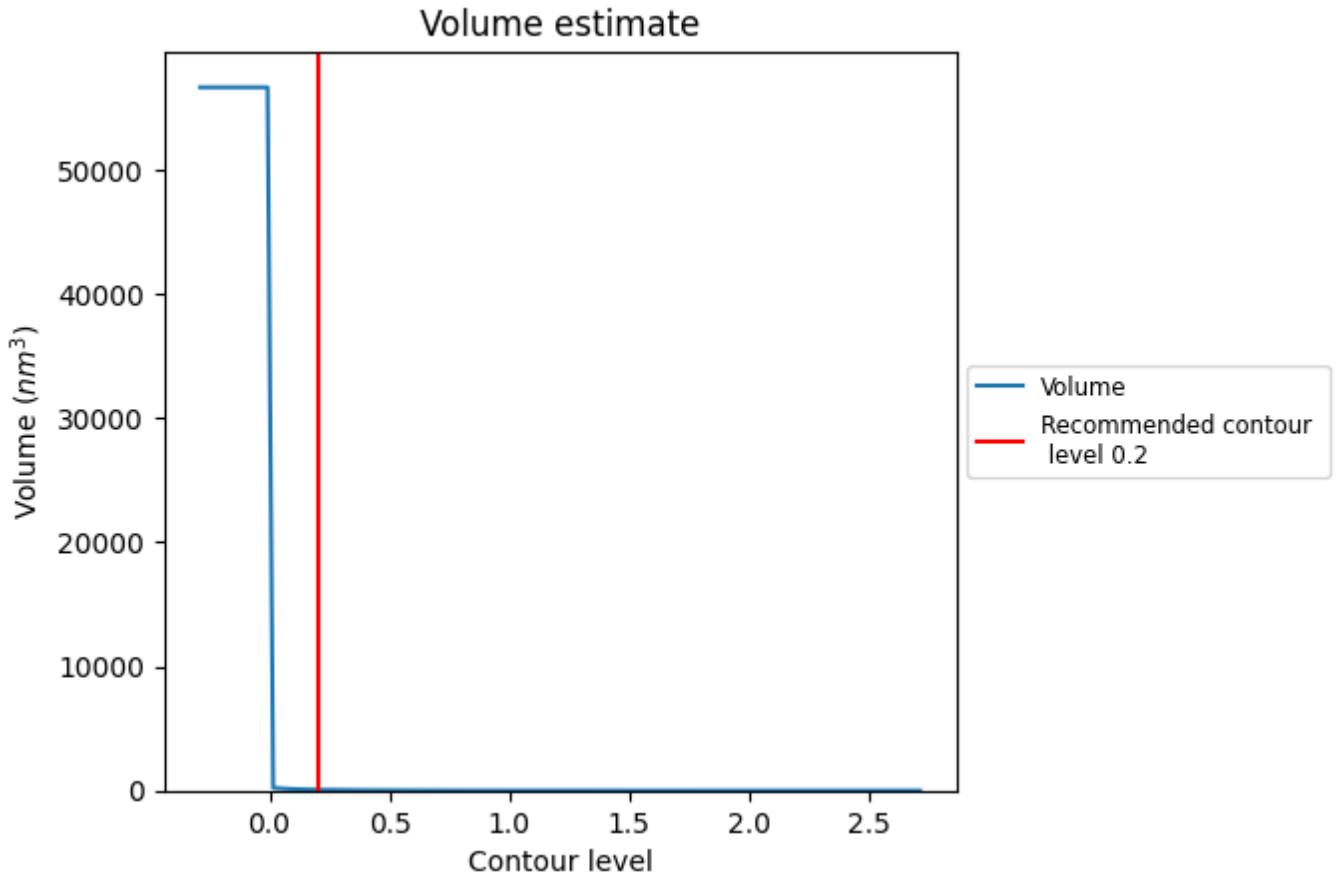
This section contains the results of statistical analysis of the map.

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.

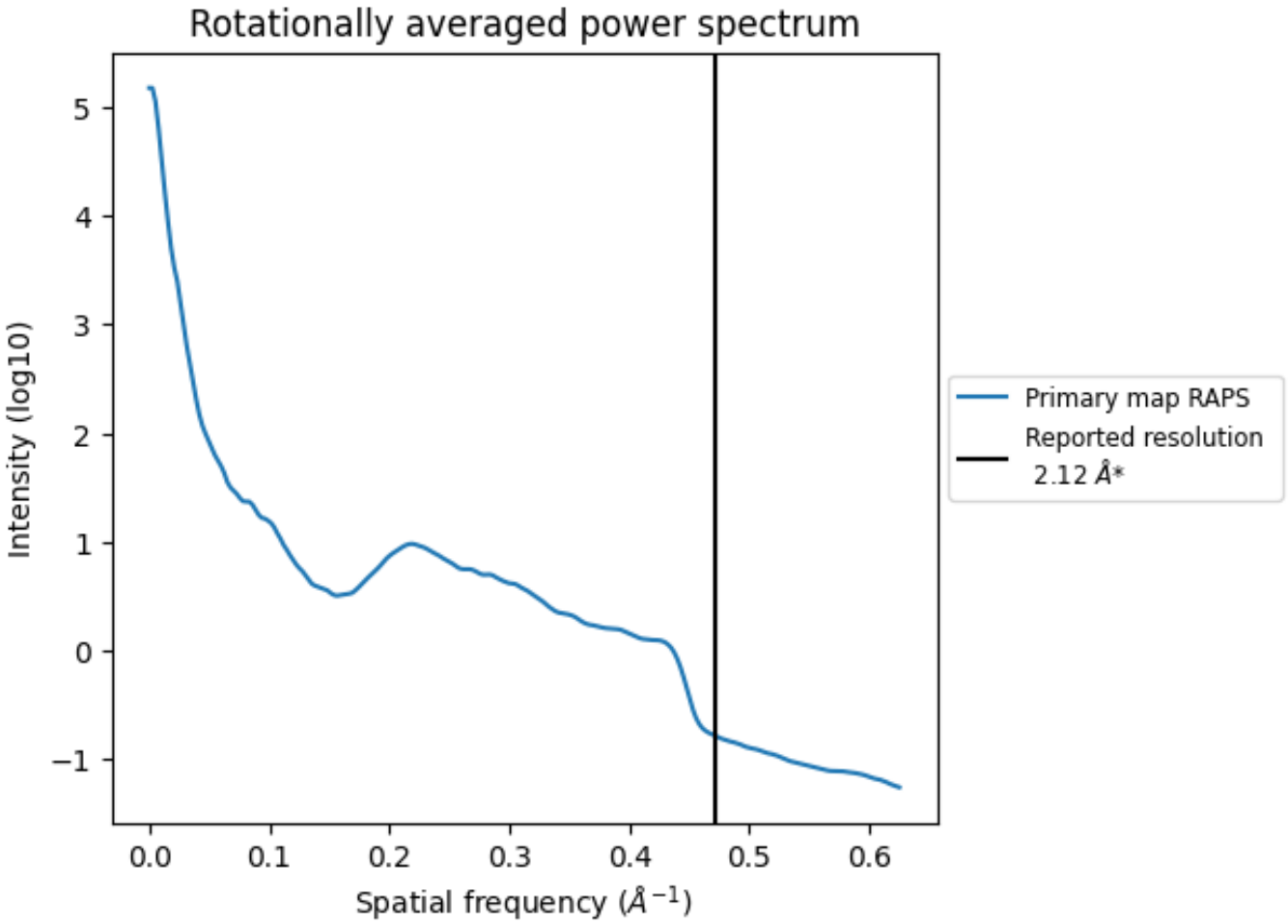
7.2 Volume estimate



The volume at the recommended contour level is 69 nm^3; this corresponds to an approximate mass of 63 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 0.472 Å^{-1}

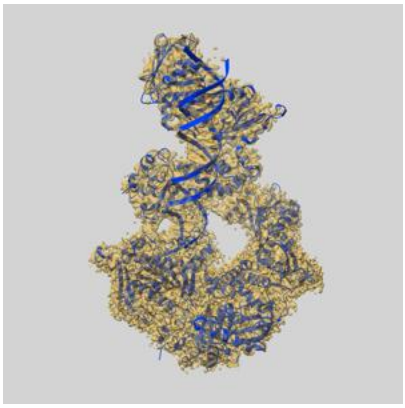
8 Fourier-Shell correlation (i)

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

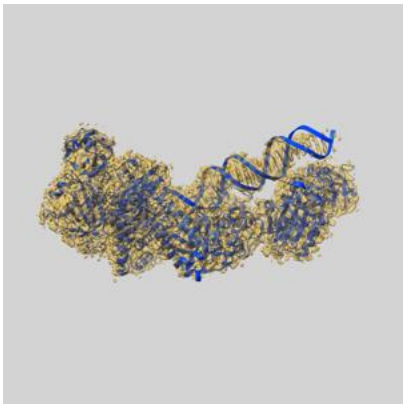
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19837 and PDB model 9ENP. Per-residue inclusion information can be found in section 3 on page 5.

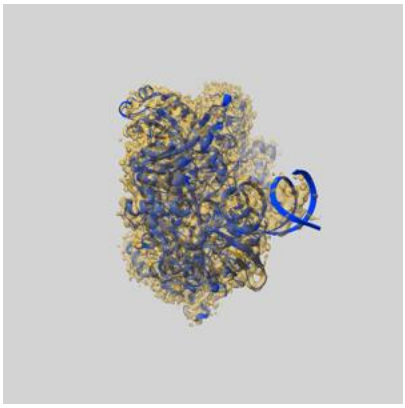
9.1 Map-model overlay



X



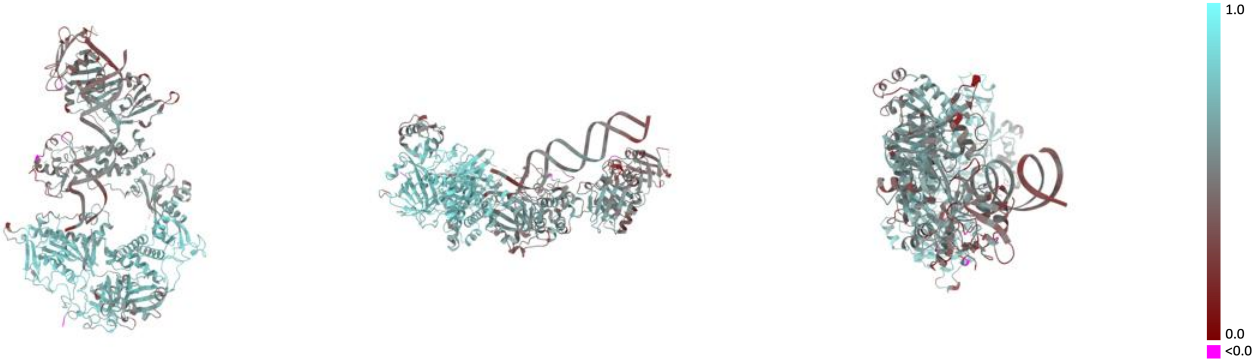
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

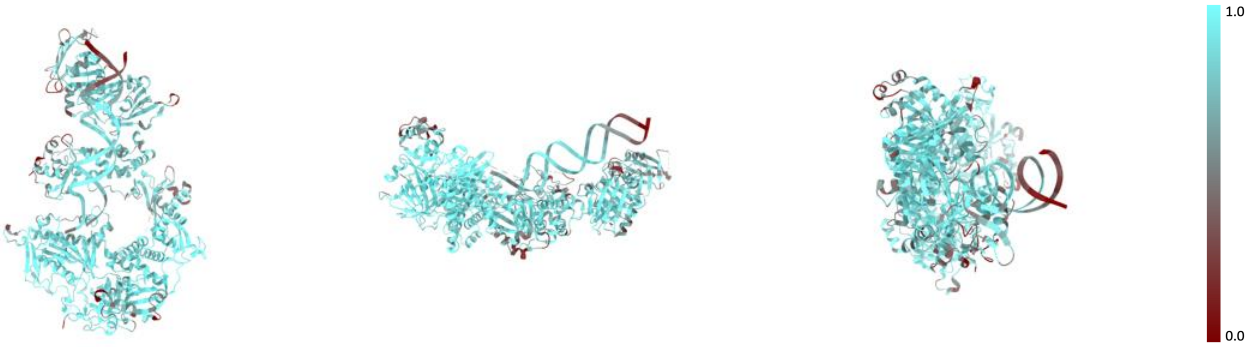
9.2 Q-score mapped to coordinate model (i)



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.

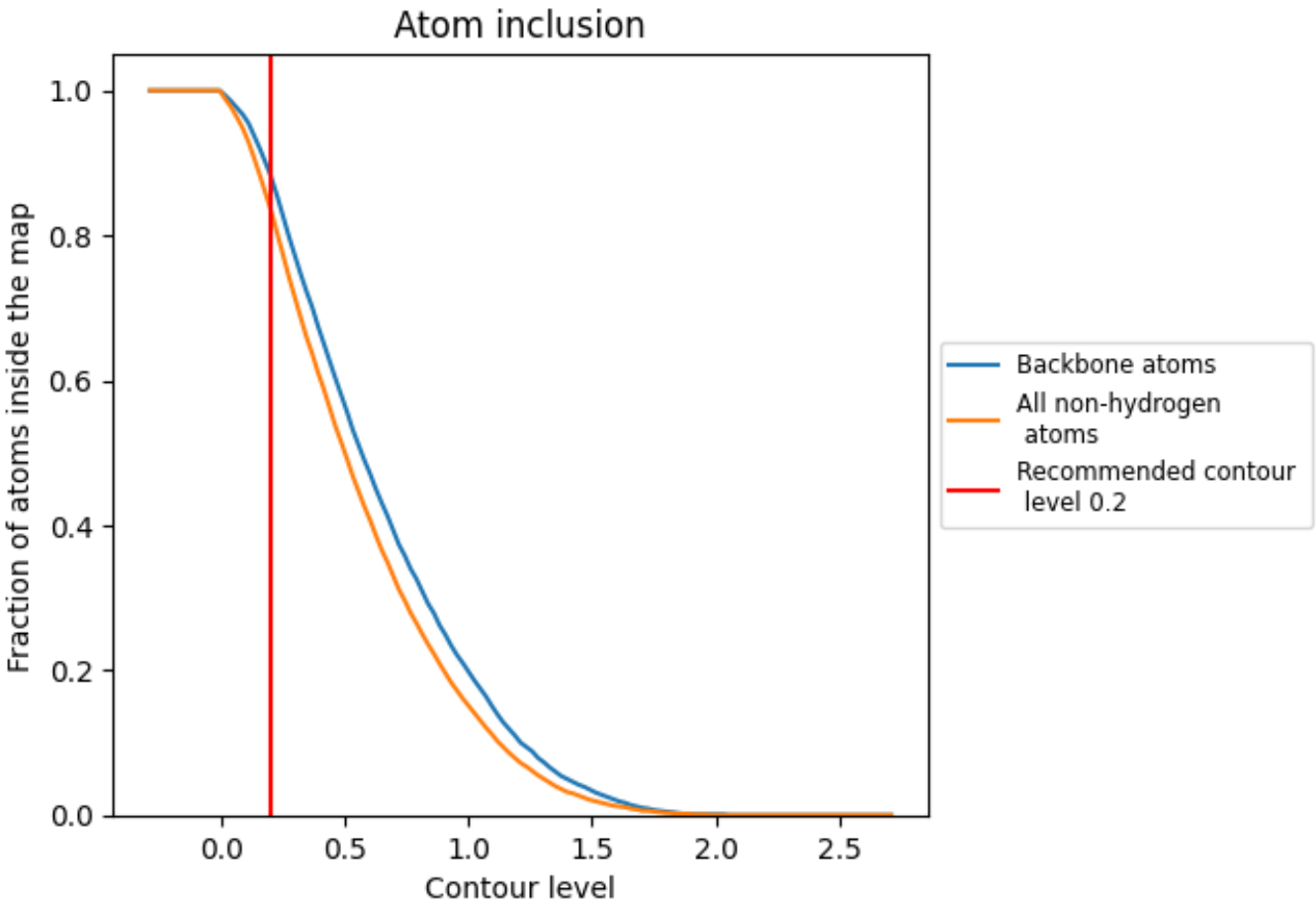
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 84% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8350	0.5880
A	0.8720	0.6360
B	0.7700	0.4680
C	0.6940	0.4070
D	0.6820	0.4420