wwPDB EM Validation Summary Report

Oct 26, 2026 – 12:09 PM EDT

PDB ID	:	9NTD / pdb_00009ntd
EMDB ID	:	EMD-49759
Title	:	Cryo-EM structure of UL5/UL8/UL52 from Herpes Simplex Virus 1 in the presence of ATP-gamma-S
Authors	:	Bermek, O.; Krahn, J.M.; Viverette, E.G.; Peele, W.; Dandey, V.P.; Borgnie, M.J.; Williams, R.S.
Deposited on	:	2025-03-18
Resolution	:	3.50 Å(reported)
Based on initial model	:	.

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:

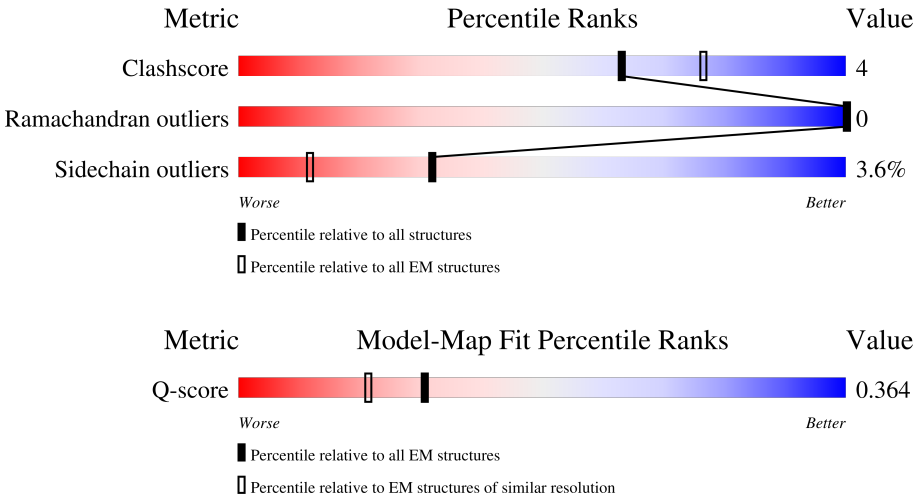
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	882	5% 39% 6% • 54%
2	B	1058	15% 66% 10% 24%
3	C	768	14% 85% 12% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15027 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 UL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	407	3248	2076	573	583	16	0	0

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A2U9A5B2
A	2	ALA	-	expression tag	UNP A0A2U9A5B2
A	3	ALA	-	expression tag	UNP A0A2U9A5B2
A	4	ALA	-	expression tag	UNP A0A2U9A5B2
A	5	GLY	-	expression tag	UNP A0A2U9A5B2
A	6	GLY	-	expression tag	UNP A0A2U9A5B2
A	7	GLU	-	expression tag	UNP A0A2U9A5B2
A	8	ARG	-	expression tag	UNP A0A2U9A5B2
A	9	GLN	-	expression tag	UNP A0A2U9A5B2
A	10	LEU	-	expression tag	UNP A0A2U9A5B2
A	11	ASP	-	expression tag	UNP A0A2U9A5B2
A	12	GLY	-	expression tag	UNP A0A2U9A5B2
A	13	GLN	-	expression tag	UNP A0A2U9A5B2
A	14	LYS	-	expression tag	UNP A0A2U9A5B2
A	15	PRO	-	expression tag	UNP A0A2U9A5B2
A	16	GLY	-	expression tag	UNP A0A2U9A5B2
A	17	PRO	-	expression tag	UNP A0A2U9A5B2
A	18	PRO	-	expression tag	UNP A0A2U9A5B2
A	19	HIS	-	expression tag	UNP A0A2U9A5B2
A	20	LEU	-	expression tag	UNP A0A2U9A5B2
A	21	GLN	-	expression tag	UNP A0A2U9A5B2
A	22	GLN	-	expression tag	UNP A0A2U9A5B2
A	23	PRO	-	expression tag	UNP A0A2U9A5B2
A	24	GLY	-	expression tag	UNP A0A2U9A5B2
A	25	ASP	-	expression tag	UNP A0A2U9A5B2
A	26	ARG	-	expression tag	UNP A0A2U9A5B2
A	27	PRO	-	expression tag	UNP A0A2U9A5B2
A	28	ALA	-	expression tag	UNP A0A2U9A5B2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	29	VAL	-	expression tag	UNP A0A2U9A5B2
A	30	PRO	-	expression tag	UNP A0A2U9A5B2
A	31	GLY	-	expression tag	UNP A0A2U9A5B2
A	32	ARG	-	expression tag	UNP A0A2U9A5B2
A	33	ALA	-	expression tag	UNP A0A2U9A5B2
A	34	GLU	-	expression tag	UNP A0A2U9A5B2
A	35	ALA	-	expression tag	UNP A0A2U9A5B2
A	36	PHE	-	expression tag	UNP A0A2U9A5B2
A	37	LEU	-	expression tag	UNP A0A2U9A5B2
A	38	ASN	-	expression tag	UNP A0A2U9A5B2
A	39	PHE	-	expression tag	UNP A0A2U9A5B2
A	40	THR	-	expression tag	UNP A0A2U9A5B2
A	41	SER	-	expression tag	UNP A0A2U9A5B2
A	205	LEU	SER	conflict	UNP A0A2U9A5B2
A	690	VAL	GLY	conflict	UNP A0A2U9A5B2

- Molecule 2 is a protein called UL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	801	Total	C	N	O	S	0	0
			6158	3909	1111	1109	29		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	129	GLU	ASP	conflict	UNP A0A2U9A692
B	166	VAL	ILE	conflict	UNP A0A2U9A692
B	385	SER	ASN	conflict	UNP A0A2U9A692
B	514	ASP	GLY	conflict	UNP A0A2U9A692
B	530	GLN	ARG	conflict	UNP A0A2U9A692
B	703	PRO	SER	conflict	UNP A0A2U9A692
B	719	ALA	THR	conflict	UNP A0A2U9A692

- Molecule 3 is a protein called UL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	746	Total	C	N	O	S	0	0
			5620	3608	996	998	18		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	MET	-	initiating methionine	UNP A0A5J6DVE7
C	-16	ARG	-	expression tag	UNP A0A5J6DVE7
C	-15	GLY	-	expression tag	UNP A0A5J6DVE7
C	-14	SER	-	expression tag	UNP A0A5J6DVE7
C	-13	HIS	-	expression tag	UNP A0A5J6DVE7
C	-12	HIS	-	expression tag	UNP A0A5J6DVE7
C	-11	HIS	-	expression tag	UNP A0A5J6DVE7
C	-10	HIS	-	expression tag	UNP A0A5J6DVE7
C	-9	HIS	-	expression tag	UNP A0A5J6DVE7
C	-8	HIS	-	expression tag	UNP A0A5J6DVE7
C	-7	GLY	-	expression tag	UNP A0A5J6DVE7
C	-6	MET	-	expression tag	UNP A0A5J6DVE7
C	-5	GLU	-	expression tag	UNP A0A5J6DVE7
C	-4	ASN	-	expression tag	UNP A0A5J6DVE7
C	-3	LEU	-	expression tag	UNP A0A5J6DVE7
C	-2	TYR	-	expression tag	UNP A0A5J6DVE7
C	-1	PHE	-	expression tag	UNP A0A5J6DVE7
C	0	GLN	-	expression tag	UNP A0A5J6DVE7
C	467	ASP	ASN	conflict	UNP A0A5J6DVE7
C	565	ASN	SER	conflict	UNP A0A5J6DVE7
C	612	GLY	CYS	conflict	UNP A0A5J6DVE7
C	634	VAL	LEU	conflict	UNP A0A5J6DVE7

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

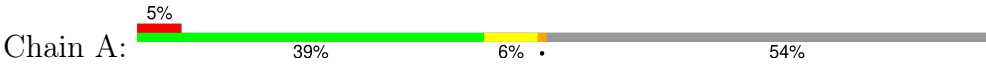
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
4	B	1	1	1	0

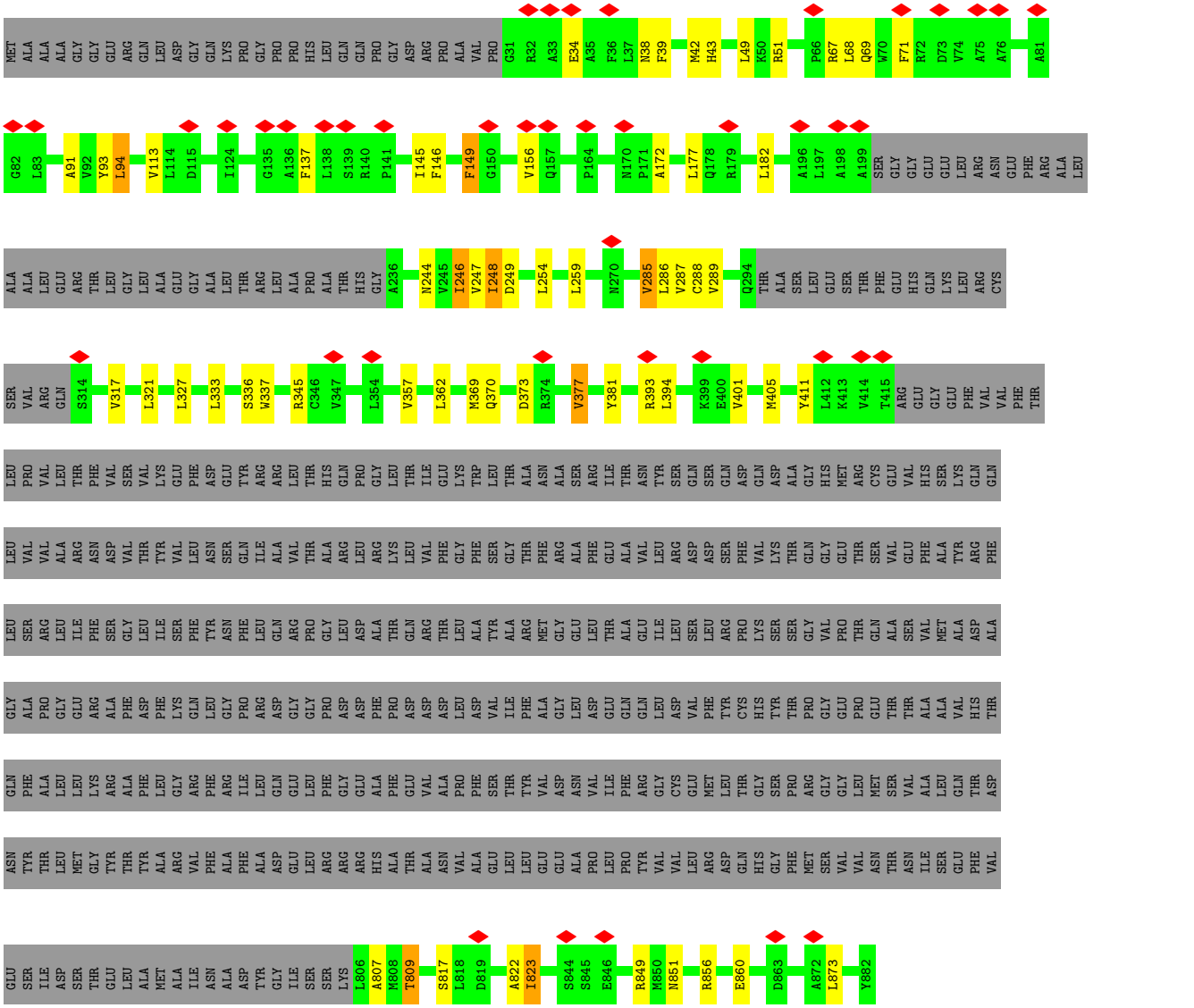
3 Residue-property plots (i)

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: UL5

Chain A:

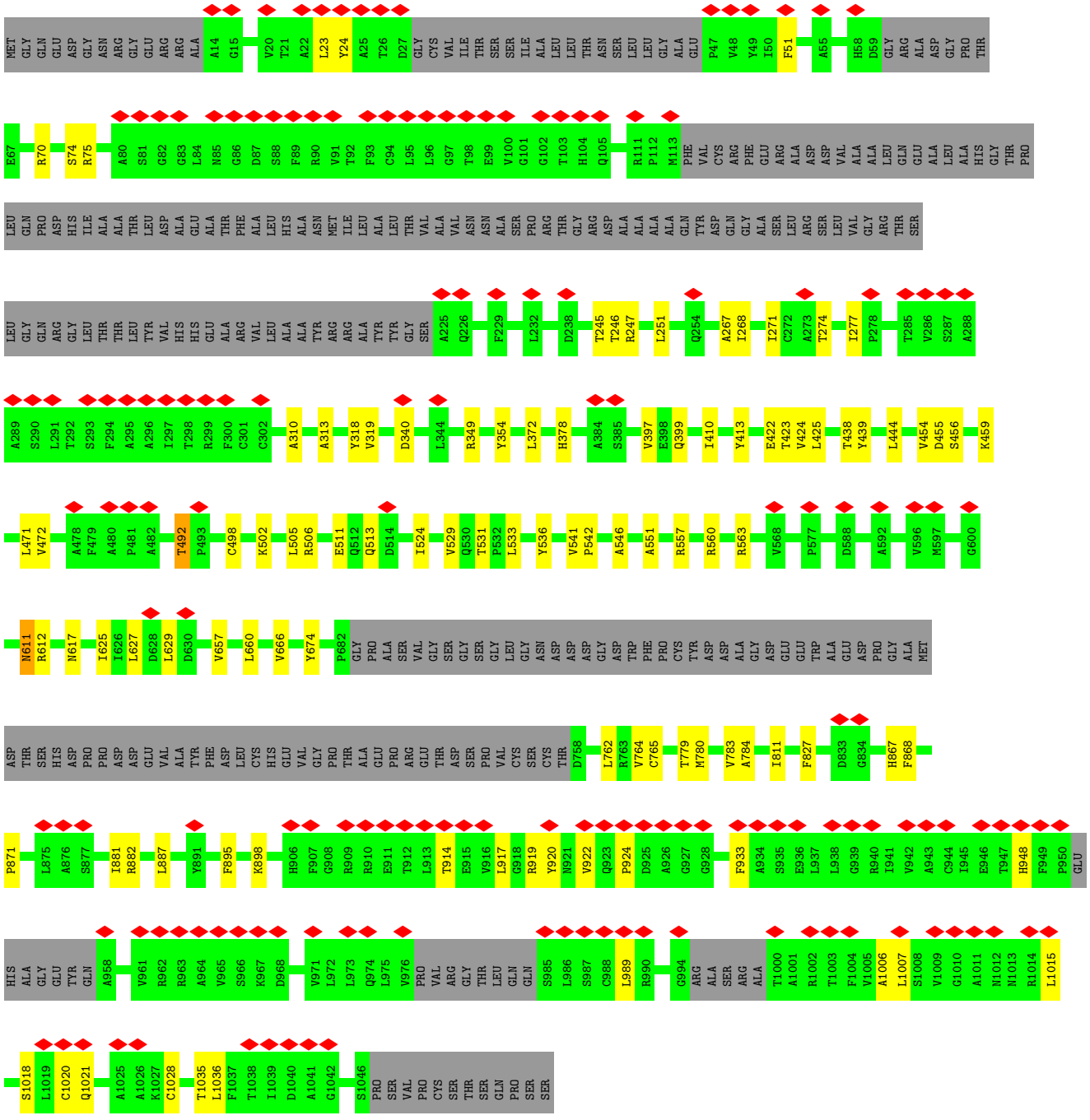




- Molecule 2: UL52

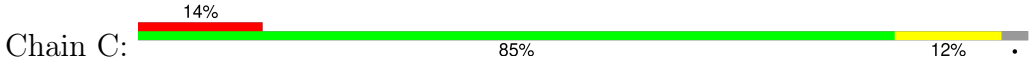
Chain B:

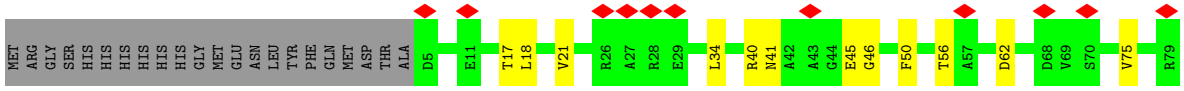


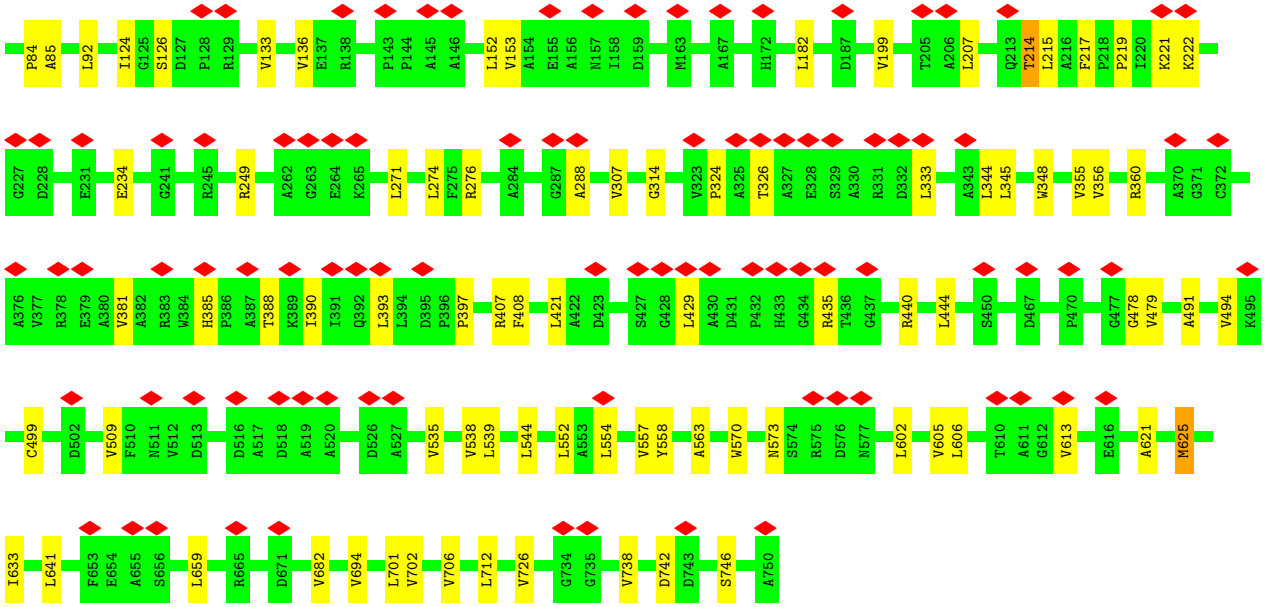


• Molecule 3: UL8

Chain C:






P84 A85 L92 I124 G125 S126 D127 P128 R129 V133 V136 E137 R138 P143 P144 A145 A146 L152 V153 A154 E155 A156 N157 I158 D159 M163 A167 H172 L182 D187 V199 T205 A206 L207 Q213 T214 L215 A216 F217 P218 P219 I220 K221 K222
G227 D228 E231 E234 G241 R245 R249 A262 G263 E264 K265 L271 L274 F275 R276 A284 G287 A288 V307 G314 V323 P324 A325 T326 A327 E328 S329 A330 R331 D332 L333 A343 L344 L345 W348 V355 V356 R360 A370 G371 C372
A376 V377 R378 E379 A380 V381 A382 R383 W384 H385 P386 A387 T388 K389 I390 I391 Q392 L393 L394 D395 P396 P397 R407 F408 L421 A422 D423 S427 G428 L429 A430 D431 P432 H433 G434 R435 T436 G437 R440 L444 S450 D467 P470 G477 G478 V479 A491 V494 K495
C499 D502 V509 F510 N511 V512 D513 D516 A517 D518 A519 A520 D526 A527 V535 V538 L539 L544 L552 A553 L554 V557 Y558 A563 W570 N573 S574 R575 D576 N577 L602 V605 L606 T610 A611 G612 V613 E616 A621 M625
I633 L641 F653 E654 A655 S656 L659 R665 D671 V682 V694 L701 V702 V706 L712 V726 G734 G735 V738 D742 D743 S746 A750

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	121471	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	56.118	Depositor
Minimum map value	-35.038	Depositor
Average map value	0.503	Depositor
Map value standard deviation	3.485	Depositor
Recommended contour level	5	Depositor
Map size (Å)	106.0342, 107.3273, 175.8616	wwPDB
Map dimensions	136, 83, 82	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2931, 1.2931, 1.2931	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.13	0/3321	0.33	0/4513
2	B	0.13	0/6310	0.35	0/8588
3	C	0.15	0/5778	0.34	0/7922
All	All	0.14	0/15409	0.34	0/21023

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	3248	0	3253	35	0
2	B	6158	0	6101	49	0
3	C	5620	0	5588	47	0
4	B	1	0	0	0	0
All	All	15027	0	14942	126	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 4.

The worst 5 of 126 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:B:674:TYR:HB2	2:B:765:CYS:O	1.88	0.74
3:C:397:PRO:HA	3:C:563:ALA:O	1.91	0.71
3:C:605:VAL:HG21	3:C:625:MET:HE3	1.78	0.64
2:B:629:LEU:HB2	2:B:762:LEU:HB2	1.78	0.63
1:A:321:LEU:HD23	1:A:327:LEU:HD21	1.82	0.61

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	399/882 (45%)	382 (96%)	17 (4%)	0	100	100
2	B	785/1058 (74%)	761 (97%)	24 (3%)	0	100	100
3	C	744/768 (97%)	729 (98%)	15 (2%)	0	100	100
All	All	1928/2708 (71%)	1872 (97%)	56 (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	351/742 (47%)	335 (95%)	16 (5%)	24	50
2	B	636/832 (76%)	614 (96%)	22 (4%)	32	57
3	C	556/575 (97%)	539 (97%)	17 (3%)	35	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1543/2149 (72%)	1488 (96%)	55 (4%)	32 57

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	454	VAL
2	B	868	PHE
3	C	738	VAL
3	C	554	LEU
2	B	472	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	902	ASN
2	B	1034	HIS
3	C	710	HIS
3	C	242	HIS
1	A	387	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)

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 1 ligands modelled in this entry, 1 is 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.

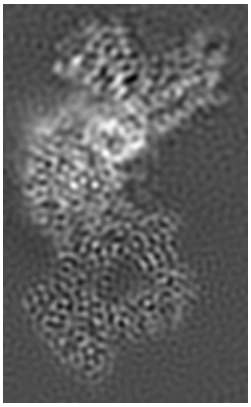
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-49759. These allow visual inspection of the internal detail of the map and identification of artifacts.

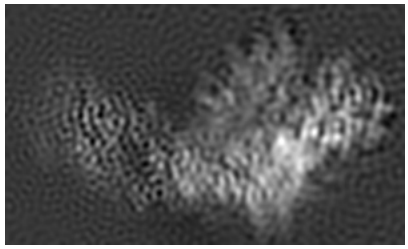
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

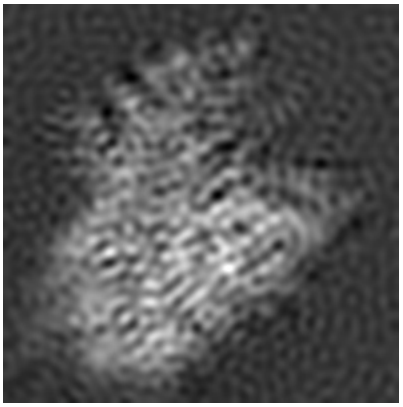
6.1.1 Primary map



X



Y

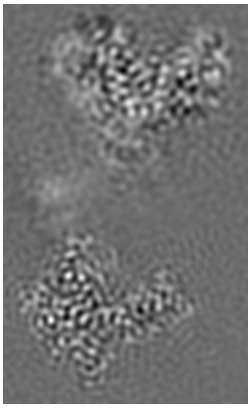


Z

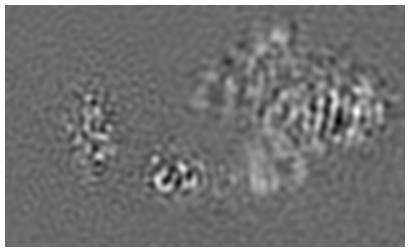
The images above show the map projected in three orthogonal directions.

6.2 Central slices

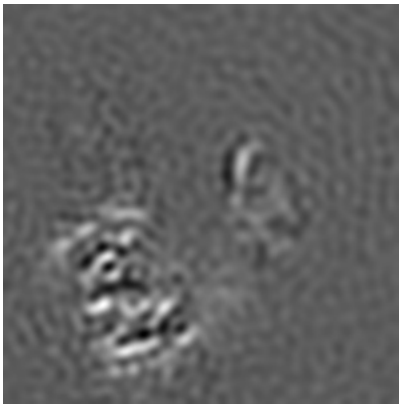
6.2.1 Primary map



X Index: 41



Y Index: 41

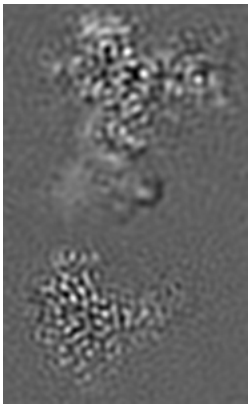


Z Index: 68

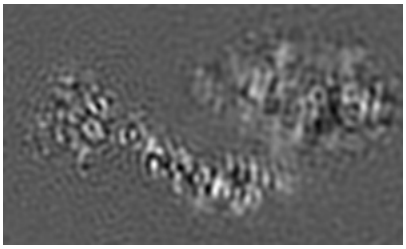
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

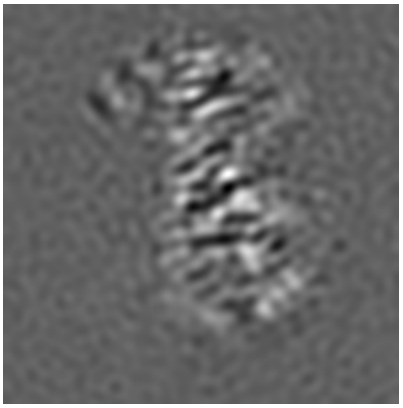
6.3.1 Primary map



X Index: 46



Y Index: 34

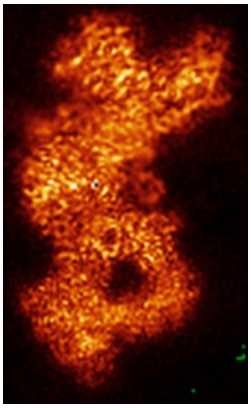


Z Index: 112

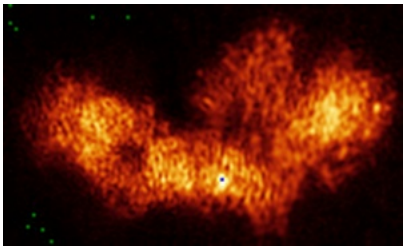
The images above show the largest variance slices of the map in three orthogonal directions.

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

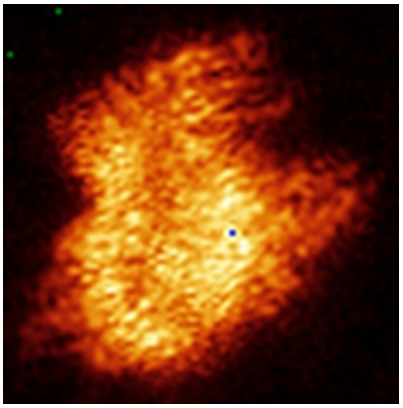
6.4.1 Primary map



X



Y

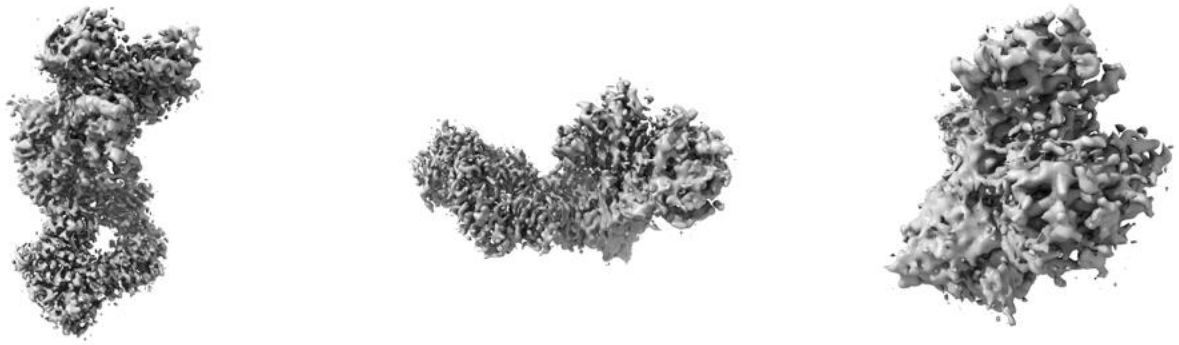


Z

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

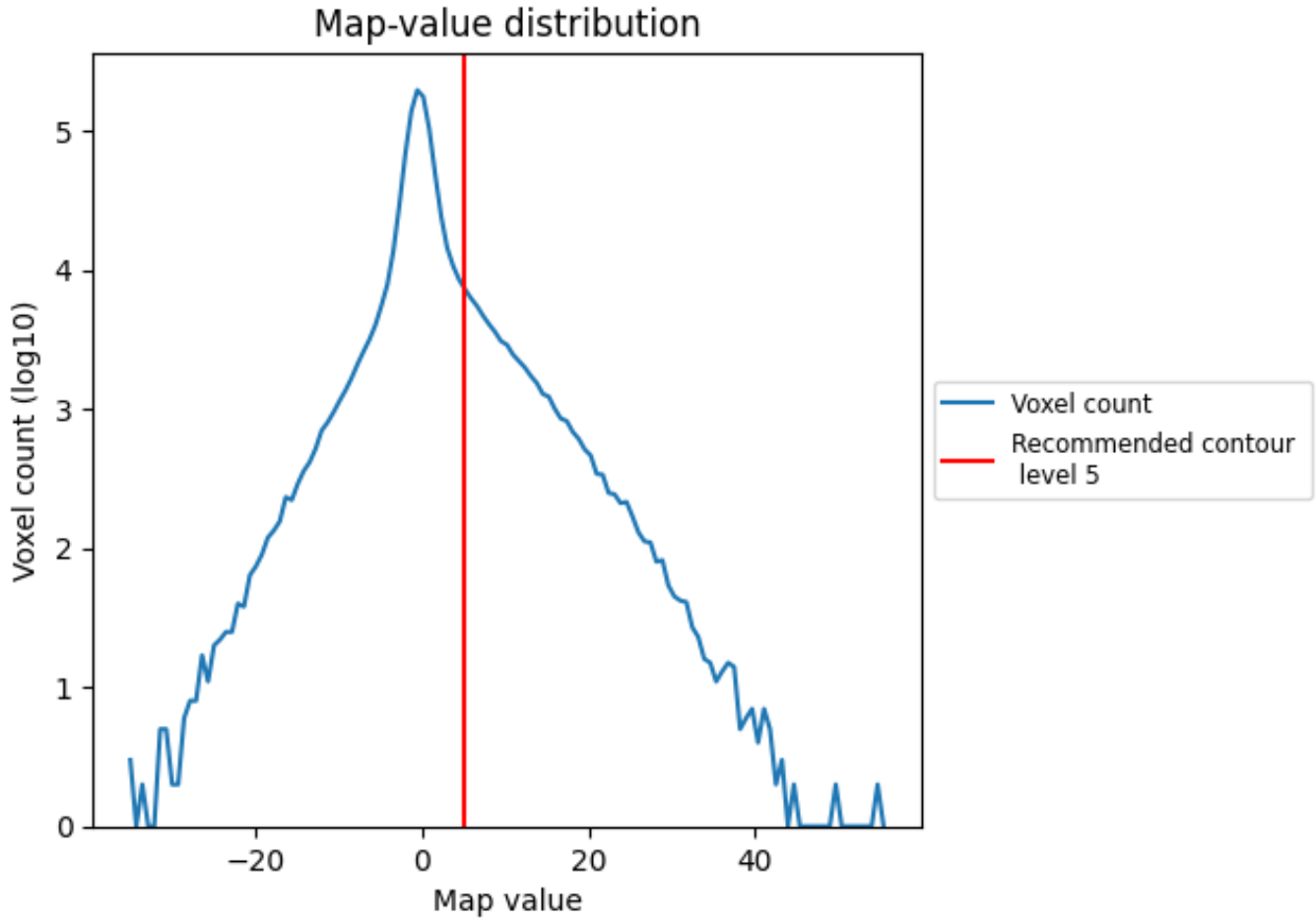
6.6 Mask visualisation (i)

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

7 Map analysis

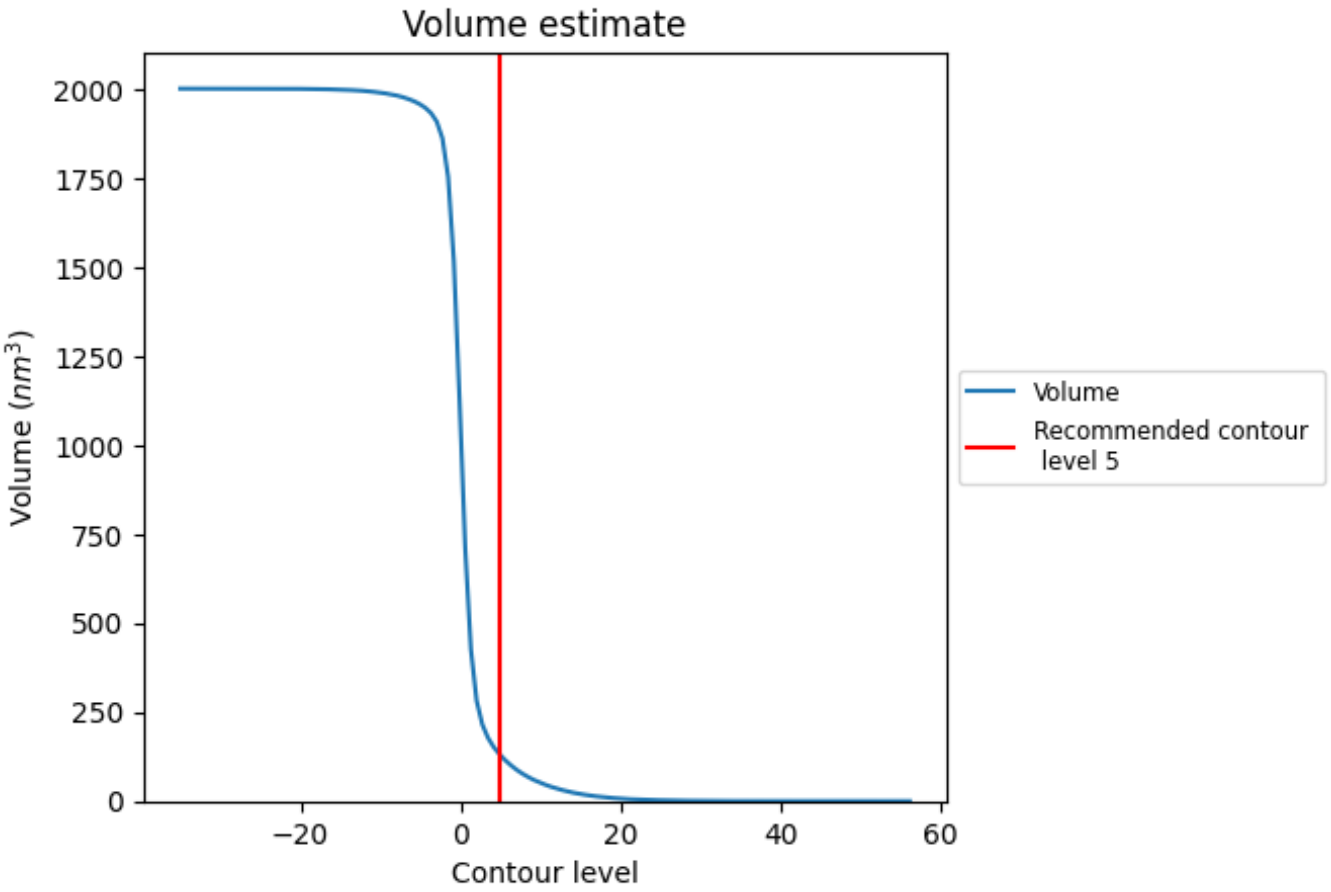
This section contains the results of statistical analysis of the map.

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 (i)



The volume at the recommended contour level is 128 nm^3; this corresponds to an approximate mass of 116 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)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

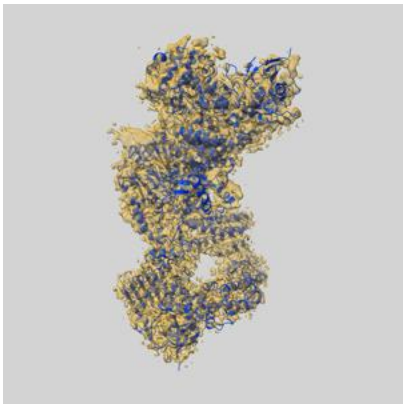
8 Fourier-Shell correlation (i)

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

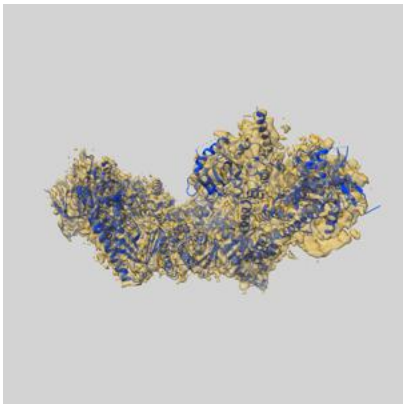
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-49759 and PDB model 9NTD. Per-residue inclusion information can be found in section 3 on page 6.

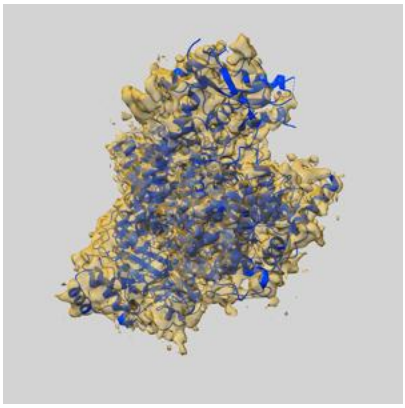
9.1 Map-model overlay



X



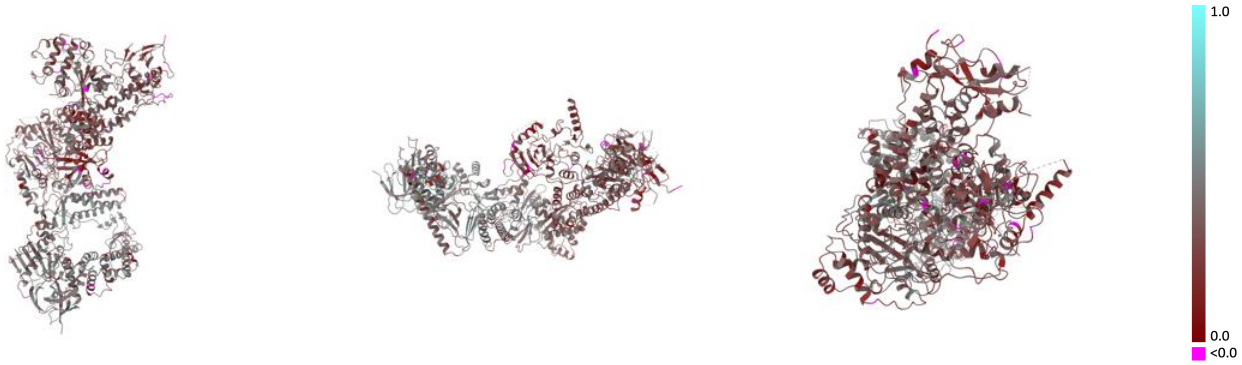
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0 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.

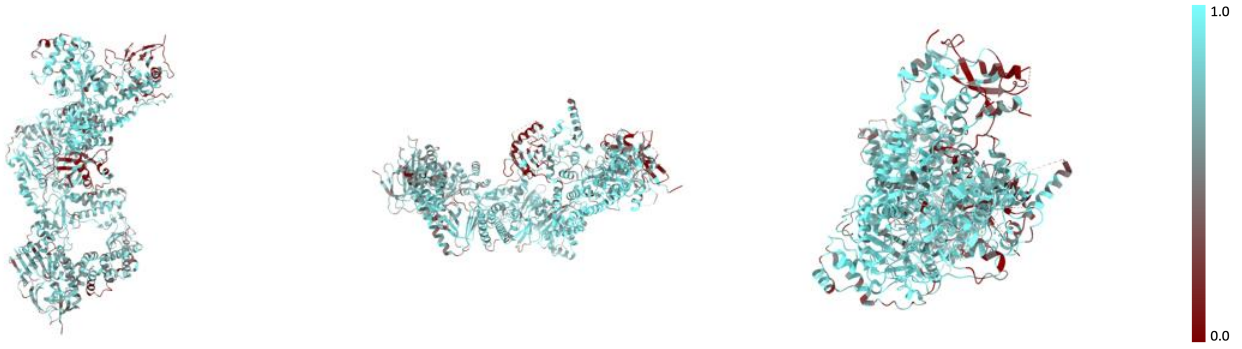
9.2 Q-score mapped to coordinate model (i)



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.

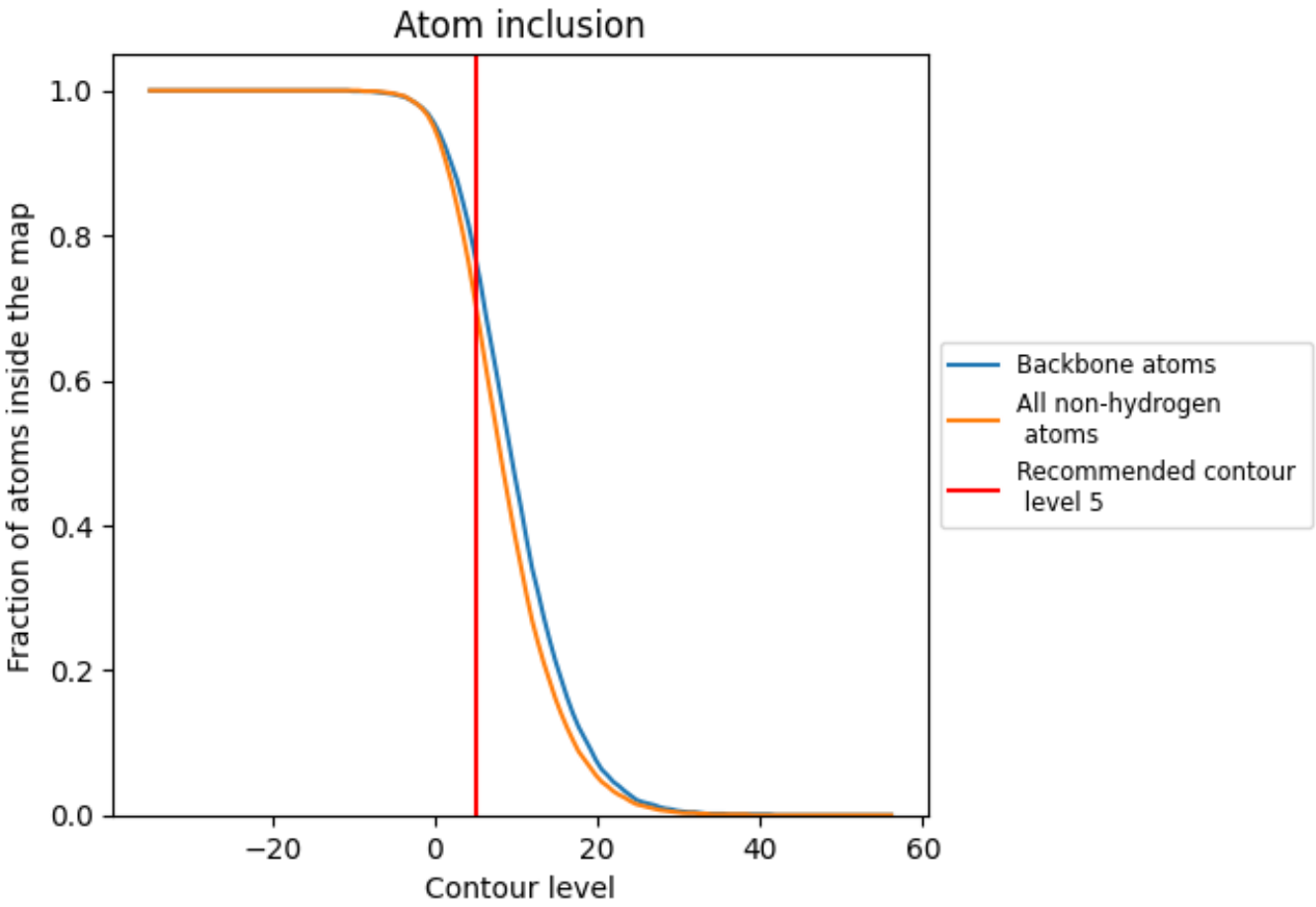
9.3 Atom inclusion mapped to coordinate model (i)



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 (5).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 71% 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 (5) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.7060	0.3640
A	0.7600	0.3290
B	0.6910	0.3200
C	0.6900	0.4330