wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 06:01 pm GMT

PDB ID	:	4BOM
EMDB ID	:	EMD-2380
Title	:	Structure of herpesvirus fusion glycoprotein B-bilayer complex revealing the protein-membrane and lateral protein-protein interaction
Authors	:	Maurer, U.E.; Zeev-Ben-Mordehai, Z.; Pandurangan, A.P.; Cairns, T.M.; Hannah, B.P.; Whitbeck, J.C.; Eisenberg, R.J.; Cohen, G.H.; Topf, M.; Huiskonen, J.T.; Grunewald, K.
Deposited on	:	2013-05-21
Resolution	:	27.00 Å(reported)
Based on initial model	:	3NWF

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 (i) 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 (i)) were used in the production of this report:

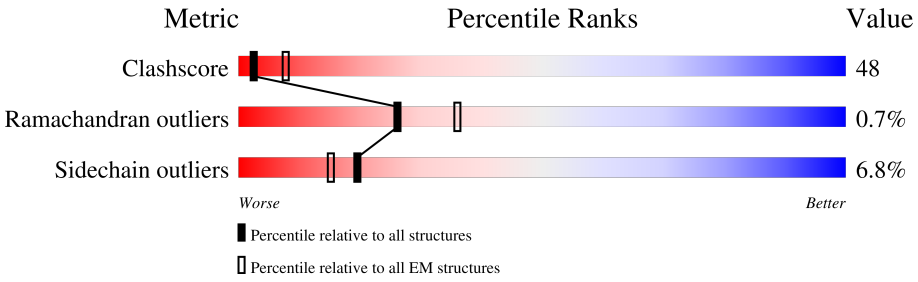
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 27.00 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	622	5% 40% 52%
1	B	622	5% 42% 51% 5%
1	C	622	5% 41% 52%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 14745 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 ENVELOPE GLYCOPROTEIN B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	608	Total	C	N	O	S	0	1
			4915	3097	869	927	22		
1	B	608	Total	C	N	O	S	0	1
			4915	3097	869	927	22		
1	C	608	Total	C	N	O	S	0	1
			4915	3097	869	927	22		

There are 6 discrepancies between the modelled and reference sequences:

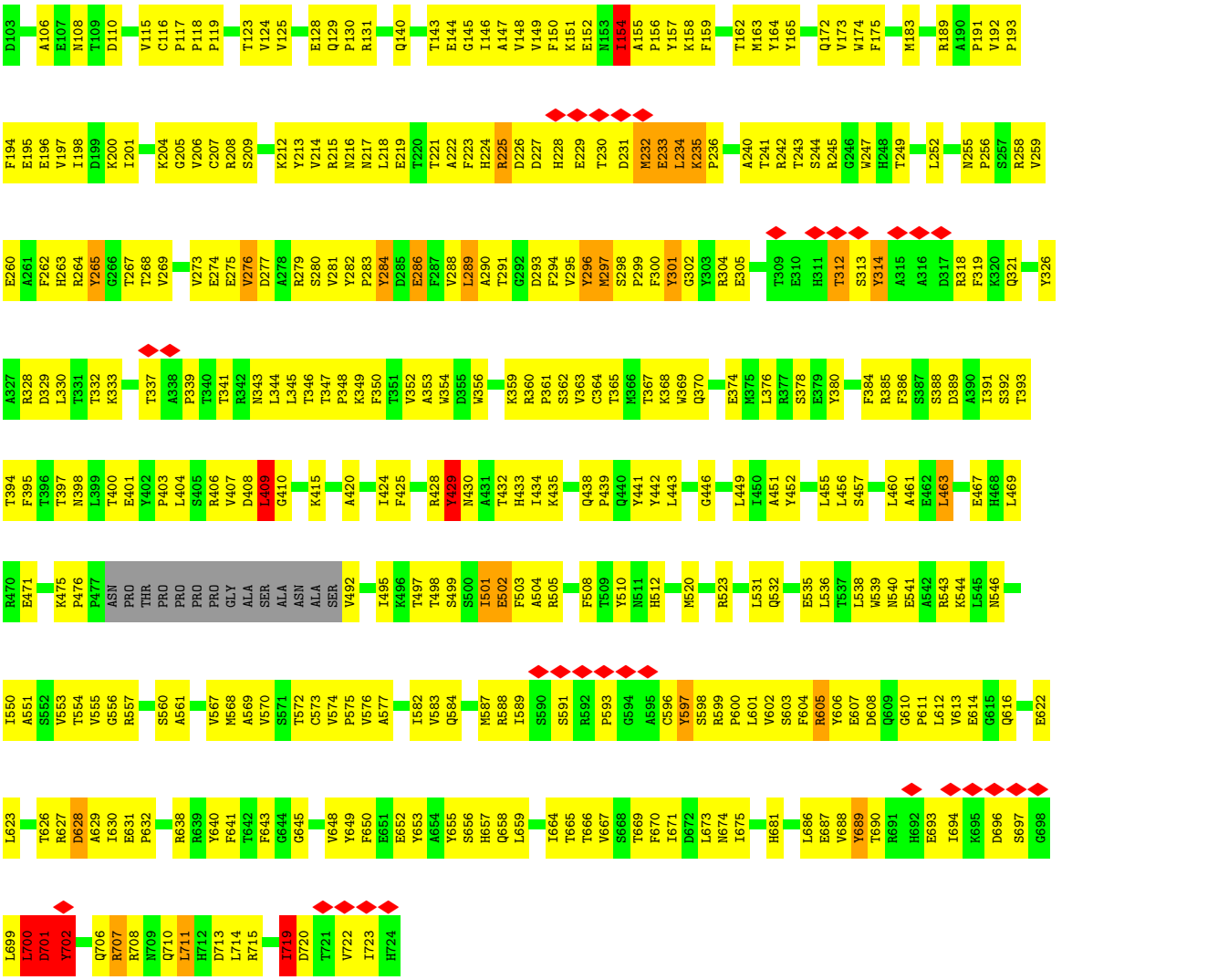
Chain	Residue	Modelled	Actual	Comment	Reference
A	313	SER	THR	conflict	UNP P06437
A	443	LEU	GLN	conflict	UNP P06437
B	313	SER	THR	conflict	UNP P06437
B	443	LEU	GLN	conflict	UNP P06437
C	313	SER	THR	conflict	UNP P06437
C	443	LEU	GLN	conflict	UNP P06437

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.

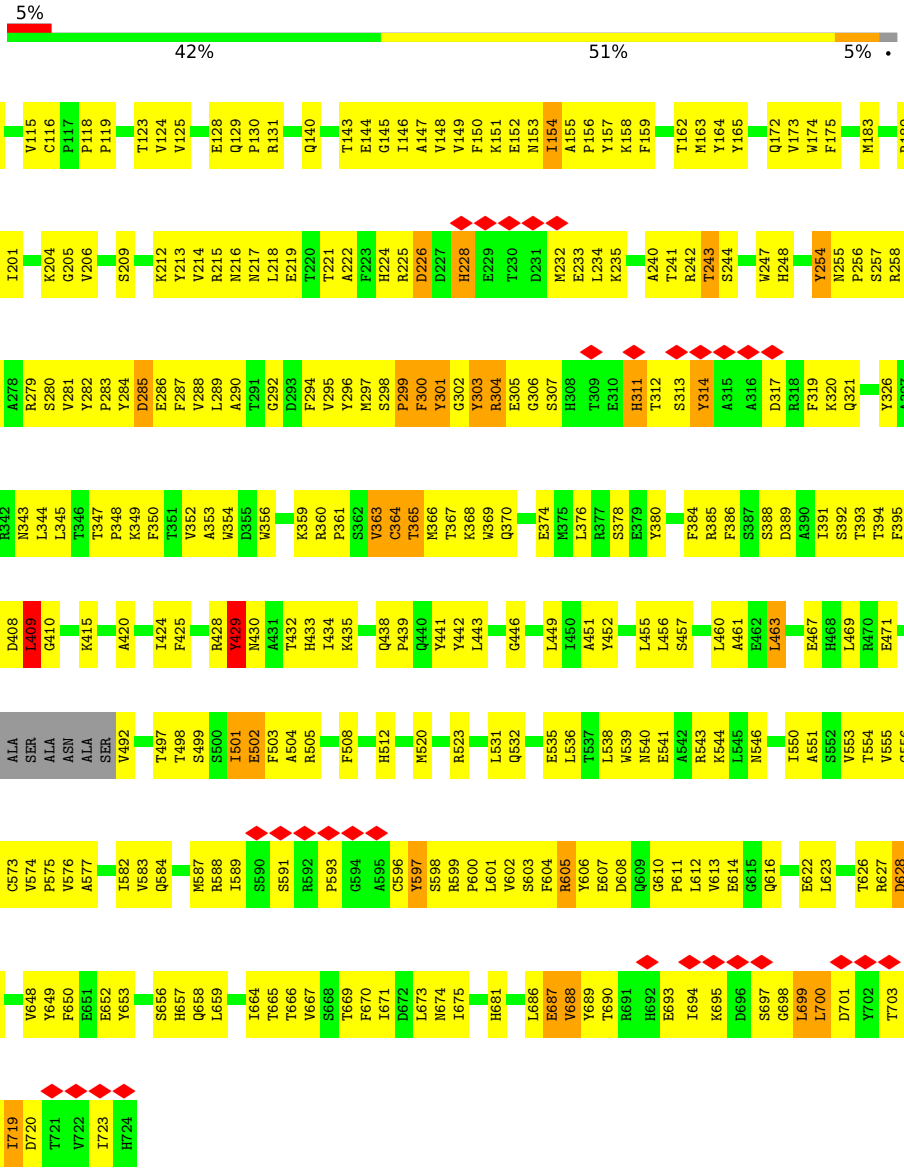
• Molecule 1: ENVELOPE GLYCOPROTEIN B

Chain A:



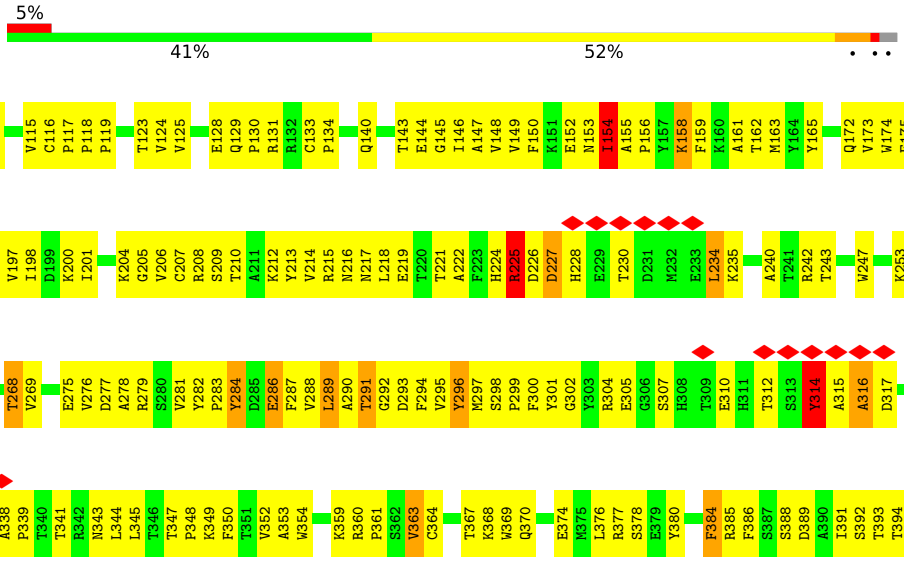
• Molecule 1: ENVELOPE GLYCOPROTEIN B

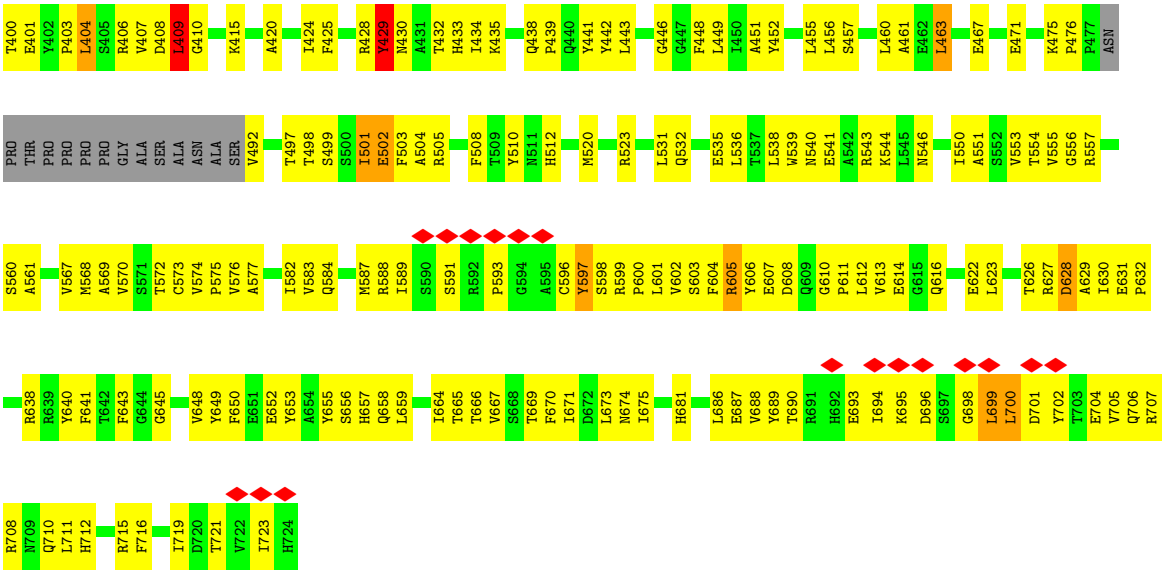
Chain B:



• Molecule 1: ENVELOPE GLYCOPROTEIN B

Chain C:




T400 E401 Y402 P403 L404 S405 R406 V407 D408 L409 G410 K415 A420 I424 F425 R428 Y429 N430 A431 T432 H433 I434 K435 Q438 P439 Q440 Y441 Y442 L443 G446 G447 F448 L449 I450 A451 Y452 L455 L456 S457 L460 A461 E462 L463 E467 E471 K475 P476 P477 ASN
PRO THR PRO PRO PRO PRO GLY ALA SER ALA ASN ALA SER V492 T497 T498 S499 S500 I501 E502 F503 A504 R505 F508 T509 Y510 N511 H512 M520 R523 L531 Q532 E535 L536 T537 L538 W539 N540 E541 A542 R543 K544 L545 N546 I550 A551 S552 V553 T554 V555 G556 R557
S560 A561 V567 M568 A569 V570 S571 T572 C573 V574 P575 V576 A577 I582 V583 Q584 M587 R588 I589 S590 S591 R592 P593 G594 A595 C596 Y597 S598 R599 P600 L601 V602 S603 F604 R605 Y606 E607 D608 Q609 G610 P611 L612 V613 E614 G615 Q616 E622 L623 T626 R627 D628 A629 I630 E631 P632
R638 R639 Y640 F641 T642 F643 G644 G645 V648 Y649 F650 E651 E652 Y653 A654 Y655 S656 H657 Q658 L659 I664 T665 T666 V667 S668 T669 F670 I671 D672 L673 N674 I675 H681 L686 E687 V688 Y689 T690 R691 H692 E693 I694 K695 D696 S697 G698 L699 L700 D701 Y702 T703 E704 V705 Q706 R707
R708 N709 Q710 L711 H712 R715 F716 I719 D720 T721 V722 I723 H724

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of tilted images used	786	Depositor
Resolution determination method	Not provided	
CTF correction method	LOW PASS FILTER TO THE FIRST ZERO CROSSING OF THE CTF	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	100	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	67000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum voxel value	18.674	Depositor
Minimum voxel value	-12.513	Depositor
Average voxel value	0.000	Depositor
Voxel value standard deviation	1.000	Depositor
Recommended contour level	2.0	Depositor
Tomogram size (Å)	460.0, 460.0, 460.0	wwPDB
Tomogram dimensions	100, 100, 100	wwPDB
Tomogram angles (°)	90.0, 90.0, 90.0	wwPDB
Grid spacing (Å)	4.6, 4.6, 4.6	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	1.04	0/5036	1.12	3/6840 (0.0%)
1	B	1.04	0/5036	1.10	1/6840 (0.0%)
1	C	1.04	0/5036	1.11	1/6840 (0.0%)
All	All	1.04	0/15108	1.11	5/20520 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	16
1	B	0	13
1	C	0	12
All	All	0	41

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	702	TYR	CA-CB-CG	-6.86	100.36	113.40
1	B	429	TYR	CA-CB-CG	-6.57	100.92	113.40
1	C	429	TYR	CA-CB-CG	-6.56	100.94	113.40
1	A	429	TYR	CA-CB-CG	-6.54	100.97	113.40
1	A	702	TYR	CB-CG-CD1	-5.92	117.45	121.00

There are no chirality outliers.

5 of 41 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	ILE	Peptide
1	A	225	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	228	HIS	Peptide
1	A	284	TYR	Peptide
1	A	362	SER	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4915	0	4740	548	0
1	B	4915	0	4740	554	0
1	C	4915	0	4740	551	0
All	All	14745	0	14220	1396	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 48.

The worst 5 of 1396 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:699:LEU:HD13	1:C:281:VAL:HG13	1.26	1.14
1:C:408:ASP:HB2	1:C:492:VAL:HG13	1.14	1.14
1:B:706:GLN:HG3	1:C:699:LEU:HD21	1.26	1.13
1:B:700:LEU:HB2	1:C:279:ARG:HG2	1.32	1.11
1:A:397:THR:HG21	1:A:442:TYR:HB3	1.33	1.11

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	604/622 (97%)	585 (97%)	14 (2%)	5 (1%)	19	60
1	B	604/622 (97%)	581 (96%)	19 (3%)	4 (1%)	22	63
1	C	604/622 (97%)	588 (97%)	13 (2%)	3 (0%)	29	69
All	All	1812/1866 (97%)	1754 (97%)	46 (2%)	12 (1%)	26	63

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	VAL
1	A	409	LEU
1	B	276	VAL
1	B	409	LEU
1	C	226	ASP

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	530/541 (98%)	493 (93%)	37 (7%)	15	40
1	B	530/541 (98%)	495 (93%)	35 (7%)	16	41
1	C	530/541 (98%)	494 (93%)	36 (7%)	16	41
All	All	1590/1623 (98%)	1482 (93%)	108 (7%)	19	41

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	392	SER
1	B	718	ASP
1	C	415	LYS
1	B	415	LYS
1	B	605	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19

such sidechains are listed below:

Mol	Chain	Res	Type
1	C	248	HIS
1	C	580	ASN
1	C	712	HIS
1	C	516	HIS
1	B	311	HIS

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

There are no such residues in this entry.

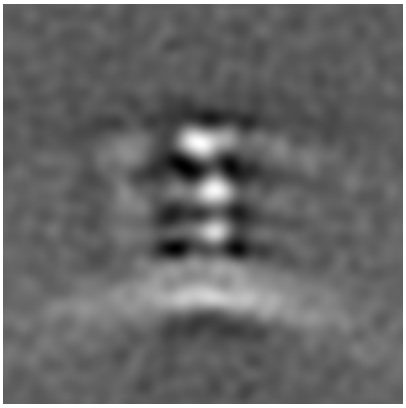
5.8 Polymer linkage issues

There are no chain breaks in this entry.

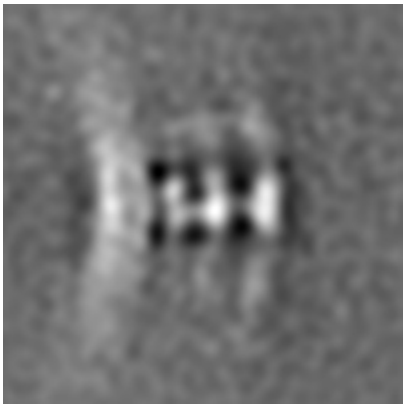
6 Tomogram visualisation

This section contains visualisations of the EMDB entry EMD-2380. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

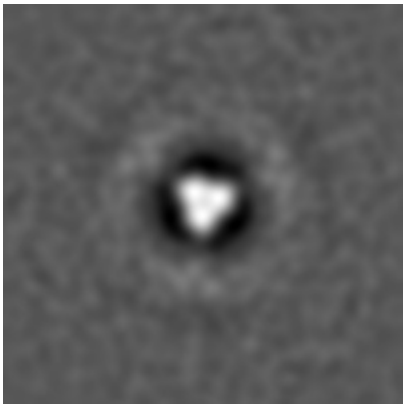
6.1 Orthogonal projections



X



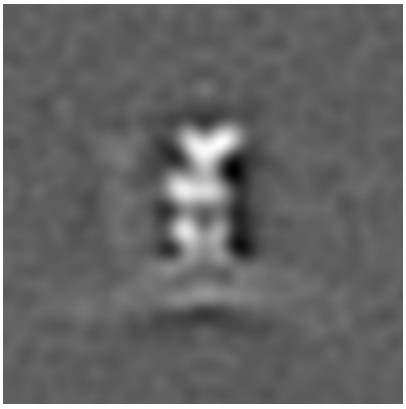
Y



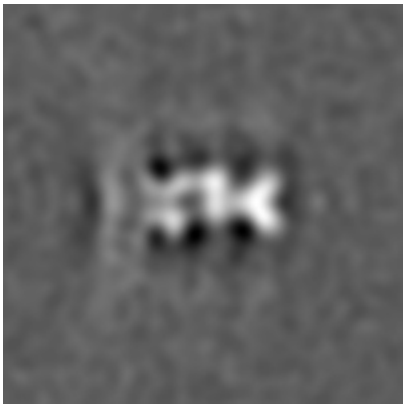
Z

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

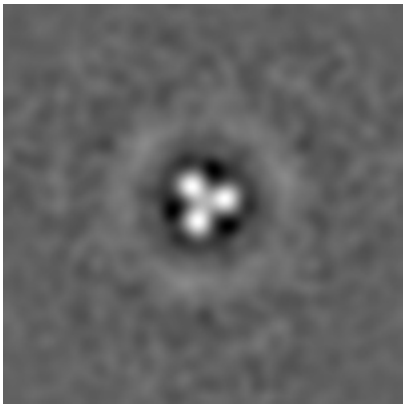
6.2 Central slices



X Index: 50



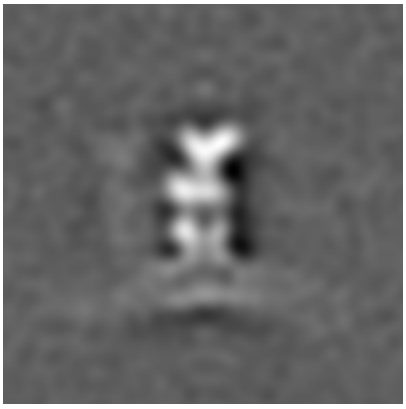
Y Index: 50



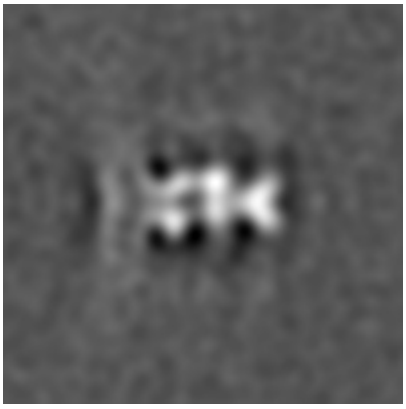
Z Index: 50

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

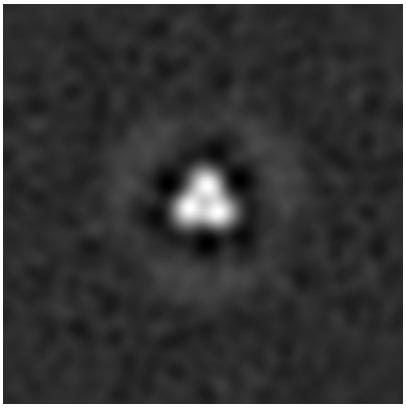
6.3 Largest variance slices (i)



X Index: 50



Y Index: 51



Z Index: 65

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

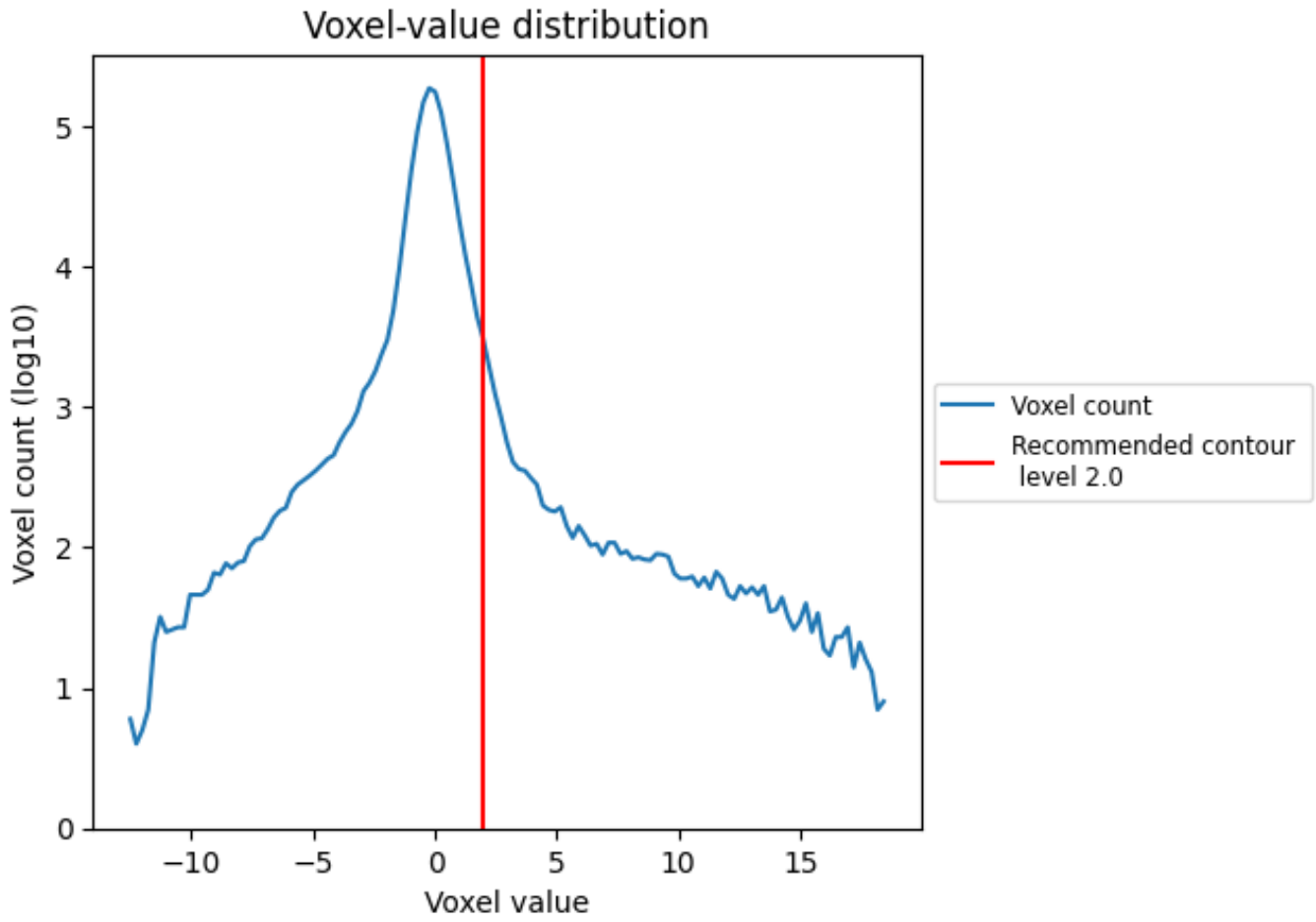
6.4 Mask visualisation (i)

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

7 Tomogram analysis (i)

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

7.1 Voxel-value distribution (i)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

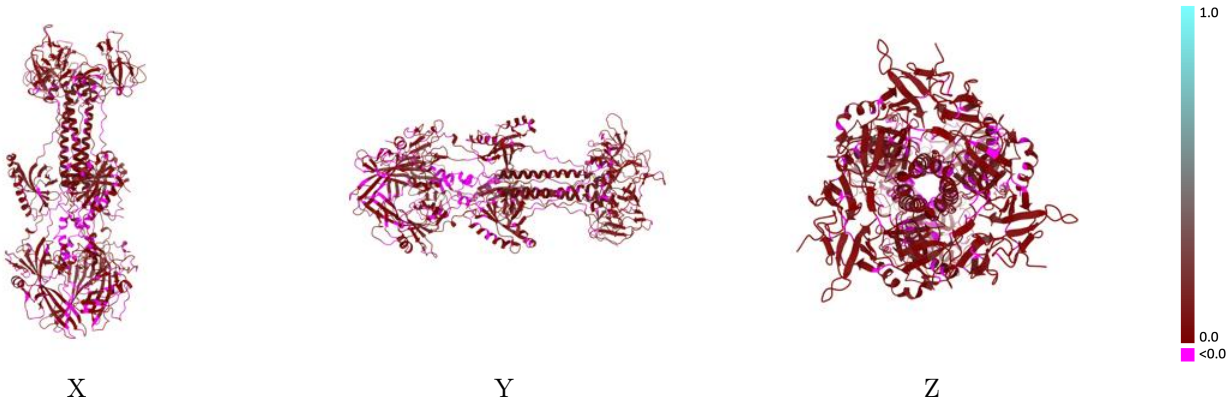
8 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2380 and PDB model 4BOM. Per-residue inclusion information can be found in section 3 on page 4.

8.1 Map-model overlay

This section was not generated.

8.2 Q-score mapped to coordinate model

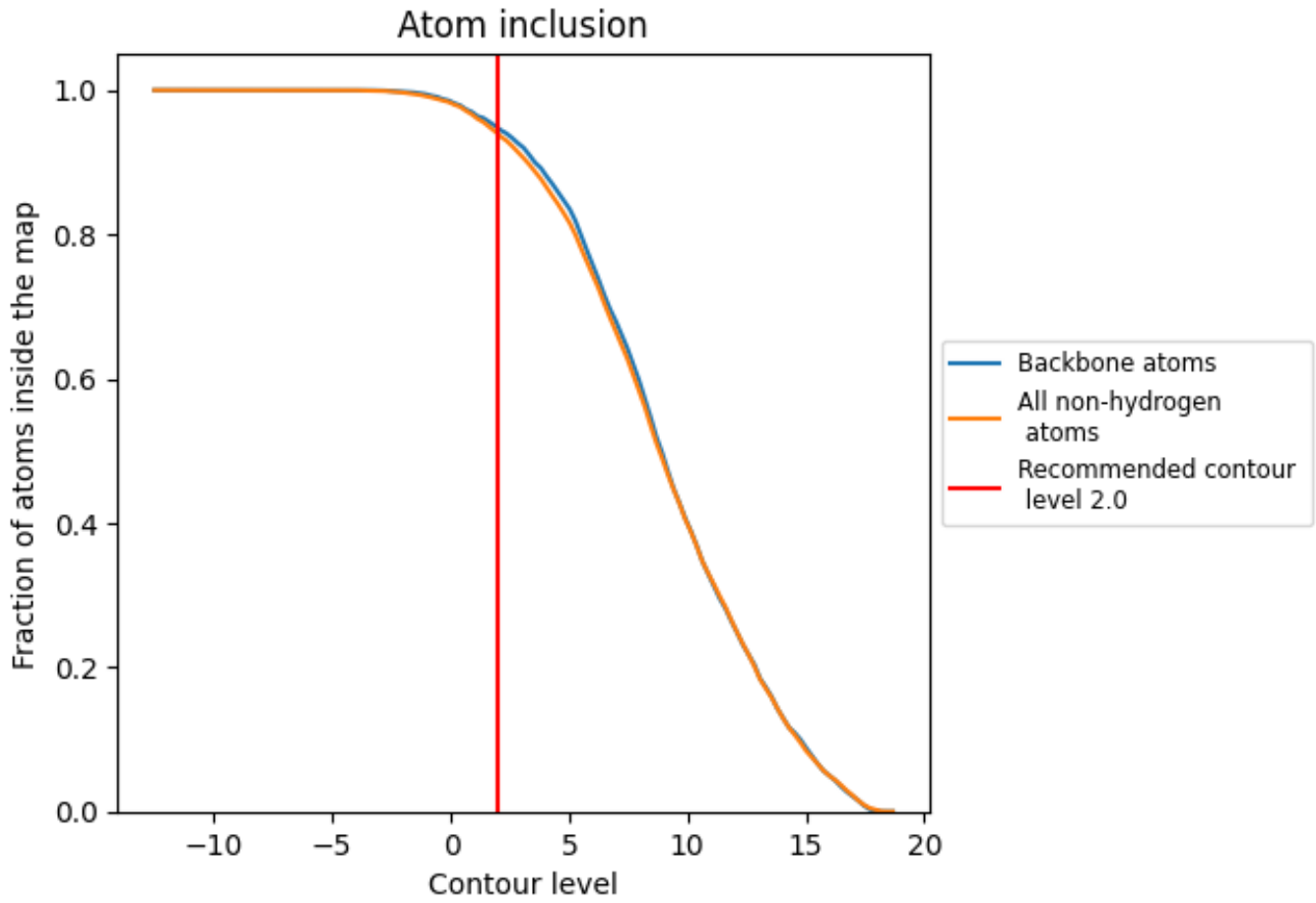


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 Atom inclusion mapped to coordinate model

This section was not generated.

8.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9393	0.0540
A	0.9372	0.0530
B	0.9403	0.0530
C	0.9403	0.0560