



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 03:20 AM UTC

PDB ID : 1Q5A / pdb_00001q5a
EMDB ID : EMD-1052
Title : S-shaped trans interactions of cadherins model based on fitting C-cadherin (1L3W) to 3D map of desmosomes obtained by electron tomography
Authors : He, W.; Cowin, P.; Stokes, D.L.
Deposited on : 2003-08-06
Resolution : 30.00 Å(reported)
Based on initial model : 1L3W

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : **FAILED**
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) : 2.49

2 Entry composition [i](#)

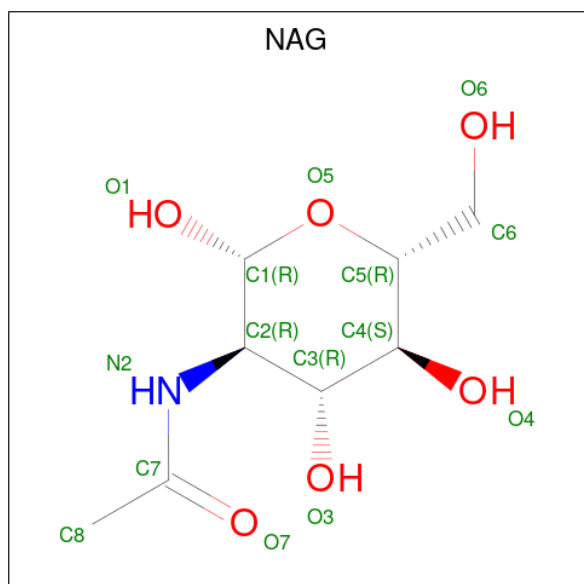
There are 4 unique types of molecules in this entry. The entry contains 8826 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 EP-cadherin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	540	Total	C	N	O	S	0	0
			4191	2635	695	850	11		
1	B	540	Total	C	N	O	S	0	0
			4191	2635	695	850	11		

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	

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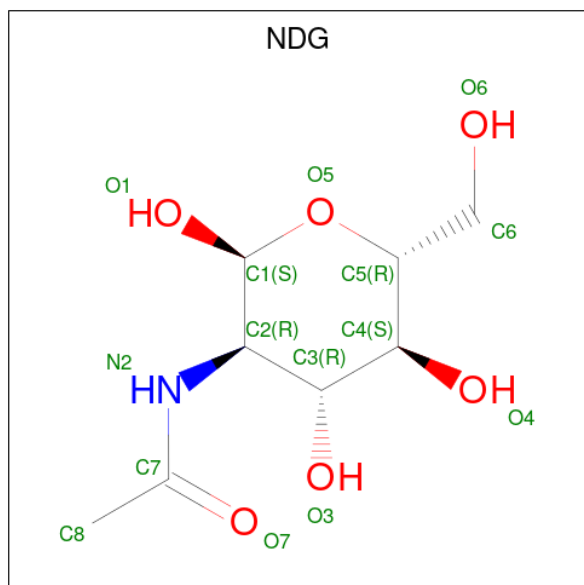
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 3 is 2-acetamido-2-deoxy- α -D-glucopyranose (CCD ID: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	A	12	Total	Ca	0
			12	12	
4	B	12	Total	Ca	0
			12	12	

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3 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	no CTF correction. Imaging at underfocus 0.4 micron with CM200FEG microscope at 50,000 magnification	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1200	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	500	Depositor
Magnification	68276	Depositor
Image detector	GENERIC GATAN	Depositor
Maximum voxel value	2603.000	Depositor
Minimum voxel value	-1866.000	Depositor
Average voxel value	1323.980	Depositor
Voxel value standard deviation	218.755	Depositor
Recommended contour level	1760	Depositor
Tomogram size ($\text{\AA}$)	3720.19, 3720.19, 617.61	wwPDB
Tomogram dimensions	512, 512, 85	wwPDB
Tomogram angles ($^\circ$)	90, 90, 90	wwPDB
Grid spacing ($\text{\AA}$)	7.266, 7.266, 7.266	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 24 are monoatomic - leaving 30 for Mogul analysis.

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	$\# Z > 2$
2	NAG	A	903	1	14,14,15	0.55	0	17,19,21	0.79	0
2	NAG	A	902	1	14,14,15	1.13	1 (7%)	17,19,21	1.09	2 (11%)
2	NAG	B	803	1	14,14,15	0.99	1 (7%)	17,19,21	1.16	2 (11%)
3	NDG	A	811	1	14,14,15	0.88	0	17,19,21	1.96	1 (5%)
2	NAG	A	809	1	14,14,15	0.75	0	17,19,21	0.94	0
2	NAG	A	808	1	14,14,15	0.65	0	17,19,21	0.70	0
2	NAG	A	801	1	14,14,15	0.70	0	17,19,21	0.97	1 (5%)
2	NAG	B	802	1	14,14,15	0.77	1 (7%)	17,19,21	0.85	0
2	NAG	B	903	1	14,14,15	0.55	0	17,19,21	0.79	0
2	NAG	B	810	1	14,14,15	0.66	0	17,19,21	1.33	4 (23%)
3	NDG	B	804	1	14,14,15	0.64	0	17,19,21	0.78	0
2	NAG	B	806	1	14,14,15	0.56	0	17,19,21	1.39	3 (17%)
2	NAG	A	812	1	14,14,15	0.83	1 (7%)	17,19,21	0.76	1 (5%)
2	NAG	B	808	1	14,14,15	0.67	0	17,19,21	0.70	0
2	NAG	B	805	1	14,14,15	0.71	0	17,19,21	1.06	1 (5%)
2	NAG	B	809	1	14,14,15	0.77	1 (7%)	17,19,21	0.94	0
2	NAG	B	801	1	14,14,15	0.70	0	17,19,21	0.98	1 (5%)
2	NAG	B	812	1	14,14,15	0.84	1 (7%)	17,19,21	0.75	1 (5%)
2	NAG	A	807	1	14,14,15	0.65	0	17,19,21	1.19	2 (11%)
3	NDG	A	804	1	14,14,15	0.65	0	17,19,21	0.78	0
2	NAG	B	807	1	14,14,15	0.64	0	17,19,21	1.19	2 (11%)
2	NAG	A	805	1	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
2	NAG	B	904	1	14,14,15	0.77	1 (7%)	17,19,21	0.70	1 (5%)
2	NAG	B	902	1	14,14,15	1.12	1 (7%)	17,19,21	1.09	1 (5%)
2	NAG	A	904	1	14,14,15	0.77	1 (7%)	17,19,21	0.70	1 (5%)
3	NDG	B	811	1	14,14,15	0.87	0	17,19,21	1.97	1 (5%)
2	NAG	A	803	1	14,14,15	0.99	1 (7%)	17,19,21	1.15	2 (11%)
2	NAG	A	806	1	14,14,15	0.56	0	17,19,21	1.39	3 (17%)
2	NAG	A	802	1	14,14,15	0.76	1 (7%)	17,19,21	0.85	0
2	NAG	A	810	1	14,14,15	0.66	0	17,19,21	1.33	4 (23%)

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
2	NAG	A	903	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	902	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	803	1	-	2/6/23/26	0/1/1/1
3	NDG	A	811	1	-	2/6/23/26	0/1/1/1
2	NAG	A	809	1	-	2/6/23/26	0/1/1/1
2	NAG	A	808	1	-	3/6/23/26	0/1/1/1
2	NAG	A	801	1	-	4/6/23/26	0/1/1/1
2	NAG	B	903	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	802	1	-	2/6/23/26	0/1/1/1
2	NAG	B	810	1	-	3/6/23/26	0/1/1/1
3	NDG	B	804	1	-	0/6/23/26	0/1/1/1
2	NAG	B	806	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	812	1	-	4/6/23/26	0/1/1/1
2	NAG	B	808	1	-	3/6/23/26	0/1/1/1
2	NAG	B	805	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	809	1	-	2/6/23/26	0/1/1/1
2	NAG	B	801	1	-	4/6/23/26	0/1/1/1
2	NAG	B	812	1	-	4/6/23/26	0/1/1/1
2	NAG	A	807	1	-	5/6/23/26	0/1/1/1
3	NDG	A	804	1	-	0/6/23/26	0/1/1/1
2	NAG	B	807	1	-	5/6/23/26	0/1/1/1
2	NAG	A	805	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	904	1	-	3/6/23/26	0/1/1/1
2	NAG	B	902	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	904	1	-	3/6/23/26	0/1/1/1
3	NDG	B	811	1	-	2/6/23/26	0/1/1/1
2	NAG	A	803	1	-	2/6/23/26	0/1/1/1
2	NAG	A	806	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	802	1	-	2/6/23/26	0/1/1/1
2	NAG	A	810	1	-	3/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	NAG	C1-C2	3.39	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	902	NAG	C1-C2	3.31	1.56	1.52
2	A	803	NAG	O5-C5	2.62	1.48	1.43
2	B	803	NAG	O5-C5	2.62	1.48	1.43
2	B	904	NAG	C1-C2	-2.42	1.49	1.52
2	A	904	NAG	C1-C2	-2.40	1.49	1.52
2	B	812	NAG	C1-C2	-2.35	1.49	1.52
2	A	812	NAG	C1-C2	-2.34	1.49	1.52
2	B	802	NAG	C1-C2	2.09	1.55	1.52
2	A	802	NAG	C1-C2	2.06	1.55	1.52
2	B	809	NAG	C1-C2	-2.01	1.49	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	811	NDG	C2-N2-C7	-7.45	112.92	122.90
3	A	811	NDG	C2-N2-C7	-7.42	112.95	122.90
2	A	806	NAG	C2-N2-C7	-3.62	118.04	122.90
2	B	806	NAG	C2-N2-C7	-3.62	118.05	122.90
2	B	805	NAG	C2-N2-C7	-3.20	118.61	122.90
2	A	805	NAG	C2-N2-C7	-3.16	118.66	122.90
2	A	807	NAG	C2-N2-C7	-3.05	118.81	122.90
2	B	807	NAG	C2-N2-C7	-3.05	118.81	122.90
2	A	803	NAG	C2-N2-C7	-2.97	118.93	122.90
2	B	803	NAG	C2-N2-C7	-2.95	118.94	122.90
2	A	810	NAG	C1-C2-N2	2.52	114.41	110.43
2	B	810	NAG	C1-C2-N2	2.51	114.38	110.43
2	B	810	NAG	C4-C3-C2	-2.46	107.42	111.02
2	A	810	NAG	C4-C3-C2	-2.45	107.42	111.02
2	B	806	NAG	C4-C3-C2	-2.44	107.44	111.02
2	A	806	NAG	C4-C3-C2	-2.44	107.44	111.02
2	B	803	NAG	C1-O5-C5	2.44	115.45	112.19
2	A	803	NAG	C1-O5-C5	2.42	115.43	112.19
2	A	810	NAG	O5-C1-C2	-2.38	107.60	111.29
2	B	810	NAG	O5-C1-C2	-2.38	107.61	111.29
2	B	810	NAG	C1-O5-C5	-2.25	109.17	112.19
2	A	810	NAG	C1-O5-C5	-2.23	109.20	112.19
2	B	902	NAG	O5-C1-C2	2.17	114.65	111.29
2	A	902	NAG	O5-C1-C2	2.16	114.63	111.29
2	A	812	NAG	C2-N2-C7	-2.16	120.01	122.90
2	A	801	NAG	C1-C2-N2	-2.14	107.06	110.43
2	B	801	NAG	C1-C2-N2	-2.14	107.06	110.43
2	B	812	NAG	C2-N2-C7	-2.13	120.04	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	807	NAG	O5-C1-C2	-2.09	108.06	111.29
2	A	807	NAG	O5-C1-C2	-2.07	108.09	111.29
2	A	902	NAG	C1-O5-C5	2.04	114.92	112.19
2	B	904	NAG	C2-N2-C7	-2.03	120.17	122.90
2	B	806	NAG	O5-C1-C2	-2.03	108.15	111.29
2	A	806	NAG	O5-C1-C2	-2.02	108.17	111.29
2	A	904	NAG	C2-N2-C7	-2.02	120.20	122.90

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	805	NAG	C1
2	A	806	NAG	C1
2	A	902	NAG	C1
2	A	903	NAG	C1
2	B	805	NAG	C1
2	B	806	NAG	C1
2	B	902	NAG	C1
2	B	903	NAG	C1

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	807	NAG	C3-C2-N2-C7
2	A	808	NAG	C1-C2-N2-C7
2	A	810	NAG	C1-C2-N2-C7
2	A	812	NAG	C1-C2-N2-C7
2	A	902	NAG	C3-C2-N2-C7
2	A	904	NAG	C3-C2-N2-C7
2	B	807	NAG	C3-C2-N2-C7
2	B	808	NAG	C1-C2-N2-C7
2	B	810	NAG	C1-C2-N2-C7
2	B	812	NAG	C1-C2-N2-C7
2	B	902	NAG	C3-C2-N2-C7
2	B	904	NAG	C3-C2-N2-C7
3	A	811	NDG	C4-C5-C6-O6
3	B	811	NDG	C4-C5-C6-O6
2	A	807	NAG	C4-C5-C6-O6
2	B	802	NAG	C4-C5-C6-O6
2	B	807	NAG	C4-C5-C6-O6
3	A	811	NDG	O5-C5-C6-O6
3	B	811	NDG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	802	NAG	C4-C5-C6-O6
2	A	809	NAG	O5-C5-C6-O6
2	B	809	NAG	O5-C5-C6-O6
2	A	809	NAG	C4-C5-C6-O6
2	B	809	NAG	C4-C5-C6-O6
2	A	807	NAG	O5-C5-C6-O6
2	B	807	NAG	O5-C5-C6-O6
2	A	807	NAG	C8-C7-N2-C2
2	B	807	NAG	C8-C7-N2-C2
2	A	805	NAG	O5-C5-C6-O6
2	B	805	NAG	O5-C5-C6-O6
2	A	802	NAG	O5-C5-C6-O6
2	B	802	NAG	O5-C5-C6-O6
2	A	904	NAG	C4-C5-C6-O6
2	B	904	NAG	C4-C5-C6-O6
2	A	805	NAG	C4-C5-C6-O6
2	B	805	NAG	C4-C5-C6-O6
2	A	810	NAG	C4-C5-C6-O6
2	B	810	NAG	C4-C5-C6-O6
2	A	812	NAG	O5-C5-C6-O6
2	B	812	NAG	O5-C5-C6-O6
2	A	807	NAG	O7-C7-N2-C2
2	B	807	NAG	O7-C7-N2-C2
2	A	803	NAG	C4-C5-C6-O6
2	B	803	NAG	C4-C5-C6-O6
2	A	810	NAG	O5-C5-C6-O6
2	B	810	NAG	O5-C5-C6-O6
2	A	904	NAG	O5-C5-C6-O6
2	B	904	NAG	O5-C5-C6-O6
2	A	801	NAG	C4-C5-C6-O6
2	B	801	NAG	C4-C5-C6-O6
2	A	803	NAG	O5-C5-C6-O6
2	B	803	NAG	O5-C5-C6-O6
2	B	903	NAG	C4-C5-C6-O6
2	A	903	NAG	C4-C5-C6-O6
2	B	806	NAG	C4-C5-C6-O6
2	A	806	NAG	C4-C5-C6-O6
2	A	808	NAG	C4-C5-C6-O6
2	B	808	NAG	C4-C5-C6-O6
2	A	801	NAG	C3-C2-N2-C7
2	A	903	NAG	C3-C2-N2-C7
2	B	801	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	B	903	NAG	C3-C2-N2-C7
2	A	801	NAG	O5-C5-C6-O6
2	B	801	NAG	O5-C5-C6-O6
2	A	801	NAG	C1-C2-N2-C7
2	A	902	NAG	C1-C2-N2-C7
2	B	801	NAG	C1-C2-N2-C7
2	B	902	NAG	C1-C2-N2-C7
2	B	806	NAG	O5-C5-C6-O6
2	A	806	NAG	O5-C5-C6-O6
2	A	808	NAG	C3-C2-N2-C7
2	A	812	NAG	C3-C2-N2-C7
2	B	808	NAG	C3-C2-N2-C7
2	B	812	NAG	C3-C2-N2-C7
2	B	812	NAG	C4-C5-C6-O6
2	A	812	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

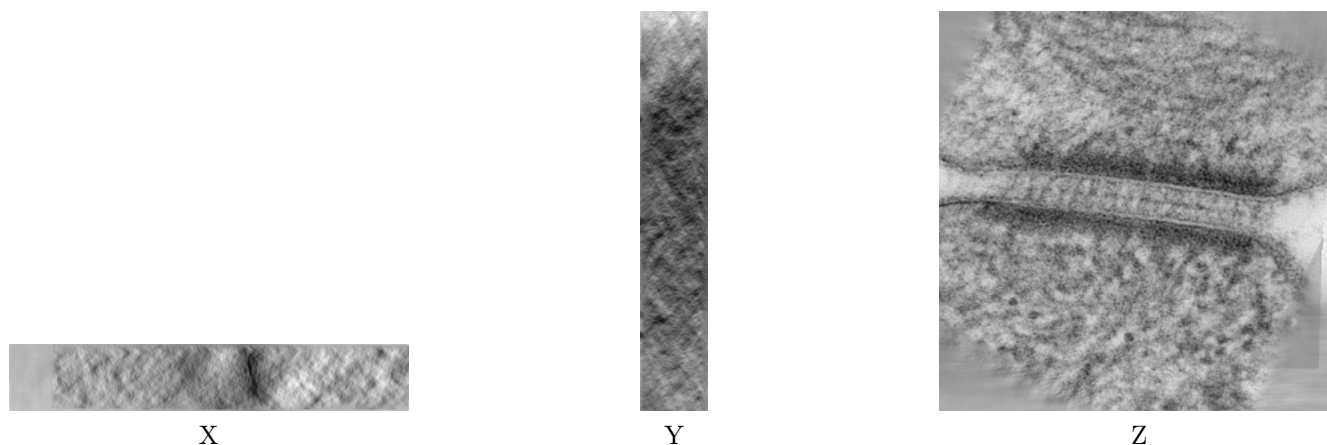
4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Tomogram visualisation [i](#)

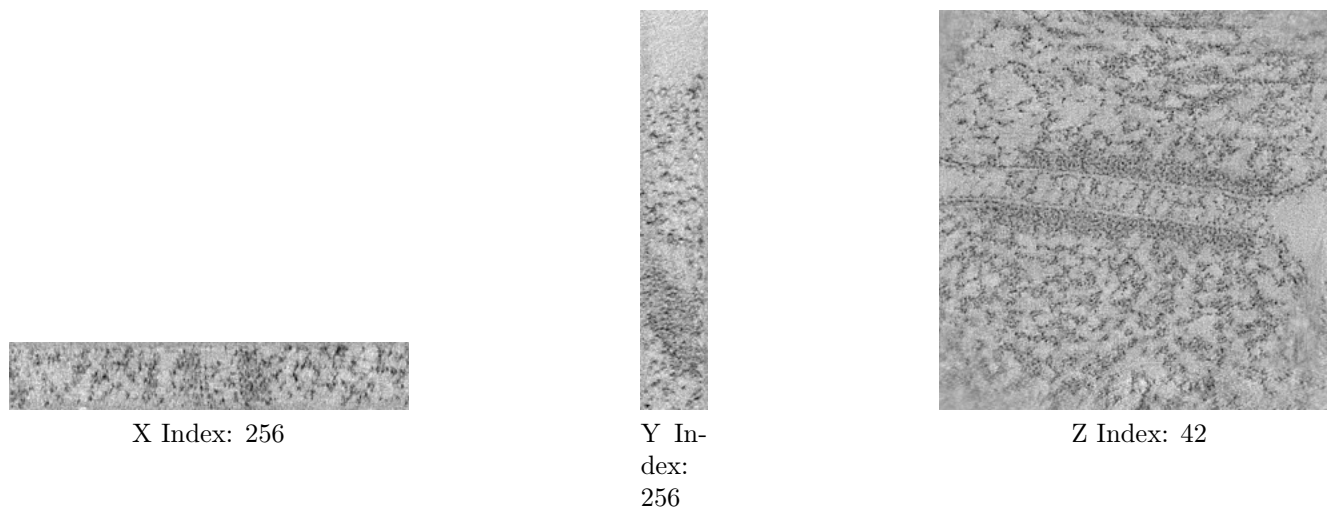
This section contains visualisations of the EMDB entry EMD-1052. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

5.1 Orthogonal projections [i](#)



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

5.2 Central slices [i](#)

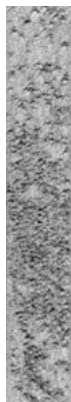
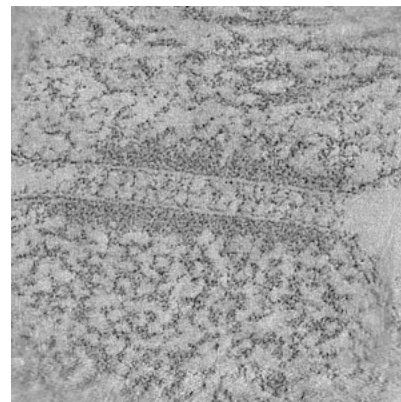


The images above show central slices of the tomogram in three orthogonal directions.

5.3 Largest variance slices [i](#)



X Index: 243

Y Index:
315

Z Index: 39

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

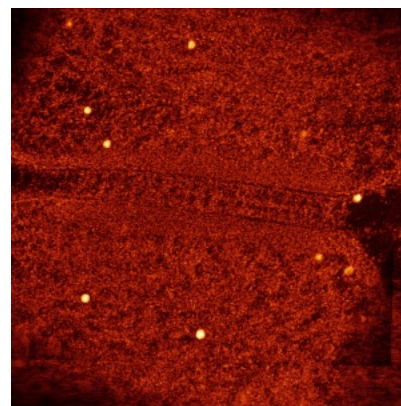
5.4 Orthogonal standard-deviation projections (False-color) [i](#)



X



Y



Z

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

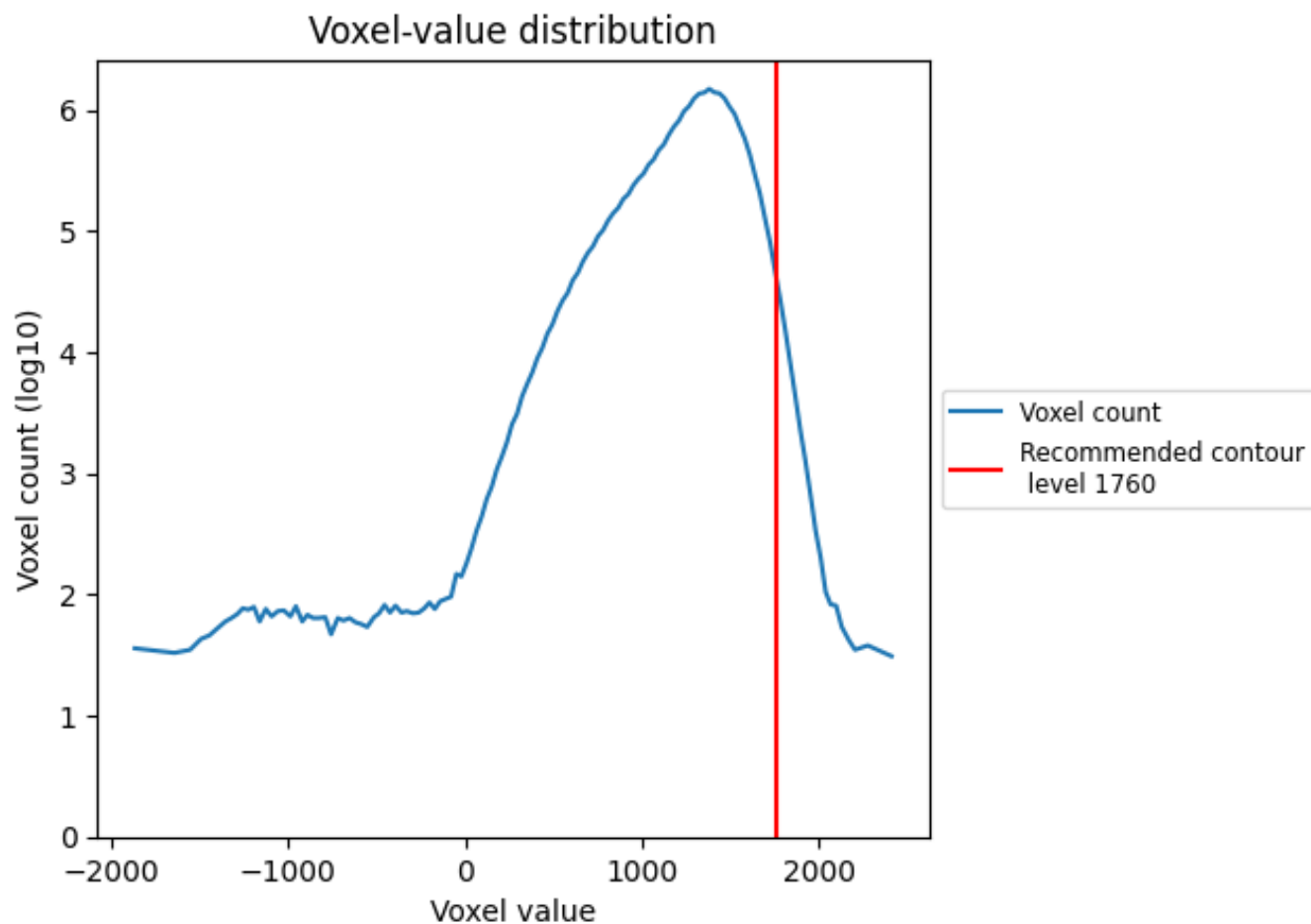
5.5 Mask visualisation [i](#)

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

6 Tomogram analysis [i](#)

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

6.1 Voxel-value distribution [i](#)



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

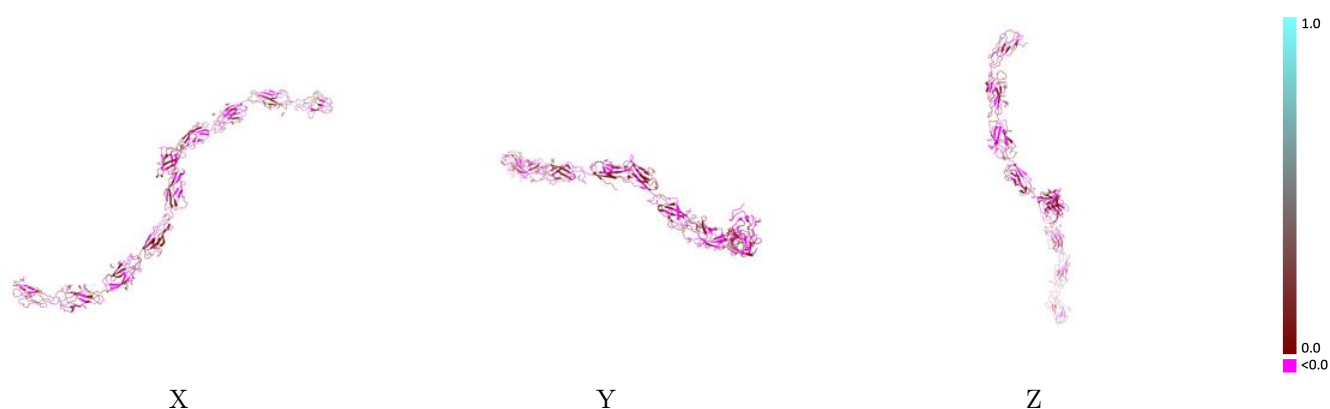
7 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1052 and PDB model 1Q5A. Per-residue inclusion information can be found in section ?? on page ??.

7.1 Map-model overlay [i](#)

This section was not generated.

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

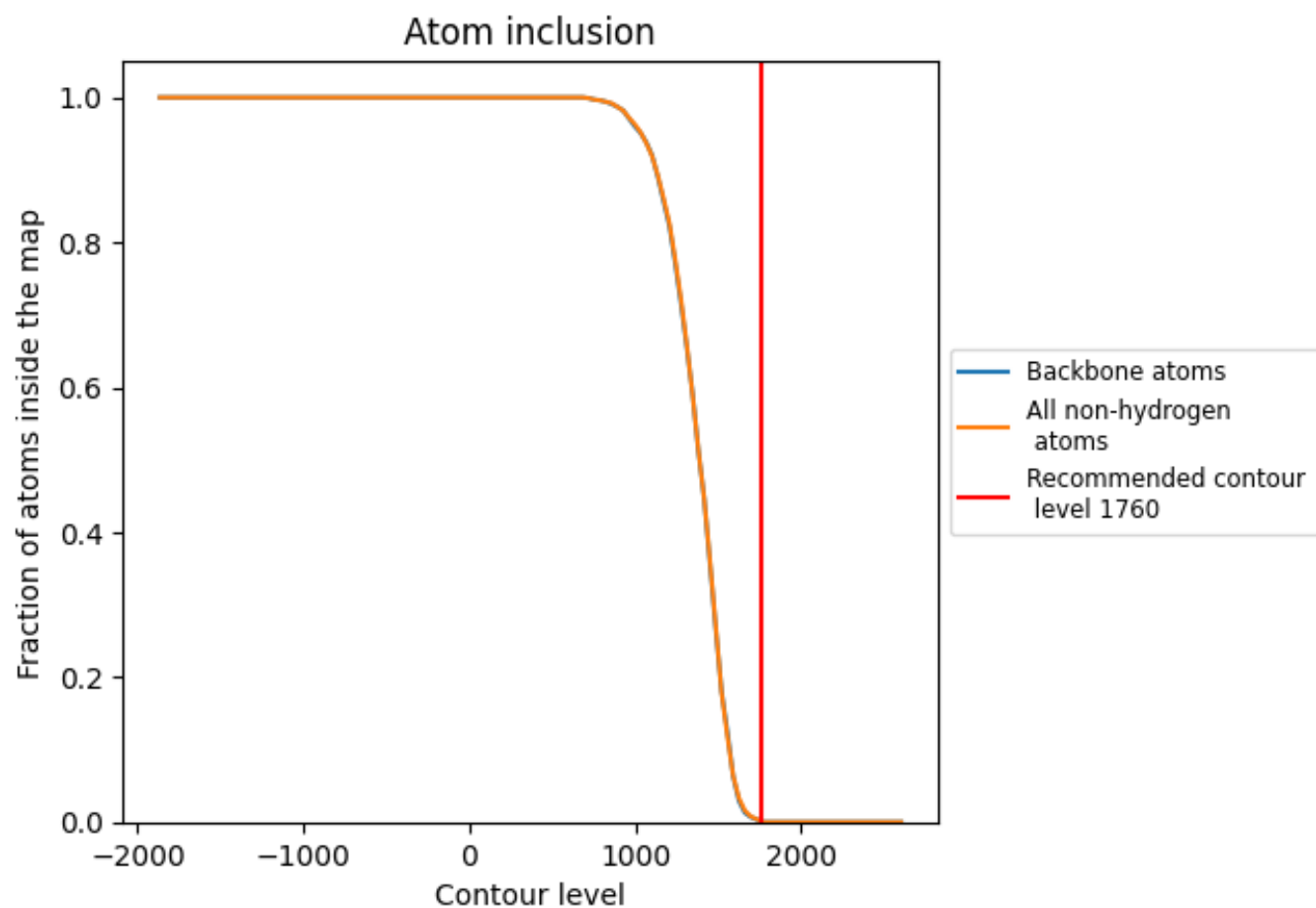


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

7.4 Atom inclusion [i](#)



At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

7.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1760) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0010	0.0050
A	0.0020	0.0070
B	0.0000	0.0030

