



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 09:36 PM EST

PDB ID : 1Q5B
EMDB ID : EMD-1052
Title : lambda-shaped TRANS and CIS 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 wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.31.3

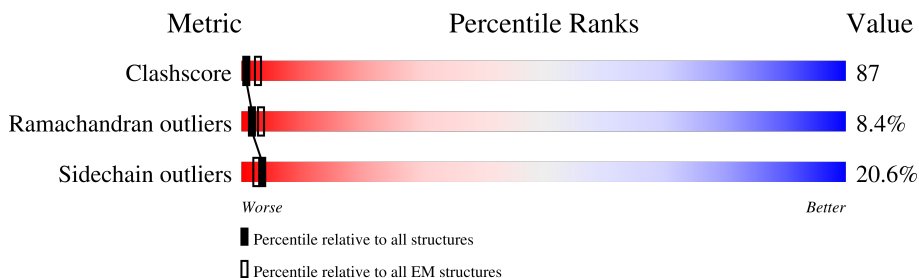
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 30.00 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 $\leq 5\%$. 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	A	880	 16% 31% 10% 61% 39%
1	B	880	 16% 31% 11% 61% 39%
1	C	880	 16% 31% 11% 61% 39%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	801	-	-	X	-
2	NAG	A	805	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	806	X	-	X	-
2	NAG	A	807	-	-	X	-
2	NAG	A	809	-	-	X	-
2	NAG	A	810	-	-	X	-
2	NAG	A	902	X	-	X	-
2	NAG	A	903	X	-	-	-
2	NAG	A	904	-	-	X	-
2	NAG	B	801	-	-	X	-
2	NAG	B	805	X	-	X	-
2	NAG	B	806	X	-	X	-
2	NAG	B	807	-	-	X	-
2	NAG	B	809	-	-	X	-
2	NAG	B	810	-	-	X	-
2	NAG	B	902	X	-	X	-
2	NAG	B	903	X	-	-	-
2	NAG	B	904	-	-	X	-
2	NAG	C	801	-	-	X	-
2	NAG	C	805	X	-	X	-
2	NAG	C	806	X	-	X	-
2	NAG	C	807	-	-	X	-
2	NAG	C	809	-	-	X	-
2	NAG	C	810	-	-	X	-
2	NAG	C	902	X	-	X	-
2	NAG	C	903	X	-	-	-
2	NAG	C	904	-	-	X	-
3	NDG	A	811	-	-	X	-
3	NDG	B	811	-	-	X	-

2 Entry composition [i](#)

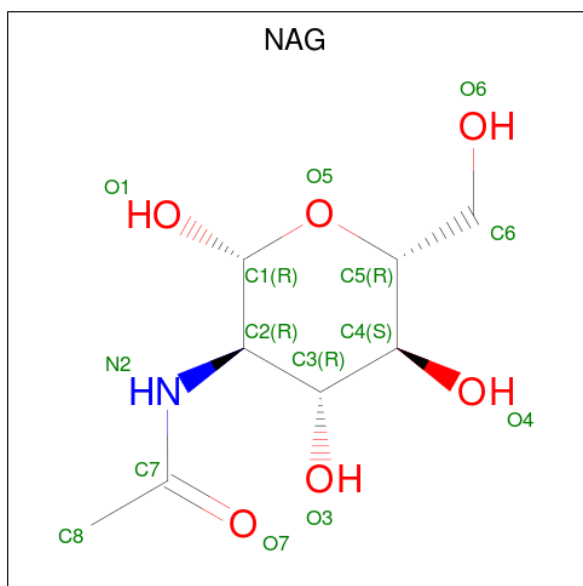
There are 4 unique types of molecules in this entry. The entry contains 13239 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S		
1	A	540	Total 4191	C 2635	N 695	O 850	S 11	0	0
1	B	540	Total 4191	C 2635	N 695	O 850	S 11	0	0
1	C	540	Total 4191	C 2635	N 695	O 850	S 11	0	0

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



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	A	1	Total 182	C 104	N 13	O 65	0
2	A	1	Total 182	C 104	N 13	O 65	0
2	A	1	Total 182	C 104	N 13	O 65	0

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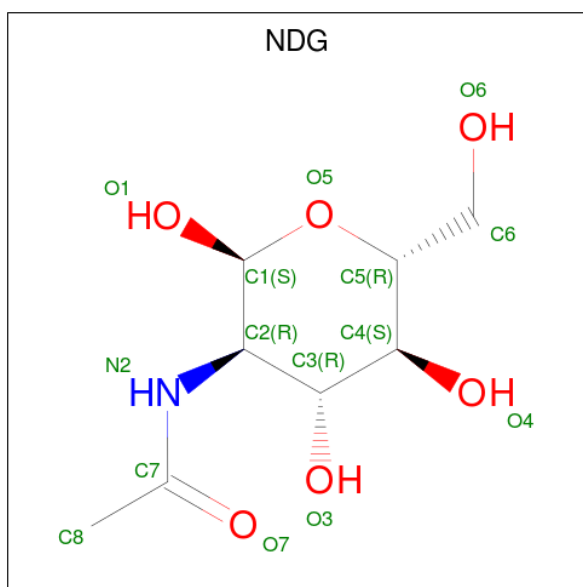
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	A	1	Total 182	C 104	N 13	O 65	0
2	A	1	Total 182	C 104	N 13	O 65	0
2	A	1	Total 182	C 104	N 13	O 65	0
2	A	1	Total 182	C 104	N 13	O 65	0
2	A	1	Total 182	C 104	N 13	O 65	0
2	A	1	Total 182	C 104	N 13	O 65	0
2	A	1	Total 182	C 104	N 13	O 65	0
2	A	1	Total 182	C 104	N 13	O 65	0
2	A	1	Total 182	C 104	N 13	O 65	0
2	A	1	Total 182	C 104	N 13	O 65	0
2	A	1	Total 182	C 104	N 13	O 65	0
2	A	1	Total 182	C 104	N 13	O 65	0
2	B	1	Total 182	C 104	N 13	O 65	0
2	B	1	Total 182	C 104	N 13	O 65	0
2	B	1	Total 182	C 104	N 13	O 65	0
2	B	1	Total 182	C 104	N 13	O 65	0
2	B	1	Total 182	C 104	N 13	O 65	0
2	B	1	Total 182	C 104	N 13	O 65	0
2	B	1	Total 182	C 104	N 13	O 65	0
2	B	1	Total 182	C 104	N 13	O 65	0
2	B	1	Total 182	C 104	N 13	O 65	0
2	B	1	Total 182	C 104	N 13	O 65	0
2	B	1	Total 182	C 104	N 13	O 65	0
2	B	1	Total 182	C 104	N 13	O 65	0
2	B	1	Total 182	C 104	N 13	O 65	0
2	B	1	Total 182	C 104	N 13	O 65	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	B	1	Total 182	C 104	N 13	O 65	0
2	B	1	Total 182	C 104	N 13	O 65	0
2	C	1	Total 182	C 104	N 13	O 65	0
2	C	1	Total 182	C 104	N 13	O 65	0
2	C	1	Total 182	C 104	N 13	O 65	0
2	C	1	Total 182	C 104	N 13	O 65	0
2	C	1	Total 182	C 104	N 13	O 65	0
2	C	1	Total 182	C 104	N 13	O 65	0
2	C	1	Total 182	C 104	N 13	O 65	0
2	C	1	Total 182	C 104	N 13	O 65	0
2	C	1	Total 182	C 104	N 13	O 65	0
2	C	1	Total 182	C 104	N 13	O 65	0
2	C	1	Total 182	C 104	N 13	O 65	0
2	C	1	Total 182	C 104	N 13	O 65	0
2	C	1	Total 182	C 104	N 13	O 65	0
2	C	1	Total 182	C 104	N 13	O 65	0

- Molecule 3 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (three-letter code: NDG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
3	A	1	28	16	2	10	0
3	A	1	28	16	2	10	0
3	B	1	28	16	2	10	0
3	B	1	28	16	2	10	0
3	C	1	28	16	2	10	0
3	C	1	28	16	2	10	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

V326	G386	T446	D506	PHE	ARG	SER
N327	I387	M447	Y507	LEU	ASN	LEU
E328	V388	C448	S508	LEU	ASP	SER
A329	T389	D449	I509	LEU	VAL	LEU
P330	G390	Q450	Y510	LEU	PRO	ASN
F331	N391	M451	V511	LEU	THR	SER
F332	G392	P452	L512	LEU	MET	SER
V333	N393	F453	L513	LYS	PRO	ASN
P334	D394	P454	S514	ARG	ALA	ASN
A335	L395	Q455	D515	LYS	PRO	ASP
V336	R396	V456	A516	VAL	HIS	GLU
S337	E397	L457	Q517	VAL	THR	HIS
R338	S398	T458	N518	LYS	ARG	ASP
V339	E399	I459	N519	GLU	PRO	TYR
D340	Y400	S460	P520	PRO	PRO	TYR
V41	V401	D461	Q521	LEU	ASN	LEU
S342	K402	A462	L522	LEU	PRO	ASP
E343	M403	D463	T523	ASP	GLU	TRP
D344	N404	I464	V524	ASP	ILE	SER
L345	T405	P465	V525	THR	GLY	ARG
S346	Y406	P466	N526	ARG	ASN	PHE
R347	T407	M467	A527	ASP	PHE	ARG
G348	V408	T468	T528	ASP	ILE	ARG
E349	I409	V469	V529	PHE	ASP	LEU
K350	M410	P470	C530	TYR	ASN	ASP
I351	L411	Y471	S531	TYR	LEU	MET
I352	V412	K472	C532	GLY	ASP	TYR
S353	T413	V473	E533	GLU	ALA	GLY
L354	D414	S474	G534	GLY	ALA	GLY
V355	D415	L475	K535	GLY	ASN	ASP
A356	G416	S476	A536	GLY	ASP	ASP
Q357	V417	H477	I537	GLU	THR	GLU
D358	S418	G478	K538	ASP	ALA	GLU
P359	V419	S479	C539	GLN	PRO	GLY
D360	G420	D480	Q540	ASP	PRO	ASP
K361	T421	L481	GLU	ASP	TYR	SER
Q362	G422	T482	LYS	LEU	ASP	LEU
Q363	T423	W483	LEU	LEU	LEU	LEU
I364	G424	K484	VAL	LEU	VAL	VAL
Q365	T425	A485	GLY	HIS	PHE	GLY
K366	L426	E486	GLY	ARG	ASP	ARG
L367	I427	L487	PHE	GLY	TYR	TYR
S368	L428	D488	ASP	LEU	GLY	GLY
Y369	H429	S489	LEU	LEU	GLY	ASP
F370	V430	K490	ILE	PRO	SER	PRO
I371	L431	G491	LEU	ASP	GLU	ASP
G372	D432	T492	VAL	ILE	ALA	ILE
N373	V433	S493	LEU	LEU	ALA	MET
D374	M434	M494	GLY	GLY	VAL	
P375	N435	L495	VAL	VAL	ALA	
A376	N436	L496	LEU	LEU	ALA	
R377	G437	S497	LEU	LEU	LEU	
W378	P438	P498	LEU	LEU	LEU	
L379	V439	T499	ILE	ILE	ILE	
T380	P440	Q500	LEU	LEU	LEU	
V381	S441	Q501	LEU	LEU	LEU	
K382	P442	L502	LEU	LEU	LEU	
D384	R443	K503	LEU	LEU	LEU	
N385	V444	K504	LEU	LEU	LEU	
	F445	G505				

4 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	1760.0	Depositor
Tomogram size (Å)	3720.19, 3720.19, 617.61	wwPDB
Tomogram dimensions	512, 512, 85	wwPDB
Tomogram angles (°)	90, 90, 90	wwPDB
Grid spacing (Å)	7.266, 7.266, 7.266	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.70	8/4276 (0.2%)	1.44	81/5839 (1.4%)
1	B	0.70	8/4276 (0.2%)	1.39	79/5839 (1.4%)
1	C	0.70	8/4276 (0.2%)	1.39	79/5839 (1.4%)
All	All	0.70	24/12828 (0.2%)	1.41	239/17517 (1.4%)

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	1	4
1	B	0	4
1	C	0	4
All	All	1	12

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ALA	CA-CB	-8.37	1.34	1.52
1	C	335	ALA	CA-CB	-8.35	1.34	1.52
1	B	335	ALA	CA-CB	-8.33	1.34	1.52
1	C	539	CYS	CB-SG	8.18	1.96	1.82
1	A	539	CYS	CB-SG	8.17	1.96	1.82

The worst 5 of 239 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	LYS	N-CA-CB	-28.44	59.41	110.60
1	A	520	PRO	CA-C-N	-13.30	87.95	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	520	PRO	CA-C-N	-13.29	87.97	117.20
1	B	520	PRO	CA-C-N	-13.28	87.99	117.20
1	C	290	PHE	N-CA-C	12.74	145.39	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	490	LYS	CA

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	PHE	Sidechain
1	A	18	PRO	Mainchain
1	A	222	ASP	Mainchain
1	A	520	PRO	Mainchain
1	B	17	PHE	Sidechain

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	4191	0	4081	823	0
1	B	4191	0	4087	811	0
1	C	4191	0	4085	859	0
2	A	182	0	169	93	0
2	B	182	0	169	92	0
2	C	182	0	169	91	0
3	A	28	0	24	9	0
3	B	28	0	24	9	0
3	C	28	0	24	8	0
4	A	12	0	0	0	0
4	B	12	0	0	0	0
4	C	12	0	0	0	0
All	All	13239	0	12832	2268	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 87.

The worst 5 of 2268 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:46:PRO:HB2	1:C:35:TYR:CE2	1.24	1.62
1:B:464:ILE:HD12	1:B:465:PRO:CD	1.30	1.58
1:C:464:ILE:HD12	1:C:465:PRO:CD	1.30	1.56
1:A:464:ILE:HD12	1:A:465:PRO:CD	1.30	1.55
1:A:87:PRO:CG	1:B:89:GLU:HB3	1.16	1.54

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	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	12
1	B	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	12
1	C	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	12
All	All	1614/2640 (61%)	1203 (74%)	276 (17%)	135 (8%)	2	12

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	PRO
1	A	155	PRO
1	A	235	ILE
1	A	347	ARG
1	A	363	GLN

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	480/779 (62%)	381 (79%)	99 (21%)	1	7
1	B	480/779 (62%)	381 (79%)	99 (21%)	1	7
1	C	480/779 (62%)	381 (79%)	99 (21%)	1	7
All	All	1440/2337 (62%)	1143 (79%)	297 (21%)	3	7

5 of 297 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	261	ILE
1	C	492	THR
1	C	284	THR
1	C	382	ASN
1	A	532	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	233	ASN
1	C	264	ASN
1	C	393	ASN
1	B	12	ASN
1	A	519	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 81 ligands modelled in this entry, 36 are monoatomic - leaving 45 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	C	808	1	14,14,15	0.65	0	17,19,21	0.68	0
2	NAG	A	903	1	14,14,15	0.53	0	17,19,21	0.76	0
2	NAG	A	809	1	14,14,15	0.72	0	17,19,21	0.92	0
2	NAG	B	803	1	14,14,15	0.96	1 (7%)	17,19,21	1.12	2 (11%)
2	NAG	C	805	1	14,14,15	0.71	0	17,19,21	1.04	1 (5%)
3	NDG	B	804	1	14,14,15	0.63	0	17,19,21	0.78	0
2	NAG	C	810	1	14,14,15	0.65	0	17,19,21	1.34	4 (23%)
2	NAG	A	803	1	14,14,15	0.96	1 (7%)	17,19,21	1.12	2 (11%)
2	NAG	A	904	1	14,14,15	0.72	1 (7%)	17,19,21	0.68	0
2	NAG	C	802	1	14,14,15	0.73	0	17,19,21	0.82	0
2	NAG	C	812	1	14,14,15	0.80	1 (7%)	17,19,21	0.73	1 (5%)
3	NDG	C	804	1	14,14,15	0.64	0	17,19,21	0.77	0
2	NAG	B	812	1	14,14,15	0.81	1 (7%)	17,19,21	0.73	1 (5%)
3	NDG	C	811	1	14,14,15	0.85	0	17,19,21	1.86	1 (5%)
2	NAG	A	801	1	14,14,15	0.68	0	17,19,21	0.94	1 (5%)
2	NAG	C	903	1	14,14,15	0.54	0	17,19,21	0.76	0
2	NAG	B	903	1	14,14,15	0.53	0	17,19,21	0.77	0
2	NAG	A	807	1	14,14,15	0.64	0	17,19,21	1.15	2 (11%)
2	NAG	C	806	1	14,14,15	0.56	0	17,19,21	1.33	2 (11%)
2	NAG	C	904	1	14,14,15	0.72	1 (7%)	17,19,21	0.68	0
2	NAG	A	902	1	14,14,15	1.07	1 (7%)	17,19,21	1.08	2 (11%)
2	NAG	A	805	1	14,14,15	0.71	0	17,19,21	1.04	1 (5%)
2	NAG	B	807	1	14,14,15	0.63	0	17,19,21	1.15	2 (11%)
2	NAG	B	802	1	14,14,15	0.73	0	17,19,21	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	902	1	14,14,15	1.06	1 (7%)	17,19,21	1.08	1 (5%)
2	NAG	C	809	1	14,14,15	0.74	0	17,19,21	0.93	0
2	NAG	B	801	1	14,14,15	0.68	0	17,19,21	0.95	1 (5%)
3	NDG	A	811	1	14,14,15	0.86	0	17,19,21	1.86	1 (5%)
2	NAG	B	810	1	14,14,15	0.65	0	17,19,21	1.34	4 (23%)
2	NAG	B	805	1	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
2	NAG	A	806	1	14,14,15	0.56	0	17,19,21	1.34	2 (11%)
2	NAG	C	801	1	14,14,15	0.68	0	17,19,21	0.95	0
2	NAG	C	803	1	14,14,15	0.97	1 (7%)	17,19,21	1.13	2 (11%)
2	NAG	A	802	1	14,14,15	0.73	0	17,19,21	0.82	0
3	NDG	B	811	1	14,14,15	0.85	0	17,19,21	1.87	1 (5%)
2	NAG	A	808	1	14,14,15	0.64	0	17,19,21	0.69	0
2	NAG	B	809	1	14,14,15	0.74	0	17,19,21	0.93	0
3	NDG	A	804	1	14,14,15	0.64	0	17,19,21	0.77	0
2	NAG	B	806	1	14,14,15	0.56	0	17,19,21	1.34	2 (11%)
2	NAG	B	808	1	14,14,15	0.66	0	17,19,21	0.69	0
2	NAG	B	904	1	14,14,15	0.72	1 (7%)	17,19,21	0.68	0
2	NAG	A	810	1	14,14,15	0.66	0	17,19,21	1.34	4 (23%)
2	NAG	C	807	1	14,14,15	0.63	0	17,19,21	1.15	2 (11%)
2	NAG	C	902	1	14,14,15	1.08	1 (7%)	17,19,21	1.08	2 (11%)
2	NAG	A	812	1	14,14,15	0.80	1 (7%)	17,19,21	0.73	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
2	NAG	C	808	1	-	3/6/23/26	0/1/1/1
2	NAG	A	903	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	809	1	-	2/6/23/26	0/1/1/1
2	NAG	B	803	1	-	2/6/23/26	0/1/1/1
2	NAG	C	805	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NDG	B	804	1	-	0/6/23/26	0/1/1/1
2	NAG	C	810	1	-	3/6/23/26	0/1/1/1
2	NAG	A	803	1	-	2/6/23/26	0/1/1/1
2	NAG	A	904	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	802	1	-	2/6/23/26	0/1/1/1
2	NAG	C	812	1	-	4/6/23/26	0/1/1/1
3	NDG	C	804	1	-	0/6/23/26	0/1/1/1
2	NAG	B	812	1	-	4/6/23/26	0/1/1/1
3	NDG	C	811	1	-	2/6/23/26	0/1/1/1
2	NAG	A	801	1	-	3/6/23/26	0/1/1/1
2	NAG	C	903	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	903	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	807	1	-	5/6/23/26	0/1/1/1
2	NAG	C	806	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	C	904	1	-	3/6/23/26	0/1/1/1
2	NAG	A	902	1	1/1/5/7	1/6/23/26	0/1/1/1
2	NAG	A	805	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	807	1	-	5/6/23/26	0/1/1/1
2	NAG	B	802	1	-	2/6/23/26	0/1/1/1
2	NAG	B	902	1	1/1/5/7	1/6/23/26	0/1/1/1
2	NAG	C	809	1	-	2/6/23/26	0/1/1/1
2	NAG	B	801	1	-	3/6/23/26	0/1/1/1
3	NDG	A	811	1	-	2/6/23/26	0/1/1/1
2	NAG	B	810	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	A	806	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	C	801	1	-	3/6/23/26	0/1/1/1
2	NAG	C	803	1	-	2/6/23/26	0/1/1/1
2	NAG	A	802	1	-	2/6/23/26	0/1/1/1
3	NDG	B	811	1	-	2/6/23/26	0/1/1/1
2	NAG	A	808	1	-	3/6/23/26	0/1/1/1
2	NAG	B	809	1	-	2/6/23/26	0/1/1/1
3	NDG	A	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	B	808	1	-	3/6/23/26	0/1/1/1
2	NAG	B	904	1	-	3/6/23/26	0/1/1/1
2	NAG	A	810	1	-	3/6/23/26	0/1/1/1
2	NAG	C	807	1	-	5/6/23/26	0/1/1/1
2	NAG	C	902	1	1/1/5/7	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	812	1	-	4/6/23/26	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	NAG	C1-C2	3.09	1.57	1.52
2	C	902	NAG	C1-C2	3.08	1.56	1.52
2	B	902	NAG	C1-C2	3.02	1.56	1.52
2	C	803	NAG	O5-C5	2.53	1.48	1.43
2	B	803	NAG	O5-C5	2.51	1.48	1.43

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	811	NDG	C2-N2-C7	-7.01	112.92	122.90
3	A	811	NDG	C2-N2-C7	-6.99	112.95	122.90
3	C	811	NDG	C2-N2-C7	-6.98	112.96	122.90
2	A	806	NAG	C2-N2-C7	-3.42	118.04	122.90
2	B	806	NAG	C2-N2-C7	-3.41	118.05	122.90

5 of 12 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

5 of 108 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	807	NAG	C3-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	902	NAG	C3-C2-N2-C7

There are no ring outliers.

39 monomers are involved in 302 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	808	NAG	2	0
2	A	809	NAG	8	0
2	B	803	NAG	4	0
2	C	805	NAG	7	0
3	B	804	NDG	2	0
2	C	810	NAG	13	0
2	A	803	NAG	4	0
2	A	904	NAG	8	0
2	C	812	NAG	3	0
3	C	804	NDG	2	0
2	B	812	NAG	3	0
3	C	811	NDG	6	0
2	A	801	NAG	21	0
2	A	807	NAG	17	0
2	C	806	NAG	12	0
2	C	904	NAG	7	0
2	A	902	NAG	8	0
2	A	805	NAG	7	0
2	B	807	NAG	16	0
2	B	902	NAG	8	0
2	C	809	NAG	8	0
2	B	801	NAG	21	0
3	A	811	NDG	7	0
2	B	810	NAG	13	0
2	B	805	NAG	7	0
2	A	806	NAG	12	0
2	C	801	NAG	20	0
2	C	803	NAG	4	0
3	B	811	NDG	7	0
2	A	808	NAG	2	0
2	B	809	NAG	8	0
3	A	804	NDG	2	0
2	B	806	NAG	12	0
2	B	808	NAG	2	0
2	B	904	NAG	8	0
2	A	810	NAG	13	0
2	C	807	NAG	17	0
2	C	902	NAG	8	0
2	A	812	NAG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

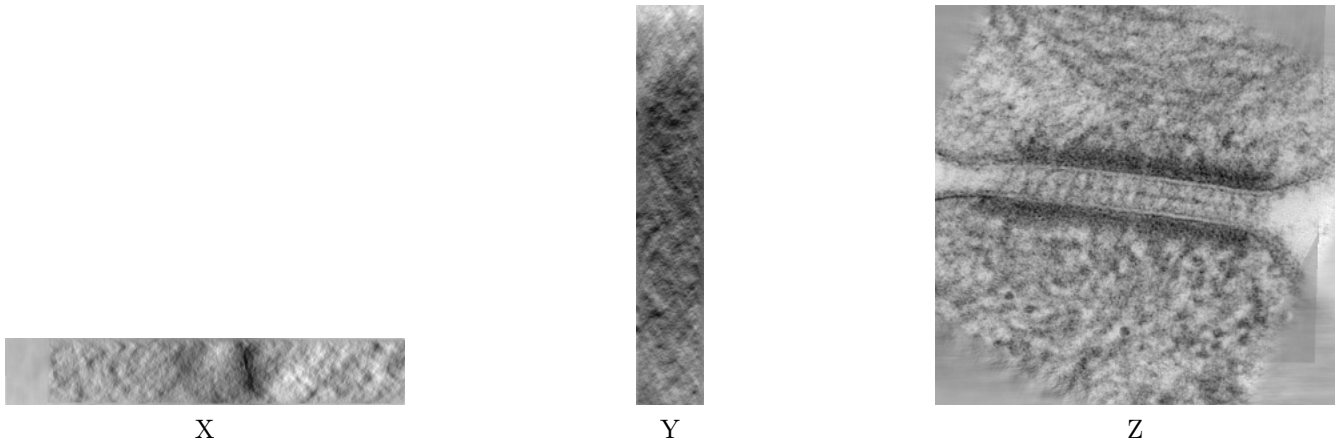
5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Tomogram visualisation [i](#)

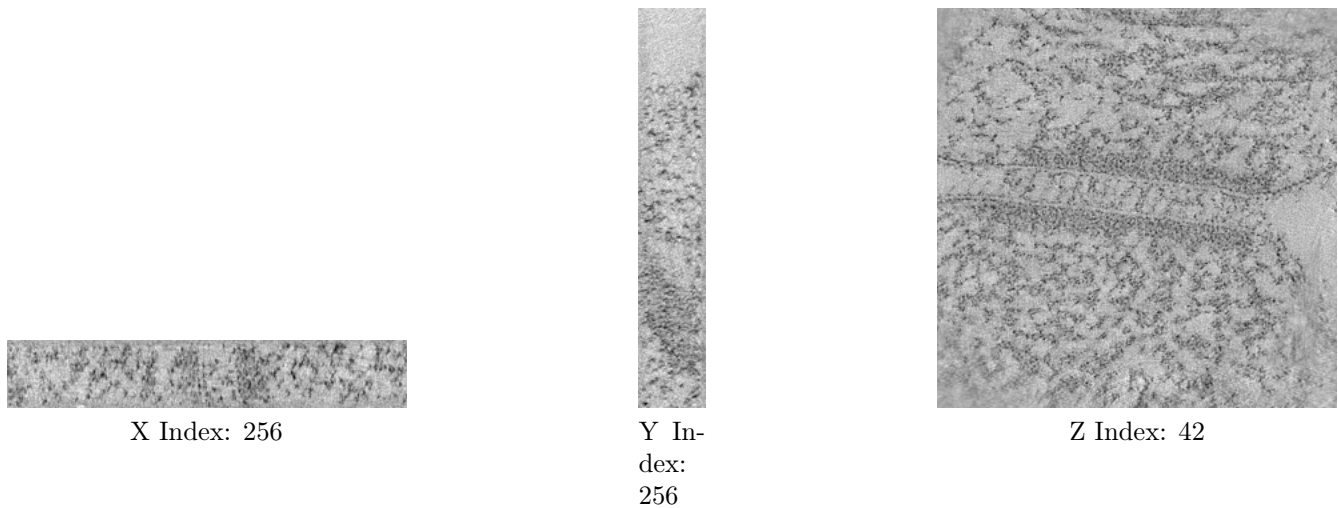
This section contains visualisations of the EMDB entry EMD-1052. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



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

6.2 Central slices [i](#)

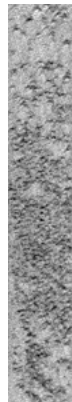


The images above show central slices of the tomogram in three orthogonal directions.

6.3 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.

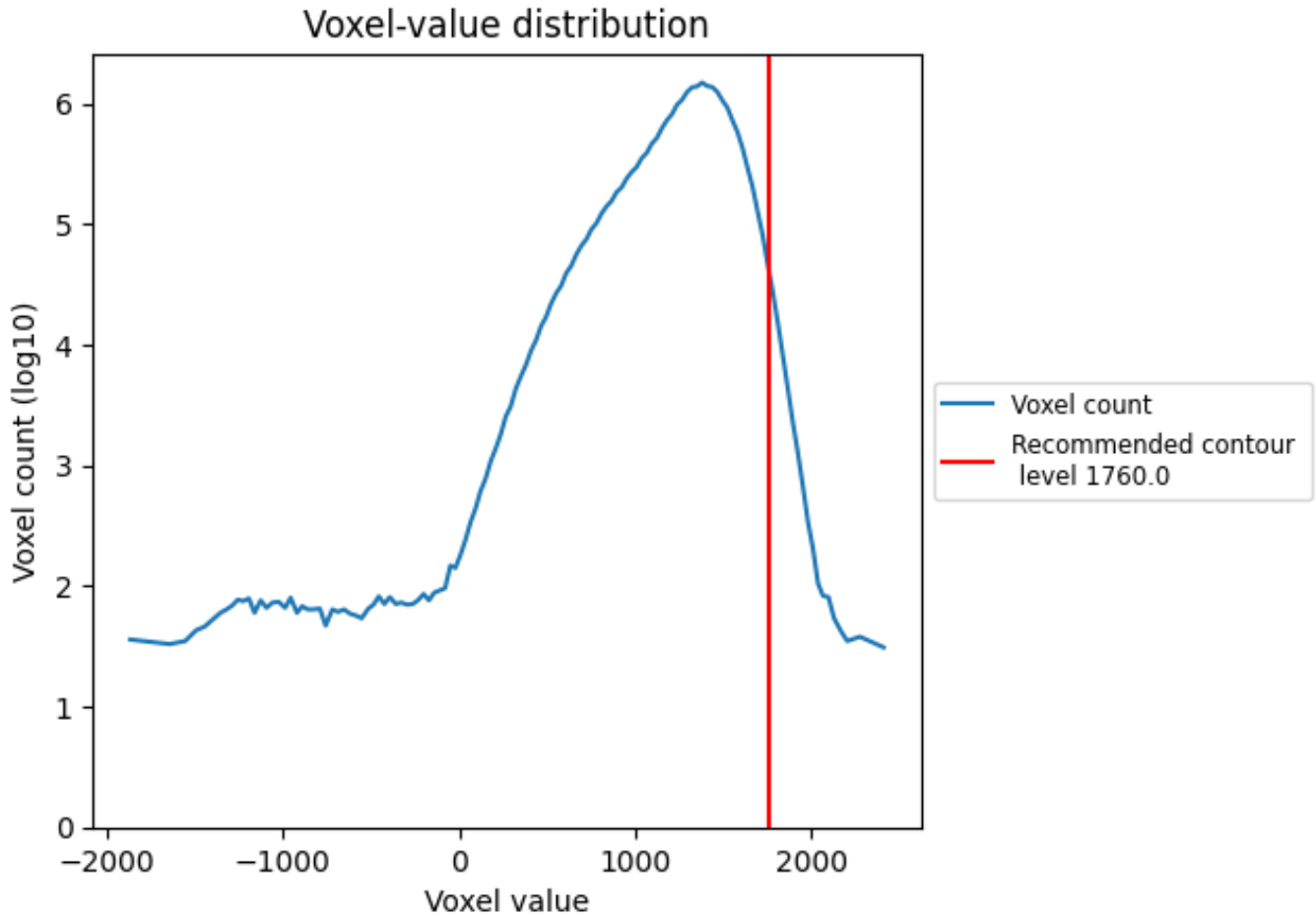
6.4 Mask visualisation [i](#)

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.

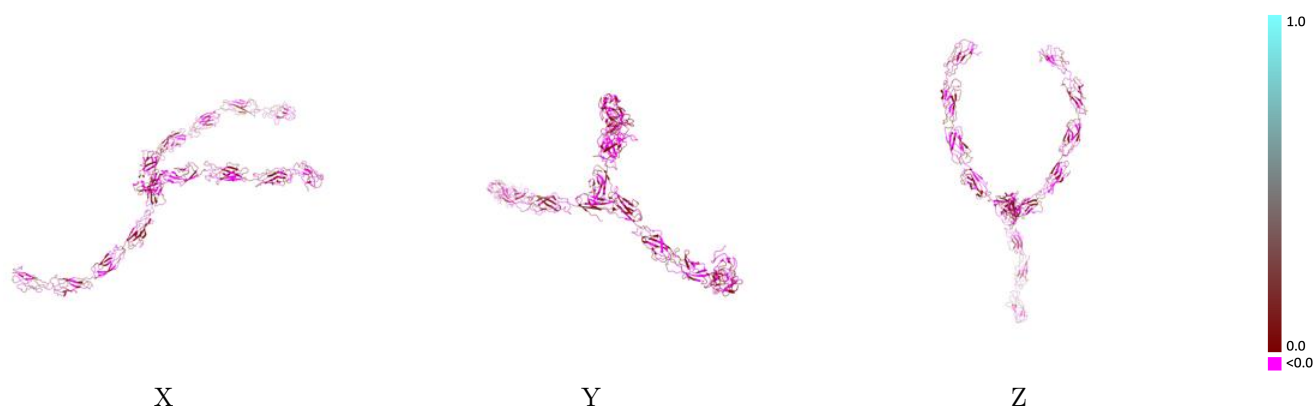
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1052 and PDB model 1Q5B. Per-residue inclusion information can be found in section 3 on page 8.

8.1 Map-model overlay [i](#)

This section was not generated.

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

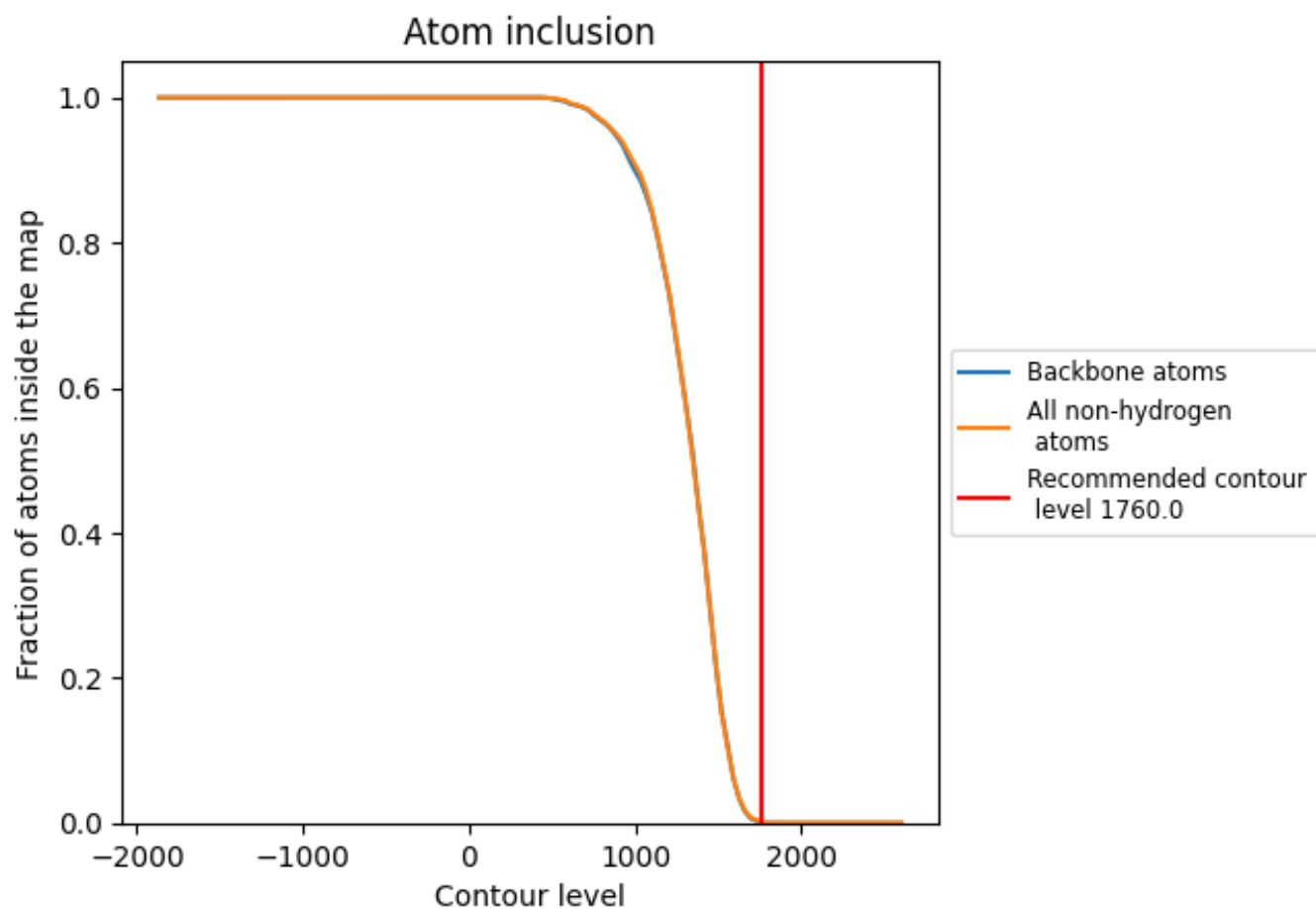


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [i](#)

This section was not generated.









8.4 Atom inclusion [i](#)



At the recommended contour level, 0% of all backbone atoms, 0% 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 (1760.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.0005	 0.0040
A	 0.0016	 0.0070
B	 0.0000	 0.0040
C	 0.0000	 0.0020

