



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 08:20 AM UTC

PDB ID : 1Q55 / pdb_00001q55
EMDB ID : EMD-1052
Title : W-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 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
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

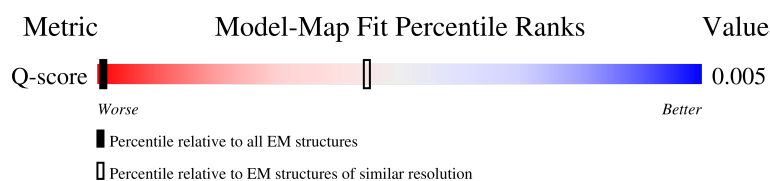
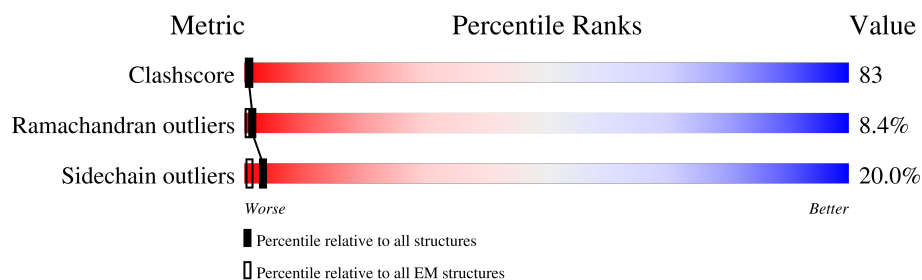
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9 (30.00 - 30.30)

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	
1	B	880	
1	C	880	
1	D	880	

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	-
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	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	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	D	801	-	-	X	-
2	NAG	D	805	X	-	X	-
2	NAG	D	806	X	-	X	-
2	NAG	D	807	-	-	X	-
2	NAG	D	809	-	-	X	-
2	NAG	D	810	-	-	X	-
2	NAG	D	902	X	-	X	-
2	NAG	D	903	X	-	-	-
3	NDG	A	811	-	-	X	-
3	NDG	B	811	-	-	X	-
3	NDG	C	811	-	-	X	-

2 Entry composition [i](#)

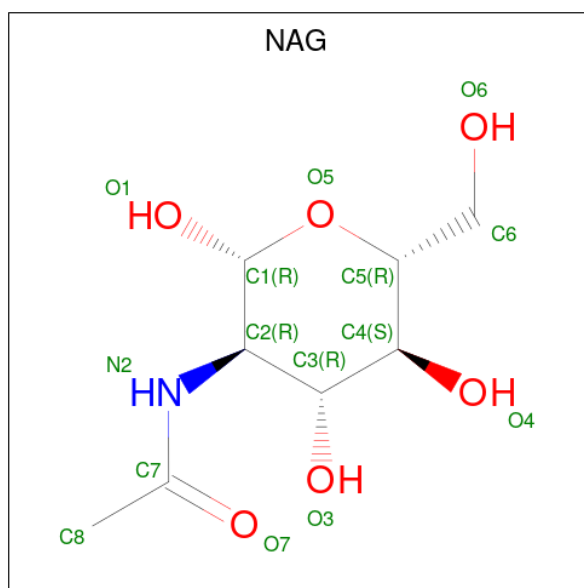
There are 4 unique types of molecules in this entry. The entry contains 17652 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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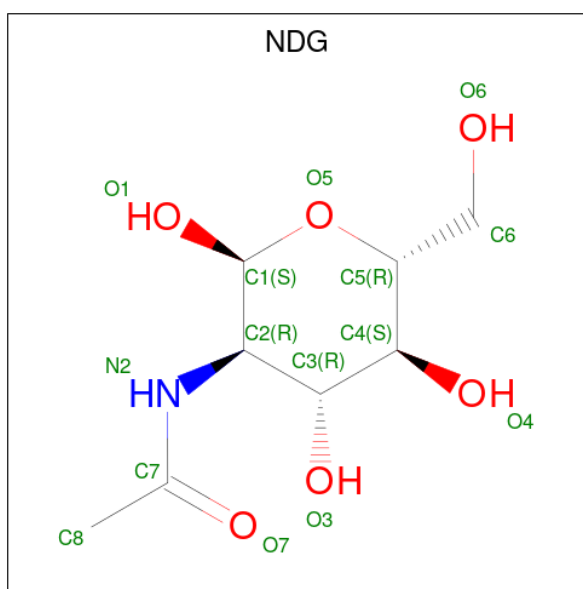
Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0
2	C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

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

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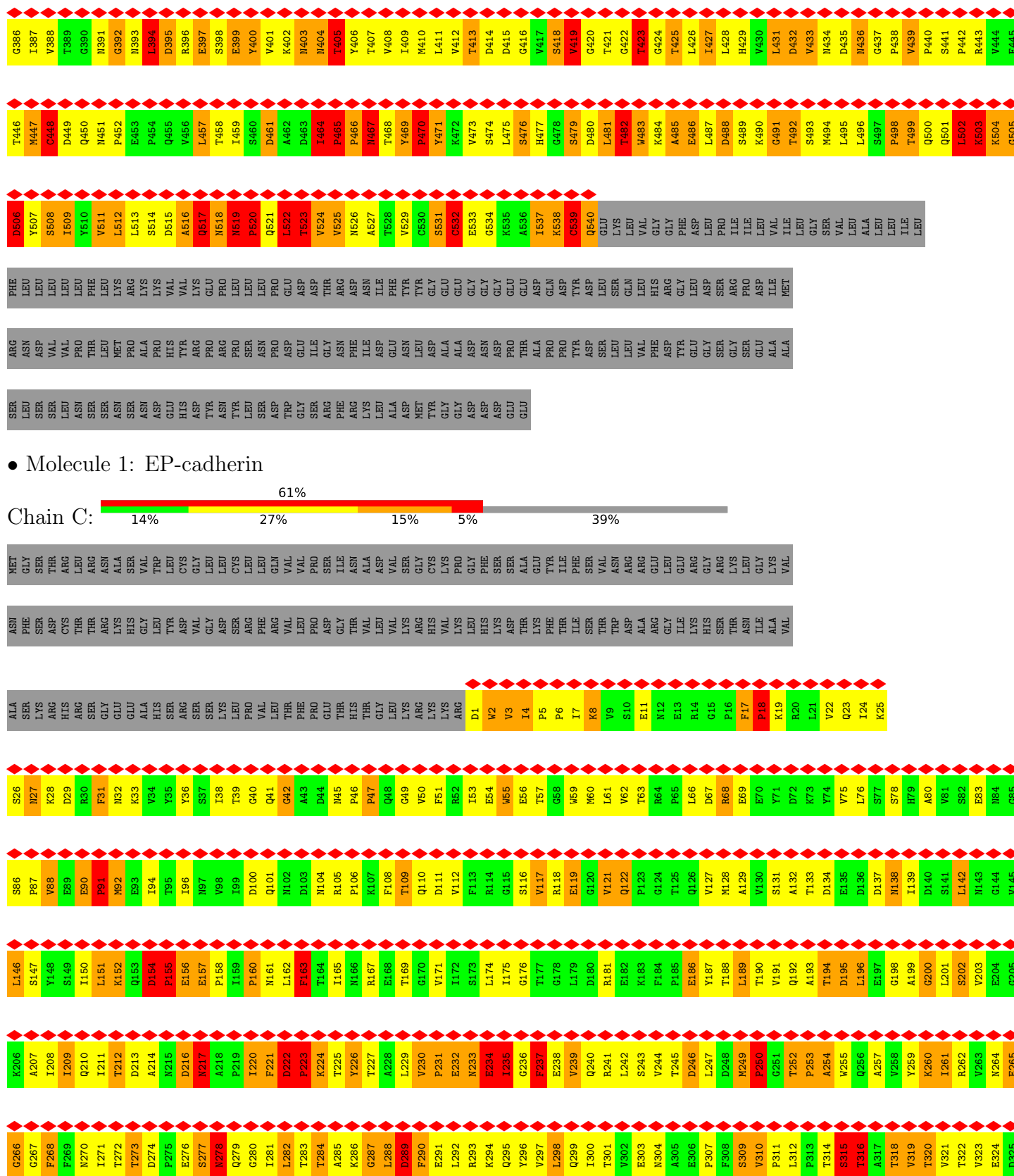
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Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

- 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	
4	C	12	Total	Ca	0
			12	12	
4	D	12	Total	Ca	0
			12	12	





• Molecule 1: EP-cadherin

SER	LEU	LEU	ASP	VAL	LEU	ASN	THR	SER	SER	ASN	ASN	ASN	ASP	GLU	HIS	GLU	HIS	ASP	ASP	TYR	ASN	ASN	TYR	SER	SER	ASN	ASP	TRP	ASP	GLY	GLY	SER	ARG	PHE	ASN	GLY	ASP	ALA	ALA	ASP	ASP	MET	LEU	TYR	GLY	GLY	ASP	ASP	ASP	GLU	GLU								
PHE	LEU	LEU	ASP	VAL	LEU	LEU	LEU	PHE	LEU	LEU	LEU	ARG	PRO	LYS	VAL	VAL	ASP	LYS	TYR	GLY	GLU	PRO	ASN	PRO	TYR	SER	ASN	ASP	PRO	ASP	GLY	GLY	THR	ASN	ASP	ASN	ASP	ASN	ASN	ASP	ASP	TYR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY								
D506	D507	S508	S509	S510	S511	S512	S513	S514	S515	S516	S517	S518	S519	S520	S521	S522	S523	S524	S525	S526	S527	S528	S529	S530	S531	S532	S533	S534	S535	S536	S537	S538	S539	S540	S541	S542	S543	S544	S545	S546	S547	S548	S549	S550	S551	S552	S553	S554											
T446	T447	C448	D449	Q450	M451	P452	E453	P454	Q455	V456	L457	T458	I459	S460	D461	L462	D463	I464	P465	P466	M467	T468	Y469	P470	L471	K472	V473	S474	L475	S476	H477	G478	S479	D480	L481	T482	M483	K484	L485	E486	L487	D488	S489	K490	G491	T492	S493	M494	L495	L496	S497	P498	T499	Q500	Q501	L502	K503	K504	C505
G386	T387	V388	T389	T390	N391	G392	N393	L394	D395	R396	E397	R398	E399	Y400	V401	K402	N403	N404	T405	Y406	T407	V408	I409	M410	L411	V412	T413	D414	D415	G416	V417	S418	V419	G420	T421	G422	T423	G424	T425	L426	I427	L428	H429	V430	L431	D432	V433	N434	D435	N436	G437	P438	V439	P440	S441	P442	R443	V444	E445
V326	N327	E328	A329	P330	F331	F332	F333	P334	A335	V336	S337	R338	V339	D340	V341	S342	E343	D344	L345	S346	R347	G348	E349	K350	L351	L352	S353	L354	V355	A356	Q357	D358	P359	D360	K361	Q362	Q363	L364	Q365	K366	L367	S368	Y369	F370	L371	G372	N373	D374	P375	A376	R377	W378	L379	T380	V381	N382	K383	D384	N385
G266	G267	F268	F269	N270	I271	T272	T273	D274	P275	E276	S277	N278	Q279	G280	I281	L282	T283	T284	A285	K286	G287	L288	D289	F290	E291	L292	K294	Q295	Y296	V297	L298	Q299	I300	T301	V302	E303	N304	A305	E306	P307	F308	S309	V310	P311	L312	P313	T314	S315	T316	A317	T318	V319	V320	V321	T322	V323	E324	N325	

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/UT	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	6038.000	Depositor
Minimum voxel value	-5609.000	Depositor
Average voxel value	1381.050	Depositor
Voxel value standard deviation	380.764	Depositor
Recommended contour level	1950	Depositor
Tomogram size ($\text{\AA}$)	4765.7, 4765.7, 484.016	wwPDB
Tomogram dimensions	512, 512, 52	wwPDB
Tomogram angles ($^\circ$)	90, 90, 90	wwPDB
Grid spacing ($\text{\AA}$)	9.308, 9.308, 9.308	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: NAG, NDG, 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	0.99	24/4276 (0.6%)	2.02	203/5839 (3.5%)
1	B	0.99	24/4276 (0.6%)	2.02	204/5839 (3.5%)
1	C	0.99	24/4276 (0.6%)	2.02	202/5839 (3.5%)
1	D	0.99	24/4276 (0.6%)	2.02	202/5839 (3.5%)
All	All	0.99	96/17104 (0.6%)	2.02	811/23356 (3.5%)

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	4
1	B	0	4
1	C	0	4
1	D	0	4
All	All	0	16

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	522	LEU	N-CA	-18.92	1.34	1.46
1	C	522	LEU	N-CA	-18.91	1.34	1.46
1	D	522	LEU	N-CA	-18.89	1.34	1.46
1	B	522	LEU	N-CA	-18.81	1.34	1.46
1	A	465	PRO	CA-C	12.07	1.58	1.51

The worst 5 of 811 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	290	PHE	N-CA-C	25.20	145.40	108.60
1	A	290	PHE	N-CA-C	25.19	145.38	108.60
1	D	290	PHE	N-CA-C	25.19	145.38	108.60
1	B	290	PHE	N-CA-C	25.17	145.35	108.60
1	A	516	ALA	N-CA-C	-20.89	88.42	114.75

There are no chirality outliers.

5 of 16 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

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	4086	777	0
1	B	4191	0	4089	770	0
1	C	4191	0	4087	743	0
1	D	4191	0	4086	733	0
2	A	182	0	169	87	0
2	B	182	0	169	88	0
2	C	182	0	169	87	0
2	D	182	0	169	88	0
3	A	28	0	24	9	0
3	B	28	0	24	9	0
3	C	28	0	24	9	0
3	D	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
4	D	12	0	0	0	0
All	All	17652	0	17120	2897	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 83.

The worst 5 of 2897 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:464:ILE:HD12	1:B:465:PRO:CD	1.30	1.61
1:D:464:ILE:HD12	1:D:465:PRO:CD	1.30	1.59
1:A:464:ILE:HD12	1:A:465:PRO:CD	1.30	1.56
1:C:464:ILE:HD12	1:C:465:PRO:CD	1.30	1.56
1:D:464:ILE:CD1	1:D:465:PRO:HD2	1.50	1.42

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%)	0	9
1	B	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	0	9
1	C	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	0	9
1	D	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	0	9
All	All	2152/3520 (61%)	1604 (74%)	368 (17%)	180 (8%)	1	9

5 of 180 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%)	384 (80%)	96 (20%)	1	7
1	B	480/779 (62%)	384 (80%)	96 (20%)	1	7
1	C	480/779 (62%)	384 (80%)	96 (20%)	1	7
1	D	480/779 (62%)	384 (80%)	96 (20%)	1	7
All	All	1920/3116 (62%)	1536 (80%)	384 (20%)	3	7

5 of 384 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	278	ASN
1	C	539	CYS
1	C	310	VAL
1	C	405	THR
1	D	121	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	240	GLN
1	D	32	ASN
1	C	278	ASN
1	C	455	GLN
1	D	110	GLN

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 108 ligands modelled in this entry, 48 are monoatomic - leaving 60 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	810	1	14,14,15	0.65	0	17,19,21	1.33	4 (23%)
2	NAG	A	805	1	14,14,15	0.72	0	17,19,21	1.05	1 (5%)
2	NAG	C	802	1	14,14,15	0.77	1 (7%)	17,19,21	0.85	0
2	NAG	C	902	1	14,14,15	1.14	1 (7%)	17,19,21	1.09	2 (11%)
2	NAG	D	805	1	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
2	NAG	A	808	1	14,14,15	0.66	0	17,19,21	0.70	0
2	NAG	A	810	1	14,14,15	0.67	0	17,19,21	1.34	4 (23%)
2	NAG	C	903	1	14,14,15	0.55	0	17,19,21	0.78	0
2	NAG	D	801	1	14,14,15	0.72	0	17,19,21	0.98	1 (5%)
2	NAG	A	904	1	14,14,15	0.77	1 (7%)	17,19,21	0.70	1 (5%)
2	NAG	B	904	1	14,14,15	0.77	1 (7%)	17,19,21	0.69	1 (5%)
2	NAG	B	802	1	14,14,15	0.78	1 (7%)	17,19,21	0.85	0
2	NAG	C	808	1	14,14,15	0.66	0	17,19,21	0.69	0
2	NAG	B	903	1	14,14,15	0.55	0	17,19,21	0.79	0
3	NDG	D	804	1	14,14,15	0.66	0	17,19,21	0.78	0
2	NAG	A	802	1	14,14,15	0.78	1 (7%)	17,19,21	0.85	0
2	NAG	C	904	1	14,14,15	0.79	1 (7%)	17,19,21	0.70	1 (5%)
3	NDG	C	811	1	14,14,15	0.87	0	17,19,21	1.95	1 (5%)
2	NAG	A	902	1	14,14,15	1.14	1 (7%)	17,19,21	1.09	1 (5%)
2	NAG	D	812	1	14,14,15	0.84	1 (7%)	17,19,21	0.76	1 (5%)
3	NDG	A	804	1	14,14,15	0.65	0	17,19,21	0.78	0
2	NAG	A	803	1	14,14,15	0.99	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	A	809	1	14,14,15	0.77	1 (7%)	17,19,21	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	806	1	14,14,15	0.56	0	17,19,21	1.38	3 (17%)
2	NAG	B	809	1	14,14,15	0.78	1 (7%)	17,19,21	0.94	0
2	NAG	B	806	1	14,14,15	0.57	0	17,19,21	1.39	3 (17%)
2	NAG	A	807	1	14,14,15	0.64	0	17,19,21	1.19	2 (11%)
3	NDG	A	811	1	14,14,15	0.87	0	17,19,21	1.96	1 (5%)
2	NAG	B	807	1	14,14,15	0.64	0	17,19,21	1.19	2 (11%)
2	NAG	D	808	1	14,14,15	0.66	0	17,19,21	0.69	0
2	NAG	D	810	1	14,14,15	0.66	0	17,19,21	1.33	4 (23%)
2	NAG	D	904	1	14,14,15	0.77	1 (7%)	17,19,21	0.70	1 (5%)
2	NAG	B	801	1	14,14,15	0.69	0	17,19,21	0.98	1 (5%)
2	NAG	C	806	1	14,14,15	0.57	0	17,19,21	1.39	3 (17%)
2	NAG	B	902	1	14,14,15	1.13	1 (7%)	17,19,21	1.09	1 (5%)
2	NAG	D	802	1	14,14,15	0.77	1 (7%)	17,19,21	0.85	0
2	NAG	B	810	1	14,14,15	0.66	0	17,19,21	1.33	4 (23%)
2	NAG	C	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.16	2 (11%)
2	NAG	D	902	1	14,14,15	1.14	1 (7%)	17,19,21	1.09	2 (11%)
2	NAG	A	801	1	14,14,15	0.70	0	17,19,21	0.98	1 (5%)
2	NAG	C	807	1	14,14,15	0.64	0	17,19,21	1.20	2 (11%)
2	NAG	B	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	D	903	1	14,14,15	0.55	0	17,19,21	0.78	0
2	NAG	C	801	1	14,14,15	0.71	0	17,19,21	0.98	1 (5%)
3	NDG	C	804	1	14,14,15	0.64	0	17,19,21	0.78	0
3	NDG	D	811	1	14,14,15	0.87	0	17,19,21	1.96	1 (5%)
2	NAG	D	809	1	14,14,15	0.77	1 (7%)	17,19,21	0.94	0
2	NAG	C	809	1	14,14,15	0.77	1 (7%)	17,19,21	0.94	0
2	NAG	C	812	1	14,14,15	0.83	1 (7%)	17,19,21	0.76	1 (5%)
2	NAG	D	807	1	14,14,15	0.64	0	17,19,21	1.19	2 (11%)
3	NDG	B	804	1	14,14,15	0.65	0	17,19,21	0.77	0
2	NAG	A	903	1	14,14,15	0.55	0	17,19,21	0.79	0
2	NAG	B	812	1	14,14,15	0.83	1 (7%)	17,19,21	0.76	1 (5%)
3	NDG	B	811	1	14,14,15	0.87	0	17,19,21	1.97	1 (5%)
2	NAG	C	805	1	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
2	NAG	A	812	1	14,14,15	0.84	1 (7%)	17,19,21	0.74	1 (5%)
2	NAG	D	806	1	14,14,15	0.56	0	17,19,21	1.39	3 (17%)
2	NAG	D	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.16	2 (11%)
2	NAG	B	808	1	14,14,15	0.67	0	17,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	805	1	14,14,15	0.72	0	17,19,21	1.05	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	902	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	805	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	C	802	1	-	2/6/23/26	0/1/1/1
2	NAG	C	810	1	-	3/6/23/26	0/1/1/1
2	NAG	D	805	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	808	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	A	810	1	-	3/6/23/26	0/1/1/1
2	NAG	D	801	1	-	4/6/23/26	0/1/1/1
2	NAG	A	904	1	-	3/6/23/26	0/1/1/1
2	NAG	B	904	1	-	3/6/23/26	0/1/1/1
2	NAG	B	802	1	-	2/6/23/26	0/1/1/1
2	NAG	C	808	1	-	3/6/23/26	0/1/1/1
2	NAG	B	903	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NDG	D	804	1	-	0/6/23/26	0/1/1/1
2	NAG	A	802	1	-	2/6/23/26	0/1/1/1
2	NAG	C	904	1	-	3/6/23/26	0/1/1/1
3	NDG	C	811	1	-	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	D	812	1	-	4/6/23/26	0/1/1/1
3	NDG	A	804	1	-	0/6/23/26	0/1/1/1
2	NAG	A	803	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	806	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	806	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
3	NDG	A	811	1	-	2/6/23/26	0/1/1/1

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	NAG	C1-C2	3.42	1.57	1.52
2	C	902	NAG	C1-C2	3.41	1.57	1.52
2	D	902	NAG	C1-C2	3.40	1.57	1.52
2	B	902	NAG	C1-C2	3.35	1.56	1.52
2	C	803	NAG	O5-C5	2.68	1.48	1.43

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	811	NDG	C2-N2-C7	-7.46	112.91	122.90
3	D	811	NDG	C2-N2-C7	-7.43	112.94	122.90
3	A	811	NDG	C2-N2-C7	-7.43	112.95	122.90
3	C	811	NDG	C2-N2-C7	-7.40	112.99	122.90
2	C	806	NAG	C2-N2-C7	-3.63	118.03	122.90

5 of 16 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 152 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

There are no ring outliers.

52 monomers are involved in 385 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	810	NAG	12	0
2	A	805	NAG	7	0
2	C	902	NAG	7	0
2	D	805	NAG	7	0
2	A	808	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	810	NAG	12	0
2	D	801	NAG	22	0
2	A	904	NAG	6	0
2	B	904	NAG	6	0
2	C	808	NAG	2	0
3	D	804	NDG	2	0
2	C	904	NAG	6	0
3	C	811	NDG	7	0
2	A	902	NAG	7	0
2	D	812	NAG	3	0
3	A	804	NDG	2	0
2	A	803	NAG	4	0
2	A	809	NAG	8	0
2	A	806	NAG	11	0
2	B	809	NAG	8	0
2	B	806	NAG	11	0
2	A	807	NAG	16	0
3	A	811	NDG	7	0
2	B	807	NAG	16	0
2	D	808	NAG	2	0
2	D	810	NAG	12	0
2	D	904	NAG	6	0
2	B	801	NAG	22	0
2	C	806	NAG	12	0
2	B	902	NAG	7	0
2	B	810	NAG	12	0
2	C	803	NAG	4	0
2	D	902	NAG	7	0
2	A	801	NAG	22	0
2	C	807	NAG	15	0
2	B	803	NAG	4	0
2	C	801	NAG	22	0
3	C	804	NDG	2	0
3	D	811	NDG	6	0
2	D	809	NAG	8	0
2	C	809	NAG	8	0
2	C	812	NAG	2	0
2	D	807	NAG	15	0
3	B	804	NDG	2	0
2	B	812	NAG	3	0
3	B	811	NDG	7	0
2	C	805	NAG	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	812	NAG	2	0
2	D	806	NAG	12	0
2	D	803	NAG	4	0
2	B	808	NAG	2	0
2	B	805	NAG	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

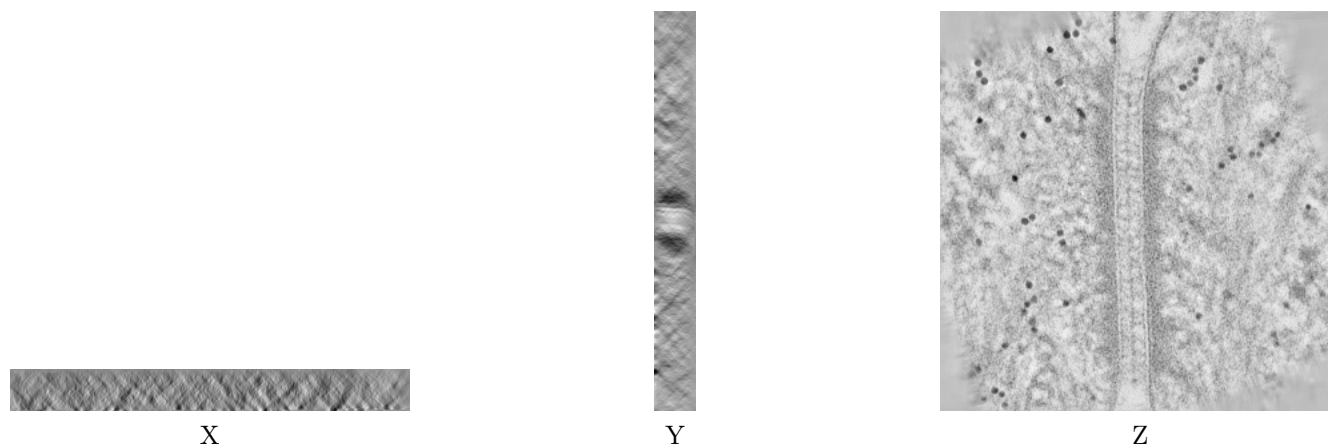
5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Tomogram visualisation [i](#)

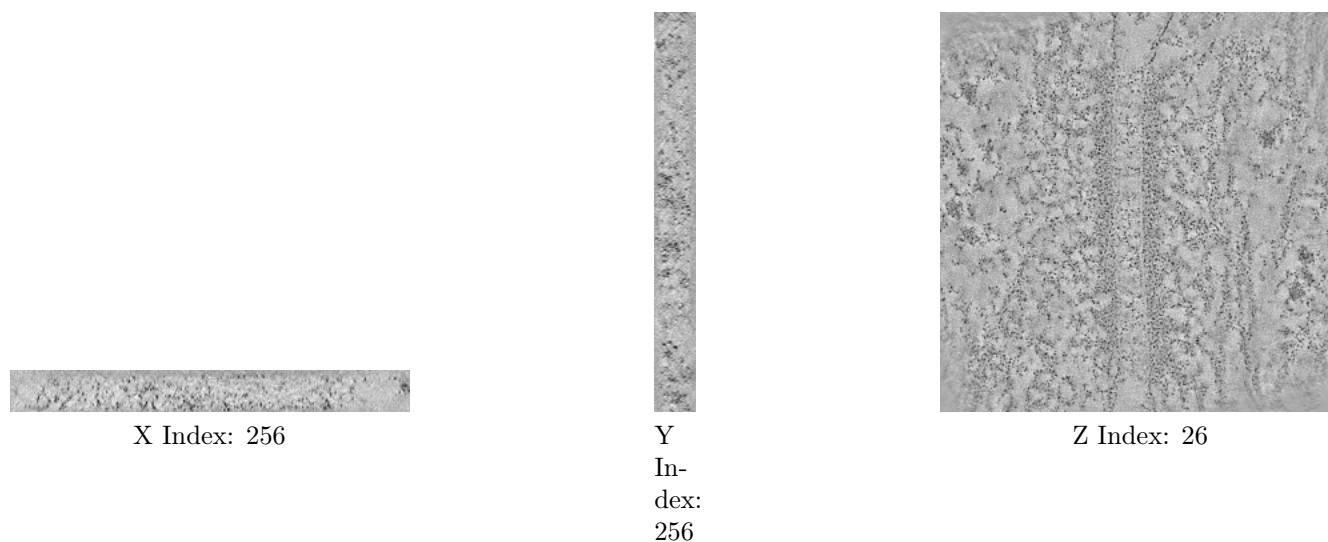
This section contains visualisations of the EMDB entry EMD-1052. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



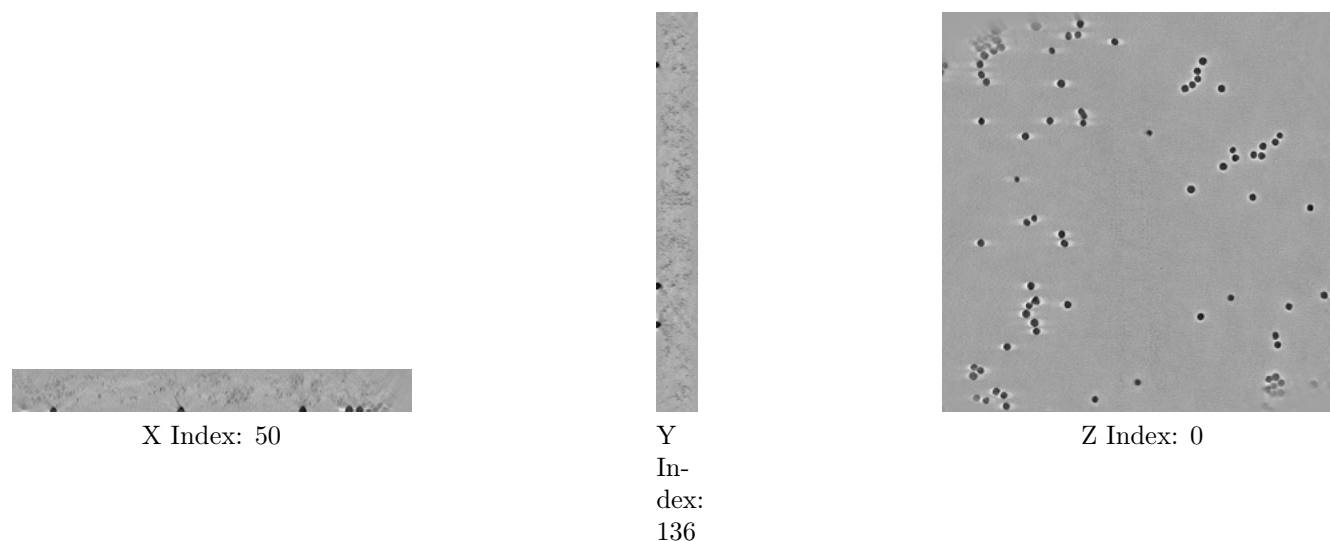
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)



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

6.3 Largest variance slices [i](#)



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

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



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

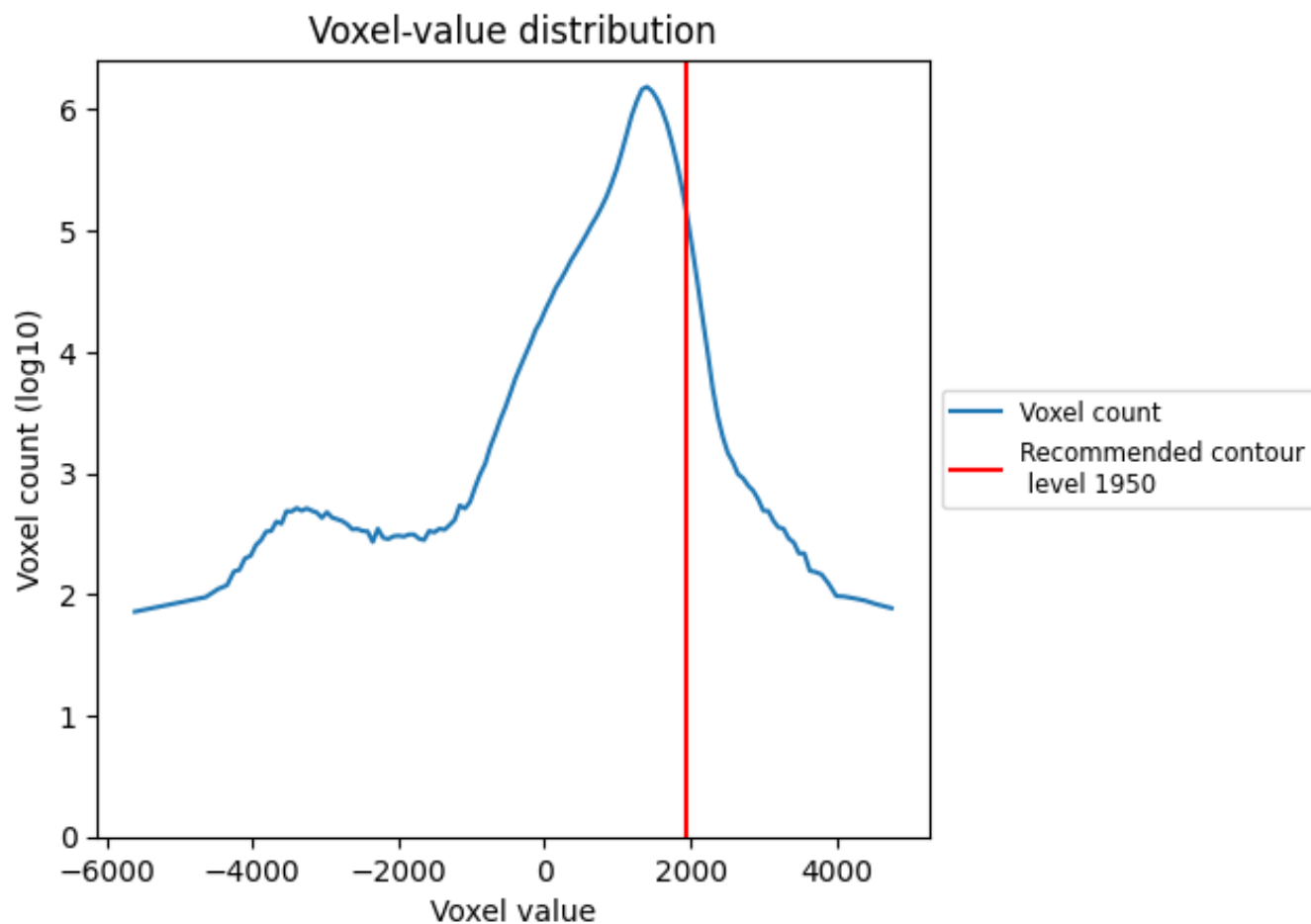
6.5 Mask visualisation [i](#)

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.

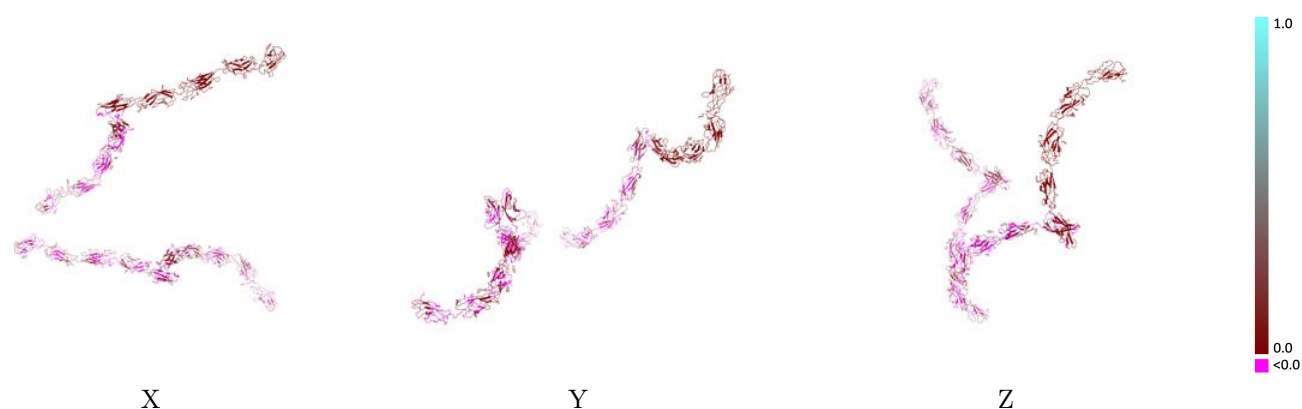
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1052 and PDB model 1Q55. Per-residue inclusion information can be found in section 3 on page 9.

8.1 Map-model overlay [i](#)

This section was not generated.

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

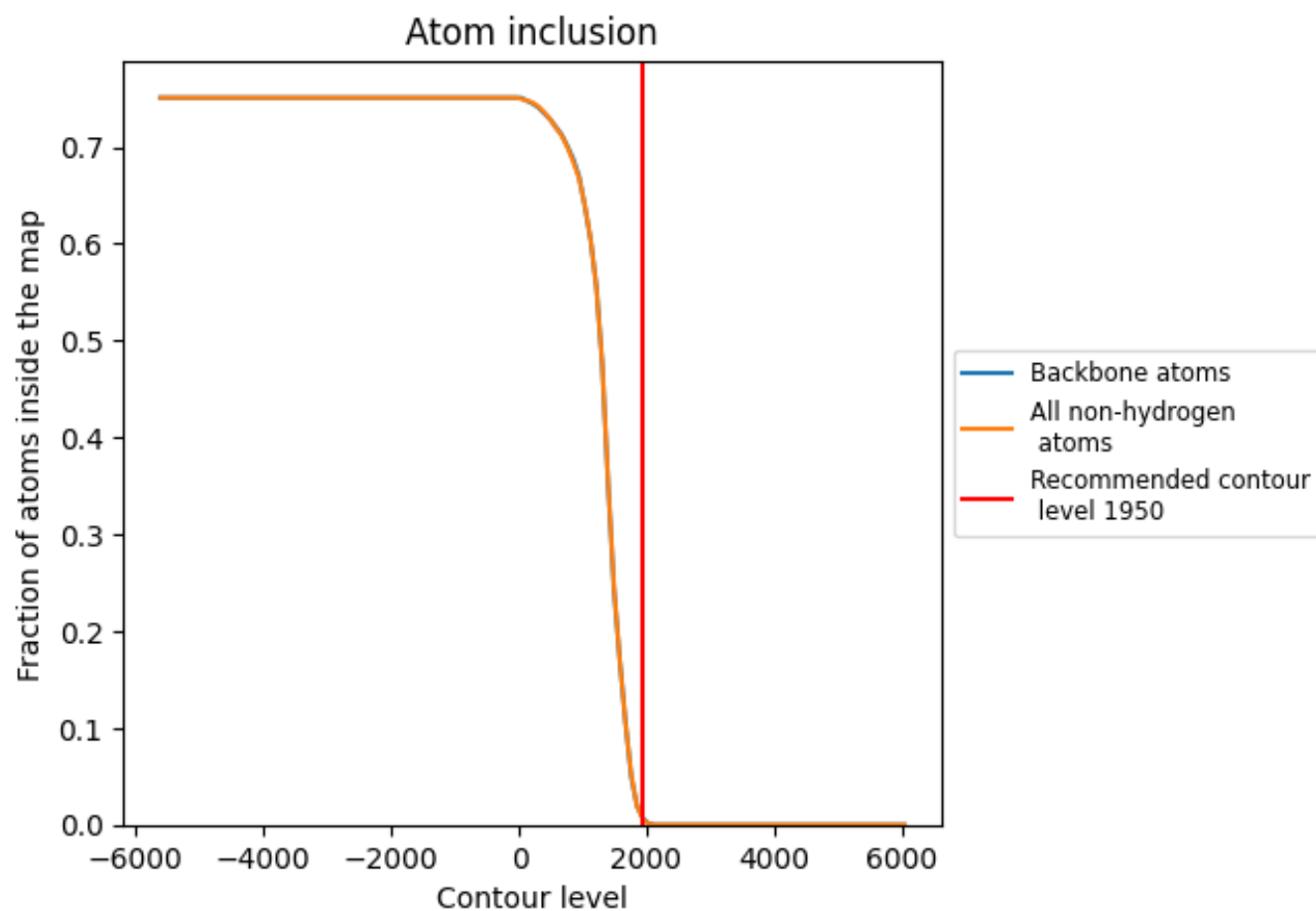


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

8.4 Atom inclusion [i](#)



At the recommended contour level, 1% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1950) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0050	0.0050
A	0.0130	0.0190
B	0.0010	-0.0010
C	0.0040	0.0010
D	0.0000	-0.0010

