



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 08:58 AM UTC

PDB ID : 1Q5C / pdb_00001q5c
EMDB ID : EMD-1052
Title : S-S-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.

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

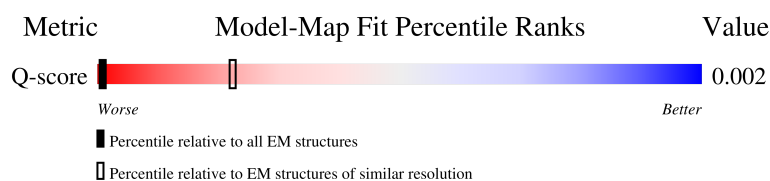
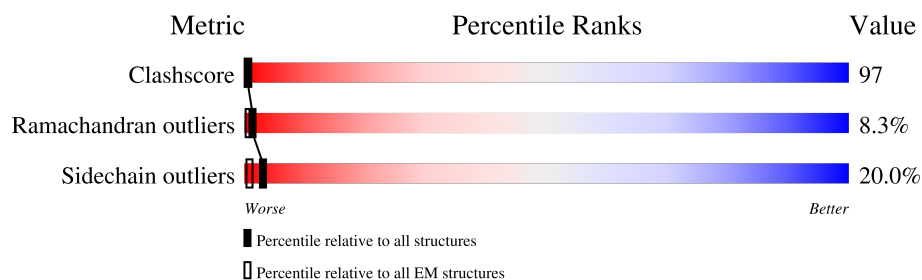
1 Overall quality at a glance i

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	60% 14% 28% 14% 5% 39%
1	B	880	61% 14% 28% 15% 5% 39%
1	C	880	61% 13% 28% 15% 5% 39%
1	D	880	60% 13% 29% 15% 5% 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	-
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	-	-	-
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	D	811	-	-	X	-

2 Entry composition [i](#)

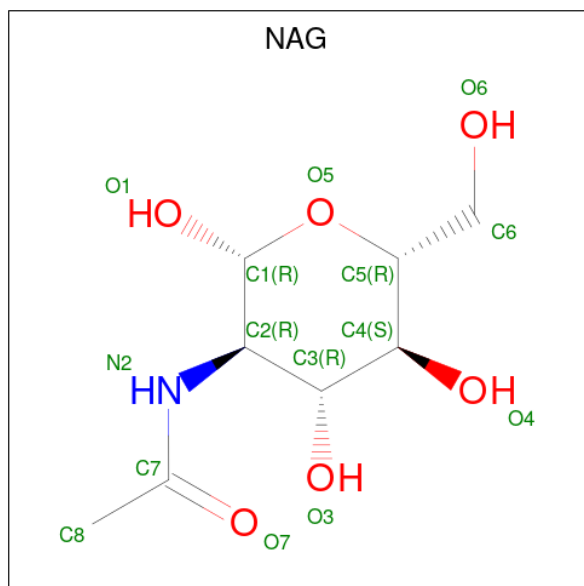
There are 4 unique types of molecules in this entry. The entry contains 17652 atoms, of which 0 are hydrogens and 0 are deuteriums.

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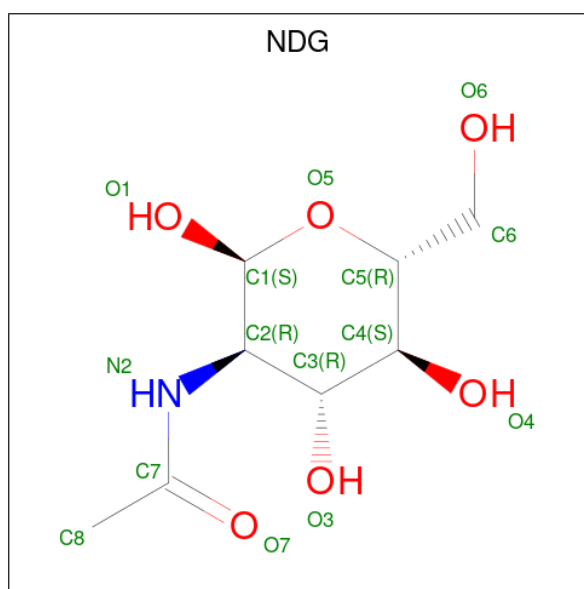
Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2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

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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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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	

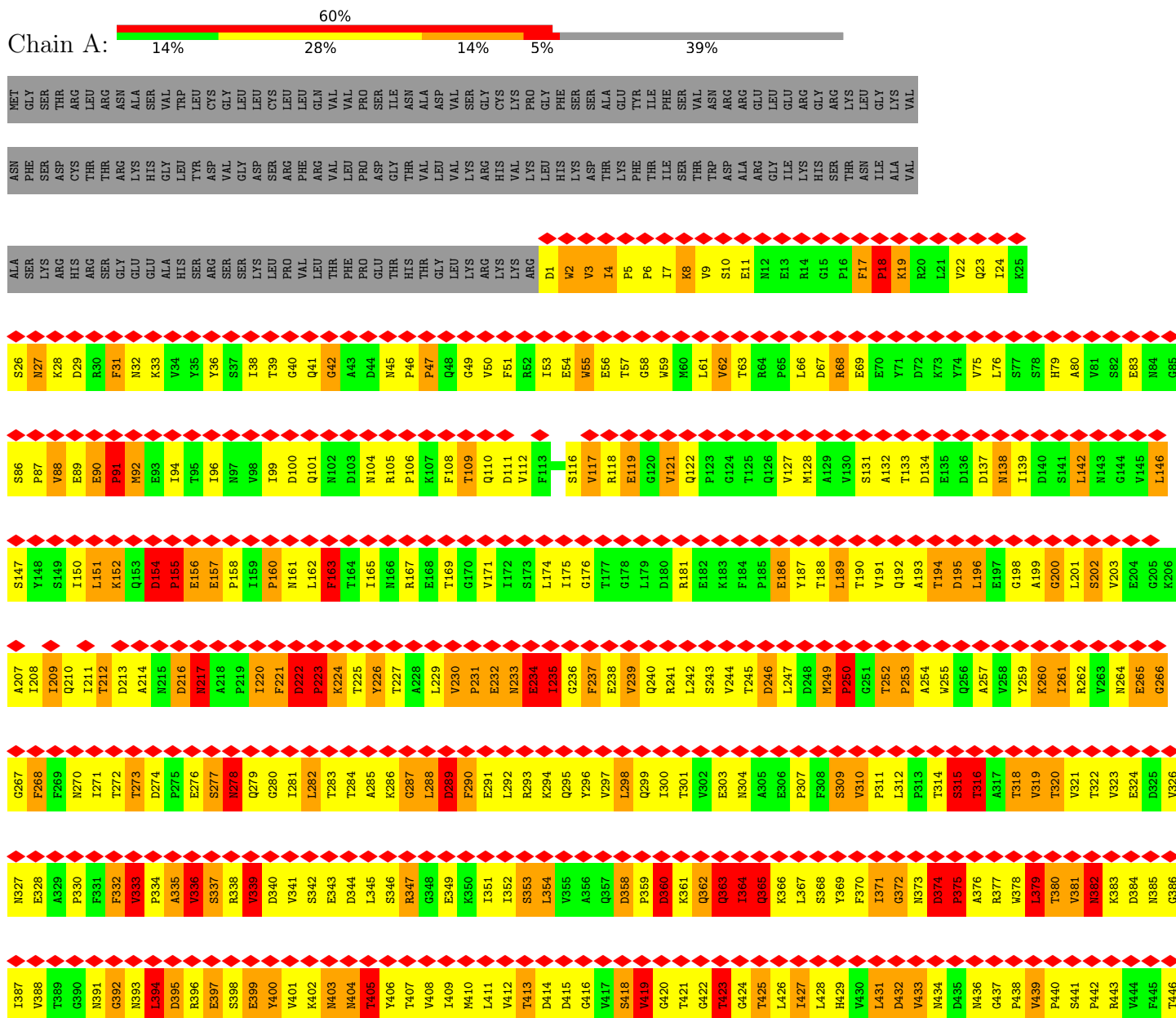
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

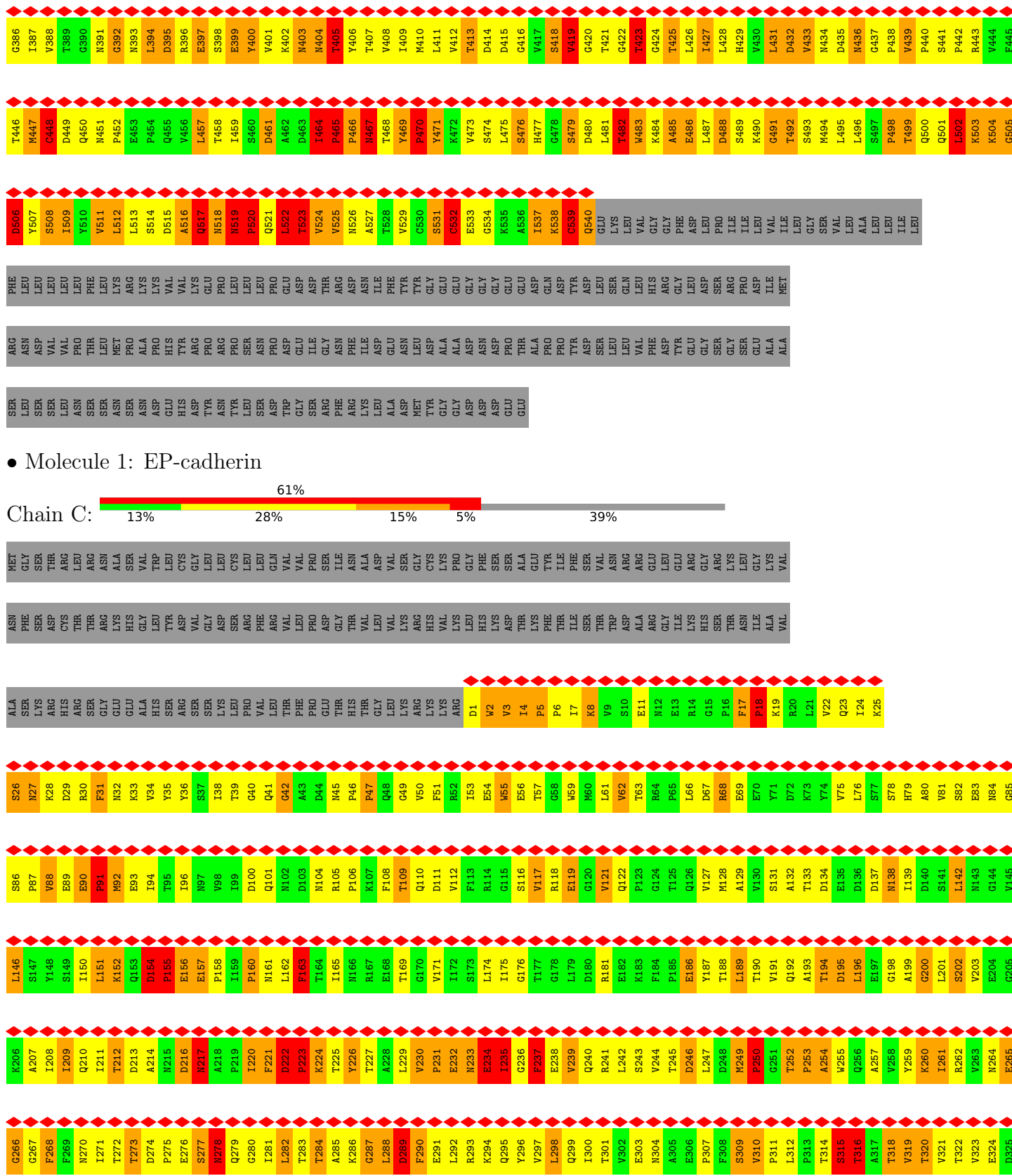
Mol	Chain	Residues	Atoms		AltConf
4	A	12	Total	Ca	0
			12	12	
4	B	12	Total	Ca	0
			12	12	
4	C	12	Total	Ca	0
			12	12	
4	D	12	Total	Ca	0
			12	12	

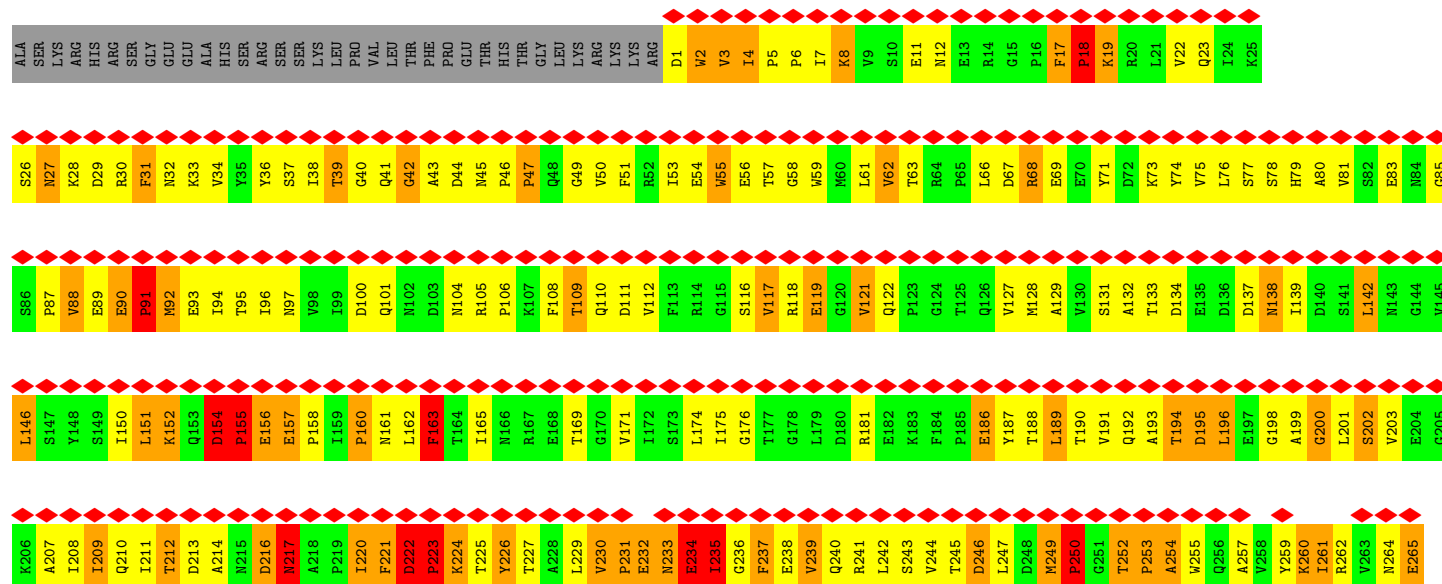
3 Residue-property plots

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: EP-cadherin







SER	ARG	PHE	D506	T446	G386	V326	G266
LEU	ASN	LEU	Y507	M447	1387	N327	G267
SER	ASP	LEU	S508	C448	V388	E328	F268
VAL	VAL	LEU	S508	D449	T389	A329	F269
LEU	PRO	LEU	Y510	Q450	F331	P330	N270
SER	THR	PHE	Y511	M451	N391	F332	I271
SER	LEU	LEU	S512	P452	G392	V333	T272
ASN	MET	LEU	S513	P452	G392	V333	T273
SER	PRO	ARG	S513	E453	N393	P334	T273
ASN	ALA	LYS	S514	P454	L394	A335	D274
ASP	PRO	LYS	D515	Q455	D395	V336	P275
GLU	HIS	VAL	D515	Q455	D395	V336	E276
HIS	TYR	VAL	A516	V456	R396	S337	E276
ASP	ARG	LYS	Q517	L457	E397	R338	S277
ASP	TYR	GLU	Q518	T457	E397	R338	S277
ASN	ARG	PRO	N518	T458	R398	V339	N278
PRO	PRO	LEU	N519	I459	E399	D340	Q279
SER	SER	LEU	F520	S460	Y400	D340	Q280
ASN	ASN	LEU	Q521	D461	V401	V341	V341
PRO	PRO	PRO	L522	D462	K402	S342	S342
TRP	ASP	GLU	L522	D462	K402	S342	L282
GLY	GLU	ASP	T523	D463	N403	D344	T283
SER	ILE	ASP	V524	I464	N404	L345	T284
ARG	GLY	THR	V525	P465	T405	S346	A285
PHE	ASN	ARG	N526	P466	Y406	S346	A285
ARG	PHE	ASP	N526	P466	Y406	R347	K286
ILE	ILE	ASN	A527	M467	T407	G348	G287
LEU	ASP	ILE	A527	M467	T407	G348	G287
ALA	GLU	PHE	T528	T468	V408	E349	L288
ASP	ASN	TYR	V529	Y469	T409	K350	D289
LEU	LEU	TYR	F530	P470	M410	I351	F290
MET	ASN	GLY	S531	Y471	L411	T352	E291
TYR	ASP	GLY	S531	Y471	L411	T352	E291
GLY	ALA	GLU	C532	K472	V412	S353	L292
ASP	GLY	GLY	E533	V473	T413	L354	R293
ASN	ASN	GLY	E534	S474	D414	V355	K294
ASP	ASP	GLY	K535	L475	D415	A356	Q295
PRO	PRO	GLU	K535	L475	D415	A356	Q295
GLU	THR	GLU	A536	S476	G416	Q357	Y296
ALA	ALA	ASP	I537	H477	V417	D358	Y297
PRO	PRO	GLN	I537	H477	V417	D358	Y297
PRO	PRO	TYR	K538	C478	S418	P359	L298
ASP	ASP	ASP	C539	S479	V419	D360	Q299
ASP	ASP	ASP	Q540	D480	G420	K361	I300
LEU	SER	LEU	Q540	D480	G420	K361	I300
LEU	LEU	SER	LYS	L481	T421	Q362	T301
LEU	LEU	GLN	LYS	T482	G422	Q363	V302
VAL	VAL	LEU	LEU	M483	T423	I364	E303
PHE	PHE	HIS	VAL	M483	T423	I364	E303
ASP	ASP	GLY	GLY	K484	G424	Q365	N304
ASP	ASP	GLY	GLY	K484	G424	Q365	N304
THR	THR	GLY	PHE	A485	T425	K366	A305
GLU	GLU	LEU	ASP	E486	L426	L367	E306
GLY	GLY	LEU	ASP	E486	L426	L367	E306
SER	SER	PRO	LEU	L487	I427	S368	P307
SER	SER	PRO	PRO	L487	I427	S368	P307
ARG	ARG	PRO	PRO	D488	H429	Y369	F308
GLY	GLY	ARG	ILE	D488	H429	Y369	F308
SER	SER	PRO	ILE	S489	V430	I371	S309
GLU	GLU	ASP	LEU	K490	V430	I371	S309
ALA	ALA	ILE	VAL	G491	L431	G372	P311
ALA	ALA	MET	ILE	T492	D432	N373	L312
			LEU	T492	V433	D374	P313
			LEU	S493	N434	P375	T314
			GLY	S493	N434	P375	T314
			SER	M494	D435	A376	S315
			VAL	M494	D435	A376	S315
			LEU	L495	N436	R377	T316
			LEU	L496	N436	R377	T316
			ALA	S497	G437	W378	A317
			LEU	S497	G437	W378	A317
			LEU	P498	P438	L379	T318
			LEU	P498	P438	L379	T318
			ILE	T499	V439	T380	V319
			LEU	T499	V439	T380	V319
				Q500	S441	V381	T320
				Q500	S441	V381	T320
				Q501	S441	N382	V321
				Q501	S441	N382	V321
				L502	P442	K383	T322
				L502	P442	K383	T322
				K503	R443	D384	V323
				K503	R443	D384	V323
				K504	F445	N385	E324
				K504	F445	N385	E324
				Q505			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	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%)	2.03	204/5839 (3.5%)
1	B	0.99	25/4276 (0.6%)	2.02	202/5839 (3.5%)
1	C	0.99	24/4276 (0.6%)	2.02	203/5839 (3.5%)
1	D	0.99	24/4276 (0.6%)	2.03	203/5839 (3.5%)
All	All	0.99	97/17104 (0.6%)	2.02	812/23356 (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 97 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	522	LEU	N-CA	-18.92	1.34	1.46
1	C	522	LEU	N-CA	-18.89	1.34	1.46
1	A	522	LEU	N-CA	-18.88	1.34	1.46
1	D	522	LEU	N-CA	-18.78	1.34	1.46
1	C	465	PRO	CA-C	12.00	1.58	1.51

The worst 5 of 812 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	290	PHE	N-CA-C	27.42	145.39	108.38
1	A	290	PHE	N-CA-C	27.41	145.38	108.38
1	C	290	PHE	N-CA-C	25.18	145.37	108.60
1	B	290	PHE	N-CA-C	25.17	145.35	108.60
1	C	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	4089	818	0
1	B	4191	0	4081	893	0
1	C	4191	0	4078	1144	0
1	D	4191	0	4082	1147	0
2	A	182	0	168	89	0
2	B	182	0	168	86	0
2	C	182	0	169	86	0
2	D	182	0	169	88	0
3	A	28	0	24	9	0
3	B	28	0	24	10	0
3	C	28	0	24	8	0
3	D	28	0	24	9	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	17100	3367	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 97.

The worst 5 of 3367 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:24:ILE:HB	1:D:2:TRP:CE2	1.18	1.70
1:C:87:PRO:HG3	1:D:43:ALA:CB	1.22	1.65
1:C:87:PRO:CG	1:D:43:ALA:CB	1.77	1.61
1:C:87:PRO:HG3	1:D:43:ALA:CA	1.16	1.58
1:C:83:GLU:HA	1:D:41:GLN:CD	1.24	1.58

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%)	402 (75%)	91 (17%)	45 (8%)	0	9
1	B	538/880 (61%)	401 (74%)	93 (17%)	44 (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%)	1605 (75%)	368 (17%)	179 (8%)	1	9

5 of 179 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	122	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	B	902	1	14,14,15	1.12	1 (7%)	17,19,21	1.09	2 (11%)
2	NAG	B	808	1	14,14,15	0.66	0	17,19,21	0.70	0
3	NDG	A	811	1	14,14,15	0.87	0	17,19,21	1.96	1 (5%)
2	NAG	D	904	1	14,14,15	0.78	1 (7%)	17,19,21	0.70	1 (5%)
2	NAG	A	809	1	14,14,15	0.77	1 (7%)	17,19,21	0.94	0
2	NAG	B	904	1	14,14,15	0.76	1 (7%)	17,19,21	0.69	0
2	NAG	D	807	1	14,14,15	0.65	0	17,19,21	1.18	2 (11%)
2	NAG	D	902	1	14,14,15	1.13	1 (7%)	17,19,21	1.08	1 (5%)
2	NAG	A	810	1	14,14,15	0.67	0	17,19,21	1.33	4 (23%)
2	NAG	D	812	1	14,14,15	0.83	1 (7%)	17,19,21	0.75	1 (5%)
2	NAG	B	810	1	14,14,15	0.67	0	17,19,21	1.33	4 (23%)
2	NAG	A	807	1	14,14,15	0.64	0	17,19,21	1.19	2 (11%)
2	NAG	A	805	1	14,14,15	0.72	0	17,19,21	1.06	1 (5%)
3	NDG	D	804	1	14,14,15	0.64	0	17,19,21	0.77	0
2	NAG	B	812	1	14,14,15	0.83	1 (7%)	17,19,21	0.76	1 (5%)
2	NAG	D	903	1	14,14,15	0.55	0	17,19,21	0.79	0
2	NAG	A	902	1	14,14,15	1.15	1 (7%)	17,19,21	1.08	2 (11%)
2	NAG	B	802	1	14,14,15	0.78	1 (7%)	17,19,21	0.85	0
2	NAG	D	806	1	14,14,15	0.55	0	17,19,21	1.38	3 (17%)
2	NAG	A	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.16	2 (11%)
2	NAG	C	801	1	14,14,15	0.70	0	17,19,21	0.98	1 (5%)
2	NAG	C	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	C	802	1	14,14,15	0.78	1 (7%)	17,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	801	1	14,14,15	0.70	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	C	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	D	805	1	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
3	NDG	B	811	1	14,14,15	0.86	0	17,19,21	1.96	1 (5%)
2	NAG	A	806	1	14,14,15	0.55	0	17,19,21	1.39	3 (17%)
3	NDG	C	804	1	14,14,15	0.64	0	17,19,21	0.78	0
2	NAG	C	807	1	14,14,15	0.63	0	17,19,21	1.19	2 (11%)
2	NAG	C	902	1	14,14,15	1.13	1 (7%)	17,19,21	1.09	2 (11%)
2	NAG	D	808	1	14,14,15	0.66	0	17,19,21	0.70	0
2	NAG	C	808	1	14,14,15	0.68	0	17,19,21	0.70	0
2	NAG	B	809	1	14,14,15	0.76	0	17,19,21	0.94	0
2	NAG	A	802	1	14,14,15	0.78	1 (7%)	17,19,21	0.85	0
3	NDG	D	811	1	14,14,15	0.87	0	17,19,21	1.96	1 (5%)
2	NAG	C	812	1	14,14,15	0.83	1 (7%)	17,19,21	0.76	1 (5%)
2	NAG	A	801	1	14,14,15	0.71	0	17,19,21	0.99	1 (5%)
2	NAG	A	808	1	14,14,15	0.67	0	17,19,21	0.70	0
3	NDG	A	804	1	14,14,15	0.65	0	17,19,21	0.78	0
2	NAG	D	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.16	2 (11%)
2	NAG	B	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	C	903	1	14,14,15	0.55	0	17,19,21	0.78	0
2	NAG	A	904	1	14,14,15	0.77	1 (7%)	17,19,21	0.70	1 (5%)
2	NAG	C	809	1	14,14,15	0.77	1 (7%)	17,19,21	0.93	0
2	NAG	D	809	1	14,14,15	0.78	1 (7%)	17,19,21	0.94	0
2	NAG	B	903	1	14,14,15	0.56	0	17,19,21	0.79	0
2	NAG	C	805	1	14,14,15	0.72	0	17,19,21	1.05	1 (5%)
2	NAG	D	802	1	14,14,15	0.79	1 (7%)	17,19,21	0.85	0
2	NAG	B	806	1	14,14,15	0.56	0	17,19,21	1.39	3 (17%)
2	NAG	D	810	1	14,14,15	0.67	0	17,19,21	1.33	4 (23%)
2	NAG	B	801	1	14,14,15	0.70	0	17,19,21	0.97	1 (5%)
2	NAG	A	903	1	14,14,15	0.55	0	17,19,21	0.79	0
2	NAG	B	805	1	14,14,15	0.72	0	17,19,21	1.05	1 (5%)
3	NDG	C	811	1	14,14,15	0.86	0	17,19,21	1.96	1 (5%)
2	NAG	C	904	1	14,14,15	0.77	1 (7%)	17,19,21	0.70	1 (5%)
2	NAG	A	812	1	14,14,15	0.84	1 (7%)	17,19,21	0.76	1 (5%)
2	NAG	B	807	1	14,14,15	0.65	0	17,19,21	1.20	2 (11%)

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

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

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	NAG	C1-C2	3.43	1.57	1.52
2	C	902	NAG	C1-C2	3.37	1.56	1.52
2	B	902	NAG	C1-C2	3.35	1.56	1.52
2	D	902	NAG	C1-C2	3.34	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	803	NAG	O5-C5	2.65	1.48	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	811	NDG	C2-N2-C7	-7.43	112.94	122.90
3	A	811	NDG	C2-N2-C7	-7.43	112.94	122.90
3	B	811	NDG	C2-N2-C7	-7.42	112.96	122.90
3	C	811	NDG	C2-N2-C7	-7.41	112.97	122.90
2	B	806	NAG	C2-N2-C7	-3.65	118.00	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	B	902	NAG	7	0
2	B	808	NAG	2	0
3	A	811	NDG	7	0
2	D	904	NAG	6	0
2	A	809	NAG	8	0
2	B	904	NAG	6	0
2	D	807	NAG	16	0
2	D	902	NAG	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	810	NAG	12	0
2	D	812	NAG	3	0
2	B	810	NAG	11	0
2	A	807	NAG	16	0
2	A	805	NAG	7	0
3	D	804	NDG	2	0
2	B	812	NAG	3	0
2	A	902	NAG	7	0
2	D	806	NAG	12	0
2	A	803	NAG	4	0
2	C	801	NAG	22	0
2	C	803	NAG	4	0
2	D	801	NAG	22	0
2	C	806	NAG	10	0
2	C	810	NAG	12	0
3	B	804	NDG	2	0
2	D	805	NAG	7	0
3	B	811	NDG	8	0
2	A	806	NAG	12	0
3	C	804	NDG	2	0
2	C	807	NAG	16	0
2	C	902	NAG	7	0
2	D	808	NAG	2	0
2	C	808	NAG	2	0
2	B	809	NAG	8	0
3	D	811	NDG	7	0
2	C	812	NAG	2	0
2	A	801	NAG	22	0
2	A	808	NAG	2	0
3	A	804	NDG	2	0
2	D	803	NAG	4	0
2	B	803	NAG	4	0
2	A	904	NAG	6	0
2	C	809	NAG	8	0
2	D	809	NAG	8	0
2	C	805	NAG	6	0
2	B	806	NAG	12	0
2	D	810	NAG	11	0
2	B	801	NAG	21	0
2	B	805	NAG	7	0
3	C	811	NDG	6	0
2	C	904	NAG	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	812	NAG	3	0
2	B	807	NAG	15	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

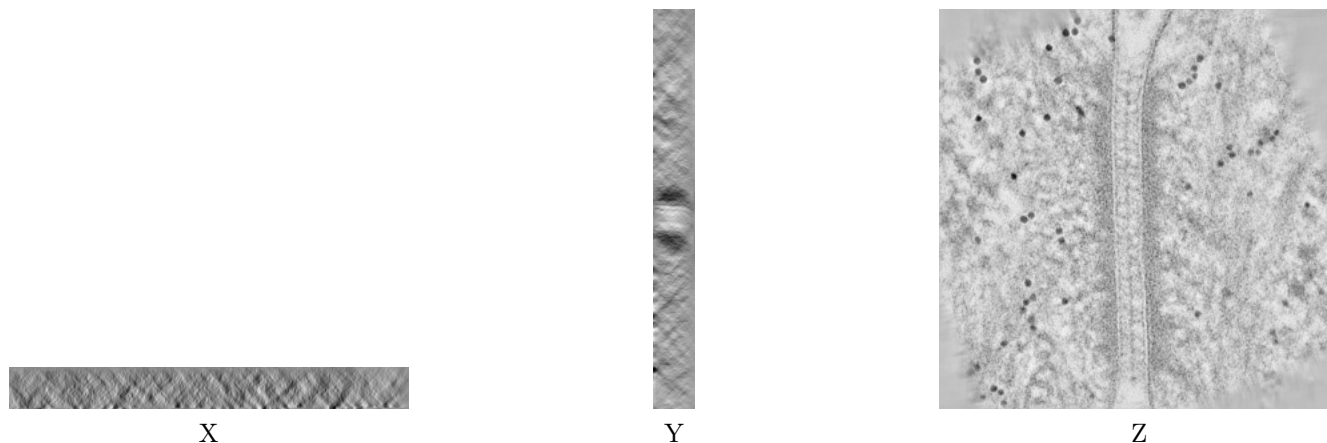
5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Tomogram visualisation [i](#)

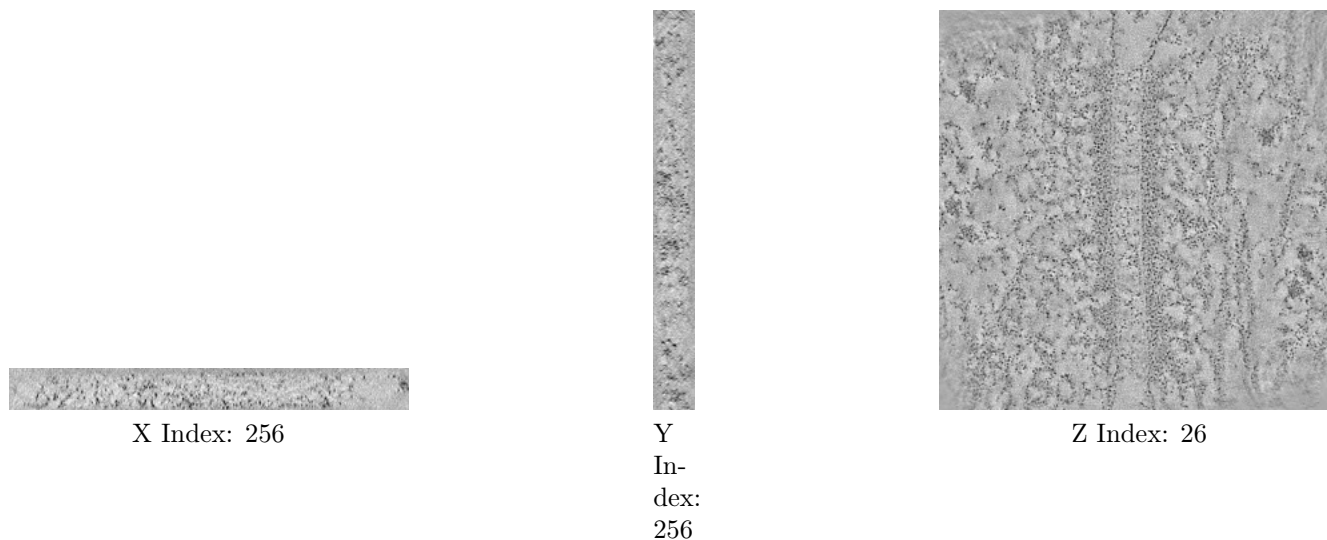
This section contains visualisations of the EMDB entry EMD-1052. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



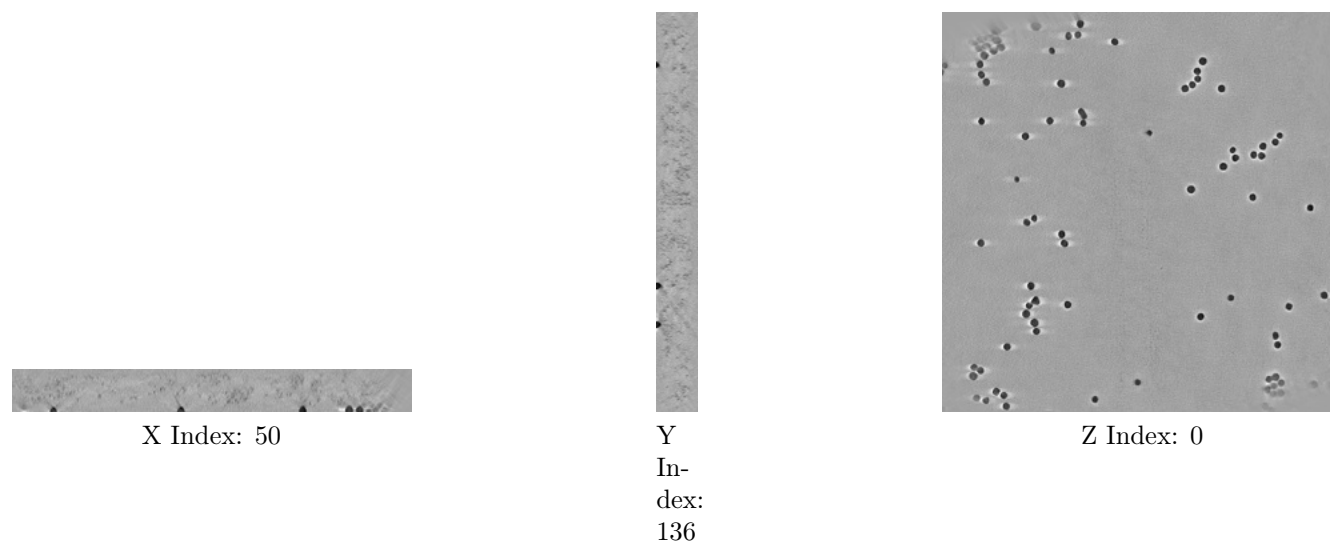
The images above show the tomogram projected in three orthogonal directions.

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.

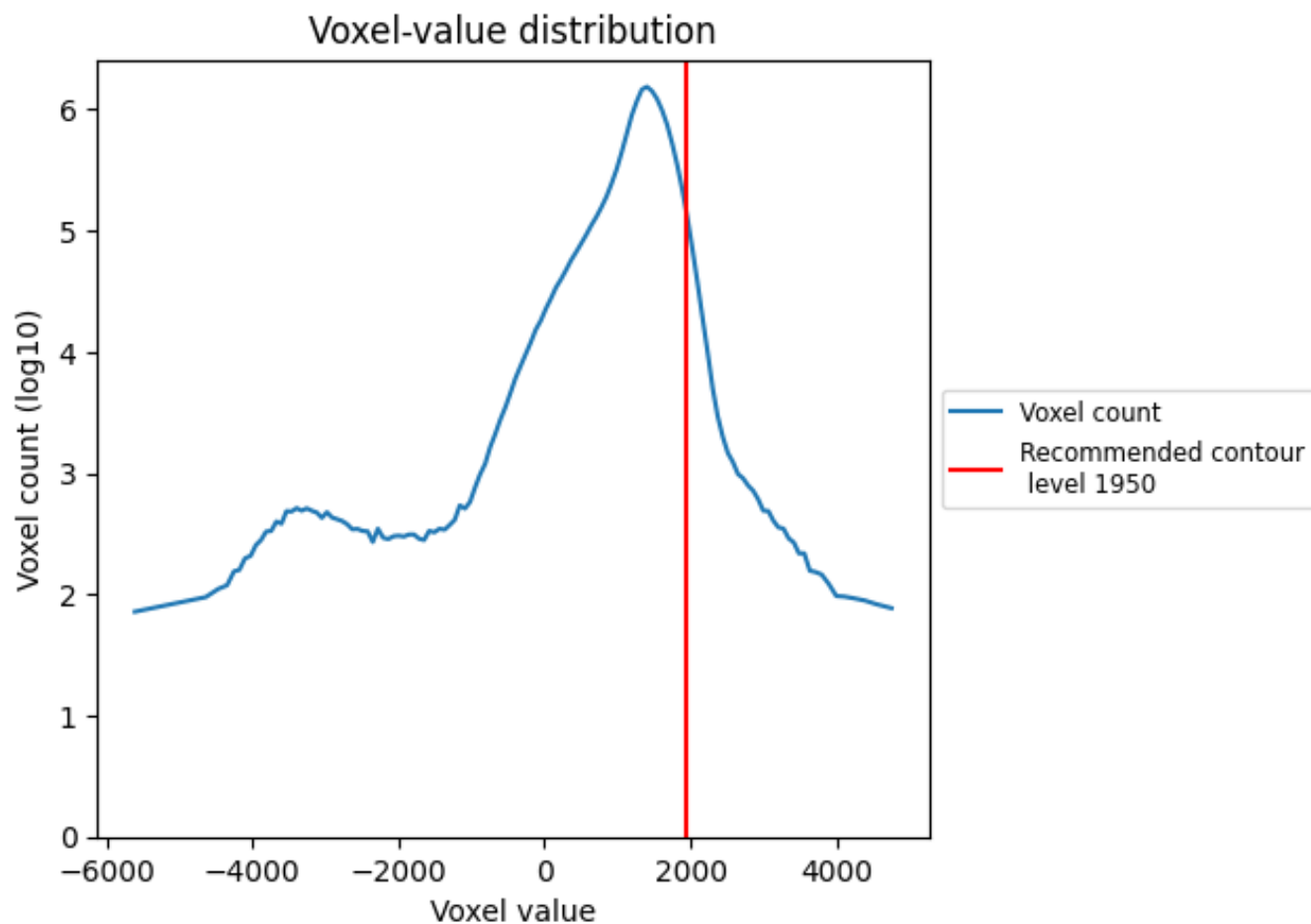
6.5 Mask visualisation [i](#)

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.

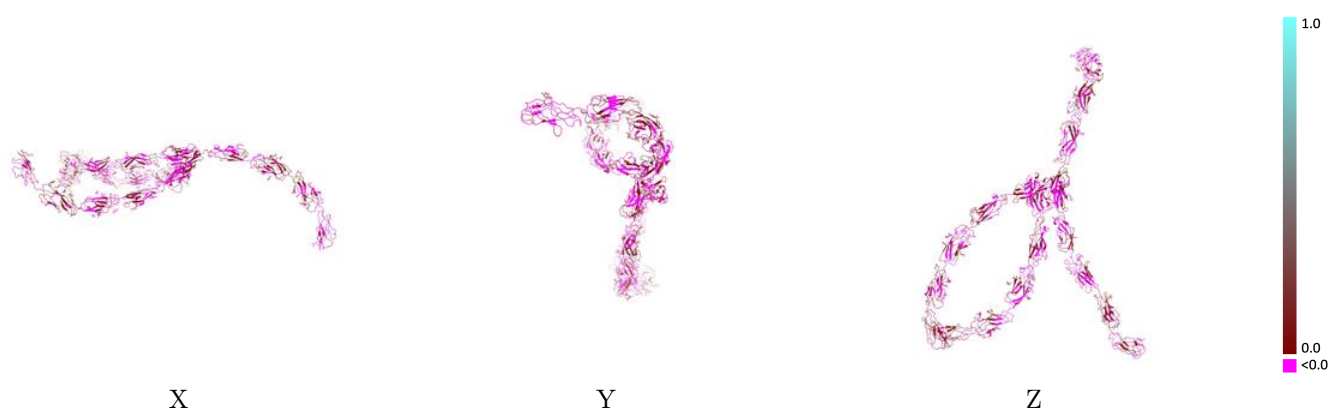
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1052 and PDB model 1Q5C. 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](#)

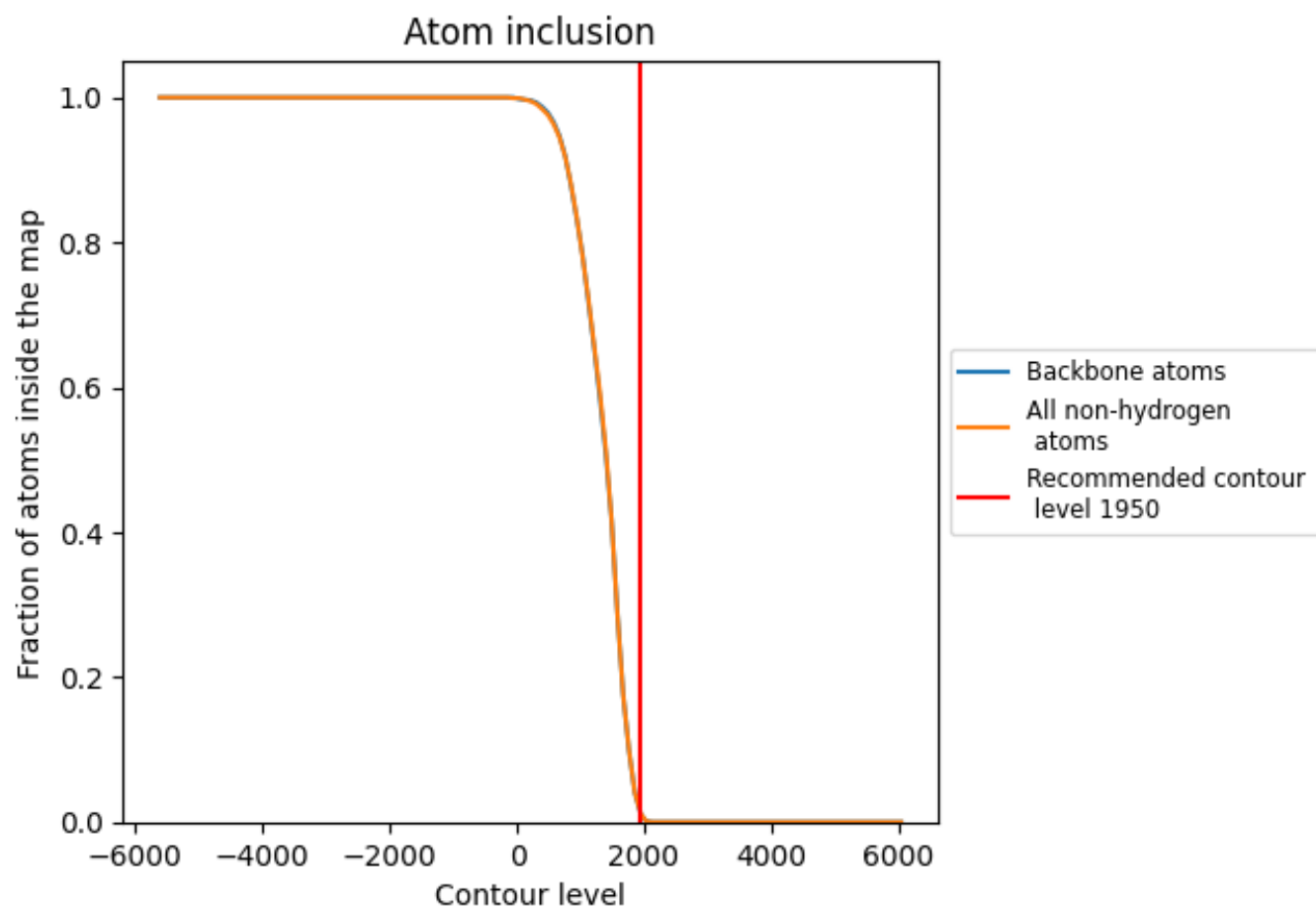


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 1% 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	0.0110	0.0020
A	0.0140	0.0090
B	0.0060	0.0060
C	0.0000	-0.0030
D	0.0240	-0.0030

