Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 02:22 pm GMT

PDB ID	:	6ZBY
EMDB ID	:	EMD-11158
Title	:	Cryo-EM structure of the nitrilase from Pseudomonas fluorescens EBC191 at 3.3 Angstroms
Authors	:	Eppinger, E.; Stolz, A.; Sewell, B.T.
Deposited on	:	2020-06-09
Resolution	:	3.10 Å(reported)

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:

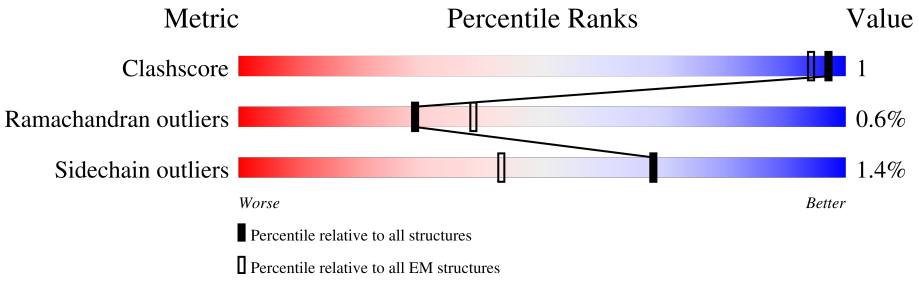
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	350	11% 84% 5% • 10%
1	B	350	15% 85% 5% 10%
1	C	350	• 86% • • 10%
1	D	350	• 85% 5% 10%
1	E	350	• 85% 5% • 10%
1	F	350	• 82% 7% • 10%
1	G	350	• 85% 5% • 10%
1	H	350	• 85% • • 10%

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Mol	Chain	Length	Quality of chain
1	I	350	
1	J	350	
1	K	350	
1	L	350	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 28836 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 NitA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	316	Total 2403	C 1536	N 412	O 443	S 12	0	0
1	B	316	Total 2403	C 1536	N 412	O 443	S 12	0	0
1	C	316	Total 2403	C 1536	N 412	O 443	S 12	0	0
1	D	316	Total 2403	C 1536	N 412	O 443	S 12	0	0
1	E	316	Total 2403	C 1536	N 412	O 443	S 12	0	0
1	F	316	Total 2403	C 1536	N 412	O 443	S 12	0	0
1	G	316	Total 2403	C 1536	N 412	O 443	S 12	0	0
1	H	316	Total 2403	C 1536	N 412	O 443	S 12	0	0
1	I	316	Total 2403	C 1536	N 412	O 443	S 12	0	0
1	J	316	Total 2403	C 1536	N 412	O 443	S 12	0	0
1	K	316	Total 2403	C 1536	N 412	O 443	S 12	0	0
1	L	316	Total 2403	C 1536	N 412	O 443	S 12	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	THR	PRO	conflict	UNP Q5EG61
B	227	THR	PRO	conflict	UNP Q5EG61
C	227	THR	PRO	conflict	UNP Q5EG61
D	227	THR	PRO	conflict	UNP Q5EG61
E	227	THR	PRO	conflict	UNP Q5EG61
F	227	THR	PRO	conflict	UNP Q5EG61

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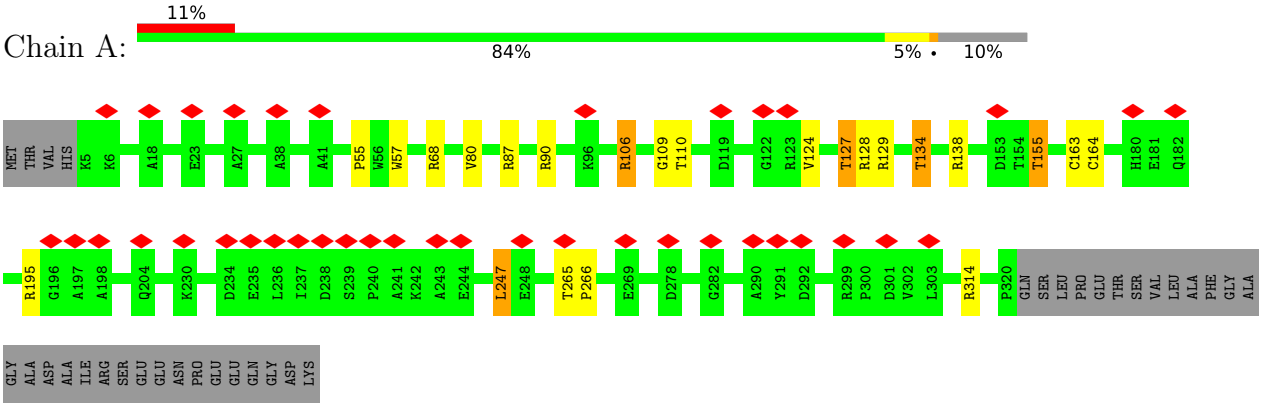
Chain	Residue	Modelled	Actual	Comment	Reference
G	227	THR	PRO	conflict	UNP Q5EG61
H	227	THR	PRO	conflict	UNP Q5EG61
I	227	THR	PRO	conflict	UNP Q5EG61
J	227	THR	PRO	conflict	UNP Q5EG61
K	227	THR	PRO	conflict	UNP Q5EG61
L	227	THR	PRO	conflict	UNP Q5EG61

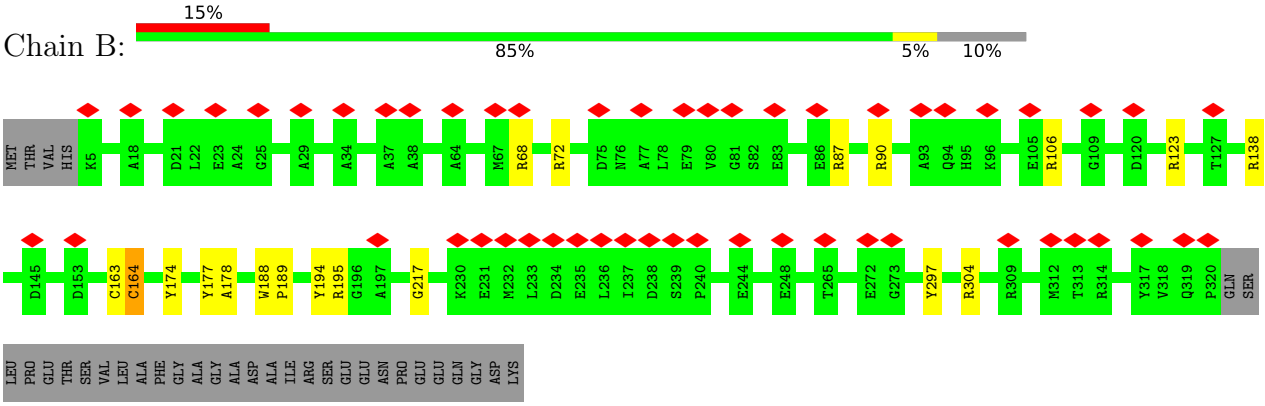
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

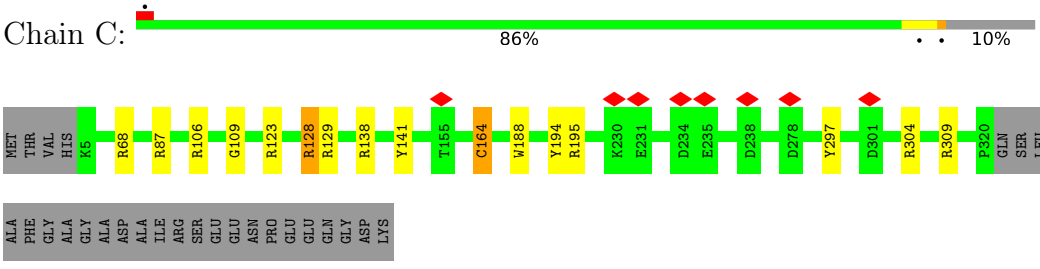
• Molecule 1: NitA



• Molecule 1: NitA

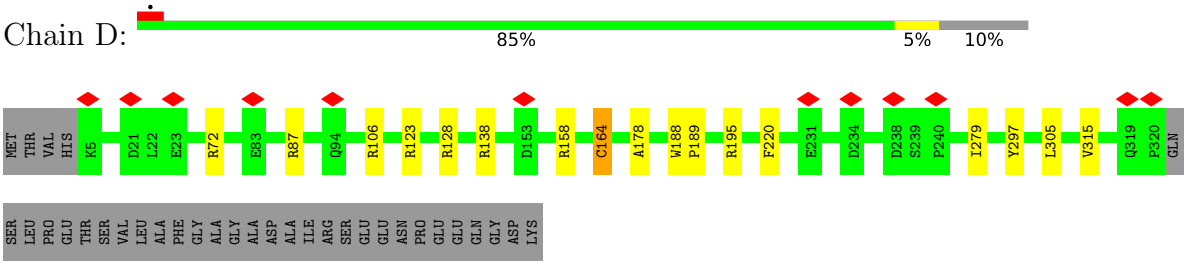


• Molecule 1: NitA



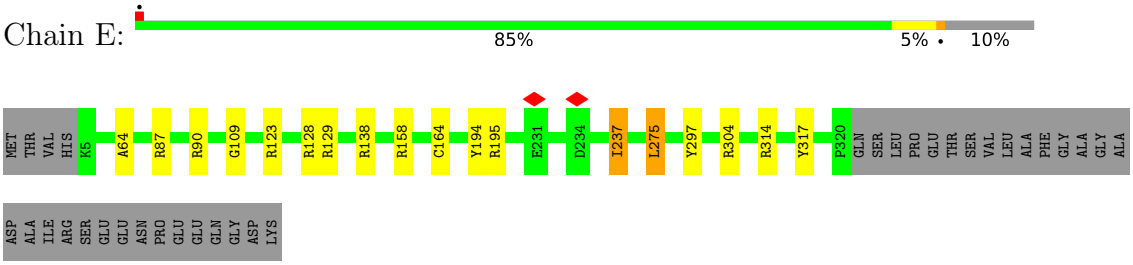
• Molecule 1: NitA

Chain D:



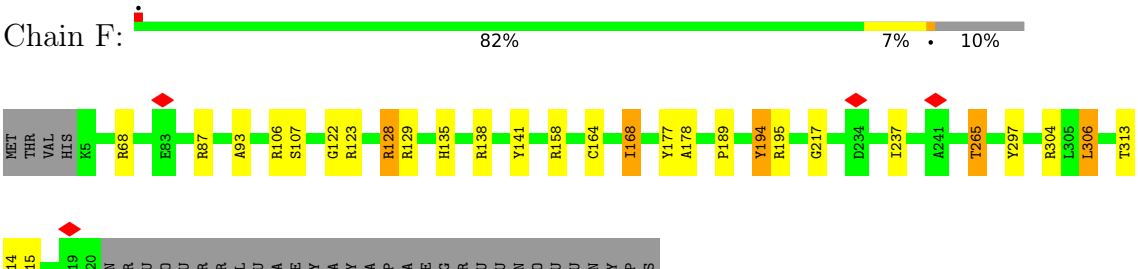
• Molecule 1: NitA

Chain E:



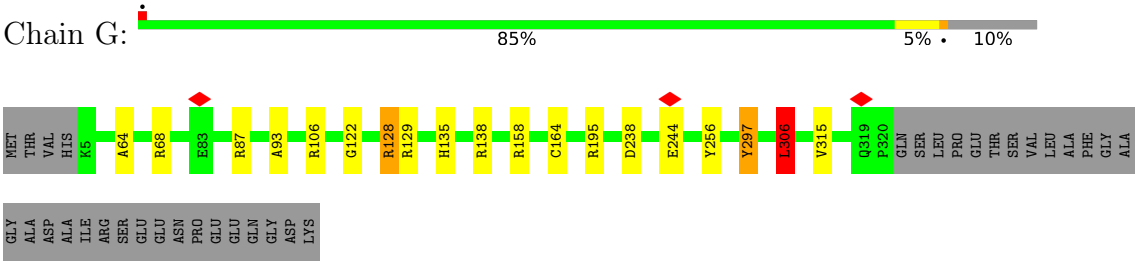
• Molecule 1: NitA

Chain F:



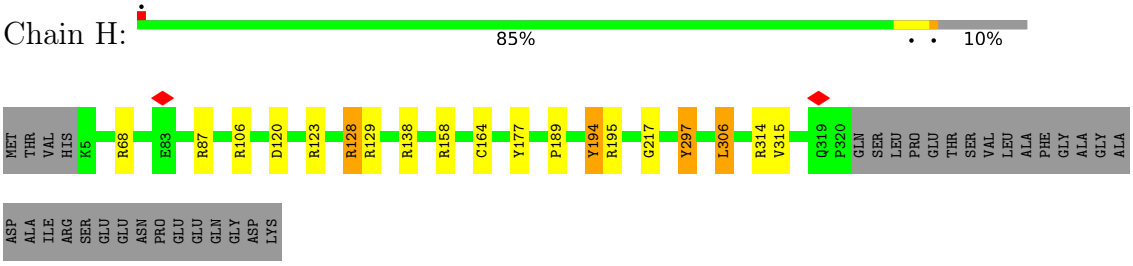
• Molecule 1: NitA

Chain G:



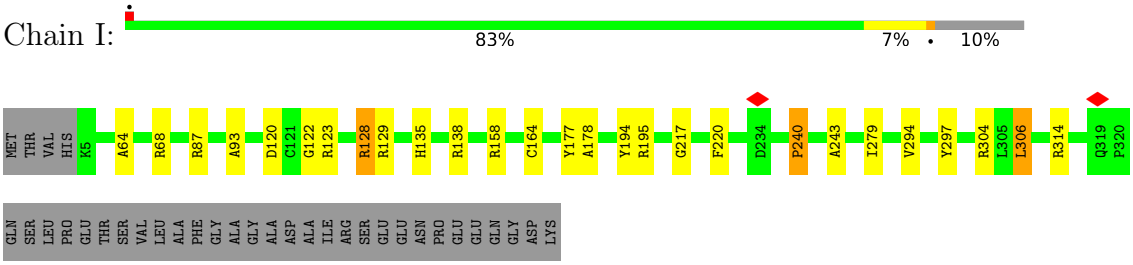
• Molecule 1: NitA

Chain H:



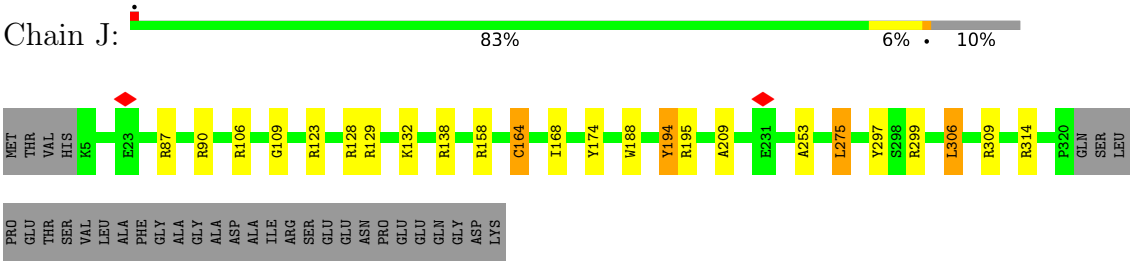
• Molecule 1: NitA

Chain I:



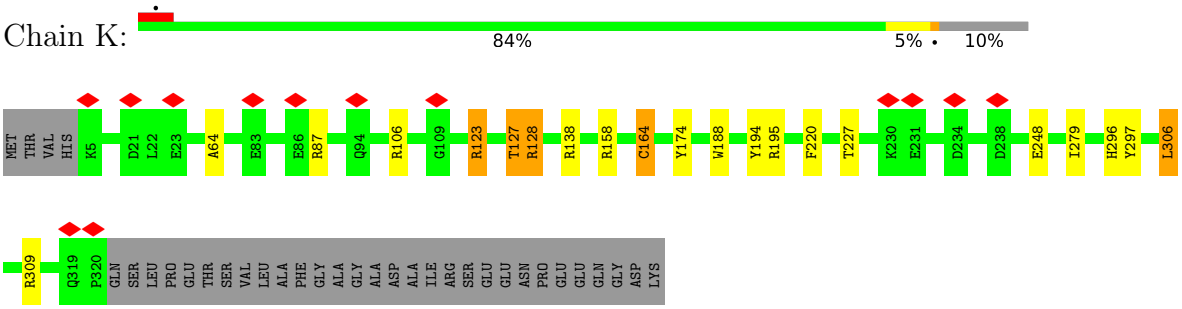
• Molecule 1: NitA

Chain J:



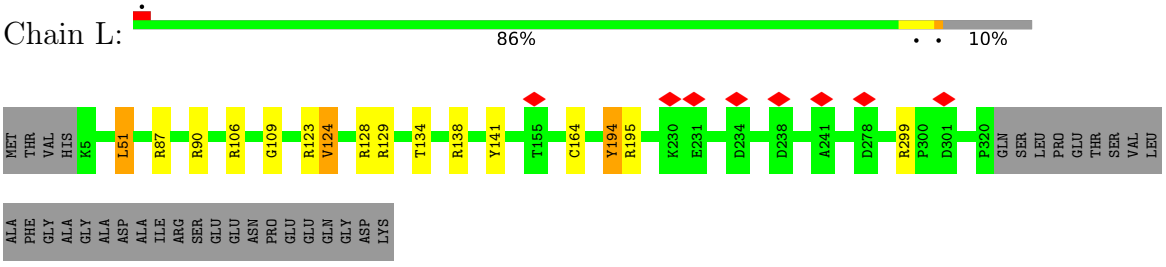
• Molecule 1: NitA

Chain K:



• Molecule 1: NitA

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-67.31°, rise=16.36 Å, axial sym=C1	Depositor
Number of segments used	91429	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	43.1	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.134	Depositor
Minimum map value	-0.082	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	139.384, 137.288, 154.056	wwPDB
Map dimensions	133, 131, 147	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.68	0/2462	1.21	15/3353 (0.4%)
1	B	0.67	0/2462	1.10	11/3353 (0.3%)
1	C	0.67	0/2462	1.11	12/3353 (0.4%)
1	D	0.65	0/2462	1.09	8/3353 (0.2%)
1	E	0.66	0/2462	1.15	14/3353 (0.4%)
1	F	0.65	0/2462	1.16	15/3353 (0.4%)
1	G	0.66	0/2462	1.13	9/3353 (0.3%)
1	H	0.66	0/2462	1.12	12/3353 (0.4%)
1	I	0.66	0/2462	1.15	14/3353 (0.4%)
1	J	0.67	0/2462	1.16	17/3353 (0.5%)
1	K	0.67	0/2462	1.13	11/3353 (0.3%)
1	L	0.65	0/2462	1.14	12/3353 (0.4%)
All	All	0.66	0/29544	1.14	150/40236 (0.4%)

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	0	2
1	B	0	1
1	C	0	3
1	D	0	1
1	E	0	1
1	F	0	2
1	G	0	2
1	H	0	1
1	J	0	1
1	K	0	1
1	L	0	1
All	All	0	16

There are no bond length outliers.

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	124	VAL	CA-CB-CG1	15.39	133.98	110.90
1	L	124	VAL	CA-CB-CG1	13.86	131.69	110.90
1	A	247	LEU	CB-CG-CD1	13.85	134.54	111.00
1	A	80	VAL	CA-CB-CG1	13.82	131.63	110.90
1	L	51	LEU	CB-CG-CD1	13.53	134.00	111.00
1	E	275	LEU	CB-CG-CD1	12.89	132.92	111.00
1	E	237	ILE	CA-CB-CG1	12.69	135.11	111.00
1	J	275	LEU	CB-CG-CD1	12.47	132.21	111.00
1	J	306	LEU	CB-CG-CD1	12.20	131.73	111.00
1	G	306	LEU	CB-CG-CD1	12.08	131.54	111.00
1	A	87	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	H	306	LEU	CB-CG-CD1	10.06	128.10	111.00
1	K	195	ARG	NE-CZ-NH2	9.88	125.24	120.30
1	L	195	ARG	NE-CZ-NH2	9.84	125.22	120.30
1	G	87	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	F	265	THR	CA-CB-OG1	9.23	128.39	109.00
1	C	304	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	A	106	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	I	304	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	B	87	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	B	72	ARG	NE-CZ-NH2	8.80	124.70	120.30
1	A	127	THR	CA-CB-OG1	8.71	127.30	109.00
1	E	195	ARG	NE-CZ-NH2	8.63	124.61	120.30
1	I	128	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	C	129	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	D	195	ARG	NE-CZ-NH2	8.43	124.52	120.30
1	K	127	THR	CA-CB-OG1	8.43	126.71	109.00
1	A	110	THR	CA-CB-OG1	8.28	126.38	109.00
1	G	158	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	C	195	ARG	NE-CZ-NH2	8.23	124.42	120.30
1	E	138	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	A	155	THR	CA-CB-OG1	8.15	126.13	109.00
1	D	106	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	L	106	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	B	304	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	L	87	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	K	87	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	B	138	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	H	87	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	G	129	ARG	NE-CZ-NH1	7.94	124.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	129	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	I	195	ARG	NE-CZ-NH2	7.93	124.26	120.30
1	E	304	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	K	138	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	134	THR	CA-CB-OG1	7.63	125.02	109.00
1	E	87	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	C	87	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	H	68	ARG	NE-CZ-NH1	7.51	124.05	120.30
1	A	138	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	E	123	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	C	106	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	J	123	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	H	129	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	I	138	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	L	299	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	J	158	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	H	158	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	J	195	ARG	NE-CZ-NH2	7.17	123.88	120.30
1	F	87	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	A	195	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	L	128	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	C	138	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	B	195	ARG	NE-CZ-NH2	7.07	123.83	120.30
1	F	138	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	G	138	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	H	106	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	F	123	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	F	195	ARG	NE-CZ-NH2	6.91	123.76	120.30
1	H	138	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	F	168	ILE	CA-CB-CG1	6.82	123.96	111.00
1	D	87	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	I	123	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	G	68	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	L	123	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	K	128	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	J	138	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	E	158	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	D	123	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	H	314	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	B	90	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	I	87	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	E	128	ARG	NE-CZ-NH1	6.45	123.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	87	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	I	129	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	D	72	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	J	106	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	F	129	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	K	309	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	B	68	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	H	128	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	68	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	K	158	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	C	309	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	G	195	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	F	158	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	E	314	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	H	195	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	L	194	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	C	123	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	C	194	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	J	309	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	F	68	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	L	129	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	106	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	K	123	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	I	194	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	F	194	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	C	304	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	F	123	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	G	128	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	D	138	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	F	314	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	I	240	PRO	N-CA-C	5.82	127.23	112.10
1	J	128	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	I	158	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	90	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	I	128	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	C	128	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	K	194	TYR	CB-CG-CD2	-5.73	117.56	121.00
1	K	106	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	E	194	TYR	CB-CG-CD2	-5.69	117.59	121.00
1	J	299	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	194	TYR	CB-CG-CD2	-5.61	117.64	121.00
1	F	304	ARG	NE-CZ-NH1	5.58	123.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	314	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C	68	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	174	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	J	194	TYR	CB-CG-CD2	-5.44	117.74	121.00
1	B	123	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	F	128	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	E	90	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	314	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	G	106	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	L	90	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	J	129	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	E	317	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	J	123	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	J	90	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	I	304	ARG	CD-NE-CZ	5.22	130.91	123.60
1	I	68	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	E	129	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	D	158	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	L	138	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	H	194	TYR	CB-CG-CD2	-5.09	117.95	121.00
1	J	174	TYR	CB-CG-CD1	-5.09	117.95	121.00
1	K	174	TYR	CB-CG-CD1	-5.06	117.97	121.00
1	J	314	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	H	123	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	D	87	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
1	F	304	ARG	CD-NE-CZ	5.00	130.60	123.60

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	ARG	Sidechain
1	A	128	ARG	Sidechain
1	B	297	TYR	Sidechain
1	C	128	ARG	Sidechain
1	C	141	TYR	Sidechain
1	C	297	TYR	Sidechain
1	D	297	TYR	Sidechain
1	E	297	TYR	Sidechain
1	F	106	ARG	Sidechain
1	F	141	TYR	Sidechain
1	G	256	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	G	297	TYR	Sidechain
1	H	297	TYR	Sidechain
1	J	297	TYR	Sidechain
1	K	297	TYR	Sidechain
1	L	141	TYR	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	2403	0	2368	2	0
1	B	2403	0	2368	3	0
1	C	2403	0	2368	1	0
1	D	2403	0	2368	5	0
1	E	2403	0	2368	1	0
1	F	2403	0	2368	7	0
1	G	2403	0	2368	5	0
1	H	2403	0	2368	4	0
1	I	2403	0	2368	10	0
1	J	2403	0	2368	6	0
1	K	2403	0	2368	5	0
1	L	2403	0	2368	1	0
All	All	28836	0	28416	36	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 1.

All (36) 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:I:240:PRO:HA	1:I:243:ALA:HB3	1.83	0.60
1:F:306:LEU:HG	1:G:306:LEU:HD11	1.91	0.52
1:I:240:PRO:HA	1:I:243:ALA:CB	2.42	0.49
1:I:93:ALA:HB2	1:I:122:GLY:HA3	1.94	0.48
1:G:93:ALA:HB2	1:G:122:GLY:HA3	1.96	0.48
1:G:64:ALA:HB2	1:H:194:TYR:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:THR:HA	1:A:266:PRO:HD3	1.76	0.47
1:F:177:TYR:CE1	1:F:217:GLY:HA3	2.51	0.46
1:G:315:VAL:HG21	1:I:178:ALA:CB	2.46	0.46
1:I:178:ALA:HA	1:I:294:VAL:HG11	1.98	0.46
1:I:220:PHE:CD2	1:I:279:ILE:HD12	2.50	0.46
1:K:164:CYS:HA	1:K:188:TRP:CZ3	2.51	0.46
1:I:64:ALA:HB2	1:J:194:TYR:CZ	2.51	0.45
1:F:178:ALA:CB	1:H:315:VAL:HG21	2.46	0.45
1:J:168:ILE:HD11	1:J:209:ALA:HB2	1.99	0.45
1:D:220:PHE:CD2	1:D:279:ILE:HD12	2.53	0.44
1:C:164:CYS:HA	1:C:188:TRP:CZ3	2.53	0.44
1:H:306:LEU:HD11	1:I:306:LEU:HG	1.98	0.44
1:J:306:LEU:HD11	1:K:306:LEU:HG	1.99	0.44
1:D:178:ALA:CB	1:F:315:VAL:HG21	2.47	0.43
1:E:64:ALA:HB2	1:F:194:TYR:CZ	2.53	0.43
1:J:253:ALA:HB3	1:J:275:LEU:HD12	2.01	0.43
1:D:164:CYS:HA	1:D:188:TRP:CZ3	2.54	0.43
1:B:177:TYR:CE1	1:B:217:GLY:HA3	2.53	0.42
1:K:220:PHE:CD2	1:K:279:ILE:HD12	2.53	0.42
1:J:132:LYS:HE2	1:K:296:HIS:O	2.20	0.42
1:I:177:TYR:CE1	1:I:217:GLY:HA3	2.55	0.42
1:J:164:CYS:HA	1:J:188:TRP:CZ3	2.55	0.42
1:A:55:PRO:HA	1:A:57:TRP:CZ3	2.55	0.42
1:F:93:ALA:HB2	1:F:122:GLY:HA3	2.01	0.42
1:K:64:ALA:HB2	1:L:194:TYR:CZ	2.54	0.41
1:D:305:LEU:HB3	1:F:315:VAL:HG22	2.03	0.41
1:H:177:TYR:CE1	1:H:217:GLY:HA3	2.55	0.41
1:G:315:VAL:HG21	1:I:178:ALA:HB1	2.03	0.41
1:B:178:ALA:CB	1:D:315:VAL:HG21	2.51	0.41
1:B:164:CYS:HB2	1:B:188:TRP:CE3	2.56	0.40

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	314/350 (90%)	300 (96%)	12 (4%)	2 (1%)	25	59
1	B	314/350 (90%)	303 (96%)	9 (3%)	2 (1%)	25	59
1	C	314/350 (90%)	297 (95%)	15 (5%)	2 (1%)	25	59
1	D	314/350 (90%)	300 (96%)	12 (4%)	2 (1%)	25	59
1	E	314/350 (90%)	295 (94%)	17 (5%)	2 (1%)	25	59
1	F	314/350 (90%)	299 (95%)	13 (4%)	2 (1%)	25	59
1	G	314/350 (90%)	297 (95%)	16 (5%)	1 (0%)	41	73
1	H	314/350 (90%)	295 (94%)	17 (5%)	2 (1%)	25	59
1	I	314/350 (90%)	301 (96%)	12 (4%)	1 (0%)	41	73
1	J	314/350 (90%)	296 (94%)	16 (5%)	2 (1%)	25	59
1	K	314/350 (90%)	302 (96%)	11 (4%)	1 (0%)	41	73
1	L	314/350 (90%)	300 (96%)	12 (4%)	2 (1%)	25	59
All	All	3768/4200 (90%)	3585 (95%)	162 (4%)	21 (1%)	29	59

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	164	CYS
1	E	164	CYS
1	F	164	CYS
1	G	164	CYS
1	H	164	CYS
1	I	164	CYS
1	J	164	CYS
1	K	164	CYS
1	A	164	CYS
1	C	164	CYS
1	D	164	CYS
1	D	189	PRO
1	F	189	PRO
1	H	189	PRO
1	L	164	CYS
1	A	109	GLY
1	B	189	PRO
1	E	109	GLY
1	C	109	GLY

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Mol	Chain	Res	Type
1	L	109	GLY
1	J	109	GLY

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	241/268 (90%)	236 (98%)	5 (2%)	53 79
1	B	241/268 (90%)	240 (100%)	1 (0%)	91 96
1	C	241/268 (90%)	241 (100%)	0	100 100
1	D	241/268 (90%)	240 (100%)	1 (0%)	91 96
1	E	241/268 (90%)	239 (99%)	2 (1%)	81 92
1	F	241/268 (90%)	232 (96%)	9 (4%)	34 66
1	G	241/268 (90%)	235 (98%)	6 (2%)	47 75
1	H	241/268 (90%)	238 (99%)	3 (1%)	71 88
1	I	241/268 (90%)	236 (98%)	5 (2%)	53 79
1	J	241/268 (90%)	241 (100%)	0	100 100
1	K	241/268 (90%)	235 (98%)	6 (2%)	47 75
1	L	241/268 (90%)	238 (99%)	3 (1%)	71 88
All	All	2892/3216 (90%)	2851 (99%)	41 (1%)	68 86

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	THR
1	A	134	THR
1	A	155	THR
1	A	163	CYS
1	A	247	LEU
1	B	163	CYS
1	D	128	ARG
1	E	237	ILE

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Mol	Chain	Res	Type
1	E	275	LEU
1	F	107	SER
1	F	128	ARG
1	F	135	HIS
1	F	168	ILE
1	F	237	ILE
1	F	265	THR
1	F	297	TYR
1	F	306	LEU
1	F	313	THR
1	G	128	ARG
1	G	135	HIS
1	G	238	ASP
1	G	244	GLU
1	G	297	TYR
1	G	306	LEU
1	H	120	ASP
1	H	128	ARG
1	H	297	TYR
1	I	120	ASP
1	I	128	ARG
1	I	135	HIS
1	I	297	TYR
1	I	306	LEU
1	K	123	ARG
1	K	127	THR
1	K	128	ARG
1	K	227	THR
1	K	248	GLU
1	K	306	LEU
1	L	51	LEU
1	L	124	VAL
1	L	134	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	115	GLN
1	E	152	HIS
1	J	152	HIS
1	K	115	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

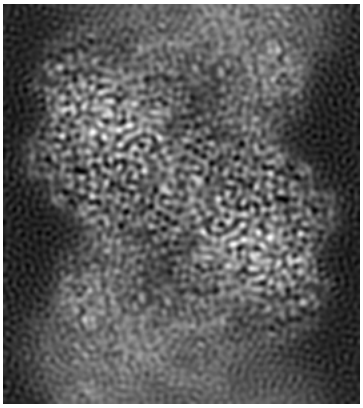
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11158. These allow visual inspection of the internal detail of the map and identification of artifacts.

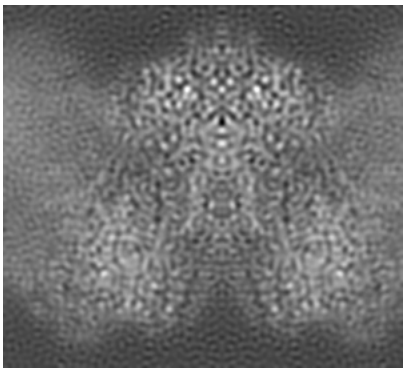
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

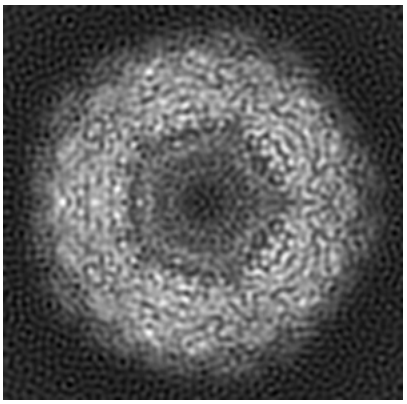
6.1.1 Primary map



X



Y

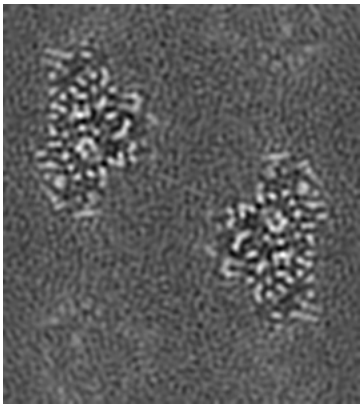


Z

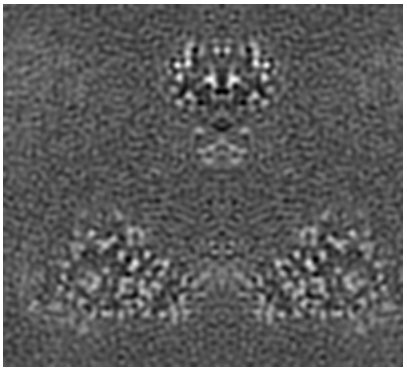
The images above show the map projected in three orthogonal directions.

6.2 Central slices

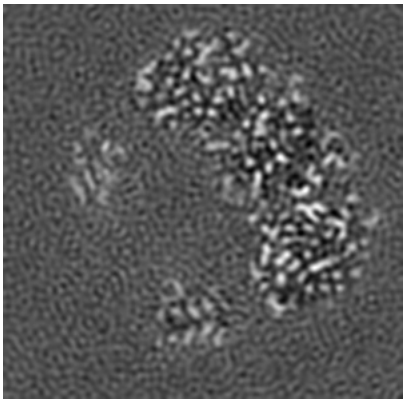
6.2.1 Primary map



X Index: 66



Y Index: 65

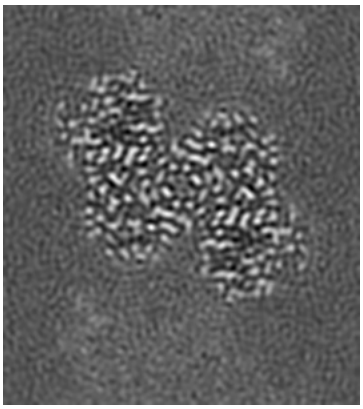


Z Index: 73

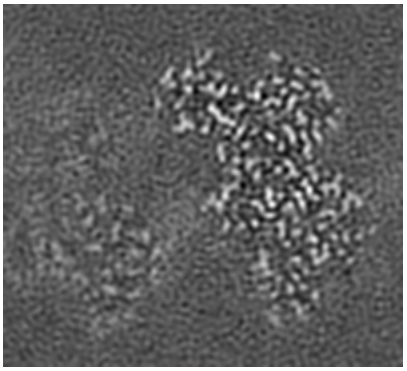
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

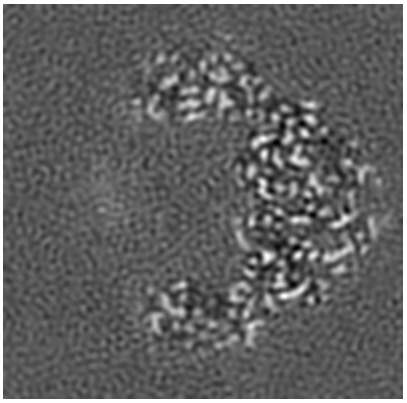
6.3.1 Primary map



X Index: 99



Y Index: 37



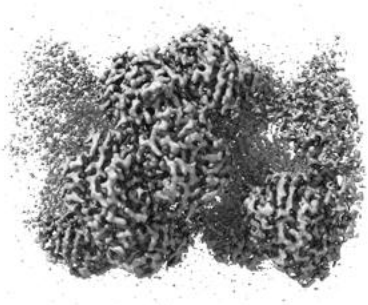
Z Index: 79

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

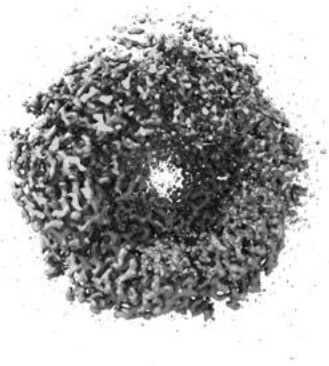
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

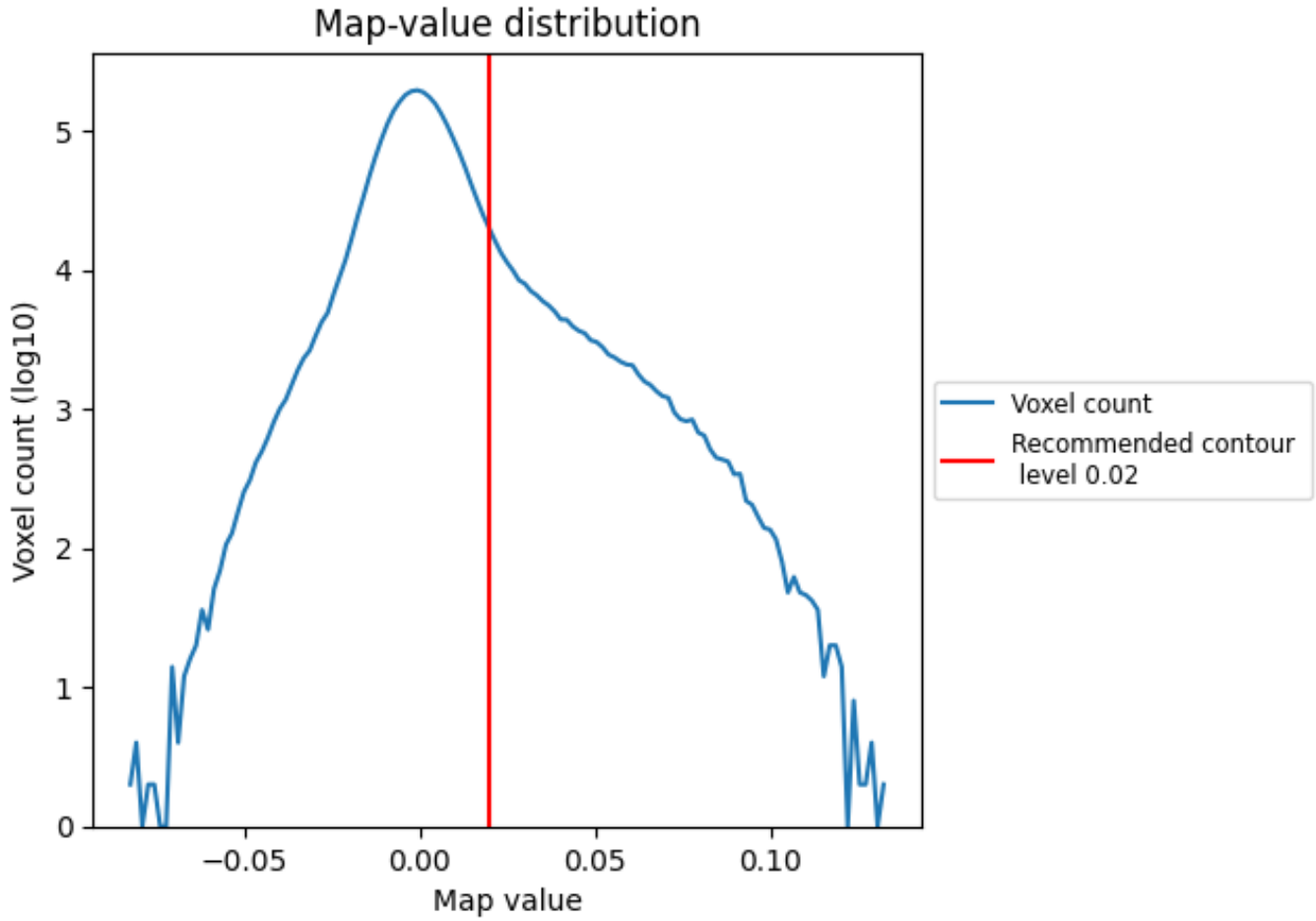
6.5 Mask visualisation (i)

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

7 Map analysis

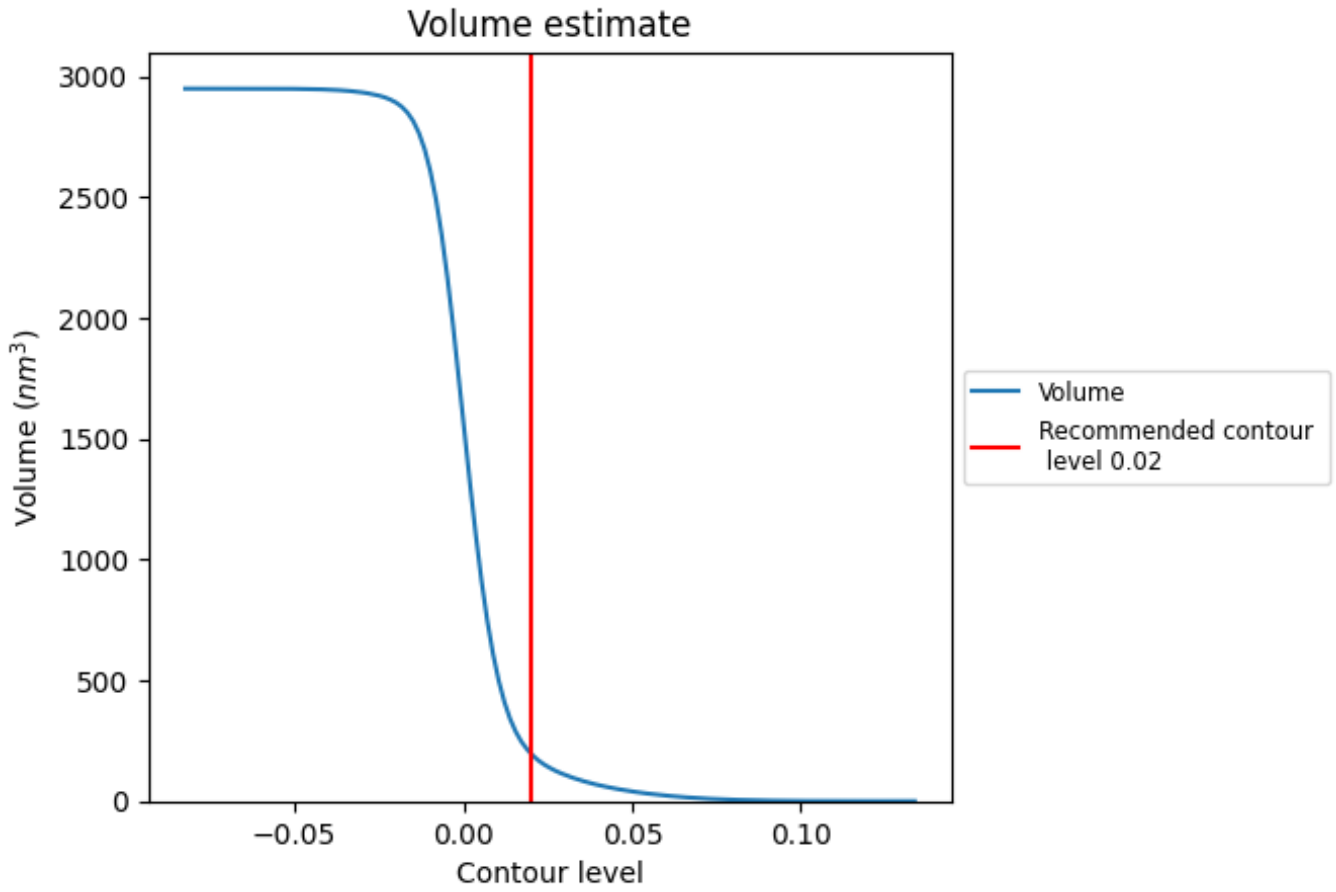
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)



The volume at the recommended contour level is 198 nm^3; this corresponds to an approximate mass of 179 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

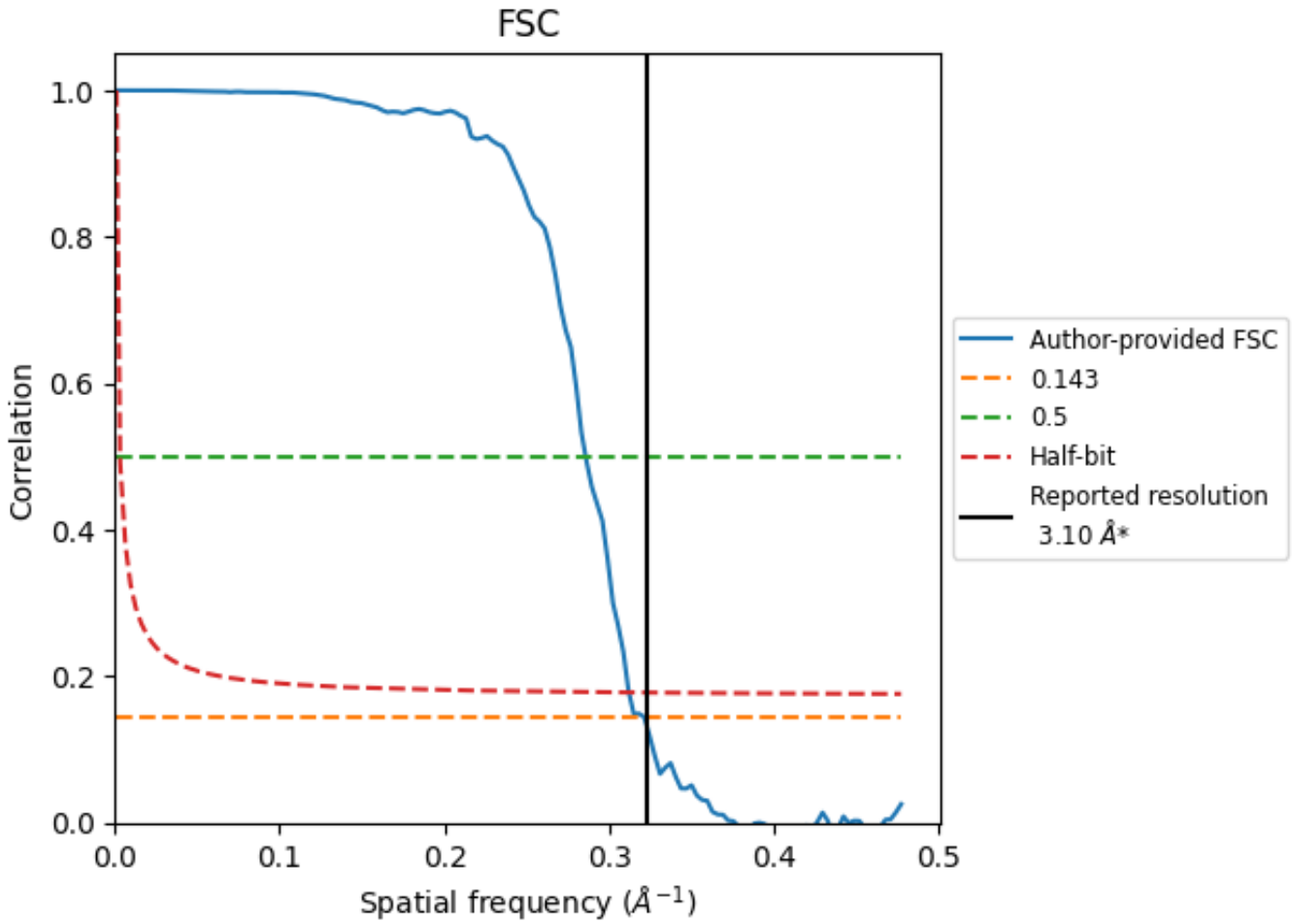
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

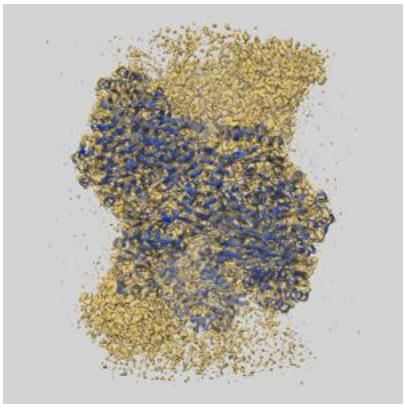
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.11	3.50	3.21
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

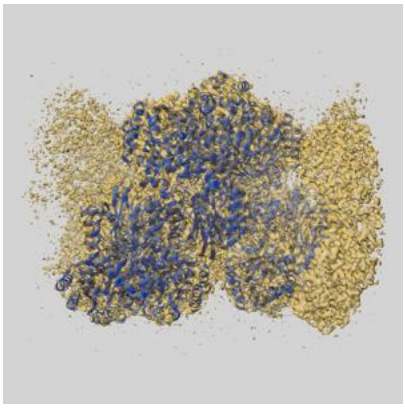
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11158 and PDB model 6ZBY. Per-residue inclusion information can be found in section 3 on page 6.

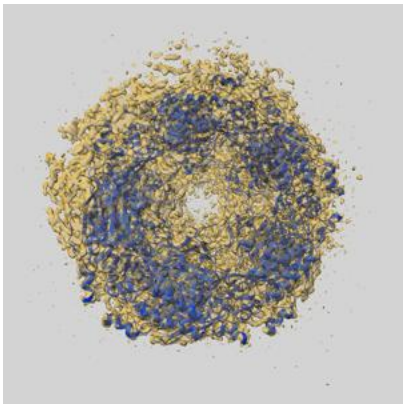
9.1 Map-model overlay



X



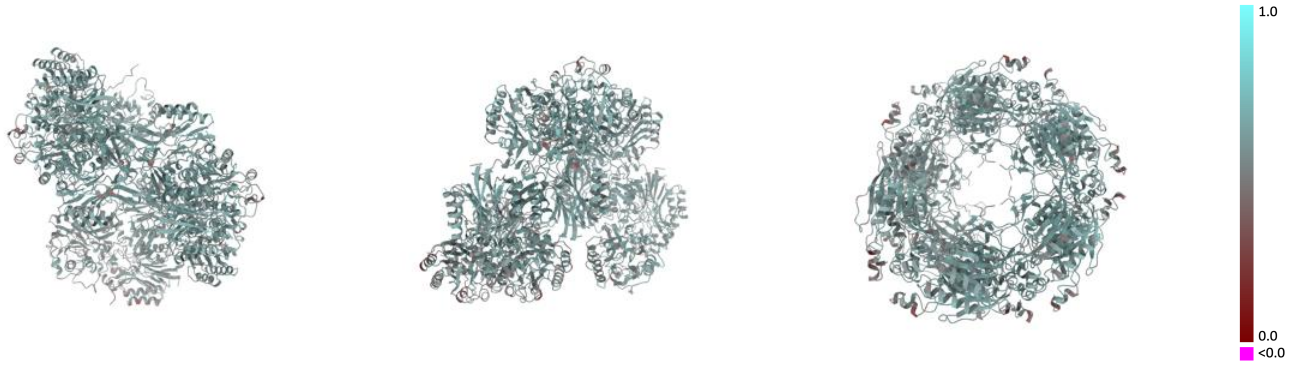
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

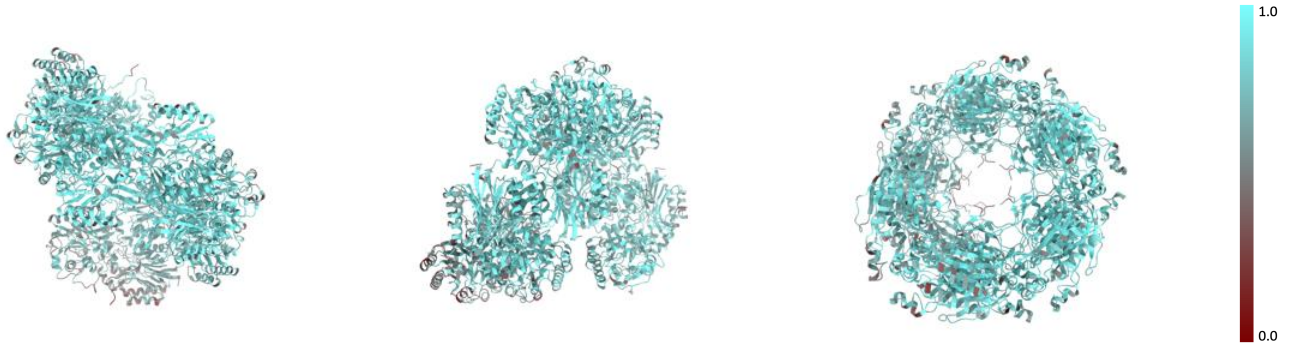
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

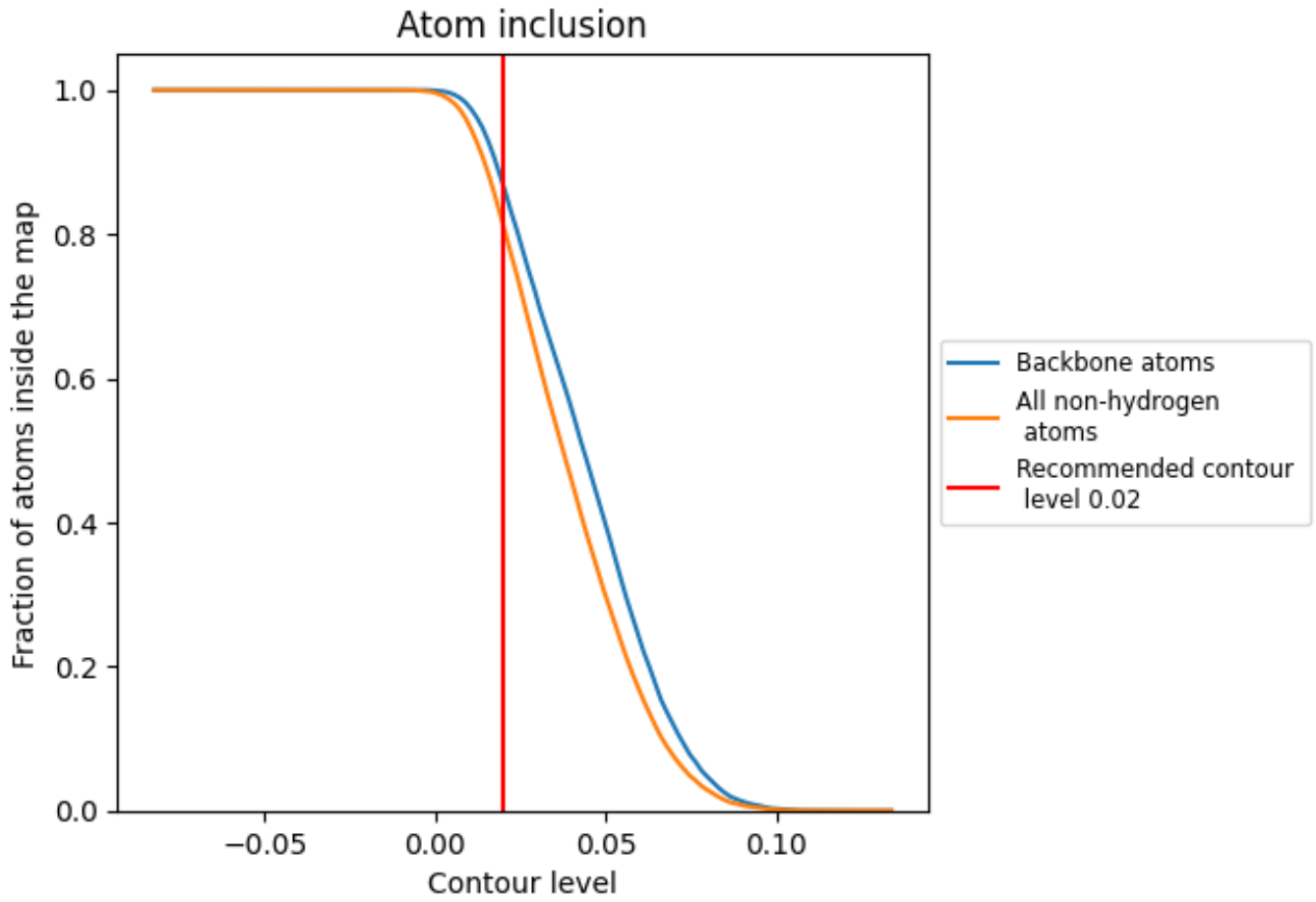
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8121	0.5720
A	0.6627	0.5180
B	0.6474	0.5260
C	0.7961	0.5600
D	0.8173	0.5770
E	0.8471	0.5830
F	0.8730	0.5940
G	0.8760	0.5930
H	0.8849	0.5930
I	0.8700	0.5930
J	0.8513	0.5850
K	0.8182	0.5790
L	0.8012	0.5610