



Full wwPDB EM Validation Report ⓘ

May 11, 2026 – 07:12 pm BST

PDB ID : 9TII / pdb_00009tii
EMDB ID : EMD-55957
Title : Phage 812 baseplate in the pre-contraction state - lower arm (segment C)
Authors : Binovsky, J.; Plevka, P.
Deposited on : 2025-12-05
Resolution : 6.00 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:

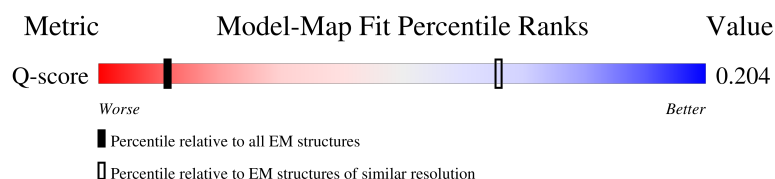
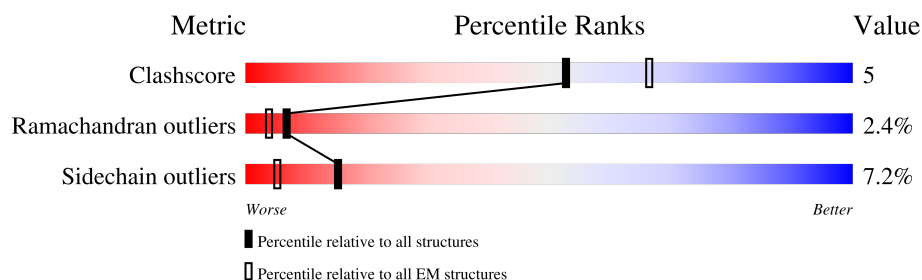
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 6.00 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	525 (5.50 - 6.50)

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	1019	
2	B	458	
2	C	458	
2	D	458	

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Mol	Chain	Length	Quality of chain
3	E	173	<div><div></div><div>24%73%22%<div><div></div><div></div><div></div></div></div></div>
3	H	173	<div><div></div><div>27%75%17%6%<div><div></div><div></div><div></div></div></div></div>
3	I	173	<div><div></div><div>16%76%18%<div><div></div><div></div><div></div></div></div></div>
3	J	173	<div><div></div><div>25%79%16%<div><div></div><div></div><div></div></div></div></div>
3	K	173	<div><div></div><div>36%82%13%<div><div></div><div></div><div></div></div></div></div>
3	L	173	<div><div></div><div>29%76%19%<div><div></div><div></div><div></div></div></div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11548 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 ORF63.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	282	Total	C	N	O	S	0	0
			2227	1414	357	454	2		

- Molecule 2 is a protein called ORF68.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	50	Total	C	N	O	S	0	0
			409	254	69	85	1		
2	C	50	Total	C	N	O	S	0	0
			409	254	69	85	1		
2	D	50	Total	C	N	O	S	0	0
			409	254	69	85	1		

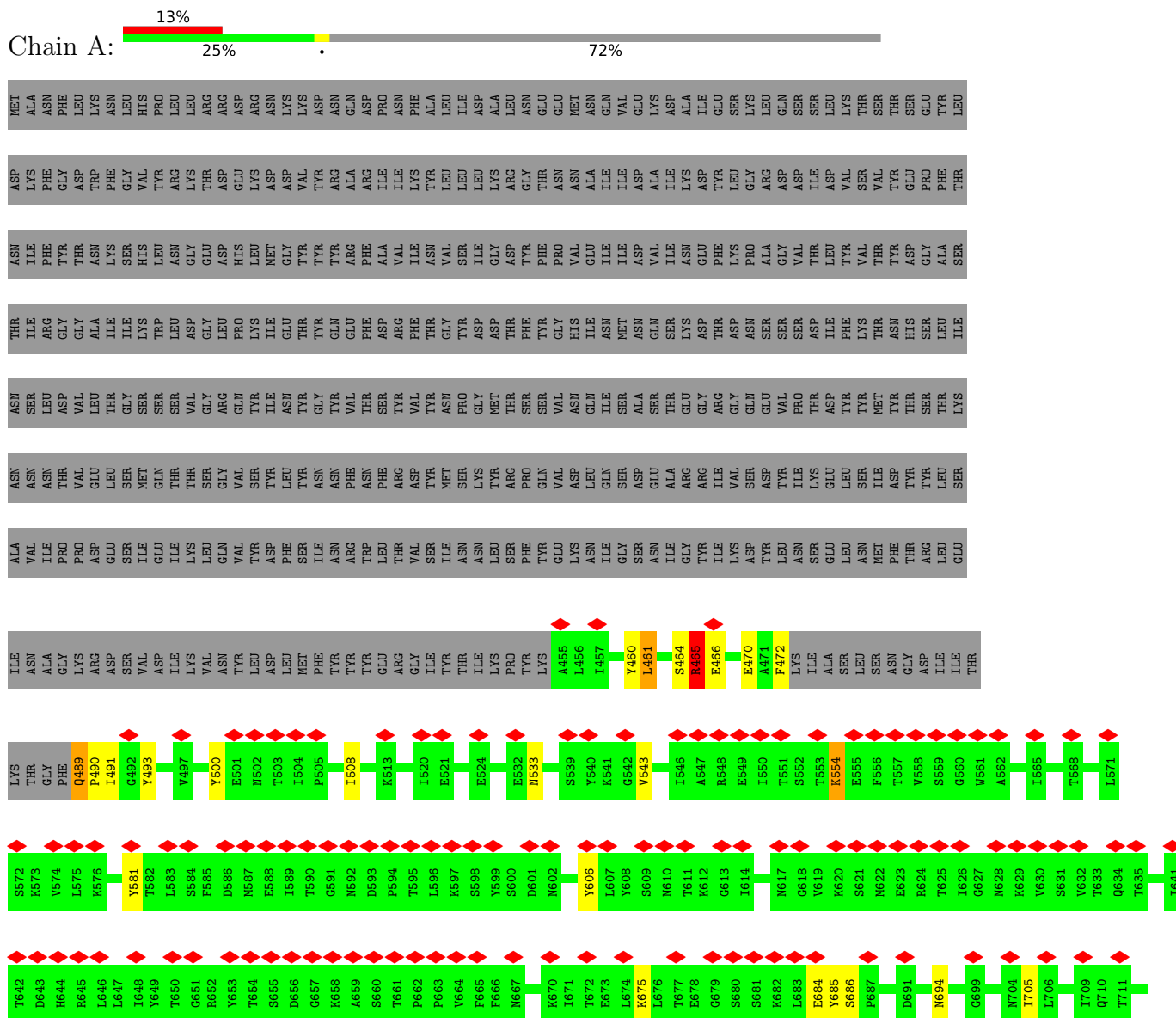
- Molecule 3 is a protein called ORF64.

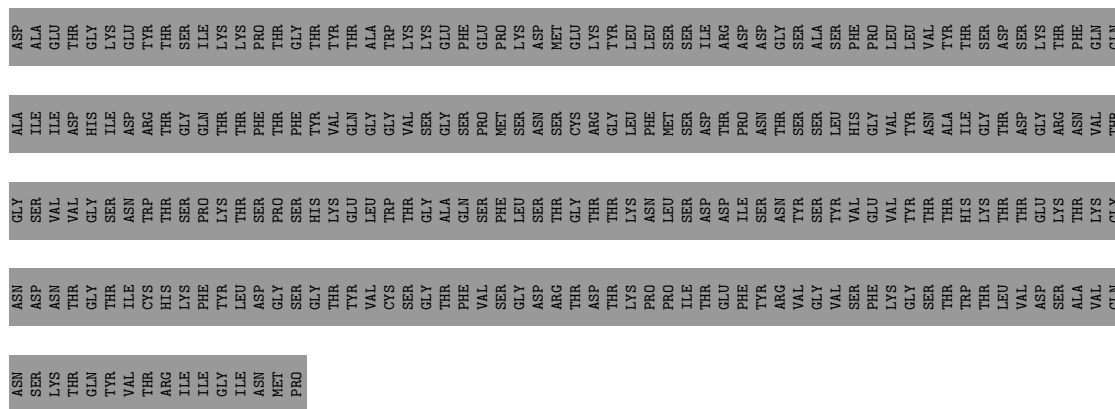
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
3	H	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
3	I	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
3	J	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
3	K	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
3	L	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		

3 Residue-property plots

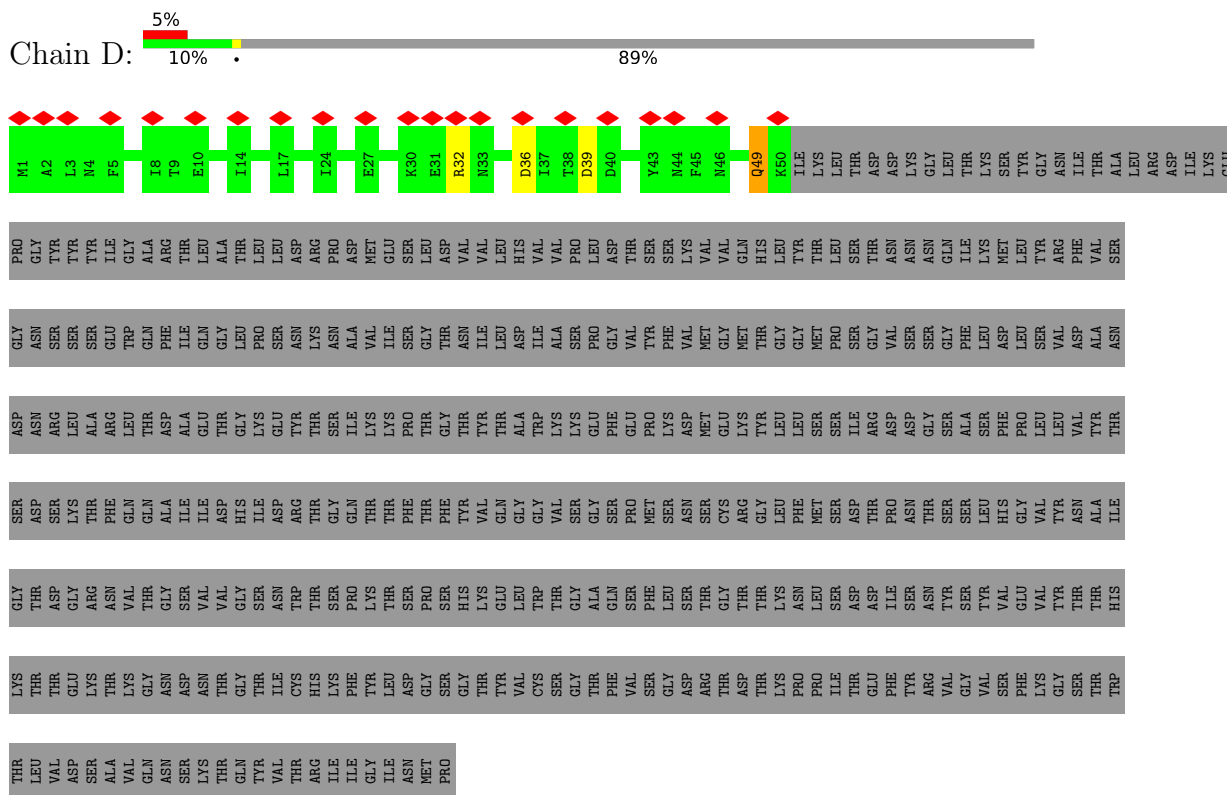
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: ORF63

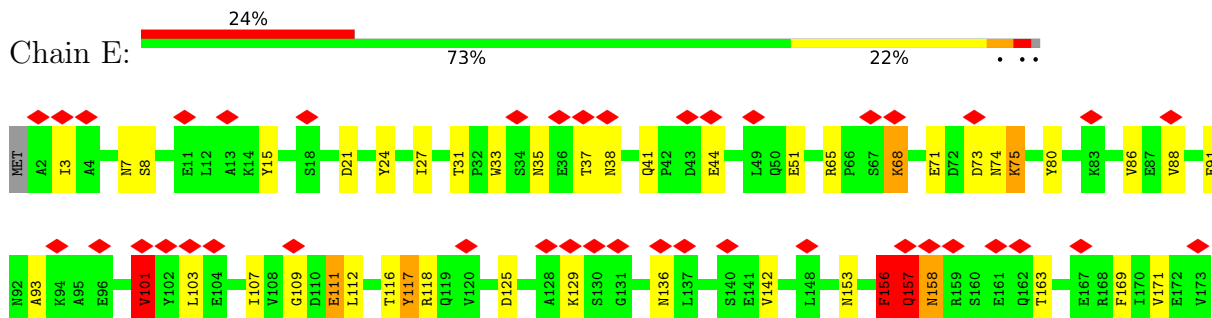





- Molecule 2: ORF68

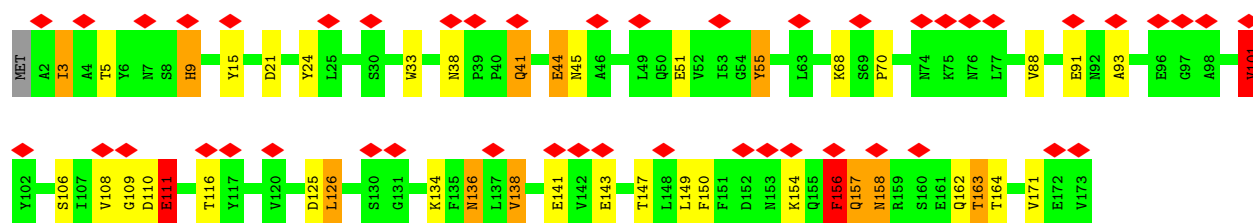


- Molecule 3: ORF64




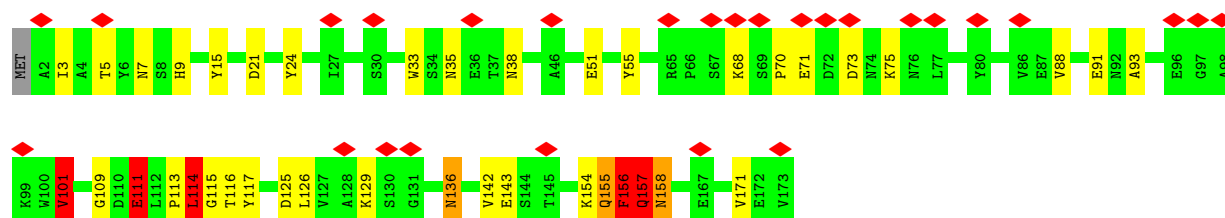
- Molecule 3: ORF64

Chain H: 




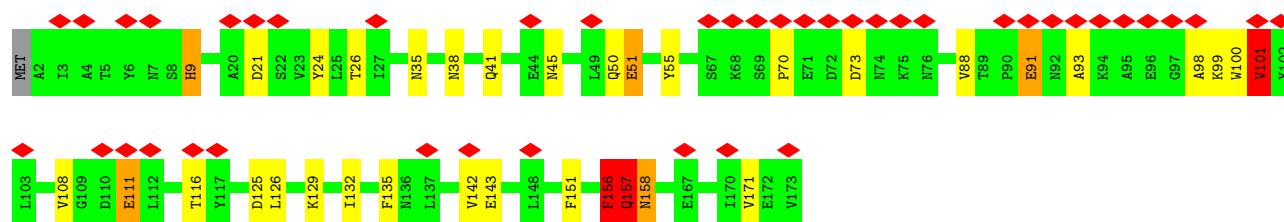
• Molecule 3: ORF64

Chain I: 




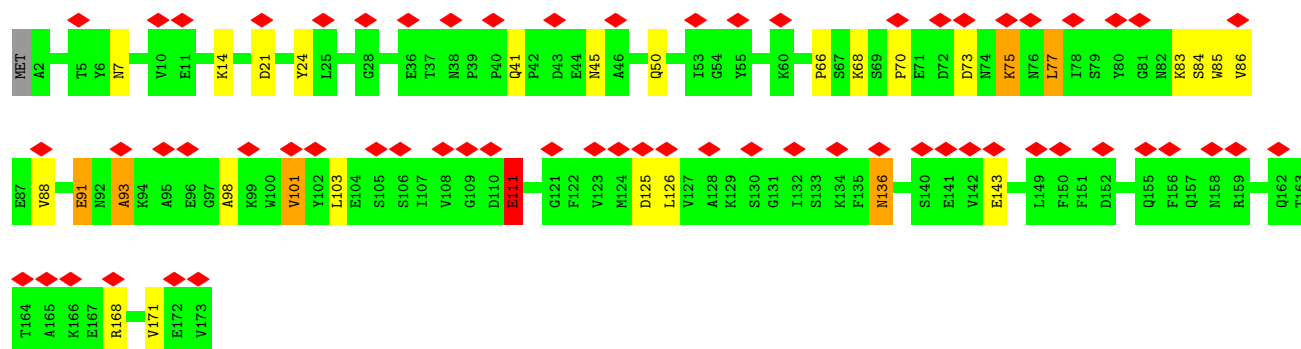
• Molecule 3: ORF64

Chain J: 




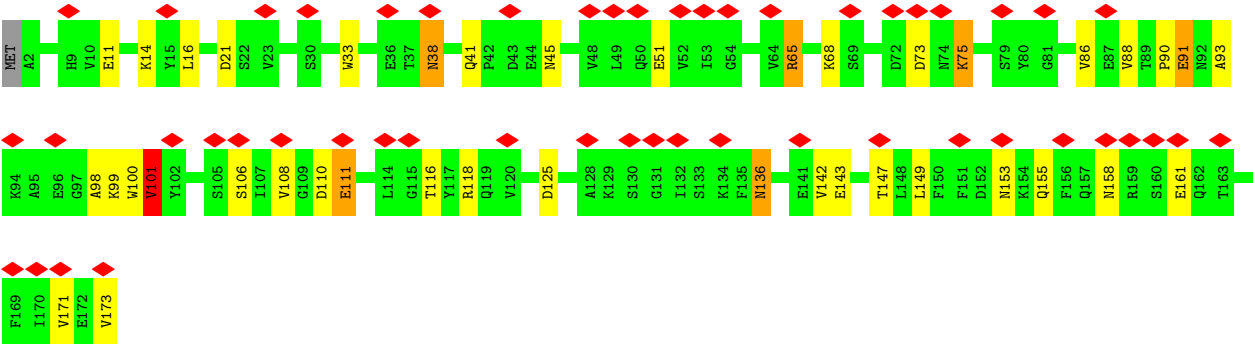
• Molecule 3: ORF64

Chain K: 



• Molecule 3: ORF64

Chain L: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	6229	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.129	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.035	Depositor
Map size (\AA)	300.096, 300.096, 300.096	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.6672001, 1.6672001, 1.6672001	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	0.76	0/2268	1.30	5/3087 (0.2%)
2	B	0.73	0/412	1.39	2/557 (0.4%)
2	C	0.75	0/412	1.44	1/557 (0.2%)
2	D	0.75	0/412	1.38	4/557 (0.7%)
3	E	0.76	0/1377	1.56	18/1872 (1.0%)
3	H	0.76	0/1377	1.62	17/1872 (0.9%)
3	I	0.74	0/1377	1.53	16/1872 (0.9%)
3	J	0.78	0/1377	1.55	14/1872 (0.7%)
3	K	0.75	0/1377	1.51	9/1872 (0.5%)
3	L	0.76	0/1377	1.53	11/1872 (0.6%)
All	All	0.76	0/11766	1.49	97/15990 (0.6%)

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	7
2	B	0	1
3	E	0	4
3	H	0	3
3	I	0	5
3	J	0	3
3	K	0	2
3	L	0	2
All	All	0	27

There are no bond length outliers.

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	101	VAL	CA-CB-CG1	12.58	131.79	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	101	VAL	CA-CB-CG1	12.52	131.68	110.40
3	J	101	VAL	CA-CB-CG1	11.62	130.16	110.40
3	L	101	VAL	CA-CB-CG1	10.86	128.87	110.40
3	L	21	ASP	CA-CB-CG	-10.53	102.07	112.60
3	K	101	VAL	CA-CB-CG1	10.50	128.25	110.40
3	J	21	ASP	CA-CB-CG	-10.18	102.42	112.60
3	E	21	ASP	CA-CB-CG	-9.20	103.40	112.60
3	I	158	ASN	OD1-CG-ND2	-9.11	113.49	122.60
3	I	158	ASN	CB-CG-ND2	8.48	129.12	116.40
3	K	21	ASP	CA-CB-CG	-8.26	104.34	112.60
3	J	156	PHE	CA-CB-CG	8.16	121.96	113.80
3	H	163	THR	CA-CB-CG2	8.15	124.36	110.50
3	H	158	ASN	OD1-CG-ND2	-8.02	114.58	122.60
3	H	158	ASN	CB-CG-ND2	7.95	128.32	116.40
3	E	158	ASN	CA-CB-CG	7.57	120.17	112.60
3	I	157	GLN	OE1-CD-NE2	-7.24	115.36	122.60
3	I	21	ASP	CA-CB-CG	-7.05	105.55	112.60
3	I	136	ASN	CA-CB-CG	6.96	119.56	112.60
2	B	32	ARG	NE-CZ-NH2	6.85	125.37	119.20
3	H	158	ASN	CA-CB-CG	6.80	119.40	112.60
3	H	156	PHE	CA-CB-CG	6.80	120.60	113.80
1	A	464	SER	N-CA-C	6.67	121.95	113.55
3	K	73	ASP	N-CA-C	6.66	121.00	112.34
3	L	143	GLU	CB-CG-CD	-6.57	101.43	112.60
3	H	21	ASP	CA-CB-CG	-6.54	106.06	112.60
3	K	136	ASN	CA-CB-CG	6.44	119.04	112.60
3	K	111	GLU	CB-CG-CD	6.19	123.12	112.60
3	E	158	ASN	N-CA-CB	6.17	118.68	110.29
3	H	158	ASN	N-CA-C	6.16	119.52	107.57
3	J	9	HIS	CA-CB-CG	6.07	119.87	113.80
3	E	65	ARG	NE-CZ-NH2	6.05	124.65	119.20
3	L	21	ASP	N-CA-C	6.02	119.72	112.38
3	L	155	GLN	OE1-CD-NE2	-6.02	116.58	122.60
3	H	136	ASN	CA-CB-CG	5.97	118.57	112.60
3	E	156	PHE	CA-CB-CG	5.91	119.71	113.80
1	A	734	TRP	N-CA-C	5.90	118.91	110.24
3	I	155	GLN	OE1-CD-NE2	-5.89	116.71	122.60
3	K	66	PRO	CB-CA-C	5.85	118.72	111.23
3	K	50	GLN	OE1-CD-NE2	-5.84	116.76	122.60
2	D	32	ARG	NE-CZ-NH2	5.82	124.43	119.20
3	E	158	ASN	CA-C-O	-5.78	115.50	122.03
3	E	153	ASN	OD1-CG-ND2	-5.77	116.83	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	136	ASN	OD1-CG-ND2	-5.76	116.84	122.60
3	H	111	GLU	CA-C-N	5.76	135.84	121.80
3	H	111	GLU	C-N-CA	5.76	135.84	121.80
3	L	106	SER	CA-C-N	5.74	127.04	121.65
3	L	106	SER	C-N-CA	5.74	127.04	121.65
1	A	461	LEU	CD1-CG-CD2	-5.73	98.19	110.80
3	E	31	THR	CA-C-N	5.67	125.67	119.89
3	E	31	THR	C-N-CA	5.67	125.67	119.89
3	K	7	ASN	CA-CB-CG	-5.65	106.95	112.60
3	L	51	GLU	CB-CG-CD	-5.57	103.14	112.60
3	E	157	GLN	OE1-CD-NE2	-5.53	117.07	122.60
3	H	106	SER	CA-C-N	5.51	126.83	121.65
3	H	106	SER	C-N-CA	5.51	126.83	121.65
3	J	157	GLN	CB-CG-CD	5.50	121.94	112.60
3	I	33	TRP	CA-CB-CG	5.49	124.03	113.60
3	L	65	ARG	NE-CZ-NH2	5.46	124.11	119.20
3	E	21	ASP	N-CA-C	5.45	119.19	112.54
3	I	21	ASP	N-CA-C	5.45	119.03	112.38
3	E	103	LEU	N-CA-CB	-5.42	101.32	110.49
3	E	65	ARG	NE-CZ-NH1	-5.39	116.11	121.50
3	E	158	ASN	OD1-CG-ND2	-5.39	117.21	122.60
3	J	51	GLU	CB-CG-CD	-5.38	103.45	112.60
3	H	9	HIS	CA-CB-CG	5.35	119.15	113.80
3	J	111	GLU	CA-C-N	5.35	134.85	121.80
3	J	111	GLU	C-N-CA	5.35	134.85	121.80
1	A	489	GLN	OE1-CD-NE2	-5.32	117.28	122.60
2	C	32	ARG	NE-CZ-NH2	5.31	123.98	119.20
3	J	157	GLN	CA-CB-CG	5.31	124.71	114.10
1	A	466	GLU	CB-CG-CD	5.30	121.62	112.60
3	E	158	ASN	CB-CG-ND2	5.30	124.35	116.40
2	D	49	GLN	OE1-CD-NE2	-5.29	117.31	122.60
3	J	35	ASN	OD1-CG-ND2	-5.29	117.31	122.60
3	I	111	GLU	CA-C-N	5.28	134.69	121.80
3	I	111	GLU	C-N-CA	5.28	134.69	121.80
3	H	138	VAL	CA-C-N	5.25	124.70	119.24
3	H	138	VAL	C-N-CA	5.25	124.70	119.24
2	D	39	ASP	CA-CB-CG	5.24	117.84	112.60
3	J	132	ILE	CB-CA-C	5.22	118.69	111.38
3	E	136	ASN	CA-CB-CG	5.22	117.82	112.60
3	J	50	GLN	OE1-CD-NE2	-5.21	117.39	122.60
3	E	169	PHE	CA-CB-CG	5.16	118.96	113.80
2	B	20	GLN	OE1-CD-NE2	-5.15	117.45	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	151	PHE	CA-CB-CG	5.15	118.95	113.80
3	L	136	ASN	CA-CB-CG	5.13	117.73	112.60
3	K	103	LEU	N-CA-CB	-5.13	101.81	110.49
3	E	101	VAL	CA-CB-CG1	5.12	119.11	110.40
3	I	114	LEU	N-CA-C	5.12	121.71	110.80
3	H	21	ASP	N-CA-C	5.08	118.74	112.54
3	I	71	GLU	CB-CG-CD	-5.06	104.00	112.60
3	J	158	ASN	N-CA-C	5.05	116.63	111.03
2	D	36	ASP	CA-CB-CG	5.04	117.64	112.60
3	I	157	GLN	CG-CD-NE2	5.03	123.94	116.40
3	L	153	ASN	OD1-CG-ND2	-5.02	117.58	122.60
3	I	35	ASN	OD1-CG-ND2	-5.02	117.58	122.60

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	460	TYR	Sidechain
1	A	465	ARG	Sidechain
1	A	493	TYR	Sidechain
1	A	500	TYR	Sidechain
1	A	581	TYR	Sidechain
1	A	606	TYR	Sidechain
1	A	726	TYR	Sidechain
2	B	32	ARG	Sidechain
3	E	117	TYR	Sidechain
3	E	156	PHE	Sidechain
3	E	24	TYR	Sidechain
3	E	80	TYR	Sidechain
3	H	156	PHE	Sidechain
3	H	55	TYR	Sidechain
3	H	9	HIS	Sidechain
3	I	117	TYR	Sidechain
3	I	15	TYR	Sidechain
3	I	24	TYR	Sidechain
3	I	55	TYR	Sidechain
3	I	9	HIS	Sidechain
3	J	135	PHE	Sidechain
3	J	24	TYR	Sidechain
3	J	9	HIS	Sidechain
3	K	168	ARG	Sidechain
3	K	24	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	L	38	ASN	Sidechain
3	L	65	ARG	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	2227	0	2212	16	0
2	B	409	0	404	0	0
2	C	409	0	404	1	0
2	D	409	0	404	0	0
3	E	1349	0	1339	44	0
3	H	1349	0	1339	41	0
3	I	1349	0	1339	33	0
3	J	1349	0	1339	28	0
3	K	1349	0	1339	10	0
3	L	1349	0	1339	15	0
All	All	11548	0	11458	122	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 5.

All (122) 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)
3:E:158:ASN:HB2	3:I:157:GLN:HA	1.36	1.06
3:E:157:GLN:HA	3:I:158:ASN:HB2	1.40	1.01
1:A:705:ILE:O	3:I:113:PRO:HB3	1.67	0.95
3:H:158:ASN:HB2	3:J:157:GLN:HA	1.52	0.90
3:E:157:GLN:HA	3:I:158:ASN:CB	2.05	0.86
3:L:101:VAL:HB	3:L:171:VAL:HG22	1.58	0.86
3:E:157:GLN:CA	3:I:158:ASN:HB2	2.06	0.85
3:K:101:VAL:HB	3:K:171:VAL:HG22	1.59	0.84
3:H:158:ASN:HB2	3:J:157:GLN:HG2	1.60	0.84
3:H:158:ASN:HB2	3:J:157:GLN:CA	2.09	0.82
3:E:7:ASN:HB3	3:H:147:THR:HG23	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:158:ASN:CB	3:J:157:GLN:HA	2.11	0.80
3:J:101:VAL:HB	3:J:171:VAL:HG22	1.64	0.79
3:I:101:VAL:HB	3:I:171:VAL:HG22	1.64	0.77
1:A:733:SER:HB3	3:E:35:ASN:OD1	1.86	0.75
1:A:733:SER:HB2	3:E:37:THR:HG23	1.69	0.74
3:E:158:ASN:CB	3:I:157:GLN:HA	2.18	0.73
3:L:101:VAL:HB	3:L:171:VAL:CG2	2.19	0.72
3:H:101:VAL:HB	3:H:171:VAL:HG22	1.72	0.71
3:K:91:GLU:CD	3:K:91:GLU:H	1.99	0.70
3:K:101:VAL:HB	3:K:171:VAL:CG2	2.21	0.70
3:E:158:ASN:HB2	3:I:157:GLN:CA	2.18	0.70
1:A:733:SER:HB3	3:E:35:ASN:CG	2.18	0.69
3:E:157:GLN:CB	3:I:158:ASN:HB2	2.23	0.68
1:A:705:ILE:HD12	3:I:115:GLY:H	1.59	0.67
1:A:554:LYS:HE2	1:A:685:TYR:CE2	2.29	0.67
3:H:158:ASN:CB	3:J:157:GLN:HG2	2.27	0.65
3:K:77:LEU:HB2	3:L:38:ASN:CG	2.23	0.63
3:E:91:GLU:H	3:E:91:GLU:CD	2.06	0.63
3:I:7:ASN:HB3	3:L:147:THR:CG2	2.29	0.62
3:L:99:LYS:HE3	3:L:100:TRP:CZ2	2.36	0.61
1:A:733:SER:HB2	3:E:37:THR:CG2	2.32	0.59
3:E:163:THR:HG21	3:I:157:GLN:HG3	1.85	0.59
3:E:158:ASN:N	3:I:158:ASN:HD22	2.01	0.58
3:H:163:THR:HG21	3:J:157:GLN:HE21	1.69	0.58
3:E:157:GLN:CG	3:I:158:ASN:HB2	2.34	0.58
1:A:461:LEU:HG	3:H:163:THR:HG22	1.87	0.56
3:H:163:THR:HG21	3:J:157:GLN:NE2	2.21	0.56
3:E:158:ASN:C	3:I:157:GLN:HG2	2.31	0.55
3:J:101:VAL:HB	3:J:171:VAL:CG2	2.35	0.55
1:A:461:LEU:CG	3:H:163:THR:HG22	2.37	0.55
3:H:158:ASN:CG	3:J:157:GLN:HA	2.31	0.55
3:H:158:ASN:O	3:J:157:GLN:HG2	2.08	0.54
3:H:158:ASN:OD1	3:J:156:PHE:CG	2.61	0.54
3:H:157:GLN:HG3	3:J:158:ASN:HB2	1.90	0.54
1:A:554:LYS:HE2	1:A:685:TYR:CD2	2.42	0.54
3:E:157:GLN:HG3	3:I:158:ASN:CB	2.38	0.53
3:J:129:LYS:HE3	3:J:142:VAL:O	2.08	0.53
3:E:158:ASN:HD22	3:I:157:GLN:CA	2.22	0.52
3:E:27:ILE:HD11	3:E:117:TYR:CE2	2.45	0.52
3:I:101:VAL:HB	3:I:171:VAL:CG2	2.39	0.52
3:I:5:THR:HG23	3:L:149:LEU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:84:SER:HB3	3:L:41:GLN:HG3	1.91	0.51
3:E:158:ASN:HB3	3:I:156:PHE:CD1	2.46	0.51
3:H:156:PHE:CG	3:J:158:ASN:ND2	2.78	0.51
3:E:157:GLN:HG3	3:I:158:ASN:HB3	1.92	0.51
3:H:149:LEU:HD23	3:H:150:PHE:CE2	2.45	0.51
3:E:157:GLN:HA	3:I:158:ASN:CG	2.36	0.51
3:E:158:ASN:HD22	3:I:157:GLN:C	2.18	0.51
3:K:75:LYS:HE2	3:K:86:VAL:CG2	2.41	0.50
1:A:705:ILE:HD12	3:I:115:GLY:N	2.26	0.50
3:H:158:ASN:HB2	3:J:157:GLN:CG	2.35	0.50
3:H:158:ASN:ND2	3:J:157:GLN:HA	2.27	0.49
3:H:157:GLN:HG2	3:J:158:ASN:H	1.78	0.49
3:H:158:ASN:HD22	3:J:157:GLN:HA	1.77	0.49
3:H:158:ASN:CA	3:J:157:GLN:HG2	2.43	0.49
3:E:157:GLN:CG	3:I:158:ASN:CB	2.91	0.48
3:E:157:GLN:C	3:I:158:ASN:HD22	2.22	0.48
3:J:41:GLN:H	3:J:41:GLN:CD	2.21	0.48
3:K:14:LYS:HE2	3:K:93:ALA:HB3	1.95	0.48
3:H:109:GLY:H	3:H:164:THR:HA	1.78	0.48
1:A:705:ILE:HB	3:I:114:LEU:N	2.29	0.48
3:L:91:GLU:CD	3:L:91:GLU:N	2.72	0.48
3:E:116:THR:HG22	3:E:158:ASN:HA	1.96	0.47
3:H:158:ASN:H	3:J:157:GLN:CD	2.22	0.47
3:J:99:LYS:HE3	3:J:100:TRP:CZ2	2.50	0.47
3:E:44:GLU:HB3	3:H:3:ILE:HG13	1.96	0.47
3:E:8:SER:HB3	3:H:149:LEU:CD1	2.45	0.47
1:A:461:LEU:CD2	3:H:163:THR:HG22	2.44	0.46
1:A:490:PRO:C	1:A:491:ILE:HG13	2.41	0.46
3:I:116:THR:HG22	3:I:158:ASN:HA	1.96	0.46
3:E:3:ILE:HD12	3:H:44:GLU:HA	1.99	0.45
3:H:158:ASN:HB2	3:J:157:GLN:CB	2.46	0.45
3:I:91:GLU:N	3:I:91:GLU:CD	2.74	0.45
3:J:116:THR:HG22	3:J:158:ASN:HA	1.98	0.45
3:E:158:ASN:HD22	3:I:157:GLN:N	2.15	0.45
3:E:101:VAL:HB	3:E:171:VAL:CG2	2.47	0.45
3:H:24:TYR:CD1	3:H:126:LEU:HD21	2.52	0.45
3:E:75:LYS:HE2	3:E:86:VAL:CG2	2.46	0.45
3:E:8:SER:HB3	3:H:149:LEU:HD12	1.99	0.45
3:H:91:GLU:CD	3:H:91:GLU:N	2.75	0.45
3:I:129:LYS:HE3	3:I:142:VAL:O	2.17	0.44
3:J:91:GLU:N	3:J:91:GLU:CD	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:75:LYS:HE2	3:L:86:VAL:CG2	2.47	0.44
3:E:7:ASN:HB3	3:H:147:THR:CG2	2.42	0.44
3:E:8:SER:CB	3:H:149:LEU:CD1	2.95	0.44
2:C:45:PHE:CE2	2:C:50:LYS:HE2	2.53	0.44
3:K:83:LYS:HB3	3:K:85:TRP:HE1	1.82	0.44
3:E:101:VAL:HB	3:E:171:VAL:HG22	1.99	0.44
3:E:129:LYS:HE3	3:E:142:VAL:O	2.18	0.43
3:I:7:ASN:HB3	3:L:147:THR:HG23	1.99	0.43
3:K:91:GLU:CD	3:K:91:GLU:N	2.73	0.43
3:H:138:VAL:H	3:H:141:GLU:CD	2.27	0.43
3:L:75:LYS:HE2	3:L:86:VAL:HG22	2.00	0.43
1:A:675:LYS:HE3	1:A:686:SER:H	1.83	0.42
3:H:41:GLN:CD	3:H:41:GLN:N	2.78	0.42
3:K:84:SER:C	3:K:85:TRP:CD1	2.98	0.42
3:L:116:THR:HG22	3:L:158:ASN:HA	2.01	0.42
3:H:158:ASN:C	3:J:157:GLN:HG2	2.45	0.42
3:J:26:THR:HB	3:J:55:TYR:CD2	2.55	0.41
3:E:15:TYR:HB2	3:H:15:TYR:CZ	2.55	0.41
3:E:156:PHE:CD2	3:I:158:ASN:ND2	2.88	0.41
3:E:33:TRP:CD1	3:E:118:ARG:HD3	2.56	0.41
1:A:684:GLU:OE1	1:A:684:GLU:HA	2.20	0.41
3:E:112:LEU:HD23	3:E:112:LEU:HA	1.92	0.41
3:E:68:LYS:HZ3	3:E:71:GLU:CD	2.28	0.41
3:H:116:THR:HG22	3:H:158:ASN:HA	2.03	0.40
3:L:33:TRP:CD1	3:L:118:ARG:HD3	2.56	0.40
3:E:44:GLU:O	3:H:5:THR:HB	2.22	0.40
3:H:134:LYS:HZ1	3:H:141:GLU:CD	2.29	0.40
3:L:16:LEU:CD1	3:L:173:VAL:HG21	2.51	0.40
3:L:14:LYS:HE2	3:L:90:PRO:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	278/1019 (27%)	262 (94%)	14 (5%)	2 (1%)	18	56
2	B	48/458 (10%)	47 (98%)	1 (2%)	0	100	100
2	C	48/458 (10%)	46 (96%)	2 (4%)	0	100	100
2	D	48/458 (10%)	45 (94%)	3 (6%)	0	100	100
3	E	170/173 (98%)	144 (85%)	22 (13%)	4 (2%)	4	27
3	H	170/173 (98%)	145 (85%)	19 (11%)	6 (4%)	3	20
3	I	170/173 (98%)	145 (85%)	18 (11%)	7 (4%)	2	17
3	J	170/173 (98%)	142 (84%)	21 (12%)	7 (4%)	2	17
3	K	170/173 (98%)	149 (88%)	17 (10%)	4 (2%)	4	27
3	L	170/173 (98%)	147 (86%)	18 (11%)	5 (3%)	3	23
All	All	1442/3431 (42%)	1272 (88%)	135 (9%)	35 (2%)	7	27

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	93	ALA
3	E	111	GLU
3	H	33	TRP
3	H	93	ALA
3	I	93	ALA
3	I	114	LEU
3	J	93	ALA
3	J	157	GLN
3	K	93	ALA
3	L	93	ALA
3	L	111	GLU
3	H	110	ASP
3	H	111	GLU
3	I	111	GLU
3	I	156	PHE
3	J	73	ASP
3	J	111	GLU
3	E	73	ASP
3	H	156	PHE
3	I	73	ASP
3	L	110	ASP
1	A	694	ASN
3	E	109	GLY
3	I	70	PRO

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Mol	Chain	Res	Type
3	J	98	ALA
1	A	465	ARG
3	J	70	PRO
3	J	156	PHE
3	K	98	ALA
3	L	73	ASP
3	K	70	PRO
3	K	111	GLU
3	L	98	ALA
3	I	109	GLY
3	H	70	PRO

5.3.2 Protein sidechains ⓘ

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	257/928 (28%)	248 (96%)	9 (4%)	32	53
2	B	48/405 (12%)	47 (98%)	1 (2%)	47	65
2	C	48/405 (12%)	48 (100%)	0	100	100
2	D	48/405 (12%)	47 (98%)	1 (2%)	47	65
3	E	152/153 (99%)	140 (92%)	12 (8%)	11	32
3	H	152/153 (99%)	133 (88%)	19 (12%)	4	16
3	I	152/153 (99%)	136 (90%)	16 (10%)	6	22
3	J	152/153 (99%)	141 (93%)	11 (7%)	13	35
3	K	152/153 (99%)	140 (92%)	12 (8%)	11	32
3	L	152/153 (99%)	139 (91%)	13 (9%)	10	29
All	All	1313/3061 (43%)	1219 (93%)	94 (7%)	15	35

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	465	ARG
1	A	470	GLU

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Mol	Chain	Res	Type
1	A	472	PHE
1	A	489	GLN
1	A	508	ILE
1	A	533	ASN
1	A	543	VAL
1	A	554	LYS
1	A	718	THR
2	B	31	GLU
2	D	49	GLN
3	E	38	ASN
3	E	41	GLN
3	E	51	GLU
3	E	68	LYS
3	E	74	ASN
3	E	75	LYS
3	E	88	VAL
3	E	101	VAL
3	E	107	ILE
3	E	111	GLU
3	E	125	ASP
3	E	157	GLN
3	H	3	ILE
3	H	38	ASN
3	H	41	GLN
3	H	44	GLU
3	H	45	ASN
3	H	51	GLU
3	H	55	TYR
3	H	68	LYS
3	H	88	VAL
3	H	101	VAL
3	H	108	VAL
3	H	111	GLU
3	H	125	ASP
3	H	126	LEU
3	H	136	ASN
3	H	143	GLU
3	H	154	LYS
3	H	157	GLN
3	H	162	GLN
3	I	3	ILE
3	I	38	ASN

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Mol	Chain	Res	Type
3	I	51	GLU
3	I	68	LYS
3	I	75	LYS
3	I	88	VAL
3	I	101	VAL
3	I	111	GLU
3	I	125	ASP
3	I	126	LEU
3	I	136	ASN
3	I	143	GLU
3	I	154	LYS
3	I	155	GLN
3	I	156	PHE
3	I	157	GLN
3	J	38	ASN
3	J	45	ASN
3	J	51	GLU
3	J	88	VAL
3	J	91	GLU
3	J	101	VAL
3	J	108	VAL
3	J	125	ASP
3	J	126	LEU
3	J	143	GLU
3	J	156	PHE
3	K	41	GLN
3	K	45	ASN
3	K	68	LYS
3	K	75	LYS
3	K	77	LEU
3	K	88	VAL
3	K	91	GLU
3	K	111	GLU
3	K	125	ASP
3	K	126	LEU
3	K	136	ASN
3	K	143	GLU
3	L	11	GLU
3	L	45	ASN
3	L	68	LYS
3	L	75	LYS
3	L	88	VAL

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Mol	Chain	Res	Type
3	L	91	GLU
3	L	101	VAL
3	L	108	VAL
3	L	111	GLU
3	L	125	ASP
3	L	136	ASN
3	L	142	VAL
3	L	161	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	49	GLN
3	E	7	ASN
3	E	38	ASN
3	E	74	ASN
3	E	153	ASN
3	E	155	GLN
3	E	157	GLN
3	E	158	ASN
3	H	38	ASN
3	H	158	ASN
3	H	162	GLN
3	I	7	ASN
3	I	38	ASN
3	I	50	GLN
3	I	119	GLN
3	I	158	ASN
3	I	162	GLN
3	J	7	ASN
3	J	38	ASN
3	J	119	GLN
3	J	153	ASN
3	K	7	ASN
3	K	153	ASN
3	L	50	GLN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

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.

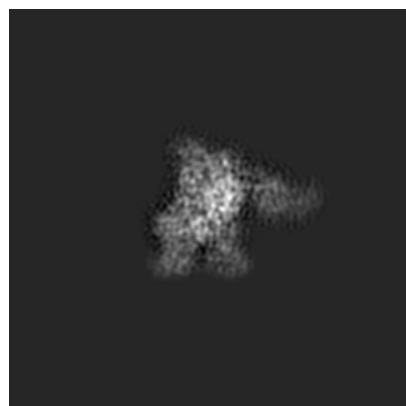
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55957. These allow visual inspection of the internal detail of the map and identification of artifacts.

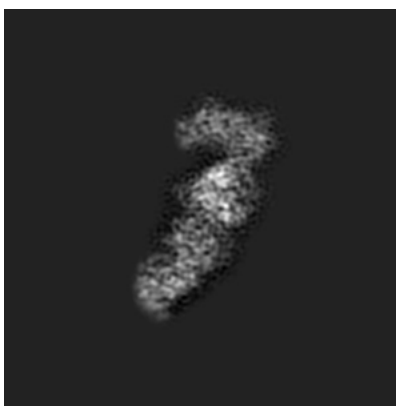
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

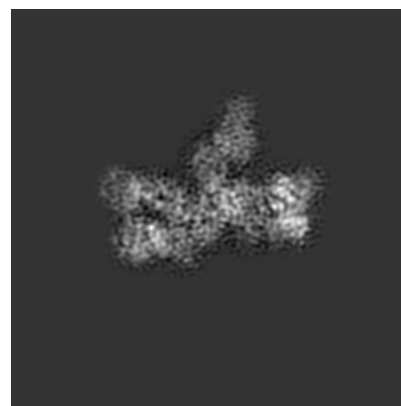
6.1.1 Primary map



X

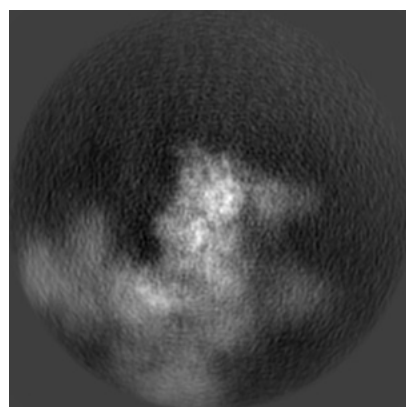


Y

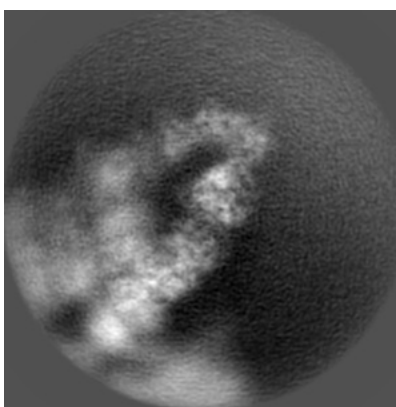


Z

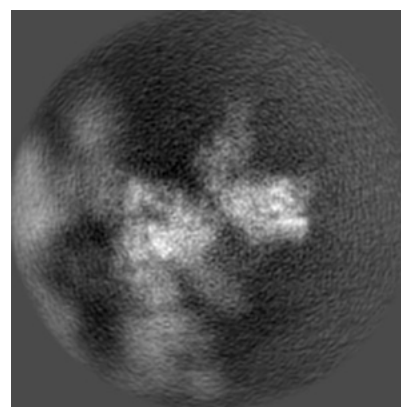
6.1.2 Raw map



X



Y

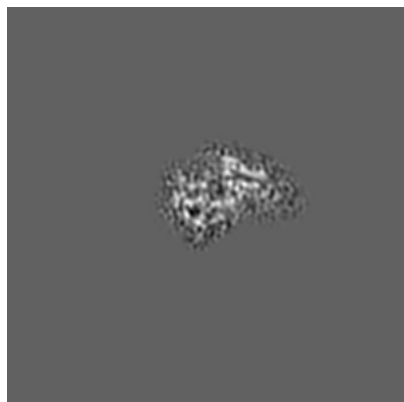


Z

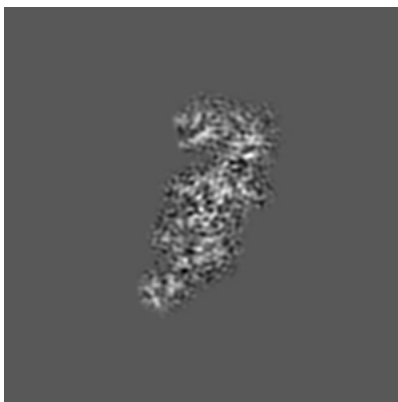
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

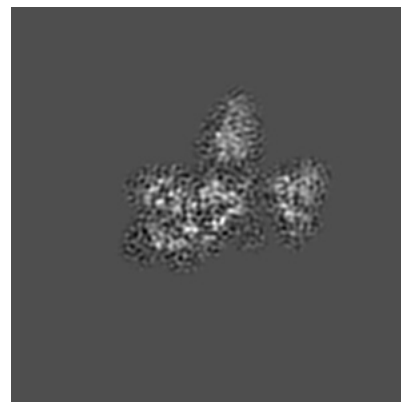
6.2.1 Primary map



X Index: 90

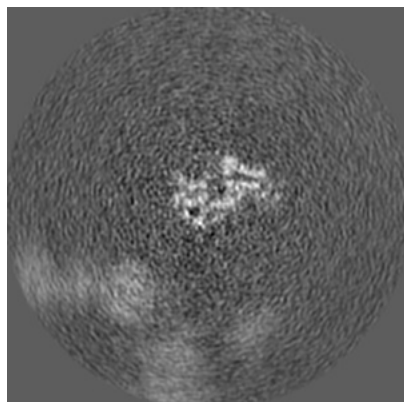


Y Index: 90

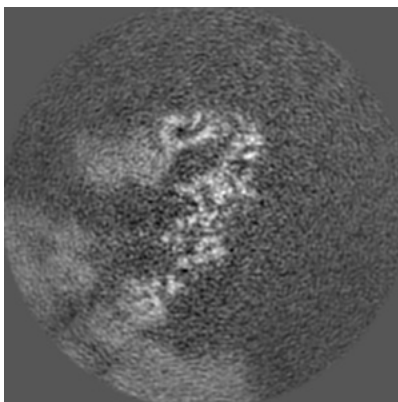


Z Index: 90

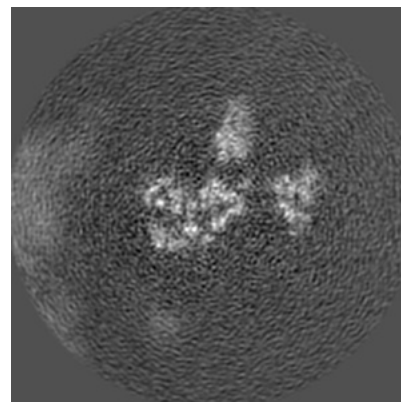
6.2.2 Raw map



X Index: 90



Y Index: 90

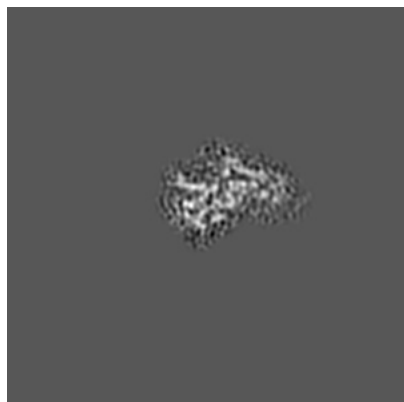


Z Index: 90

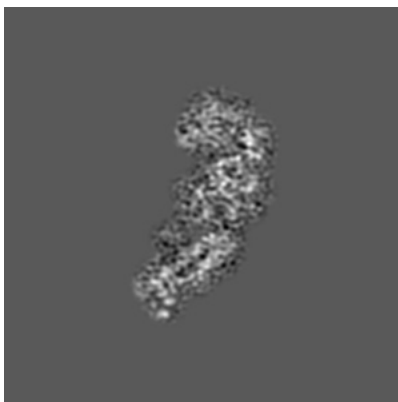
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

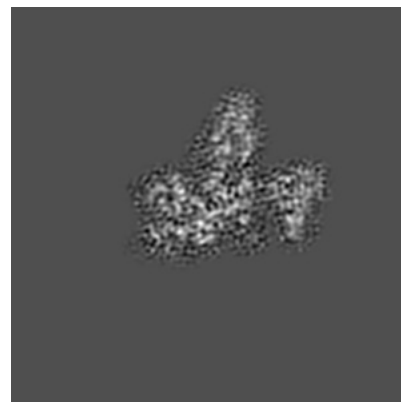
6.3.1 Primary map



X Index: 91

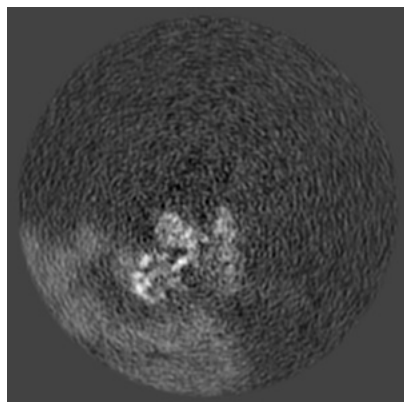


Y Index: 97

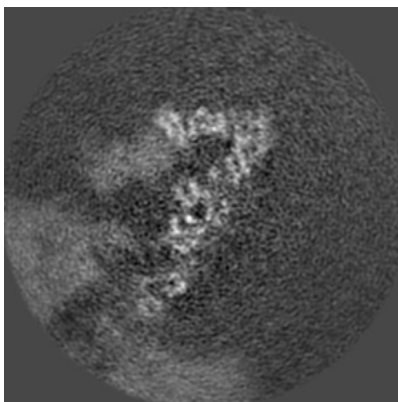


Z Index: 93

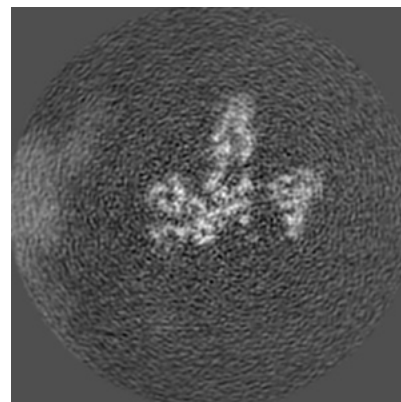
6.3.2 Raw map



X Index: 57



Y Index: 85

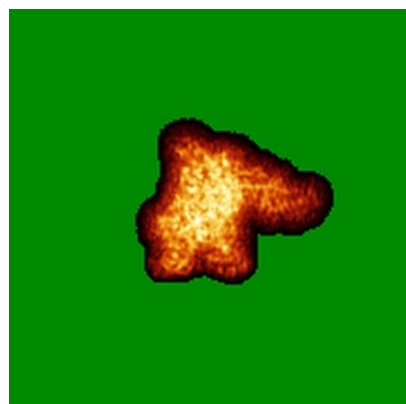


Z Index: 93

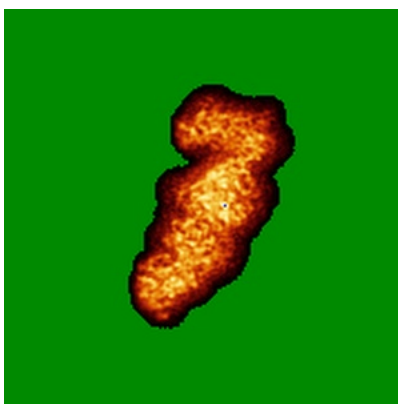
The images above show the largest variance slices of the map in three orthogonal directions.

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

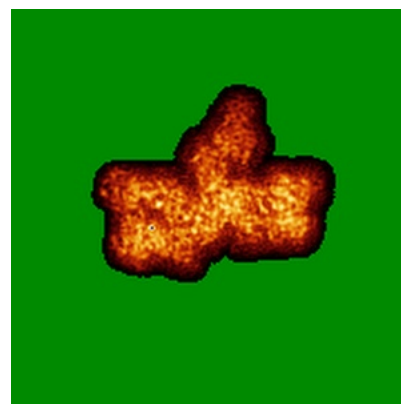
6.4.1 Primary map



X

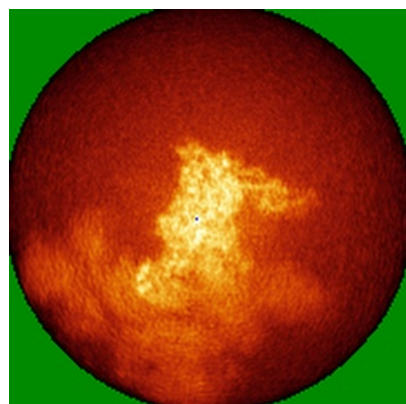


Y

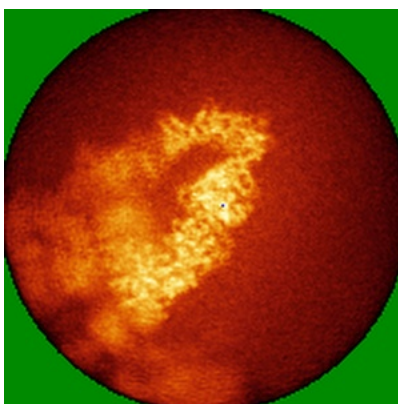


Z

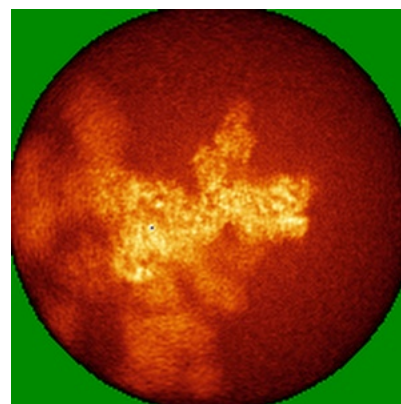
6.4.2 Raw map



X



Y

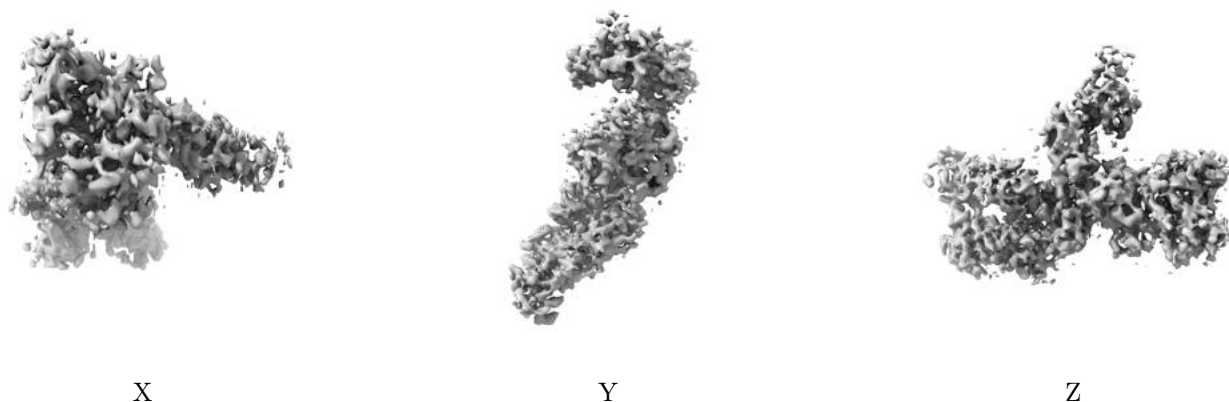


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

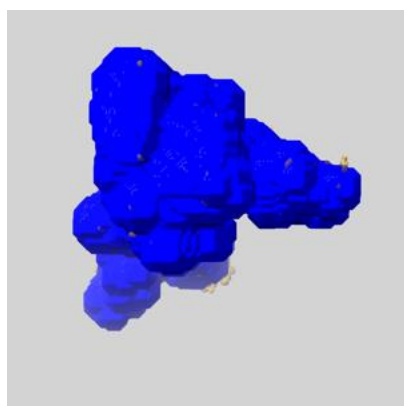
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

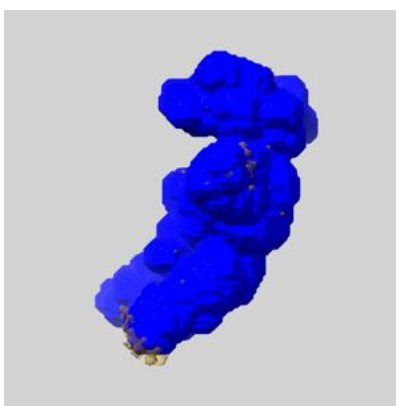
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

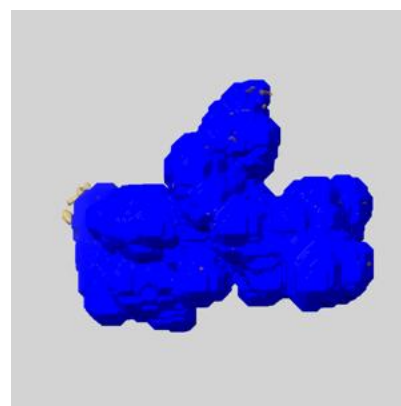
6.6.1 emd_55957_msk_1.map [i](#)



X



Y

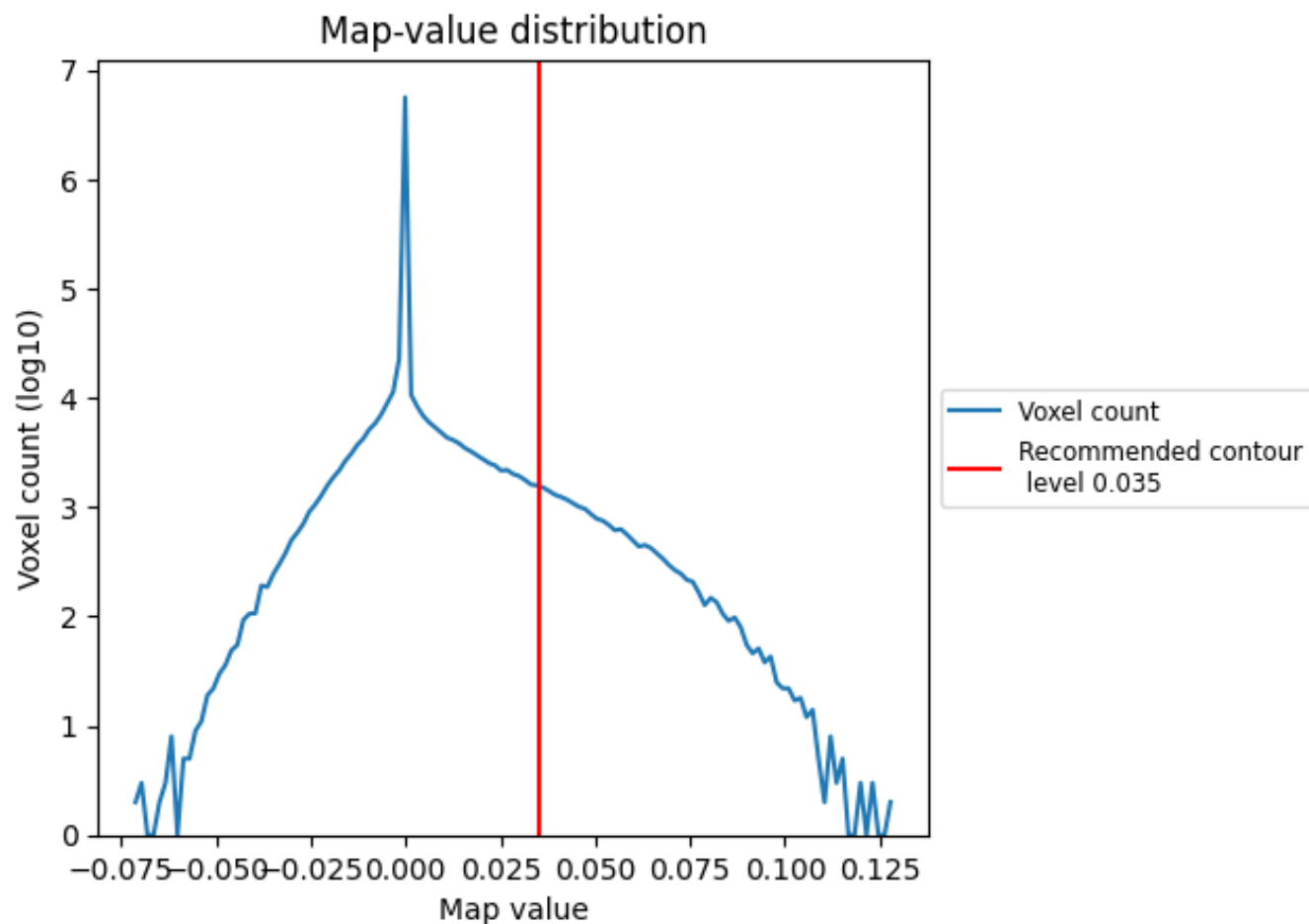


Z

7 Map analysis [i](#)

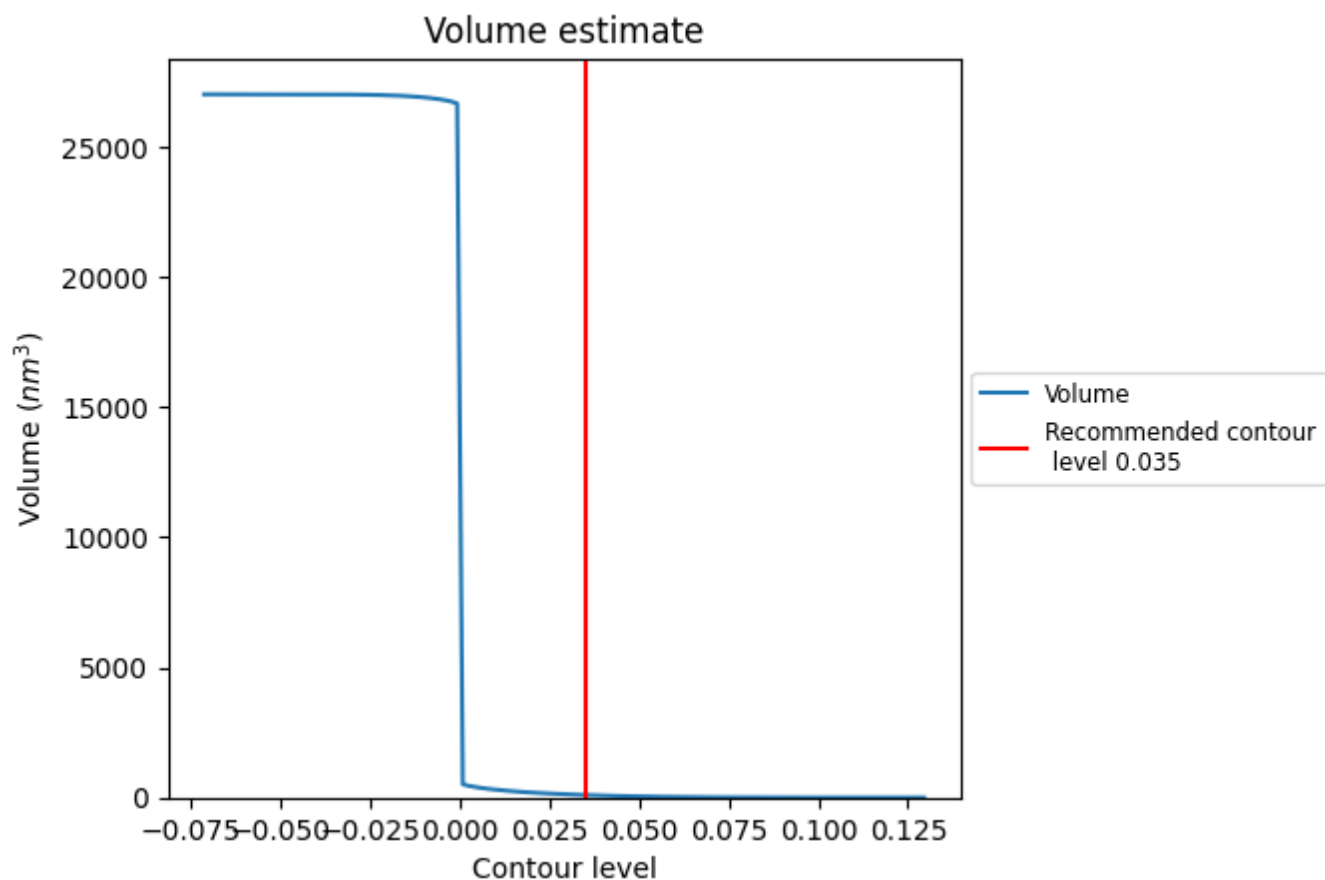
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

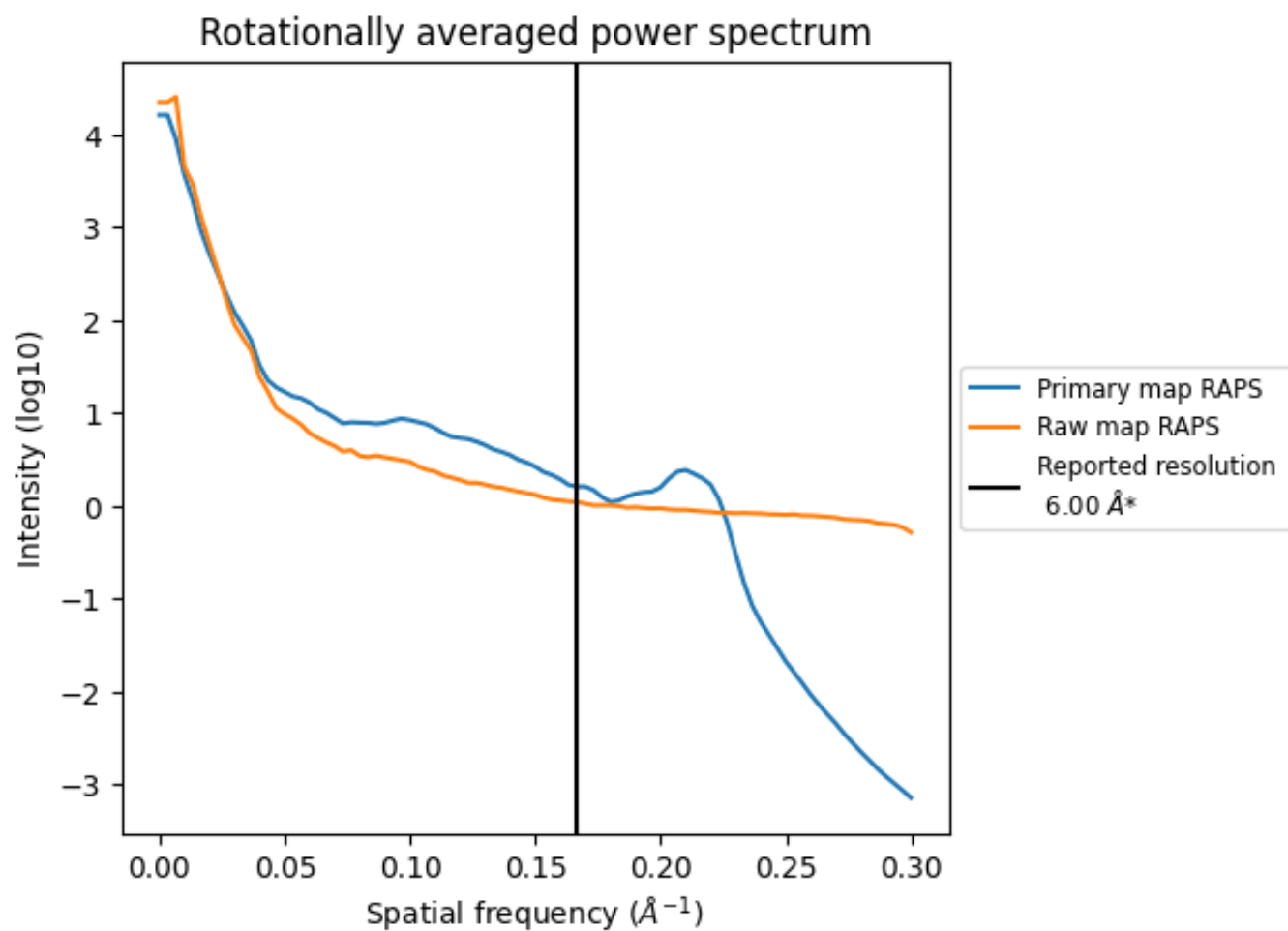
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 97 nm^3 ; this corresponds to an approximate mass of 88 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 ⓘ

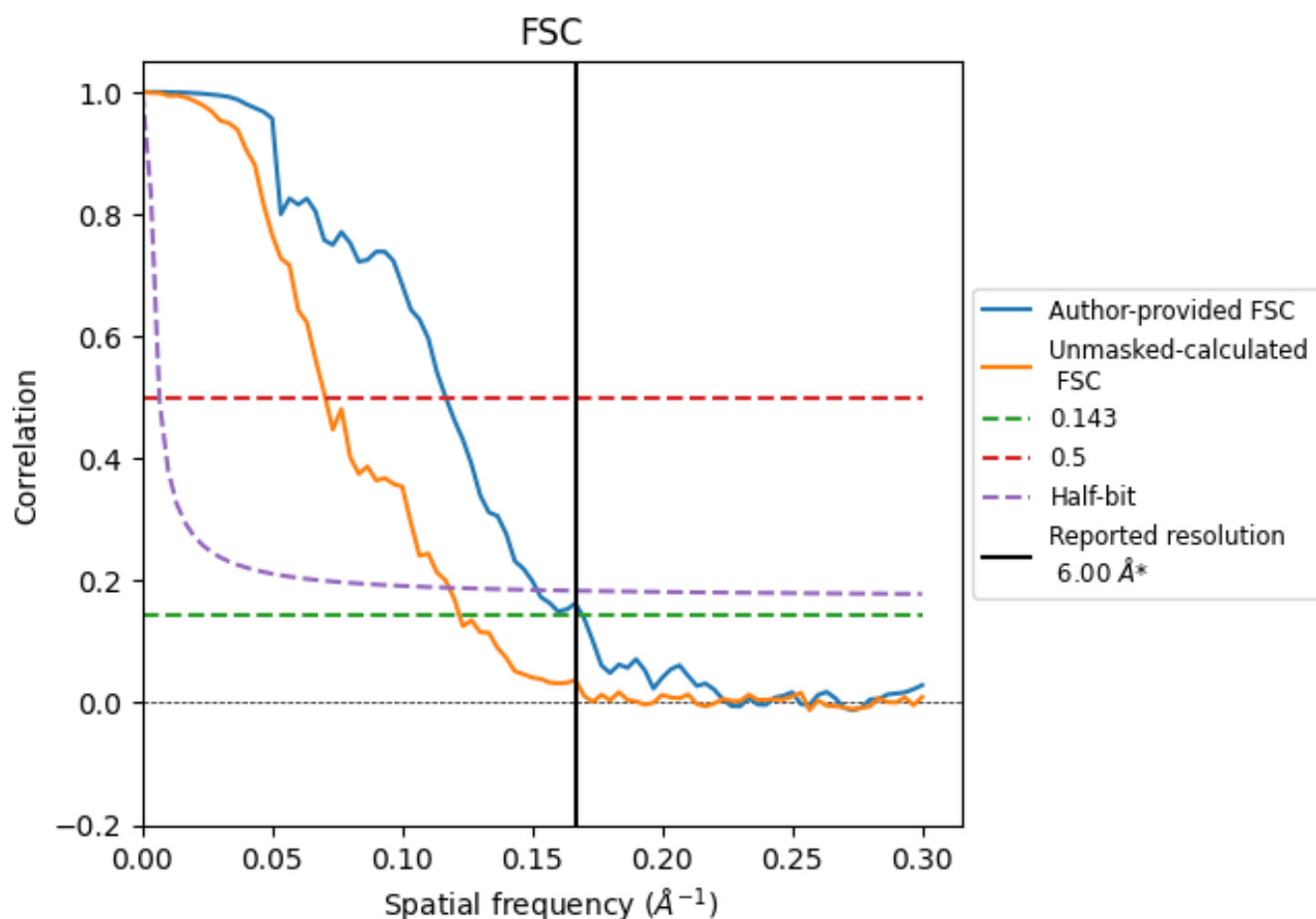


*Reported resolution corresponds to spatial frequency of 0.167 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.167 \AA^{-1}

8.2 Resolution estimates [i](#)

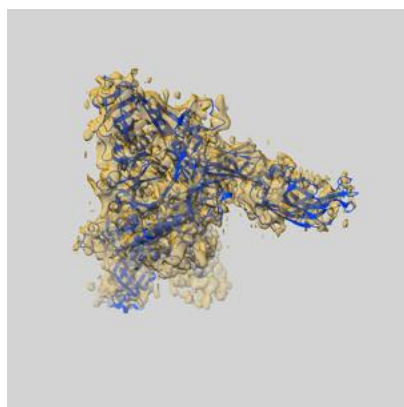
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.00	-	-
Author-provided FSC curve	5.91	8.57	6.58
Unmasked-calculated*	8.20	14.22	8.47

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.20 differs from the reported value 6.0 by more than 10 %

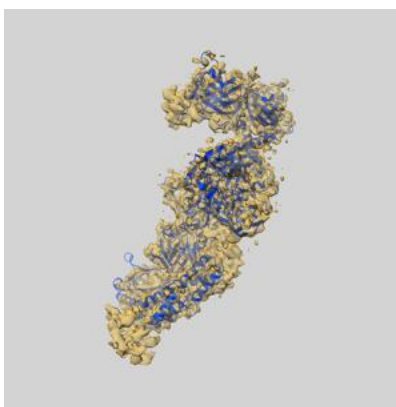
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55957 and PDB model 9TII. Per-residue inclusion information can be found in section [3](#) on page [5](#).

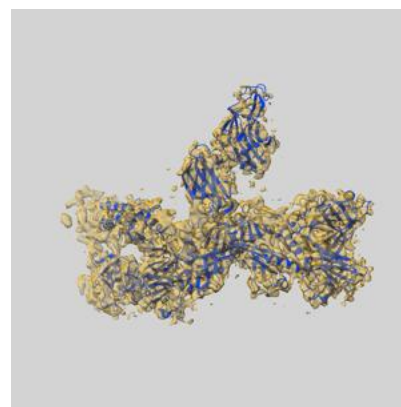
9.1 Map-model overlay [i](#)



X



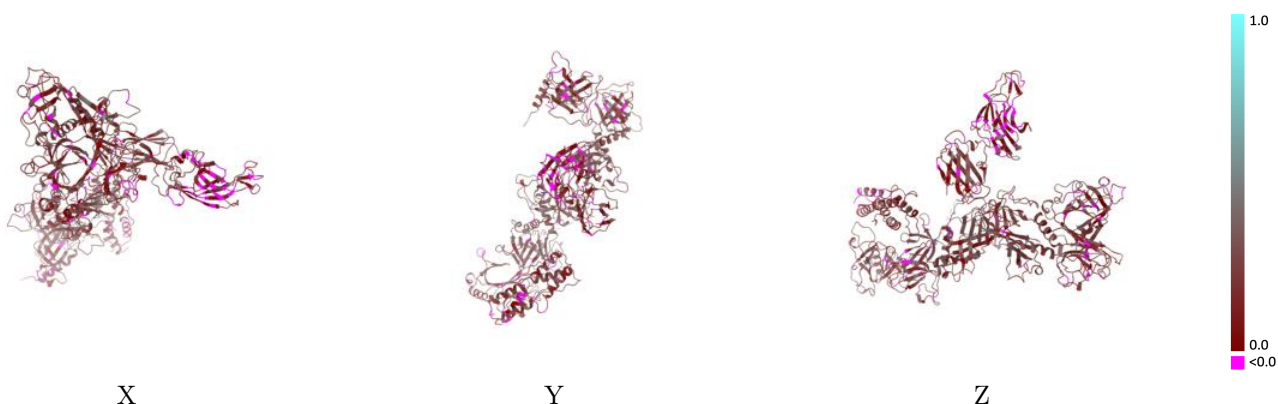
Y



Z

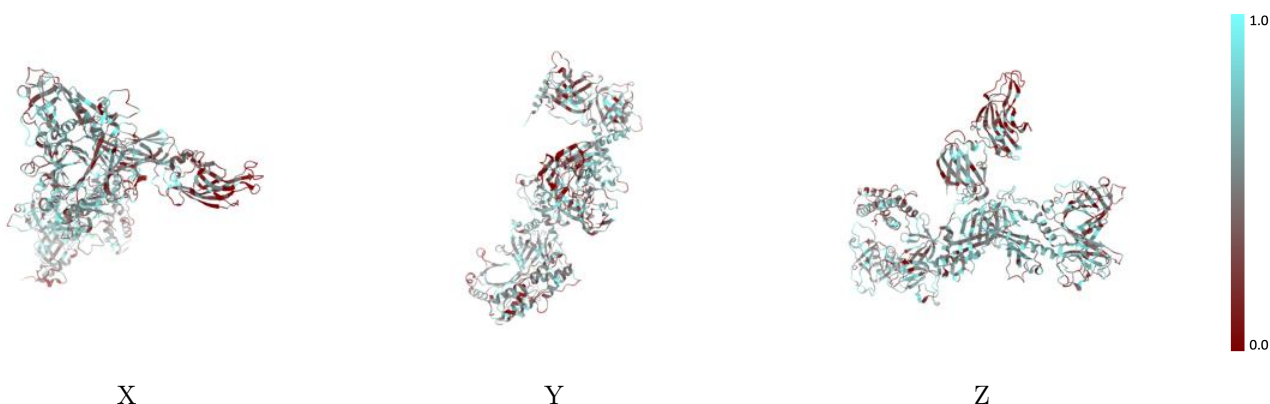
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



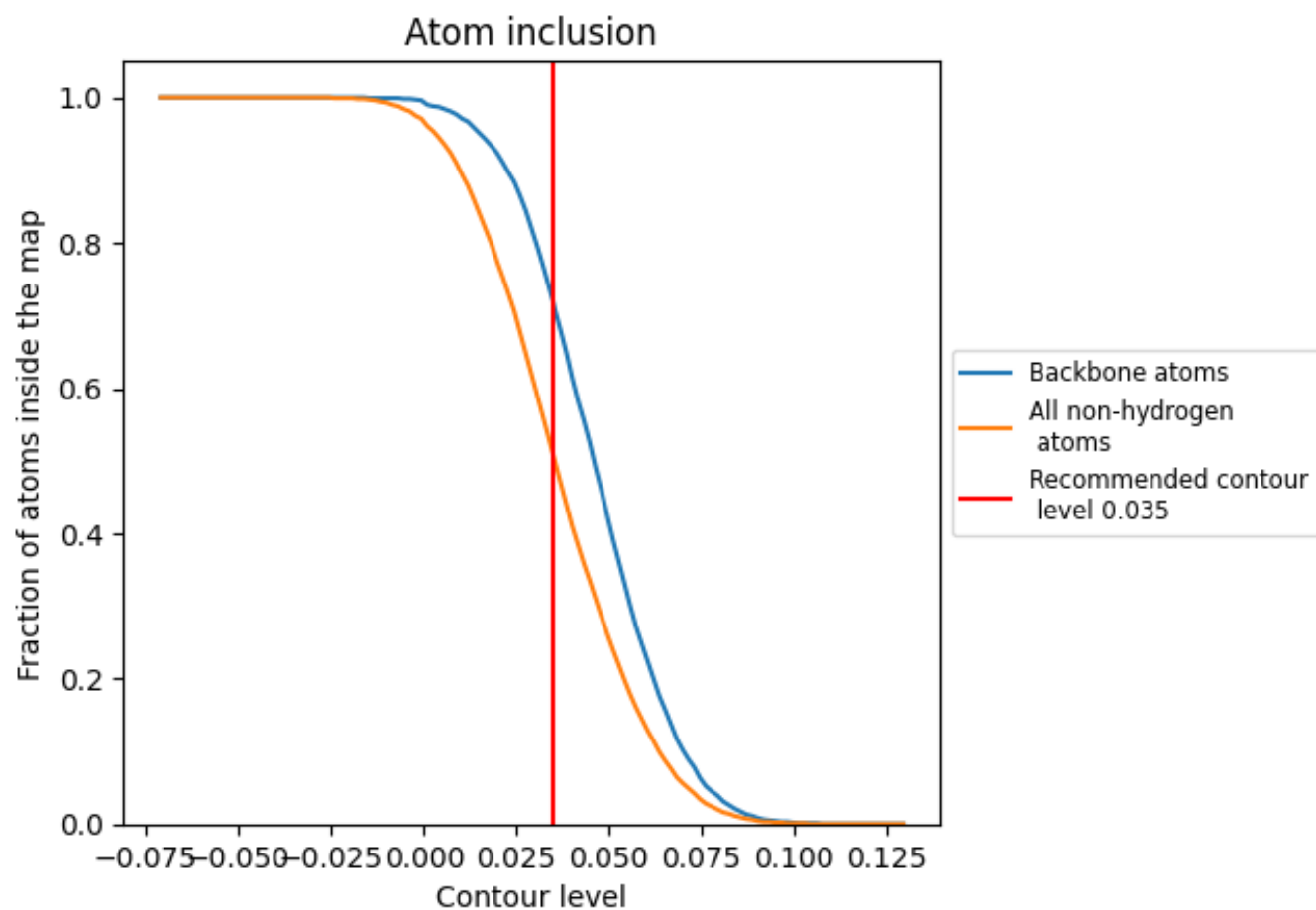
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 51% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5070	<div></div> 0.2040
A	<div></div> 0.4070	<div></div> 0.1520
B	<div></div> 0.4700	<div></div> 0.1950
C	<div></div> 0.4750	<div></div> 0.1600
D	<div></div> 0.4460	<div></div> 0.1670
E	<div></div> 0.5700	<div></div> 0.2510
H	<div></div> 0.5380	<div></div> 0.2200
I	<div></div> 0.6000	<div></div> 0.2470
J	<div></div> 0.5100	<div></div> 0.1960
K	<div></div> 0.4990	<div></div> 0.1980
L	<div></div> 0.5270	<div></div> 0.2270

