



Full wwPDB EM Validation Report ⓘ

Apr 18, 2023 – 10:33 AM EDT

PDB ID : 8FCK
EMDB ID : EMD-28981
Title : Structure of the vertebrate augmin complex
Authors : Travis, S.M.; Huang, W.; Zhang, R.; Petry, S.
Deposited on : 2022-12-01
Resolution : 6.88 Å (reported)

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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.dev50
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) : 2.32.2

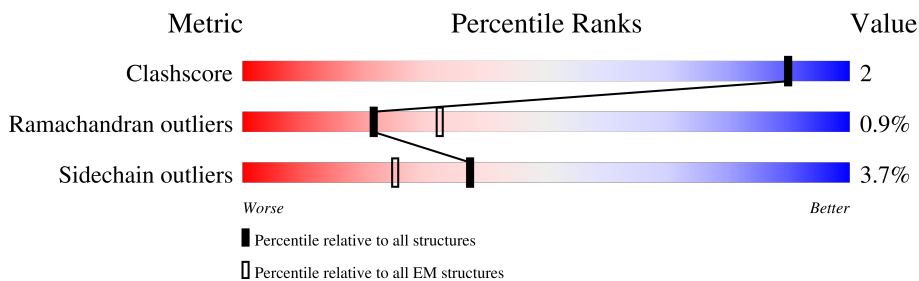
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.88 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	286	
2	B	597	
3	C	353	
4	D	666	
5	E	472	
6	F	442	
7	G	348	
8	H	367	

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 24717 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 HAUS augmin-like complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	286	2281	1435	378	455	13	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	GLN	ARG	conflict	UNP A0A8J1L9M8

- Molecule 2 is a protein called HAUS augmin-like complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	597	4756	2980	811	942	23	0	0

- Molecule 3 is a protein called HAUS augmin like complex subunit 4 L homeolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	353	2886	1807	508	555	16	0	0

- Molecule 4 is a protein called HAUS augmin-like complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	666	5416	3362	1000	1023	31	0	0

- Molecule 5 is a protein called HAUS augmin like complex subunit 2 L homeolog, Green fluorescent protein chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	222	1755	1098	302	342	13	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	223	VAL	-	linker	UNP Q6INL9
E	224	ASP	-	linker	UNP Q6INL9
E	225	MET	-	linker	UNP Q6INL9
E	226	VAL	-	linker	UNP Q6INL9
E	289	LEU	PHE	conflict	UNP P42212
E	290	THR	SER	conflict	UNP P42212
E	446	LYS	LEU	conflict	UNP P42212
E	456	LEU	HIS	conflict	UNP P42212
E	464	VAL	-	expression tag	UNP P42212
E	465	ASP	-	expression tag	UNP P42212
E	466	HIS	-	expression tag	UNP P42212
E	467	HIS	-	expression tag	UNP P42212
E	468	HIS	-	expression tag	UNP P42212
E	469	HIS	-	expression tag	UNP P42212
E	470	HIS	-	expression tag	UNP P42212
E	471	HIS	-	expression tag	UNP P42212
E	472	HIS	-	expression tag	UNP P42212

- Molecule 6 is a protein called HAUS augmin like complex subunit 6 L homeolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	393	3211	2039	581	571	20	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-11	GLY	-	expression tag	UNP A0JPI0
F	-10	PRO	-	expression tag	UNP A0JPI0
F	-9	ALA	-	expression tag	UNP A0JPI0
F	-8	SER	-	expression tag	UNP A0JPI0
F	-7	GLY	-	expression tag	UNP A0JPI0
F	-6	SER	-	expression tag	UNP A0JPI0
F	-5	THR	-	expression tag	UNP A0JPI0
F	-4	ARG	-	expression tag	UNP A0JPI0
F	-3	GLY	-	expression tag	UNP A0JPI0
F	-2	ALA	-	expression tag	UNP A0JPI0
F	-1	GLU	-	expression tag	UNP A0JPI0
F	0	PHE	-	expression tag	UNP A0JPI0

- Molecule 7 is a protein called HAUS augmin like complex subunit 7 S homeolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	332	2627	1655	435	517	20	0	0

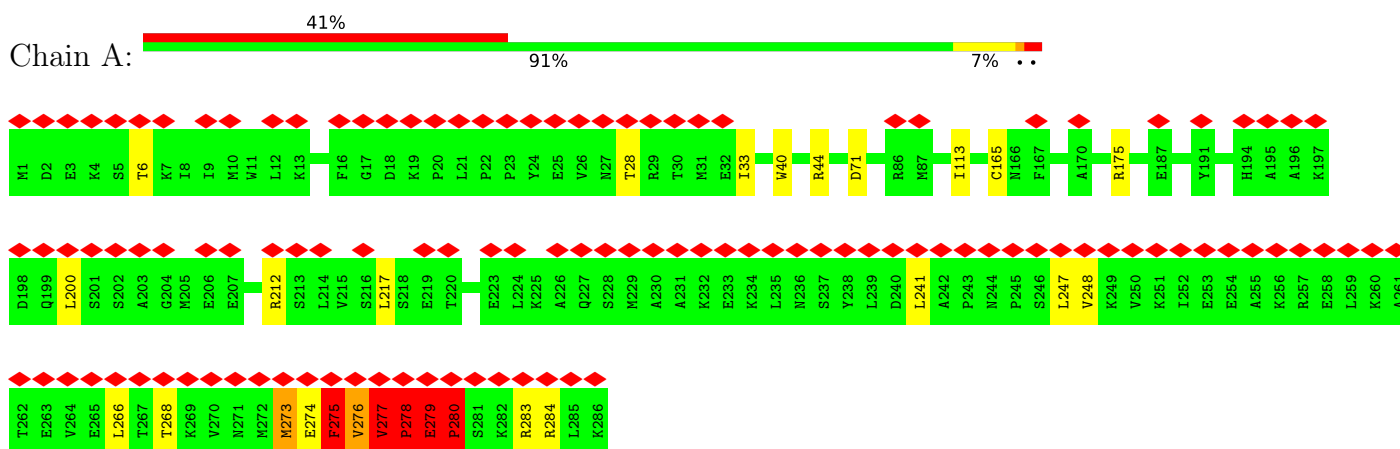
- Molecule 8 is a protein called HAUS augmin-like complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	218	1785	1122	305	351	7	0	0

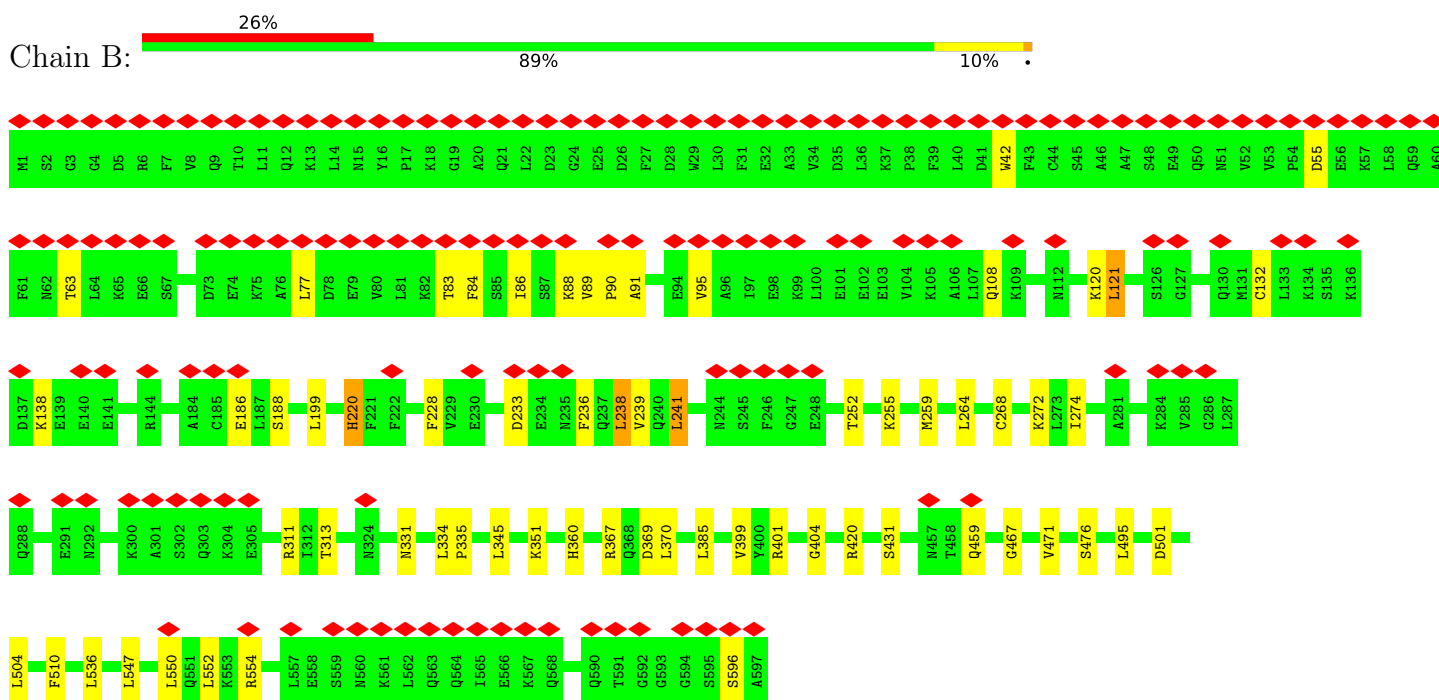
3 Residue-property plots

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.

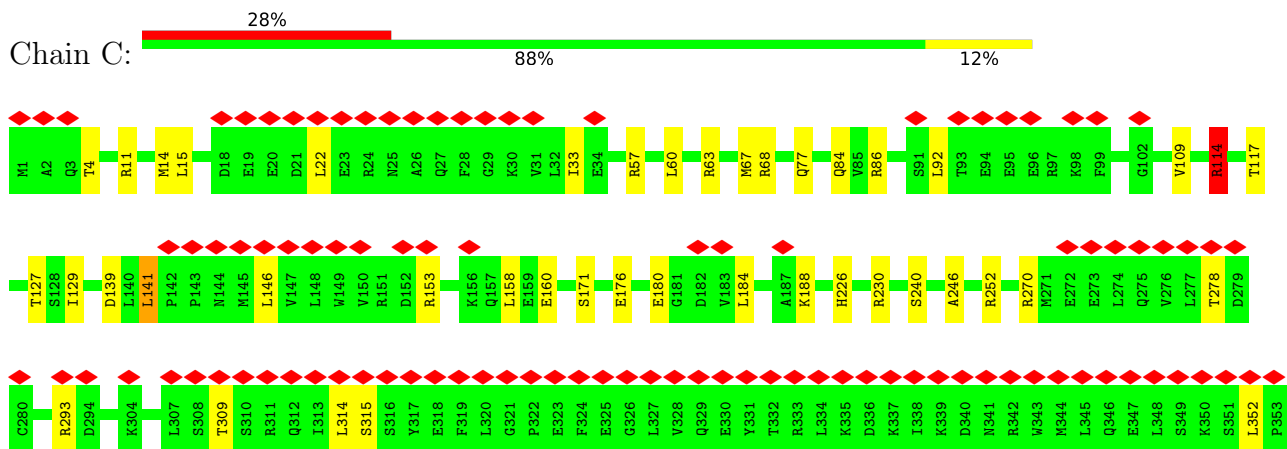
- Molecule 1: HAUS augmin-like complex subunit 1



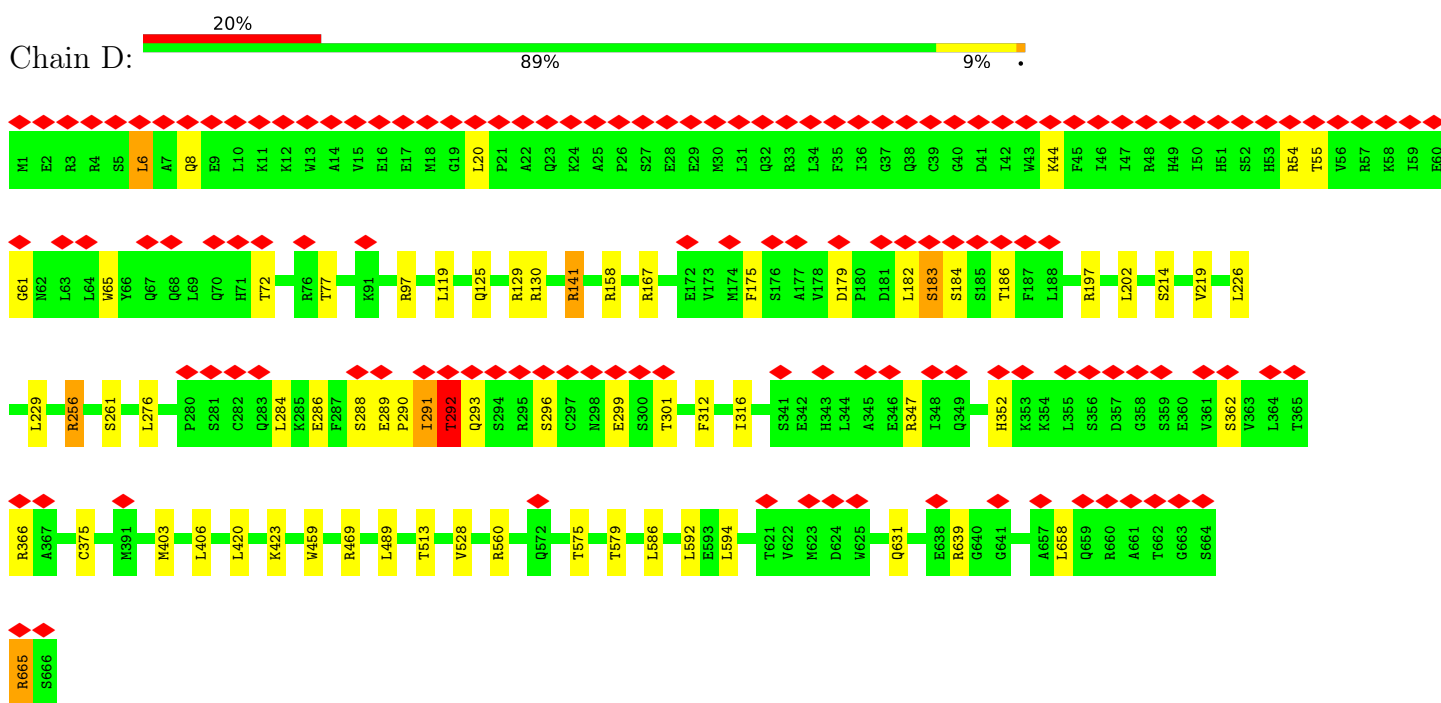
- Molecule 2: HAUS augmin-like complex subunit 3



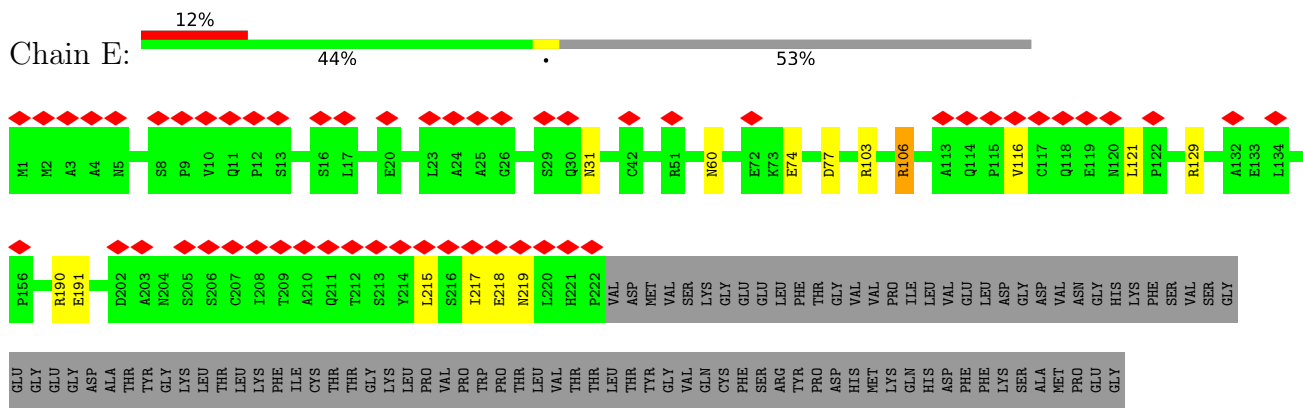
- Molecule 3: HAUS augmin like complex subunit 4 L homeolog



• Molecule 4: HAUS augmin-like complex subunit 5



• Molecule 5: HAUS augmin like complex subunit 2 L homeolog, Green fluorescent protein chimera



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	114000	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 ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	10105	Depositor
Maximum defocus (nm)	39903	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.224	Depositor
Minimum map value	-0.749	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.161	Depositor
Map size (Å)	712.4, 712.4, 712.4	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality i

5.1 Standard geometry i

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	0.62	0/2308	0.91	5/3100 (0.2%)
2	B	0.61	0/4821	0.86	6/6477 (0.1%)
3	C	0.65	0/2921	0.94	12/3925 (0.3%)
4	D	0.63	0/5504	0.95	16/7400 (0.2%)
5	E	0.63	0/1783	0.98	4/2416 (0.2%)
6	F	0.94	5/3270 (0.2%)	1.11	20/4392 (0.5%)
7	G	0.65	0/2678	0.96	6/3622 (0.2%)
8	H	0.66	0/1809	1.04	10/2440 (0.4%)
All	All	0.68	5/25094 (0.0%)	0.96	79/33772 (0.2%)

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	12
2	B	0	2
3	C	0	4
4	D	0	8
5	E	0	3
6	F	0	5
7	G	0	1
8	H	0	3
All	All	0	38

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	293	HIS	CD2-NE2	19.01	1.81	1.42
6	F	293	HIS	CG-CD2	18.79	1.67	1.35
6	F	293	HIS	CG-ND1	16.37	1.74	1.38
6	F	293	HIS	CE1-NE2	14.40	1.65	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	293	HIS	ND1-CE1	12.77	1.66	1.34

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	326	ARG	NE-CZ-NH1	10.89	125.74	120.30
3	C	114	ARG	NE-CZ-NH2	-10.68	114.96	120.30
6	F	238	ARG	NE-CZ-NH1	9.97	125.29	120.30
6	F	287	ARG	NE-CZ-NH1	9.32	124.96	120.30
4	D	97	ARG	NE-CZ-NH1	9.10	124.85	120.30
8	H	324	ARG	NE-CZ-NH1	8.89	124.74	120.30
3	C	68	ARG	NE-CZ-NH1	8.78	124.69	120.30
4	D	141	ARG	NE-CZ-NH1	8.58	124.59	120.30
6	F	6	ARG	NE-CZ-NH1	8.14	124.37	120.30
3	C	114	ARG	NE-CZ-NH1	8.12	124.36	120.30
7	G	239	ARG	NE-CZ-NH1	7.96	124.28	120.30
4	D	469	ARG	NE-CZ-NH1	7.82	124.21	120.30
4	D	560	ARG	NE-CZ-NH1	7.73	124.16	120.30
6	F	170	ARG	NE-CZ-NH1	7.69	124.15	120.30
6	F	194	ARG	NE-CZ-NH1	7.63	124.11	120.30
2	B	220	HIS	CA-CB-CG	7.57	126.47	113.60
6	F	383	ARG	NE-CZ-NH1	7.43	124.02	120.30
7	G	16	ARG	NE-CZ-NH1	7.39	124.00	120.30
7	G	100	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	A	279	GLU	CA-CB-CG	7.18	129.20	113.40
2	B	401	ARG	NE-CZ-NH1	6.97	123.78	120.30
8	H	221	ARG	NE-CZ-NH2	-6.93	116.83	120.30
6	F	87	ARG	NE-CZ-NH1	6.88	123.74	120.30
5	E	129	ARG	NE-CZ-NH1	6.87	123.74	120.30
3	C	252	ARG	NE-CZ-NH1	6.82	123.71	120.30
3	C	153	ARG	NE-CZ-NH2	6.79	123.70	120.30
2	B	311	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	A	277	VAL	CG1-CB-CG2	-6.69	100.19	110.90
6	F	144	ARG	NE-CZ-NH1	6.62	123.61	120.30
5	E	190	ARG	NE-CZ-NH1	6.61	123.60	120.30
8	H	221	ARG	NE-CZ-NH1	6.55	123.58	120.30
4	D	347	ARG	NE-CZ-NH1	6.51	123.55	120.30
3	C	86	ARG	NE-CZ-NH1	6.46	123.53	120.30
8	H	211	ARG	NE-CZ-NH1	6.42	123.51	120.30
6	F	359	ARG	NE-CZ-NH1	6.24	123.42	120.30
7	G	310	ARG	NE-CZ-NH1	6.21	123.40	120.30
8	H	218	ARG	NE-CZ-NH1	6.14	123.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	54	ARG	NE-CZ-NH2	-6.00	117.30	120.30
8	H	183	ARG	NE-CZ-NH1	5.96	123.28	120.30
4	D	97	ARG	NH1-CZ-NH2	-5.96	112.85	119.40
4	D	197	ARG	NE-CZ-NH1	5.93	123.27	120.30
7	G	335	ARG	NE-CZ-NH1	5.91	123.25	120.30
3	C	57	ARG	NE-CZ-NH1	5.81	123.20	120.30
6	F	356	ARG	NE-CZ-NH2	-5.80	117.40	120.30
6	F	175	ARG	NE-CZ-NH1	5.78	123.19	120.30
6	F	379	ARG	NE-CZ-NH1	5.77	123.19	120.30
6	F	326	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	175	ARG	NE-CZ-NH1	5.75	123.17	120.30
3	C	11	ARG	NE-CZ-NH1	5.73	123.16	120.30
6	F	207	ARG	NE-CZ-NH1	5.70	123.15	120.30
5	E	106	ARG	NE-CZ-NH1	5.55	123.07	120.30
8	H	190	ARG	NE-CZ-NH1	5.51	123.06	120.30
6	F	263	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	280	PRO	CA-N-CD	-5.47	103.83	111.50
6	F	71	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	B	554	ARG	NE-CZ-NH1	5.45	123.03	120.30
4	D	528	VAL	CG1-CB-CG2	-5.45	102.18	110.90
8	H	358	ARG	NE-CZ-NH1	5.45	123.02	120.30
4	D	256	ARG	NE-CZ-NH1	5.42	123.01	120.30
8	H	274	ARG	NE-CZ-NH1	5.39	123.00	120.30
5	E	103	ARG	NE-CZ-NH1	5.37	122.98	120.30
7	G	147	ARG	NE-CZ-NH1	5.36	122.98	120.30
3	C	139	ASP	CB-CG-OD2	-5.36	113.48	118.30
6	F	57	TYR	CB-CG-CD2	-5.33	117.80	121.00
2	B	220	HIS	CB-CA-C	5.31	121.02	110.40
3	C	270	ARG	NE-CZ-NH1	5.29	122.95	120.30
4	D	167	ARG	NE-CZ-NH1	5.29	122.94	120.30
4	D	183	SER	C-N-CA	5.28	134.90	121.70
6	F	356	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	277	VAL	CA-CB-CG2	5.26	118.78	110.90
3	C	153	ARG	NH1-CZ-NH2	-5.23	113.65	119.40
8	H	221	ARG	CD-NE-CZ	5.22	130.91	123.60
4	D	639	ARG	NE-CZ-NH1	5.21	122.91	120.30
3	C	293	ARG	NE-CZ-NH2	-5.20	117.70	120.30
6	F	238	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
4	D	129	ARG	NE-CZ-NH1	5.19	122.89	120.30
4	D	130	ARG	NE-CZ-NH1	5.16	122.88	120.30
4	D	469	ARG	NH1-CZ-NH2	-5.08	113.81	119.40
2	B	311	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	212	ARG	Sidechain
1	A	273	MET	Peptide
1	A	274	GLU	Peptide
1	A	275	PHE	Peptide
1	A	276	VAL	Peptide
1	A	277	VAL	Peptide
1	A	278	PRO	Peptide
1	A	279	GLU	Peptide
1	A	280	PRO	Peptide
1	A	283	ARG	Mainchain,Peptide
1	A	284	ARG	Peptide
2	B	367	ARG	Sidechain
2	B	596	SER	Peptide
3	C	114	ARG	Sidechain
3	C	117	THR	Peptide
3	C	230	ARG	Sidechain
3	C	63	ARG	Sidechain
4	D	288	SER	Peptide
4	D	289	GLU	Peptide
4	D	290	PRO	Peptide
4	D	291	ILE	Peptide
4	D	292	THR	Peptide
4	D	296	SER	Peptide
4	D	299	GLU	Peptide
4	D	665	ARG	Peptide
5	E	106	ARG	Sidechain
5	E	217	ILE	Peptide
5	E	218	GLU	Peptide
6	F	13	ARG	Sidechain
6	F	225	ARG	Sidechain
6	F	263	ARG	Peptide
6	F	269	TYR	Sidechain
6	F	71	ARG	Sidechain
7	G	310	ARG	Sidechain
8	H	172	TYR	Sidechain
8	H	272	ARG	Sidechain
8	H	366	LEU	Peptide

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	2281	0	2360	21	0
2	B	4756	0	4769	36	0
3	C	2886	0	2957	15	0
4	D	5416	0	5455	21	0
5	E	1755	0	1763	6	0
6	F	3211	0	3280	7	0
7	G	2627	0	2592	0	0
8	H	1785	0	1807	22	0
All	All	24717	0	24983	82	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 2.

All (82) 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)
6:F:293:HIS:ND1	6:F:293:HIS:CG	1.74	1.52
6:F:293:HIS:NE2	6:F:293:HIS:CD2	1.81	1.46
2:B:268:CYS:SG	8:H:345:GLN:HA	1.91	1.11
5:E:60:ASN:HB3	8:H:207:HIS:CD2	1.85	1.10
5:E:60:ASN:HB3	8:H:207:HIS:NE2	1.83	0.92
2:B:268:CYS:HG	8:H:345:GLN:HA	1.36	0.91
2:B:331:ASN:HB3	8:H:356:LEU:HD11	1.62	0.82
1:A:279:GLU:HB3	1:A:280:PRO:HD3	1.63	0.81
1:A:278:PRO:HD2	1:A:279:GLU:HB2	1.63	0.80
2:B:335:PRO:CB	8:H:360:TRP:NE1	2.45	0.79
3:C:129:ILE:HD11	4:D:489:LEU:HD22	1.67	0.76
6:F:293:HIS:CG	6:F:293:HIS:CE1	2.76	0.73
6:F:293:HIS:CD2	6:F:293:HIS:CE1	2.78	0.72
2:B:335:PRO:HB3	8:H:360:TRP:CE2	2.26	0.71
2:B:335:PRO:HB2	8:H:360:TRP:NE1	2.04	0.70
1:A:278:PRO:CD	1:A:279:GLU:HB2	2.22	0.70
2:B:335:PRO:CB	8:H:360:TRP:CE2	2.78	0.67
1:A:277:VAL:HG12	1:A:278:PRO:HD3	1.77	0.65
1:A:279:GLU:CB	1:A:280:PRO:HD3	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:335:PRO:CG	8:H:360:TRP:CZ2	2.84	0.61
2:B:331:ASN:O	8:H:356:LEU:HD21	2.03	0.59
4:D:352:HIS:CD2	4:D:366:ARG:HE	2.21	0.58
1:A:277:VAL:CB	1:A:278:PRO:HD3	2.33	0.58
3:C:4:THR:HG23	3:C:33:ILE:HD11	1.86	0.57
2:B:77:LEU:HD21	4:D:61:GLY:HA3	1.87	0.56
2:B:268:CYS:SG	8:H:345:GLN:CA	2.82	0.56
2:B:272:LYS:HE3	8:H:348:VAL:CG2	2.35	0.56
2:B:238:LEU:HD12	4:D:403:MET:CE	2.36	0.55
8:H:263:ILE:HD12	8:H:272:ARG:HH12	1.71	0.55
1:A:277:VAL:CG1	1:A:278:PRO:HD3	2.37	0.54
5:E:60:ASN:CB	8:H:207:HIS:NE2	2.67	0.54
1:A:278:PRO:HD2	1:A:279:GLU:CB	2.37	0.54
2:B:404:GLY:HA2	4:D:459:TRP:CH2	2.43	0.53
5:E:60:ASN:CB	8:H:207:HIS:CD2	2.77	0.52
3:C:129:ILE:HD11	4:D:489:LEU:CD2	2.38	0.52
1:A:279:GLU:HB3	1:A:280:PRO:CD	2.39	0.51
1:A:275:PHE:HB3	1:A:276:VAL:HG23	1.94	0.50
2:B:84:PHE:CE2	4:D:65:TRP:CZ3	2.99	0.50
5:E:74:GLU:CG	6:F:238:ARG:HH22	2.24	0.50
2:B:138:LYS:HE2	3:C:84:GLN:NE2	2.27	0.49
2:B:241:LEU:HD11	2:B:259:MET:HG3	1.94	0.49
2:B:274:ILE:HG21	2:B:334:LEU:HD11	1.95	0.49
4:D:6:LEU:HD11	4:D:44:LYS:HE3	1.93	0.48
2:B:351:LYS:HA	4:D:406:LEU:HD21	1.94	0.48
2:B:272:LYS:HE3	8:H:348:VAL:HG22	1.96	0.47
2:B:335:PRO:CG	8:H:360:TRP:CE2	2.98	0.47
5:E:121:LEU:HG	8:H:263:ILE:HD11	1.97	0.46
1:A:71:ASP:HB3	3:C:114:ARG:NH2	2.29	0.46
2:B:399:VAL:HA	4:D:158:ARG:HH12	1.80	0.46
3:C:77:GLN:NE2	4:D:125:GLN:HE22	2.13	0.46
2:B:120:LYS:HZ1	3:C:171:SER:HB2	1.79	0.46
6:F:236:LYS:HZ3	8:H:230:ASP:CG	2.19	0.45
1:A:71:ASP:HB3	3:C:114:ARG:HH22	1.81	0.45
1:A:113:ILE:CG2	2:B:121:LEU:HD11	2.46	0.45
2:B:335:PRO:HG2	8:H:360:TRP:CZ2	2.52	0.45
1:A:241:LEU:HD22	1:A:248:VAL:HG13	1.99	0.45
3:C:4:THR:CG2	3:C:33:ILE:HD11	2.45	0.45
4:D:291:ILE:HG22	4:D:292:THR:HA	1.99	0.44
1:A:40:TRP:CH2	3:C:14:MET:HG3	2.53	0.44
4:D:175:PHE:HB2	4:D:256:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:352:HIS:CG	4:D:366:ARG:HH21	2.36	0.43
2:B:399:VAL:HA	4:D:158:ARG:NH1	2.33	0.43
3:C:109:VAL:HG11	3:C:141:LEU:HD12	2.00	0.43
1:A:277:VAL:HB	1:A:278:PRO:HD3	1.99	0.43
2:B:420:ARG:NH2	4:D:141:ARG:HH22	2.16	0.43
2:B:89:VAL:N	2:B:90:PRO:HD2	2.33	0.43
1:A:33:ILE:HG23	3:C:15:LEU:HD22	1.99	0.42
2:B:510:PHE:CE1	4:D:586:LEU:HB3	2.54	0.42
4:D:175:PHE:HB2	4:D:256:ARG:CZ	2.49	0.42
2:B:255:LYS:HG2	4:D:312:PHE:CE1	2.54	0.42
1:A:279:GLU:CG	1:A:280:PRO:HD3	2.50	0.41
2:B:467:GLY:O	2:B:471:VAL:HG23	2.20	0.41
1:A:40:TRP:CZ2	3:C:14:MET:SD	3.13	0.41
2:B:91:ALA:O	2:B:95:VAL:HG23	2.20	0.41
2:B:274:ILE:HD13	2:B:334:LEU:HD11	2.03	0.41
1:A:165:CYS:SG	3:C:246:ALA:HB1	2.60	0.41
6:F:93:LYS:HZ3	6:F:97:GLU:CD	2.23	0.41
1:A:278:PRO:CG	1:A:279:GLU:HB2	2.50	0.41
3:C:180:GLU:CD	3:C:188:LYS:HZ2	2.23	0.41
2:B:335:PRO:HG3	8:H:360:TRP:CZ2	2.55	0.41
2:B:42:TRP:CD2	4:D:20:LEU:HD13	2.56	0.41
2:B:369:ASP:CG	4:D:423:LYS:HZ3	2.25	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	284/286 (99%)	274 (96%)	7 (2%)	3 (1%)	14	52
2	B	595/597 (100%)	578 (97%)	9 (2%)	8 (1%)	12	48
3	C	351/353 (99%)	344 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	664/666 (100%)	634 (96%)	21 (3%)	9 (1%)	11	46
5	E	220/472 (47%)	210 (96%)	9 (4%)	1 (0%)	29	69
6	F	391/442 (88%)	364 (93%)	27 (7%)	0	100	100
7	G	328/348 (94%)	305 (93%)	19 (6%)	4 (1%)	13	50
8	H	216/367 (59%)	207 (96%)	7 (3%)	2 (1%)	17	57
All	All	3049/3531 (86%)	2916 (96%)	106 (4%)	27 (1%)	21	57

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	GLU
1	A	280	PRO
2	B	186	GLU
4	D	184	SER
7	G	2	THR
1	A	278	PRO
2	B	86	ILE
2	B	239	VAL
4	D	284	LEU
4	D	286	GLU
4	D	665	ARG
7	G	125	ILE
8	H	240	LYS
2	B	88	LYS
2	B	236	PHE
2	B	241	LEU
4	D	183	SER
4	D	186	THR
4	D	293	GLN
4	D	301	THR
7	G	196	LYS
8	H	259	HIS
2	B	188	SER
2	B	459	GLN
5	E	116	VAL
4	D	219	VAL
7	G	129	VAL

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	260/260 (100%)	249 (96%)	11 (4%)	30	54
2	B	538/541 (99%)	511 (95%)	27 (5%)	24	49
3	C	326/326 (100%)	308 (94%)	18 (6%)	21	47
4	D	605/605 (100%)	579 (96%)	26 (4%)	29	53
5	E	195/415 (47%)	190 (97%)	5 (3%)	46	66
6	F	347/387 (90%)	342 (99%)	5 (1%)	67	80
7	G	306/320 (96%)	301 (98%)	5 (2%)	62	79
8	H	205/328 (62%)	199 (97%)	6 (3%)	42	64
All	All	2782/3182 (87%)	2679 (96%)	103 (4%)	37	58

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	28	THR
1	A	44	ARG
1	A	200	LEU
1	A	217	LEU
1	A	247	LEU
1	A	266	LEU
1	A	268	THR
1	A	273	MET
1	A	275	PHE
1	A	277	VAL
2	B	55	ASP
2	B	63	THR
2	B	83	THR
2	B	108	GLN
2	B	121	LEU
2	B	132	CYS
2	B	199	LEU
2	B	220	HIS

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Mol	Chain	Res	Type
2	B	228	PHE
2	B	233	ASP
2	B	238	LEU
2	B	252	THR
2	B	264	LEU
2	B	313	THR
2	B	345	LEU
2	B	360	HIS
2	B	370	LEU
2	B	385	LEU
2	B	431	SER
2	B	476	SER
2	B	495	LEU
2	B	501	ASP
2	B	504	LEU
2	B	536	LEU
2	B	547	LEU
2	B	550	LEU
2	B	552	LEU
3	C	22	LEU
3	C	60	LEU
3	C	67	MET
3	C	92	LEU
3	C	127	THR
3	C	141	LEU
3	C	146	LEU
3	C	158	LEU
3	C	160	GLU
3	C	176	GLU
3	C	184	LEU
3	C	226	HIS
3	C	240	SER
3	C	278	THR
3	C	309	THR
3	C	314	LEU
3	C	315	SER
3	C	352	LEU
4	D	6	LEU
4	D	8	GLN
4	D	55	THR
4	D	72	THR
4	D	77	THR

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Mol	Chain	Res	Type
4	D	119	LEU
4	D	179	ASP
4	D	182	LEU
4	D	202	LEU
4	D	214	SER
4	D	226	LEU
4	D	229	LEU
4	D	261	SER
4	D	276	LEU
4	D	292	THR
4	D	316	ILE
4	D	362	SER
4	D	375	CYS
4	D	420	LEU
4	D	513	THR
4	D	575	THR
4	D	579	THR
4	D	592	LEU
4	D	594	LEU
4	D	631	GLN
4	D	658	LEU
5	E	31	ASN
5	E	77	ASP
5	E	191	GLU
5	E	215	LEU
5	E	219	ASN
6	F	214	GLN
6	F	229	ASP
6	F	256	ASP
6	F	259	ASP
6	F	266	ILE
7	G	185	GLU
7	G	230	ASP
7	G	274	MET
7	G	293	GLU
7	G	307	ASP
8	H	198	GLN
8	H	218	ARG
8	H	258	ARG
8	H	278	GLU
8	H	299	SER
8	H	359	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	220	HIS
2	B	244	ASN
2	B	386	GLN
3	C	77	GLN
3	C	84	GLN
4	D	49	HIS
4	D	125	GLN
4	D	161	GLN
4	D	211	HIS
4	D	272	GLN
4	D	426	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

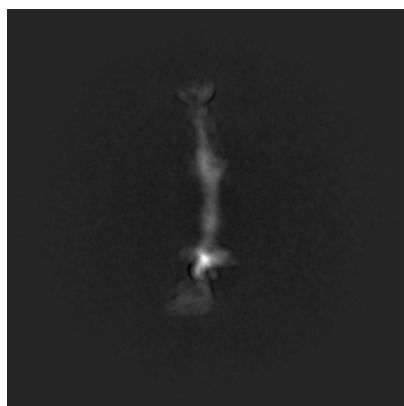
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28981. These allow visual inspection of the internal detail of the map and identification of artifacts.

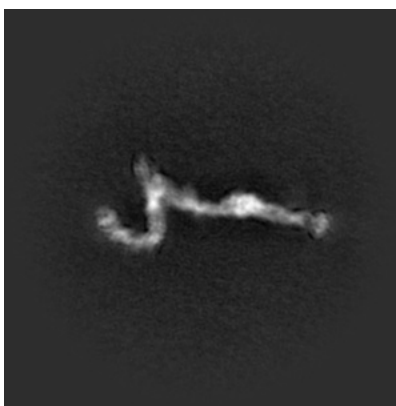
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

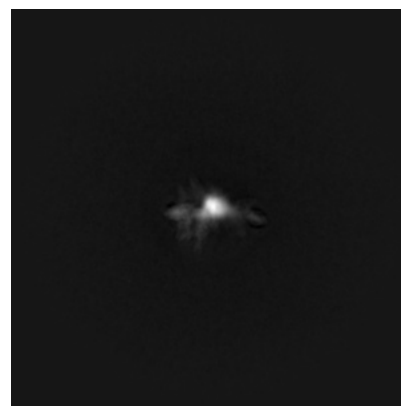
6.1.1 Primary map



X

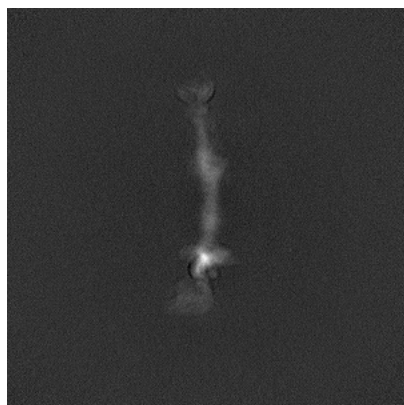


Y

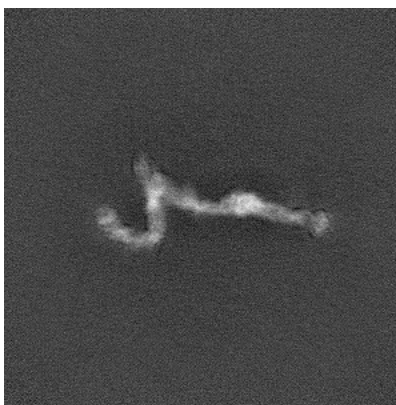


Z

6.1.2 Raw map



X



Y

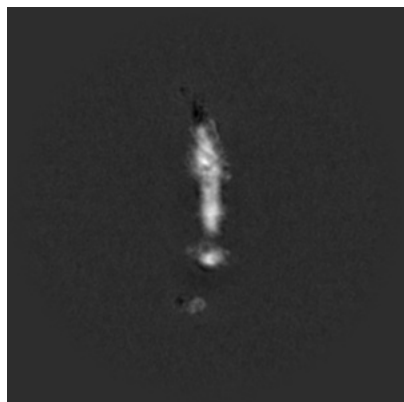


Z

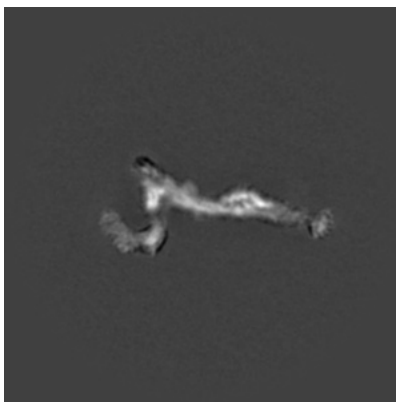
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

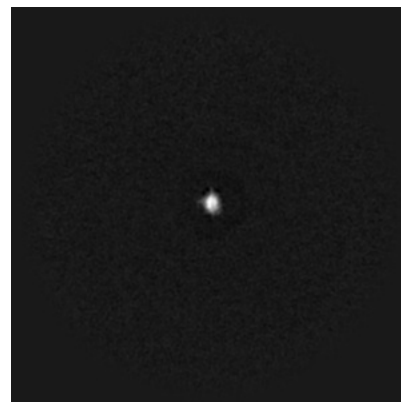
6.2.1 Primary map



X Index: 260

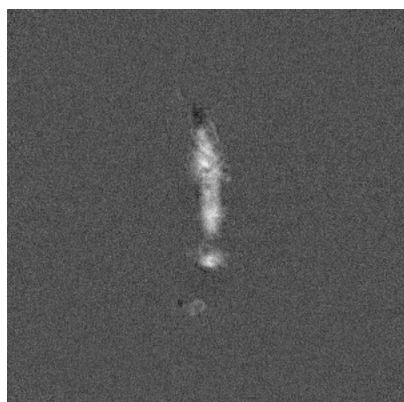


Y Index: 260

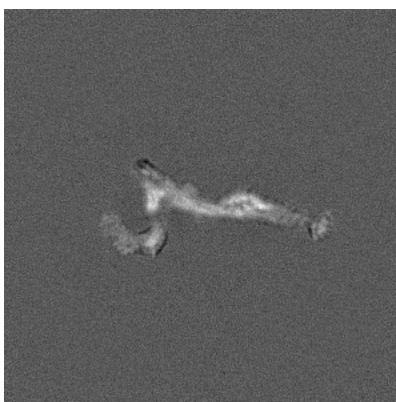


Z Index: 260

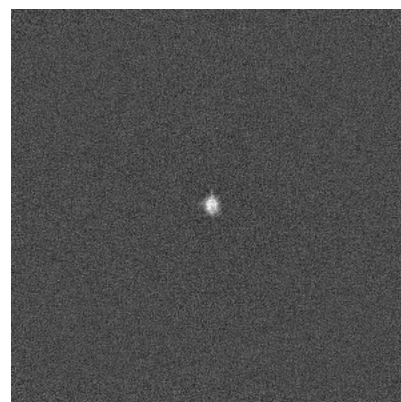
6.2.2 Raw map



X Index: 260



Y Index: 260

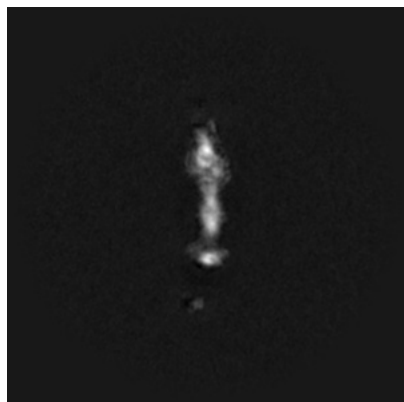


Z Index: 260

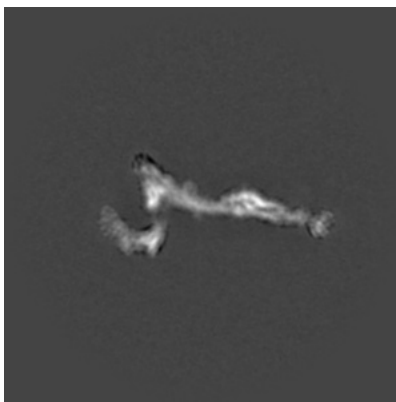
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

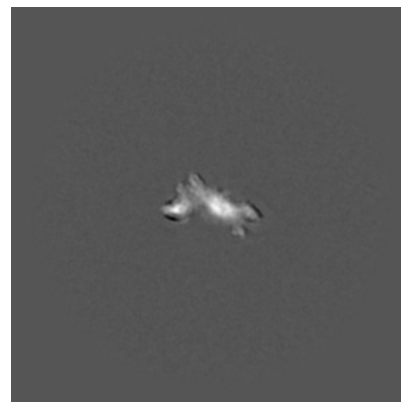
6.3.1 Primary map



X Index: 263



Y Index: 257



Z Index: 194

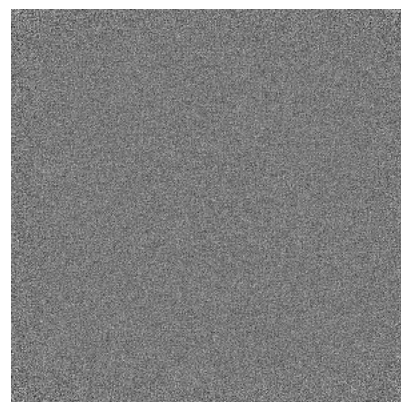
6.3.2 Raw map



X Index: 263



Y Index: 257

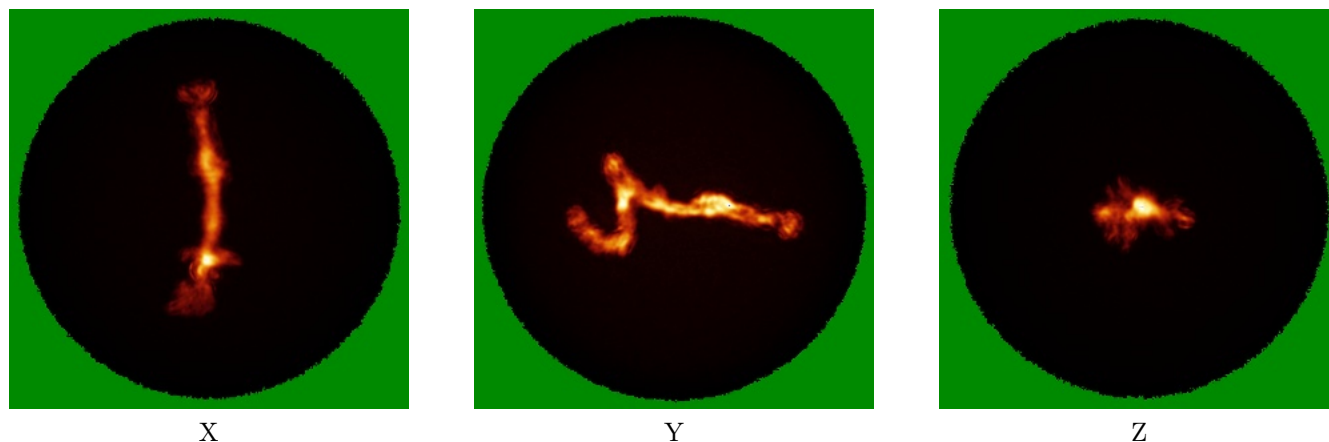


Z Index: 0

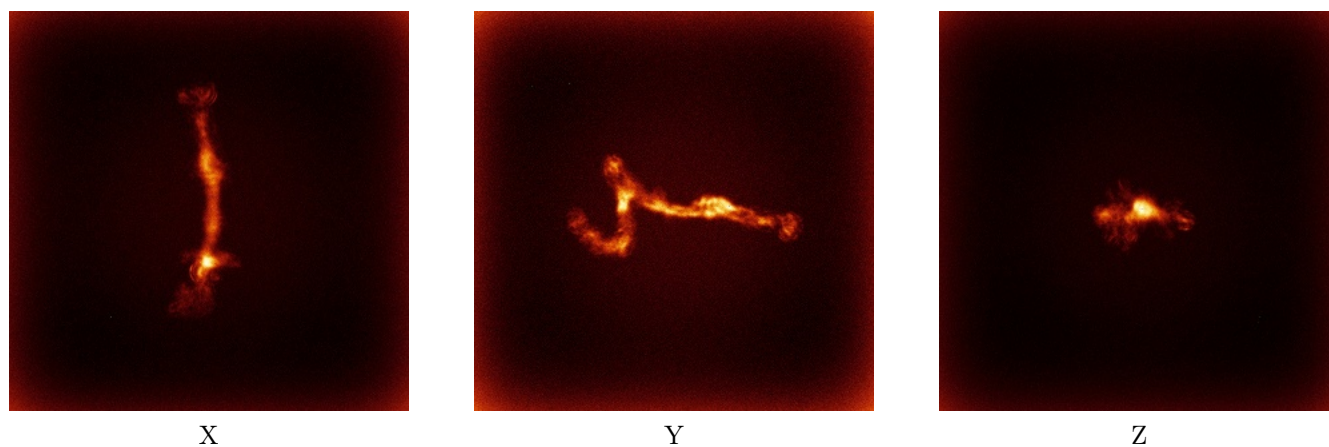
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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.

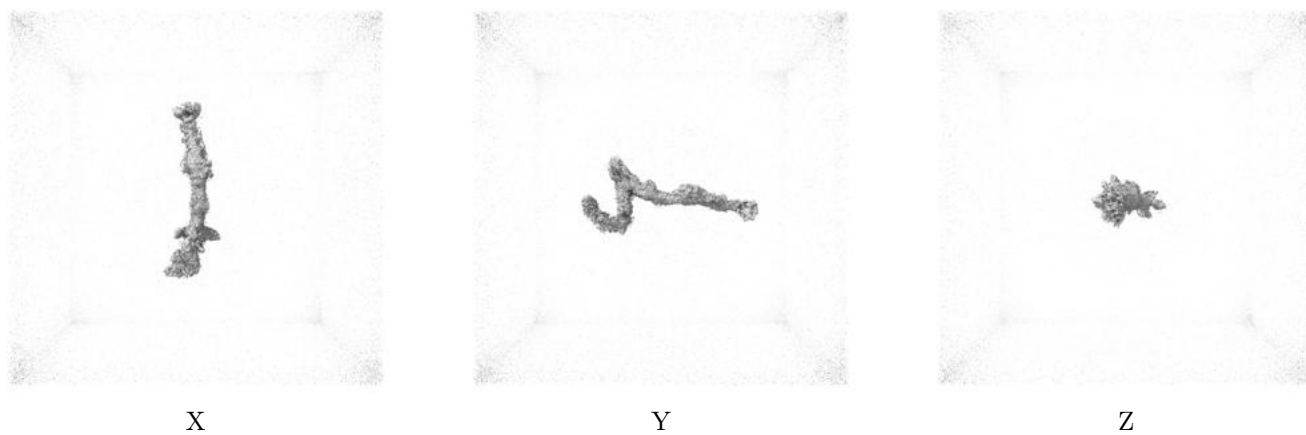
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.161. 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.

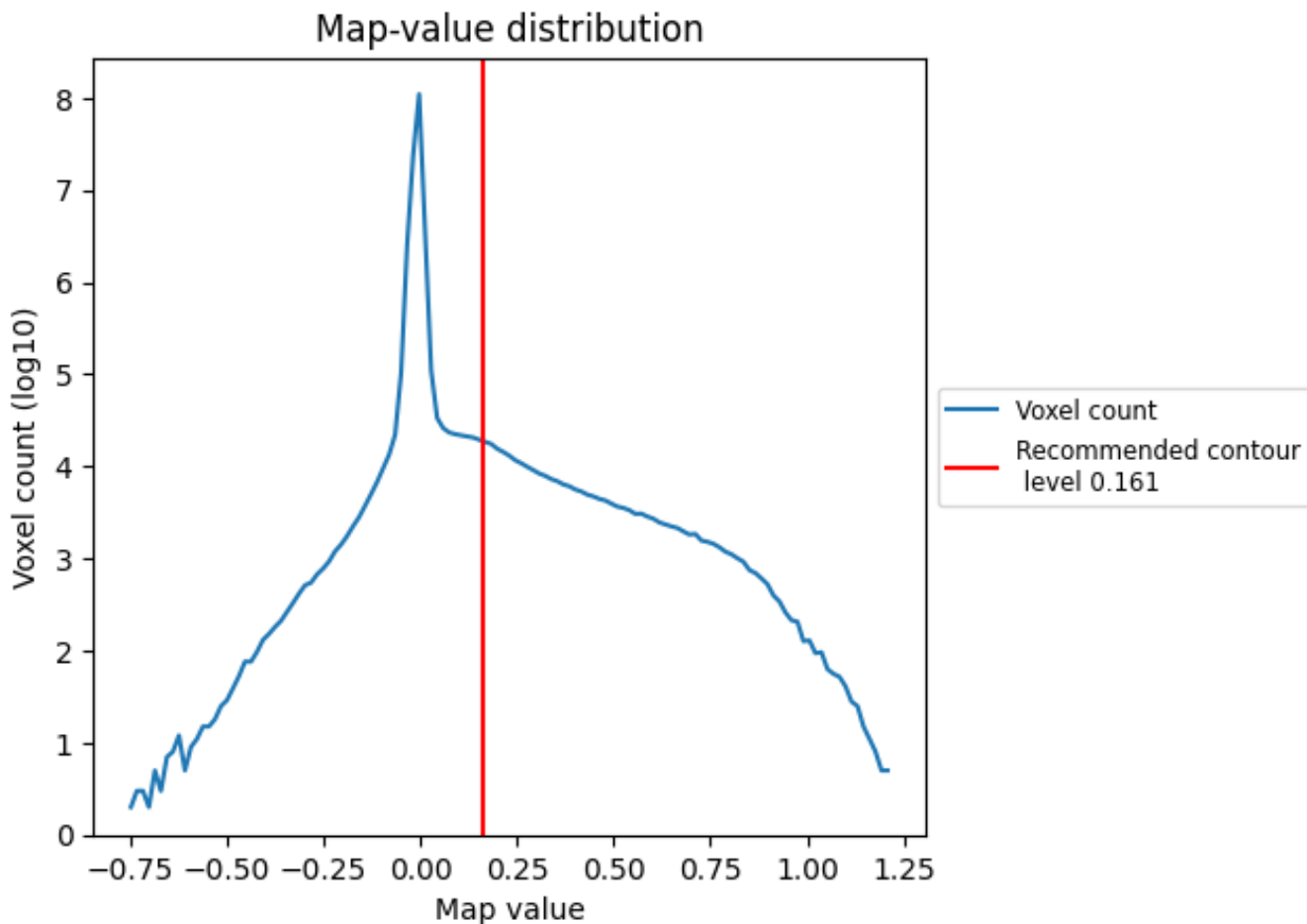
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

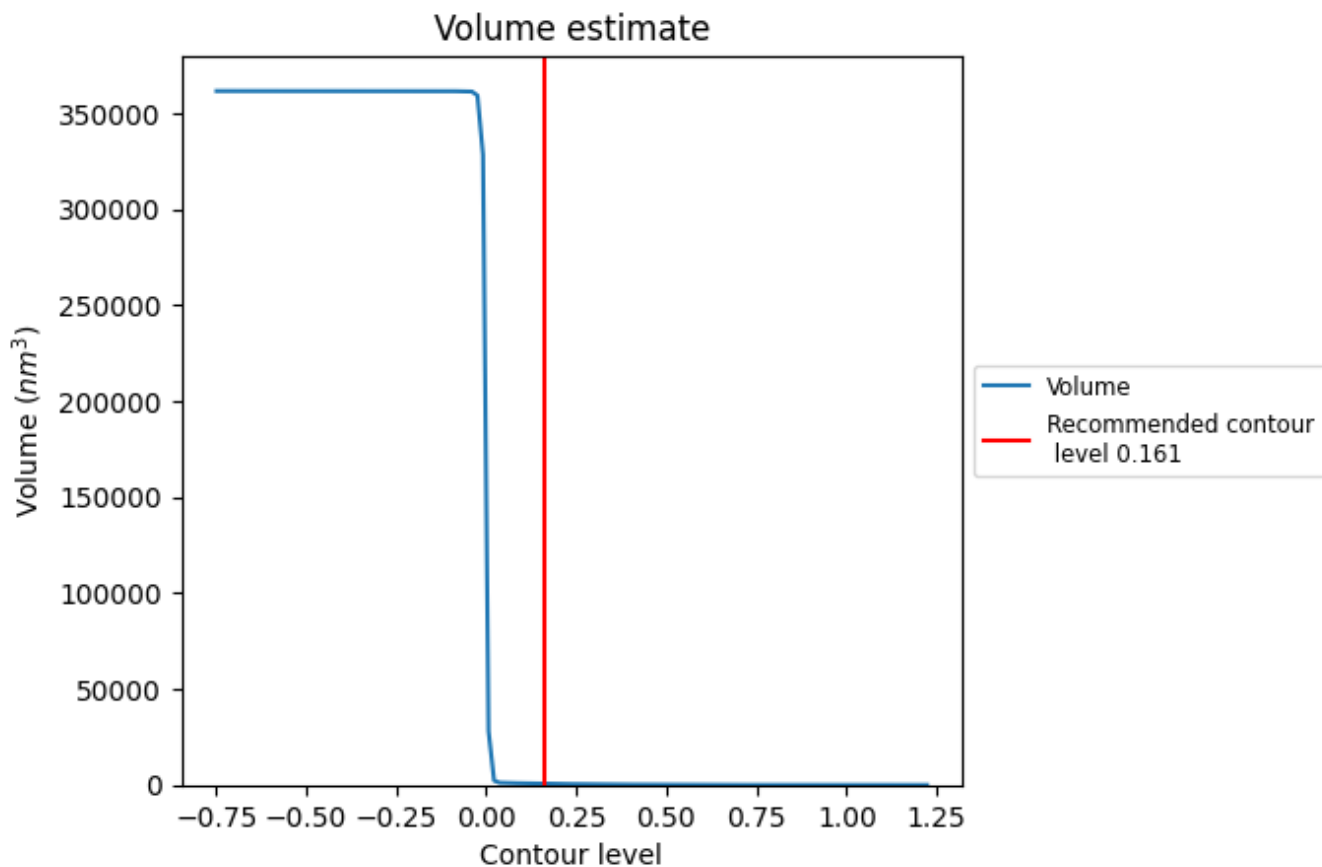
This section contains the results of statistical analysis of the map.

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.

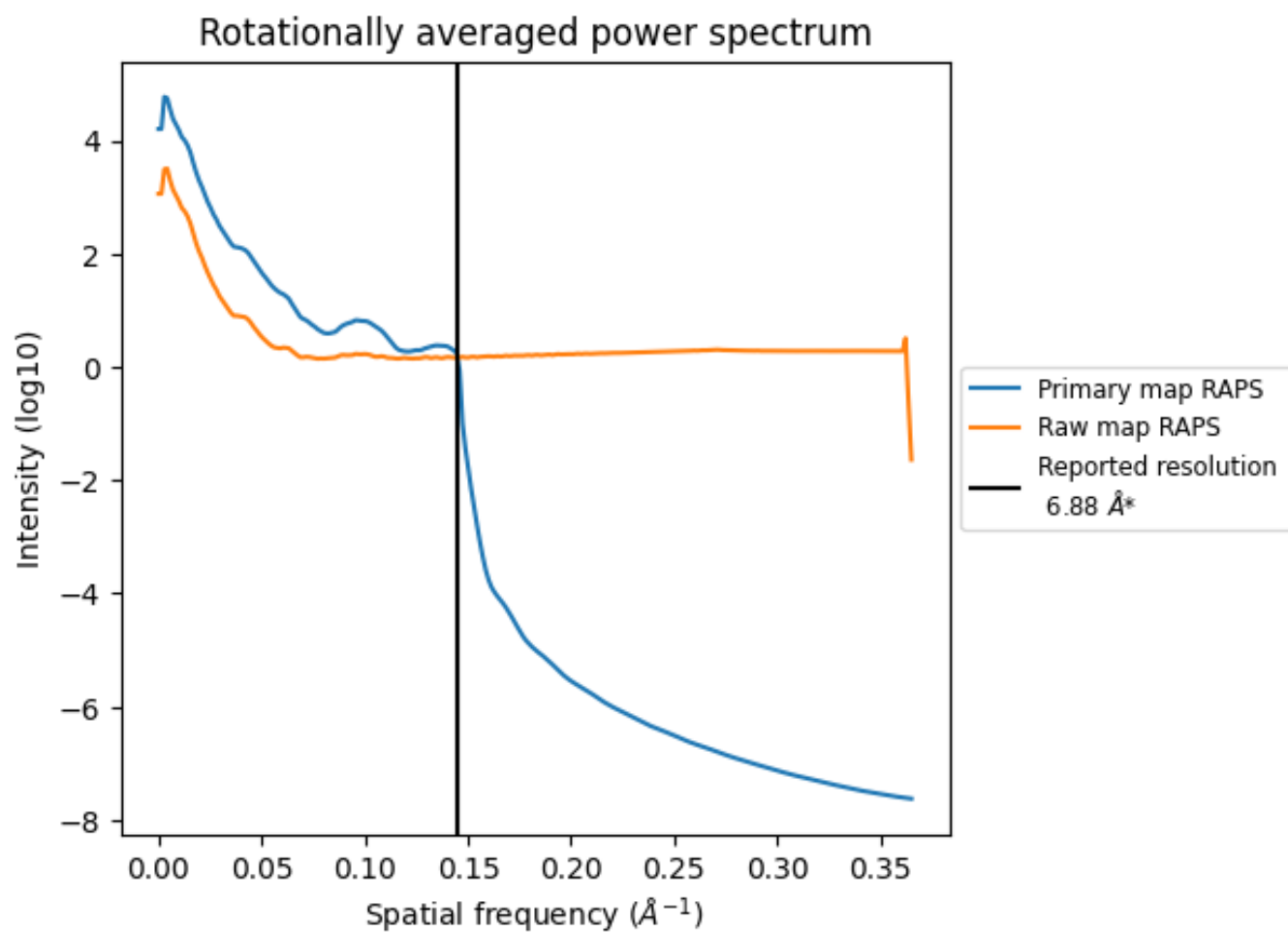
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 661 nm^3 ; this corresponds to an approximate mass of 597 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

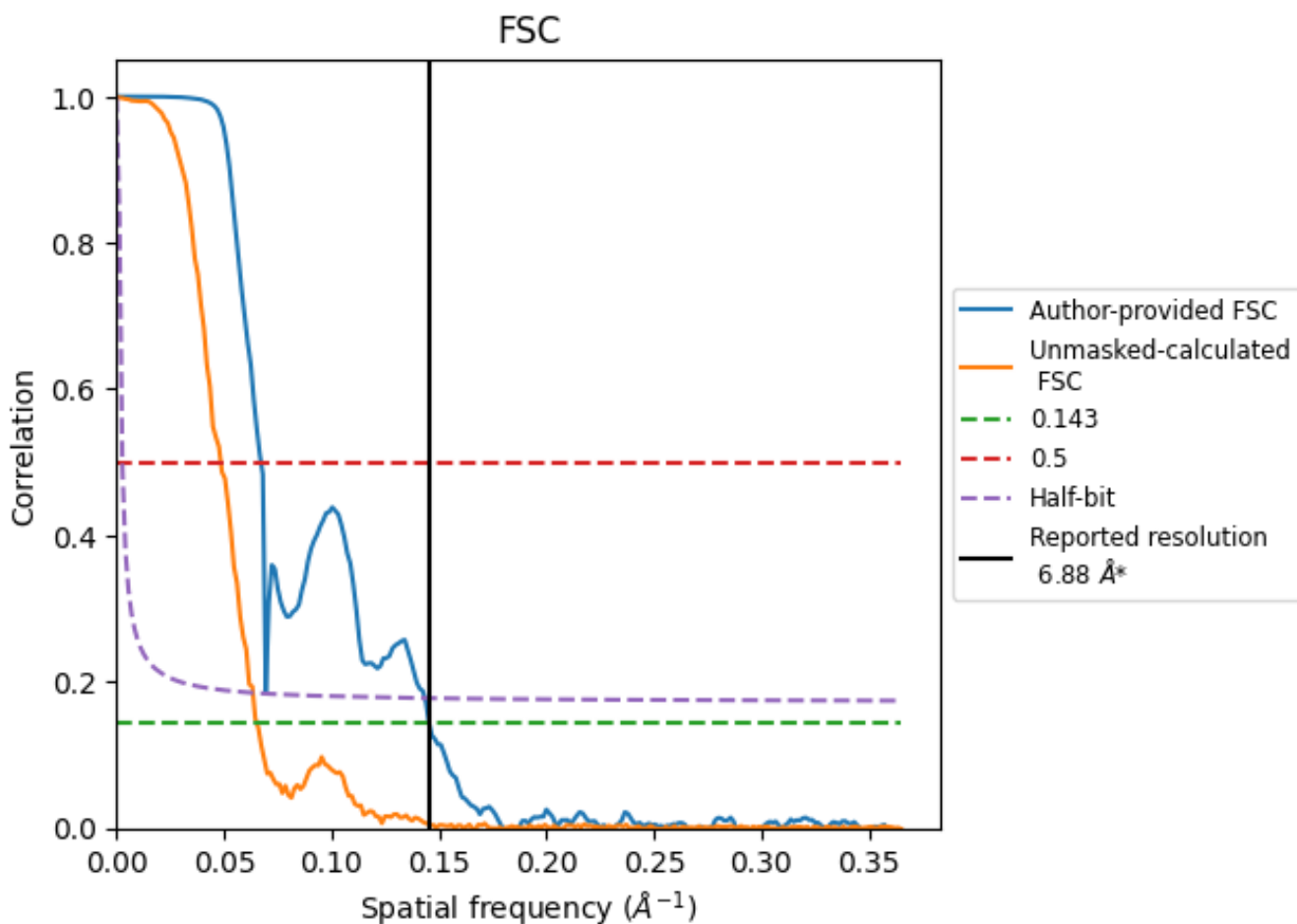


*Reported resolution corresponds to spatial frequency of 0.145 Å⁻¹

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 0.145 Å⁻¹

8.2 Resolution estimates [i](#)

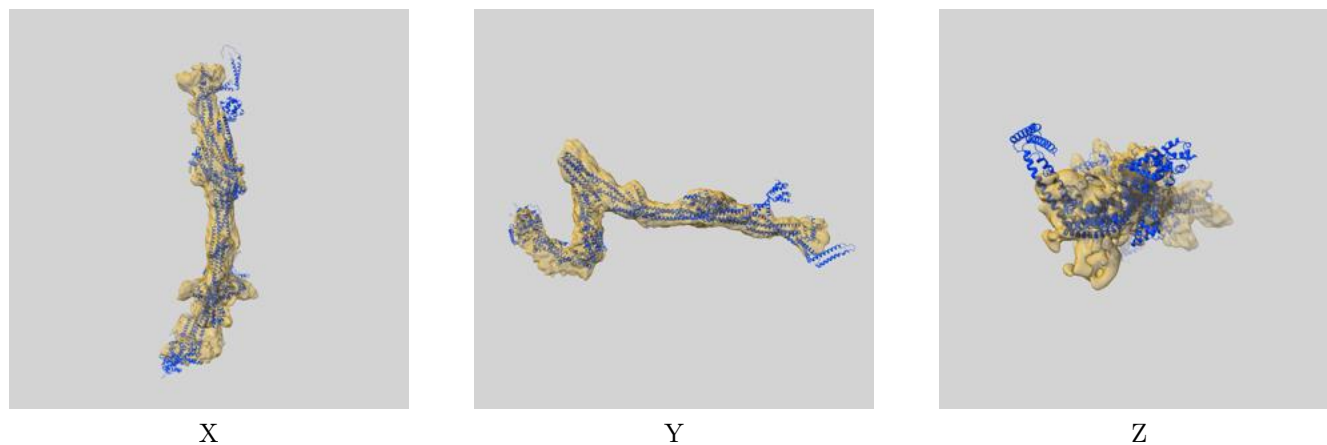
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.88	-	-
Author-provided FSC curve	6.88	14.88	6.97
Unmasked-calculated*	15.31	20.58	15.77

*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 15.31 differs from the reported value 6.88 by more than 10 %

9 Map-model fit [i](#)

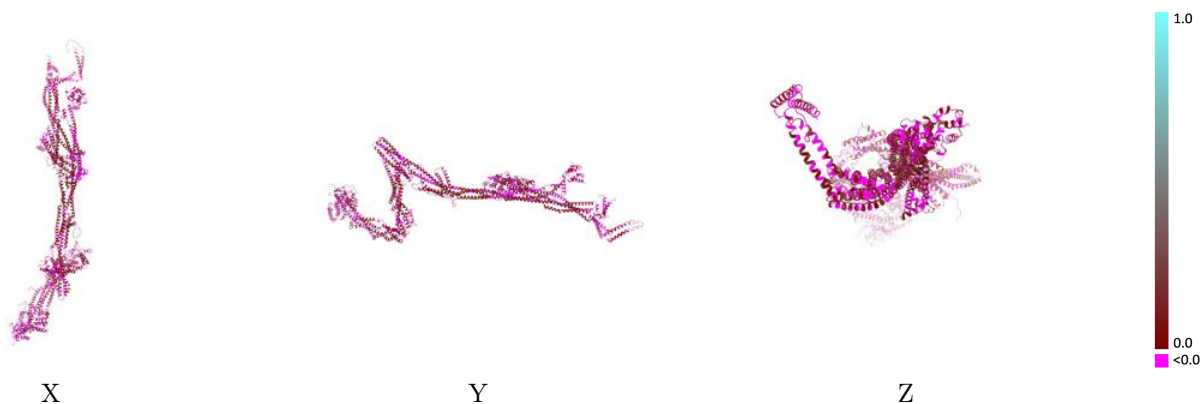
This section contains information regarding the fit between EMDB map EMD-28981 and PDB model 8FCK. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



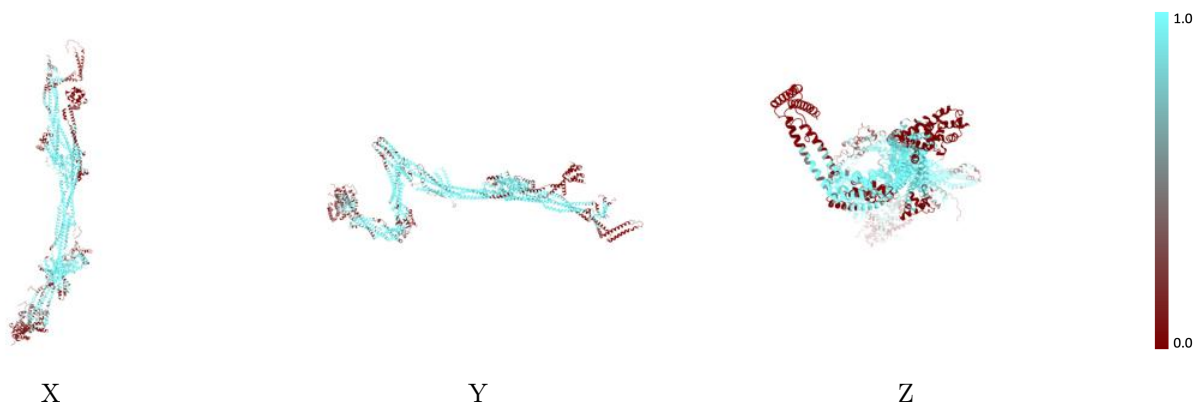
The images above show the 3D surface view of the map at the recommended contour level 0.161 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



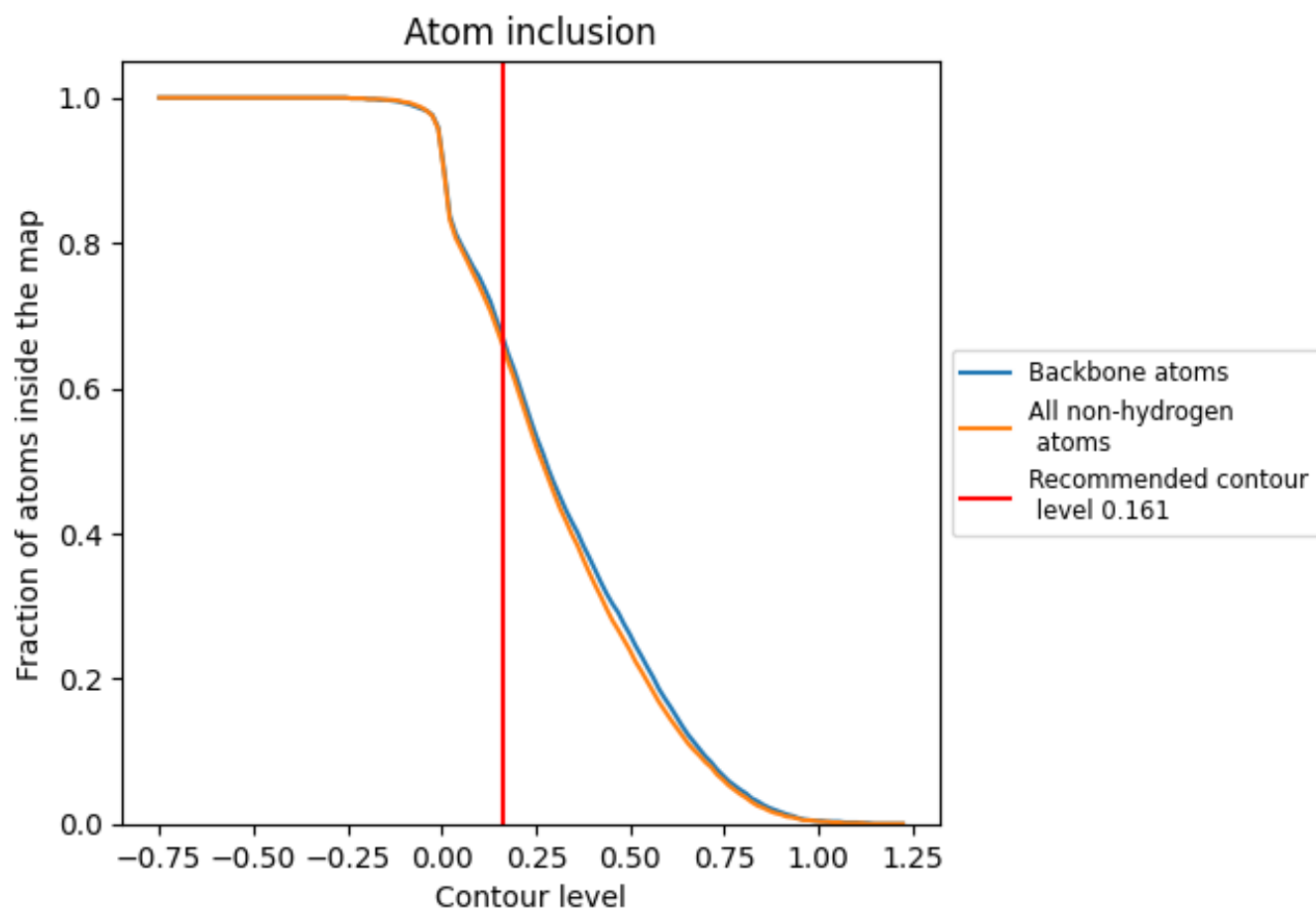
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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 (0.161).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 66% 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 (0.161) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6610	 0.0350
A	 0.5820	 0.0470
B	 0.7120	 0.0240
C	 0.6800	 0.0350
D	 0.7680	 0.0530
E	 0.7380	 0.0430
F	 0.4320	 0.0210
G	 0.5600	 0.0230
H	 0.7500	 0.0280

