



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:58 AM UTC

PDB ID : 8W20 / pdb_00008w20
EMDB ID : EMD-43736
Title : Umb1 umbrella toxin particle
Authors : Park, Y.J.; Zhao, Q.; Seattle Structural Genomics Center for Infectious Disease (SSGCID); DiMaio, F.; Mougous, J.D.; Veesler, D.
Deposited on : 2024-02-19
Resolution : 4.30 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

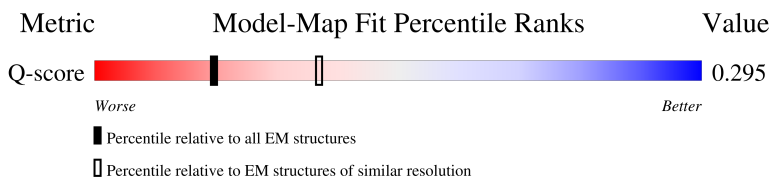
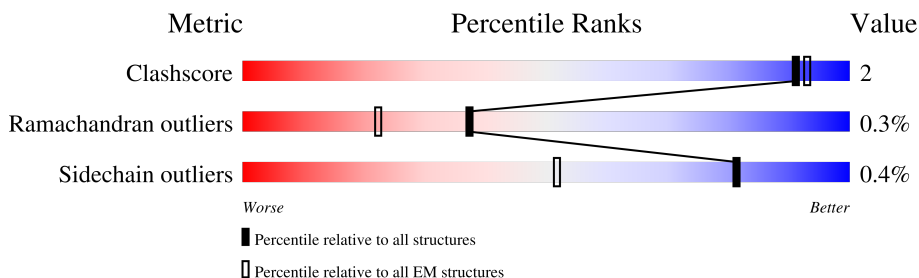
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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	4585 (3.80 - 4.80)

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	B	166	
1	D	166	
1	F	166	
1	H	166	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	J	166	
2	C	515	
2	E	515	
2	G	515	
2	I	515	
2	K	515	
3	A	1368	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15412 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 Secreted protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	124	Total	C	N	O	S	0	0
			768	494	139	129	6		
1	D	122	Total	C	N	O	S	0	0
			756	479	140	131	6		
1	F	121	Total	C	N	O	S	0	0
			696	440	127	126	3		
1	H	124	Total	C	N	O	S	0	0
			728	458	136	130	4		
1	J	122	Total	C	N	O	S	0	0
			698	442	126	126	4		

- Molecule 2 is a protein called Secreted esterase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	405	Total	C	N	O	S	0	0
			2091	1268	410	409	4		
2	E	221	Total	C	N	O	S	0	0
			1125	678	222	221	4		
2	G	219	Total	C	N	O	S	0	0
			1115	672	220	219	4		
2	I	405	Total	C	N	O	S	0	0
			2044	1226	409	405	4		
2	K	219	Total	C	N	O	S	0	0
			1112	669	220	219	4		

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	506	GLY	-	expression tag	UNP Q9ACV4
C	507	SER	-	expression tag	UNP Q9ACV4
C	508	HIS	-	expression tag	UNP Q9ACV4
C	509	HIS	-	expression tag	UNP Q9ACV4
C	510	HIS	-	expression tag	UNP Q9ACV4
C	511	HIS	-	expression tag	UNP Q9ACV4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	512	HIS	-	expression tag	UNP Q9ACV4
C	513	HIS	-	expression tag	UNP Q9ACV4
C	514	HIS	-	expression tag	UNP Q9ACV4
C	515	HIS	-	expression tag	UNP Q9ACV4
E	506	GLY	-	expression tag	UNP Q9ACV4
E	507	SER	-	expression tag	UNP Q9ACV4
E	508	HIS	-	expression tag	UNP Q9ACV4
E	509	HIS	-	expression tag	UNP Q9ACV4
E	510	HIS	-	expression tag	UNP Q9ACV4
E	511	HIS	-	expression tag	UNP Q9ACV4
E	512	HIS	-	expression tag	UNP Q9ACV4
E	513	HIS	-	expression tag	UNP Q9ACV4
E	514	HIS	-	expression tag	UNP Q9ACV4
E	515	HIS	-	expression tag	UNP Q9ACV4
G	506	GLY	-	expression tag	UNP Q9ACV4
G	507	SER	-	expression tag	UNP Q9ACV4
G	508	HIS	-	expression tag	UNP Q9ACV4
G	509	HIS	-	expression tag	UNP Q9ACV4
G	510	HIS	-	expression tag	UNP Q9ACV4
G	511	HIS	-	expression tag	UNP Q9ACV4
G	512	HIS	-	expression tag	UNP Q9ACV4
G	513	HIS	-	expression tag	UNP Q9ACV4
G	514	HIS	-	expression tag	UNP Q9ACV4
G	515	HIS	-	expression tag	UNP Q9ACV4
I	506	GLY	-	expression tag	UNP Q9ACV4
I	507	SER	-	expression tag	UNP Q9ACV4
I	508	HIS	-	expression tag	UNP Q9ACV4
I	509	HIS	-	expression tag	UNP Q9ACV4
I	510	HIS	-	expression tag	UNP Q9ACV4
I	511	HIS	-	expression tag	UNP Q9ACV4
I	512	HIS	-	expression tag	UNP Q9ACV4
I	513	HIS	-	expression tag	UNP Q9ACV4
I	514	HIS	-	expression tag	UNP Q9ACV4
I	515	HIS	-	expression tag	UNP Q9ACV4
K	506	GLY	-	expression tag	UNP Q9ACV4
K	507	SER	-	expression tag	UNP Q9ACV4
K	508	HIS	-	expression tag	UNP Q9ACV4
K	509	HIS	-	expression tag	UNP Q9ACV4
K	510	HIS	-	expression tag	UNP Q9ACV4
K	511	HIS	-	expression tag	UNP Q9ACV4
K	512	HIS	-	expression tag	UNP Q9ACV4
K	513	HIS	-	expression tag	UNP Q9ACV4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	514	HIS	-	expression tag	UNP Q9ACV4
K	515	HIS	-	expression tag	UNP Q9ACV4

- Molecule 3 is a protein called Intein C-terminal splicing domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	732	Total	C	N	O	S	0	0
			4279	2636	851	785	7		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9ACV2
A	2	ARG	-	expression tag	UNP Q9ACV2
A	3	ARG	-	expression tag	UNP Q9ACV2
A	4	ARG	-	expression tag	UNP Q9ACV2
A	5	ILE	-	expression tag	UNP Q9ACV2
A	6	PRO	-	expression tag	UNP Q9ACV2
A	7	SER	-	expression tag	UNP Q9ACV2
A	8	ARG	-	expression tag	UNP Q9ACV2
A	9	THR	-	expression tag	UNP Q9ACV2
A	10	PRO	-	expression tag	UNP Q9ACV2
A	11	GLY	-	expression tag	UNP Q9ACV2
A	12	SER	-	expression tag	UNP Q9ACV2
A	13	GLY	-	expression tag	UNP Q9ACV2
A	14	ALA	-	expression tag	UNP Q9ACV2
A	15	LYS	-	expression tag	UNP Q9ACV2
A	16	GLN	-	expression tag	UNP Q9ACV2
A	17	LYS	-	expression tag	UNP Q9ACV2
A	18	SER	-	expression tag	UNP Q9ACV2
A	19	TRP	-	expression tag	UNP Q9ACV2
A	20	PHE	-	expression tag	UNP Q9ACV2
A	21	PRO	-	expression tag	UNP Q9ACV2
A	22	ARG	-	expression tag	UNP Q9ACV2
A	23	ARG	-	expression tag	UNP Q9ACV2
A	24	SER	-	expression tag	UNP Q9ACV2
A	25	LEU	-	expression tag	UNP Q9ACV2
A	26	GLN	-	expression tag	UNP Q9ACV2
A	27	VAL	-	expression tag	UNP Q9ACV2
A	28	LEU	-	expression tag	UNP Q9ACV2
A	29	LEU	-	expression tag	UNP Q9ACV2
A	30	SER	-	expression tag	UNP Q9ACV2

Continued on next page...

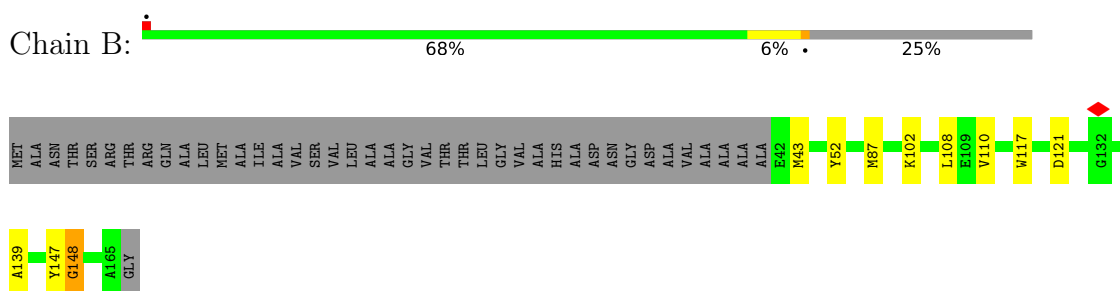
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	ALA	-	expression tag	UNP Q9ACV2
A	32	GLY	-	expression tag	UNP Q9ACV2

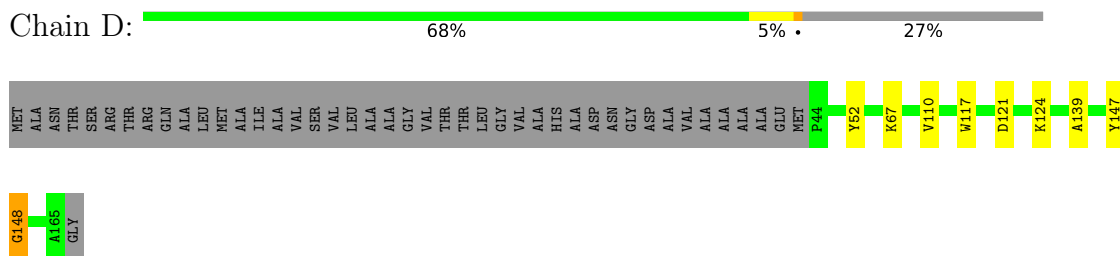
3 Residue-property plots

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.

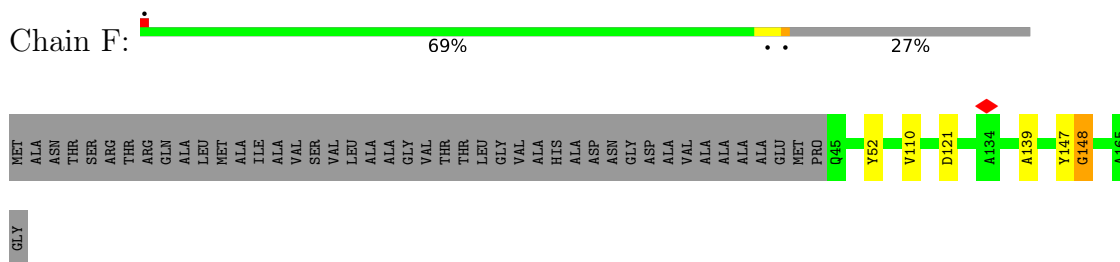
- Molecule 1: Secreted protein



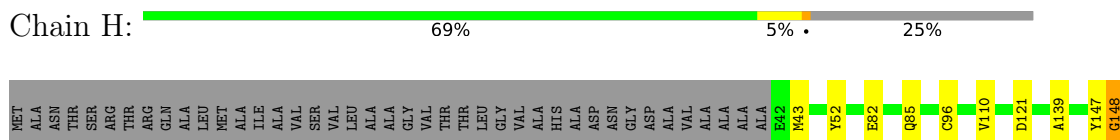
- Molecule 1: Secreted protein



- Molecule 1: Secreted protein



- Molecule 1: Secreted protein



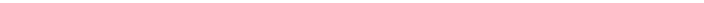
[illegible]

- Molecule 2: Secreted esterase

Chain G:  40% 57%

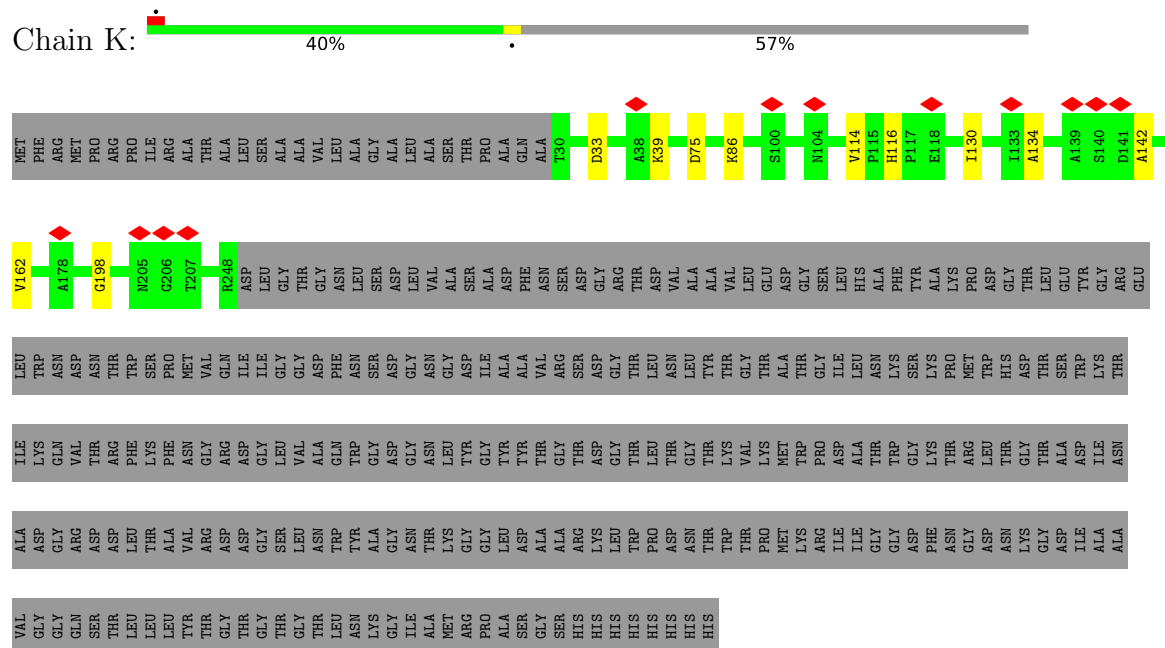
[illegible]

- Molecule 2: Secreted esterase

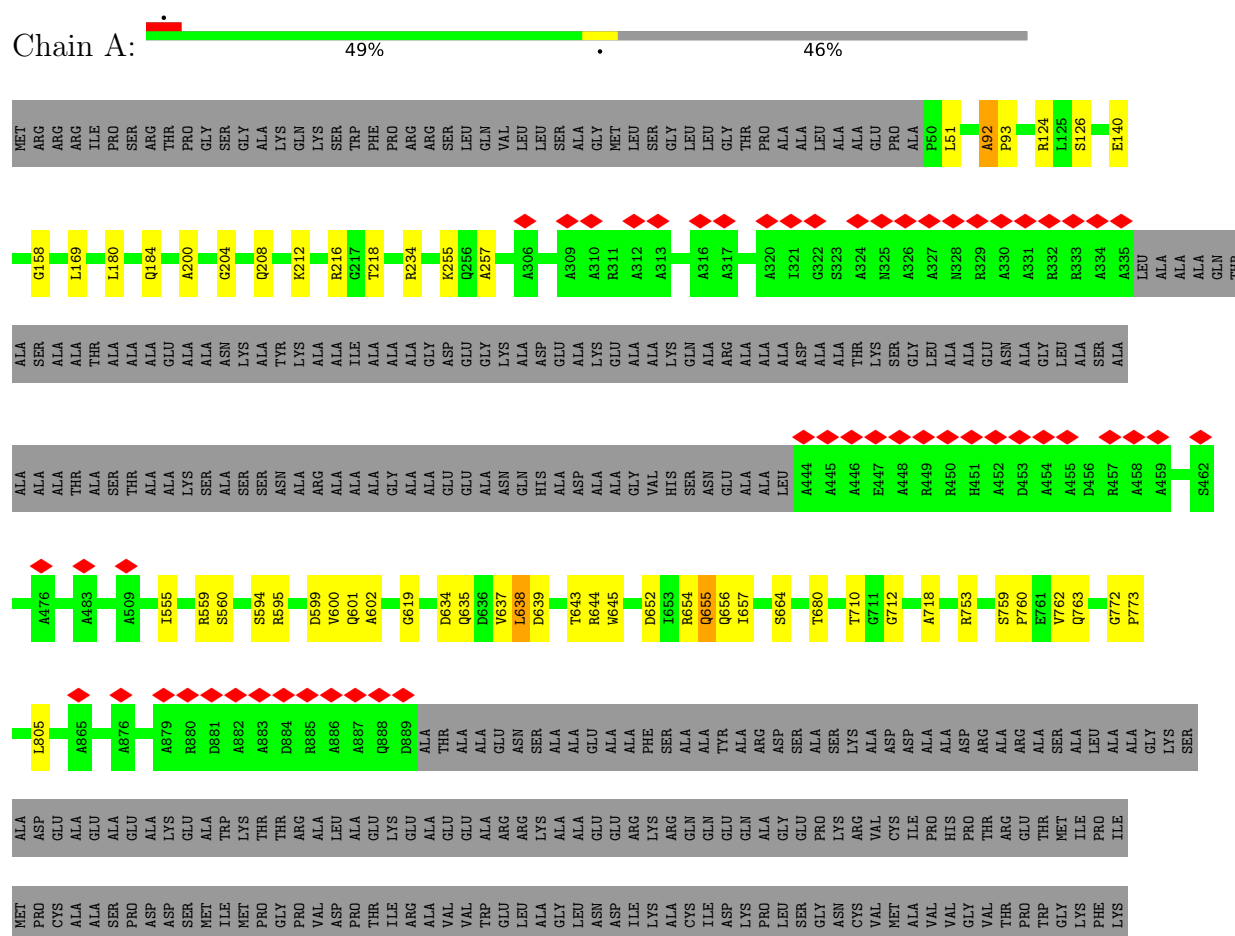
Chain I:  28% 75% 21%

HIS HIS HIS HIS	K449	L450	W451	P452	D453	W454	T455	T457	P458	W459	L462	I463	G464	GLY	ASP	PHE	ASN	GLY	ASP	ASN	ASN	ASN	LYS	G473	D474	I475	ALA	A477	V478	G479	T483	L484	L486	Y487	THR	GLY	THR	GLY	THR	GLY	THR	LEU	ASN	LYS	G498	T499	A500	W501	R502	P503	A504	SER	GLY	SER	HIS	HIS	HIS	
	S256	D257	L258	V259	A260	S261	A262	D263	F264	N265	S266	D267	G268	R269	T270	E277	D278	G279	S280	Y285	A286	K287	PRO	ASP	GLY	THR	L292	R296	E297	LEU	TRP	ASN	ASP	ASN	THR	THR	PRO	M307	V308	Q309	T310	I311	F315	N316	S317	D318	G319	N320	G321	D322	I323	ALA	VAL	VAL	ARG			
	SER	GLY	THR	L332	N333	L334	G337	T338	A339	T340	G341	L342	L343	N344	K345	S346	K347	P348	M349	W350	H351	ASP	THR	SER	THR	K356	T357	L358	K359	Q360	V361	T362	K363	F364	K365	F366	N367	G368	R369	ASP	G371	L372	V373	A374	Q375	W376	G377	D378	G379	N380	L381	Y382	G383	Y384	Y385	THR	GLY	THR
	ASP	GLY	THR	LEU	THR	GLY	T395	K396	V397	K398	M399	W400	P401	D402	A403	T404	W405	GLY	LYS	T408	R409	L410	T411	G412	T413	A414	D415	T416	W417	ALA	ASP	GLY	ARG	ASP	D423	L424	T425	A426	W427	R428	D429	D430	G431	S432	L433	W434	W435	Y436	A437	GLY	ASN	LYS	GLY	GLY	LEU	ASP	ALA	A447
MET	PHE	ARG	MET	PRO	ARG	PRO	ILE	ARG	ALA	LEU	SER	ALA	VAL	LEU	ALA	GLY	LEU	ALA	ALA	SER	SER	THR	PRO	ALA	GLN	ALA	T30	D33	K39	D75	K36	V114	P115	H116	I130	A134	S140	D141	A142	V162	G198	N205	T252	G253														

- Molecule 2: Secreted esterase



- Molecule 3: Intein C-terminal splicing domain-containing protein



HIS	VAL	ALA	ASP	THR	LEU
TYR	ALA	TRP	THR	PRO	VAL
PRO	HIS	LYS	LEU	THR	SER
GLY	HIS	LYS	ARG	THR	LYS
SER	ALA	LEU	THR	GLY	GLY
ASP	ALA	PRO	PRO	THR	ASN
ALA	LYS	ARG	GLN	GLY	GLY
LEU	ILE	LYS	THR	ALA	LEU
GLU	ALA	SER	ALA	ARG	ASP
LEU	TRP	GLY	VAL	THR	ALA
LYS	GLU	ASP	VAL	VAL	VAL
GLY	MET	PRO	ILE	THR	LYS
THR	ARG	THR	ALA	ARG	ASP
ALA	THR	SER	ALA	THR	ALA
LYS	ALA	GLY	THR	ILE	ARG
ARG	MET	TYR	HIS	GLY	GLY
	GLY	VAL	ASP	THR	ALA
	LYS	PHE	TRP	PRO	ARG
	GLY	GLU	PRO	ASP	ARG
	LYS	ALA	GLY	ASP	THR
	LEU	GLY	GLN	ASN	ALA
	HIS	THR	ASP	PHE	CYS
	ILE	LEU	ALA	THR	LEU
	VAL	VAL	TYR	ASP	THR
	ILE	TRP	ASP	VAL	GLY
	ASN	ASP	LEU	ALA	ALA
	THR	SER	THR	LEU	ALA
	ASN	VAL	VAL	ALA	HIS
	TYR	LEU	GLY	ASP	SER
	VAL	THR	GLY	GLY	PHE
	CYS	SER	PHE	SER	PRO
	PRO	GLY	HIS	THR	ALA
	LYS	ARG	SER	LEU	GLY
	VAL	SER	TYR	THR	THR
	SER	PRO	TYR	SER	ARG
	SER	LEU	VAL	THR	VAL
	PRO	SER	SER	THR	LEU
	ASN	GLU	THR	HIS	MET
	SER	ASP	GLY	HIS	ALA
	MET	ILE	THR	PRO	ASP
	GLY	SER	THR	TYR	GLY
	CYS	ALA	ASP	TRP	THR
	LYS	PHE	VAL	SER	ARG
	GLN	LEU	GLN	GLN	ARG
	ALA	LYS	VAL	ASN	SER
	VAL	GLY	HIS	ASP	ILE
	PRO	SER	ASN	GLN	GLU
	ALA	PRO	ASN	THR	GLN
	ILE	ASP	ASP	THR	ILE
	TYR	PHE	ASN	LYS	GLY
	LEU	PRO	PRO	ASN	ALA
	GLU	ASN	CYS	ALA	GLY
	ASP	PHE	PRO	GLY	ASP
	GLN	PRO	ASP	LEU	LEU
	THR	GLY	TRP	THR	VAL
	LEU	TYR	VAL	GLU	THR
	VAL	ALA	SER	ALA	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	386275	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	13.808	Depositor
Minimum map value	-11.234	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.110	Depositor
Recommended contour level	0.7	Depositor
Map size ($\text{\AA}$)	512.544, 512.544, 512.544	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.686, 1.686, 1.686	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	B	0.58	1/785 (0.1%)	1.05	10/1077 (0.9%)
1	D	0.61	1/773 (0.1%)	1.06	9/1057 (0.9%)
1	F	0.45	0/710	1.02	8/981 (0.8%)
1	H	0.46	0/743	1.04	10/1023 (1.0%)
1	J	0.50	0/714	1.05	9/987 (0.9%)
2	C	0.45	0/2103	1.04	29/2905 (1.0%)
2	E	0.44	0/1138	1.13	21/1587 (1.3%)
2	G	0.44	0/1128	1.14	21/1573 (1.3%)
2	I	0.45	0/2051	1.05	29/2834 (1.0%)
2	K	0.43	0/1125	1.14	21/1569 (1.3%)
3	A	0.55	3/4324 (0.1%)	0.95	44/5951 (0.7%)
All	All	0.50	5/15594 (0.0%)	1.04	211/21544 (1.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	102	LYS	C-O	-8.79	1.12	1.24
3	A	234	ARG	CA-C	-7.35	1.43	1.52
1	D	124	LYS	C-O	-5.48	1.17	1.24
3	A	599	ASP	N-CA	5.42	1.49	1.46
3	A	638	LEU	CA-C	5.28	1.59	1.52

All (211) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	645	TRP	N-CA-C	-9.83	100.55	111.07
3	A	639	ASP	N-CA-C	9.55	122.89	111.33
3	A	637	VAL	N-CA-C	-8.75	101.46	111.00
3	A	619	GLY	CA-C-N	8.30	128.78	119.32
3	A	619	GLY	C-N-CA	8.30	128.78	119.32
3	A	257	ALA	N-CA-C	-8.25	102.36	111.36
3	A	643	THR	N-CA-C	7.89	122.82	112.72
3	A	204	GLY	CA-C-N	7.86	127.41	119.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	204	GLY	C-N-CA	7.86	127.41	119.24
2	K	114	VAL	CA-C-N	7.77	127.69	119.85
2	K	114	VAL	C-N-CA	7.77	127.69	119.85
2	I	114	VAL	CA-C-N	7.74	127.67	119.85
2	I	114	VAL	C-N-CA	7.74	127.67	119.85
2	C	114	VAL	CA-C-N	7.72	127.65	119.85
2	C	114	VAL	C-N-CA	7.72	127.65	119.85
2	G	114	VAL	CA-C-N	7.69	127.61	119.85
2	G	114	VAL	C-N-CA	7.69	127.61	119.85
2	E	114	VAL	CA-C-N	7.67	127.59	119.85
2	E	114	VAL	C-N-CA	7.67	127.59	119.85
3	A	657	ILE	N-CA-C	-7.46	103.19	110.72
3	A	656	GLN	N-CA-C	7.31	121.46	112.54
1	B	43	MET	CA-C-N	7.31	127.26	120.03
1	B	43	MET	C-N-CA	7.31	127.26	120.03
2	K	142	ALA	CA-C-N	7.24	127.24	119.78
2	K	142	ALA	C-N-CA	7.24	127.24	119.78
3	A	772	GLY	CA-C-N	7.23	127.83	120.38
3	A	772	GLY	C-N-CA	7.23	127.83	120.38
3	A	158	GLY	CA-C-N	7.20	127.53	119.32
3	A	158	GLY	C-N-CA	7.20	127.53	119.32
2	C	142	ALA	CA-C-N	7.18	127.18	119.78
2	C	142	ALA	C-N-CA	7.18	127.18	119.78
2	I	142	ALA	CA-C-N	7.16	127.16	119.78
2	I	142	ALA	C-N-CA	7.16	127.16	119.78
2	E	142	ALA	CA-C-N	7.14	127.14	119.78
2	E	142	ALA	C-N-CA	7.14	127.14	119.78
2	G	142	ALA	CA-C-N	7.14	127.13	119.78
2	G	142	ALA	C-N-CA	7.14	127.13	119.78
1	J	110	VAL	CA-C-N	7.04	127.02	119.76
1	J	110	VAL	C-N-CA	7.04	127.02	119.76
1	F	110	VAL	CA-C-N	7.02	127.01	119.78
1	F	110	VAL	C-N-CA	7.02	127.01	119.78
1	D	110	VAL	CA-C-N	6.96	126.92	119.76
1	D	110	VAL	C-N-CA	6.96	126.92	119.76
2	C	502	ARG	CA-C-N	6.93	126.89	120.03
2	C	502	ARG	C-N-CA	6.93	126.89	120.03
1	H	110	VAL	CA-C-N	6.92	126.90	119.78
1	H	110	VAL	C-N-CA	6.92	126.90	119.78
2	G	134	ALA	CA-C-N	6.89	127.34	120.52
2	G	134	ALA	C-N-CA	6.89	127.34	120.52
2	C	134	ALA	CA-C-N	6.89	127.34	120.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	134	ALA	C-N-CA	6.89	127.34	120.52
1	B	110	VAL	CA-C-N	6.88	126.86	119.78
1	B	110	VAL	C-N-CA	6.88	126.86	119.78
2	I	502	ARG	CA-C-N	6.87	126.83	120.03
2	I	502	ARG	C-N-CA	6.87	126.83	120.03
3	A	645	TRP	N-CA-CB	6.86	119.95	110.01
2	K	134	ALA	CA-C-N	6.86	127.31	120.52
2	K	134	ALA	C-N-CA	6.86	127.31	120.52
2	I	134	ALA	CA-C-N	6.85	127.31	120.52
2	I	134	ALA	C-N-CA	6.85	127.31	120.52
1	H	139	ALA	CA-C-N	6.81	126.77	120.03
1	H	139	ALA	C-N-CA	6.81	126.77	120.03
2	E	134	ALA	CA-C-N	6.80	127.25	120.52
2	E	134	ALA	C-N-CA	6.80	127.25	120.52
1	B	139	ALA	CA-C-N	6.76	126.72	120.03
1	B	139	ALA	C-N-CA	6.76	126.72	120.03
3	A	773	PRO	CA-C-N	6.74	127.28	119.47
3	A	773	PRO	C-N-CA	6.74	127.28	119.47
3	A	712	GLY	CA-C-N	6.72	126.98	119.32
3	A	712	GLY	C-N-CA	6.72	126.98	119.32
2	G	75	ASP	CA-C-N	6.71	126.40	119.56
2	G	75	ASP	C-N-CA	6.71	126.40	119.56
3	A	126	SER	CA-C-N	6.71	126.22	119.24
3	A	126	SER	C-N-CA	6.71	126.22	119.24
3	A	664	SER	CA-C-N	6.67	126.80	119.87
3	A	664	SER	C-N-CA	6.67	126.80	119.87
2	C	75	ASP	CA-C-N	6.65	126.34	119.56
2	C	75	ASP	C-N-CA	6.65	126.34	119.56
2	I	451	TRP	CA-C-N	6.65	126.90	119.32
2	I	451	TRP	C-N-CA	6.65	126.90	119.32
2	G	130	ILE	CA-C-N	6.65	126.78	119.87
2	G	130	ILE	C-N-CA	6.65	126.78	119.87
2	C	451	TRP	CA-C-N	6.64	126.89	119.32
2	C	451	TRP	C-N-CA	6.64	126.89	119.32
3	A	255	LYS	N-CA-C	6.64	118.18	111.07
2	E	130	ILE	CA-C-N	6.64	126.78	119.87
2	E	130	ILE	C-N-CA	6.64	126.78	119.87
2	G	198	GLY	CA-C-N	6.63	126.54	119.85
2	G	198	GLY	C-N-CA	6.63	126.54	119.85
2	K	130	ILE	CA-C-N	6.63	126.76	119.87
2	K	130	ILE	C-N-CA	6.63	126.76	119.87
2	I	75	ASP	CA-C-N	6.62	126.25	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	75	ASP	C-N-CA	6.62	126.25	119.56
2	E	75	ASP	CA-C-N	6.61	126.30	119.56
2	E	75	ASP	C-N-CA	6.61	126.30	119.56
2	E	116	HIS	CA-C-N	6.60	126.22	119.56
2	E	116	HIS	C-N-CA	6.60	126.22	119.56
2	G	116	HIS	CA-C-N	6.60	126.22	119.56
2	G	116	HIS	C-N-CA	6.60	126.22	119.56
2	I	130	ILE	CA-C-N	6.60	126.73	119.87
2	I	130	ILE	C-N-CA	6.60	126.73	119.87
2	C	130	ILE	CA-C-N	6.58	126.72	119.87
2	C	130	ILE	C-N-CA	6.58	126.72	119.87
2	I	400	TRP	CA-C-N	6.58	127.10	119.47
2	I	400	TRP	C-N-CA	6.58	127.10	119.47
2	K	116	HIS	CA-C-N	6.57	126.20	119.56
2	K	116	HIS	C-N-CA	6.57	126.20	119.56
2	K	198	GLY	CA-C-N	6.56	126.47	119.85
2	K	198	GLY	C-N-CA	6.56	126.47	119.85
2	C	400	TRP	CA-C-N	6.55	127.07	119.47
2	C	400	TRP	C-N-CA	6.55	127.07	119.47
1	F	139	ALA	CA-C-N	6.55	126.51	120.03
1	F	139	ALA	C-N-CA	6.55	126.51	120.03
1	H	121	ASP	CA-C-N	6.55	126.52	119.78
1	H	121	ASP	C-N-CA	6.55	126.52	119.78
1	B	121	ASP	CA-C-N	6.51	126.47	119.76
1	B	121	ASP	C-N-CA	6.51	126.47	119.76
1	F	121	ASP	CA-C-N	6.49	126.45	119.76
1	F	121	ASP	C-N-CA	6.49	126.45	119.76
2	I	116	HIS	CA-C-N	6.48	126.11	119.56
2	I	116	HIS	C-N-CA	6.48	126.11	119.56
2	K	75	ASP	CA-C-N	6.48	126.17	119.56
2	K	75	ASP	C-N-CA	6.48	126.17	119.56
2	C	162	VAL	CA-C-N	6.47	126.44	120.03
2	C	162	VAL	C-N-CA	6.47	126.44	120.03
1	J	139	ALA	CA-C-N	6.47	126.39	119.85
1	J	139	ALA	C-N-CA	6.47	126.39	119.85
2	C	116	HIS	CA-C-N	6.46	126.14	119.56
2	C	116	HIS	C-N-CA	6.46	126.14	119.56
2	K	162	VAL	CA-C-N	6.45	126.63	120.31
2	K	162	VAL	C-N-CA	6.45	126.63	120.31
2	I	162	VAL	CA-C-N	6.44	126.62	120.31
2	I	162	VAL	C-N-CA	6.44	126.62	120.31
2	G	162	VAL	CA-C-N	6.44	126.62	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	162	VAL	C-N-CA	6.44	126.62	120.31
1	H	43	MET	CA-C-N	6.44	126.97	120.14
1	H	43	MET	C-N-CA	6.44	126.97	120.14
2	C	33	ASP	CA-C-N	6.44	126.39	119.76
2	C	33	ASP	C-N-CA	6.44	126.39	119.76
1	D	139	ALA	CA-C-N	6.43	126.34	119.85
1	D	139	ALA	C-N-CA	6.43	126.34	119.85
3	A	51	LEU	CA-C-N	6.42	126.37	119.76
3	A	51	LEU	C-N-CA	6.42	126.37	119.76
1	J	121	ASP	CA-C-N	6.42	126.37	119.76
1	J	121	ASP	C-N-CA	6.42	126.37	119.76
2	E	162	VAL	CA-C-N	6.39	126.57	120.31
2	E	162	VAL	C-N-CA	6.39	126.57	120.31
2	K	33	ASP	CA-C-N	6.37	126.32	119.76
2	K	33	ASP	C-N-CA	6.37	126.32	119.76
2	I	86	LYS	CA-C-N	6.36	126.31	119.76
2	I	86	LYS	C-N-CA	6.36	126.31	119.76
2	G	33	ASP	CA-C-N	6.30	126.25	119.76
2	G	33	ASP	C-N-CA	6.30	126.25	119.76
2	E	33	ASP	CA-C-N	6.29	126.24	119.76
2	E	33	ASP	C-N-CA	6.29	126.24	119.76
2	C	347	LYS	CA-C-N	6.29	126.32	119.90
2	C	347	LYS	C-N-CA	6.29	126.32	119.90
2	E	86	LYS	CA-C-N	6.29	126.24	119.76
2	E	86	LYS	C-N-CA	6.29	126.24	119.76
1	D	121	ASP	CA-C-N	6.29	126.24	119.76
1	D	121	ASP	C-N-CA	6.29	126.24	119.76
2	G	86	LYS	CA-C-N	6.26	126.21	119.76
2	G	86	LYS	C-N-CA	6.26	126.21	119.76
2	C	86	LYS	CA-C-N	6.26	126.21	119.76
2	C	86	LYS	C-N-CA	6.26	126.21	119.76
2	K	86	LYS	CA-C-N	6.25	126.20	119.76
2	K	86	LYS	C-N-CA	6.25	126.20	119.76
2	I	33	ASP	CA-C-N	6.21	126.16	119.76
2	I	33	ASP	C-N-CA	6.21	126.16	119.76
2	I	347	LYS	CA-C-N	6.21	126.23	119.90
2	I	347	LYS	C-N-CA	6.21	126.23	119.90
2	C	198	GLY	CA-C-N	6.17	126.68	120.14
2	C	198	GLY	C-N-CA	6.17	126.68	120.14
1	J	105	TYR	CB-CA-C	-6.14	96.86	109.94
1	F	52	TYR	CA-C-N	6.14	126.46	119.83
1	F	52	TYR	C-N-CA	6.14	126.46	119.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	198	GLY	CA-C-N	6.13	126.64	120.14
2	I	198	GLY	C-N-CA	6.13	126.64	120.14
3	A	654	ARG	N-CA-C	-6.12	104.61	111.28
3	A	257	ALA	N-CA-CB	6.12	119.21	110.16
1	H	52	TYR	CA-C-N	6.08	126.39	119.83
1	H	52	TYR	C-N-CA	6.08	126.39	119.83
1	D	52	TYR	CA-C-N	6.06	126.37	119.83
1	D	52	TYR	C-N-CA	6.06	126.37	119.83
1	J	52	TYR	CA-C-N	6.06	126.38	119.83
1	J	52	TYR	C-N-CA	6.06	126.38	119.83
2	E	198	GLY	CA-C-N	6.04	126.55	120.14
2	E	198	GLY	C-N-CA	6.04	126.55	120.14
3	A	718	ALA	N-CA-C	5.98	117.80	111.28
1	B	52	TYR	CA-C-N	5.97	126.28	119.83
1	B	52	TYR	C-N-CA	5.97	126.28	119.83
1	D	67	LYS	N-CA-C	5.88	117.48	108.30
3	A	680	THR	CA-C-N	5.86	126.00	119.32
3	A	680	THR	C-N-CA	5.86	126.00	119.32
3	A	218	THR	CA-C-N	5.75	125.88	119.32
3	A	218	THR	C-N-CA	5.75	125.88	119.32
3	A	560	SER	N-CA-C	5.62	117.41	111.28
3	A	759	SER	CA-C-N	5.61	126.85	119.84
3	A	759	SER	C-N-CA	5.61	126.85	119.84
3	A	762	VAL	O-C-N	5.54	127.47	121.87
3	A	140	GLU	CA-C-N	5.39	125.47	119.32
3	A	140	GLU	C-N-CA	5.39	125.47	119.32
3	A	92	ALA	CA-C-N	5.37	125.03	119.56
3	A	92	ALA	C-N-CA	5.37	125.03	119.56
2	C	39	LYS	N-CA-C	-5.36	107.40	114.04
3	A	655	GLN	N-CA-C	5.28	117.45	111.11
2	K	39	LYS	N-CA-C	-5.26	107.52	114.04
2	G	39	LYS	N-CA-C	-5.23	107.55	114.04
2	E	39	LYS	N-CA-C	-5.17	107.64	114.04
2	I	39	LYS	N-CA-C	-5.08	107.74	114.04
3	A	644	ARG	CB-CA-C	-5.06	99.73	110.31

There are no chirality outliers.

There are no planarity outliers.

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	B	768	0	609	12	0
1	D	756	0	579	4	0
1	F	696	0	470	1	0
1	H	728	0	515	3	0
1	J	698	0	460	3	0
2	C	2091	0	1185	2	0
2	E	1125	0	639	0	0
2	G	1115	0	635	0	0
2	I	2044	0	1109	2	0
2	K	1112	0	626	0	0
3	A	4279	0	3333	28	0
All	All	15412	0	10160	41	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 (41) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:TRP:CZ2	3:A:169:LEU:HD23	1.77	1.20
1:B:87:MET:HE1	3:A:169:LEU:HD21	1.31	1.06
1:B:87:MET:CE	3:A:169:LEU:HD21	1.86	1.06
1:B:117:TRP:HZ2	3:A:169:LEU:HD23	1.20	0.99
1:B:87:MET:HE1	3:A:169:LEU:CD2	2.02	0.88
3:A:555:ILE:O	3:A:559:ARG:HG2	1.74	0.86
1:B:117:TRP:HZ2	3:A:169:LEU:CD2	1.90	0.85
1:B:117:TRP:CZ2	3:A:169:LEU:CD2	2.62	0.80
3:A:600:VAL:C	3:A:602:ALA:H	1.95	0.74
1:H:85:GLN:HG2	1:H:96:CYS:SG	2.30	0.72
3:A:634:ASP:O	3:A:638:LEU:HG	1.89	0.71
3:A:635:GLN:HA	3:A:638:LEU:HD12	1.74	0.70
1:H:82:GLU:CB	1:H:85:GLN:OE1	2.40	0.70
3:A:600:VAL:O	3:A:602:ALA:N	2.28	0.64
1:B:87:MET:HE2	3:A:169:LEU:HD21	1.80	0.61
3:A:200:ALA:O	3:A:208:GLN:HG3	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:TYR:O	1:F:148:GLY:C	2.49	0.55
1:H:147:TYR:O	1:H:148:GLY:C	2.50	0.54
3:A:216:ARG:HG3	1:D:117:TRP:CH2	2.43	0.54
1:D:147:TYR:O	1:D:148:GLY:C	2.51	0.54
3:A:760:PRO:O	3:A:763:GLN:HB3	2.09	0.52
1:B:147:TYR:O	1:B:148:GLY:C	2.52	0.51
3:A:92:ALA:N	3:A:93:PRO:CD	2.74	0.51
3:A:216:ARG:CG	1:D:117:TRP:CH2	2.93	0.51
1:J:147:TYR:O	1:J:148:GLY:C	2.54	0.51
3:A:652:ASP:O	3:A:655:GLN:HB3	2.11	0.51
3:A:600:VAL:C	3:A:602:ALA:N	2.62	0.50
1:B:87:MET:HE1	3:A:169:LEU:HD11	1.94	0.49
2:C:457:THR:N	2:C:458:PRO:CD	2.77	0.47
2:I:457:THR:N	2:I:458:PRO:CD	2.77	0.47
3:A:216:ARG:HD2	1:D:117:TRP:CZ3	2.51	0.46
3:A:208:GLN:O	3:A:212:LYS:HG3	2.15	0.46
2:C:457:THR:N	2:C:458:PRO:HD2	2.33	0.43
1:B:87:MET:HE1	3:A:169:LEU:CD1	2.48	0.43
2:I:457:THR:N	2:I:458:PRO:HD2	2.33	0.43
3:A:805:LEU:HA	3:A:805:LEU:HD23	1.33	0.42
3:A:180:LEU:HD12	3:A:184:GLN:NE2	2.35	0.42
3:A:124:ARG:HD2	1:J:117:TRP:CZ2	2.56	0.41
1:J:52:TYR:HA	1:J:53:PRO:HD3	1.90	0.41
3:A:594:SER:O	3:A:595:ARG:C	2.64	0.40
1:B:108:LEU:H	1:B:108:LEU:HD23	1.86	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	B	122/166 (74%)	114 (93%)	7 (6%)	1 (1%)	16 52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	120/166 (72%)	113 (94%)	6 (5%)	1 (1%)	16	52
1	F	119/166 (72%)	113 (95%)	5 (4%)	1 (1%)	16	52
1	H	122/166 (74%)	116 (95%)	5 (4%)	1 (1%)	16	52
1	J	120/166 (72%)	113 (94%)	6 (5%)	1 (1%)	16	52
2	C	379/515 (74%)	372 (98%)	7 (2%)	0	100	100
2	E	219/515 (42%)	213 (97%)	6 (3%)	0	100	100
2	G	217/515 (42%)	212 (98%)	5 (2%)	0	100	100
2	I	379/515 (74%)	371 (98%)	8 (2%)	0	100	100
2	K	217/515 (42%)	211 (97%)	6 (3%)	0	100	100
3	A	728/1368 (53%)	716 (98%)	10 (1%)	2 (0%)	36	71
All	All	2742/4773 (57%)	2664 (97%)	71 (3%)	7 (0%)	37	71

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	148	GLY
1	F	148	GLY
1	J	148	GLY
1	B	148	GLY
3	A	601	GLN
3	A	710	THR
1	H	148	GLY

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	B	42/123 (34%)	42 (100%)	0	100	100
1	D	40/123 (32%)	40 (100%)	0	100	100
1	F	26/123 (21%)	26 (100%)	0	100	100
1	H	31/123 (25%)	31 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	25/123 (20%)	24 (96%)	1 (4%)	28	49
2	C	36/395 (9%)	36 (100%)	0	100	100
2	E	19/395 (5%)	19 (100%)	0	100	100
2	G	19/395 (5%)	19 (100%)	0	100	100
2	I	26/395 (7%)	26 (100%)	0	100	100
2	K	18/395 (5%)	18 (100%)	0	100	100
3	A	167/961 (17%)	166 (99%)	1 (1%)	78	80
All	All	449/3551 (13%)	447 (100%)	2 (0%)	81	82

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	753	ARG
1	J	105	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	184	GLN
3	A	188	GLN
3	A	655	GLN
3	A	692	GLN
3	A	739	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 oligosaccharides 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.

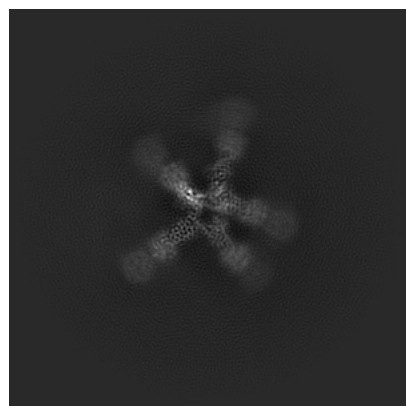
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43736. These allow visual inspection of the internal detail of the map and identification of artifacts.

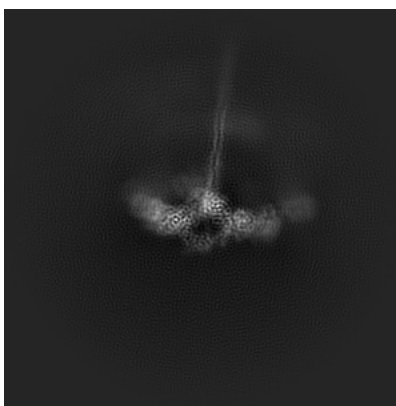
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

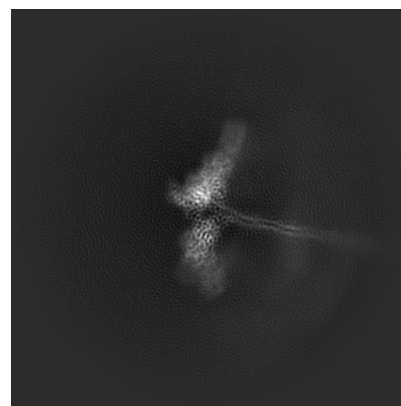
6.1.1 Primary map



X

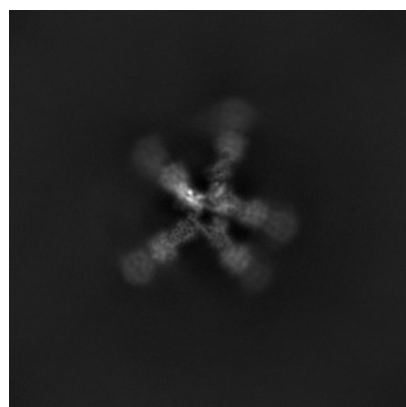


Y

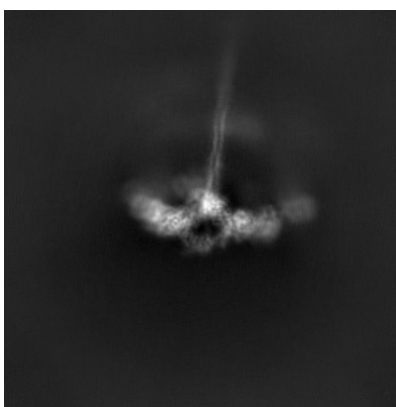


Z

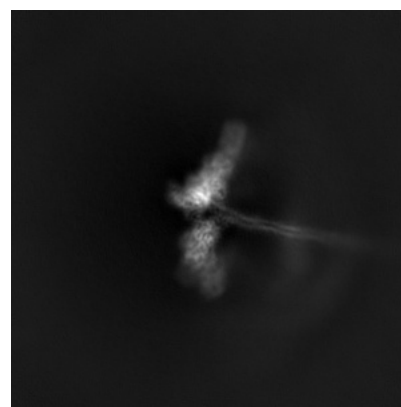
6.1.2 Raw map



X



Y

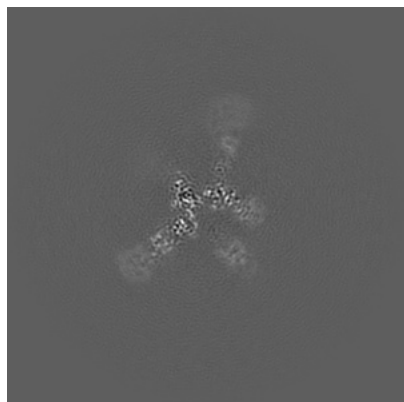


Z

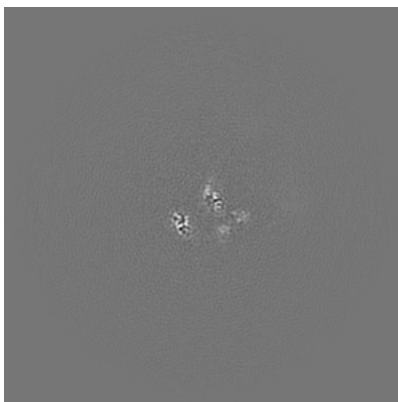
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

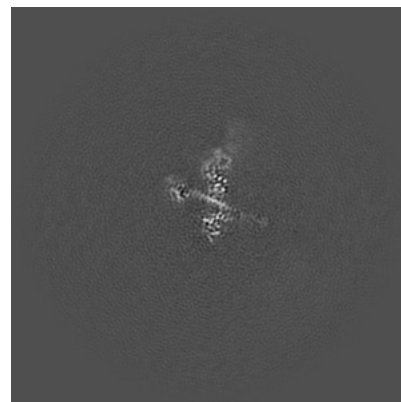
6.2.1 Primary map



X Index: 152

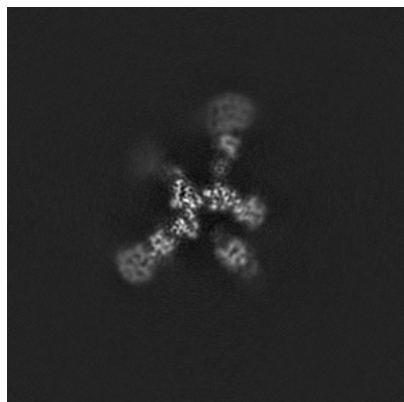


Y Index: 152

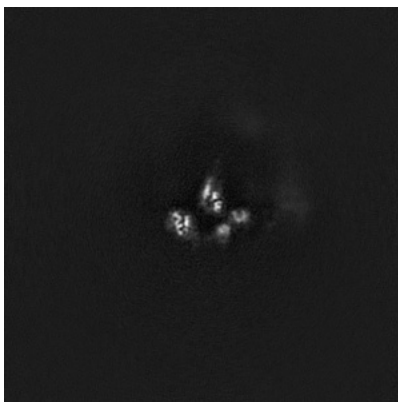


Z Index: 152

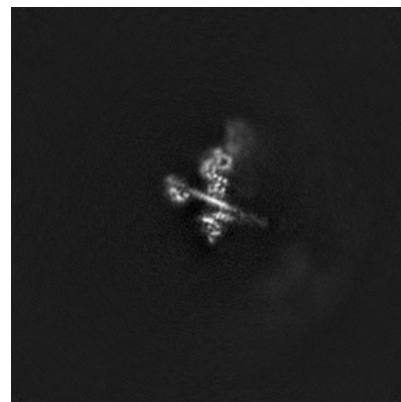
6.2.2 Raw map



X Index: 152



Y Index: 152

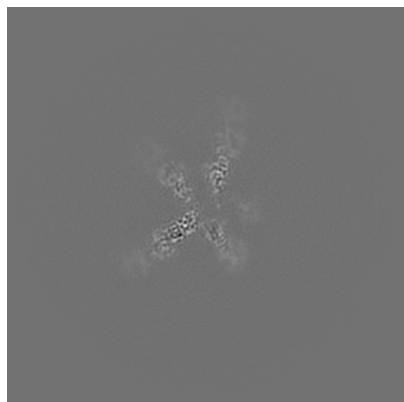


Z Index: 152

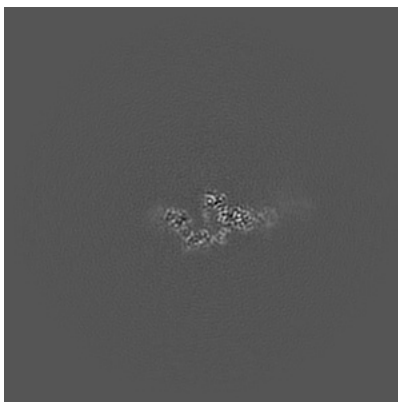
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 145

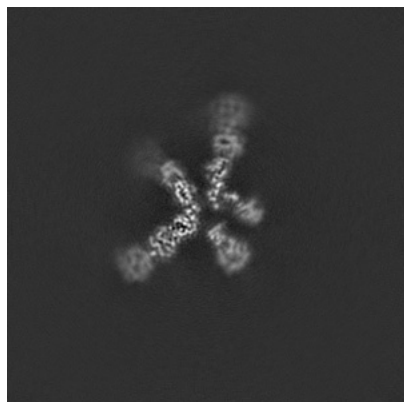


Y Index: 160

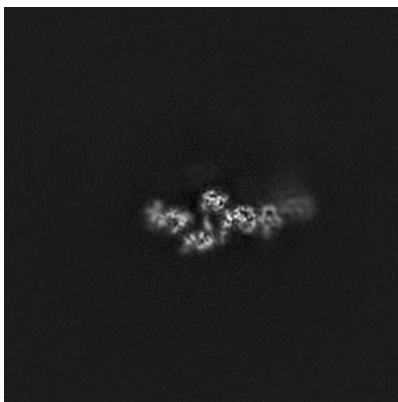


Z Index: 161

6.3.2 Raw map



X Index: 148



Y Index: 163

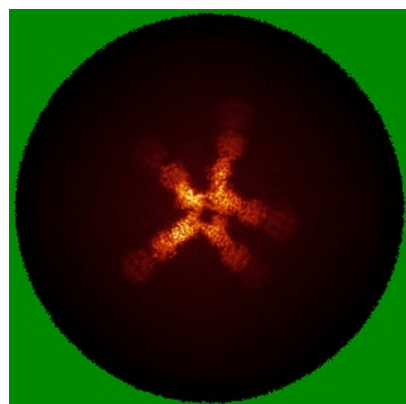


Z Index: 161

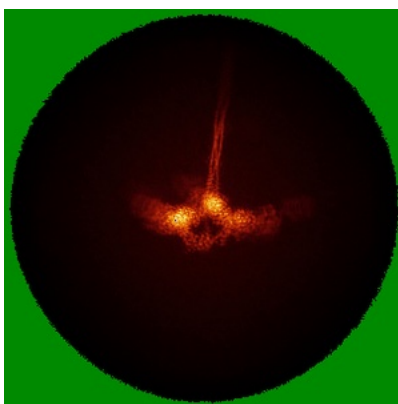
The images above show the largest variance slices of the map in three orthogonal directions.

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

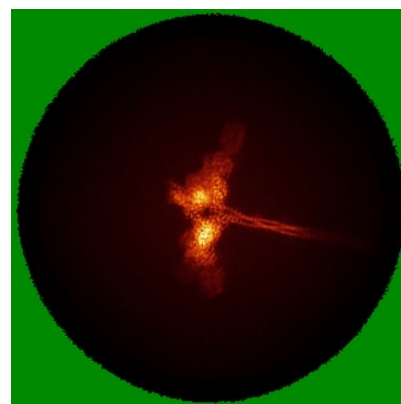
6.4.1 Primary map



X

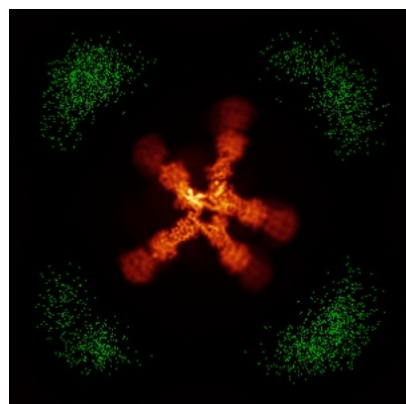


Y

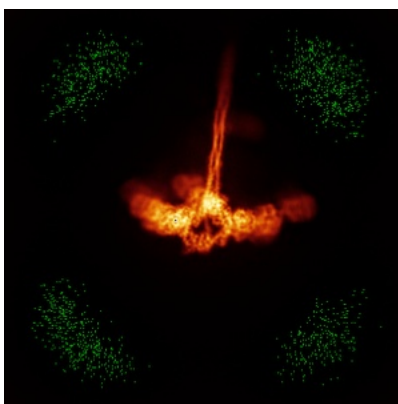


Z

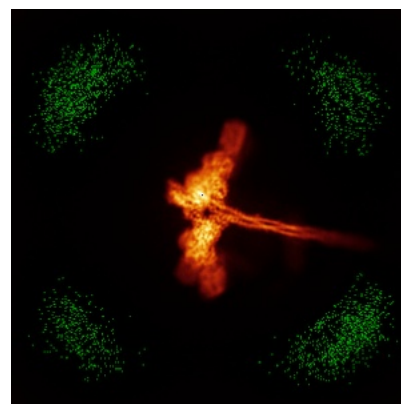
6.4.2 Raw map



X



Y

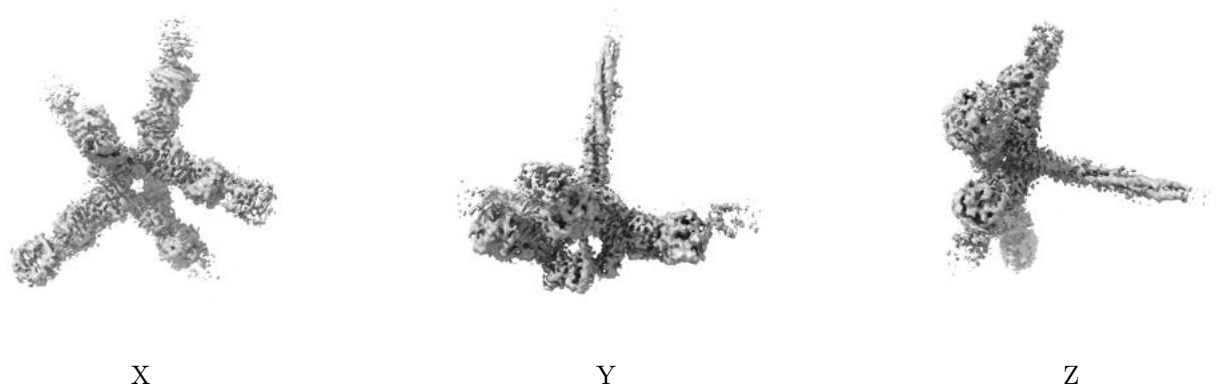


Z

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 0.7. 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.

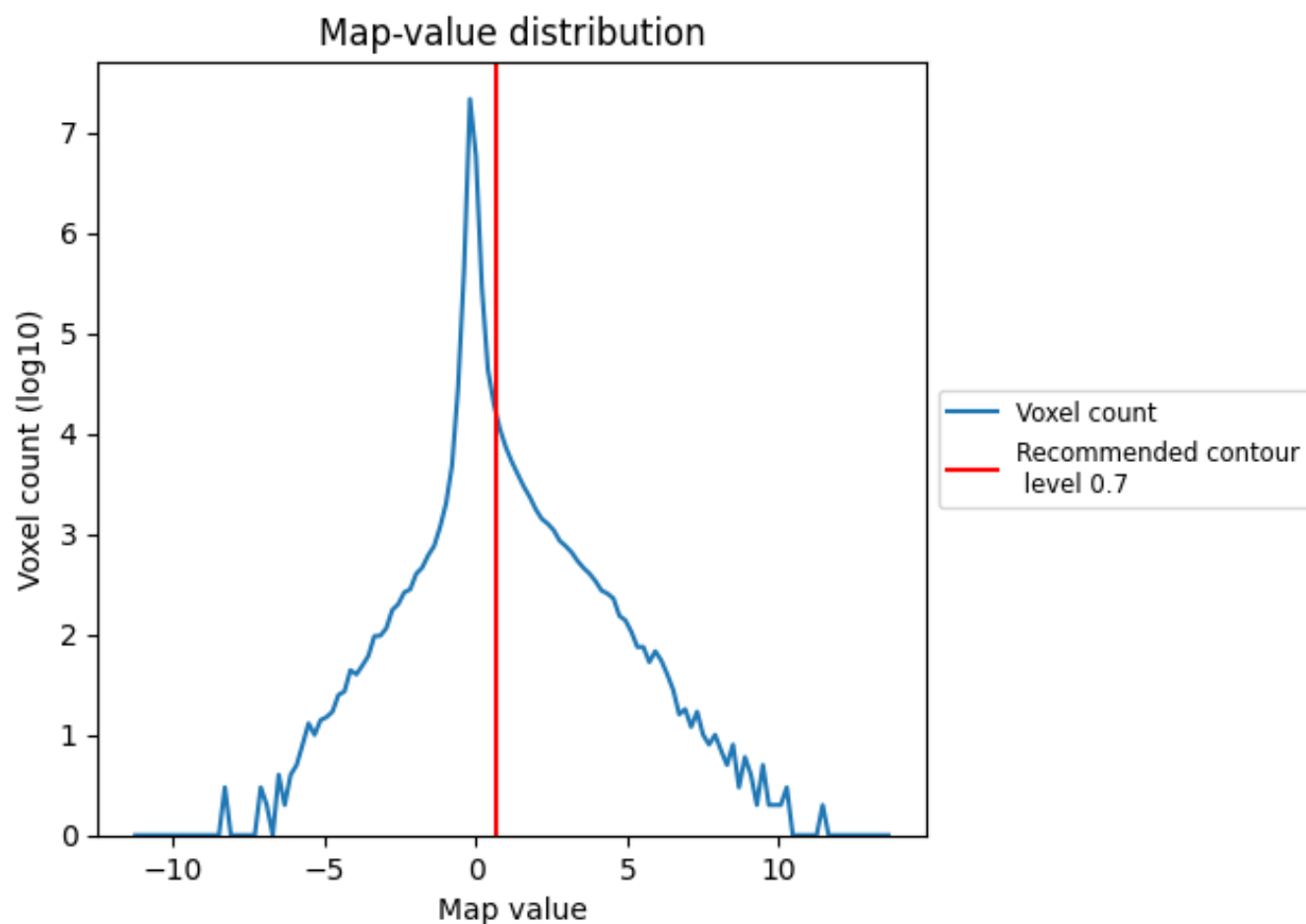
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

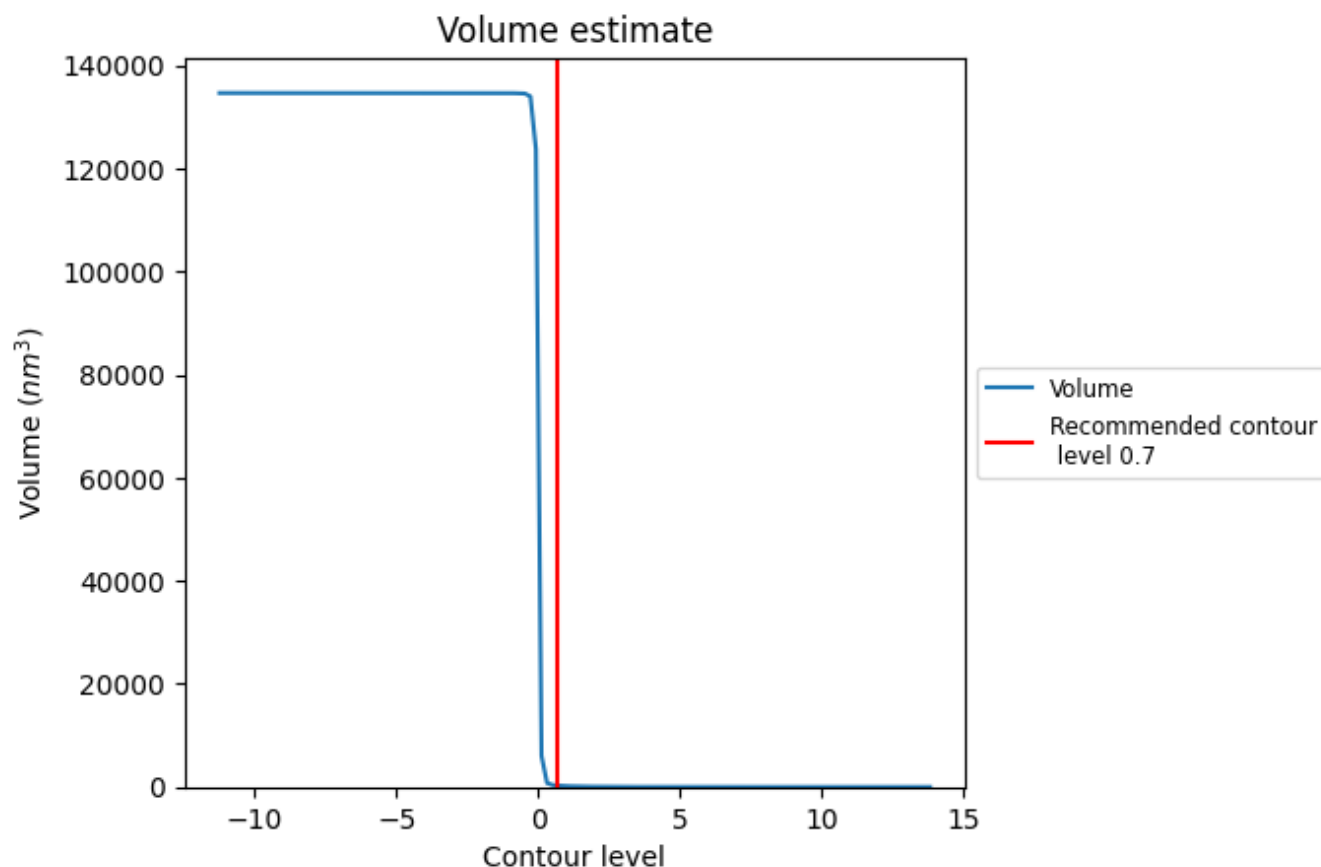
This section contains the results of statistical analysis of the map.

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.

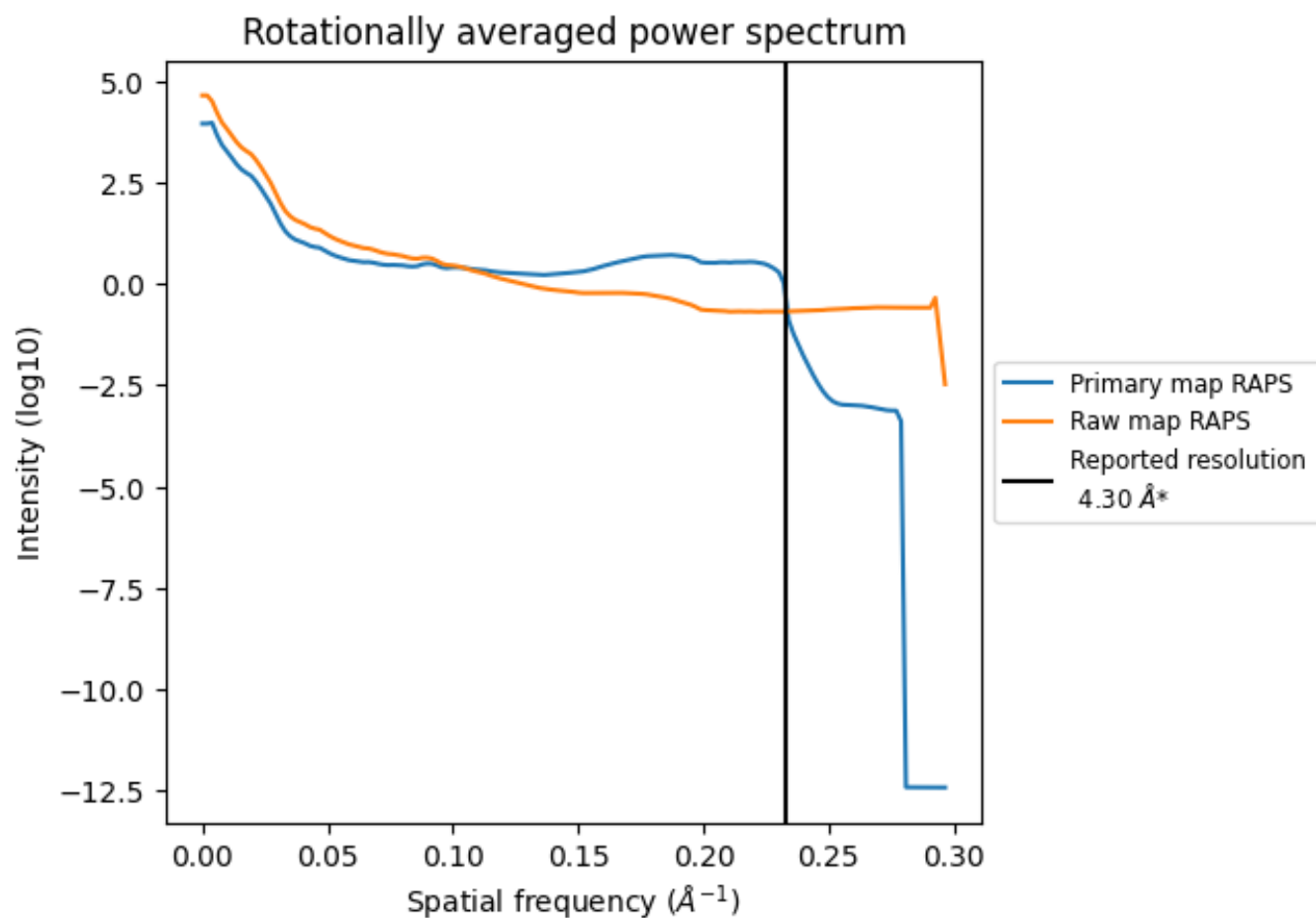
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 249 nm^3 ; this corresponds to an approximate mass of 225 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 ⓘ

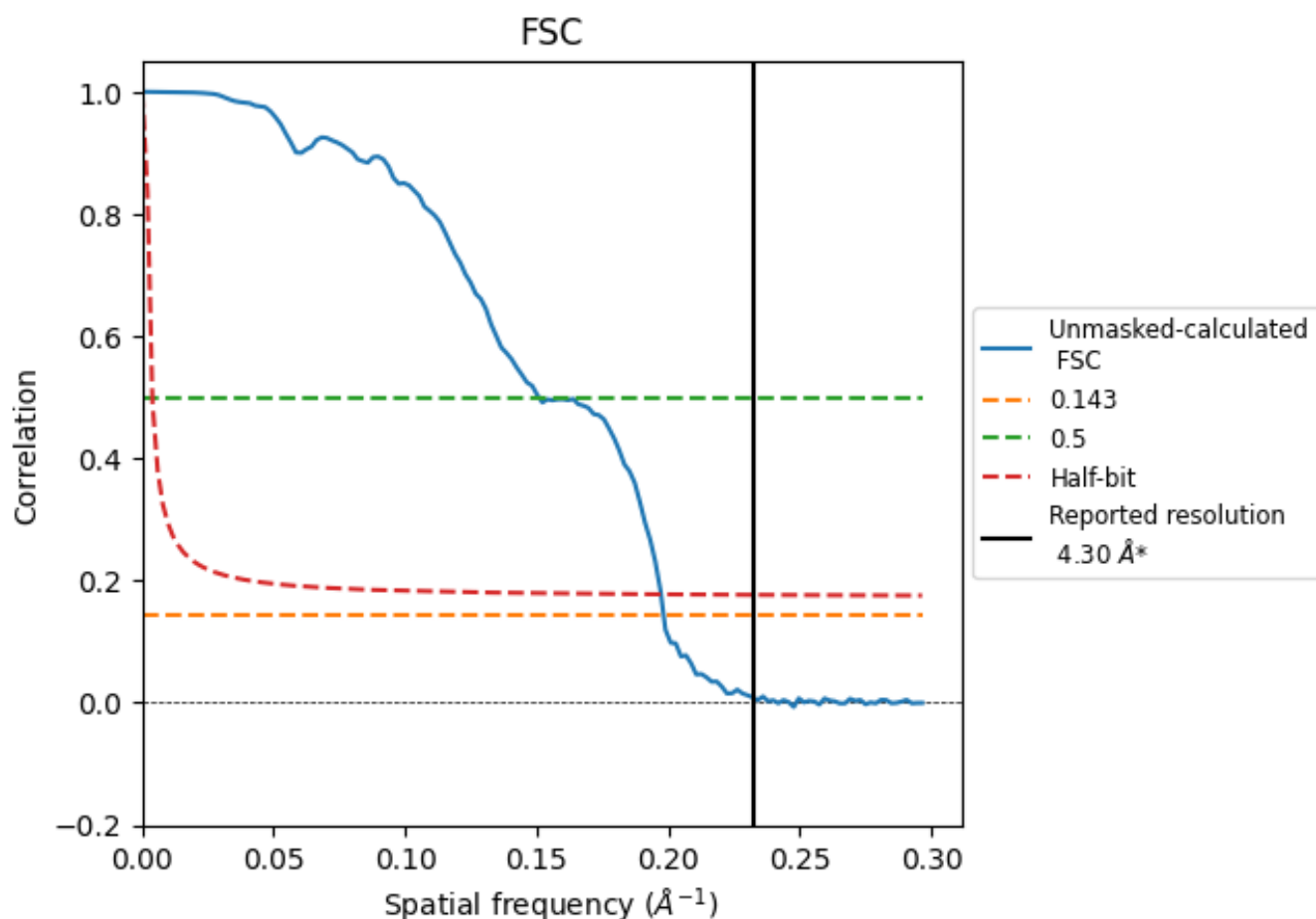


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

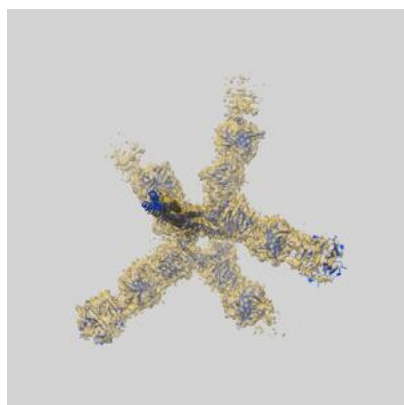
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.04	6.63	5.07

*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 5.04 differs from the reported value 4.3 by more than 10 %

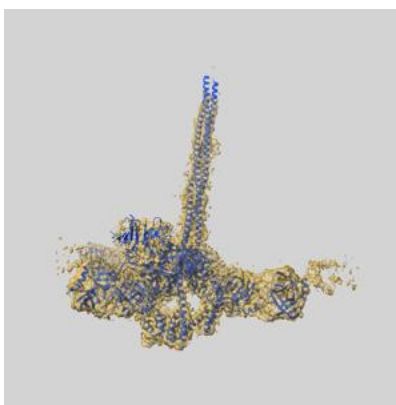
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43736 and PDB model 8W20. Per-residue inclusion information can be found in section [3](#) on page [8](#).

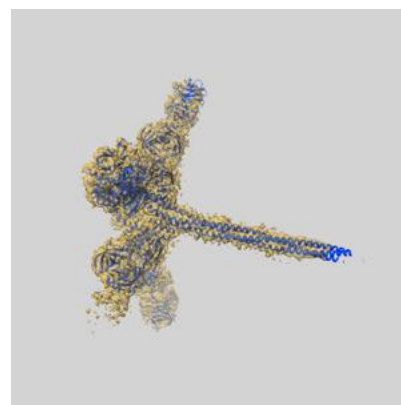
9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7 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](#)

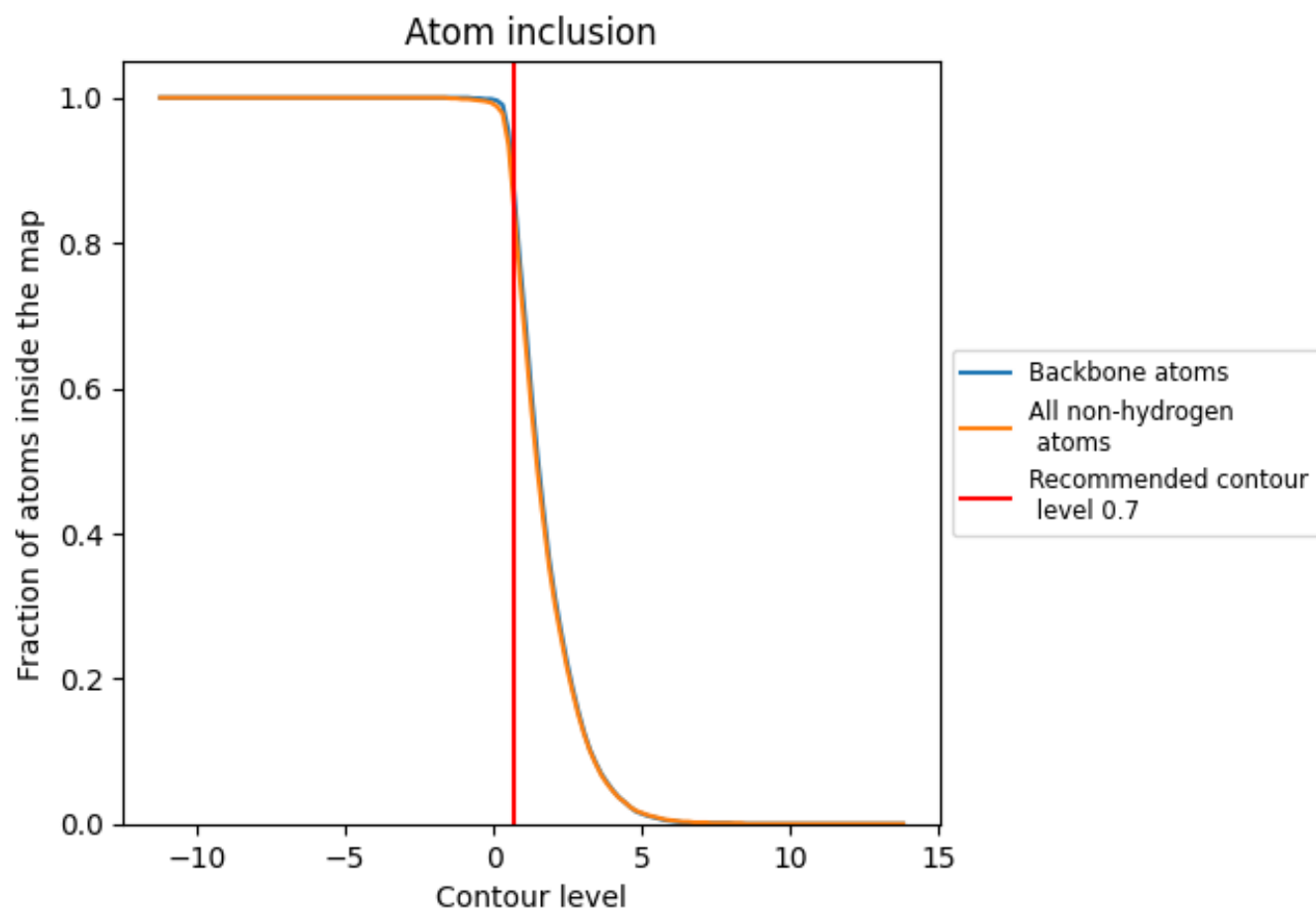


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 84% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8440	 0.2950
A	 0.8780	 0.3040
B	 0.9460	 0.4050
C	 0.7660	 0.2620
D	 0.9380	 0.4010
E	 0.9180	 0.3020
F	 0.9410	 0.3700
G	 0.8380	 0.2170
H	 0.9490	 0.3960
I	 0.6160	 0.2100
J	 0.9490	 0.3780
K	 0.8860	 0.2300

