



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:00 PM UTC

PDB ID : 9IXI / pdb\_00009ixi  
EMDB ID : EMD-60970  
Title : VLP structure of Chikungunya virus, 2f block.  
Authors : Han, X.; Ji, C.; Wang, F.; Tian, S.; Gao, F.G.; Yan, J.  
Deposited on : 2024-07-28  
Resolution : 3.01 Å(reported)  
Based on initial models : 8FCG, 6JO8

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

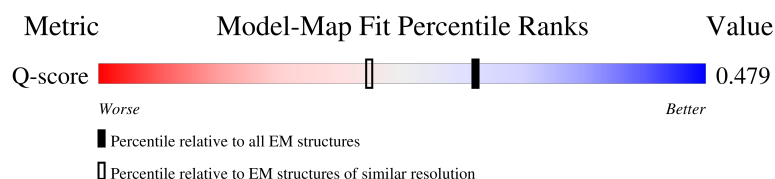
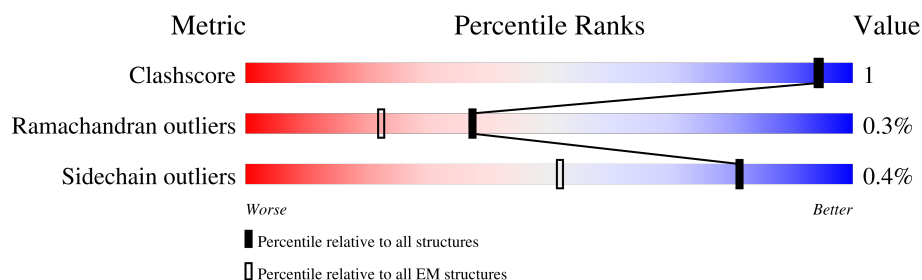
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 3.01 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	13882 ( 2.51 - 3.51 )

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  $\geq 3$ , 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	439	91% 8% .
1	B	439	92% 8% .
1	C	439	93% 7%
1	D	439	93% 6%

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Mol	Chain	Length	Quality of chain
2	E	423	
2	F	423	
2	G	423	
2	H	423	
3	I	151	
3	J	151	
3	K	151	
3	L	151	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 31120 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 CHIKV E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	439	Total	C	N	O	S	0	0
			3325	2107	558	634	26		
1	B	439	Total	C	N	O	S	0	0
			3325	2107	558	634	26		
1	C	439	Total	C	N	O	S	0	0
			3325	2107	558	634	26		
1	D	439	Total	C	N	O	S	0	0
			3325	2107	558	634	26		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	LYS	GLU	conflict	UNP A0A286S4J4
B	211	LYS	GLU	conflict	UNP A0A286S4J4
C	211	LYS	GLU	conflict	UNP A0A286S4J4
D	211	LYS	GLU	conflict	UNP A0A286S4J4

- Molecule 2 is a protein called CHIKV E2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	421	Total	C	N	O	S	0	0
			3299	2072	587	611	29		
2	F	421	Total	C	N	O	S	0	0
			3299	2072	587	611	29		
2	G	421	Total	C	N	O	S	0	0
			3299	2072	587	611	29		
2	H	421	Total	C	N	O	S	0	0
			3299	2072	587	611	29		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	103	ALA	THR	conflict	UNP A0A8A4JNF6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	211	THR	ILE	conflict	UNP A0A8A4JNF6
E	312	MET	THR	conflict	UNP A0A8A4JNF6
F	103	ALA	THR	conflict	UNP A0A8A4JNF6
F	211	THR	ILE	conflict	UNP A0A8A4JNF6
F	312	MET	THR	conflict	UNP A0A8A4JNF6
G	103	ALA	THR	conflict	UNP A0A8A4JNF6
G	211	THR	ILE	conflict	UNP A0A8A4JNF6
G	312	MET	THR	conflict	UNP A0A8A4JNF6
H	103	ALA	THR	conflict	UNP A0A8A4JNF6
H	211	THR	ILE	conflict	UNP A0A8A4JNF6
H	312	MET	THR	conflict	UNP A0A8A4JNF6

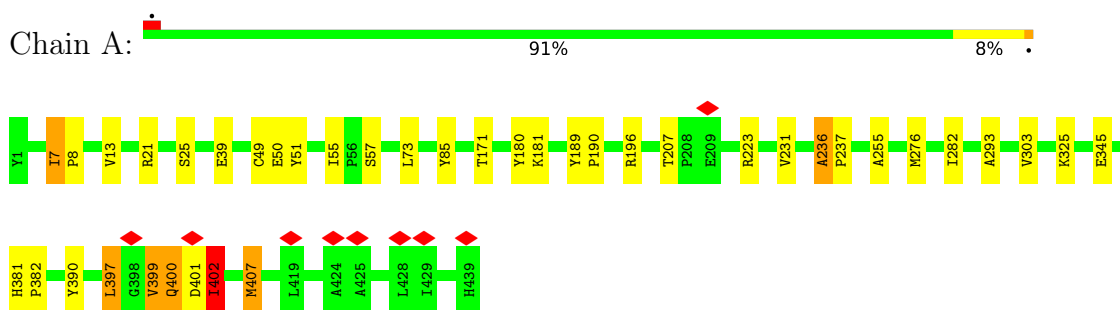
- Molecule 3 is a protein called CHIKV capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	151	Total	C	N	O	S	0	0
			1156	730	204	217	5		
3	J	151	Total	C	N	O	S	0	0
			1156	730	204	217	5		
3	K	151	Total	C	N	O	S	0	0
			1156	730	204	217	5		
3	L	151	Total	C	N	O	S	0	0
			1156	730	204	217	5		

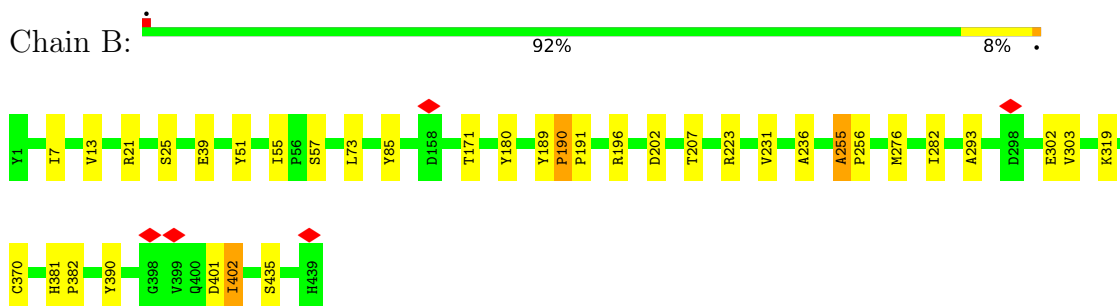
### 3 Residue-property plots [i](#)

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

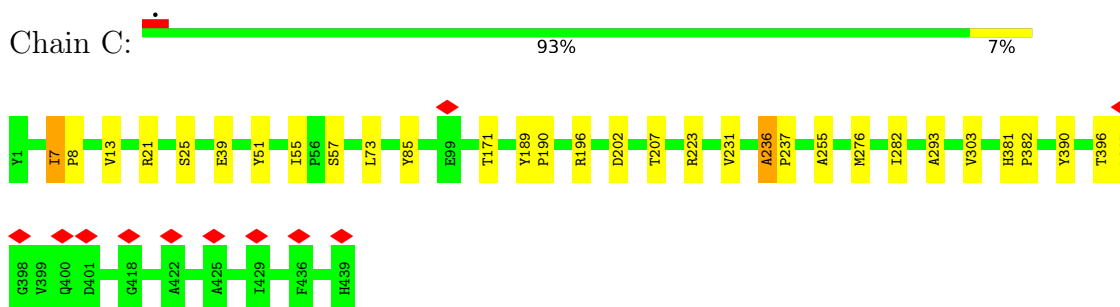
#### • Molecule 1: CHIKV E1



#### • Molecule 1: CHIKV E1

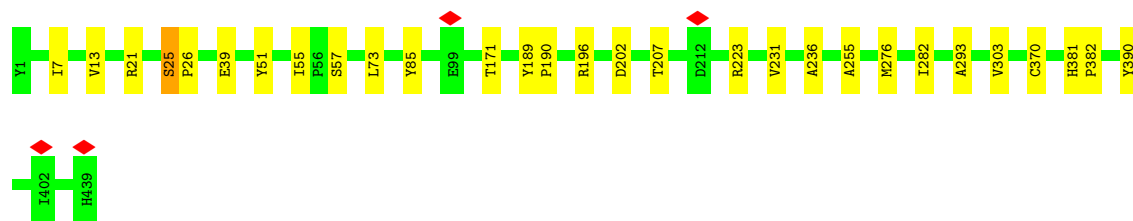


#### • Molecule 1: CHIKV E1

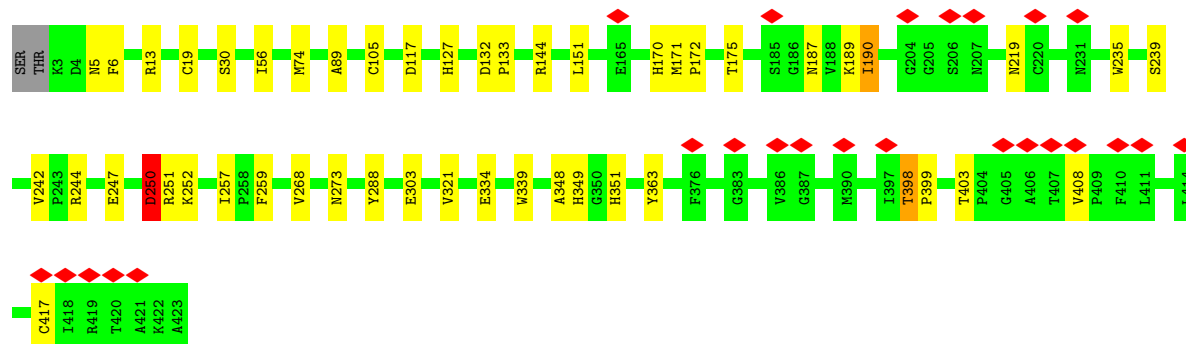


#### • Molecule 1: CHIKV E1

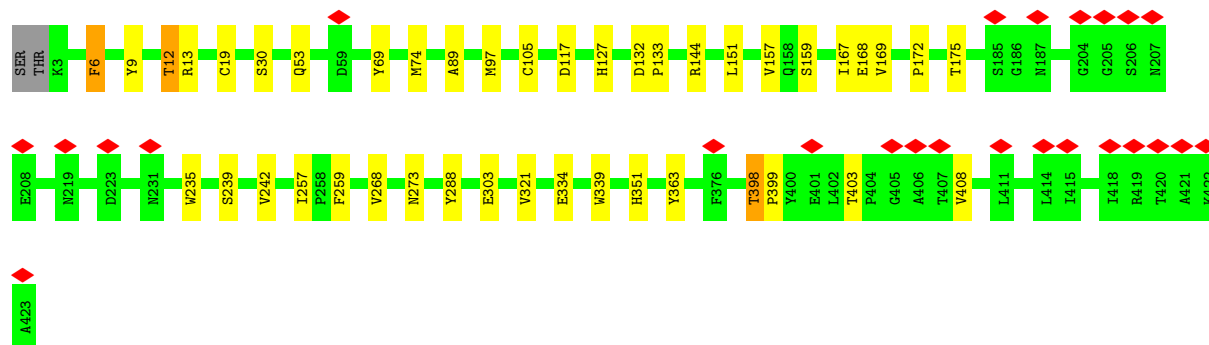
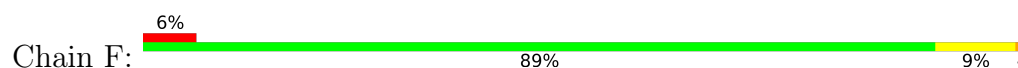




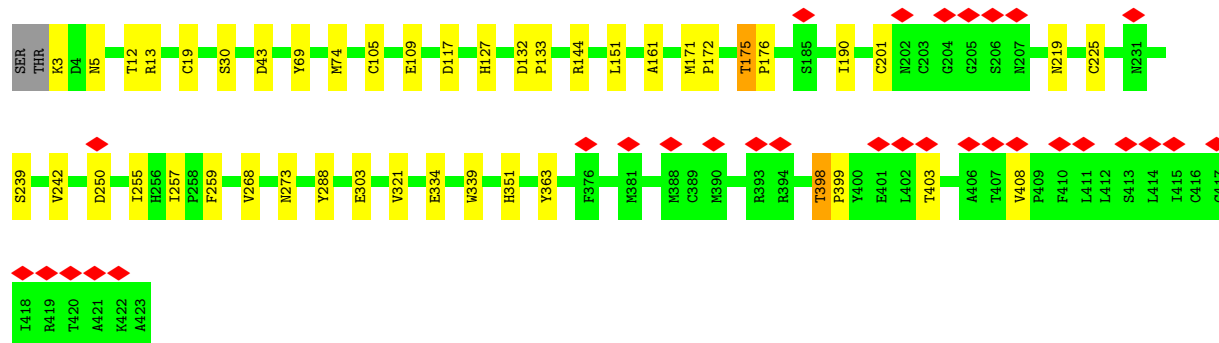
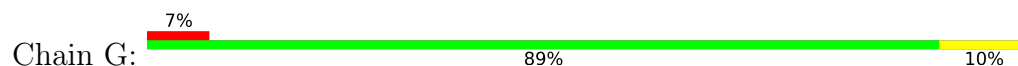
• Molecule 2: CHIKV E2




• Molecule 2: CHIKV E2

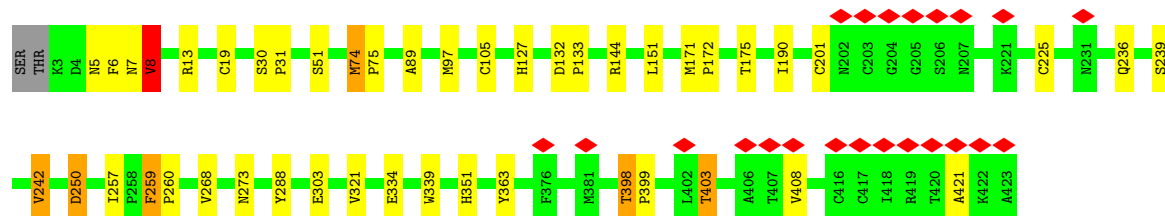


• Molecule 2: CHIKV E2



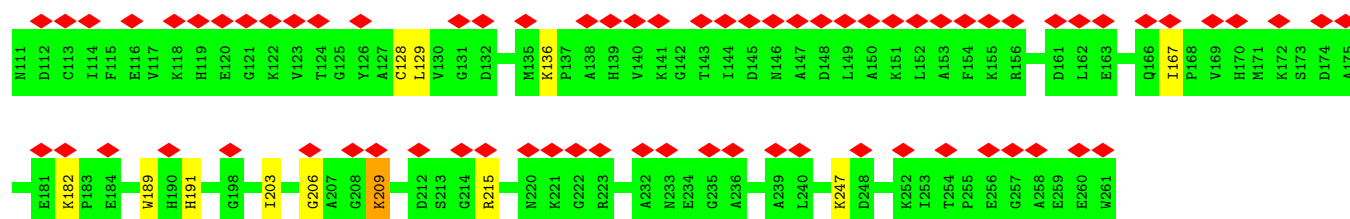
- Molecule 2: CHIKV E2

Chain H: 

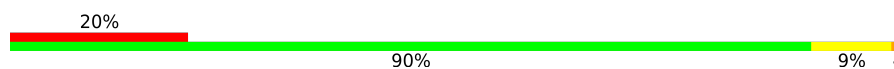


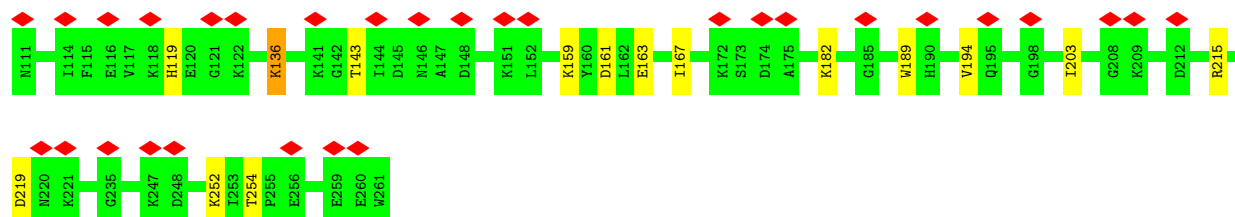
- Molecule 3: CHIKV capsid protein

Chain I: 



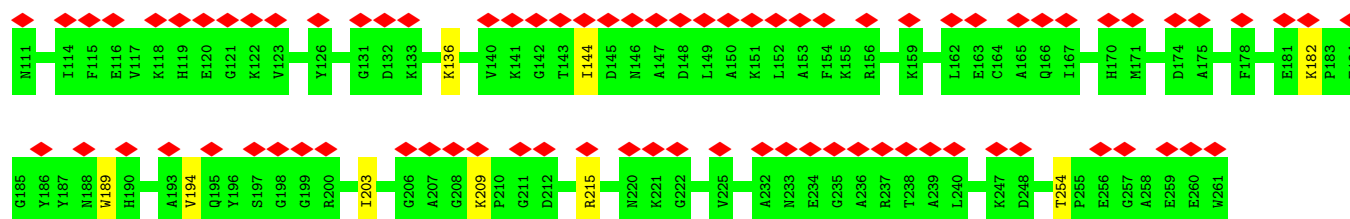
- Molecule 3: CHIKV capsid protein

Chain J: 



- Molecule 3: CHIKV capsid protein

Chain K: 



- Molecule 3: CHIKV capsid protein

Chain L: 





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	240393	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.720	Depositor
Minimum map value	-0.362	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.095	Depositor
Map size ( $\text{\AA}$ )	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.04, 1.04, 1.04	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	0.60	1/3407 (0.0%)	1.05	55/4649 (1.2%)
1	B	0.56	0/3407	1.02	50/4649 (1.1%)
1	C	0.55	0/3407	1.01	50/4649 (1.1%)
1	D	0.55	0/3407	1.00	50/4649 (1.1%)
2	E	0.58	0/3386	1.06	63/4611 (1.4%)
2	F	0.60	1/3386 (0.0%)	1.06	60/4611 (1.3%)
2	G	0.61	1/3386 (0.0%)	1.07	57/4611 (1.2%)
2	H	0.60	0/3386	1.11	61/4611 (1.3%)
3	I	0.57	0/1184	0.91	12/1599 (0.8%)
3	J	0.58	0/1184	0.94	12/1599 (0.8%)
3	K	0.58	0/1184	0.92	12/1599 (0.8%)
3	L	0.58	0/1184	0.92	12/1599 (0.8%)
All	All	0.58	3/31908 (0.0%)	1.03	494/43436 (1.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	172	PRO	CA-C	6.50	1.56	1.52
1	A	397	LEU	CA-C	-6.42	1.46	1.53
2	G	172	PRO	CA-C	5.26	1.57	1.52

All (494) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	TYR	N-CA-C	-10.92	94.23	109.95
2	H	250	ASP	N-CA-C	10.48	122.79	111.36
2	H	5	ASN	N-CA-C	-10.30	100.25	112.92
2	H	8	VAL	N-CA-C	-9.64	103.75	113.10
1	C	189	TYR	CA-C-N	9.51	126.50	119.66
1	C	189	TYR	C-N-CA	9.51	126.50	119.66
2	H	132	ASP	CA-C-N	9.45	126.56	119.66
2	H	132	ASP	C-N-CA	9.45	126.56	119.66
2	G	132	ASP	CA-C-N	9.34	126.48	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	132	ASP	C-N-CA	9.34	126.48	119.66
2	G	172	PRO	N-CA-C	9.22	121.95	110.70
1	B	189	TYR	CA-C-N	9.08	126.20	119.66
1	B	189	TYR	C-N-CA	9.08	126.20	119.66
1	A	397	LEU	N-CA-C	-9.04	99.26	110.65
1	D	189	TYR	CA-C-N	9.01	126.24	119.66
1	D	189	TYR	C-N-CA	9.01	126.24	119.66
1	A	402	ILE	N-CA-C	8.94	119.74	110.62
1	A	189	TYR	CA-C-N	8.91	126.07	119.66
1	A	189	TYR	C-N-CA	8.91	126.07	119.66
1	B	381	HIS	CA-C-N	8.78	125.98	119.66
1	B	381	HIS	C-N-CA	8.78	125.98	119.66
2	F	168	GLU	N-CA-C	8.56	122.57	108.96
2	H	105	CYS	N-CA-C	8.16	122.46	110.14
2	H	172	PRO	CA-C-N	7.97	127.92	120.03
2	H	172	PRO	C-N-CA	7.97	127.92	120.03
1	A	382	PRO	CA-C-N	7.97	127.92	120.03
1	A	382	PRO	C-N-CA	7.97	127.92	120.03
2	G	144	ARG	CA-C-N	7.90	128.05	120.31
2	G	144	ARG	C-N-CA	7.90	128.05	120.31
2	F	105	CYS	CA-C-N	7.83	127.84	119.78
2	F	105	CYS	C-N-CA	7.83	127.84	119.78
2	E	105	CYS	CA-C-N	7.78	127.79	119.78
2	E	105	CYS	C-N-CA	7.78	127.79	119.78
2	E	321	VAL	CA-C-N	7.77	127.72	120.03
2	E	321	VAL	C-N-CA	7.77	127.72	120.03
1	A	400	GLN	N-CA-C	-7.76	103.54	113.16
2	E	172	PRO	CA-C-N	7.73	127.68	120.03
2	E	172	PRO	C-N-CA	7.73	127.68	120.03
2	F	257	ILE	CA-C-N	7.68	127.58	120.21
2	F	257	ILE	C-N-CA	7.68	127.58	120.21
2	F	144	ARG	CA-C-N	7.65	127.81	120.31
2	F	144	ARG	C-N-CA	7.65	127.81	120.31
2	H	363	TYR	CA-C-N	7.63	127.27	119.56
2	H	363	TYR	C-N-CA	7.63	127.27	119.56
2	F	13	ARG	CA-C-N	7.63	127.64	119.78
2	F	13	ARG	C-N-CA	7.63	127.64	119.78
1	C	382	PRO	CA-C-N	7.60	127.56	120.03
1	C	382	PRO	C-N-CA	7.60	127.56	120.03
2	E	363	TYR	CA-C-N	7.54	127.25	119.56
2	E	363	TYR	C-N-CA	7.54	127.25	119.56
1	D	255	ALA	CA-C-N	7.53	127.97	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	255	ALA	C-N-CA	7.53	127.97	119.92
1	D	382	PRO	CA-C-N	7.52	127.44	119.85
1	D	382	PRO	C-N-CA	7.52	127.44	119.85
1	C	255	ALA	CA-C-N	7.51	127.95	120.52
1	C	255	ALA	C-N-CA	7.51	127.95	120.52
1	A	255	ALA	CA-C-N	7.50	127.95	119.92
1	A	255	ALA	C-N-CA	7.50	127.95	119.92
1	B	255	ALA	CA-C-N	7.45	127.89	119.92
1	B	255	ALA	C-N-CA	7.45	127.89	119.92
2	G	363	TYR	CA-C-N	7.43	127.06	119.56
2	G	363	TYR	C-N-CA	7.43	127.06	119.56
2	H	257	ILE	CA-C-N	7.41	127.32	120.21
2	H	257	ILE	C-N-CA	7.41	127.32	120.21
2	G	30	SER	CA-C-N	7.39	127.56	119.87
2	G	30	SER	C-N-CA	7.39	127.56	119.87
1	C	190	PRO	CA-C-N	7.35	127.35	119.78
1	C	190	PRO	C-N-CA	7.35	127.35	119.78
3	K	215	ARG	CA-C-N	7.35	127.31	120.03
3	K	215	ARG	C-N-CA	7.35	127.31	120.03
2	E	13	ARG	CA-C-N	7.33	127.33	119.78
2	E	13	ARG	C-N-CA	7.33	127.33	119.78
2	F	172	PRO	N-CA-C	7.31	118.40	110.58
2	H	30	SER	CA-C-N	7.30	127.46	119.87
2	H	30	SER	C-N-CA	7.30	127.46	119.87
1	B	382	PRO	CA-C-N	7.28	127.21	119.85
1	B	382	PRO	C-N-CA	7.28	127.21	119.85
3	L	215	ARG	CA-C-N	7.28	127.45	120.31
3	L	215	ARG	C-N-CA	7.28	127.45	120.31
1	A	85	TYR	CA-C-N	7.24	127.16	119.85
1	A	85	TYR	C-N-CA	7.24	127.16	119.85
1	C	85	TYR	CA-C-N	7.23	127.15	119.85
1	C	85	TYR	C-N-CA	7.23	127.15	119.85
2	E	144	ARG	CA-C-N	7.23	127.39	120.31
2	E	144	ARG	C-N-CA	7.23	127.39	120.31
2	H	259	PHE	CA-C-N	7.21	127.14	119.85
2	H	259	PHE	C-N-CA	7.21	127.14	119.85
2	F	30	SER	CA-C-N	7.21	126.84	119.56
2	F	30	SER	C-N-CA	7.21	126.84	119.56
1	D	85	TYR	CA-C-N	7.21	127.13	119.85
1	D	85	TYR	C-N-CA	7.21	127.13	119.85
2	G	105	CYS	CA-C-N	7.21	127.13	119.85
2	G	105	CYS	C-N-CA	7.21	127.13	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	407	MET	N-CA-C	-7.19	102.81	112.94
3	L	209	LYS	CA-C-N	7.19	127.16	119.76
3	L	209	LYS	C-N-CA	7.19	127.16	119.76
1	D	190	PRO	CA-C-N	7.18	127.18	119.78
1	D	190	PRO	C-N-CA	7.18	127.18	119.78
1	C	55	ILE	CA-C-N	7.16	127.16	119.78
1	C	55	ILE	C-N-CA	7.16	127.16	119.78
2	H	133	PRO	CA-C-N	7.14	127.06	119.85
2	H	133	PRO	C-N-CA	7.14	127.06	119.85
2	E	30	SER	CA-C-N	7.10	126.73	119.56
2	E	30	SER	C-N-CA	7.10	126.73	119.56
2	G	74	MET	CA-C-N	7.08	127.08	119.78
2	G	74	MET	C-N-CA	7.08	127.08	119.78
1	B	55	ILE	CA-C-N	7.07	127.07	119.78
1	B	55	ILE	C-N-CA	7.07	127.07	119.78
1	A	7	ILE	CA-C-N	7.03	127.02	119.78
1	A	7	ILE	C-N-CA	7.03	127.02	119.78
2	E	268	VAL	CA-C-N	7.03	126.99	120.03
2	E	268	VAL	C-N-CA	7.03	126.99	120.03
1	D	196	ARG	CA-C-N	7.03	126.79	119.76
1	D	196	ARG	C-N-CA	7.03	126.79	119.76
2	E	250	ASP	N-CA-C	7.03	119.02	111.36
2	H	268	VAL	CA-C-N	7.03	126.99	120.03
2	H	268	VAL	C-N-CA	7.03	126.99	120.03
1	B	85	TYR	CA-C-N	7.02	126.94	119.85
1	B	85	TYR	C-N-CA	7.02	126.94	119.85
2	G	273	ASN	CA-C-N	7.02	126.98	120.03
2	G	273	ASN	C-N-CA	7.02	126.98	120.03
1	C	196	ARG	CA-C-N	7.01	126.98	119.76
1	C	196	ARG	C-N-CA	7.01	126.98	119.76
2	F	74	MET	CA-C-N	7.00	126.96	120.03
2	F	74	MET	C-N-CA	7.00	126.96	120.03
2	E	133	PRO	CA-C-N	6.99	126.91	119.85
2	E	133	PRO	C-N-CA	6.99	126.91	119.85
2	F	133	PRO	CA-C-N	6.98	126.90	119.85
2	F	133	PRO	C-N-CA	6.98	126.90	119.85
2	G	133	PRO	CA-C-N	6.98	126.90	119.85
2	G	133	PRO	C-N-CA	6.98	126.90	119.85
1	A	223	ARG	CA-C-N	6.97	126.96	119.78
1	A	223	ARG	C-N-CA	6.97	126.96	119.78
2	E	242	VAL	CA-C-N	6.97	126.96	119.78
2	E	242	VAL	C-N-CA	6.97	126.96	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	268	VAL	CA-C-N	6.97	126.93	120.03
2	G	268	VAL	C-N-CA	6.97	126.93	120.03
2	G	175	THR	CA-C-N	6.95	126.92	119.76
2	G	175	THR	C-N-CA	6.95	126.92	119.76
2	G	257	ILE	CA-C-N	6.95	126.91	120.03
2	G	257	ILE	C-N-CA	6.95	126.91	120.03
1	B	196	ARG	CA-C-N	6.95	126.92	119.76
1	B	196	ARG	C-N-CA	6.95	126.92	119.76
2	F	268	VAL	CA-C-N	6.94	126.90	120.03
2	F	268	VAL	C-N-CA	6.94	126.90	120.03
1	B	7	ILE	CA-C-N	6.92	126.91	119.78
1	B	7	ILE	C-N-CA	6.92	126.91	119.78
1	B	282	ILE	CA-C-N	6.92	126.88	119.76
1	B	282	ILE	C-N-CA	6.92	126.88	119.76
1	C	171	THR	CA-C-N	6.91	126.54	119.56
1	C	171	THR	C-N-CA	6.91	126.54	119.56
2	H	74	MET	CA-C-N	6.91	126.89	119.78
2	H	74	MET	C-N-CA	6.91	126.89	119.78
2	E	403	THR	CA-C-N	6.89	126.59	119.56
2	E	403	THR	C-N-CA	6.89	126.59	119.56
2	H	144	ARG	CA-C-N	6.89	127.34	120.52
2	H	144	ARG	C-N-CA	6.89	127.34	120.52
1	D	223	ARG	CA-C-N	6.89	126.81	119.85
1	D	223	ARG	C-N-CA	6.89	126.81	119.85
2	H	13	ARG	CA-C-N	6.89	126.85	120.03
2	H	13	ARG	C-N-CA	6.89	126.85	120.03
2	E	257	ILE	CA-C-N	6.88	126.84	120.03
2	E	257	ILE	C-N-CA	6.88	126.84	120.03
1	C	223	ARG	CA-C-N	6.88	126.84	120.03
1	C	223	ARG	C-N-CA	6.88	126.84	120.03
2	E	175	THR	CA-C-N	6.87	126.83	119.76
2	E	175	THR	C-N-CA	6.87	126.83	119.76
2	G	259	PHE	CA-C-N	6.87	126.83	120.03
2	G	259	PHE	C-N-CA	6.87	126.83	120.03
1	D	73	LEU	CA-C-N	6.87	127.15	119.32
1	D	73	LEU	C-N-CA	6.87	127.15	119.32
2	H	239	SER	CA-C-N	6.86	127.00	119.87
2	H	239	SER	C-N-CA	6.86	127.00	119.87
3	K	209	LYS	CA-C-N	6.85	126.77	119.85
3	K	209	LYS	C-N-CA	6.85	126.77	119.85
1	A	303	VAL	CA-C-N	6.85	126.48	119.56
1	A	303	VAL	C-N-CA	6.85	126.48	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	273	ASN	CA-C-N	6.85	126.81	120.03
2	H	273	ASN	C-N-CA	6.85	126.81	120.03
1	B	73	LEU	CA-C-N	6.84	127.12	119.32
1	B	73	LEU	C-N-CA	6.84	127.12	119.32
1	B	223	ARG	CA-C-N	6.84	126.76	119.85
1	B	223	ARG	C-N-CA	6.84	126.76	119.85
2	H	321	VAL	CA-C-N	6.83	127.28	120.52
2	H	321	VAL	C-N-CA	6.83	127.28	120.52
1	A	196	ARG	CA-C-N	6.82	126.79	119.76
1	A	196	ARG	C-N-CA	6.82	126.79	119.76
2	E	259	PHE	CA-C-N	6.82	126.73	119.85
2	E	259	PHE	C-N-CA	6.82	126.73	119.85
1	D	171	THR	CA-C-N	6.82	126.44	119.56
1	D	171	THR	C-N-CA	6.82	126.44	119.56
2	F	321	VAL	CA-C-N	6.82	127.27	120.52
2	F	321	VAL	C-N-CA	6.82	127.27	120.52
2	F	363	TYR	CA-C-N	6.81	126.44	119.56
2	F	363	TYR	C-N-CA	6.81	126.44	119.56
1	D	7	ILE	CA-C-N	6.81	126.80	119.78
1	D	7	ILE	C-N-CA	6.81	126.80	119.78
1	C	57	SER	CA-C-N	6.81	126.57	119.76
1	C	57	SER	C-N-CA	6.81	126.57	119.76
2	F	334	GLU	CA-C-N	6.81	126.79	119.78
2	F	334	GLU	C-N-CA	6.81	126.79	119.78
2	G	321	VAL	CA-C-N	6.81	127.26	120.52
2	G	321	VAL	C-N-CA	6.81	127.26	120.52
3	K	254	THR	CA-C-N	6.80	126.79	119.78
3	K	254	THR	C-N-CA	6.80	126.79	119.78
1	A	190	PRO	CA-C-N	6.80	126.78	119.78
1	A	190	PRO	C-N-CA	6.80	126.78	119.78
2	G	408	VAL	CA-C-N	6.80	126.78	119.78
2	G	408	VAL	C-N-CA	6.80	126.78	119.78
1	D	57	SER	CA-C-N	6.79	126.76	120.03
1	D	57	SER	C-N-CA	6.79	126.76	120.03
3	I	167	ILE	CA-C-N	6.79	126.75	119.76
3	I	167	ILE	C-N-CA	6.79	126.75	119.76
3	J	215	ARG	CA-C-N	6.79	126.77	119.78
3	J	215	ARG	C-N-CA	6.79	126.77	119.78
1	A	39	GLU	CA-C-N	6.77	126.68	119.85
1	A	39	GLU	C-N-CA	6.77	126.68	119.85
2	E	74	MET	CA-C-N	6.76	126.75	119.78
2	E	74	MET	C-N-CA	6.76	126.75	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	ILE	CA-C-N	6.75	126.72	119.76
1	A	282	ILE	C-N-CA	6.75	126.72	119.76
1	C	73	LEU	CA-C-N	6.75	127.01	119.32
1	C	73	LEU	C-N-CA	6.75	127.01	119.32
1	A	390	TYR	CA-C-N	6.74	126.66	119.85
1	A	390	TYR	C-N-CA	6.74	126.66	119.85
2	G	334	GLU	CA-C-N	6.74	126.72	119.78
2	G	334	GLU	C-N-CA	6.74	126.72	119.78
2	H	175	THR	CA-C-N	6.73	126.69	119.76
2	H	175	THR	C-N-CA	6.73	126.69	119.76
1	A	276	MET	CA-C-N	6.73	126.69	119.76
1	A	276	MET	C-N-CA	6.73	126.69	119.76
2	E	334	GLU	CA-C-N	6.72	126.70	119.78
2	E	334	GLU	C-N-CA	6.72	126.70	119.78
2	G	239	SER	CA-C-N	6.72	126.86	119.87
2	G	239	SER	C-N-CA	6.72	126.86	119.87
1	A	171	THR	CA-C-N	6.72	126.35	119.56
1	A	171	THR	C-N-CA	6.72	126.35	119.56
2	E	273	ASN	CA-C-N	6.71	126.63	119.85
2	E	273	ASN	C-N-CA	6.71	126.63	119.85
1	D	293	ALA	CA-C-N	6.70	126.66	119.76
1	D	293	ALA	C-N-CA	6.70	126.66	119.76
1	D	303	VAL	CA-C-N	6.69	126.32	119.56
1	D	303	VAL	C-N-CA	6.69	126.32	119.56
2	F	151	LEU	CA-C-N	6.69	126.65	119.76
2	F	151	LEU	C-N-CA	6.69	126.65	119.76
1	C	236	ALA	CA-C-N	6.68	126.66	119.78
1	C	236	ALA	C-N-CA	6.68	126.66	119.78
2	F	239	SER	CA-C-N	6.68	126.82	119.87
2	F	239	SER	C-N-CA	6.68	126.82	119.87
3	J	254	THR	CA-C-N	6.68	126.64	119.76
3	J	254	THR	C-N-CA	6.68	126.64	119.76
3	L	182	LYS	CA-C-N	6.68	126.60	119.85
3	L	182	LYS	C-N-CA	6.68	126.60	119.85
1	B	390	TYR	CA-C-N	6.68	126.59	119.85
1	B	390	TYR	C-N-CA	6.68	126.59	119.85
1	C	282	ILE	CA-C-N	6.67	126.65	119.78
1	C	282	ILE	C-N-CA	6.67	126.65	119.78
2	E	239	SER	CA-C-N	6.66	126.79	119.87
2	E	239	SER	C-N-CA	6.66	126.79	119.87
1	A	55	ILE	CA-C-N	6.65	126.62	119.78
1	A	55	ILE	C-N-CA	6.65	126.62	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	276	MET	CA-C-N	6.64	126.61	119.76
1	D	276	MET	C-N-CA	6.64	126.61	119.76
1	C	276	MET	CA-C-N	6.64	126.60	119.76
1	C	276	MET	C-N-CA	6.64	126.60	119.76
1	C	390	TYR	CA-C-N	6.64	126.56	119.85
1	C	390	TYR	C-N-CA	6.64	126.56	119.85
1	C	293	ALA	CA-C-N	6.63	126.59	119.76
1	C	293	ALA	C-N-CA	6.63	126.59	119.76
2	G	242	VAL	CA-C-N	6.63	126.66	119.90
2	G	242	VAL	C-N-CA	6.63	126.66	119.90
2	F	339	TRP	CA-C-N	6.62	126.54	119.85
2	F	339	TRP	C-N-CA	6.62	126.54	119.85
2	G	303	GLU	CA-C-N	6.62	126.25	119.56
2	G	303	GLU	C-N-CA	6.62	126.25	119.56
1	B	190	PRO	CA-C-N	6.61	126.59	119.78
1	B	190	PRO	C-N-CA	6.61	126.59	119.78
2	G	151	LEU	CA-C-N	6.61	126.57	119.76
2	G	151	LEU	C-N-CA	6.61	126.57	119.76
1	A	293	ALA	CA-C-N	6.61	126.56	119.76
1	A	293	ALA	C-N-CA	6.61	126.56	119.76
2	F	259	PHE	CA-C-N	6.61	126.57	120.03
2	F	259	PHE	C-N-CA	6.61	126.57	120.03
2	F	167	ILE	O-C-N	-6.60	116.25	123.18
1	B	171	THR	CA-C-N	6.60	126.22	119.56
1	B	171	THR	C-N-CA	6.60	126.22	119.56
1	A	73	LEU	CA-C-N	6.60	126.84	119.32
1	A	73	LEU	C-N-CA	6.60	126.84	119.32
2	G	13	ARG	N-CA-C	6.59	121.01	109.48
3	L	254	THR	CA-C-N	6.58	126.54	119.76
3	L	254	THR	C-N-CA	6.58	126.54	119.76
2	H	334	GLU	CA-C-N	6.58	126.53	119.76
2	H	334	GLU	C-N-CA	6.58	126.53	119.76
2	H	303	GLU	CA-C-N	6.56	126.19	119.56
2	H	303	GLU	C-N-CA	6.56	126.19	119.56
2	F	273	ASN	CA-C-N	6.56	126.52	120.03
2	F	273	ASN	C-N-CA	6.56	126.52	120.03
1	C	303	VAL	CA-C-N	6.55	126.79	119.32
1	C	303	VAL	C-N-CA	6.55	126.79	119.32
3	I	215	ARG	CA-C-N	6.55	127.08	120.14
3	I	215	ARG	C-N-CA	6.55	127.08	120.14
2	H	19	CYS	CA-C-N	6.54	126.17	119.56
2	H	19	CYS	C-N-CA	6.54	126.17	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	SER	CA-C-N	6.53	126.44	119.85
1	A	25	SER	C-N-CA	6.53	126.44	119.85
1	B	39	GLU	CA-C-N	6.52	126.44	119.85
1	B	39	GLU	C-N-CA	6.52	126.44	119.85
1	A	57	SER	CA-C-N	6.51	126.42	119.85
1	A	57	SER	C-N-CA	6.51	126.42	119.85
1	B	293	ALA	CA-C-N	6.51	126.46	119.76
1	B	293	ALA	C-N-CA	6.51	126.46	119.76
2	G	339	TRP	CA-C-N	6.50	126.41	119.85
2	G	339	TRP	C-N-CA	6.50	126.41	119.85
2	E	151	LEU	CA-C-N	6.49	126.44	119.76
2	E	151	LEU	C-N-CA	6.49	126.44	119.76
2	F	175	THR	CA-C-N	6.49	126.40	119.85
2	F	175	THR	C-N-CA	6.49	126.40	119.85
3	J	182	LYS	CA-C-N	6.48	126.46	119.78
3	J	182	LYS	C-N-CA	6.48	126.46	119.78
1	C	231	VAL	CA-C-N	6.48	126.39	119.85
1	C	231	VAL	C-N-CA	6.48	126.39	119.85
1	D	390	TYR	CA-C-N	6.48	126.39	119.85
1	D	390	TYR	C-N-CA	6.48	126.39	119.85
2	F	19	CYS	CA-C-N	6.46	126.39	119.28
2	F	19	CYS	C-N-CA	6.46	126.39	119.28
2	E	171	MET	CA-C-N	6.45	127.03	120.38
2	E	171	MET	C-N-CA	6.45	127.03	120.38
2	F	242	VAL	CA-C-N	6.45	126.36	119.85
2	F	242	VAL	C-N-CA	6.45	126.36	119.85
3	K	203	ILE	CA-C-N	6.44	126.39	119.76
3	K	203	ILE	C-N-CA	6.44	126.39	119.76
2	E	303	GLU	CA-C-N	6.44	126.06	119.56
2	E	303	GLU	C-N-CA	6.44	126.06	119.56
3	I	182	LYS	CA-C-N	6.44	126.41	119.78
3	I	182	LYS	C-N-CA	6.44	126.41	119.78
1	A	13	VAL	CA-C-N	6.43	126.35	119.85
1	A	13	VAL	C-N-CA	6.43	126.35	119.85
3	K	182	LYS	CA-C-N	6.43	126.39	120.03
3	K	182	LYS	C-N-CA	6.43	126.39	120.03
1	C	7	ILE	CA-C-N	6.42	126.37	119.76
1	C	7	ILE	C-N-CA	6.42	126.37	119.76
1	D	55	ILE	CA-C-N	6.39	126.57	120.31
1	D	55	ILE	C-N-CA	6.39	126.57	120.31
3	L	203	ILE	CA-C-N	6.38	126.34	119.76
3	L	203	ILE	C-N-CA	6.38	126.34	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	57	SER	CA-C-N	6.38	126.14	119.76
1	B	57	SER	C-N-CA	6.38	126.14	119.76
1	C	13	VAL	CA-C-N	6.37	126.28	119.85
1	C	13	VAL	C-N-CA	6.37	126.28	119.85
2	H	288	TYR	CA-C-N	6.36	126.28	119.85
2	H	288	TYR	C-N-CA	6.36	126.28	119.85
2	H	151	LEU	CA-C-N	6.36	126.31	119.76
2	H	151	LEU	C-N-CA	6.36	126.31	119.76
3	J	167	ILE	CA-C-N	6.35	126.30	119.76
3	J	167	ILE	C-N-CA	6.35	126.30	119.76
2	F	303	GLU	CA-C-N	6.33	126.01	119.56
2	F	303	GLU	C-N-CA	6.33	126.01	119.56
2	H	408	VAL	CA-C-N	6.32	126.35	119.90
2	H	408	VAL	C-N-CA	6.32	126.35	119.90
3	K	136	LYS	CA-C-N	6.32	126.27	119.76
3	K	136	LYS	C-N-CA	6.32	126.27	119.76
2	G	19	CYS	CA-C-N	6.31	126.23	119.28
2	G	19	CYS	C-N-CA	6.31	126.23	119.28
1	D	13	VAL	CA-C-N	6.31	126.07	119.76
1	D	13	VAL	C-N-CA	6.31	126.07	119.76
1	D	236	ALA	CA-C-N	6.30	126.27	119.78
1	D	236	ALA	C-N-CA	6.30	126.27	119.78
1	D	282	ILE	CA-C-N	6.30	126.21	119.85
1	D	282	ILE	C-N-CA	6.30	126.21	119.85
2	G	171	MET	CA-C-N	-6.30	113.89	120.38
2	G	171	MET	C-N-CA	-6.30	113.89	120.38
1	B	13	VAL	CA-C-N	6.28	126.20	119.85
1	B	13	VAL	C-N-CA	6.28	126.20	119.85
1	B	303	VAL	CA-C-N	6.25	126.44	119.32
1	B	303	VAL	C-N-CA	6.25	126.44	119.32
1	B	236	ALA	CA-C-N	6.24	126.20	119.78
1	B	236	ALA	C-N-CA	6.24	126.20	119.78
2	F	288	TYR	CA-C-N	6.24	126.15	119.85
2	F	288	TYR	C-N-CA	6.24	126.15	119.85
1	A	21	ARG	CA-C-N	6.23	126.25	119.90
1	A	21	ARG	C-N-CA	6.23	126.25	119.90
1	D	39	GLU	CA-C-N	6.23	126.14	119.85
1	D	39	GLU	C-N-CA	6.23	126.14	119.85
1	C	39	GLU	CA-C-N	6.21	126.12	119.85
1	C	39	GLU	C-N-CA	6.21	126.12	119.85
2	E	19	CYS	CA-C-N	6.20	126.10	119.28
2	E	19	CYS	C-N-CA	6.20	126.10	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	242	VAL	CA-C-N	6.19	126.10	119.85
2	H	242	VAL	C-N-CA	6.19	126.10	119.85
3	I	136	LYS	CA-C-N	6.18	126.13	119.76
3	I	136	LYS	C-N-CA	6.18	126.13	119.76
1	A	231	VAL	CA-C-N	6.17	126.68	120.14
1	A	231	VAL	C-N-CA	6.17	126.68	120.14
1	A	236	ALA	CA-C-N	6.17	126.13	119.78
1	A	236	ALA	C-N-CA	6.17	126.13	119.78
2	E	288	TYR	CA-C-N	6.16	126.07	119.85
2	E	288	TYR	C-N-CA	6.16	126.07	119.85
2	F	351	HIS	CA-C-N	6.16	126.34	119.32
2	F	351	HIS	C-N-CA	6.16	126.34	119.32
2	F	408	VAL	CA-C-N	6.15	126.06	119.85
2	F	408	VAL	C-N-CA	6.15	126.06	119.85
1	B	276	MET	CA-C-N	6.14	126.46	119.83
1	B	276	MET	C-N-CA	6.14	126.46	119.83
2	E	408	VAL	CA-C-N	6.13	126.07	119.76
2	E	408	VAL	C-N-CA	6.13	126.07	119.76
2	G	288	TYR	CA-C-N	6.12	125.89	119.76
2	G	288	TYR	C-N-CA	6.12	125.89	119.76
1	A	207	THR	CA-C-N	6.12	126.01	119.28
1	A	207	THR	C-N-CA	6.12	126.01	119.28
2	E	132	ASP	CA-C-N	6.10	126.66	120.38
2	E	132	ASP	C-N-CA	6.10	126.66	120.38
1	B	25	SER	CA-C-N	6.09	126.11	119.90
1	B	25	SER	C-N-CA	6.09	126.11	119.90
2	F	132	ASP	CA-C-N	6.08	126.64	120.38
2	F	132	ASP	C-N-CA	6.08	126.64	120.38
1	D	231	VAL	CA-C-N	6.04	126.55	120.14
1	D	231	VAL	C-N-CA	6.04	126.55	120.14
1	C	25	SER	CA-C-N	6.03	126.05	119.90
1	C	25	SER	C-N-CA	6.03	126.05	119.90
1	D	207	THR	CA-C-N	6.03	125.91	119.28
1	D	207	THR	C-N-CA	6.03	125.91	119.28
3	J	136	LYS	CA-C-N	6.01	125.96	119.76
3	J	136	LYS	C-N-CA	6.01	125.96	119.76
3	J	203	ILE	CA-C-N	6.01	125.95	119.76
3	J	203	ILE	C-N-CA	6.01	125.95	119.76
1	B	231	VAL	CA-C-N	5.99	126.49	120.14
1	B	231	VAL	C-N-CA	5.99	126.49	120.14
3	I	209	LYS	CA-C-N	5.95	125.96	119.90
3	I	209	LYS	C-N-CA	5.95	125.96	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	172	PRO	CA-C-O	-5.88	116.08	120.73
2	G	351	HIS	CA-C-N	5.88	126.02	119.32
2	G	351	HIS	C-N-CA	5.88	126.02	119.32
2	H	403	THR	CA-C-N	5.87	125.63	119.76
2	H	403	THR	C-N-CA	5.87	125.63	119.76
3	I	203	ILE	CA-C-N	5.85	125.79	119.76
3	I	203	ILE	C-N-CA	5.85	125.79	119.76
2	E	351	HIS	CA-C-N	5.82	125.95	119.32
2	E	351	HIS	C-N-CA	5.82	125.95	119.32
2	H	351	HIS	CA-C-N	5.80	125.93	119.32
2	H	351	HIS	C-N-CA	5.80	125.93	119.32
2	H	89	ALA	CA-C-N	5.77	125.79	119.90
2	H	89	ALA	C-N-CA	5.77	125.79	119.90
2	E	127	HIS	CA-C-N	5.76	125.52	119.76
2	E	127	HIS	C-N-CA	5.76	125.52	119.76
2	E	339	TRP	CA-C-N	5.76	126.24	120.14
2	E	339	TRP	C-N-CA	5.76	126.24	120.14
2	G	127	HIS	CA-C-N	5.74	125.50	119.76
2	G	127	HIS	C-N-CA	5.74	125.50	119.76
1	C	21	ARG	CA-C-N	5.71	126.04	119.93
1	C	21	ARG	C-N-CA	5.71	126.04	119.93
2	H	398	THR	CA-C-N	5.69	125.36	119.56
2	H	398	THR	C-N-CA	5.69	125.36	119.56
2	H	339	TRP	CA-C-N	5.67	126.16	120.14
2	H	339	TRP	C-N-CA	5.67	126.16	120.14
2	E	398	THR	CA-C-N	5.66	125.33	119.56
2	E	398	THR	C-N-CA	5.66	125.33	119.56
2	F	403	THR	CA-C-N	5.66	125.67	119.90
2	F	403	THR	C-N-CA	5.66	125.67	119.90
2	F	89	ALA	CA-C-N	5.66	125.67	119.90
2	F	89	ALA	C-N-CA	5.66	125.67	119.90
1	B	21	ARG	CA-C-N	5.61	125.94	119.93
1	B	21	ARG	C-N-CA	5.61	125.94	119.93
2	G	250	ASP	N-CA-C	5.61	117.39	111.28
1	D	25	SER	CA-C-N	5.61	125.93	119.93
1	D	25	SER	C-N-CA	5.61	125.93	119.93
1	D	21	ARG	CA-C-N	5.57	125.89	119.93
1	D	21	ARG	C-N-CA	5.57	125.89	119.93
2	E	89	ALA	CA-C-N	5.54	125.55	119.90
2	E	89	ALA	C-N-CA	5.54	125.55	119.90
1	C	381	HIS	CA-C-N	5.46	126.00	120.38
1	C	381	HIS	C-N-CA	5.46	126.00	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	127	HIS	CA-C-N	5.43	125.70	119.83
2	H	127	HIS	C-N-CA	5.43	125.70	119.83
2	H	421	ALA	CB-CA-C	-5.43	110.29	116.54
3	L	136	LYS	CA-C-N	5.43	125.70	119.83
3	L	136	LYS	C-N-CA	5.43	125.70	119.83
1	A	381	HIS	CA-C-N	5.42	125.97	120.38
1	A	381	HIS	C-N-CA	5.42	125.97	120.38
1	D	381	HIS	CA-C-N	5.42	125.96	120.38
1	D	381	HIS	C-N-CA	5.42	125.96	120.38
2	F	127	HIS	CA-C-N	5.40	125.32	119.76
2	F	127	HIS	C-N-CA	5.40	125.32	119.76
1	C	207	THR	CA-C-N	5.39	125.73	119.47
1	C	207	THR	C-N-CA	5.39	125.73	119.47
1	B	207	THR	CA-C-N	5.33	125.66	119.47
1	B	207	THR	C-N-CA	5.33	125.66	119.47
2	E	417	CYS	CB-CA-C	-5.28	110.51	116.63
2	E	235	TRP	N-CA-C	5.27	117.67	110.55
2	F	398	THR	CA-C-N	5.19	124.99	119.28
2	F	398	THR	C-N-CA	5.19	124.99	119.28
2	G	403	THR	CA-C-N	5.14	125.30	119.90
2	G	403	THR	C-N-CA	5.14	125.30	119.90
2	G	398	THR	CA-C-N	5.03	124.82	119.28
2	G	398	THR	C-N-CA	5.03	124.82	119.28

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	A	3325	0	3254	8	0
1	B	3325	0	3254	7	0
1	C	3325	0	3254	5	0
1	D	3325	0	3254	3	0
2	E	3299	0	3236	10	0
2	F	3299	0	3239	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	3299	0	3239	8	0
2	H	3299	0	3239	10	0
3	I	1156	0	1133	3	0
3	J	1156	0	1135	6	0
3	K	1156	0	1135	1	0
3	L	1156	0	1135	6	0
All	All	31120	0	30507	73	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (73) 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)
2:H:171:MET:HB3	2:H:250:ASP:OD2	1.91	0.69
2:H:6:PHE:CZ	2:H:97:MET:HG2	2.31	0.66
2:E:170:HIS:HB2	2:E:250:ASP:HB2	1.78	0.65
2:F:12:THR:HG23	2:F:53:GLN:HE22	1.67	0.59
2:G:69:TYR:OH	2:G:117:ASP:OD1	2.16	0.56
2:G:5:ASN:CG	2:G:161:ALA:HB2	2.36	0.51
1:A:325:LYS:NZ	1:A:345:GLU:OE2	2.43	0.51
2:H:6:PHE:C	2:H:8:VAL:H	2.19	0.51
1:A:49:CYS:SG	1:A:50:GLU:N	2.85	0.50
2:F:9:TYR:O	2:F:12:THR:HG22	2.11	0.50
1:B:435:SER:O	3:J:159:LYS:NZ	2.44	0.50
2:F:398:THR:N	2:F:399:PRO:CD	2.74	0.49
2:H:403:THR:OG1	3:L:250:VAL:N	2.45	0.49
3:J:136:LYS:NZ	3:J:163:GLU:OE1	2.38	0.49
2:H:398:THR:N	2:H:399:PRO:CD	2.76	0.48
1:A:402:ILE:H	1:A:402:ILE:HG12	1.43	0.48
1:D:202:ASP:N	1:D:202:ASP:OD1	2.45	0.48
2:F:69:TYR:OH	2:F:117:ASP:OD1	2.11	0.48
1:A:399:VAL:HG12	1:A:401:ASP:H	1.78	0.48
3:L:119:HIS:CG	3:L:120:GLU:H	2.33	0.47
2:F:169:VAL:HB	2:F:235:TRP:HB3	1.96	0.47
2:E:348:ALA:C	2:E:349:HIS:CG	2.92	0.47
2:E:187:ASN:OD1	2:E:219:ASN:N	2.48	0.46
2:E:398:THR:N	2:E:399:PRO:CD	2.77	0.46
2:E:251:ARG:O	2:E:252:LYS:HB2	2.15	0.46
1:B:302:GLU:OE1	1:B:319:LYS:NZ	2.48	0.46
2:E:251:ARG:HA	2:E:251:ARG:HD3	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:119:HIS:ND1	3:L:120:GLU:N	2.64	0.46
3:L:119:HIS:CG	3:L:120:GLU:N	2.84	0.46
1:A:399:VAL:HB	1:A:402:ILE:HG12	1.98	0.45
3:J:161:ASP:OD2	3:J:252:LYS:NZ	2.47	0.45
2:G:398:THR:N	2:G:399:PRO:CD	2.79	0.45
2:G:109:GLU:N	2:G:109:GLU:OE1	2.50	0.45
2:E:189:LYS:O	2:E:190:ILE:C	2.60	0.45
2:H:236:GLN:NE2	2:H:242:VAL:HG11	2.32	0.45
1:B:51:TYR:CD1	1:B:51:TYR:C	2.95	0.44
1:B:402:ILE:H	1:B:402:ILE:HD13	1.82	0.44
1:C:51:TYR:CD1	1:C:51:TYR:C	2.96	0.44
2:E:117:ASP:OD1	2:E:117:ASP:C	2.58	0.44
1:D:51:TYR:C	1:D:51:TYR:CD1	2.95	0.44
2:F:157:VAL:HG12	2:F:159:SER:H	1.83	0.44
2:H:201:CYS:HB3	2:H:225:CYS:HA	1.99	0.44
3:J:189:TRP:CD1	3:J:194:VAL:HG23	2.53	0.44
2:E:6:PHE:HD2	2:E:56:ILE:HD11	1.82	0.44
1:A:51:TYR:C	1:A:51:TYR:CD1	2.95	0.43
3:I:128:CYS:SG	3:I:129:LEU:N	2.91	0.43
2:E:244:ARG:NH2	2:E:247:GLU:O	2.52	0.43
2:G:12:THR:HG21	2:G:255:ILE:HD11	2.00	0.43
1:B:190:PRO:HA	1:B:191:PRO:HD3	1.82	0.42
2:H:259:PHE:N	2:H:260:PRO:CD	2.82	0.42
2:G:201:CYS:HB3	2:G:225:CYS:HA	2.01	0.42
1:B:202:ASP:N	1:B:202:ASP:OD1	2.52	0.42
1:B:255:ALA:HA	1:B:256:PRO:HD3	1.86	0.42
1:C:202:ASP:N	1:C:202:ASP:OD1	2.50	0.42
3:J:119:HIS:O	3:J:143:THR:N	2.52	0.42
3:J:219:ASP:OD1	3:J:219:ASP:C	2.63	0.42
3:I:206:GLY:O	3:I:209:LYS:NZ	2.53	0.41
1:C:7:ILE:HA	1:C:8:PRO:HD3	1.93	0.41
3:L:145:ASP:OD1	3:L:146:ASN:N	2.54	0.41
1:A:236:ALA:HA	1:A:237:PRO:HD3	1.90	0.41
2:H:31:PRO:O	2:H:51:SER:OG	2.39	0.41
3:L:209:LYS:HA	3:L:210:PRO:HD3	1.94	0.41
3:K:189:TRP:CD1	3:K:194:VAL:HG23	2.55	0.41
1:D:25:SER:HA	1:D:26:PRO:HD3	1.90	0.40
2:G:43:ASP:OD1	2:G:43:ASP:C	2.65	0.40
1:A:7:ILE:HA	1:A:8:PRO:HD3	1.91	0.40
2:F:398:THR:HB	2:F:399:PRO:HD3	2.04	0.40
2:H:74:MET:HA	2:H:75:PRO:HD3	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:189:TRP:NE1	3:I:191:HIS:O	2.55	0.40
1:C:236:ALA:HA	1:C:237:PRO:HD3	1.92	0.40
1:C:396:THR:OG1	1:C:397:LEU:N	2.54	0.40
2:F:6:PHE:CE1	2:F:97:MET:SD	3.15	0.40
2:G:175:THR:HA	2:G:176:PRO:HD3	1.86	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	437/439 (100%)	434 (99%)	3 (1%)	0	100	100
1	B	437/439 (100%)	429 (98%)	5 (1%)	3 (1%)	18	51
1	C	437/439 (100%)	430 (98%)	7 (2%)	0	100	100
1	D	437/439 (100%)	431 (99%)	5 (1%)	1 (0%)	43	75
2	E	419/423 (99%)	406 (97%)	12 (3%)	1 (0%)	43	75
2	F	419/423 (99%)	409 (98%)	10 (2%)	0	100	100
2	G	419/423 (99%)	406 (97%)	11 (3%)	2 (0%)	24	59
2	H	419/423 (99%)	413 (99%)	4 (1%)	2 (0%)	24	59
3	I	149/151 (99%)	147 (99%)	1 (1%)	1 (1%)	18	51
3	J	149/151 (99%)	147 (99%)	2 (1%)	0	100	100
3	K	149/151 (99%)	146 (98%)	2 (1%)	1 (1%)	18	51
3	L	149/151 (99%)	146 (98%)	3 (2%)	0	100	100
All	All	4020/4052 (99%)	3944 (98%)	65 (2%)	11 (0%)	37	68

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	401	ASP
1	B	180	TYR
2	H	7	ASN
3	I	247	LYS
3	K	144	ILE
1	B	370	CYS
1	D	370	CYS
2	G	190	ILE
2	G	219	ASN
2	E	190	ILE
2	H	190	ILE

### 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	366/366 (100%)	360 (98%)	6 (2%)	55	78
1	B	366/366 (100%)	365 (100%)	1 (0%)	86	90
1	C	366/366 (100%)	366 (100%)	0	100	100
1	D	366/366 (100%)	366 (100%)	0	100	100
2	E	371/373 (100%)	369 (100%)	2 (0%)	81	88
2	F	371/373 (100%)	369 (100%)	2 (0%)	81	88
2	G	371/373 (100%)	370 (100%)	1 (0%)	86	90
2	H	371/373 (100%)	370 (100%)	1 (0%)	86	90
3	I	120/120 (100%)	120 (100%)	0	100	100
3	J	120/120 (100%)	120 (100%)	0	100	100
3	K	120/120 (100%)	120 (100%)	0	100	100
3	L	120/120 (100%)	120 (100%)	0	100	100
All	All	3428/3436 (100%)	3415 (100%)	13 (0%)	81	89

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	LYS
1	A	397	LEU
1	A	399	VAL
1	A	400	GLN
1	A	402	ILE
1	A	407	MET
1	B	402	ILE
2	E	5	ASN
2	E	250	ASP
2	F	6	PHE
2	F	12	THR
2	G	3	LYS
2	H	8	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	331	HIS
1	D	331	HIS
1	D	349	ASN
2	E	29	HIS
2	E	146	GLN
2	E	158	GLN
2	E	195	GLN
2	E	333	ASN
2	F	5	ASN
2	F	62	HIS
2	F	72	ASN
2	F	146	GLN
2	F	184	GLN
2	F	187	ASN
2	G	5	ASN
2	G	184	GLN
2	G	218	ASN
2	G	219	ASN
2	H	207	ASN
2	H	333	ASN
3	K	139	HIS

### 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.

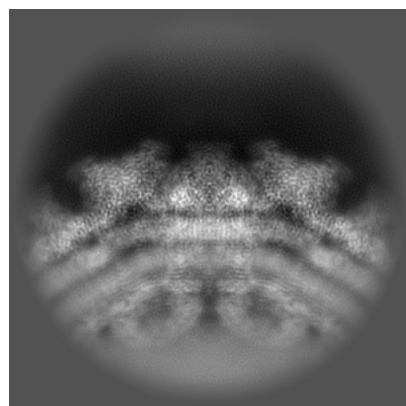
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60970. These allow visual inspection of the internal detail of the map and identification of artifacts.

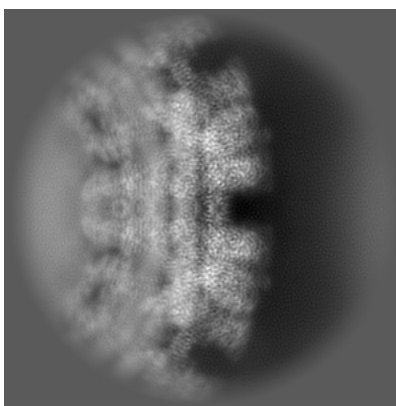
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

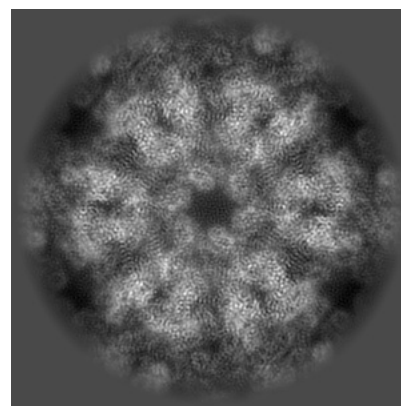
#### 6.1.1 Primary map



X

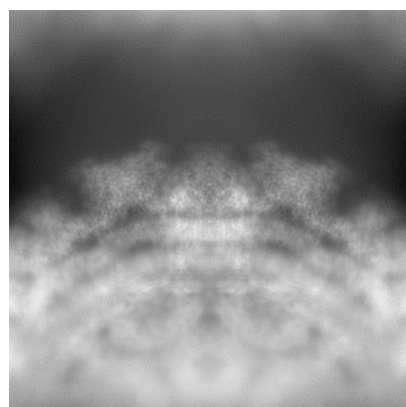


Y

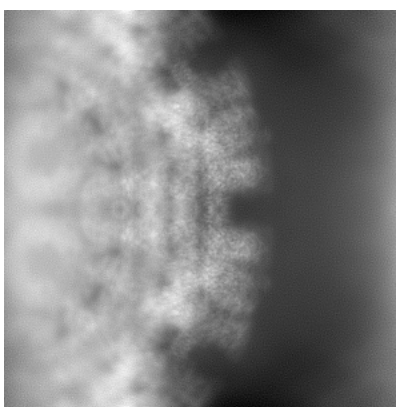


Z

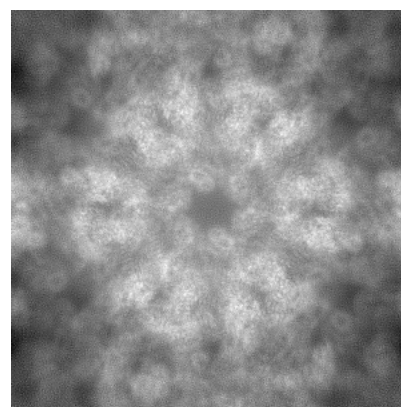
#### 6.1.2 Raw map



X



Y

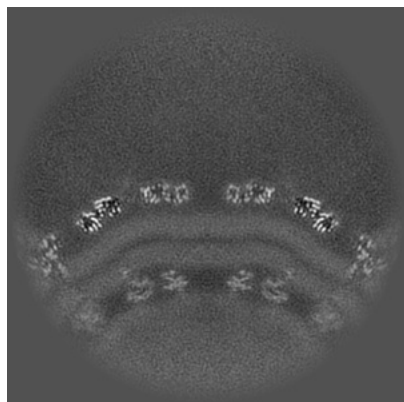


Z

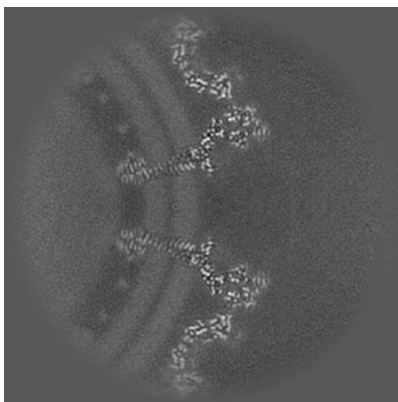
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

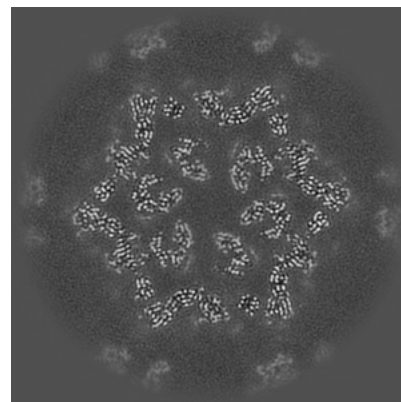
### 6.2.1 Primary map



X Index: 200

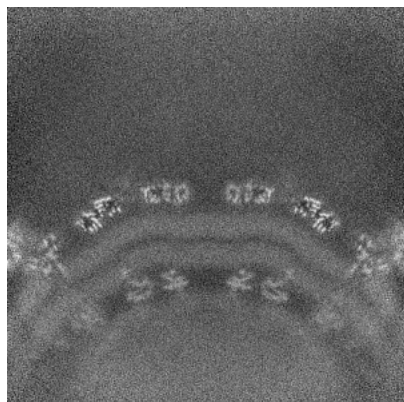


Y Index: 200

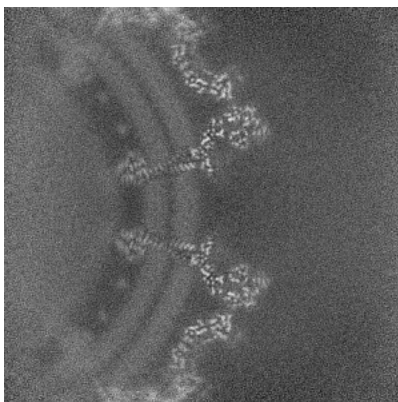


Z Index: 200

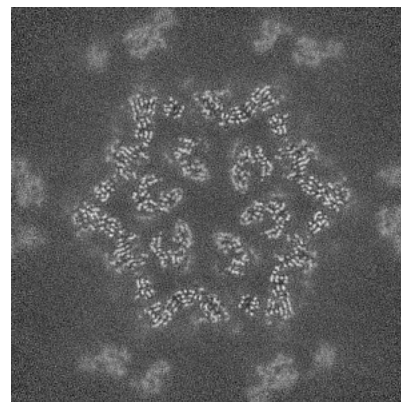
### 6.2.2 Raw map



X Index: 200



Y Index: 200



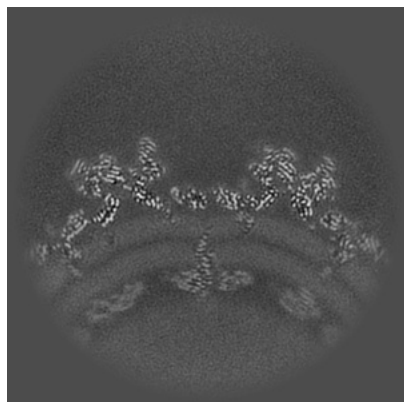
Z Index: 200

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

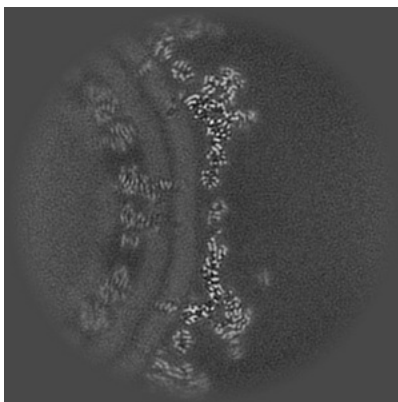


## 6.3 Largest variance slices [i](#)

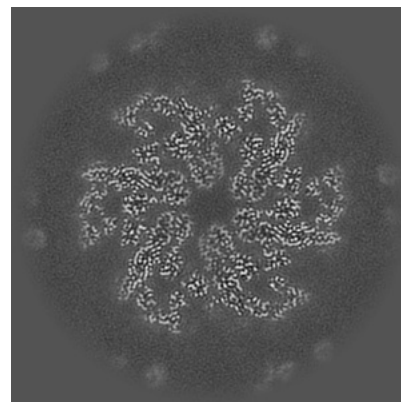
### 6.3.1 Primary map



X Index: 234

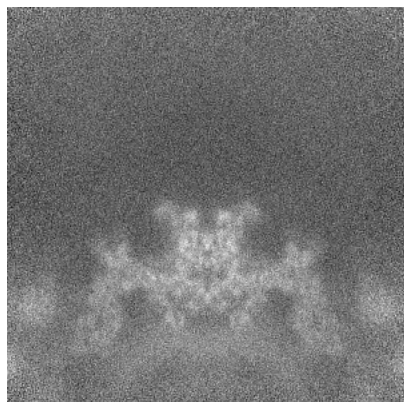


Y Index: 223

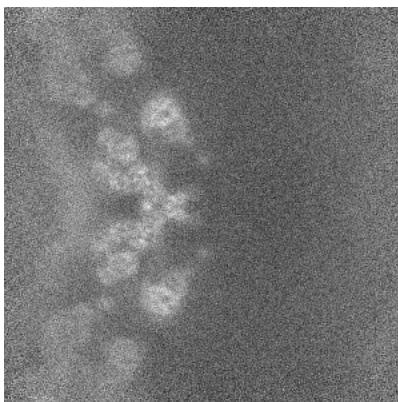


Z Index: 209

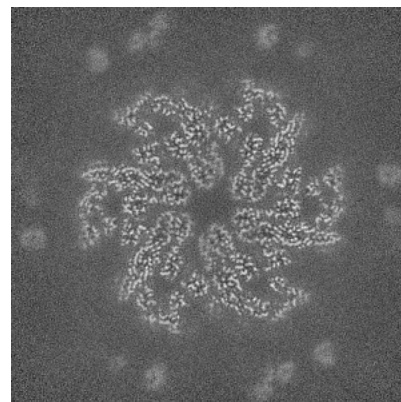
### 6.3.2 Raw map



X Index: 0



Y Index: 0



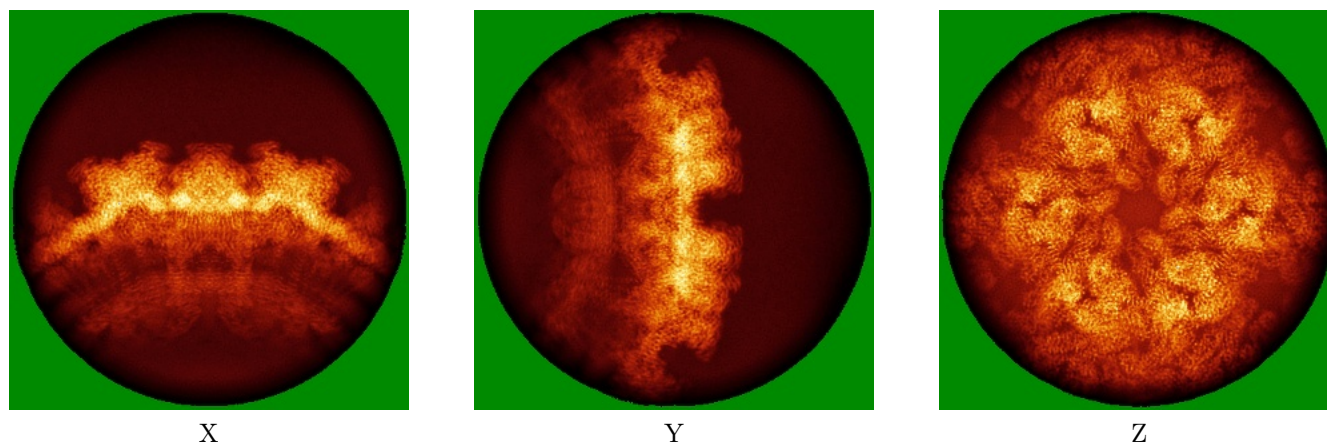
Z Index: 209

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

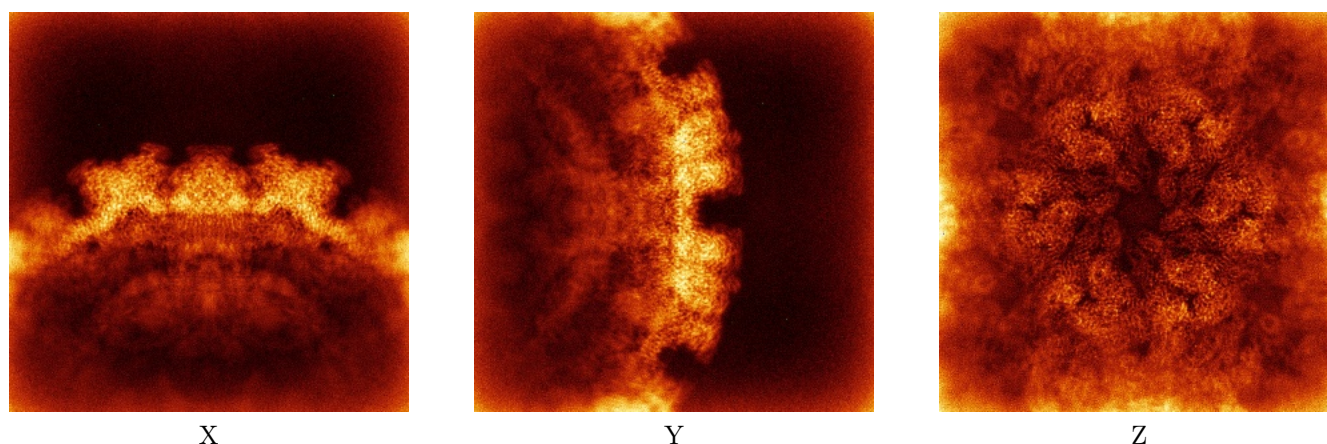


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 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](#)

This section was not generated.

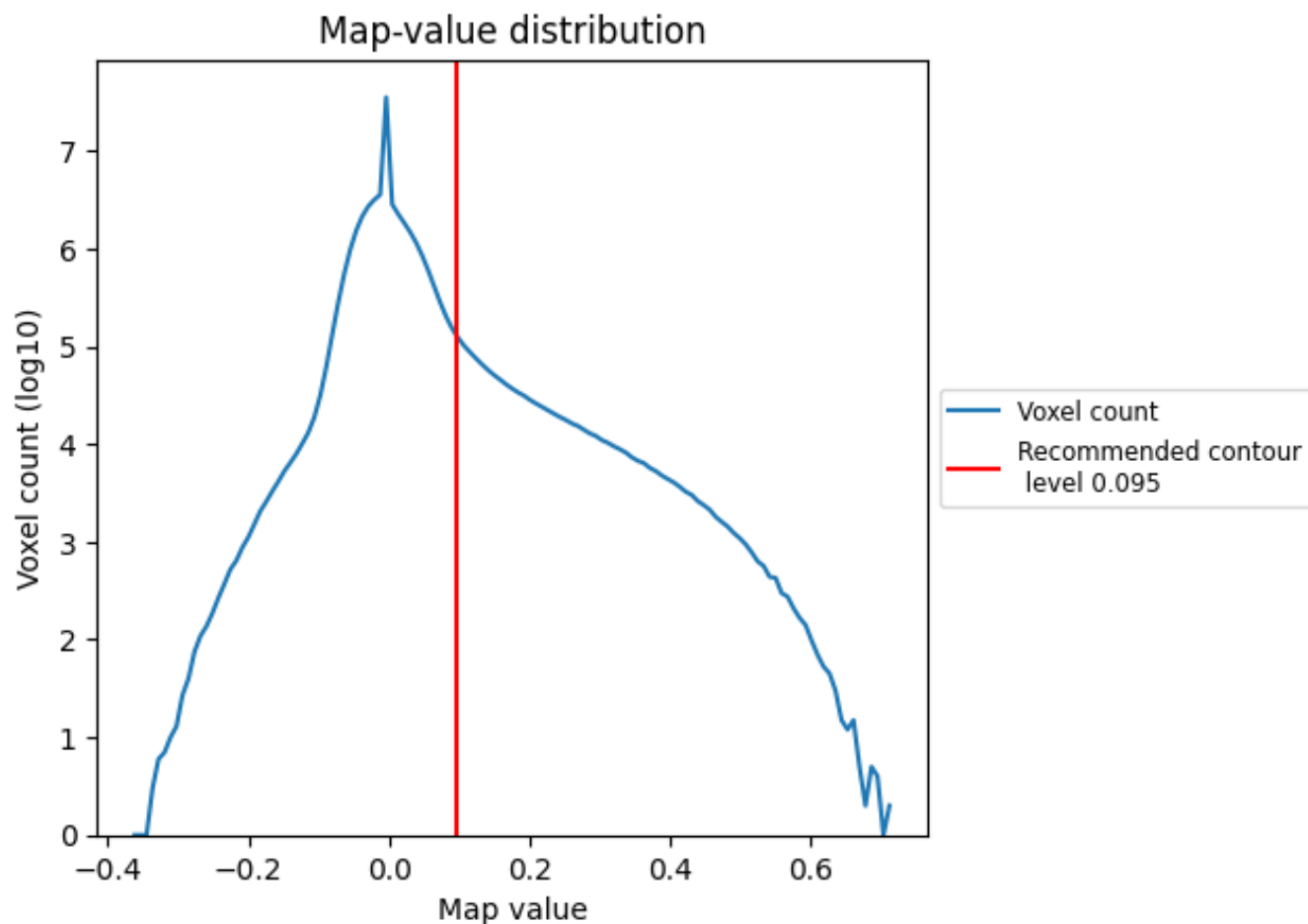
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

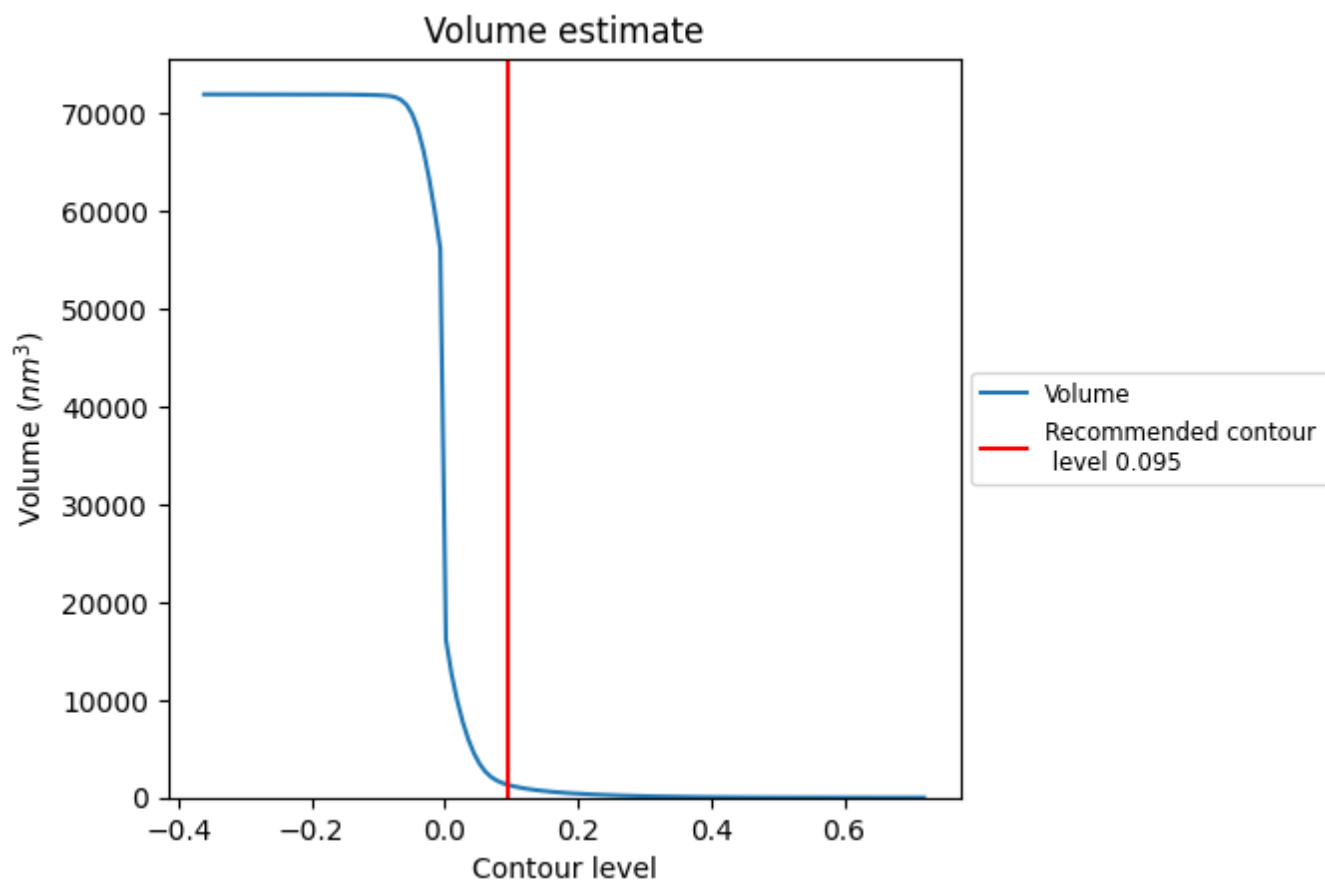
This section contains the results of statistical analysis of the map.

### 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.

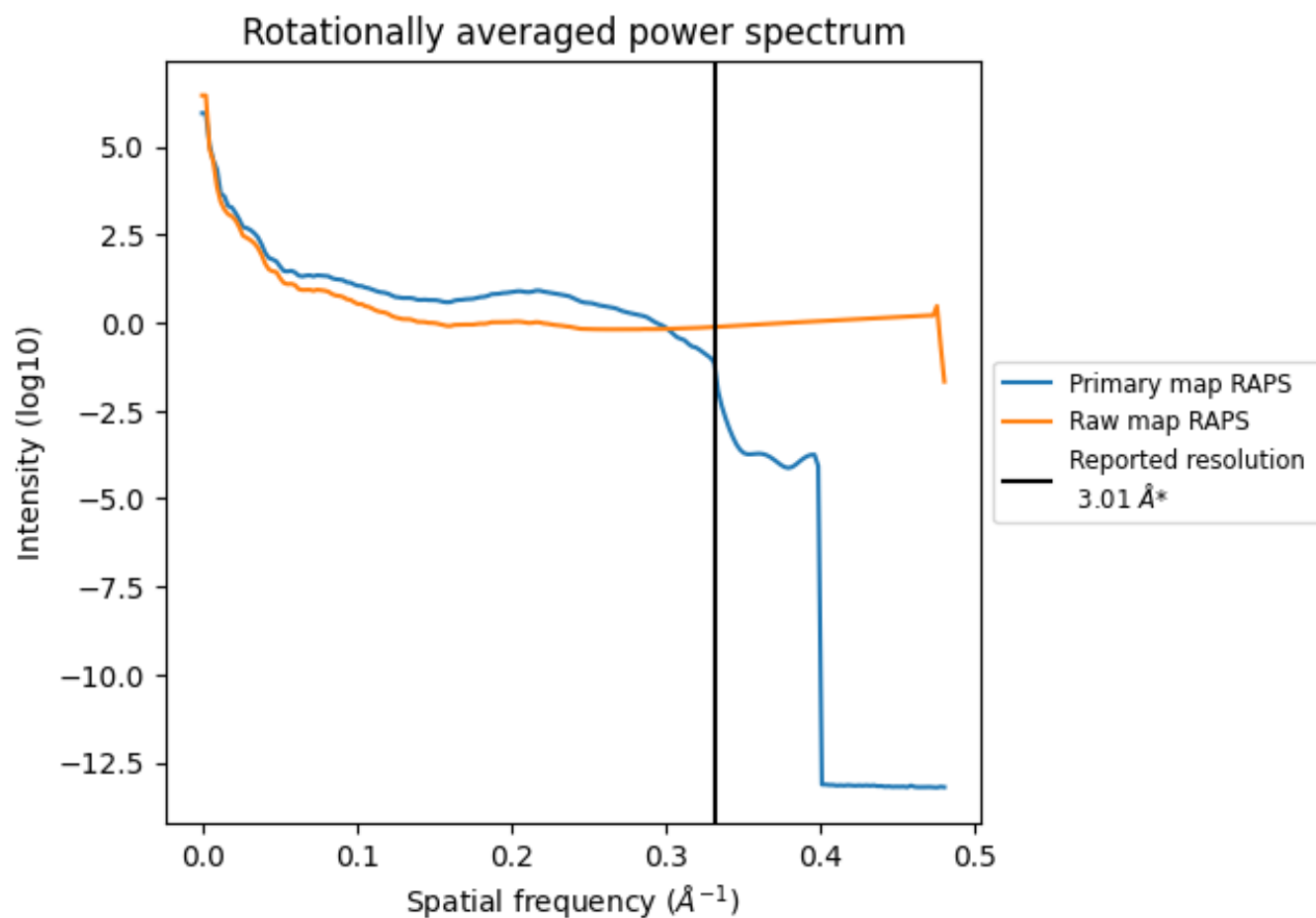
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1298 nm<sup>3</sup>; this corresponds to an approximate mass of 1173 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 ⓘ

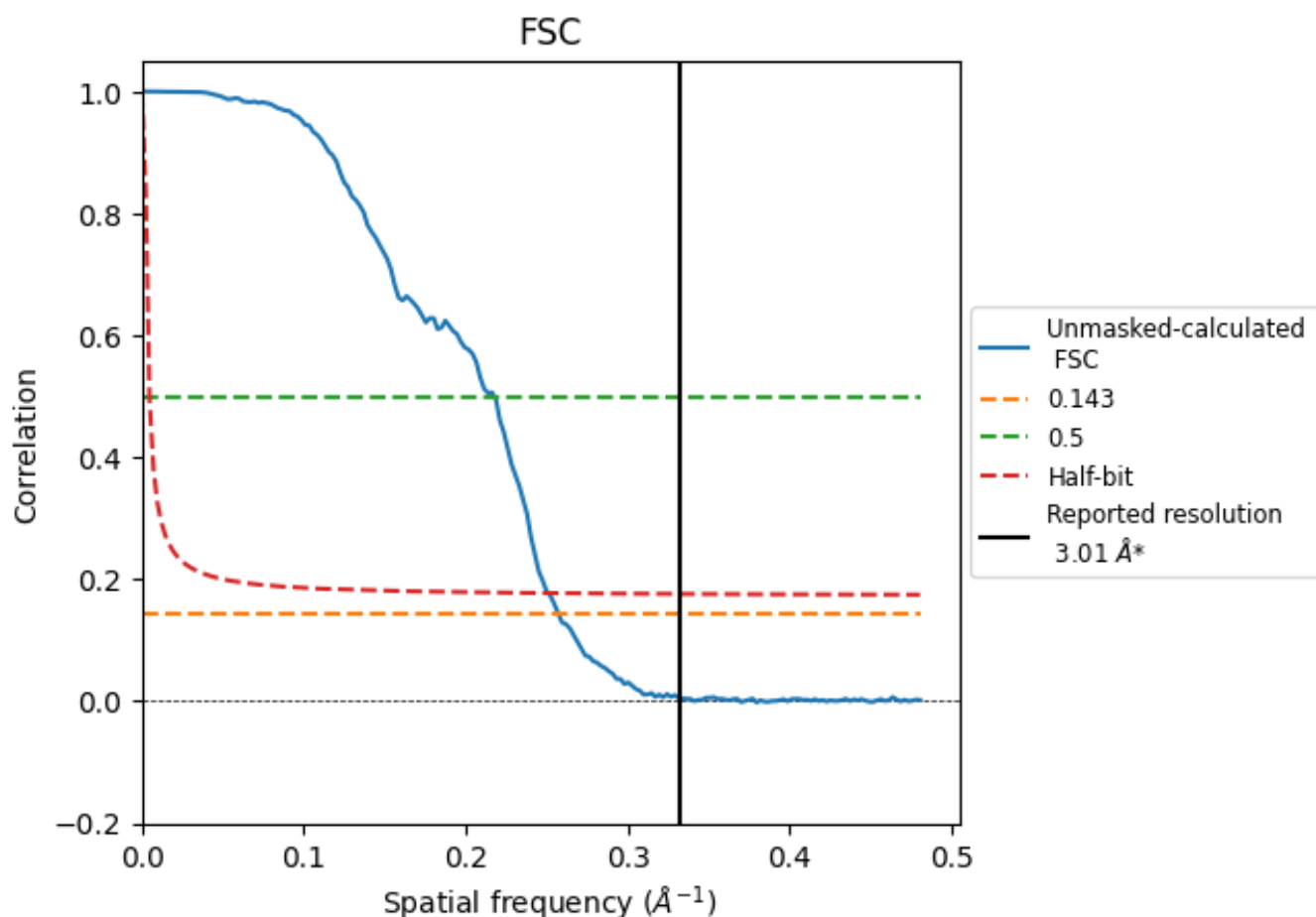


\*Reported resolution corresponds to spatial frequency of 0.332  $\text{\AA}^{-1}$

## 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 0.332  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.88	4.60	3.98

\*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 3.88 differs from the reported value 3.01 by more than 10 %

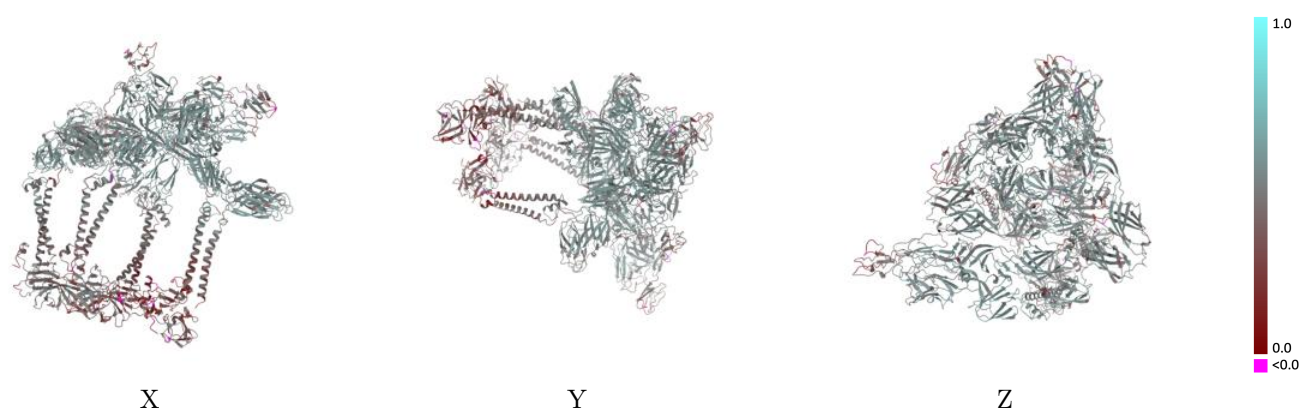
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60970 and PDB model 9IXI. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)

This section was not generated.

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

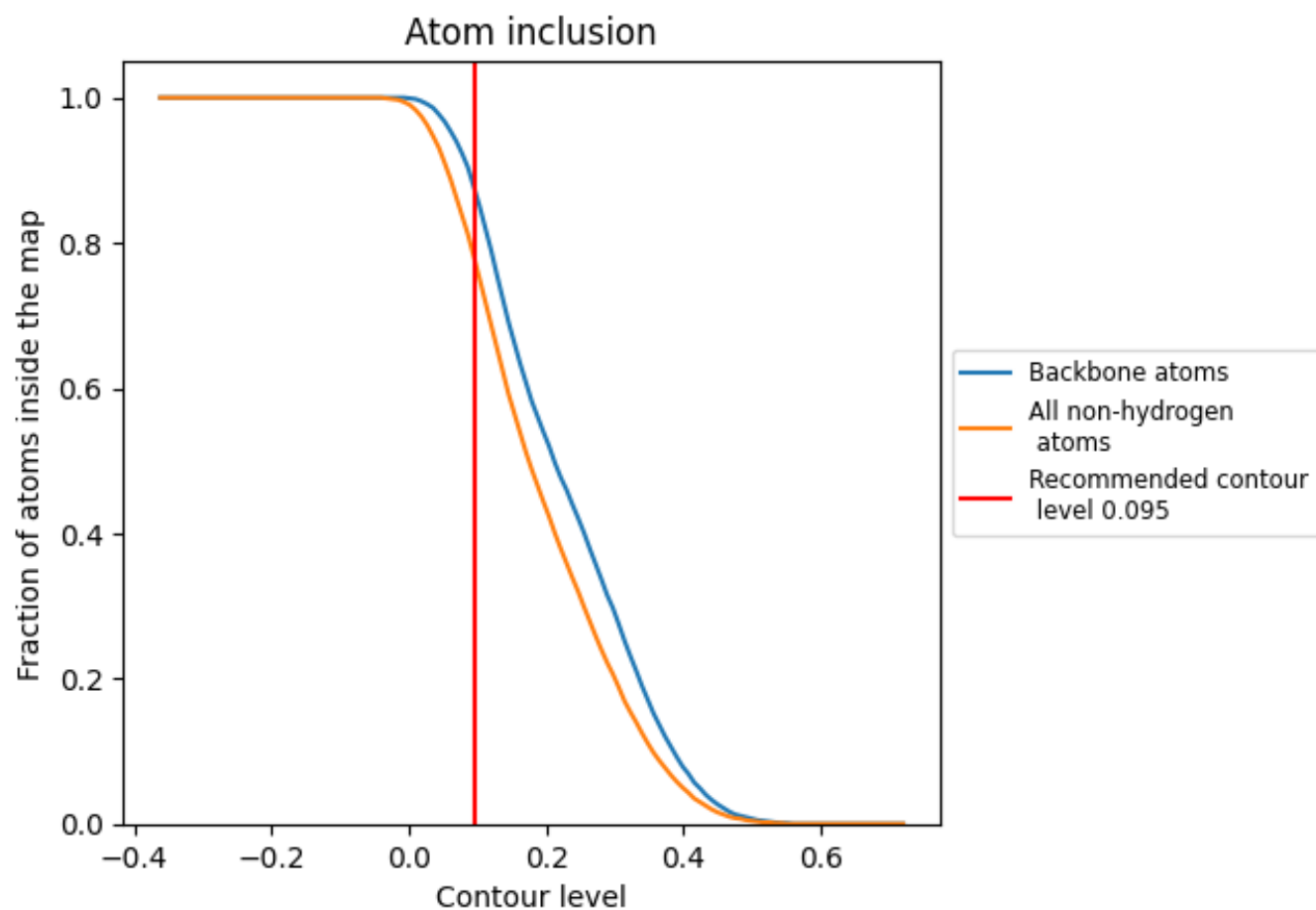


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 88% of all backbone atoms, 78% 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 (0.095) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7800	<div></div> 0.4790
A	<div></div> 0.8450	<div></div> 0.5110
B	<div></div> 0.8380	<div></div> 0.5070
C	<div></div> 0.8360	<div></div> 0.5060
D	<div></div> 0.8580	<div></div> 0.5200
E	<div></div> 0.8250	<div></div> 0.4860
F	<div></div> 0.8250	<div></div> 0.4920
G	<div></div> 0.8240	<div></div> 0.4900
H	<div></div> 0.8230	<div></div> 0.4910
I	<div></div> 0.4110	<div></div> 0.2940
J	<div></div> 0.5630	<div></div> 0.3950
K	<div></div> 0.3690	<div></div> 0.3140
L	<div></div> 0.5320	<div></div> 0.4120

