



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:29 AM UTC

PDB ID : 9HVM / pdb_00009hvm
EMDB ID : EMD-52438
Title : In-cell Structure of Pyrenoid Rubisco
Authors : Nadav, E.; Zhen, H.; Maud, D.; Alireza, R.; Juan R, P.; Peijun, P.
Deposited on : 2024-12-30
Resolution : 8.10 Å(reported)
Based on initial models : 1EJ7, 1GK8

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

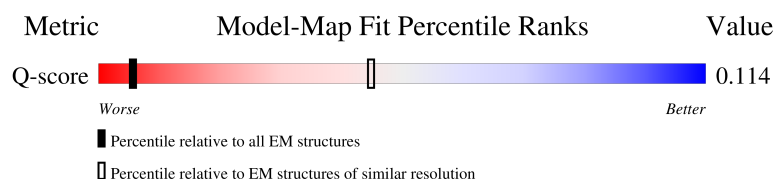
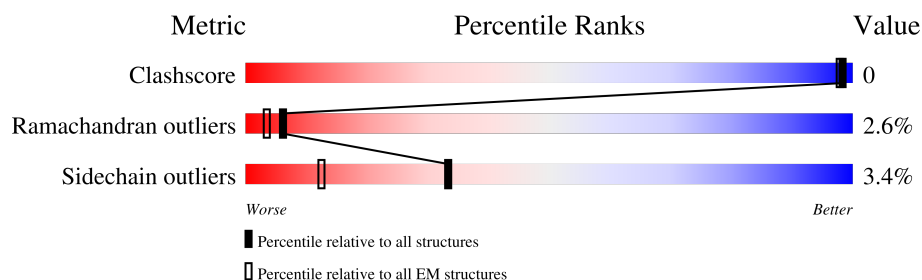
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

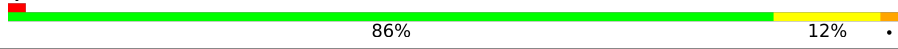
The reported resolution of this entry is 8.10 Å.

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



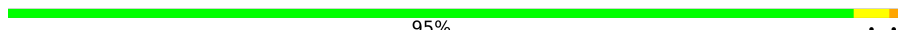
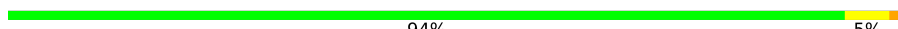
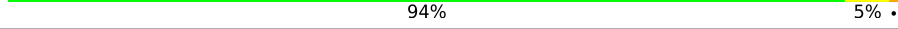
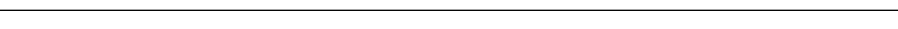
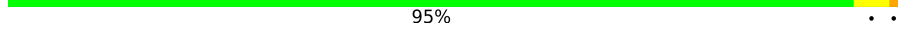
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	342 (7.60 - 8.60)

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	469	 86% 13% .
1	C	469	 85% 13% .
1	E	469	 86% 12% .
1	G	469	 86% 12% .

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Mol	Chain	Length	Quality of chain
1	I	469	 85%14%
1	K	469	 84%15%
1	M	469	 85%13%
1	O	469	 87%12%
2	B	132	 95%5%
2	D	132	 94%5%
2	F	132	 94%5%
2	H	132	 95%5%
2	J	132	 95%5%
2	L	132	 92%7%
2	N	132	 92%7%
2	P	132	 92%7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 37816 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 Ribulose biphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	469	Total	C	N	O	S	0	0
			3647	2308	642	673	24		
1	C	469	Total	C	N	O	S	0	0
			3647	2308	642	673	24		
1	E	469	Total	C	N	O	S	0	0
			3647	2308	642	673	24		
1	G	469	Total	C	N	O	S	0	0
			3647	2308	642	673	24		
1	I	469	Total	C	N	O	S	0	0
			3647	2308	642	673	24		
1	K	469	Total	C	N	O	S	0	0
			3647	2308	642	673	24		
1	M	469	Total	C	N	O	S	0	0
			3647	2308	642	673	24		
1	O	469	Total	C	N	O	S	0	0
			3647	2308	642	673	24		

- Molecule 2 is a protein called Ribulose biphosphate carboxylase small subunit, chloroplastic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	132	Total	C	N	O	S	0	0
			1080	701	176	192	11		
2	D	132	Total	C	N	O	S	0	0
			1080	701	176	192	11		
2	F	132	Total	C	N	O	S	0	0
			1080	701	176	192	11		
2	H	132	Total	C	N	O	S	0	0
			1080	701	176	192	11		
2	J	132	Total	C	N	O	S	0	0
			1080	701	176	192	11		
2	L	132	Total	C	N	O	S	0	0
			1080	701	176	192	11		

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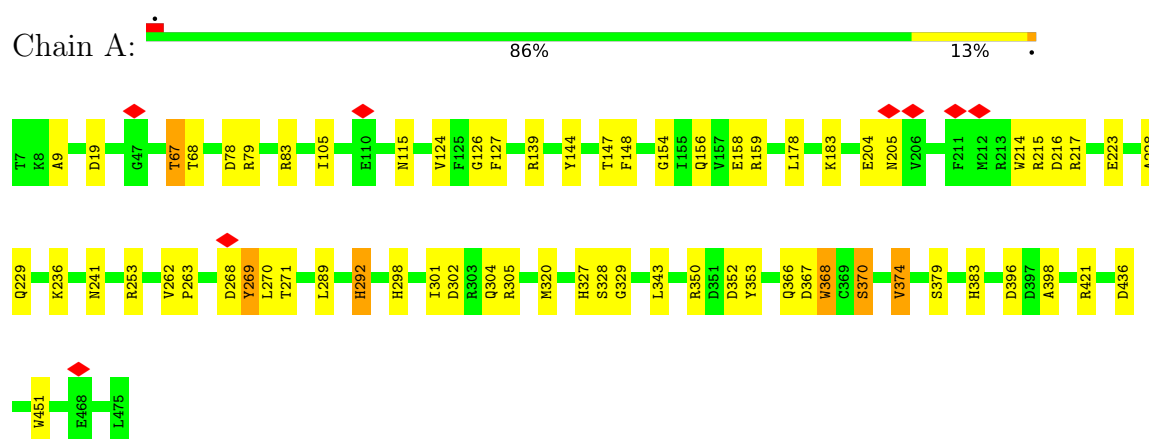
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	132	Total	C	N	O	S	0	0
			1080	701	176	192	11		
2	P	132	Total	C	N	O	S	0	0
			1080	701	176	192	11		

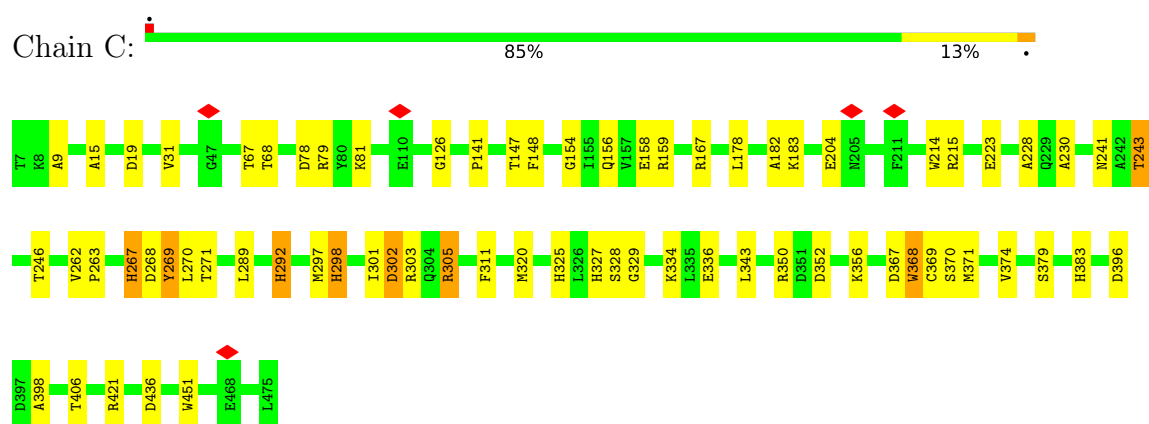
3 Residue-property plots

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.

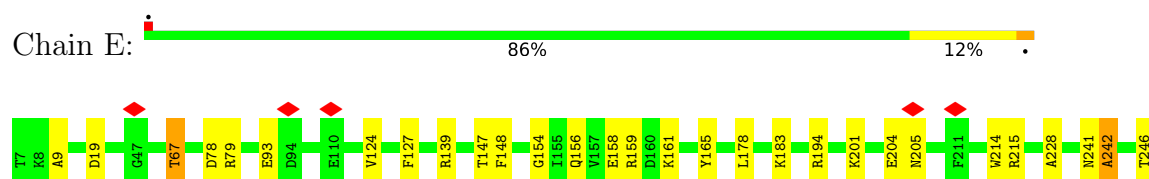
- Molecule 1: Ribulose biphosphate carboxylase large chain

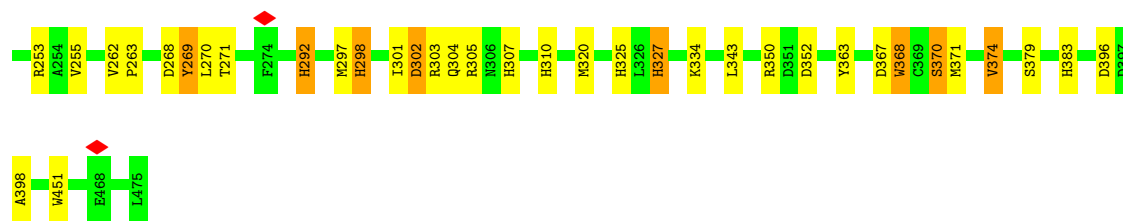


- Molecule 1: Ribulose biphosphate carboxylase large chain



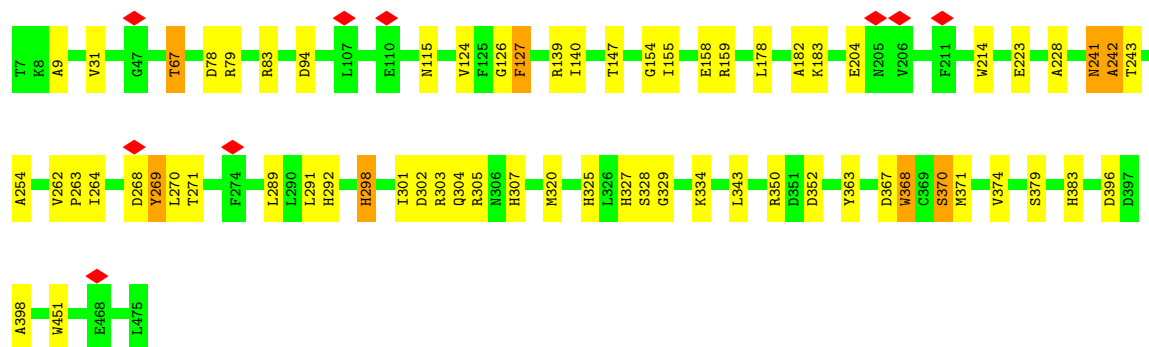
- Molecule 1: Ribulose biphosphate carboxylase large chain





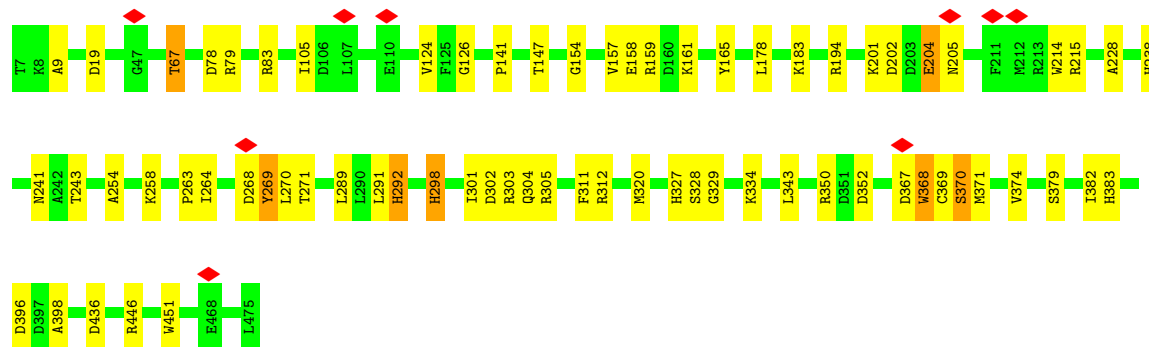
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain G: 86% 12%



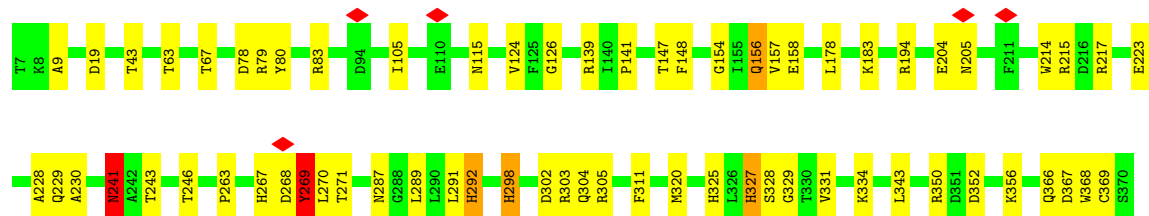
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain I: 85% 14%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain K: 84% 15%





- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain M: 85% 13%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain O: 87% 12%



- Molecule 2: Ribulose biphosphate carboxylase small subunit, chloroplastic 1

Chain B: 95% 5%



- Molecule 2: Ribulose biphosphate carboxylase small subunit, chloroplastic 1

Chain D: 94% 5%



- Molecule 2: Ribulose biphosphate carboxylase small subunit, chloroplastic 1

Chain F: 94% 5%



- Molecule 2: Ribulose biphosphate carboxylase small subunit, chloroplastic 1



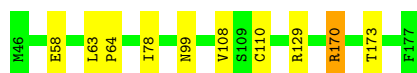
- Molecule 2: Ribulose biphosphate carboxylase small subunit, chloroplastic 1



- Molecule 2: Ribulose biphosphate carboxylase small subunit, chloroplastic 1



- Molecule 2: Ribulose biphosphate carboxylase small subunit, chloroplastic 1



- Molecule 2: Ribulose biphosphate carboxylase small subunit, chloroplastic 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, D4	Depositor
Number of subtomograms used	17713	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	120	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	29.887	Depositor
Minimum map value	-14.231	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.926	Depositor
Recommended contour level	4	Depositor
Map size ($\text{\AA}$)	504.32, 504.32, 504.32	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.97, 1.97, 1.97	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.88	0/3733	1.56	37/5054 (0.7%)
1	C	0.89	0/3733	1.58	37/5054 (0.7%)
1	E	0.88	0/3733	1.57	37/5054 (0.7%)
1	G	0.88	0/3733	1.57	38/5054 (0.8%)
1	I	0.88	0/3733	1.57	36/5054 (0.7%)
1	K	0.88	0/3733	1.57	39/5054 (0.8%)
1	M	0.88	0/3733	1.57	43/5054 (0.9%)
1	O	0.89	0/3733	1.57	30/5054 (0.6%)
2	B	0.84	0/1111	1.42	2/1509 (0.1%)
2	D	0.84	0/1111	1.44	3/1509 (0.2%)
2	F	0.85	0/1111	1.45	5/1509 (0.3%)
2	H	0.85	0/1111	1.44	7/1509 (0.5%)
2	J	0.84	0/1111	1.43	2/1509 (0.1%)
2	L	0.84	0/1111	1.43	6/1509 (0.4%)
2	N	0.85	0/1111	1.44	8/1509 (0.5%)
2	P	0.85	1/1111 (0.1%)	1.47	5/1509 (0.3%)
All	All	0.87	1/38752 (0.0%)	1.54	335/52504 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	19
1	C	0	16
1	E	0	20
1	G	0	18
1	I	0	20
1	K	0	19
1	M	0	18
1	O	0	19
2	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
2	F	0	1
2	H	0	2
2	J	0	1
2	L	0	2
2	N	0	2
2	P	0	2
All	All	0	161

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	64	PRO	CA-C	5.12	1.54	1.51

All (335) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	334	LYS	N-CA-C	9.59	121.74	111.28
1	K	334	LYS	N-CA-C	9.23	121.34	111.28
1	I	334	LYS	N-CA-C	8.25	120.27	111.28
1	E	292	HIS	CA-CB-CG	7.91	121.71	113.80
1	A	262	VAL	N-CA-C	7.77	117.50	108.96
1	E	262	VAL	N-CA-C	7.76	117.50	108.96
2	F	170	ARG	O-C-N	-7.74	116.76	121.71
1	O	271	THR	N-CA-C	-7.62	104.51	113.88
1	A	271	THR	N-CA-C	-7.55	104.60	113.88
1	O	350	ARG	N-CA-C	7.33	119.06	111.14
1	A	343	LEU	CA-C-N	7.32	128.07	119.94
1	A	343	LEU	C-N-CA	7.32	128.07	119.94
1	E	334	LYS	N-CA-C	7.29	119.22	111.28
1	G	271	THR	N-CA-C	-7.28	104.93	113.88
1	C	398	ALA	CA-C-N	7.25	134.76	121.70
1	C	398	ALA	C-N-CA	7.25	134.76	121.70
1	I	271	THR	N-CA-C	-7.24	104.97	113.88
1	M	271	THR	N-CA-C	-7.22	105.00	113.88
1	C	301	ILE	CA-C-N	7.21	129.94	120.28
1	C	301	ILE	C-N-CA	7.21	129.94	120.28
1	A	292	HIS	CA-CB-CG	7.19	120.99	113.80
1	K	398	ALA	CA-C-N	7.13	134.54	121.70
1	K	398	ALA	C-N-CA	7.13	134.54	121.70
1	M	262	VAL	N-CA-C	7.13	116.80	108.96
1	K	241	ASN	CA-CB-CG	7.12	119.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	398	ALA	CA-C-N	7.10	134.48	121.70
1	I	398	ALA	C-N-CA	7.10	134.48	121.70
1	M	271	THR	CA-C-N	7.07	127.64	119.94
1	M	271	THR	C-N-CA	7.07	127.64	119.94
1	M	398	ALA	CA-C-N	7.06	134.40	121.70
1	M	398	ALA	C-N-CA	7.06	134.40	121.70
1	G	398	ALA	CA-C-N	7.04	134.38	121.70
1	G	398	ALA	C-N-CA	7.04	134.38	121.70
1	A	214	TRP	CA-C-N	7.01	129.67	120.28
1	A	214	TRP	C-N-CA	7.01	129.67	120.28
1	O	398	ALA	CA-C-N	7.00	134.31	121.70
1	O	398	ALA	C-N-CA	7.00	134.31	121.70
1	O	334	LYS	N-CA-C	6.97	121.54	112.89
1	E	271	THR	N-CA-C	-6.97	105.31	113.88
1	C	343	LEU	CA-C-N	6.91	127.61	119.94
1	C	343	LEU	C-N-CA	6.91	127.61	119.94
2	N	63	LEU	CA-C-N	6.88	124.69	119.66
2	N	63	LEU	C-N-CA	6.88	124.69	119.66
1	C	298	HIS	CA-CB-CG	6.86	120.66	113.80
1	K	271	THR	N-CA-C	-6.81	105.50	113.88
1	K	311	PHE	N-CA-C	6.79	118.68	111.28
1	C	214	TRP	CA-C-N	6.78	129.37	120.28
1	C	214	TRP	C-N-CA	6.78	129.37	120.28
1	K	325	HIS	CA-CB-CG	6.78	120.58	113.80
1	K	292	HIS	CA-CB-CG	6.77	120.57	113.80
1	M	127	PHE	CA-CB-CG	-6.77	107.03	113.80
1	C	292	HIS	CA-CB-CG	6.76	120.56	113.80
1	C	271	THR	N-CA-C	-6.74	105.59	113.88
1	I	292	HIS	CA-CB-CG	6.73	120.53	113.80
1	M	352	ASP	CA-CB-CG	6.70	119.30	112.60
1	K	343	LEU	CA-C-N	6.70	127.37	119.94
1	K	343	LEU	C-N-CA	6.70	127.37	119.94
1	M	473	ASP	N-CA-C	6.70	119.72	110.35
1	K	352	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	352	ASP	CA-CB-CG	6.65	119.25	112.60
1	C	262	VAL	N-CA-C	6.64	116.26	108.96
1	E	398	ALA	CA-C-N	6.60	133.58	121.70
1	E	398	ALA	C-N-CA	6.60	133.58	121.70
1	A	398	ALA	CA-C-N	6.54	133.47	121.70
1	A	398	ALA	C-N-CA	6.54	133.47	121.70
1	O	292	HIS	CA-CB-CG	6.53	120.33	113.80
1	I	352	ASP	CA-CB-CG	6.52	119.12	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	271	THR	CA-C-N	6.52	127.05	119.94
1	G	271	THR	C-N-CA	6.52	127.05	119.94
1	G	343	LEU	CA-C-N	6.49	127.14	119.94
1	G	343	LEU	C-N-CA	6.49	127.14	119.94
1	M	325	HIS	CA-CB-CG	6.46	120.26	113.80
1	I	271	THR	CA-C-N	6.44	126.96	119.94
1	I	271	THR	C-N-CA	6.44	126.96	119.94
1	I	343	LEU	CA-C-N	6.43	127.08	119.94
1	I	343	LEU	C-N-CA	6.43	127.08	119.94
1	G	124	VAL	N-CA-C	6.40	116.57	110.42
1	K	271	THR	CA-C-N	6.37	126.89	119.94
1	K	271	THR	C-N-CA	6.37	126.89	119.94
1	M	334	LYS	N-CA-C	6.37	120.79	112.89
1	O	271	THR	CA-C-N	6.36	126.87	119.94
1	O	271	THR	C-N-CA	6.36	126.87	119.94
1	G	292	HIS	CA-CB-CG	6.36	120.16	113.80
1	E	301	ILE	CA-C-N	6.35	128.79	120.28
1	E	301	ILE	C-N-CA	6.35	128.79	120.28
1	K	214	TRP	CA-C-N	6.34	128.77	120.28
1	K	214	TRP	C-N-CA	6.34	128.77	120.28
1	M	343	LEU	CA-C-N	6.32	126.96	119.94
1	M	343	LEU	C-N-CA	6.32	126.96	119.94
1	E	214	TRP	CA-C-N	6.32	128.75	120.28
1	E	214	TRP	C-N-CA	6.32	128.75	120.28
1	E	350	ARG	N-CA-C	6.31	117.82	111.07
1	G	214	TRP	CA-C-N	6.30	128.72	120.28
1	G	214	TRP	C-N-CA	6.30	128.72	120.28
2	B	170	ARG	O-C-N	-6.27	117.46	121.85
1	C	271	THR	CA-C-N	6.25	126.75	119.94
1	C	271	THR	C-N-CA	6.25	126.75	119.94
1	M	214	TRP	CA-C-N	6.24	128.63	120.28
1	M	214	TRP	C-N-CA	6.24	128.63	120.28
2	H	170	ARG	O-C-N	-6.22	117.50	121.85
1	E	310	HIS	CA-C-N	6.21	128.61	120.28
1	E	310	HIS	C-N-CA	6.21	128.61	120.28
2	L	170	ARG	O-C-N	-6.20	117.51	121.85
1	K	298	HIS	N-CA-C	6.16	118.00	111.28
2	P	170	ARG	O-C-N	-6.15	117.55	121.85
1	E	19	ASP	CA-CB-CG	6.14	118.74	112.60
2	N	170	ARG	O-C-N	-6.08	117.60	121.85
1	I	214	TRP	CA-C-N	6.08	128.42	120.28
1	I	214	TRP	C-N-CA	6.08	128.42	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	SER	N-CA-CB	6.06	120.73	110.49
1	M	292	HIS	CA-CB-CG	6.04	119.84	113.80
1	G	301	ILE	CA-C-N	6.00	128.32	120.28
1	G	301	ILE	C-N-CA	6.00	128.32	120.28
1	C	352	ASP	CA-CB-CG	5.98	118.58	112.60
1	C	19	ASP	CA-CB-CG	5.98	118.58	112.60
1	I	124	VAL	N-CA-C	5.97	116.15	110.42
1	G	298	HIS	CA-CB-CG	5.96	119.76	113.80
1	A	350	ARG	N-CA-C	5.96	117.44	111.07
1	M	205	ASN	CA-CB-CG	-5.96	106.64	112.60
1	A	19	ASP	CA-CB-CG	5.94	118.54	112.60
1	C	334	LYS	N-CA-C	5.94	120.25	112.89
1	I	350	ARG	N-CA-C	5.93	117.42	111.07
2	P	63	LEU	CA-C-N	5.93	123.99	119.66
2	P	63	LEU	C-N-CA	5.93	123.99	119.66
1	C	350	ARG	N-CA-C	5.92	117.41	111.07
1	E	298	HIS	CA-CB-CG	5.92	119.72	113.80
1	O	214	TRP	CA-C-N	5.90	128.19	120.28
1	O	214	TRP	C-N-CA	5.90	128.19	120.28
1	E	93	GLU	CA-C-N	5.88	128.16	120.28
1	E	93	GLU	C-N-CA	5.88	128.16	120.28
1	G	31	VAL	N-CA-C	5.85	117.58	109.80
1	C	398	ALA	O-C-N	-5.83	114.83	122.59
1	G	370	SER	N-CA-CB	5.82	120.33	110.49
1	E	271	THR	CA-C-N	5.82	126.28	119.94
1	E	271	THR	C-N-CA	5.82	126.28	119.94
2	D	170	ARG	O-C-N	-5.81	117.78	121.85
1	A	301	ILE	CA-C-N	5.80	128.06	120.28
1	A	301	ILE	C-N-CA	5.80	128.06	120.28
1	A	271	THR	CA-C-N	5.80	126.26	119.94
1	A	271	THR	C-N-CA	5.80	126.26	119.94
1	K	19	ASP	CA-CB-CG	5.79	118.39	112.60
1	G	350	ARG	N-CA-C	5.78	117.26	111.07
1	I	311	PHE	N-CA-C	5.75	117.55	111.28
1	E	352	ASP	CA-CB-CG	5.75	118.34	112.60
1	K	205	ASN	CA-CB-CG	-5.74	106.86	112.60
1	G	127	PHE	CA-CB-CG	-5.73	108.07	113.80
1	O	398	ALA	O-C-N	-5.73	114.97	122.59
1	A	398	ALA	O-C-N	-5.73	114.97	122.59
2	D	110	CYS	N-CA-C	5.72	119.08	111.30
1	K	298	HIS	CA-CB-CG	5.72	119.52	113.80
1	M	350	ARG	N-CA-C	5.72	117.31	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	105	ILE	CA-C-N	5.71	128.72	120.38
1	M	105	ILE	C-N-CA	5.71	128.72	120.38
1	G	398	ALA	O-C-N	-5.70	115.01	122.59
1	I	19	ASP	CA-CB-CG	5.69	118.29	112.60
1	M	124	VAL	N-CA-C	5.69	115.88	110.42
1	E	370	SER	N-CA-CB	5.69	120.10	110.49
1	G	241	ASN	CA-CB-CG	5.68	118.28	112.60
1	O	343	LEU	CA-C-N	5.68	126.24	119.94
1	O	343	LEU	C-N-CA	5.68	126.24	119.94
1	E	124	VAL	N-CA-C	5.66	115.86	110.42
1	A	115	ASN	CA-CB-CG	5.66	118.26	112.60
1	O	167	ARG	N-CA-C	-5.65	100.14	108.79
1	G	352	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	298	HIS	CA-CB-CG	5.62	119.42	113.80
1	E	398	ALA	O-C-N	-5.59	115.15	122.59
1	O	105	ILE	CA-C-N	5.58	128.53	120.38
1	O	105	ILE	C-N-CA	5.58	128.53	120.38
1	E	368	TRP	N-CA-C	5.57	122.67	110.80
1	I	370	SER	N-CA-CB	5.57	119.90	110.49
1	O	304	GLN	CA-C-N	5.57	132.17	121.54
1	O	304	GLN	C-N-CA	5.57	132.17	121.54
1	I	67	THR	N-CA-CB	5.56	119.89	110.49
1	E	343	LEU	CA-C-N	5.55	126.10	119.94
1	E	343	LEU	C-N-CA	5.55	126.10	119.94
1	M	298	HIS	CA-CB-CG	5.55	119.35	113.80
1	C	141	PRO	CA-C-O	-5.54	116.91	120.90
1	A	124	VAL	N-CA-C	5.54	115.74	110.42
2	F	81	ASN	CA-CB-CG	-5.54	107.06	112.60
1	G	115	ASN	CA-CB-CG	5.52	118.12	112.60
1	A	67	THR	N-CA-CB	5.52	119.82	110.49
1	O	113	VAL	N-CA-C	5.51	116.29	110.72
1	O	124	VAL	N-CA-C	5.51	115.71	110.42
1	K	350	ARG	N-CA-C	5.50	117.08	111.14
1	K	217	ARG	CA-C-N	5.49	127.63	120.28
1	K	217	ARG	C-N-CA	5.49	127.63	120.28
1	G	262	VAL	N-CA-C	5.48	114.98	108.96
1	K	398	ALA	O-C-N	-5.48	115.31	122.59
2	B	166	PHE	O-C-N	-5.47	116.41	122.86
1	O	217	ARG	CA-C-N	5.46	127.60	120.28
1	O	217	ARG	C-N-CA	5.46	127.60	120.28
1	I	398	ALA	O-C-N	-5.46	115.33	122.59
1	M	398	ALA	O-C-N	-5.46	115.33	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	155	ILE	N-CA-C	5.46	116.19	110.62
1	C	31	VAL	N-CA-C	5.45	118.39	109.78
1	O	325	HIS	CA-CB-CG	5.44	119.24	113.80
1	E	253	ARG	NE-CZ-NH1	5.43	126.93	121.50
2	P	130	ASP	CA-CB-CG	5.42	118.03	112.60
1	O	352	ASP	CA-CB-CG	5.41	118.01	112.60
2	N	108	VAL	CA-C-N	5.40	131.42	121.70
2	N	108	VAL	C-N-CA	5.40	131.42	121.70
1	G	368	TRP	N-CA-C	5.40	122.30	110.80
1	I	436	ASP	CA-C-N	5.40	127.78	120.38
1	I	436	ASP	C-N-CA	5.40	127.78	120.38
1	A	353	TYR	N-CA-C	5.38	117.75	111.02
2	L	166	PHE	O-C-N	-5.37	116.52	122.86
1	I	298	HIS	N-CA-C	5.36	117.12	111.28
1	M	81	LYS	CA-C-N	5.34	125.05	119.92
1	M	81	LYS	C-N-CA	5.34	125.05	119.92
2	H	110	CYS	N-CA-C	5.33	118.55	111.30
1	I	105	ILE	CA-C-N	5.33	127.96	120.28
1	I	105	ILE	C-N-CA	5.33	127.96	120.28
1	I	157	VAL	CA-C-N	5.31	127.83	120.29
1	I	157	VAL	C-N-CA	5.31	127.83	120.29
1	G	67	THR	N-CA-CB	5.30	119.45	110.49
1	K	230	ALA	N-CA-C	5.30	117.06	111.28
1	E	242	ALA	N-CA-C	5.29	122.07	110.80
1	M	368	TRP	N-CA-C	5.29	122.07	110.80
1	C	311	PHE	N-CA-C	5.29	117.04	111.28
1	A	105	ILE	CA-C-N	5.28	128.09	120.38
1	A	105	ILE	C-N-CA	5.28	128.09	120.38
1	M	327	HIS	CA-CB-CG	5.28	119.08	113.80
2	L	108	VAL	CA-C-N	5.28	131.19	121.70
2	L	108	VAL	C-N-CA	5.28	131.19	121.70
2	N	64	PRO	CA-C-O	-5.28	117.10	120.90
1	K	291	LEU	N-CA-C	5.27	117.25	108.02
1	O	141	PRO	CA-C-O	-5.27	117.10	120.90
2	H	108	VAL	CA-C-N	5.27	131.18	121.70
2	H	108	VAL	C-N-CA	5.27	131.18	121.70
1	A	205	ASN	CA-CB-CG	-5.26	107.34	112.60
1	M	217	ARG	CA-C-N	5.26	127.33	120.28
1	M	217	ARG	C-N-CA	5.26	127.33	120.28
1	G	298	HIS	N-CA-C	5.26	117.01	111.28
1	A	144	TYR	N-CA-C	-5.25	107.00	113.41
1	I	205	ASN	CA-CB-CG	-5.25	107.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	304	GLN	CA-C-N	5.25	131.56	121.54
1	E	304	GLN	C-N-CA	5.25	131.56	121.54
2	H	166	PHE	O-C-N	-5.25	116.67	122.86
1	M	67	THR	N-CA-CB	5.25	119.36	110.49
1	O	241	ASN	CA-CB-CG	5.24	117.84	112.60
1	I	368	TRP	N-CA-C	5.24	121.96	110.80
1	I	298	HIS	CA-CB-CG	5.24	119.04	113.80
1	E	302	ASP	CA-CB-CG	5.23	117.83	112.60
2	F	108	VAL	CA-C-N	5.23	131.12	121.70
2	F	108	VAL	C-N-CA	5.23	131.12	121.70
1	M	207	ASN	CA-CB-CG	5.23	117.83	112.60
1	C	230	ALA	N-CA-C	5.23	116.98	111.28
1	A	216	ASP	CA-CB-CG	-5.22	107.38	112.60
1	C	167	ARG	N-CA-C	-5.22	100.81	108.79
1	K	387	MET	CA-C-N	5.21	124.66	119.24
1	K	387	MET	C-N-CA	5.21	124.66	119.24
1	E	205	ASN	CA-CB-CG	-5.21	107.39	112.60
1	E	67	THR	N-CA-CB	5.20	119.28	110.49
1	G	325	HIS	CA-CB-CG	5.20	119.00	113.80
2	N	110	CYS	N-CA-C	5.20	118.37	111.30
1	M	387	MET	CA-C-N	5.20	124.64	119.24
1	M	387	MET	C-N-CA	5.20	124.64	119.24
1	E	325	HIS	CA-CB-CG	5.19	118.99	113.80
1	E	161	LYS	N-CA-C	5.18	116.93	111.28
1	G	343	LEU	N-CA-C	-5.17	105.26	112.45
2	P	144	ALA	N-CA-C	5.16	116.99	111.36
1	O	368	TRP	N-CA-C	5.16	121.79	110.80
1	A	368	TRP	N-CA-C	5.16	121.78	110.80
1	O	437	LEU	N-CA-C	5.15	116.89	111.28
1	C	325	HIS	CA-CB-CG	5.15	118.95	113.80
2	L	166	PHE	CA-C-N	5.13	130.94	121.70
2	L	166	PHE	C-N-CA	5.13	130.94	121.70
1	G	242	ALA	N-CA-C	5.13	121.73	110.80
1	M	253	ARG	NE-CZ-NH1	5.13	126.63	121.50
1	I	291	LEU	N-CA-C	5.13	116.99	108.02
1	K	229	GLN	N-CA-C	5.13	119.42	112.04
1	C	302	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	311	PHE	CA-CB-CG	-5.12	108.68	113.80
1	C	356	LYS	N-CA-C	5.12	117.31	110.35
1	C	368	TRP	N-CA-C	5.12	121.71	110.80
1	M	140	ILE	CA-C-N	5.12	123.34	119.66
1	M	140	ILE	C-N-CA	5.12	123.34	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	67	THR	N-CA-CB	5.11	119.13	110.49
1	C	182	ALA	N-CA-C	5.11	116.85	111.28
1	G	304	GLN	CA-C-N	5.11	131.29	121.54
1	G	304	GLN	C-N-CA	5.11	131.29	121.54
1	K	157	VAL	CA-C-N	5.10	127.53	120.29
1	K	157	VAL	C-N-CA	5.10	127.53	120.29
1	C	436	ASP	CA-C-N	5.10	127.11	120.28
1	C	436	ASP	C-N-CA	5.10	127.11	120.28
1	C	336	GLU	N-CA-C	5.09	117.10	110.43
1	K	115	ASN	CA-CB-CG	5.09	117.69	112.60
1	M	161	LYS	N-CA-C	5.09	116.83	111.28
1	C	298	HIS	N-CA-C	5.09	117.49	111.33
1	E	255	VAL	N-CA-CB	5.09	119.06	110.56
1	G	140	ILE	CA-C-N	5.09	123.33	119.66
1	G	140	ILE	C-N-CA	5.09	123.33	119.66
1	M	304	GLN	CA-C-N	5.09	131.26	121.54
1	M	304	GLN	C-N-CA	5.09	131.26	121.54
1	A	217	ARG	CA-C-N	5.08	127.09	120.28
1	A	217	ARG	C-N-CA	5.08	127.09	120.28
1	G	291	LEU	N-CA-C	5.08	116.91	108.02
2	H	166	PHE	CA-C-N	5.08	130.84	121.70
2	H	166	PHE	C-N-CA	5.08	130.84	121.70
1	I	301	ILE	CA-C-N	5.08	127.08	120.28
1	I	301	ILE	C-N-CA	5.08	127.08	120.28
1	K	124	VAL	N-CA-C	5.08	115.30	110.42
1	K	287	ASN	CA-CB-CG	-5.08	107.53	112.60
1	A	436	ASP	CA-C-N	5.07	127.33	120.38
1	A	436	ASP	C-N-CA	5.07	127.33	120.38
1	I	161	LYS	N-CA-C	5.07	116.80	111.28
1	A	229	GLN	N-CA-C	5.06	119.33	112.04
1	A	304	GLN	CA-C-N	5.06	131.20	121.54
1	A	304	GLN	C-N-CA	5.06	131.20	121.54
2	F	108	VAL	O-C-N	-5.06	117.30	122.82
1	A	253	ARG	NE-CZ-NH1	5.05	126.56	121.50
1	K	304	GLN	CA-C-N	5.05	131.19	121.54
1	K	304	GLN	C-N-CA	5.05	131.19	121.54
1	I	141	PRO	CA-C-O	-5.04	116.75	120.73
2	N	108	VAL	O-C-N	-5.04	117.32	122.82
1	G	182	ALA	N-CA-C	5.03	116.77	111.28
1	M	393	ILE	N-CA-C	5.03	115.26	110.53
1	K	105	ILE	CA-C-N	5.03	127.52	120.28
1	K	105	ILE	C-N-CA	5.03	127.52	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	108	VAL	O-C-N	-5.03	117.34	123.02
1	G	94	ASP	N-CA-C	5.03	116.76	111.28
1	M	298	HIS	N-CA-C	5.02	116.75	111.28
1	O	355	GLU	N-CA-C	5.02	117.58	110.50
1	K	141	PRO	CA-C-O	-5.02	117.29	120.90
1	K	356	LYS	N-CA-C	5.02	117.51	110.23
1	M	157	VAL	CA-C-N	5.01	127.41	120.29
1	M	157	VAL	C-N-CA	5.01	127.41	120.29
1	I	304	GLN	CA-C-N	5.01	131.10	121.54
1	I	304	GLN	C-N-CA	5.01	131.10	121.54
2	J	166	PHE	CA-C-N	5.01	130.71	121.70
2	J	166	PHE	C-N-CA	5.01	130.71	121.70
1	E	327	HIS	CA-CB-CG	5.00	118.81	113.80
1	C	15	ALA	N-CA-C	5.00	116.75	110.24
1	C	81	LYS	CA-C-N	5.00	124.85	120.10
1	C	81	LYS	C-N-CA	5.00	124.85	120.10

There are no chirality outliers.

All (161) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	ARG	Sidechain
1	A	147	THR	Peptide
1	A	178	LEU	Peptide
1	A	215	ARG	Sidechain
1	A	228	ALA	Peptide
1	A	236	LYS	Peptide
1	A	263	PRO	Peptide
1	A	268	ASP	Peptide
1	A	269	TYR	Sidechain
1	A	320	MET	Peptide
1	A	327	HIS	Peptide
1	A	367	ASP	Peptide
1	A	374	VAL	Peptide
1	A	379	SER	Peptide
1	A	383	HIS	Peptide
1	A	396	ASP	Peptide
1	A	421	ARG	Sidechain
1	A	451	TRP	Peptide
1	A	83	ARG	Sidechain
2	B	129	ARG	Sidechain
1	C	147	THR	Peptide

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Mol	Chain	Res	Type	Group
1	C	178	LEU	Peptide
1	C	215	ARG	Sidechain
1	C	228	ALA	Peptide
1	C	241	ASN	Peptide
1	C	263	PRO	Peptide
1	C	268	ASP	Peptide
1	C	305	ARG	Sidechain
1	C	320	MET	Peptide
1	C	327	HIS	Peptide
1	C	367	ASP	Peptide
1	C	379	SER	Peptide
1	C	383	HIS	Peptide
1	C	396	ASP	Peptide
1	C	421	ARG	Sidechain
1	C	451	TRP	Peptide
2	D	129	ARG	Sidechain
1	E	139	ARG	Sidechain
1	E	147	THR	Peptide
1	E	178	LEU	Peptide
1	E	194	ARG	Sidechain
1	E	215	ARG	Sidechain
1	E	228	ALA	Peptide
1	E	241	ASN	Peptide
1	E	263	PRO	Peptide
1	E	268	ASP	Peptide
1	E	269	TYR	Sidechain
1	E	320	MET	Peptide
1	E	327	HIS	Sidechain,Peptide
1	E	363	TYR	Sidechain
1	E	367	ASP	Peptide
1	E	374	VAL	Peptide
1	E	379	SER	Peptide
1	E	383	HIS	Peptide
1	E	396	ASP	Peptide
1	E	451	TRP	Peptide
2	F	129	ARG	Sidechain
1	G	139	ARG	Sidechain
1	G	147	THR	Peptide
1	G	178	LEU	Peptide
1	G	228	ALA	Peptide
1	G	241	ASN	Peptide
1	G	254	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	G	263	PRO	Peptide
1	G	268	ASP	Peptide
1	G	269	TYR	Sidechain
1	G	320	MET	Peptide
1	G	327	HIS	Peptide
1	G	363	TYR	Sidechain
1	G	367	ASP	Peptide
1	G	379	SER	Peptide
1	G	383	HIS	Peptide
1	G	396	ASP	Peptide
1	G	451	TRP	Peptide
1	G	83	ARG	Sidechain
2	H	117	TYR	Sidechain
2	H	129	ARG	Sidechain
1	I	147	THR	Peptide
1	I	178	LEU	Peptide
1	I	194	ARG	Sidechain
1	I	215	ARG	Sidechain
1	I	228	ALA	Peptide
1	I	241	ASN	Peptide
1	I	254	ALA	Mainchain
1	I	263	PRO	Peptide
1	I	268	ASP	Peptide
1	I	269	TYR	Sidechain
1	I	312	ARG	Sidechain
1	I	320	MET	Peptide
1	I	327	HIS	Peptide
1	I	367	ASP	Peptide
1	I	379	SER	Peptide
1	I	383	HIS	Peptide
1	I	396	ASP	Peptide
1	I	446	ARG	Sidechain
1	I	451	TRP	Peptide
1	I	83	ARG	Sidechain
2	J	129	ARG	Sidechain
1	K	139	ARG	Sidechain
1	K	147	THR	Peptide
1	K	178	LEU	Peptide
1	K	194	ARG	Sidechain
1	K	215	ARG	Sidechain
1	K	228	ALA	Peptide
1	K	241	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	K	263	PRO	Peptide
1	K	268	ASP	Peptide
1	K	269	TYR	Sidechain
1	K	320	MET	Peptide
1	K	327	HIS	Peptide
1	K	367	ASP	Peptide
1	K	379	SER	Peptide
1	K	383	HIS	Peptide
1	K	396	ASP	Peptide
1	K	451	TRP	Peptide
1	K	80	TYR	Sidechain
1	K	83	ARG	Sidechain
2	L	117	TYR	Sidechain
2	L	129	ARG	Sidechain
1	M	100	TYR	Sidechain
1	M	147	THR	Peptide
1	M	159	ARG	Sidechain
1	M	178	LEU	Peptide
1	M	215	ARG	Sidechain
1	M	228	ALA	Peptide
1	M	241	ASN	Peptide
1	M	263	PRO	Peptide
1	M	268	ASP	Peptide
1	M	269	TYR	Sidechain
1	M	320	MET	Peptide
1	M	327	HIS	Peptide
1	M	367	ASP	Peptide
1	M	379	SER	Peptide
1	M	383	HIS	Peptide
1	M	396	ASP	Peptide
1	M	41	ARG	Sidechain
1	M	451	TRP	Peptide
2	N	129	ARG	Sidechain
2	N	170	ARG	Sidechain
1	O	139	ARG	Sidechain
1	O	147	THR	Peptide
1	O	178	LEU	Peptide
1	O	194	ARG	Sidechain
1	O	215	ARG	Sidechain
1	O	228	ALA	Peptide
1	O	241	ASN	Peptide
1	O	263	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	O	268	ASP	Peptide
1	O	269	TYR	Sidechain
1	O	320	MET	Peptide
1	O	327	HIS	Peptide
1	O	367	ASP	Peptide
1	O	379	SER	Peptide
1	O	383	HIS	Peptide
1	O	396	ASP	Peptide
1	O	421	ARG	Sidechain
1	O	451	TRP	Peptide
1	O	83	ARG	Sidechain
2	P	129	ARG	Sidechain
2	P	170	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3647	0	3570	1	0
1	C	3647	0	3570	2	0
1	E	3647	0	3570	2	0
1	G	3647	0	3570	2	0
1	I	3647	0	3570	4	0
1	K	3647	0	3570	4	0
1	M	3647	0	3570	3	0
1	O	3647	0	3570	1	0
2	B	1080	0	1052	0	0
2	D	1080	0	1052	0	0
2	F	1080	0	1052	0	0
2	H	1080	0	1052	0	0
2	J	1080	0	1052	1	0
2	L	1080	0	1052	0	0
2	N	1080	0	1052	0	0
2	P	1080	0	1052	0	0
All	All	37816	0	36976	19	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 0.

All (19) 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:E:307:HIS:CE1	1:G:307:HIS:CE1	2.99	0.51
1:I:202:ASP:OD2	1:I:238:HIS:HE1	1.97	0.48
1:M:298:HIS:CE1	1:M:303:ARG:HD2	2.50	0.47
1:G:298:HIS:CE1	1:G:303:ARG:HD2	2.50	0.47
1:I:298:HIS:CE1	1:I:303:ARG:HD2	2.51	0.46
1:M:267:HIS:CD2	1:M:269:TYR:CD1	3.03	0.46
1:K:267:HIS:CD2	1:K:269:TYR:CD1	3.04	0.46
1:O:298:HIS:CE1	1:O:303:ARG:HD2	2.53	0.44
1:I:204:GLU:H	1:I:204:GLU:CD	2.26	0.44
1:C:298:HIS:CE1	1:C:303:ARG:HD2	2.52	0.44
1:C:267:HIS:CD2	1:C:269:TYR:CD1	3.07	0.43
1:K:156:GLN:CD	1:K:156:GLN:H	2.26	0.43
1:K:298:HIS:CE1	1:K:303:ARG:HD2	2.54	0.43
2:J:83:TRP:CZ3	2:J:156:ASP:HB2	2.55	0.42
1:I:202:ASP:OD2	1:I:238:HIS:CE1	2.73	0.41
1:K:366:GLN:H	1:K:366:GLN:CD	2.28	0.41
1:A:366:GLN:CD	1:A:366:GLN:H	2.30	0.40
1:E:298:HIS:CE1	1:E:303:ARG:HD2	2.56	0.40
1:M:366:GLN:H	1:M:366:GLN:CD	2.29	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	467/469 (100%)	420 (90%)	33 (7%)	14 (3%)	3	23
1	C	467/469 (100%)	420 (90%)	30 (6%)	17 (4%)	2	20
1	E	467/469 (100%)	418 (90%)	36 (8%)	13 (3%)	4	24
1	G	467/469 (100%)	419 (90%)	33 (7%)	15 (3%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	467/469 (100%)	416 (89%)	36 (8%)	15 (3%)	3	21
1	K	467/469 (100%)	425 (91%)	28 (6%)	14 (3%)	3	23
1	M	467/469 (100%)	420 (90%)	33 (7%)	14 (3%)	3	23
1	O	467/469 (100%)	418 (90%)	34 (7%)	15 (3%)	3	21
2	B	130/132 (98%)	118 (91%)	10 (8%)	2 (2%)	8	40
2	D	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	16	54
2	F	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	16	54
2	H	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
2	J	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	16	54
2	L	130/132 (98%)	118 (91%)	11 (8%)	1 (1%)	16	54
2	N	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
2	P	130/132 (98%)	120 (92%)	8 (6%)	2 (2%)	8	40
All	All	4776/4808 (99%)	4314 (90%)	337 (7%)	125 (3%)	6	25

All (125) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ALA
1	A	67	THR
1	A	78	ASP
1	A	269	TYR
1	A	305	ARG
1	A	368	TRP
1	A	370	SER
1	C	9	ALA
1	C	67	THR
1	C	78	ASP
1	C	269	TYR
1	C	305	ARG
1	C	368	TRP
1	E	9	ALA
1	E	67	THR
1	E	78	ASP
1	E	242	ALA
1	E	269	TYR
1	E	305	ARG
1	E	368	TRP
1	E	370	SER

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Mol	Chain	Res	Type
1	G	9	ALA
1	G	67	THR
1	G	269	TYR
1	G	305	ARG
1	G	368	TRP
1	G	370	SER
1	I	9	ALA
1	I	67	THR
1	I	78	ASP
1	I	269	TYR
1	I	305	ARG
1	I	368	TRP
1	I	370	SER
1	K	9	ALA
1	K	78	ASP
1	K	269	TYR
1	K	305	ARG
1	K	368	TRP
1	M	9	ALA
1	M	67	THR
1	M	78	ASP
1	M	269	TYR
1	M	305	ARG
1	M	368	TRP
1	O	9	ALA
1	O	67	THR
1	O	78	ASP
1	O	269	TYR
1	O	305	ARG
1	O	368	TRP
1	A	154	GLY
1	A	328	SER
1	A	329	GLY
1	C	243	THR
1	C	328	SER
1	C	329	GLY
1	E	154	GLY
1	G	78	ASP
1	G	154	GLY
1	G	328	SER
1	G	329	GLY
1	I	165	TYR

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Mol	Chain	Res	Type
1	I	329	GLY
1	K	328	SER
1	K	329	GLY
1	K	369	CYS
1	M	328	SER
1	M	329	GLY
1	O	154	GLY
1	O	328	SER
1	O	329	GLY
1	C	370	SER
2	D	50	THR
1	E	127	PHE
1	E	148	PHE
1	E	165	TYR
1	G	127	PHE
1	I	154	GLY
1	I	369	CYS
1	K	67	THR
1	K	148	PHE
1	K	154	GLY
1	K	289	LEU
1	M	154	GLY
1	M	165	TYR
1	M	297	MET
1	O	165	TYR
1	O	243	THR
1	O	297	MET
1	A	148	PHE
1	C	154	GLY
1	C	289	LEU
1	C	297	MET
1	C	406	THR
1	E	297	MET
1	G	242	ALA
1	I	264	ILE
1	I	289	LEU
1	I	328	SER
1	M	148	PHE
1	O	148	PHE
2	P	175	ARG
1	A	126	GLY
1	A	127	PHE

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Mol	Chain	Res	Type
2	B	175	ARG
1	C	148	PHE
1	G	126	GLY
1	G	289	LEU
2	L	50	THR
2	P	50	THR
1	A	289	LEU
1	C	126	GLY
1	C	369	CYS
2	F	50	THR
1	G	264	ILE
1	I	126	GLY
1	K	126	GLY
1	O	126	GLY
1	O	264	ILE
2	B	50	THR
2	J	50	THR
1	M	126	GLY
1	K	331	VAL
1	M	263	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	375/375 (100%)	362 (96%)	13 (4%)	32	53
1	C	375/375 (100%)	359 (96%)	16 (4%)	26	47
1	E	375/375 (100%)	362 (96%)	13 (4%)	32	53
1	G	375/375 (100%)	364 (97%)	11 (3%)	37	58
1	I	375/375 (100%)	361 (96%)	14 (4%)	30	51
1	K	375/375 (100%)	358 (96%)	17 (4%)	24	46
1	M	375/375 (100%)	363 (97%)	12 (3%)	34	56
1	O	375/375 (100%)	363 (97%)	12 (3%)	34	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	116/116 (100%)	114 (98%)	2 (2%)	53	69
2	D	116/116 (100%)	112 (97%)	4 (3%)	32	54
2	F	116/116 (100%)	112 (97%)	4 (3%)	32	54
2	H	116/116 (100%)	115 (99%)	1 (1%)	70	79
2	J	116/116 (100%)	114 (98%)	2 (2%)	53	69
2	L	116/116 (100%)	111 (96%)	5 (4%)	26	47
2	N	116/116 (100%)	112 (97%)	4 (3%)	32	54
2	P	116/116 (100%)	112 (97%)	4 (3%)	32	54
All	All	3928/3928 (100%)	3794 (97%)	134 (3%)	33	54

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	THR
1	A	79	ARG
1	A	156	GLN
1	A	158	GLU
1	A	159	ARG
1	A	183	LYS
1	A	204	GLU
1	A	223	GLU
1	A	241	ASN
1	A	270	LEU
1	A	292	HIS
1	A	302	ASP
1	A	374	VAL
2	B	50	THR
2	B	58	GLU
1	C	68	THR
1	C	79	ARG
1	C	156	GLN
1	C	158	GLU
1	C	159	ARG
1	C	183	LYS
1	C	204	GLU
1	C	223	GLU
1	C	243	THR
1	C	246	THR
1	C	267	HIS

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Mol	Chain	Res	Type
1	C	270	LEU
1	C	292	HIS
1	C	302	ASP
1	C	371	MET
1	C	374	VAL
2	D	50	THR
2	D	58	GLU
2	D	78	ILE
2	D	99	ASN
1	E	79	ARG
1	E	156	GLN
1	E	158	GLU
1	E	159	ARG
1	E	183	LYS
1	E	201	LYS
1	E	204	GLU
1	E	246	THR
1	E	270	LEU
1	E	292	HIS
1	E	302	ASP
1	E	371	MET
1	E	374	VAL
2	F	50	THR
2	F	58	GLU
2	F	78	ILE
2	F	99	ASN
1	G	79	ARG
1	G	158	GLU
1	G	159	ARG
1	G	183	LYS
1	G	204	GLU
1	G	223	GLU
1	G	243	THR
1	G	270	LEU
1	G	302	ASP
1	G	371	MET
1	G	374	VAL
2	H	58	GLU
1	I	79	ARG
1	I	158	GLU
1	I	159	ARG
1	I	183	LYS

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Mol	Chain	Res	Type
1	I	201	LYS
1	I	204	GLU
1	I	243	THR
1	I	258	LYS
1	I	270	LEU
1	I	292	HIS
1	I	302	ASP
1	I	371	MET
1	I	374	VAL
1	I	382	ILE
2	J	50	THR
2	J	58	GLU
1	K	43	THR
1	K	63	THR
1	K	79	ARG
1	K	156	GLN
1	K	158	GLU
1	K	183	LYS
1	K	204	GLU
1	K	223	GLU
1	K	241	ASN
1	K	243	THR
1	K	246	THR
1	K	270	LEU
1	K	292	HIS
1	K	302	ASP
1	K	327	HIS
1	K	371	MET
1	K	374	VAL
2	L	50	THR
2	L	58	GLU
2	L	78	ILE
2	L	99	ASN
2	L	173	THR
1	M	79	ARG
1	M	158	GLU
1	M	183	LYS
1	M	204	GLU
1	M	243	THR
1	M	246	THR
1	M	258	LYS
1	M	267	HIS

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Mol	Chain	Res	Type
1	M	270	LEU
1	M	302	ASP
1	M	371	MET
1	M	374	VAL
2	N	58	GLU
2	N	78	ILE
2	N	99	ASN
2	N	173	THR
1	O	68	THR
1	O	79	ARG
1	O	158	GLU
1	O	159	ARG
1	O	183	LYS
1	O	204	GLU
1	O	223	GLU
1	O	243	THR
1	O	267	HIS
1	O	292	HIS
1	O	371	MET
1	O	374	VAL
2	P	50	THR
2	P	58	GLU
2	P	78	ILE
2	P	99	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	184	ASN
1	A	241	ASN
2	B	74	GLN
2	B	99	ASN
1	C	95	ASN
1	C	267	HIS
1	C	294	HIS
1	C	306	ASN
1	C	386	HIS
2	D	99	ASN
2	D	158	GLN
1	E	184	ASN
1	E	386	HIS

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Mol	Chain	Res	Type
1	G	298	HIS
1	G	386	HIS
1	G	429	GLN
2	H	74	GLN
2	H	160	GLN
1	I	386	HIS
1	I	432	ASN
2	J	99	ASN
1	K	241	ASN
1	K	267	HIS
1	K	292	HIS
1	K	294	HIS
1	K	298	HIS
1	K	386	HIS
2	L	74	GLN
2	L	99	ASN
2	L	160	GLN
1	M	292	HIS
1	M	294	HIS
1	M	298	HIS
1	M	307	HIS
1	M	432	ASN
2	N	99	ASN
1	O	207	ASN
1	O	294	HIS
1	O	306	ASN
1	O	386	HIS
2	P	74	GLN
2	P	99	ASN

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.

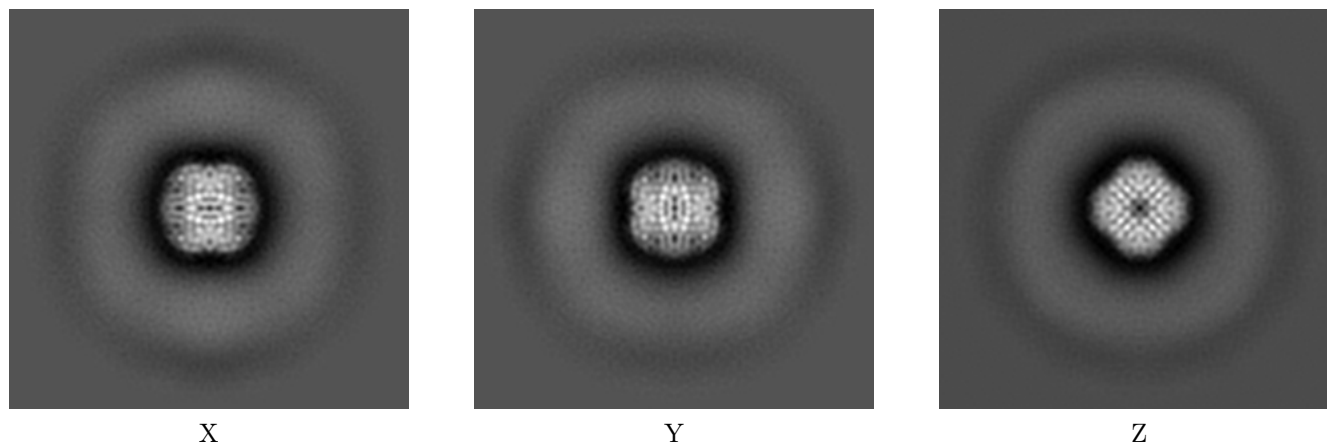
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52438. These allow visual inspection of the internal detail of the map and identification of artifacts.

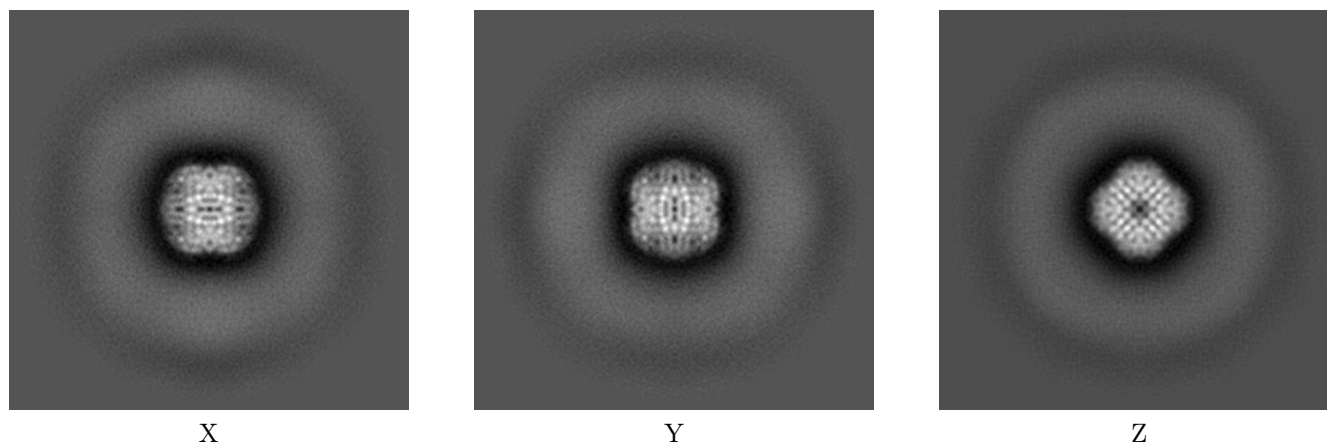
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



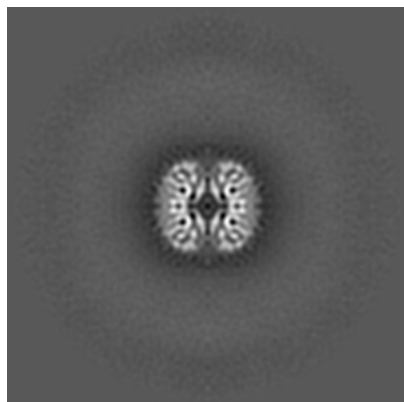
6.1.2 Raw map



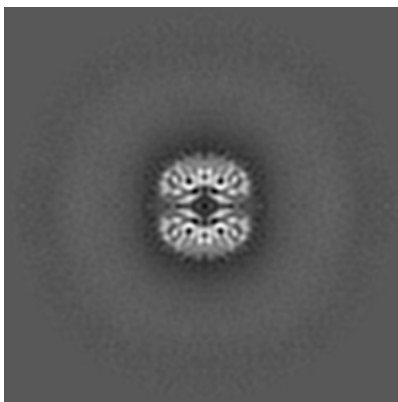
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

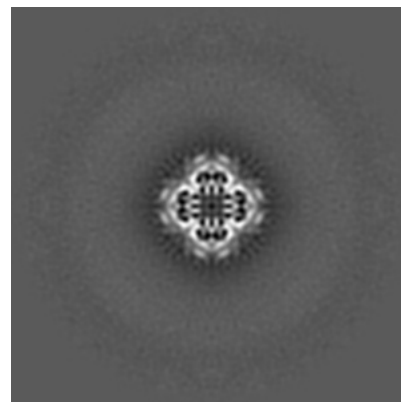
6.2.1 Primary map



X Index: 128

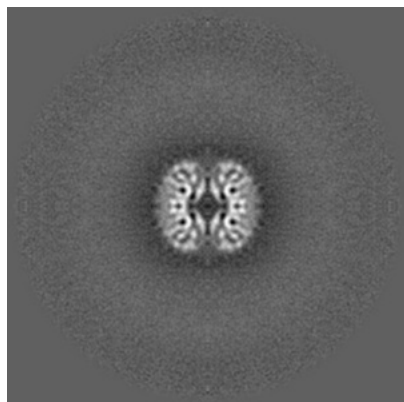


Y Index: 128

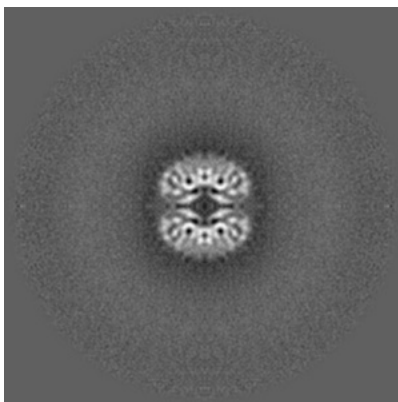


Z Index: 128

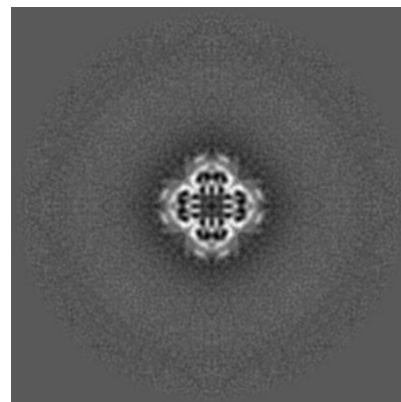
6.2.2 Raw map



X Index: 128



Y Index: 128

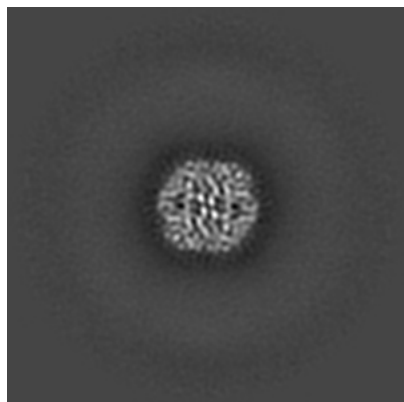


Z Index: 128

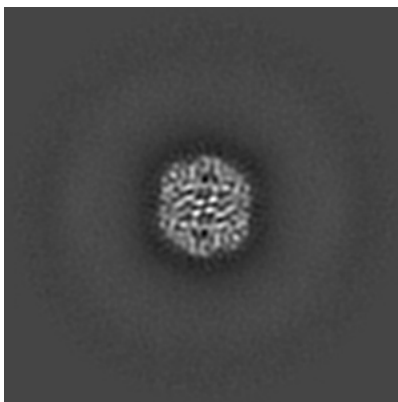
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

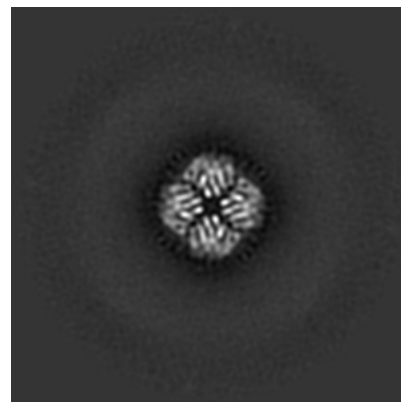
6.3.1 Primary map



X Index: 120

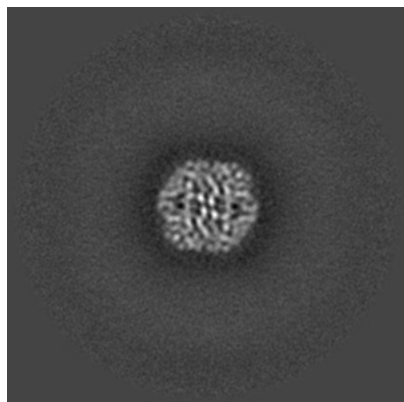


Y Index: 120

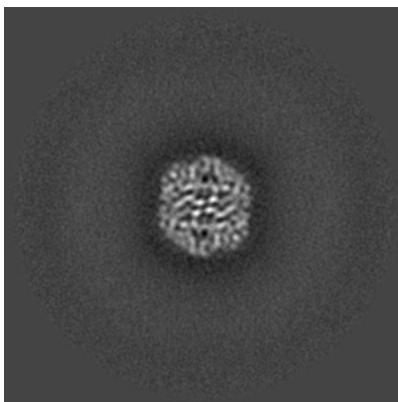


Z Index: 125

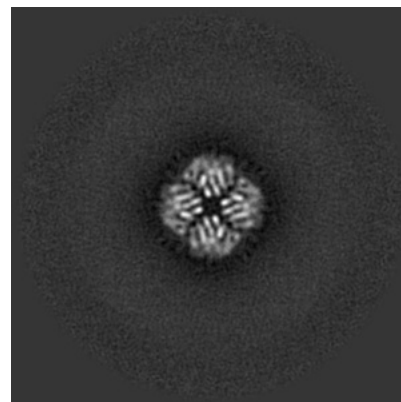
6.3.2 Raw map



X Index: 120



Y Index: 120

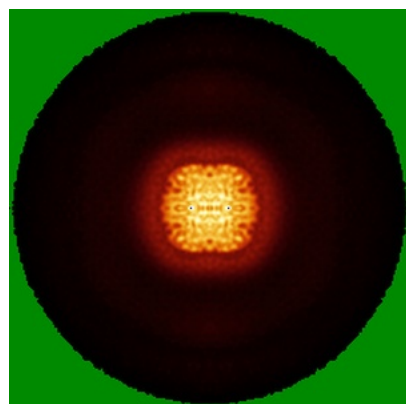


Z Index: 125

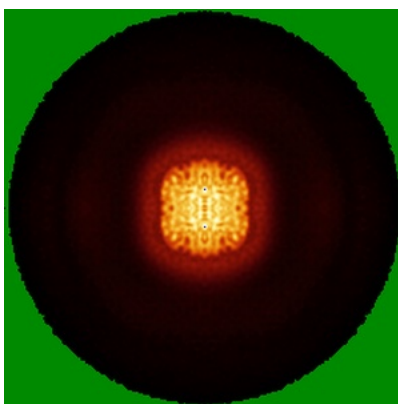
The images above show the largest variance slices of the map in three orthogonal directions.

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

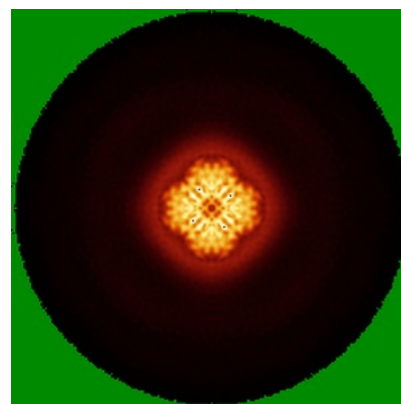
6.4.1 Primary map



X

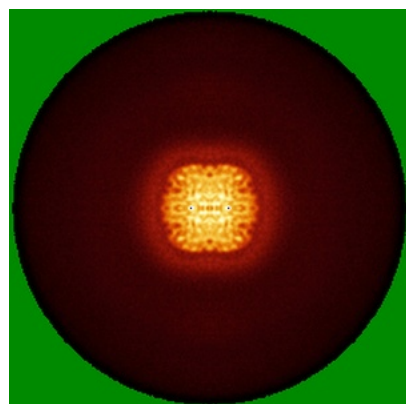


Y

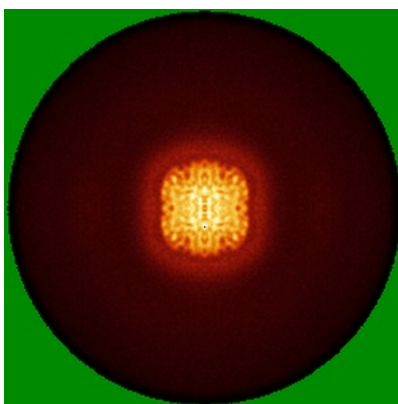


Z

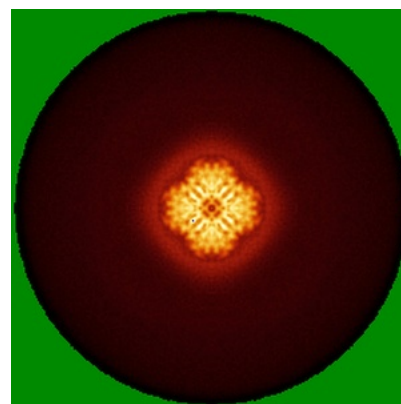
6.4.2 Raw map



X



Y

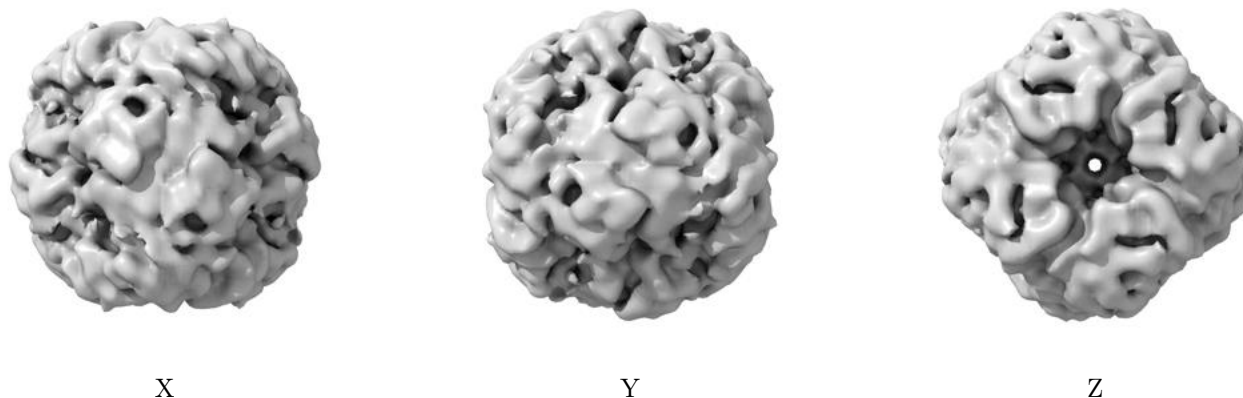


Z

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.

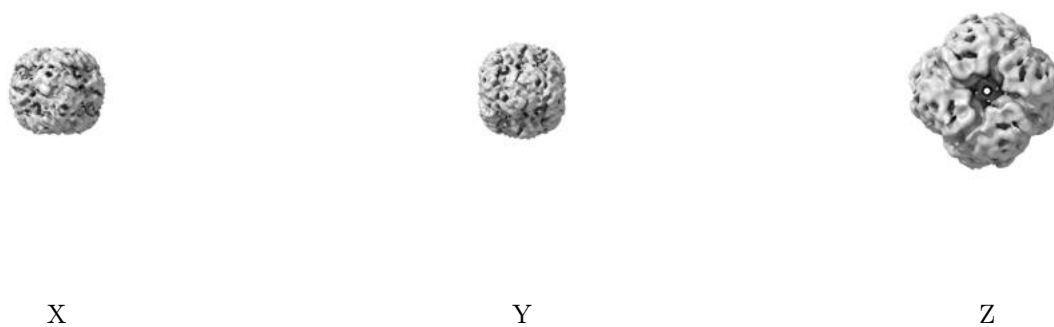
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

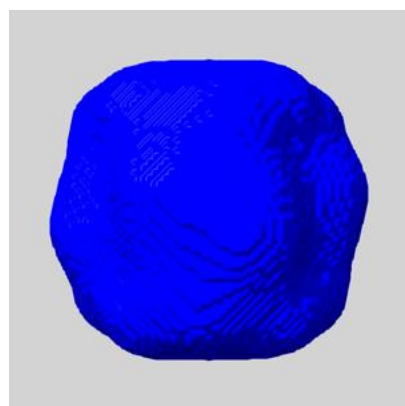
6.6 Mask visualisation [i](#)

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

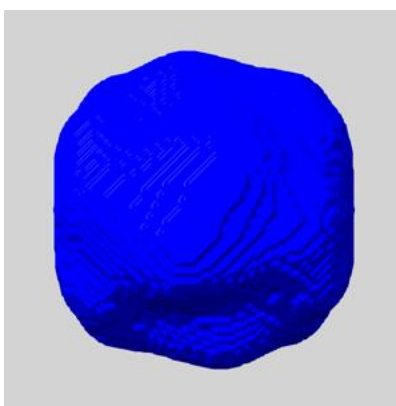
A mask typically either:

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

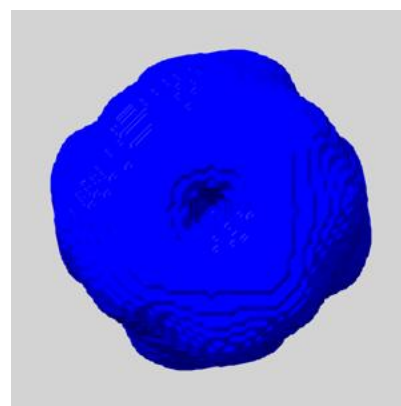
6.6.1 emd_52438_msk_1.map [i](#)



X



Y

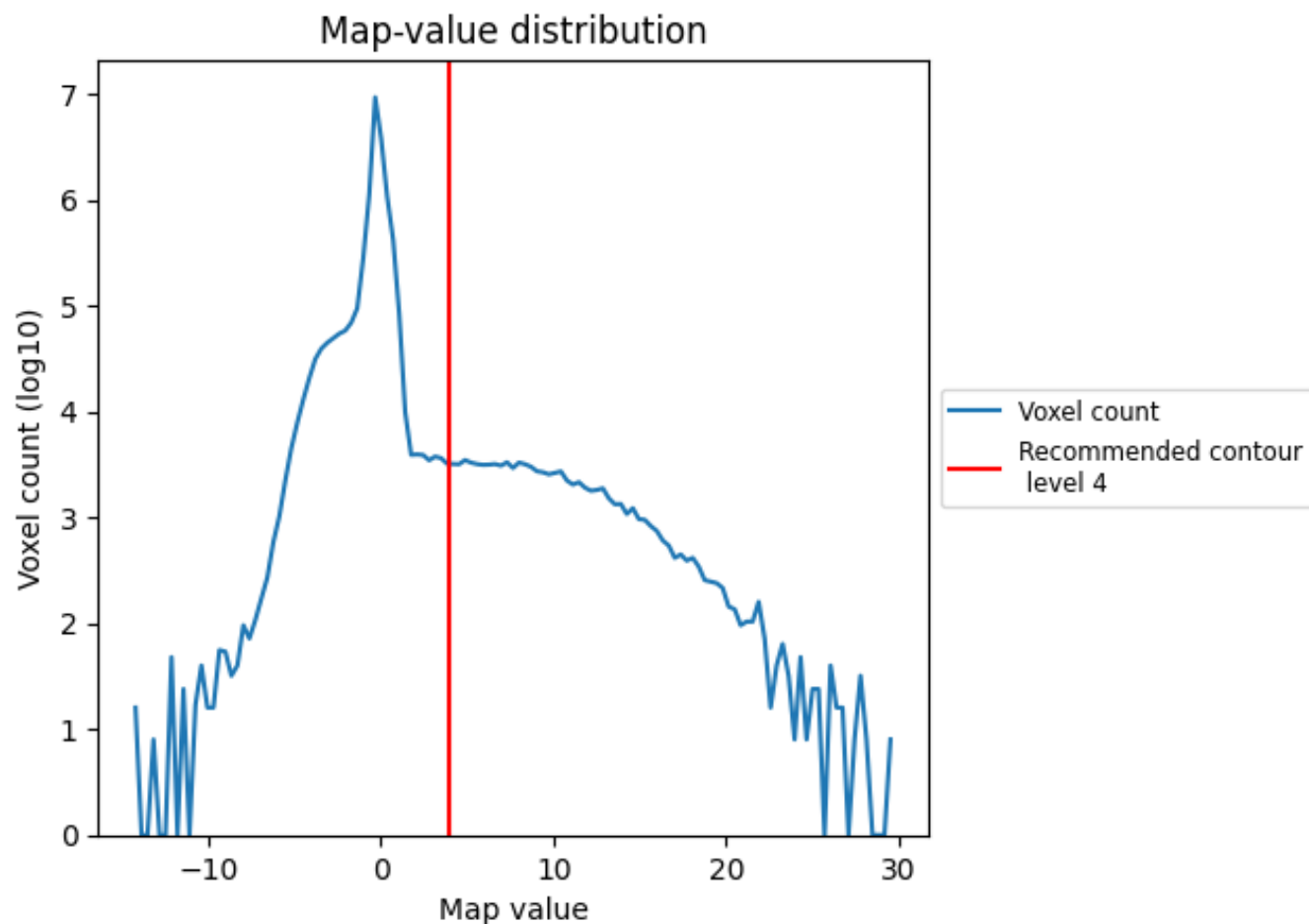


Z

7 Map analysis [i](#)

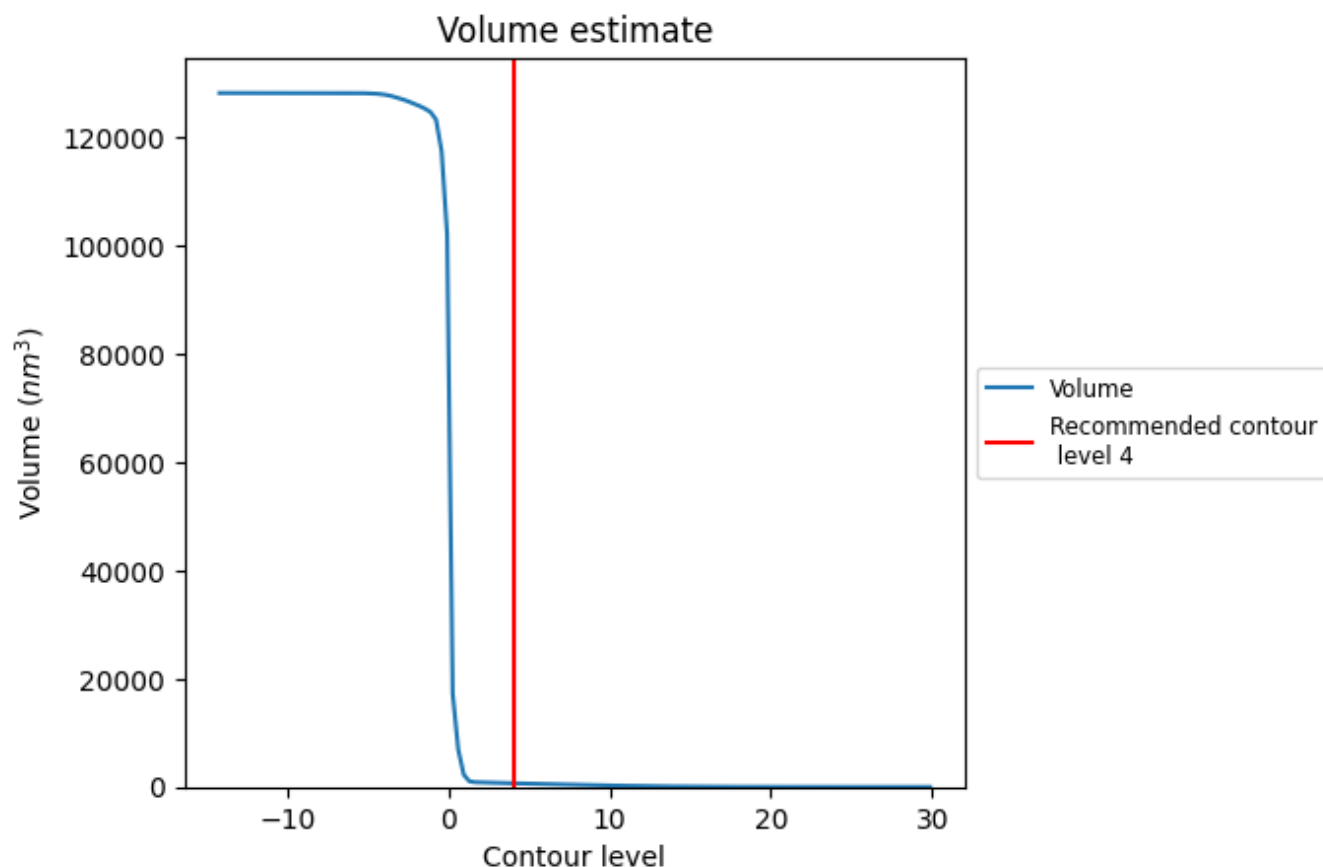
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

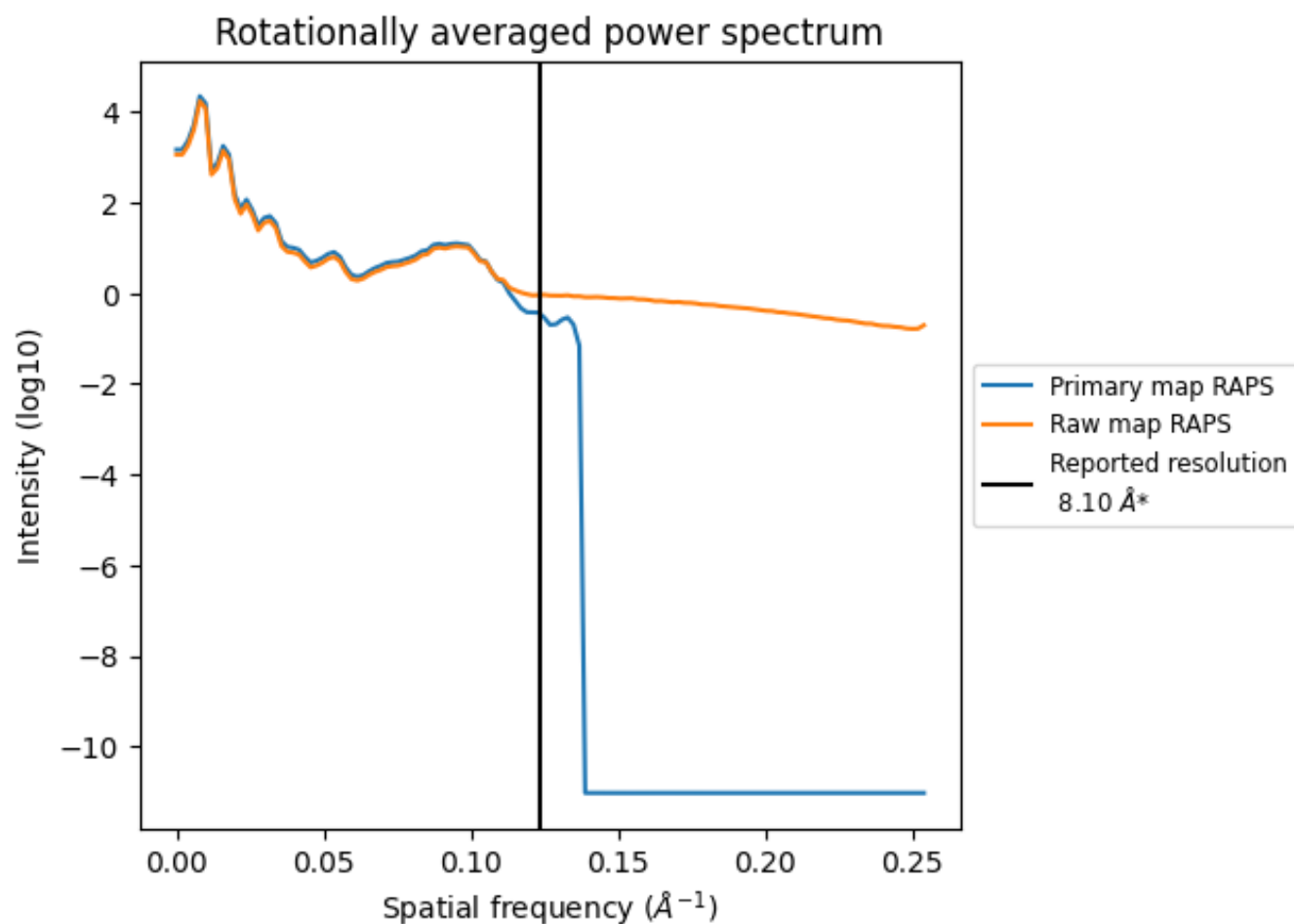
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 681 nm^3 ; this corresponds to an approximate mass of 616 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 ⓘ

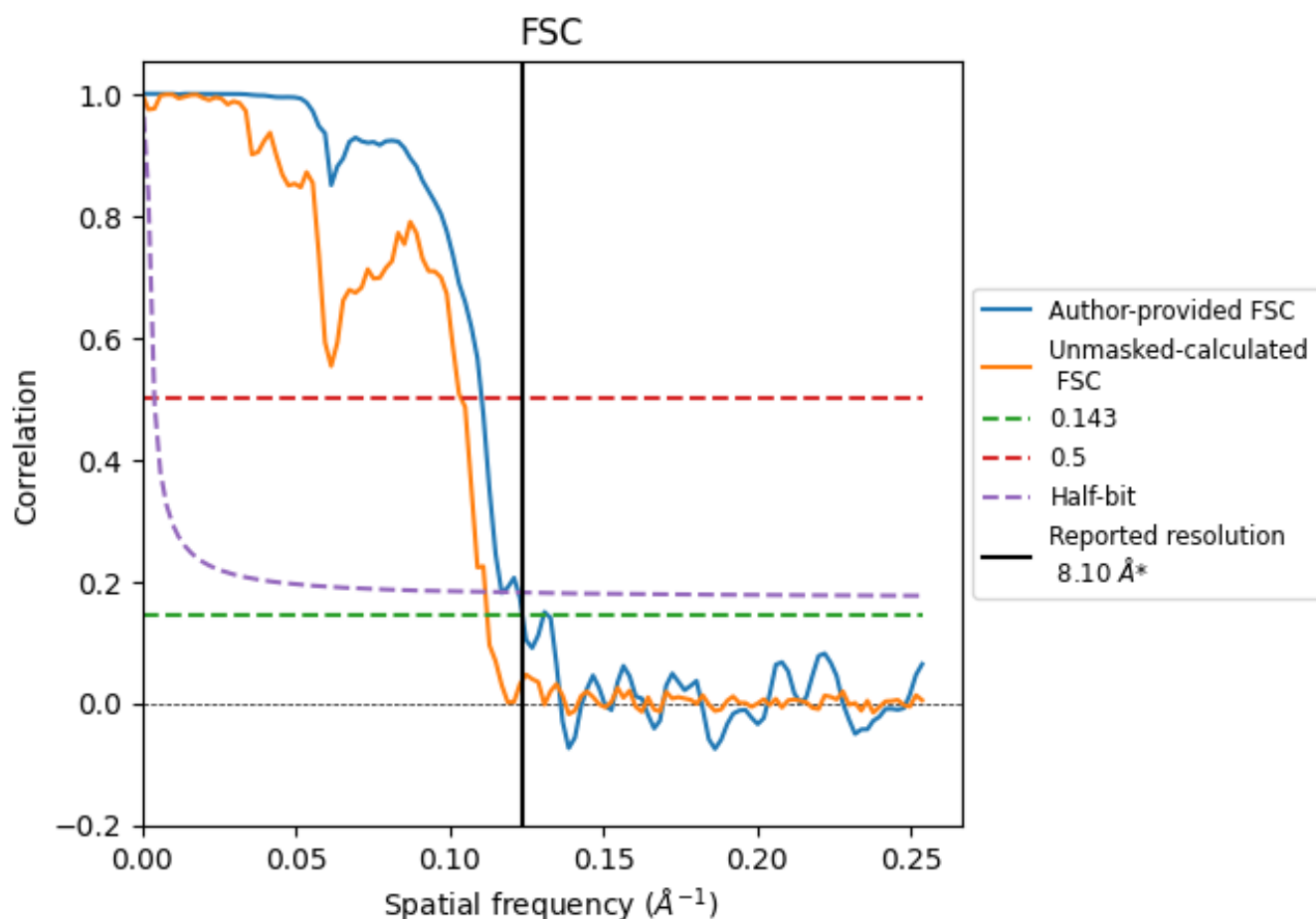


*Reported resolution corresponds to spatial frequency of 0.123 Å⁻¹

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 0.123 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

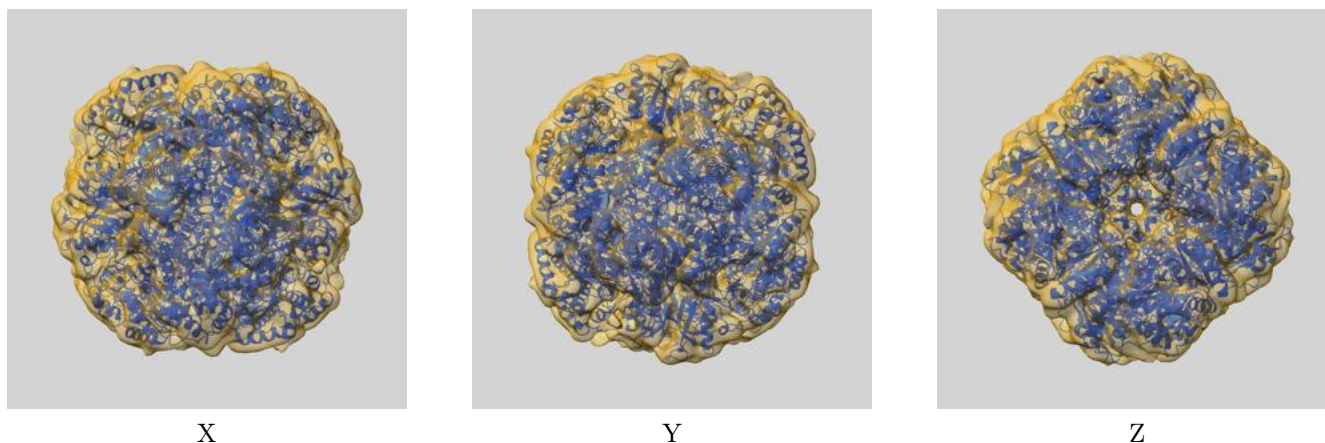
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.10	-	-
Author-provided FSC curve	8.08	9.05	8.55
Unmasked-calculated*	8.90	9.63	8.95

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

9 Map-model fit [i](#)

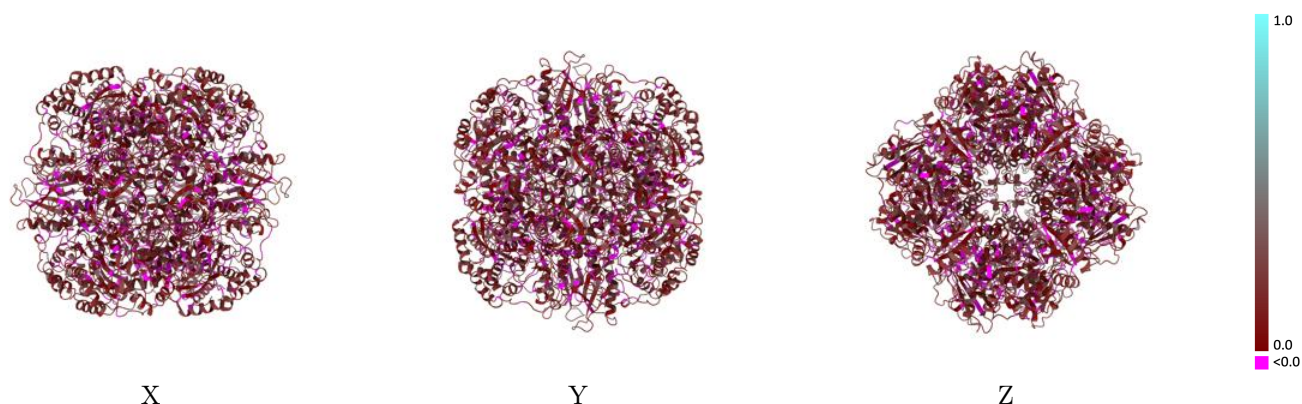
This section contains information regarding the fit between EMDB map EMD-52438 and PDB model 9HVM. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



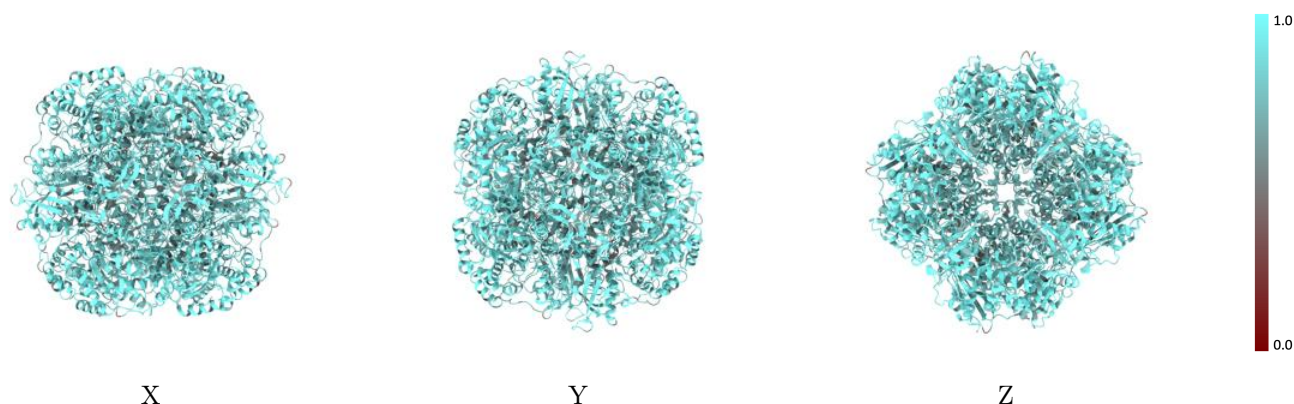
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



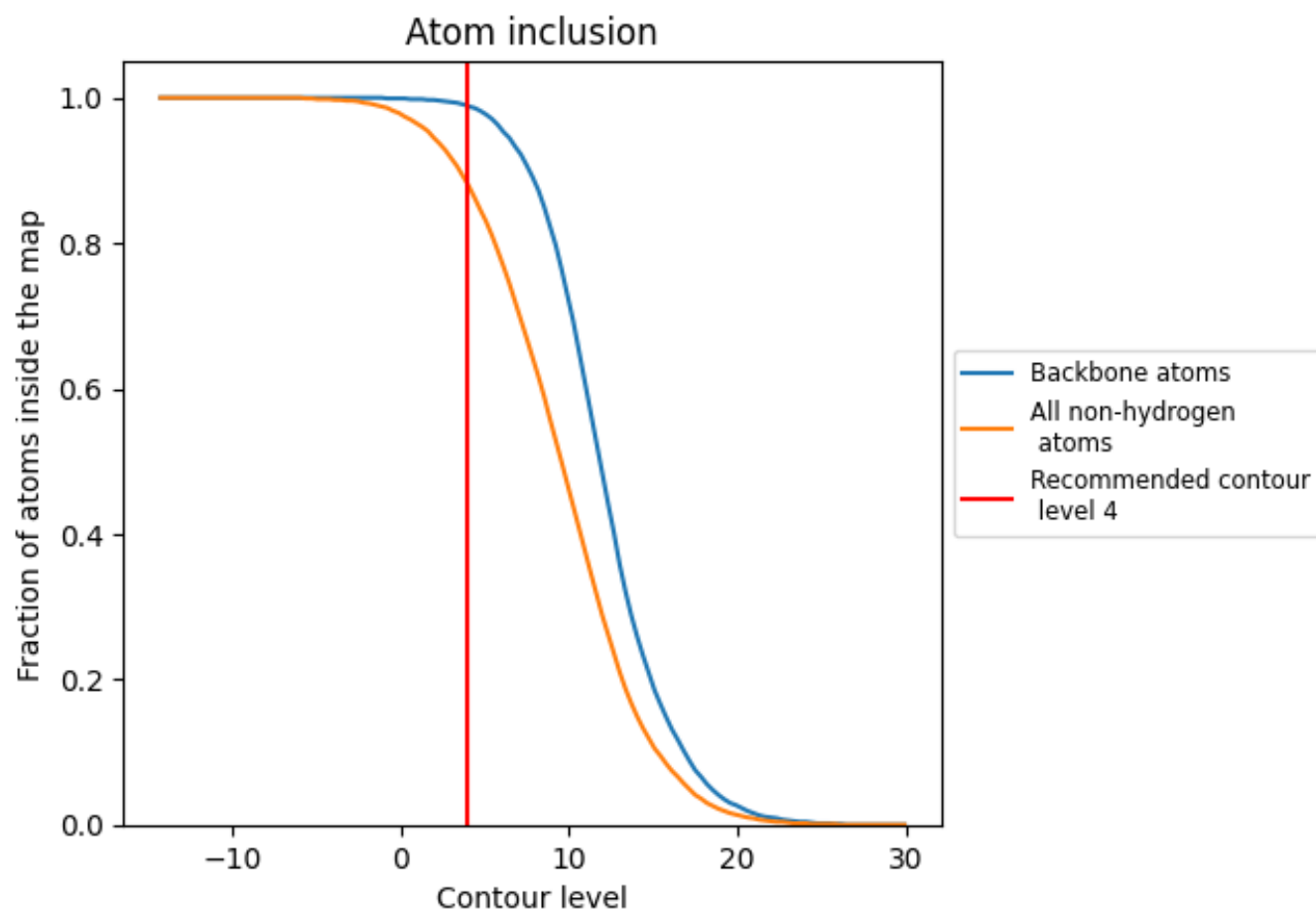
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 88% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8810	 0.1140
A	 0.8740	 0.1100
B	 0.9080	 0.1310
C	 0.8730	 0.1110
D	 0.8980	 0.1290
E	 0.8720	 0.1080
F	 0.9050	 0.1290
G	 0.8720	 0.1100
H	 0.9060	 0.1280
I	 0.8750	 0.1080
J	 0.9080	 0.1250
K	 0.8740	 0.1070
L	 0.9060	 0.1260
M	 0.8750	 0.1090
N	 0.8970	 0.1300
O	 0.8750	 0.1090
P	 0.9170	 0.1320

