



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 05:33 AM UTC

PDB ID : 8P2M / pdb_00008p2m
EMDB ID : EMD-17370
Title : C. elegans TIR-1 protein.
Authors : Isupov, M.N.; Opatowsky, Y.
Deposited on : 2023-05-16
Resolution : 3.82 Å(reported)
Based on initial model : .

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:

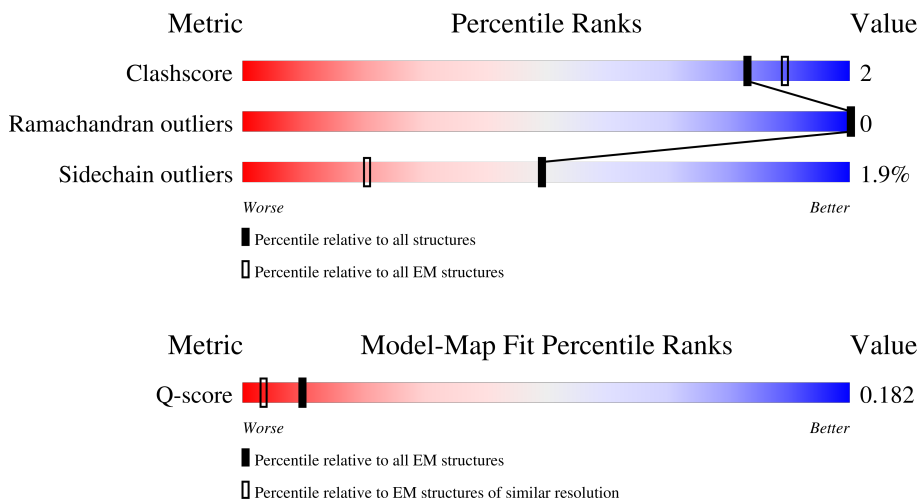
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.82 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	9152 (3.32 - 4.32)

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	738	
1	B	738	
1	C	738	
1	D	738	

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Mol	Chain	Length	Quality of chain
1	E	738	40% 79% 7% 13%
1	F	738	21% 79% 7% 13%
1	G	738	28% 77% 10% 13%
1	H	738	43% 78% 8% 13%
1	I	738	24% 78% 8% 13%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 46702 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 NAD(+) hydrolase tir-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	659	Total	C	N	O	S	0	0
			5286	3376	894	981	35		
1	B	645	Total	C	N	O	S	0	0
			5177	3308	878	957	34		
1	C	645	Total	C	N	O	S	0	0
			5177	3308	878	957	34		
1	D	645	Total	C	N	O	S	0	0
			5177	3308	878	957	34		
1	E	645	Total	C	N	O	S	0	0
			5177	3308	878	957	34		
1	F	645	Total	C	N	O	S	0	0
			5177	3308	878	957	34		
1	G	645	Total	C	N	O	S	0	0
			5177	3308	878	957	34		
1	H	645	Total	C	N	O	S	0	0
			5177	3308	878	957	34		
1	I	645	Total	C	N	O	S	0	0
			5177	3308	878	957	34		

There are 243 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	MET	-	initiating methionine	UNP Q86DA5
A	136	SER	-	expression tag	UNP Q86DA5
A	137	TYR	-	expression tag	UNP Q86DA5
A	138	HIS	-	expression tag	UNP Q86DA5
A	139	HIS	-	expression tag	UNP Q86DA5
A	140	HIS	-	expression tag	UNP Q86DA5
A	141	HIS	-	expression tag	UNP Q86DA5
A	142	HIS	-	expression tag	UNP Q86DA5
A	143	HIS	-	expression tag	UNP Q86DA5
A	144	ASP	-	expression tag	UNP Q86DA5
A	145	TYR	-	expression tag	UNP Q86DA5
A	146	ASP	-	expression tag	UNP Q86DA5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	147	ILE	-	expression tag	UNP Q86DA5
A	148	PRO	-	expression tag	UNP Q86DA5
A	149	THR	-	expression tag	UNP Q86DA5
A	150	THR	-	expression tag	UNP Q86DA5
A	151	GLU	-	expression tag	UNP Q86DA5
A	152	ASN	-	expression tag	UNP Q86DA5
A	153	LEU	-	expression tag	UNP Q86DA5
A	154	TYR	-	expression tag	UNP Q86DA5
A	155	PHE	-	expression tag	UNP Q86DA5
A	156	GLN	-	expression tag	UNP Q86DA5
A	157	GLY	-	expression tag	UNP Q86DA5
A	158	ALA	-	expression tag	UNP Q86DA5
A	159	MET	-	expression tag	UNP Q86DA5
A	160	GLY	-	expression tag	UNP Q86DA5
A	161	SER	-	expression tag	UNP Q86DA5
B	135	MET	-	initiating methionine	UNP Q86DA5
B	136	SER	-	expression tag	UNP Q86DA5
B	137	TYR	-	expression tag	UNP Q86DA5
B	138	HIS	-	expression tag	UNP Q86DA5
B	139	HIS	-	expression tag	UNP Q86DA5
B	140	HIS	-	expression tag	UNP Q86DA5
B	141	HIS	-	expression tag	UNP Q86DA5
B	142	HIS	-	expression tag	UNP Q86DA5
B	143	HIS	-	expression tag	UNP Q86DA5
B	144	ASP	-	expression tag	UNP Q86DA5
B	145	TYR	-	expression tag	UNP Q86DA5
B	146	ASP	-	expression tag	UNP Q86DA5
B	147	ILE	-	expression tag	UNP Q86DA5
B	148	PRO	-	expression tag	UNP Q86DA5
B	149	THR	-	expression tag	UNP Q86DA5
B	150	THR	-	expression tag	UNP Q86DA5
B	151	GLU	-	expression tag	UNP Q86DA5
B	152	ASN	-	expression tag	UNP Q86DA5
B	153	LEU	-	expression tag	UNP Q86DA5
B	154	TYR	-	expression tag	UNP Q86DA5
B	155	PHE	-	expression tag	UNP Q86DA5
B	156	GLN	-	expression tag	UNP Q86DA5
B	157	GLY	-	expression tag	UNP Q86DA5
B	158	ALA	-	expression tag	UNP Q86DA5
B	159	MET	-	expression tag	UNP Q86DA5
B	160	GLY	-	expression tag	UNP Q86DA5
B	161	SER	-	expression tag	UNP Q86DA5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	135	MET	-	initiating methionine	UNP Q86DA5
C	136	SER	-	expression tag	UNP Q86DA5
C	137	TYR	-	expression tag	UNP Q86DA5
C	138	HIS	-	expression tag	UNP Q86DA5
C	139	HIS	-	expression tag	UNP Q86DA5
C	140	HIS	-	expression tag	UNP Q86DA5
C	141	HIS	-	expression tag	UNP Q86DA5
C	142	HIS	-	expression tag	UNP Q86DA5
C	143	HIS	-	expression tag	UNP Q86DA5
C	144	ASP	-	expression tag	UNP Q86DA5
C	145	TYR	-	expression tag	UNP Q86DA5
C	146	ASP	-	expression tag	UNP Q86DA5
C	147	ILE	-	expression tag	UNP Q86DA5
C	148	PRO	-	expression tag	UNP Q86DA5
C	149	THR	-	expression tag	UNP Q86DA5
C	150	THR	-	expression tag	UNP Q86DA5
C	151	GLU	-	expression tag	UNP Q86DA5
C	152	ASN	-	expression tag	UNP Q86DA5
C	153	LEU	-	expression tag	UNP Q86DA5
C	154	TYR	-	expression tag	UNP Q86DA5
C	155	PHE	-	expression tag	UNP Q86DA5
C	156	GLN	-	expression tag	UNP Q86DA5
C	157	GLY	-	expression tag	UNP Q86DA5
C	158	ALA	-	expression tag	UNP Q86DA5
C	159	MET	-	expression tag	UNP Q86DA5
C	160	GLY	-	expression tag	UNP Q86DA5
C	161	SER	-	expression tag	UNP Q86DA5
D	135	MET	-	initiating methionine	UNP Q86DA5
D	136	SER	-	expression tag	UNP Q86DA5
D	137	TYR	-	expression tag	UNP Q86DA5
D	138	HIS	-	expression tag	UNP Q86DA5
D	139	HIS	-	expression tag	UNP Q86DA5
D	140	HIS	-	expression tag	UNP Q86DA5
D	141	HIS	-	expression tag	UNP Q86DA5
D	142	HIS	-	expression tag	UNP Q86DA5
D	143	HIS	-	expression tag	UNP Q86DA5
D	144	ASP	-	expression tag	UNP Q86DA5
D	145	TYR	-	expression tag	UNP Q86DA5
D	146	ASP	-	expression tag	UNP Q86DA5
D	147	ILE	-	expression tag	UNP Q86DA5
D	148	PRO	-	expression tag	UNP Q86DA5
D	149	THR	-	expression tag	UNP Q86DA5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	150	THR	-	expression tag	UNP Q86DA5
D	151	GLU	-	expression tag	UNP Q86DA5
D	152	ASN	-	expression tag	UNP Q86DA5
D	153	LEU	-	expression tag	UNP Q86DA5
D	154	TYR	-	expression tag	UNP Q86DA5
D	155	PHE	-	expression tag	UNP Q86DA5
D	156	GLN	-	expression tag	UNP Q86DA5
D	157	GLY	-	expression tag	UNP Q86DA5
D	158	ALA	-	expression tag	UNP Q86DA5
D	159	MET	-	expression tag	UNP Q86DA5
D	160	GLY	-	expression tag	UNP Q86DA5
D	161	SER	-	expression tag	UNP Q86DA5
E	135	MET	-	initiating methionine	UNP Q86DA5
E	136	SER	-	expression tag	UNP Q86DA5
E	137	TYR	-	expression tag	UNP Q86DA5
E	138	HIS	-	expression tag	UNP Q86DA5
E	139	HIS	-	expression tag	UNP Q86DA5
E	140	HIS	-	expression tag	UNP Q86DA5
E	141	HIS	-	expression tag	UNP Q86DA5
E	142	HIS	-	expression tag	UNP Q86DA5
E	143	HIS	-	expression tag	UNP Q86DA5
E	144	ASP	-	expression tag	UNP Q86DA5
E	145	TYR	-	expression tag	UNP Q86DA5
E	146	ASP	-	expression tag	UNP Q86DA5
E	147	ILE	-	expression tag	UNP Q86DA5
E	148	PRO	-	expression tag	UNP Q86DA5
E	149	THR	-	expression tag	UNP Q86DA5
E	150	THR	-	expression tag	UNP Q86DA5
E	151	GLU	-	expression tag	UNP Q86DA5
E	152	ASN	-	expression tag	UNP Q86DA5
E	153	LEU	-	expression tag	UNP Q86DA5
E	154	TYR	-	expression tag	UNP Q86DA5
E	155	PHE	-	expression tag	UNP Q86DA5
E	156	GLN	-	expression tag	UNP Q86DA5
E	157	GLY	-	expression tag	UNP Q86DA5
E	158	ALA	-	expression tag	UNP Q86DA5
E	159	MET	-	expression tag	UNP Q86DA5
E	160	GLY	-	expression tag	UNP Q86DA5
E	161	SER	-	expression tag	UNP Q86DA5
F	135	MET	-	initiating methionine	UNP Q86DA5
F	136	SER	-	expression tag	UNP Q86DA5
F	137	TYR	-	expression tag	UNP Q86DA5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	138	HIS	-	expression tag	UNP Q86DA5
F	139	HIS	-	expression tag	UNP Q86DA5
F	140	HIS	-	expression tag	UNP Q86DA5
F	141	HIS	-	expression tag	UNP Q86DA5
F	142	HIS	-	expression tag	UNP Q86DA5
F	143	HIS	-	expression tag	UNP Q86DA5
F	144	ASP	-	expression tag	UNP Q86DA5
F	145	TYR	-	expression tag	UNP Q86DA5
F	146	ASP	-	expression tag	UNP Q86DA5
F	147	ILE	-	expression tag	UNP Q86DA5
F	148	PRO	-	expression tag	UNP Q86DA5
F	149	THR	-	expression tag	UNP Q86DA5
F	150	THR	-	expression tag	UNP Q86DA5
F	151	GLU	-	expression tag	UNP Q86DA5
F	152	ASN	-	expression tag	UNP Q86DA5
F	153	LEU	-	expression tag	UNP Q86DA5
F	154	TYR	-	expression tag	UNP Q86DA5
F	155	PHE	-	expression tag	UNP Q86DA5
F	156	GLN	-	expression tag	UNP Q86DA5
F	157	GLY	-	expression tag	UNP Q86DA5
F	158	ALA	-	expression tag	UNP Q86DA5
F	159	MET	-	expression tag	UNP Q86DA5
F	160	GLY	-	expression tag	UNP Q86DA5
F	161	SER	-	expression tag	UNP Q86DA5
G	135	MET	-	initiating methionine	UNP Q86DA5
G	136	SER	-	expression tag	UNP Q86DA5
G	137	TYR	-	expression tag	UNP Q86DA5
G	138	HIS	-	expression tag	UNP Q86DA5
G	139	HIS	-	expression tag	UNP Q86DA5
G	140	HIS	-	expression tag	UNP Q86DA5
G	141	HIS	-	expression tag	UNP Q86DA5
G	142	HIS	-	expression tag	UNP Q86DA5
G	143	HIS	-	expression tag	UNP Q86DA5
G	144	ASP	-	expression tag	UNP Q86DA5
G	145	TYR	-	expression tag	UNP Q86DA5
G	146	ASP	-	expression tag	UNP Q86DA5
G	147	ILE	-	expression tag	UNP Q86DA5
G	148	PRO	-	expression tag	UNP Q86DA5
G	149	THR	-	expression tag	UNP Q86DA5
G	150	THR	-	expression tag	UNP Q86DA5
G	151	GLU	-	expression tag	UNP Q86DA5
G	152	ASN	-	expression tag	UNP Q86DA5

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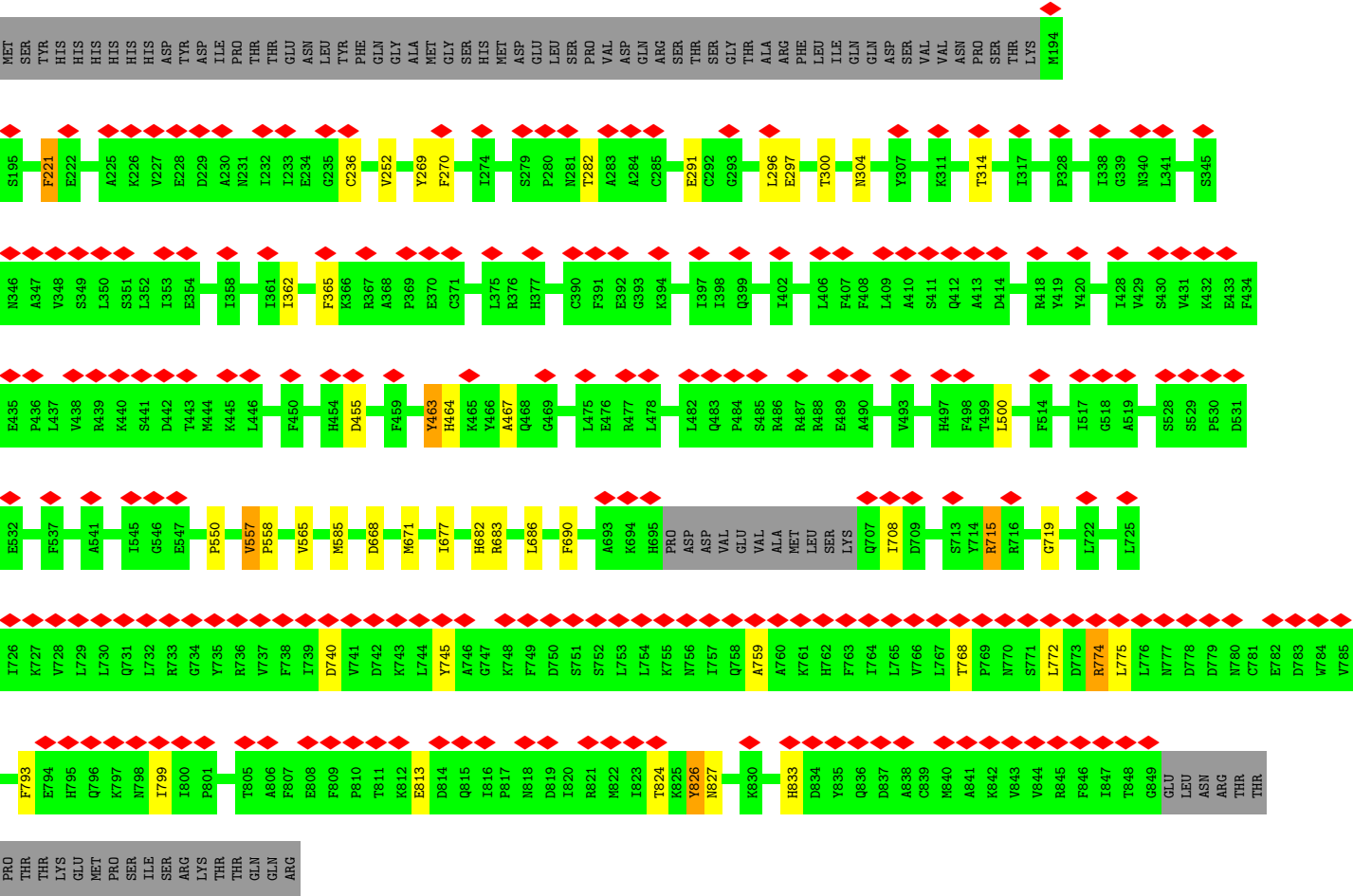
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Chain	Residue	Modelled	Actual	Comment	Reference
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G	154	TYR	-	expression tag	UNP Q86DA5
G	155	PHE	-	expression tag	UNP Q86DA5
G	156	GLN	-	expression tag	UNP Q86DA5
G	157	GLY	-	expression tag	UNP Q86DA5
G	158	ALA	-	expression tag	UNP Q86DA5
G	159	MET	-	expression tag	UNP Q86DA5
G	160	GLY	-	expression tag	UNP Q86DA5
G	161	SER	-	expression tag	UNP Q86DA5
H	135	MET	-	initiating methionine	UNP Q86DA5
H	136	SER	-	expression tag	UNP Q86DA5
H	137	TYR	-	expression tag	UNP Q86DA5
H	138	HIS	-	expression tag	UNP Q86DA5
H	139	HIS	-	expression tag	UNP Q86DA5
H	140	HIS	-	expression tag	UNP Q86DA5
H	141	HIS	-	expression tag	UNP Q86DA5
H	142	HIS	-	expression tag	UNP Q86DA5
H	143	HIS	-	expression tag	UNP Q86DA5
H	144	ASP	-	expression tag	UNP Q86DA5
H	145	TYR	-	expression tag	UNP Q86DA5
H	146	ASP	-	expression tag	UNP Q86DA5
H	147	ILE	-	expression tag	UNP Q86DA5
H	148	PRO	-	expression tag	UNP Q86DA5
H	149	THR	-	expression tag	UNP Q86DA5
H	150	THR	-	expression tag	UNP Q86DA5
H	151	GLU	-	expression tag	UNP Q86DA5
H	152	ASN	-	expression tag	UNP Q86DA5
H	153	LEU	-	expression tag	UNP Q86DA5
H	154	TYR	-	expression tag	UNP Q86DA5
H	155	PHE	-	expression tag	UNP Q86DA5
H	156	GLN	-	expression tag	UNP Q86DA5
H	157	GLY	-	expression tag	UNP Q86DA5
H	158	ALA	-	expression tag	UNP Q86DA5
H	159	MET	-	expression tag	UNP Q86DA5
H	160	GLY	-	expression tag	UNP Q86DA5
H	161	SER	-	expression tag	UNP Q86DA5
I	135	MET	-	initiating methionine	UNP Q86DA5
I	136	SER	-	expression tag	UNP Q86DA5
I	137	TYR	-	expression tag	UNP Q86DA5
I	138	HIS	-	expression tag	UNP Q86DA5
I	139	HIS	-	expression tag	UNP Q86DA5
I	140	HIS	-	expression tag	UNP Q86DA5

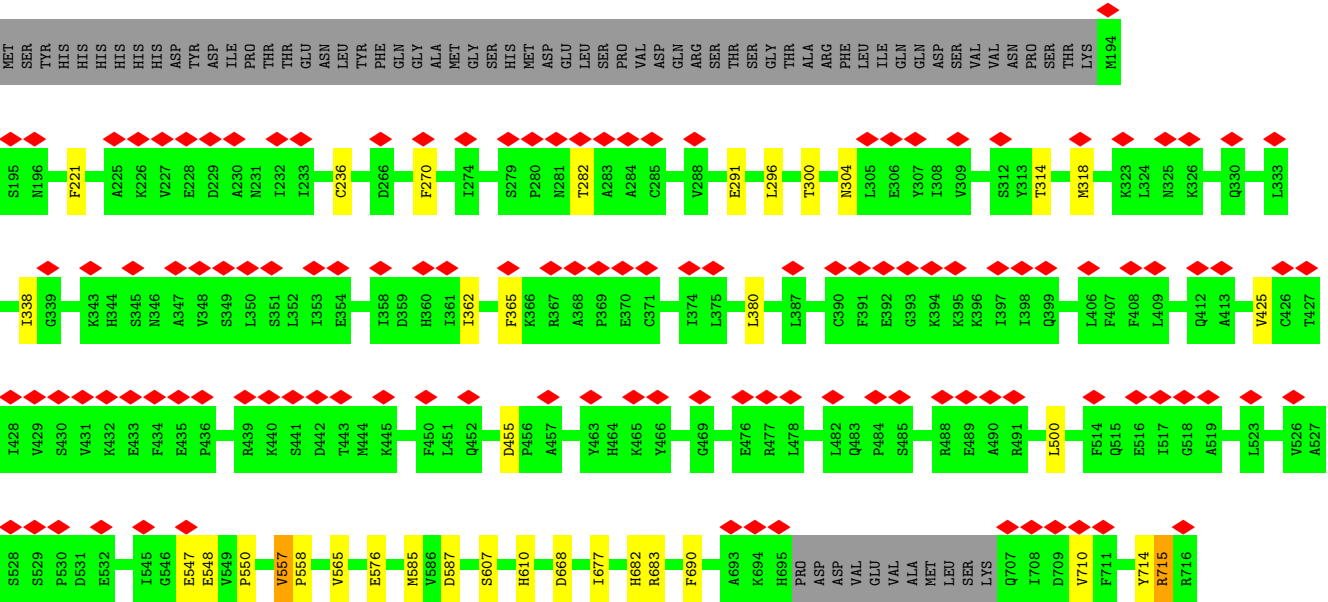
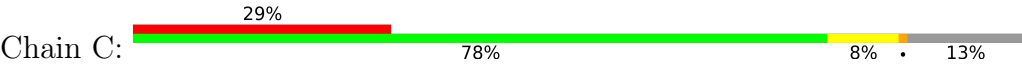
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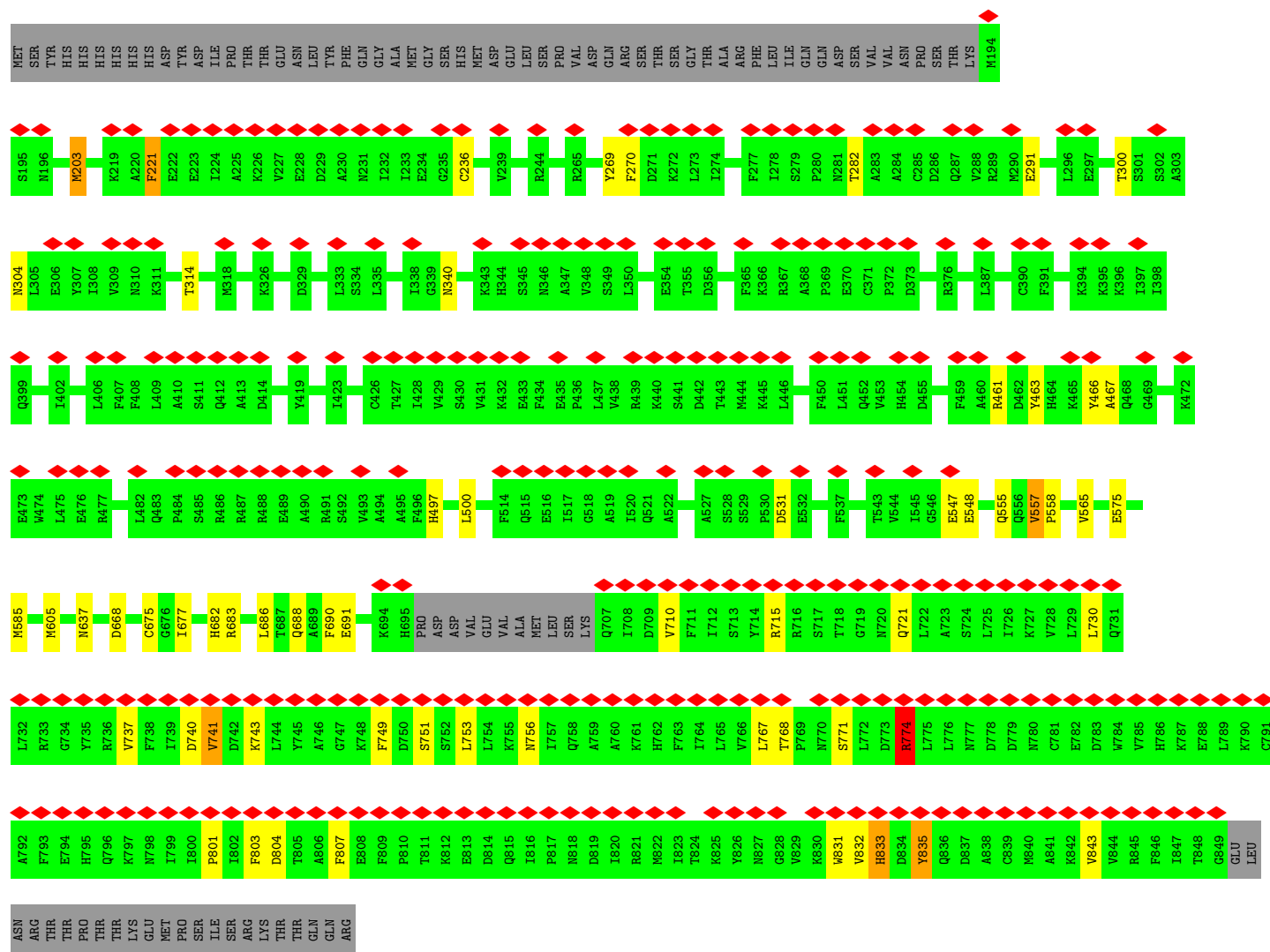
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Chain	Residue	Modelled	Actual	Comment	Reference
I	141	HIS	-	expression tag	UNP Q86DA5
I	142	HIS	-	expression tag	UNP Q86DA5
I	143	HIS	-	expression tag	UNP Q86DA5
I	144	ASP	-	expression tag	UNP Q86DA5
I	145	TYR	-	expression tag	UNP Q86DA5
I	146	ASP	-	expression tag	UNP Q86DA5
I	147	ILE	-	expression tag	UNP Q86DA5
I	148	PRO	-	expression tag	UNP Q86DA5
I	149	THR	-	expression tag	UNP Q86DA5
I	150	THR	-	expression tag	UNP Q86DA5
I	151	GLU	-	expression tag	UNP Q86DA5
I	152	ASN	-	expression tag	UNP Q86DA5
I	153	LEU	-	expression tag	UNP Q86DA5
I	154	TYR	-	expression tag	UNP Q86DA5
I	155	PHE	-	expression tag	UNP Q86DA5
I	156	GLN	-	expression tag	UNP Q86DA5
I	157	GLY	-	expression tag	UNP Q86DA5
I	158	ALA	-	expression tag	UNP Q86DA5
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I	161	SER	-	expression tag	UNP Q86DA5

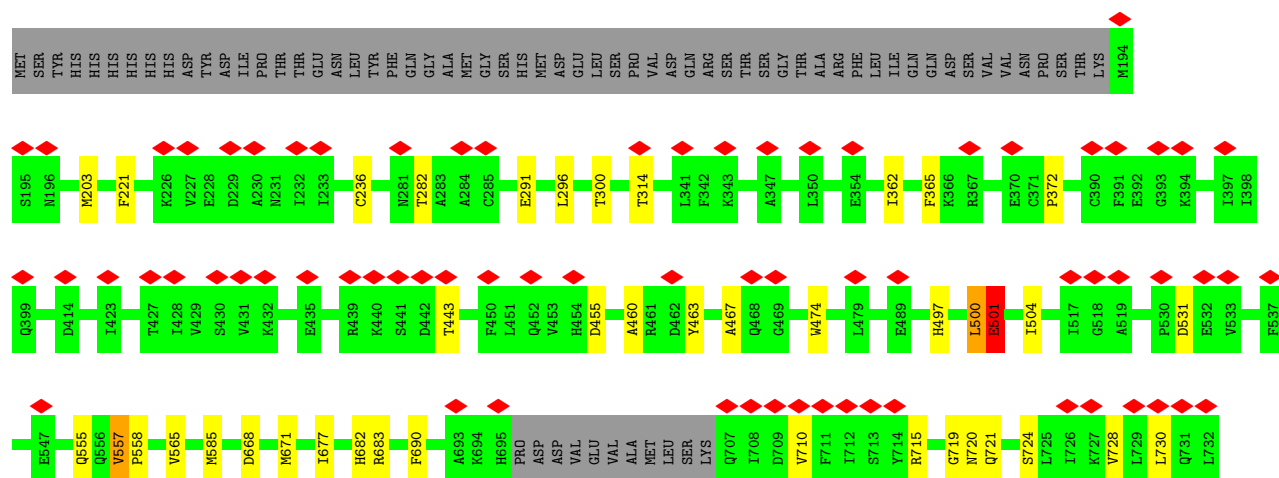
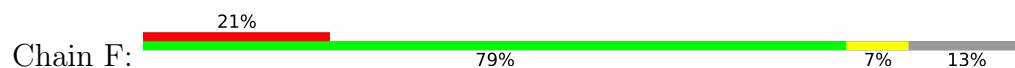


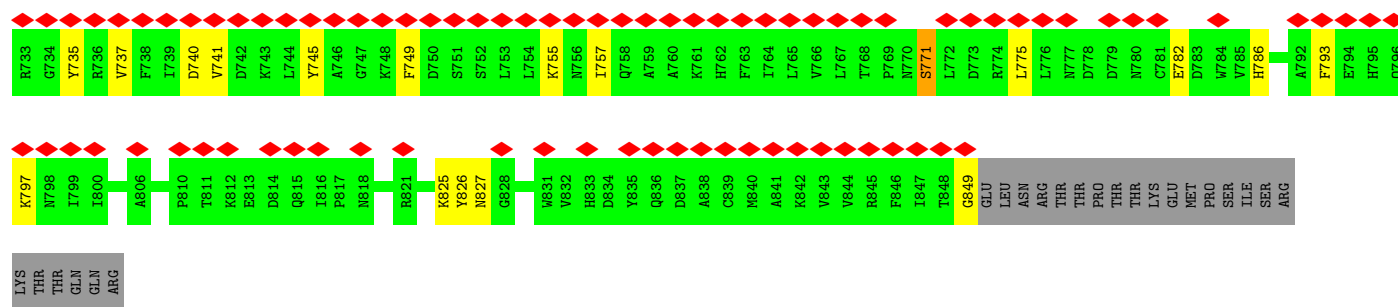
● Molecule 1: NAD(+) hydrolase tir-1



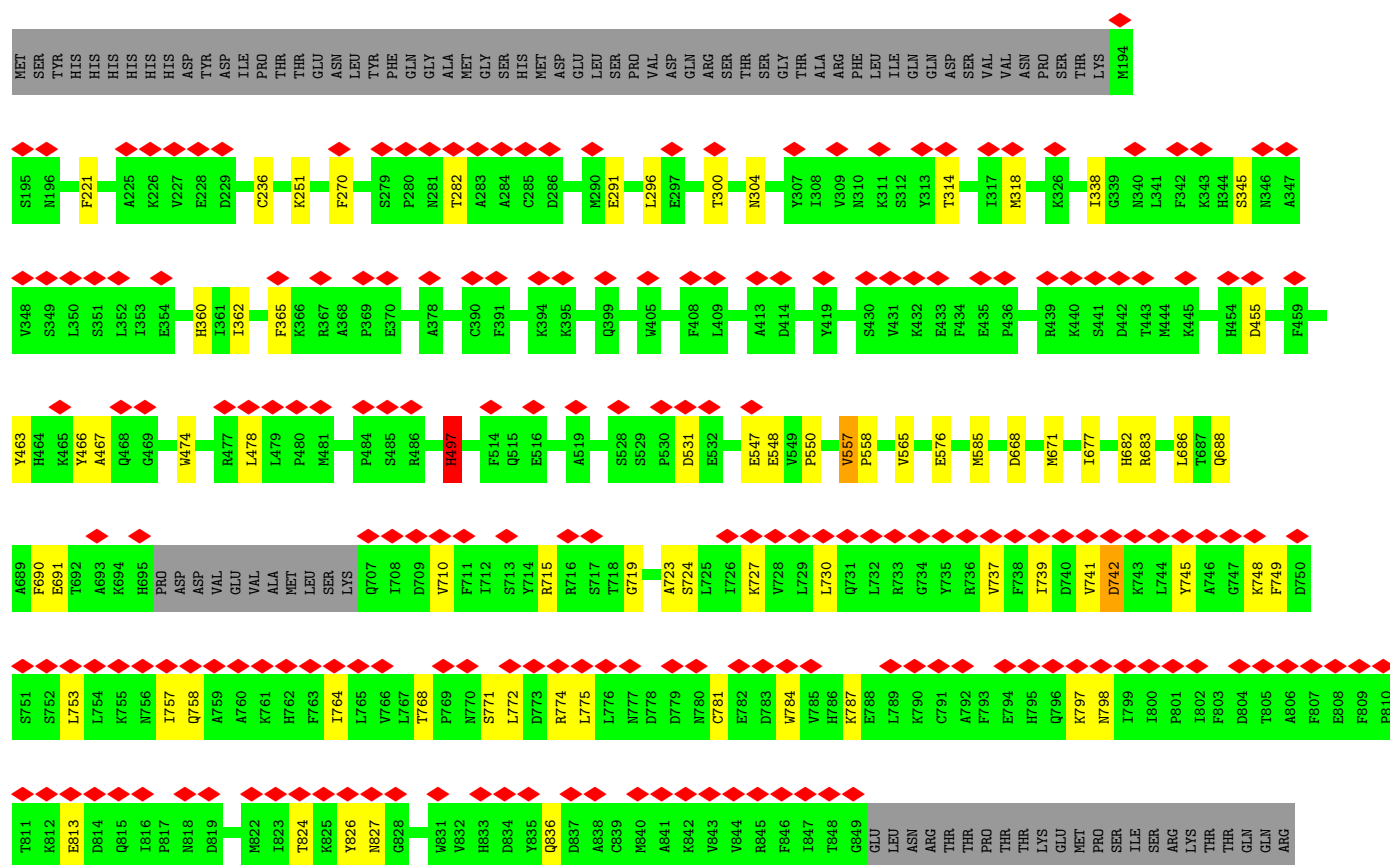
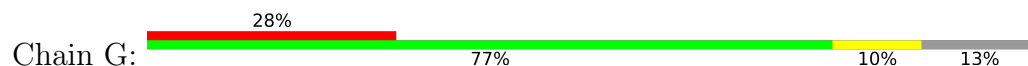


• Molecule 1: NAD(+) hydrolase tir-1

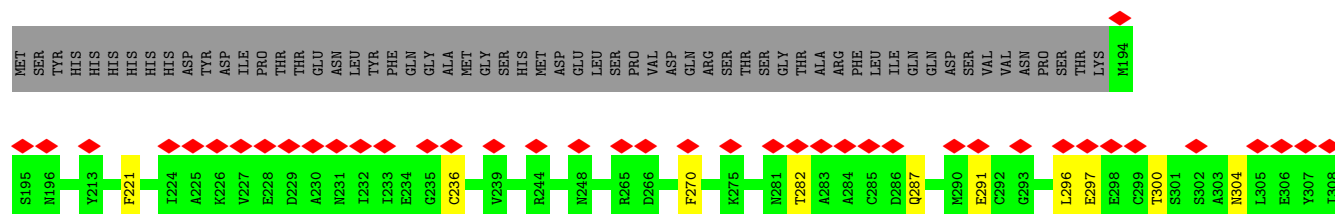
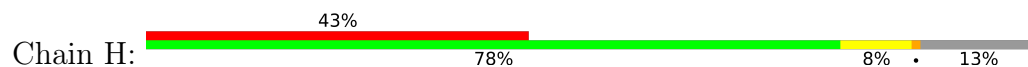


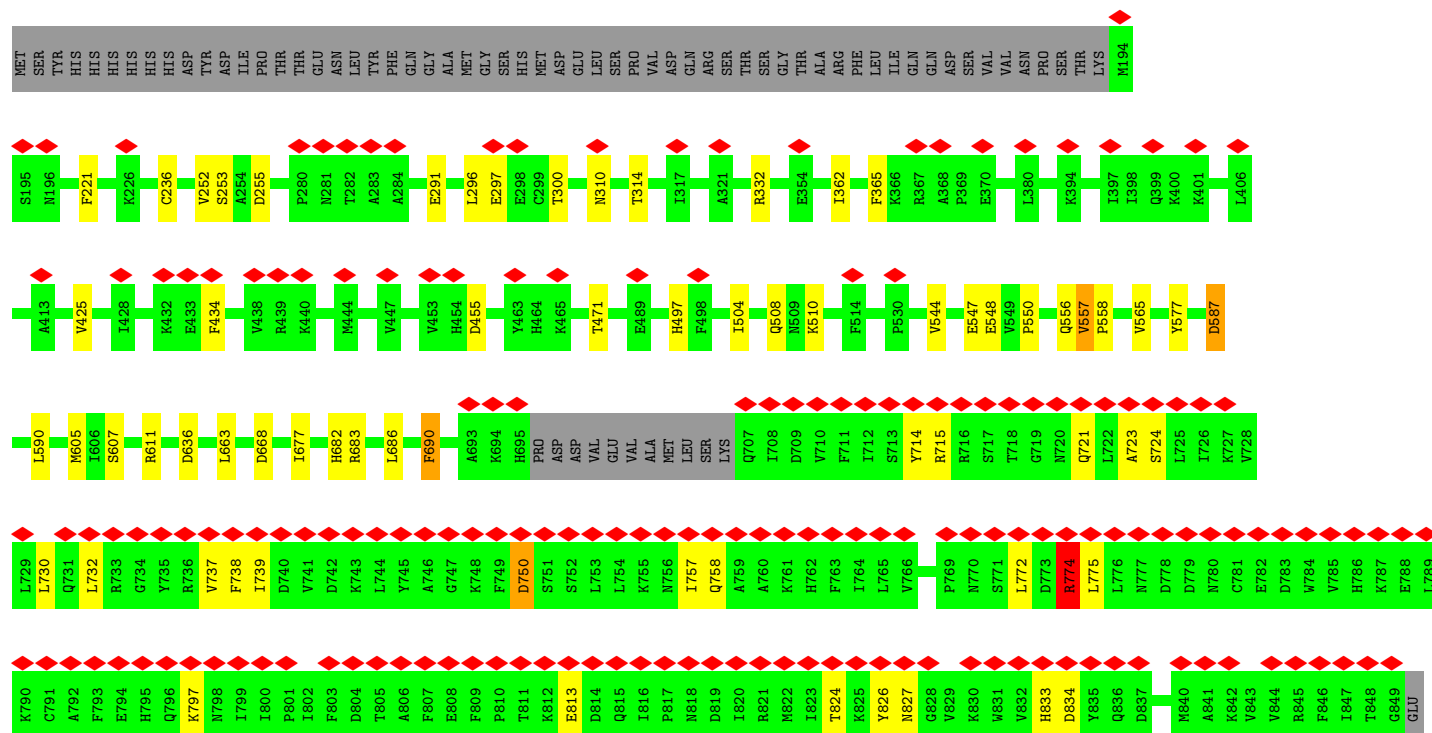


• Molecule 1: NAD(+) hydrolase tir-1



• Molecule 1: NAD(+) hydrolase tir-1





LEU
ASN
ARG
THR
THR
PRO
THR
THR
LYS
GLU
MET
PRO
SER
ILE
SER
SER
ARG
LYS
THR
THR
GLN
GLN
ARG

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	121487	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 ($e^-/\text{\AA}^2$)	41.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.511	Depositor
Minimum map value	-0.201	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	268.8, 268.8, 268.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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	0.85	1/5385 (0.0%)	1.39	16/7275 (0.2%)
1	B	0.69	0/5273	1.28	11/7120 (0.2%)
1	C	0.76	2/5273 (0.0%)	1.36	22/7120 (0.3%)
1	D	0.68	2/5273 (0.0%)	1.28	12/7120 (0.2%)
1	E	0.74	3/5273 (0.1%)	1.32	20/7120 (0.3%)
1	F	0.76	3/5273 (0.1%)	1.38	19/7120 (0.3%)
1	G	0.70	3/5273 (0.1%)	1.29	9/7120 (0.1%)
1	H	0.69	0/5273	1.28	18/7120 (0.3%)
1	I	0.73	1/5273 (0.0%)	1.29	19/7120 (0.3%)
All	All	0.73	15/47569 (0.0%)	1.32	146/64235 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	1
1	C	0	3
1	E	0	1
1	F	0	2
1	H	0	1
1	I	0	2
All	All	0	15

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	831	TRP	C-O	-7.50	1.14	1.23
1	C	840	MET	C-O	-7.19	1.15	1.24
1	F	501	GLU	CD-OE2	-7.04	1.11	1.25
1	G	360	HIS	CE1-NE2	6.62	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	679	ASN	CG-OD1	-6.06	1.12	1.23
1	E	497	HIS	CE1-NE2	5.94	1.38	1.32
1	D	771	SER	C-O	5.86	1.29	1.23
1	F	497	HIS	CE1-NE2	5.40	1.38	1.32
1	C	786	HIS	CD2-NE2	-5.29	1.32	1.37
1	F	719	GLY	C-O	-5.26	1.17	1.23
1	D	691	GLU	CD-OE1	5.25	1.35	1.25
1	G	497	HIS	CE1-NE2	5.17	1.37	1.32
1	I	255	ASP	CG-OD1	5.07	1.34	1.25
1	E	203	MET	CG-SD	5.06	1.93	1.80
1	G	497	HIS	CG-ND1	-5.04	1.32	1.38

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	501	GLU	CG-CD-OE1	19.71	163.73	118.40
1	F	501	GLU	CG-CD-OE2	-14.63	84.75	118.40
1	F	501	GLU	OE1-CD-OE2	-12.45	93.02	122.90
1	D	836	GLN	CB-CA-C	10.86	133.00	110.31
1	C	455	ASP	CA-CB-CG	10.28	122.88	112.60
1	H	834	ASP	CA-CB-CG	8.93	121.53	112.60
1	F	501	GLU	CB-CG-CD	8.50	127.04	112.60
1	A	471	THR	CA-CB-CG2	8.29	124.58	110.50
1	G	221	PHE	CA-CB-CG	-8.18	105.62	113.80
1	C	833	HIS	CA-C-N	7.82	131.54	120.28
1	C	833	HIS	C-N-CA	7.82	131.54	120.28
1	F	720	ASN	CA-C-N	7.75	131.00	120.38
1	F	720	ASN	C-N-CA	7.75	131.00	120.38
1	D	550	PRO	N-CA-CB	7.67	111.31	103.25
1	I	690	PHE	CA-CB-CG	-7.36	106.44	113.80
1	H	690	PHE	CA-CB-CG	-7.35	106.45	113.80
1	G	742	ASP	CB-CA-C	7.34	124.93	111.06
1	A	304	ASN	OD1-CG-ND2	-7.30	115.30	122.60
1	H	833	HIS	CA-CB-CG	-7.26	106.54	113.80
1	B	690	PHE	CA-CB-CG	-7.25	106.55	113.80
1	I	556	GLN	OE1-CD-NE2	-7.23	115.37	122.60
1	D	500	LEU	CB-CA-C	-7.22	99.55	110.88
1	B	500	LEU	CB-CA-C	-7.14	99.67	110.88
1	F	690	PHE	CA-CB-CG	-7.09	106.70	113.80
1	I	221	PHE	CA-CB-CG	-7.06	106.74	113.80
1	C	221	PHE	CA-CB-CG	-7.04	106.76	113.80
1	G	690	PHE	CA-CB-CG	-6.97	106.83	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	690	PHE	CA-CB-CG	-6.94	106.86	113.80
1	A	589	ASP	CA-CB-CG	6.94	119.54	112.60
1	D	461	ARG	CG-CD-NE	6.93	127.26	112.00
1	H	550	PRO	N-CA-CB	6.89	110.48	103.25
1	G	531	ASP	CA-CB-CG	6.84	119.44	112.60
1	A	656	ASN	OD1-CG-ND2	-6.83	115.77	122.60
1	C	715	ARG	NE-CZ-NH1	-6.79	114.71	121.50
1	G	455	ASP	CA-CB-CG	-6.79	105.81	112.60
1	F	531	ASP	CA-CB-CG	6.77	119.37	112.60
1	E	531	ASP	CA-CB-CG	6.70	119.30	112.60
1	C	773	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	509	ASN	CA-CB-CG	-6.62	105.98	112.60
1	C	727	LYS	O-C-N	-6.60	114.50	122.22
1	C	690	PHE	CA-CB-CG	-6.59	107.21	113.80
1	C	380	LEU	CD1-CG-CD2	-6.58	96.33	110.80
1	B	455	ASP	CA-CB-CG	6.53	119.13	112.60
1	I	497	HIS	CA-CB-CG	-6.51	107.28	113.80
1	F	740	ASP	CA-CB-CG	6.51	119.11	112.60
1	D	740	ASP	CA-CB-CG	6.49	119.09	112.60
1	E	221	PHE	CA-CB-CG	-6.46	107.34	113.80
1	C	550	PRO	N-CA-CB	6.45	110.02	103.25
1	A	279	SER	N-CA-C	6.38	117.42	109.57
1	F	221	PHE	CA-CB-CG	-6.32	107.48	113.80
1	H	221	PHE	CA-CB-CG	-6.32	107.48	113.80
1	B	464	HIS	CA-C-N	6.31	129.59	120.38
1	B	464	HIS	C-N-CA	6.31	129.59	120.38
1	H	584	GLN	OE1-CD-NE2	-6.28	116.32	122.60
1	D	221	PHE	CA-CB-CG	-6.23	107.57	113.80
1	E	833	HIS	CB-CA-C	6.22	120.81	110.92
1	C	740	ASP	CA-CB-CG	6.17	118.77	112.60
1	B	550	PRO	N-CA-CB	6.16	109.72	103.25
1	F	372	PRO	N-CA-CB	6.15	110.10	103.33
1	C	733	ARG	CA-C-O	-6.14	114.05	121.05
1	H	434	PHE	CA-CB-CG	6.13	119.93	113.80
1	D	455	ASP	CA-CB-CG	6.12	118.72	112.60
1	G	550	PRO	N-CA-CB	6.10	109.66	103.25
1	C	821	ARG	NE-CZ-NH1	-6.08	115.42	121.50
1	F	455	ASP	CA-CB-CG	6.04	118.64	112.60
1	I	332	ARG	NE-CZ-NH1	-6.03	115.47	121.50
1	E	461	ARG	CG-CD-NE	5.99	125.18	112.00
1	D	721	GLN	CB-CG-CD	5.96	122.73	112.60
1	B	221	PHE	CA-CB-CG	-5.95	107.85	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	LYS	CA-C-N	5.95	123.99	120.24
1	A	401	LYS	C-N-CA	5.95	123.99	120.24
1	I	455	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	565	VAL	CA-CB-CG1	5.83	120.31	110.40
1	C	727	LYS	CA-C-N	5.77	132.35	121.97
1	C	727	LYS	C-N-CA	5.77	132.35	121.97
1	F	755	LYS	CA-C-N	5.72	127.94	120.28
1	F	755	LYS	C-N-CA	5.72	127.94	120.28
1	B	774	ARG	CG-CD-NE	5.70	124.55	112.00
1	E	774	ARG	CG-CD-NE	5.70	124.54	112.00
1	D	298	GLU	CB-CG-CD	5.69	122.27	112.60
1	H	774	ARG	CG-CD-NE	5.68	124.51	112.00
1	I	252	VAL	CA-C-N	5.67	130.21	121.19
1	I	252	VAL	C-N-CA	5.67	130.21	121.19
1	E	575	GLU	CA-C-N	5.66	128.65	120.38
1	E	575	GLU	C-N-CA	5.66	128.65	120.38
1	E	637	ASN	CA-CB-CG	-5.66	106.94	112.60
1	E	637	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	A	595	THR	CA-CB-CG2	5.65	120.11	110.50
1	E	756	ASN	OD1-CG-ND2	-5.64	116.96	122.60
1	H	597	ASN	CB-CG-OD1	5.63	132.07	120.80
1	F	771	SER	N-CA-C	5.63	117.89	111.02
1	I	471	THR	OG1-CB-CG2	-5.60	98.11	109.30
1	I	774	ARG	CG-CD-NE	5.60	124.31	112.00
1	F	849	GLY	CA-C-O	5.59	132.54	120.80
1	D	464	HIS	CA-C-N	5.58	128.53	120.38
1	D	464	HIS	C-N-CA	5.58	128.53	120.38
1	B	740	ASP	CB-CA-C	5.56	120.92	110.63
1	I	750	ASP	CB-CA-C	5.56	122.31	110.19
1	C	839	CYS	CA-C-N	5.52	127.94	120.38
1	C	839	CYS	C-N-CA	5.52	127.94	120.38
1	A	221	PHE	CA-CB-CG	-5.50	108.30	113.80
1	H	455	ASP	CA-CB-CG	5.49	118.09	112.60
1	E	835	TYR	CA-C-N	5.45	131.95	121.54
1	E	835	TYR	C-N-CA	5.45	131.95	121.54
1	A	287	GLN	CB-CG-CD	5.44	121.85	112.60
1	E	340	ASN	OD1-CG-ND2	5.43	128.03	122.60
1	H	445	LYS	CA-C-N	5.43	128.56	120.31
1	H	445	LYS	C-N-CA	5.43	128.56	120.31
1	C	801	PRO	N-CA-CB	5.42	108.15	103.27
1	A	650	THR	OG1-CB-CG2	-5.41	98.48	109.30
1	F	474	TRP	CA-CB-CG	5.40	123.86	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	740	ASP	CA-CB-CG	5.40	118.00	112.60
1	G	474	TRP	CA-CB-CG	5.38	123.82	113.60
1	I	544	VAL	CA-CB-CG2	5.36	119.52	110.40
1	I	550	PRO	N-CA-CB	5.35	108.87	103.25
1	H	287	GLN	CB-CG-CD	5.34	121.67	112.60
1	I	587	ASP	CA-C-N	5.31	125.98	120.03
1	I	587	ASP	C-N-CA	5.31	125.98	120.03
1	G	345	SER	CA-C-N	5.29	127.68	120.54
1	G	345	SER	C-N-CA	5.29	127.68	120.54
1	E	843	VAL	CA-CB-CG2	5.26	119.33	110.40
1	H	442	ASP	CA-CB-CG	5.26	117.86	112.60
1	E	740	ASP	CA-CB-CG	5.21	117.81	112.60
1	H	345	SER	CA-C-N	5.19	127.54	120.54
1	H	345	SER	C-N-CA	5.19	127.54	120.54
1	F	749	PHE	CB-CA-C	5.18	118.94	110.96
1	D	690	PHE	CA-CB-CG	-5.16	108.64	113.80
1	F	443	THR	N-CA-CB	5.16	117.70	110.12
1	A	708	ILE	O-C-N	-5.13	118.05	123.03
1	A	455	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	832	VAL	CA-CB-CG1	5.11	119.09	110.40
1	I	434	PHE	CA-CB-CG	5.11	118.91	113.80
1	C	730	LEU	N-CA-C	-5.08	107.58	112.97
1	I	834	ASP	CA-CB-CG	5.08	117.67	112.60
1	E	721	GLN	CB-CA-C	5.07	120.41	110.67
1	I	636	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	690	PHE	CA-CB-CG	-5.05	108.75	113.80
1	I	738	PHE	CB-CA-C	5.05	120.86	110.40
1	B	715	ARG	CA-C-N	5.04	127.28	120.38
1	B	715	ARG	C-N-CA	5.04	127.28	120.38
1	E	751	SER	CA-C-N	5.03	127.27	120.38
1	E	751	SER	C-N-CA	5.03	127.27	120.38
1	H	470	ASN	CA-CB-CG	5.02	117.62	112.60
1	C	587	ASP	CA-C-N	5.02	125.65	120.03
1	C	587	ASP	C-N-CA	5.02	125.65	120.03
1	E	741	VAL	CA-CB-CG1	5.01	118.92	110.40

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	MET	Mainchain
1	A	567	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	573	GLY	Mainchain
1	A	768	THR	Peptide
1	A	833	HIS	Mainchain
1	B	463	TYR	Sidechain
1	C	748	LYS	Peptide
1	C	768	THR	Peptide
1	C	810	PRO	Peptide
1	E	804	ASP	Peptide
1	F	501	GLU	Sidechain
1	F	745	TYR	Peptide
1	H	745	TYR	Peptide
1	I	504	ILE	Mainchain
1	I	714	TYR	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	5286	0	5365	16	0
1	B	5177	0	5253	30	0
1	C	5177	0	5253	31	0
1	D	5177	0	5253	21	0
1	E	5177	0	5253	28	0
1	F	5177	0	5253	27	0
1	G	5177	0	5253	40	0
1	H	5177	0	5253	39	0
1	I	5177	0	5253	37	0
All	All	46702	0	47389	230	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (230) 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:H:724:SER:OG	1:I:833:HIS:HE1	1.30	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:724:SER:OG	1:I:833:HIS:CE1	2.19	0.94
1:H:833:HIS:CE1	1:I:724:SER:HB3	2.18	0.79
1:B:833:HIS:NE2	1:G:741:VAL:HG22	2.04	0.73
1:F:730:LEU:HB3	1:F:737:VAL:HG21	1.74	0.70
1:G:798:ASN:OD1	1:H:746:ALA:HB1	1.91	0.70
1:H:720:ASN:HB2	1:I:833:HIS:CD2	2.27	0.69
1:E:730:LEU:HB3	1:E:737:VAL:HG21	1.73	0.69
1:B:826:TYR:CE1	1:C:748:LYS:HA	2.27	0.69
1:G:827:ASN:OD1	1:H:744:LEU:HB3	1.93	0.68
1:H:722:LEU:HD22	1:I:721:GLN:NE2	2.09	0.67
1:C:732:LEU:HD12	1:F:728:VAL:HG13	1.78	0.66
1:C:835:TYR:HB3	1:E:835:TYR:OH	1.95	0.66
1:H:732:LEU:HD21	1:I:732:LEU:CD2	2.26	0.66
1:F:730:LEU:CB	1:F:737:VAL:HG21	2.26	0.66
1:B:833:HIS:CE1	1:G:741:VAL:HG22	2.32	0.64
1:D:605:MET:HE1	1:D:610:HIS:HB2	1.79	0.64
1:G:827:ASN:CG	1:H:744:LEU:HB3	2.22	0.64
1:H:605:MET:HE1	1:H:610:HIS:HB2	1.80	0.64
1:C:832:VAL:HB	1:C:839:CYS:SG	2.38	0.63
1:B:833:HIS:CE1	1:G:741:VAL:CG2	2.84	0.61
1:E:688:GLN:OE1	1:E:691:GLU:OE1	2.19	0.60
1:E:730:LEU:CB	1:E:737:VAL:HG21	2.30	0.60
1:E:203:MET:SD	1:E:555:GLN:HB3	2.41	0.59
1:B:715:ARG:NH1	1:B:774:ARG:NH2	2.51	0.59
1:I:715:ARG:NH1	1:I:774:ARG:NH2	2.52	0.57
1:A:591:LEU:HD12	1:A:594:LEU:HD12	1.84	0.57
1:H:715:ARG:NH1	1:H:774:ARG:NH2	2.51	0.57
1:E:715:ARG:NH1	1:E:774:ARG:NH2	2.51	0.57
1:A:354:GLU:OE2	1:I:310:ASN:CG	2.48	0.57
1:F:203:MET:SD	1:F:555:GLN:HB3	2.45	0.57
1:B:715:ARG:HH22	1:B:774:ARG:HB2	1.70	0.56
1:G:753:LEU:HD23	1:G:784:TRP:CE3	2.40	0.56
1:C:834:ASP:O	1:F:741:VAL:HG13	2.06	0.56
1:A:596:GLU:HG3	1:A:611:ARG:HE	1.73	0.54
1:F:827:ASN:ND2	1:G:745:TYR:O	2.41	0.54
1:H:722:LEU:HD22	1:I:721:GLN:HE22	1.71	0.54
1:B:827:ASN:ND2	1:C:750:ASP:HB2	2.23	0.53
1:A:463:TYR:CD2	1:A:467:ALA:HB2	2.43	0.53
1:H:715:ARG:HH22	1:H:774:ARG:HB2	1.72	0.53
1:E:715:ARG:HH22	1:E:774:ARG:HB2	1.72	0.53
1:I:715:ARG:HH22	1:I:774:ARG:HB2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:781:CYS:SG	1:G:787:LYS:HG2	2.49	0.53
1:A:650:THR:HG22	1:A:654:LEU:HD12	1.91	0.52
1:D:710:VAL:HG11	1:D:764:ILE:HD12	1.92	0.52
1:F:757:ILE:O	1:F:797:LYS:HE3	2.09	0.52
1:G:757:ILE:O	1:G:797:LYS:HE3	2.09	0.52
1:C:757:ILE:O	1:C:797:LYS:HE3	2.09	0.52
1:H:715:ARG:CZ	1:H:774:ARG:CZ	2.88	0.52
1:D:296:LEU:O	1:D:300:THR:HG23	2.09	0.52
1:D:757:ILE:O	1:D:797:LYS:HE3	2.09	0.52
1:H:720:ASN:HB2	1:I:833:HIS:CG	2.44	0.52
1:A:296:LEU:O	1:A:300:THR:HG23	2.09	0.52
1:B:715:ARG:CZ	1:B:774:ARG:CZ	2.88	0.52
1:C:296:LEU:O	1:C:300:THR:HG23	2.10	0.52
1:F:467:ALA:HB1	1:F:504:ILE:HD13	1.92	0.52
1:I:715:ARG:CZ	1:I:774:ARG:CZ	2.88	0.52
1:B:296:LEU:O	1:B:300:THR:HG23	2.10	0.51
1:E:715:ARG:CZ	1:E:774:ARG:CZ	2.88	0.51
1:H:757:ILE:O	1:H:797:LYS:HE3	2.10	0.51
1:H:296:LEU:O	1:H:300:THR:HG23	2.10	0.51
1:I:757:ILE:O	1:I:797:LYS:HE3	2.11	0.51
1:F:460:ALA:HB2	1:F:500:LEU:HD12	1.92	0.51
1:B:793:PHE:CD1	1:B:799:ILE:HD13	2.46	0.50
1:B:719:GLY:HA2	1:B:768:THR:HG21	1.93	0.50
1:C:728:VAL:HG12	1:F:728:VAL:CG1	2.42	0.50
1:D:710:VAL:HB	1:D:737:VAL:HG22	1.93	0.50
1:H:602:ASP:OD2	1:I:607:SER:HB3	2.12	0.50
1:G:296:LEU:O	1:G:300:THR:HG23	2.11	0.50
1:B:827:ASN:HD21	1:C:750:ASP:HB2	1.76	0.49
1:C:722:LEU:N	1:F:721:GLN:OE1	2.45	0.49
1:G:715:ARG:HD3	1:G:771:SER:O	2.12	0.49
1:I:296:LEU:O	1:I:300:THR:HG23	2.11	0.49
1:G:715:ARG:NH1	1:G:774:ARG:HB2	2.27	0.49
1:H:758:GLN:O	1:H:797:LYS:NZ	2.40	0.48
1:C:710:VAL:HG11	1:C:764:ILE:HD12	1.95	0.48
1:F:775:LEU:HD22	1:F:786:HIS:HB2	1.95	0.48
1:H:714:TYR:CE2	1:H:720:ASN:HA	2.49	0.48
1:F:710:VAL:HB	1:F:737:VAL:HG22	1.95	0.48
1:D:730:LEU:HB3	1:D:737:VAL:HG21	1.95	0.48
1:D:758:GLN:O	1:D:797:LYS:NZ	2.42	0.48
1:B:827:ASN:HD21	1:C:750:ASP:CB	2.26	0.48
1:E:767:LEU:HD12	1:E:803:PHE:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:798:ASN:CG	1:H:746:ALA:HB1	2.38	0.48
1:H:762:HIS:CD2	1:H:847:ILE:HG23	2.49	0.48
1:F:296:LEU:O	1:F:300:THR:HG23	2.14	0.47
1:D:766:VAL:HG12	1:D:768:THR:HG23	1.96	0.47
1:G:677:ILE:HD11	1:G:682:HIS:HB3	1.96	0.47
1:F:677:ILE:HD11	1:F:682:HIS:HB3	1.97	0.47
1:I:547:GLU:HG2	1:I:548:GLU:N	2.29	0.47
1:F:793:PHE:HE1	1:F:826:TYR:CZ	2.32	0.47
1:I:758:GLN:O	1:I:797:LYS:NZ	2.42	0.47
1:G:730:LEU:HB3	1:G:737:VAL:HG21	1.96	0.47
1:E:767:LEU:HB3	1:E:807:PHE:CE1	2.50	0.47
1:I:730:LEU:HB3	1:I:737:VAL:HG21	1.97	0.47
1:G:688:GLN:OE1	1:G:691:GLU:OE1	2.33	0.46
1:B:708:ILE:HD12	1:B:759:ALA:HB3	1.97	0.46
1:G:727:LYS:HD2	1:G:739:ILE:CG2	2.45	0.46
1:A:354:GLU:CD	1:I:310:ASN:HA	2.40	0.46
1:B:677:ILE:HD11	1:B:682:HIS:HB3	1.98	0.46
1:B:833:HIS:CE1	1:G:741:VAL:HG21	2.51	0.46
1:F:362:ILE:HA	1:F:365:PHE:CE2	2.50	0.46
1:F:825:LYS:O	1:G:749:PHE:HB2	2.15	0.46
1:E:677:ILE:HD11	1:E:682:HIS:HB3	1.97	0.46
1:C:832:VAL:HG12	1:C:835:TYR:H	1.81	0.46
1:D:833:HIS:CD2	1:E:741:VAL:HG21	2.51	0.46
1:E:743:LYS:HE3	1:E:743:LYS:HA	1.96	0.46
1:H:460:ALA:HB2	1:H:500:LEU:HD12	1.97	0.46
1:C:715:ARG:HD3	1:C:771:SER:HA	1.98	0.46
1:E:236:CYS:HB2	1:E:291:GLU:HB3	1.96	0.46
1:G:723:ALA:HB1	1:G:739:ILE:CD1	2.45	0.46
1:I:772:LEU:HD22	1:I:775:LEU:HD12	1.98	0.46
1:G:710:VAL:HB	1:G:737:VAL:HG22	1.97	0.45
1:G:758:GLN:O	1:G:797:LYS:NZ	2.42	0.45
1:H:463:TYR:CD2	1:H:467:ALA:HB2	2.51	0.45
1:C:714:TYR:CE1	1:C:740:ASP:HB3	2.52	0.45
1:D:236:CYS:HB2	1:D:291:GLU:HB3	1.98	0.45
1:E:463:TYR:CE1	1:E:466:TYR:HB2	2.51	0.45
1:G:463:TYR:CD2	1:G:467:ALA:HB2	2.51	0.45
1:H:730:LEU:HB2	1:H:737:VAL:HG21	1.99	0.45
1:D:719:GLY:HA2	1:D:768:THR:HG21	1.98	0.45
1:B:813:GLU:HG3	1:B:824:THR:HG21	1.98	0.45
1:C:362:ILE:HA	1:C:365:PHE:CE2	2.51	0.45
1:B:772:LEU:HD22	1:B:775:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:724:SER:O	1:F:728:VAL:HG23	2.16	0.45
1:H:715:ARG:NH1	1:H:774:ARG:CZ	2.80	0.45
1:D:362:ILE:HA	1:D:365:PHE:CE2	2.52	0.45
1:G:362:ILE:HA	1:G:365:PHE:CE2	2.52	0.45
1:E:767:LEU:HD11	1:E:801:PRO:HB2	1.98	0.45
1:C:839:CYS:SG	1:E:835:TYR:CZ	3.03	0.45
1:G:719:GLY:HA2	1:G:768:THR:HG21	1.99	0.45
1:G:772:LEU:HD22	1:G:775:LEU:HD12	1.99	0.44
1:I:715:ARG:NH1	1:I:774:ARG:CZ	2.80	0.44
1:B:715:ARG:NH1	1:B:774:ARG:CZ	2.80	0.44
1:B:745:TYR:O	1:I:827:ASN:HB3	2.17	0.44
1:D:730:LEU:CB	1:D:737:VAL:HG21	2.46	0.44
1:B:362:ILE:HA	1:B:365:PHE:CE2	2.52	0.44
1:H:677:ILE:HD11	1:H:682:HIS:HB3	1.99	0.44
1:H:772:LEU:HD22	1:H:775:LEU:HD12	1.98	0.44
1:B:668:ASP:CG	1:B:683:ARG:HE	2.26	0.44
1:E:715:ARG:NH1	1:E:774:ARG:CZ	2.80	0.44
1:D:668:ASP:CG	1:D:683:ARG:HE	2.26	0.44
1:I:236:CYS:HB2	1:I:291:GLU:HB3	1.98	0.44
1:I:668:ASP:CG	1:I:683:ARG:HE	2.26	0.44
1:B:826:TYR:CD1	1:C:748:LYS:HA	2.51	0.44
1:C:236:CYS:HB2	1:C:291:GLU:HB3	1.99	0.44
1:E:547:GLU:HG2	1:E:548:GLU:N	2.33	0.44
1:G:318:MET:SD	1:G:338:ILE:HG12	2.58	0.44
1:I:362:ILE:HA	1:I:365:PHE:CE2	2.53	0.44
1:A:668:ASP:CG	1:A:683:ARG:HE	2.26	0.43
1:D:677:ILE:HD11	1:D:682:HIS:HB3	2.00	0.43
1:H:362:ILE:HA	1:H:365:PHE:CE2	2.53	0.43
1:A:354:GLU:OE2	1:I:310:ASN:OD1	2.35	0.43
1:G:236:CYS:HB2	1:G:291:GLU:HB3	2.00	0.43
1:H:762:HIS:NE2	1:H:847:ILE:HG23	2.33	0.43
1:B:221:PHE:CZ	1:B:269:TYR:HB3	2.54	0.43
1:B:236:CYS:HB2	1:B:291:GLU:HB3	2.01	0.43
1:C:668:ASP:CG	1:C:683:ARG:HE	2.25	0.43
1:A:596:GLU:HG3	1:A:611:ARG:NE	2.33	0.43
1:E:749:PHE:CE1	1:E:753:LEU:HD22	2.53	0.43
1:G:668:ASP:CG	1:G:683:ARG:HE	2.26	0.43
1:G:813:GLU:HG3	1:G:824:THR:HG21	2.00	0.43
1:C:677:ILE:HD11	1:C:682:HIS:HB3	2.00	0.43
1:C:710:VAL:HB	1:C:737:VAL:HG22	1.99	0.43
1:G:547:GLU:HG2	1:G:548:GLU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:663:LEU:HB2	1:I:690:PHE:CZ	2.54	0.43
1:G:730:LEU:CB	1:G:737:VAL:HG21	2.49	0.43
1:F:463:TYR:CD2	1:F:467:ALA:HB2	2.54	0.43
1:H:236:CYS:HB2	1:H:291:GLU:HB3	2.01	0.43
1:D:805:THR:HG23	1:D:830:LYS:NZ	2.33	0.43
1:E:668:ASP:CG	1:E:683:ARG:HE	2.26	0.43
1:F:236:CYS:HB2	1:F:291:GLU:HB3	2.01	0.43
1:G:710:VAL:HG11	1:G:764:ILE:HD12	2.00	0.43
1:C:778:ASP:O	1:C:786:HIS:ND1	2.52	0.43
1:I:723:ALA:HB1	1:I:739:ILE:HD11	2.01	0.43
1:E:463:TYR:CD2	1:E:467:ALA:HB2	2.54	0.42
1:H:668:ASP:CG	1:H:683:ARG:HE	2.25	0.42
1:H:813:GLU:HG3	1:H:824:THR:HG21	2.00	0.42
1:H:833:HIS:CE1	1:I:724:SER:CB	2.97	0.42
1:C:270:PHE:CZ	1:C:304:ASN:HB3	2.55	0.42
1:I:677:ILE:HD11	1:I:682:HIS:HB3	2.02	0.42
1:I:730:LEU:CB	1:I:737:VAL:HG21	2.49	0.42
1:F:826:TYR:CE1	1:G:748:LYS:HG3	2.53	0.42
1:A:270:PHE:CZ	1:A:304:ASN:HB3	2.55	0.42
1:F:668:ASP:CG	1:F:683:ARG:HE	2.26	0.42
1:H:579:GLU:HG3	1:H:580:LYS:N	2.35	0.42
1:B:463:TYR:CD2	1:B:467:ALA:HB2	2.53	0.42
1:B:827:ASN:CG	1:C:744:LEU:HB3	2.45	0.42
1:I:813:GLU:HG3	1:I:824:THR:HG21	2.01	0.42
1:D:557:VAL:N	1:D:558:PRO:CD	2.83	0.42
1:F:735:TYR:HB2	1:F:737:VAL:HG23	2.02	0.42
1:G:463:TYR:CE1	1:G:466:TYR:HB2	2.55	0.42
1:C:749:PHE:CZ	1:C:784:TRP:CD1	3.07	0.41
1:H:805:THR:HG23	1:H:830:LYS:NZ	2.35	0.41
1:C:607:SER:HB2	1:C:610:HIS:HB2	2.02	0.41
1:A:221:PHE:CZ	1:A:269:TYR:HB3	2.55	0.41
1:C:557:VAL:N	1:C:558:PRO:CD	2.84	0.41
1:I:605:MET:HE3	1:I:611:ARG:HG2	2.01	0.41
1:D:720:ASN:HB2	1:E:833:HIS:CG	2.54	0.41
1:F:557:VAL:N	1:F:558:PRO:CD	2.84	0.41
1:F:715:ARG:HB2	1:F:771:SER:HA	2.02	0.41
1:G:270:PHE:CZ	1:G:304:ASN:HB3	2.55	0.41
1:A:405:TRP:CE2	1:A:732:LEU:HD11	2.55	0.41
1:C:547:GLU:HG2	1:C:548:GLU:N	2.36	0.41
1:E:270:PHE:CZ	1:E:304:ASN:HB3	2.55	0.41
1:I:577:TYR:CE1	1:I:605:MET:HG2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:PHE:CZ	1:E:269:TYR:HB3	2.56	0.41
1:A:557:VAL:N	1:A:558:PRO:CD	2.83	0.41
1:A:772:LEU:HD12	1:A:810:PRO:HD3	2.03	0.41
1:F:671:MET:O	1:F:677:ILE:HG22	2.21	0.41
1:I:557:VAL:N	1:I:558:PRO:CD	2.84	0.41
1:B:270:PHE:CZ	1:B:304:ASN:HB3	2.55	0.41
1:B:557:VAL:N	1:B:558:PRO:CD	2.84	0.41
1:C:318:MET:SD	1:C:338:ILE:HG12	2.61	0.41
1:D:221:PHE:CZ	1:D:269:TYR:HB3	2.56	0.41
1:H:270:PHE:CZ	1:H:304:ASN:HB3	2.55	0.41
1:I:587:ASP:H	1:I:590:LEU:HB2	1.85	0.41
1:E:557:VAL:N	1:E:558:PRO:CD	2.84	0.41
1:G:557:VAL:N	1:G:558:PRO:CD	2.84	0.41
1:E:710:VAL:HB	1:E:737:VAL:HG22	2.03	0.40
1:E:768:THR:OG1	1:E:771:SER:HB3	2.21	0.40
1:A:650:THR:HG22	1:A:654:LEU:CD1	2.52	0.40
1:B:671:MET:O	1:B:677:ILE:HG22	2.21	0.40
1:G:478:LEU:HD13	1:G:497:HIS:CE1	2.56	0.40
1:D:463:TYR:CE2	1:D:467:ALA:HB2	2.57	0.40
1:D:406:LEU:HB3	1:D:425:VAL:HG13	2.04	0.40
1:G:671:MET:O	1:G:677:ILE:HG22	2.22	0.40
1:H:557:VAL:N	1:H:558:PRO:CD	2.84	0.40
1:H:607:SER:HB2	1:H:610:HIS:HB2	2.03	0.40
1:I:508:GLN:NE2	1:I:510:LYS:HE3	2.35	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	657/738 (89%)	629 (96%)	28 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	641/738 (87%)	613 (96%)	28 (4%)	0	100	100
1	C	641/738 (87%)	608 (95%)	33 (5%)	0	100	100
1	D	641/738 (87%)	610 (95%)	31 (5%)	0	100	100
1	E	641/738 (87%)	607 (95%)	34 (5%)	0	100	100
1	F	641/738 (87%)	614 (96%)	27 (4%)	0	100	100
1	G	641/738 (87%)	613 (96%)	28 (4%)	0	100	100
1	H	641/738 (87%)	618 (96%)	23 (4%)	0	100	100
1	I	641/738 (87%)	613 (96%)	28 (4%)	0	100	100
All	All	5785/6642 (87%)	5525 (96%)	260 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	586/660 (89%)	579 (99%)	7 (1%)	63	71
1	B	572/660 (87%)	563 (98%)	9 (2%)	55	68
1	C	572/660 (87%)	555 (97%)	17 (3%)	36	57
1	D	572/660 (87%)	560 (98%)	12 (2%)	47	64
1	E	572/660 (87%)	560 (98%)	12 (2%)	47	64
1	F	572/660 (87%)	564 (99%)	8 (1%)	59	70
1	G	572/660 (87%)	559 (98%)	13 (2%)	44	63
1	H	572/660 (87%)	562 (98%)	10 (2%)	53	67
1	I	572/660 (87%)	562 (98%)	10 (2%)	53	67
All	All	5162/5940 (87%)	5064 (98%)	98 (2%)	49	66

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	SER
1	A	297	GLU
1	A	314	THR
1	A	442	ASP
1	A	471	THR
1	A	473	GLU
1	A	598	ASP
1	B	252	VAL
1	B	282	THR
1	B	297	GLU
1	B	314	THR
1	B	557	VAL
1	B	565	VAL
1	B	585	MET
1	B	686	LEU
1	B	826	TYR
1	C	282	THR
1	C	314	THR
1	C	425	VAL
1	C	500	LEU
1	C	557	VAL
1	C	565	VAL
1	C	576	GLU
1	C	585	MET
1	C	721	GLN
1	C	735	TYR
1	C	750	ASP
1	C	769	PRO
1	C	822	MET
1	C	826	TYR
1	C	833	HIS
1	C	834	ASP
1	C	836	GLN
1	D	282	THR
1	D	314	THR
1	D	557	VAL
1	D	565	VAL
1	D	585	MET
1	D	605	MET
1	D	612	LYS
1	D	686	LEU
1	D	721	GLN
1	D	782	GLU

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Mol	Chain	Res	Type
1	D	826	TYR
1	D	836	GLN
1	E	282	THR
1	E	300	THR
1	E	314	THR
1	E	500	LEU
1	E	557	VAL
1	E	565	VAL
1	E	585	MET
1	E	605	MET
1	E	675	CYS
1	E	686	LEU
1	E	774	ARG
1	E	832	VAL
1	F	282	THR
1	F	314	THR
1	F	500	LEU
1	F	501	GLU
1	F	557	VAL
1	F	565	VAL
1	F	585	MET
1	F	782	GLU
1	G	251	LYS
1	G	282	THR
1	G	314	THR
1	G	497	HIS
1	G	557	VAL
1	G	565	VAL
1	G	576	GLU
1	G	585	MET
1	G	686	LEU
1	G	724	SER
1	G	742	ASP
1	G	826	TYR
1	G	836	GLN
1	H	282	THR
1	H	297	GLU
1	H	314	THR
1	H	500	LEU
1	H	557	VAL
1	H	565	VAL
1	H	602	ASP

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Mol	Chain	Res	Type
1	H	605	MET
1	H	774	ARG
1	H	826	TYR
1	I	253	SER
1	I	297	GLU
1	I	314	THR
1	I	425	VAL
1	I	557	VAL
1	I	565	VAL
1	I	686	LEU
1	I	750	ASP
1	I	774	ARG
1	I	826	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	199	GLN
1	A	331	GLN
1	A	464	HIS
1	A	468	GLN
1	A	509	ASN
1	A	555	GLN
1	A	597	ASN
1	A	707	GLN
1	A	720	ASN
1	A	777	ASN
1	B	231	ASN
1	B	331	GLN
1	B	593	GLN
1	B	770	ASN
1	B	777	ASN
1	B	815	GLN
1	C	331	GLN
1	C	707	GLN
1	D	331	GLN
1	D	707	GLN
1	D	777	ASN
1	D	795	HIS
1	E	281	ASN
1	E	331	GLN

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Mol	Chain	Res	Type
1	E	464	HIS
1	E	468	GLN
1	E	508	GLN
1	E	777	ASN
1	E	798	ASN
1	E	815	GLN
1	F	196	ASN
1	F	331	GLN
1	F	673	ASN
1	F	756	ASN
1	F	777	ASN
1	G	331	GLN
1	G	464	HIS
1	G	497	HIS
1	G	770	ASN
1	G	777	ASN
1	H	331	GLN
1	H	468	GLN
1	H	593	GLN
1	H	770	ASN
1	H	777	ASN
1	H	815	GLN
1	I	231	ASN
1	I	331	GLN
1	I	468	GLN
1	I	508	GLN
1	I	721	GLN
1	I	770	ASN
1	I	777	ASN
1	I	833	HIS

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 [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.

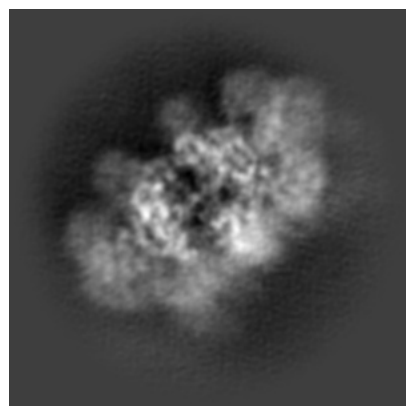
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17370. These allow visual inspection of the internal detail of the map and identification of artifacts.

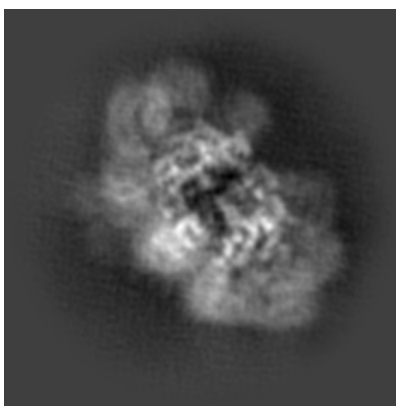
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

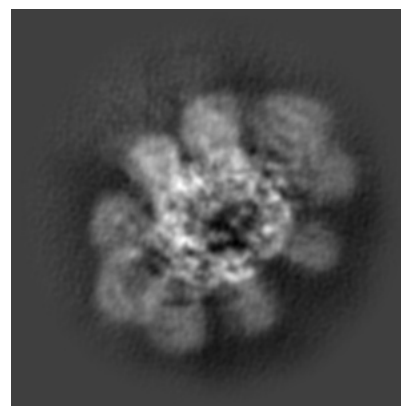
6.1.1 Primary map



X

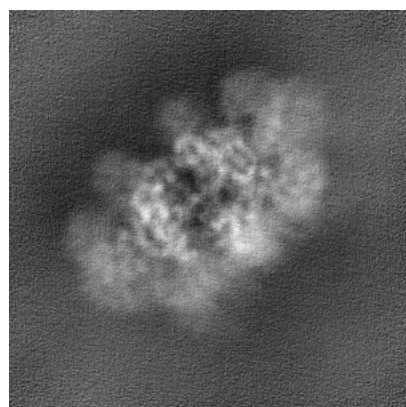


Y

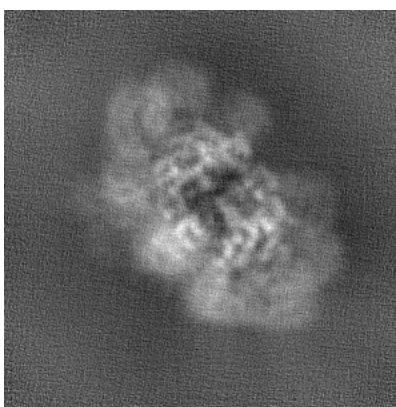


Z

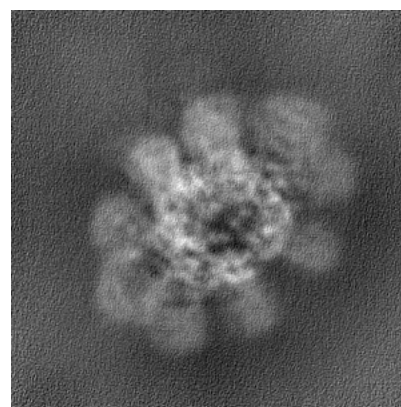
6.1.2 Raw map



X



Y

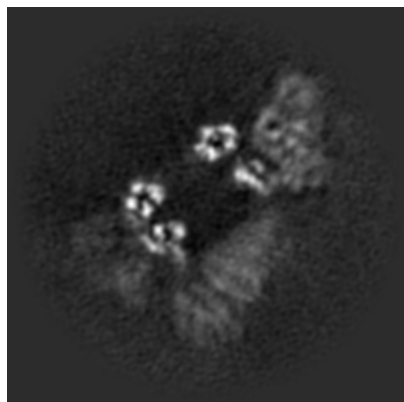


Z

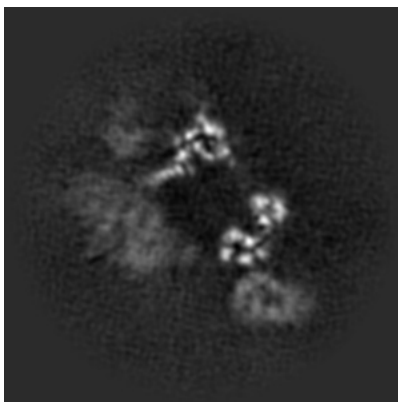
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

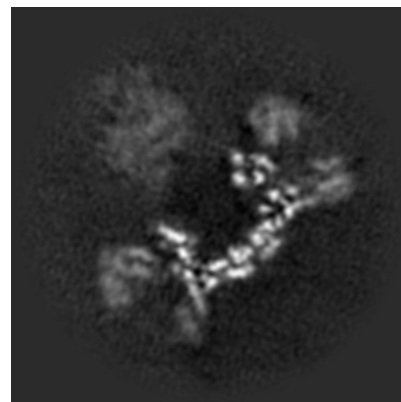
6.2.1 Primary map



X Index: 160

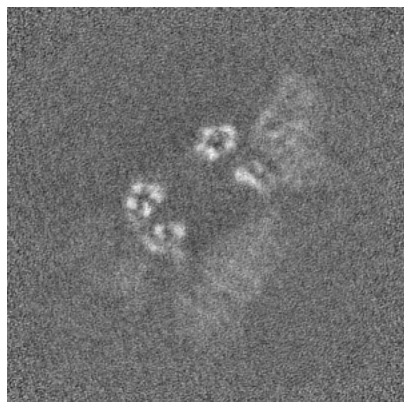


Y Index: 160

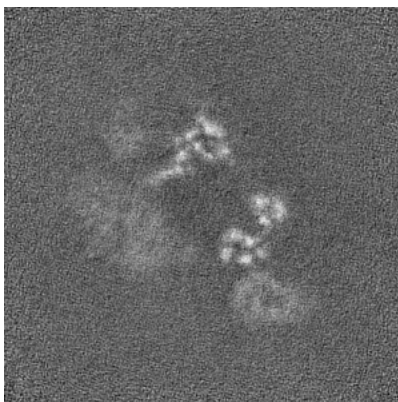


Z Index: 160

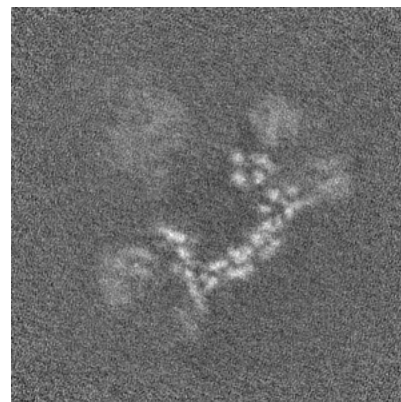
6.2.2 Raw map



X Index: 160



Y Index: 160

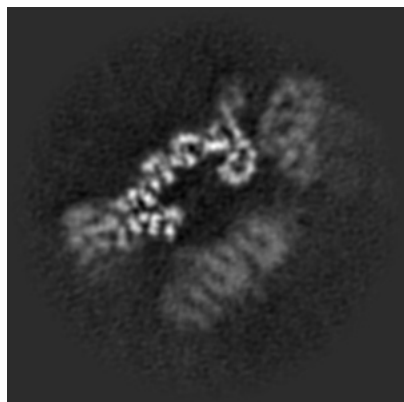


Z Index: 160

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

6.3 Largest variance slices [i](#)

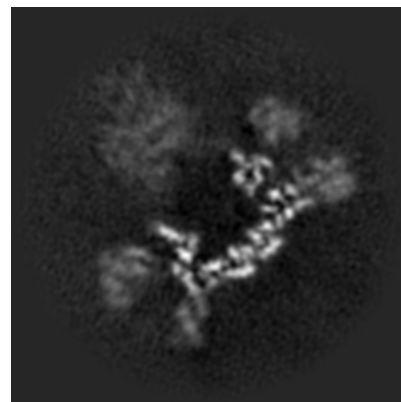
6.3.1 Primary map



X Index: 147

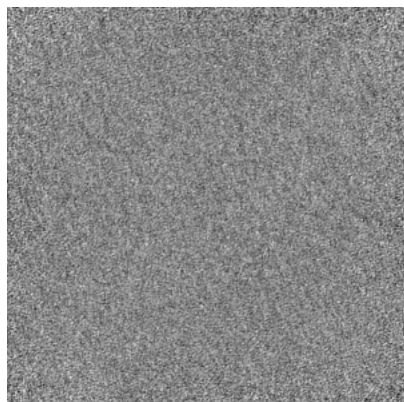


Y Index: 183

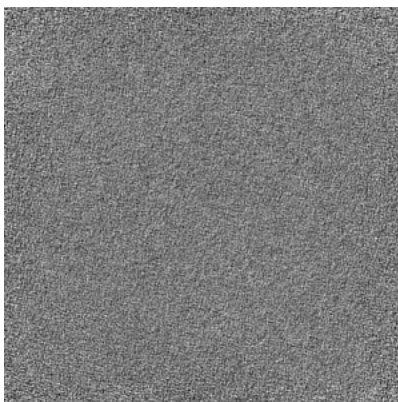


Z Index: 158

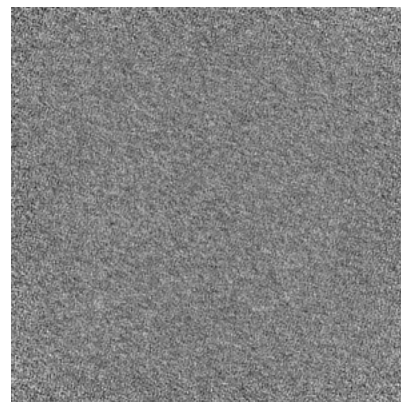
6.3.2 Raw map



X Index: 0



Y Index: 0

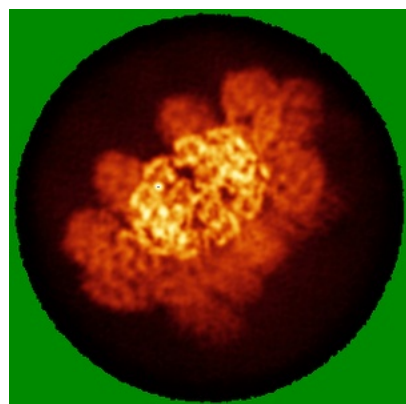


Z Index: 0

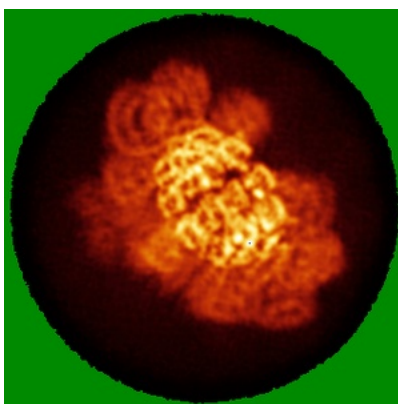
The images above show the largest variance slices of the map in three orthogonal directions.

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

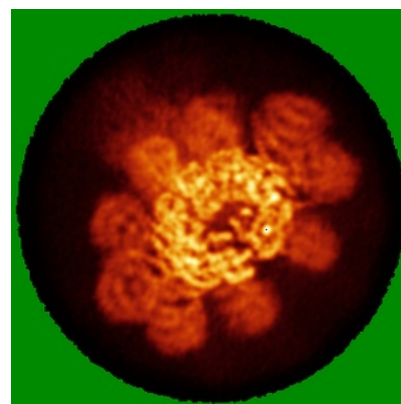
6.4.1 Primary map



X

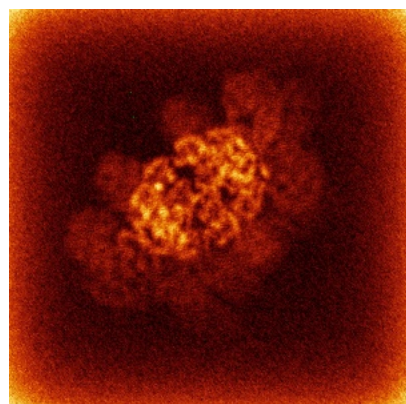


Y

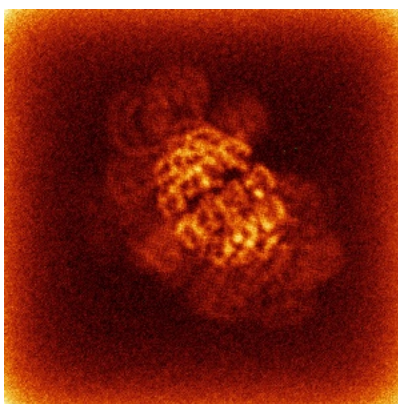


Z

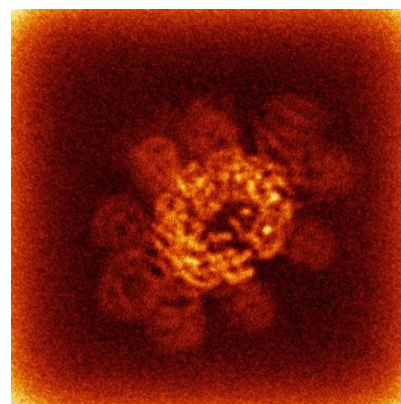
6.4.2 Raw map



X



Y

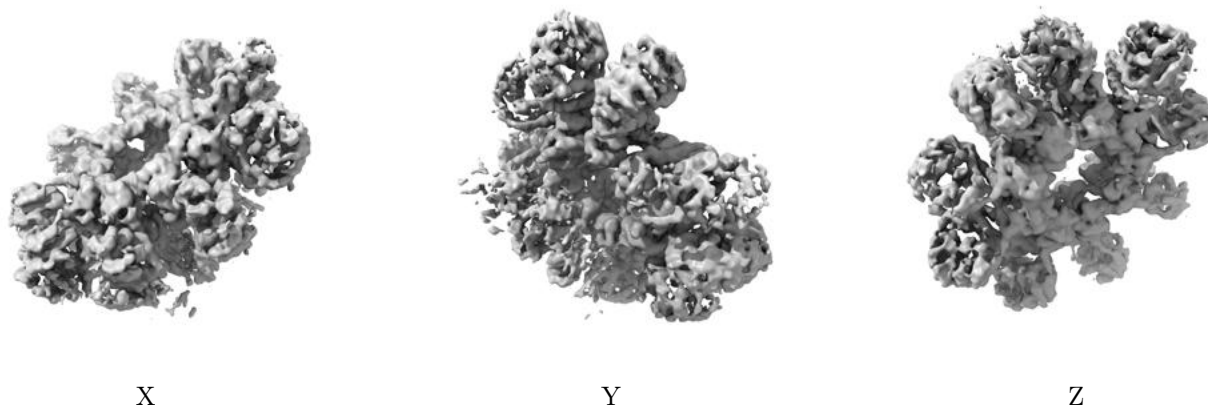


Z

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

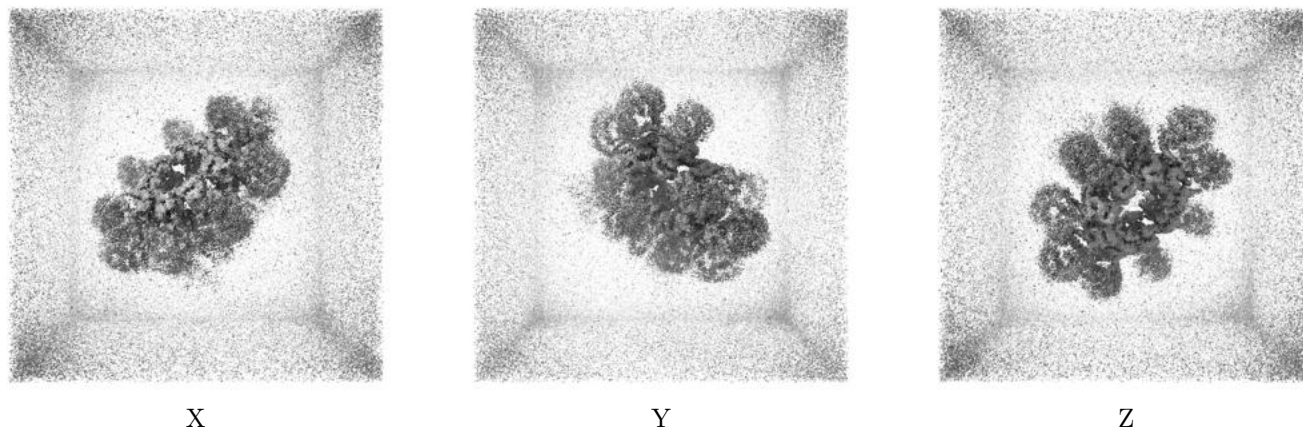
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

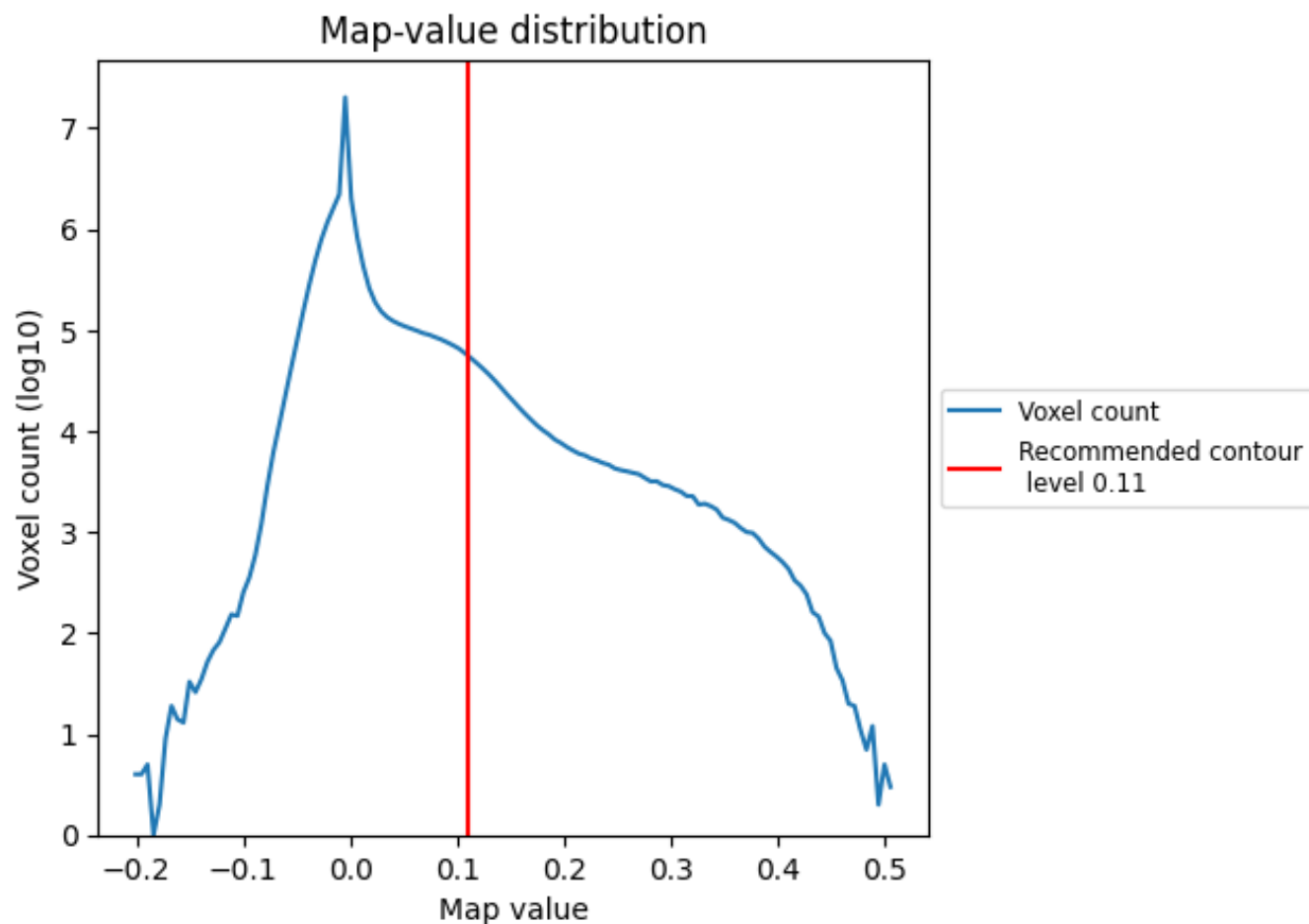
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

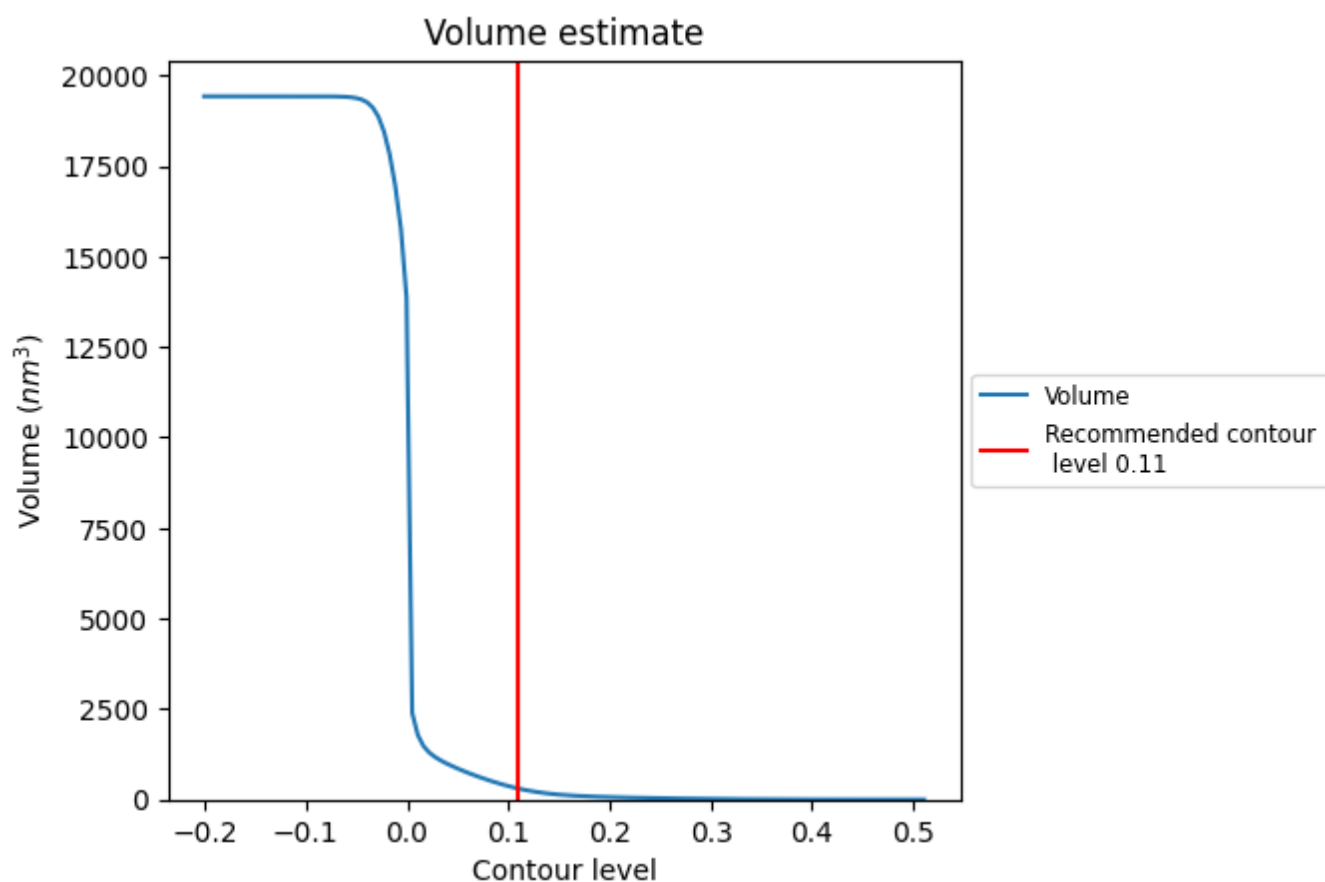
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

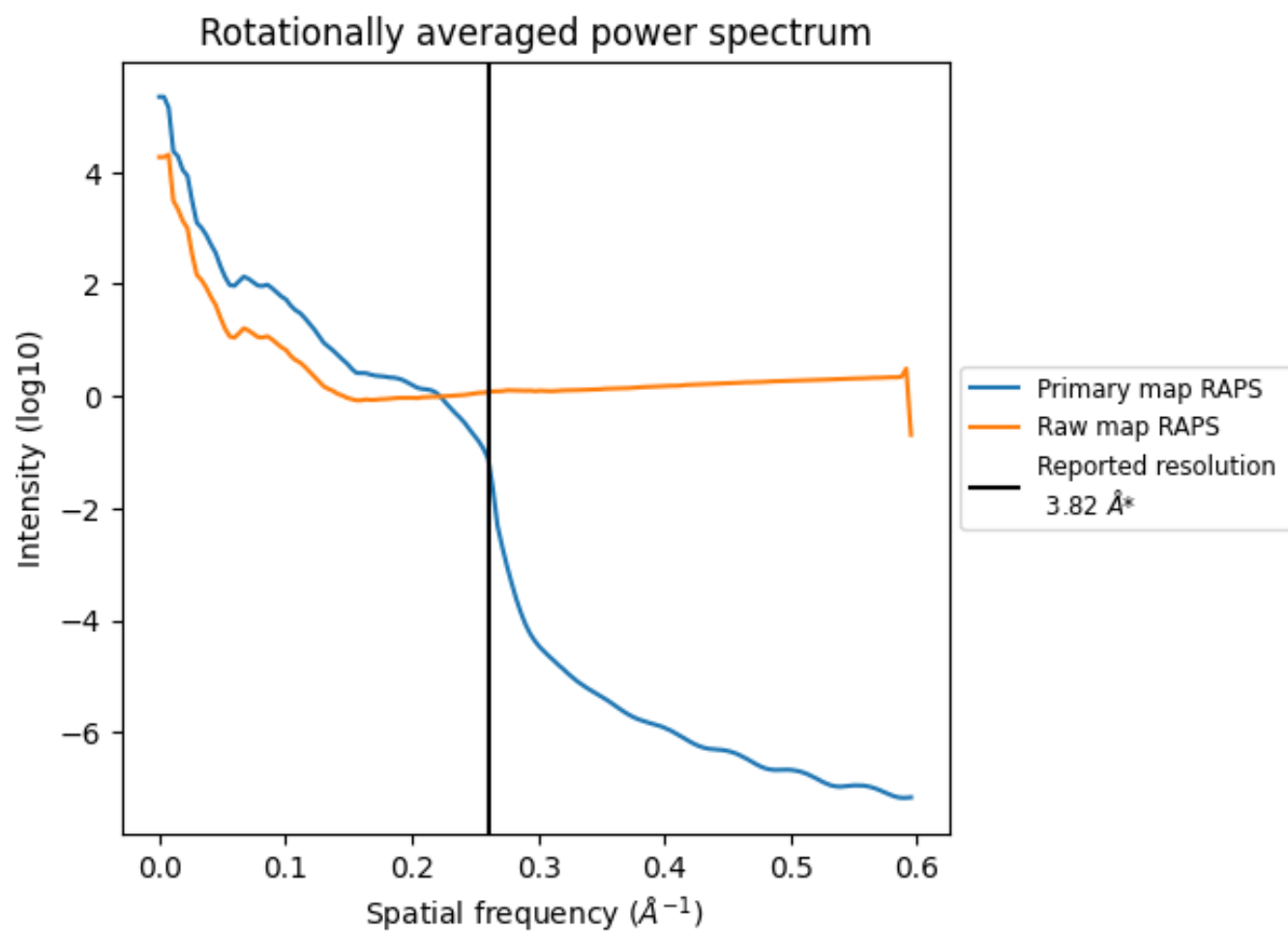
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 304 nm³; this corresponds to an approximate mass of 275 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 ⓘ

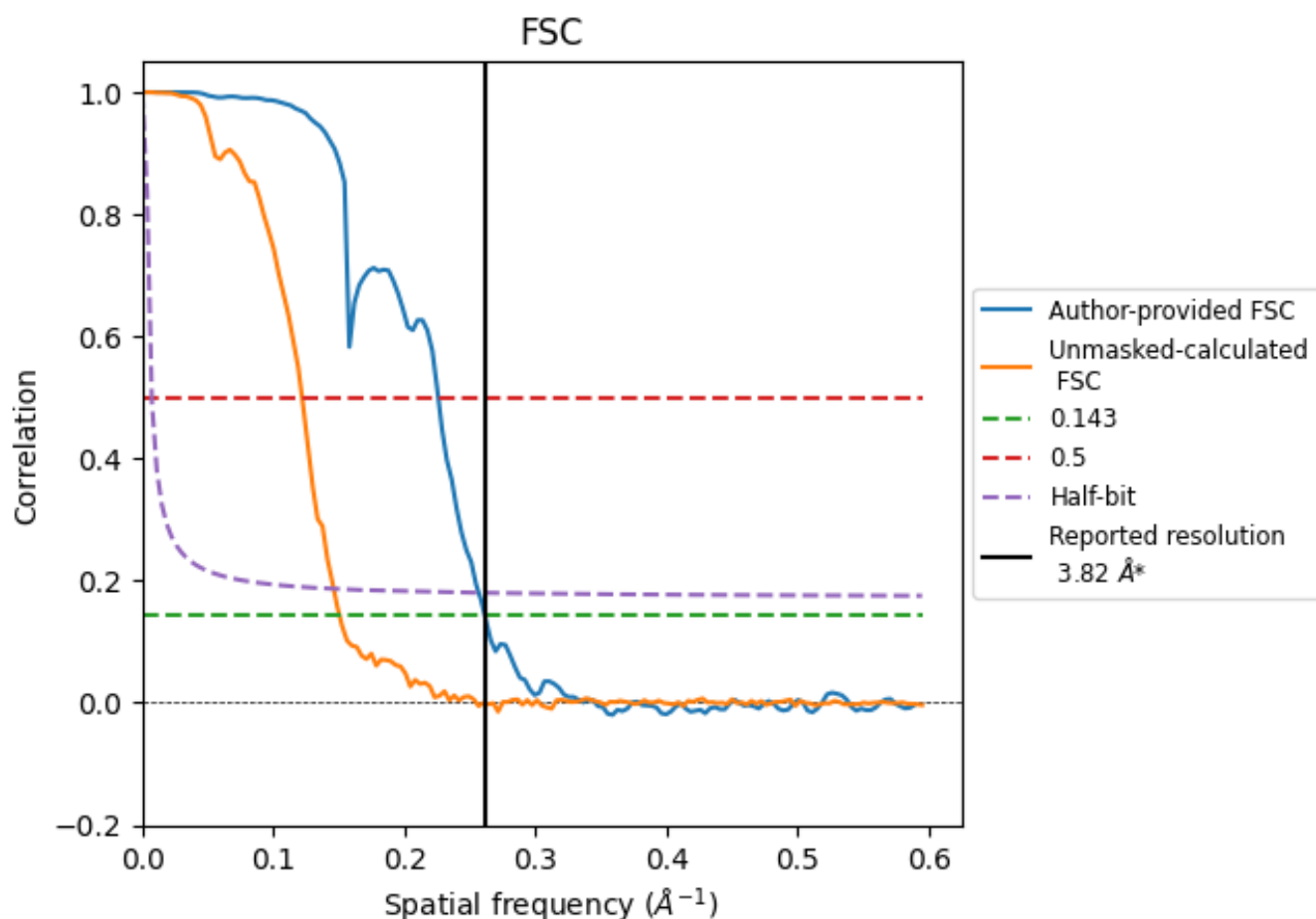


*Reported resolution corresponds to spatial frequency of 0.262 $\text{\AA}^{-1}$

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 0.262 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

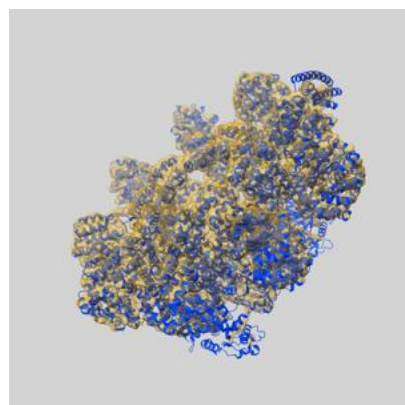
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.82	-	-
Author-provided FSC curve	3.83	4.43	3.89
Unmasked-calculated*	6.64	8.20	6.84

*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 6.64 differs from the reported value 3.82 by more than 10 %

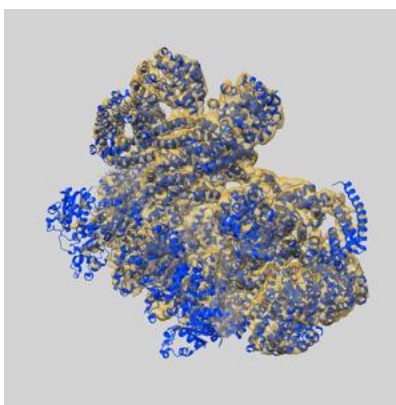
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17370 and PDB model 8P2M. Per-residue inclusion information can be found in section 3 on page 11.

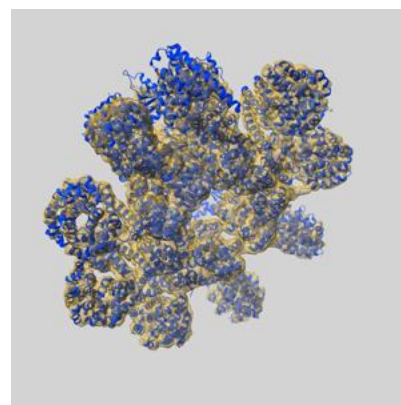
9.1 Map-model overlay [i](#)



X



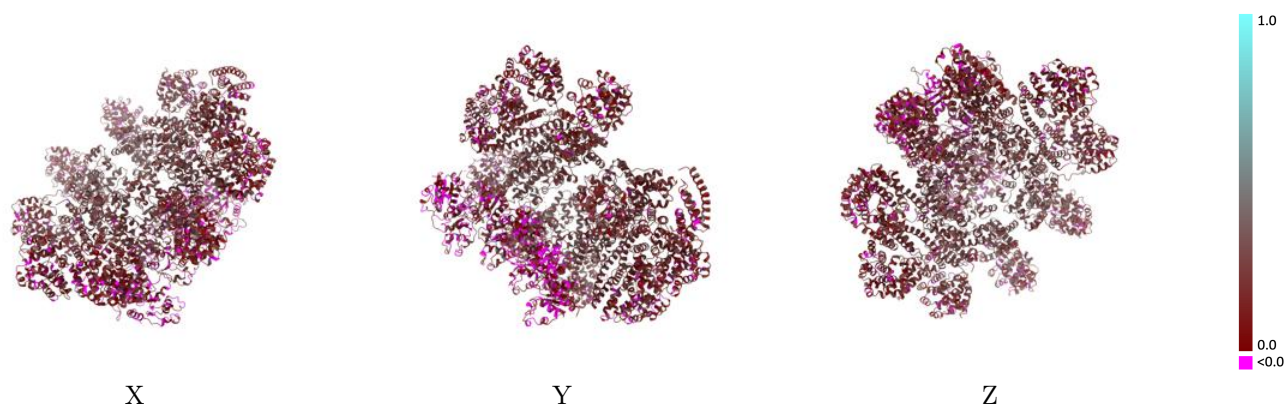
Y



Z

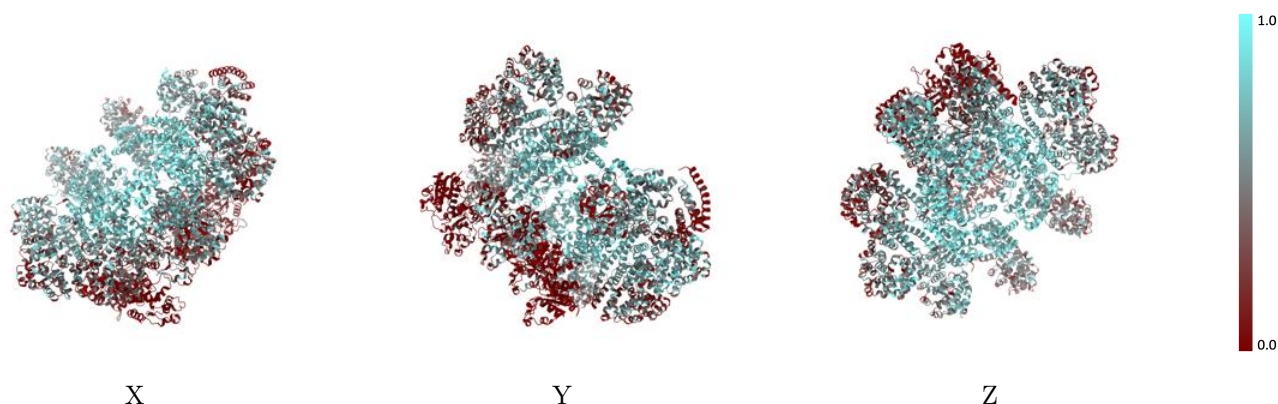
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



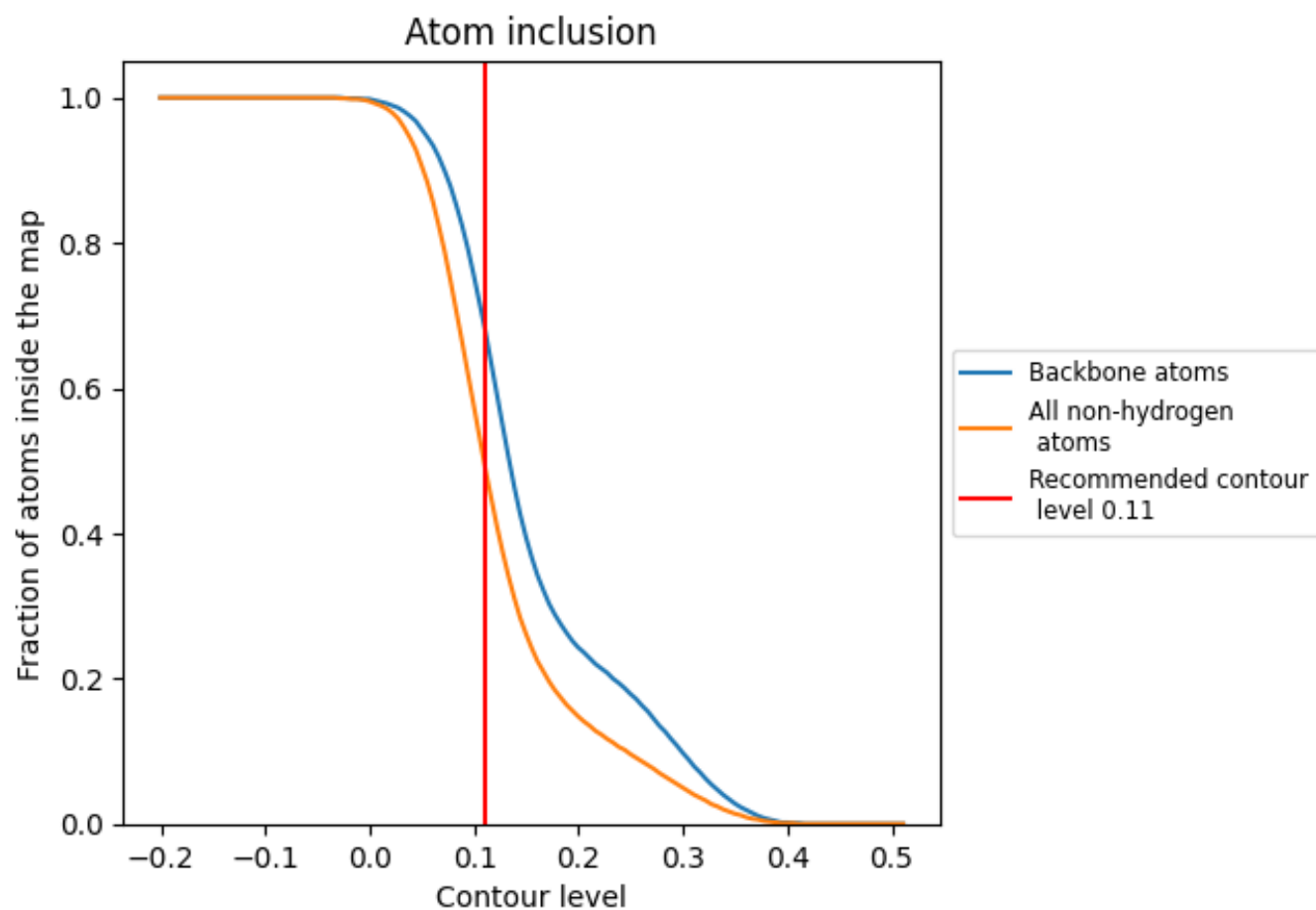
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 49% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4940	0.1820
A	0.4640	0.2100
B	0.5200	0.1810
C	0.5230	0.1940
D	0.3950	0.1650
E	0.4460	0.1720
F	0.5910	0.1940
G	0.5330	0.1840
H	0.4150	0.1660
I	0.5550	0.1720

1.0

0.0

<0.0