



Full wwPDB EM Validation Report (i)

Aug 29, 2023 – 02:04 pm BST

PDB ID : 8P2M
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 (i) 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 \(i\)](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev50
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

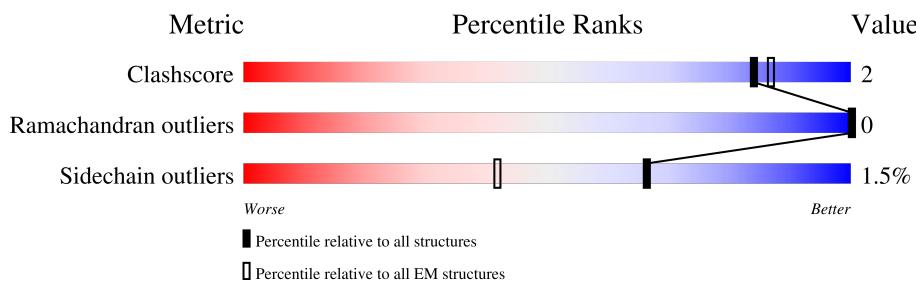
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

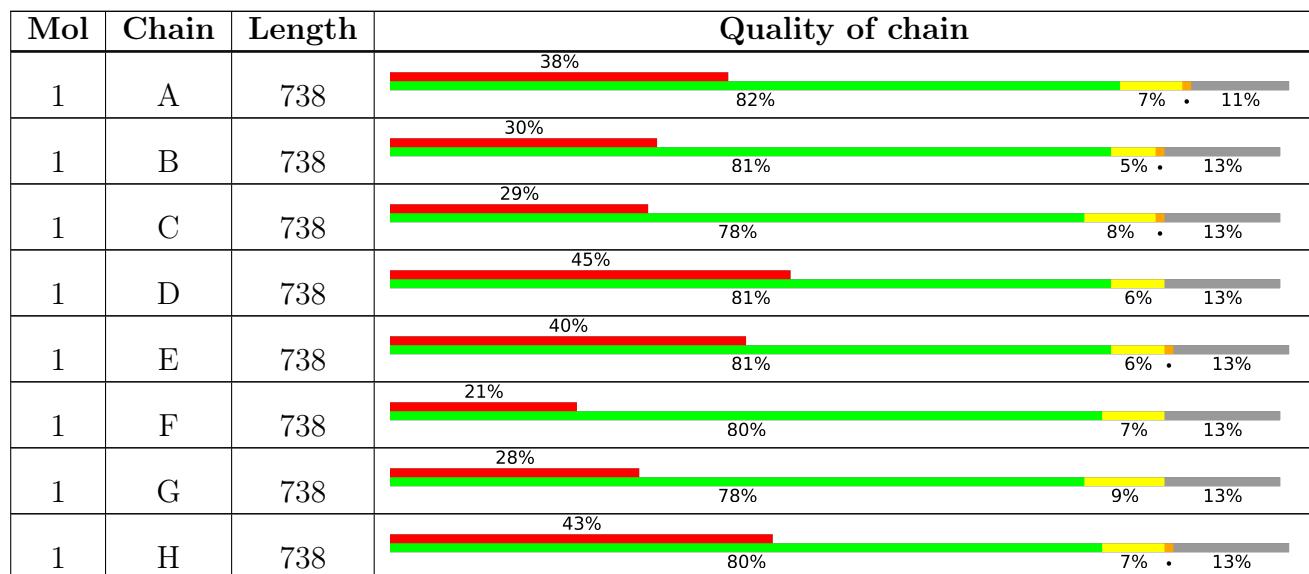
The reported resolution of this entry is 3.82 Å.

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.



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Mol	Chain	Length	Quality of chain		
1	I	738	24%	79%	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
			Total	C	N	O	S		
1	A	659	5286	3376	894	981	35	0	0
1	B	645	5177	3308	878	957	34	0	0
1	C	645	5177	3308	878	957	34	0	0
1	D	645	5177	3308	878	957	34	0	0
1	E	645	5177	3308	878	957	34	0	0
1	F	645	5177	3308	878	957	34	0	0
1	G	645	5177	3308	878	957	34	0	0
1	H	645	5177	3308	878	957	34	0	0
1	I	645	5177	3308	878	957	34	0	0

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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Chain	Residue	Modelled	Actual	Comment	Reference
G	153	LEU	-	expression tag	UNP Q86DA5
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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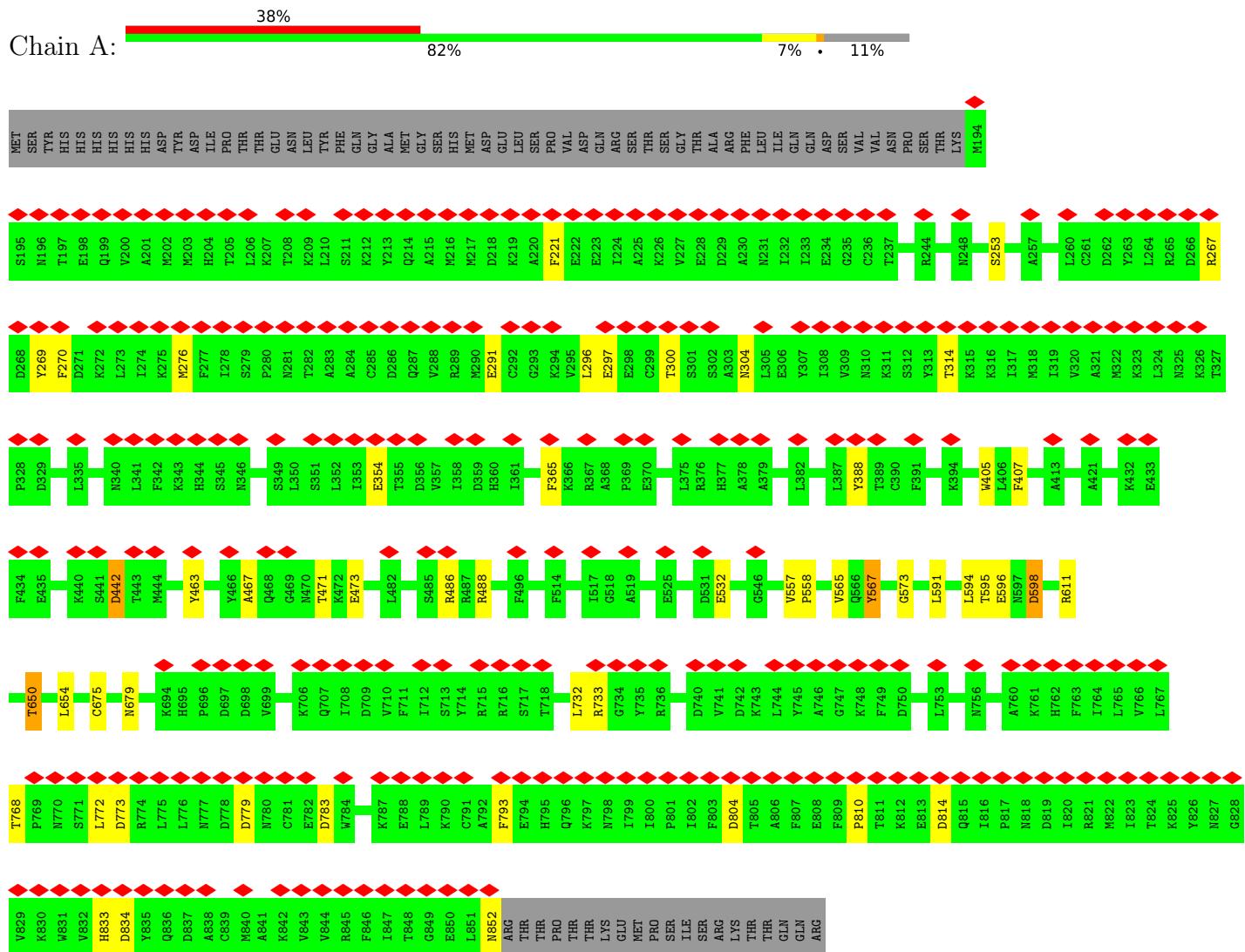
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Chain	Residue	Modelled	Actual	Comment	Reference
I	141	HIS	-	expression tag	UNP Q86DA5
I	142	HIS	-	expression tag	UNP Q86DA5
I	143	HIS	-	expression tag	UNP Q86DA5
I	144	ASP	-	expression tag	UNP Q86DA5
I	145	TYR	-	expression tag	UNP Q86DA5
I	146	ASP	-	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
I	159	MET	-	expression tag	UNP Q86DA5
I	160	GLY	-	expression tag	UNP Q86DA5
I	161	SER	-	expression tag	UNP Q86DA5

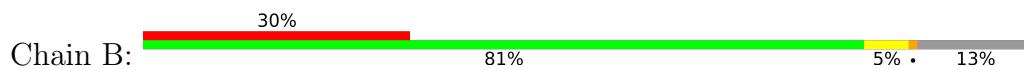
3 Residue-property plots [\(i\)](#)

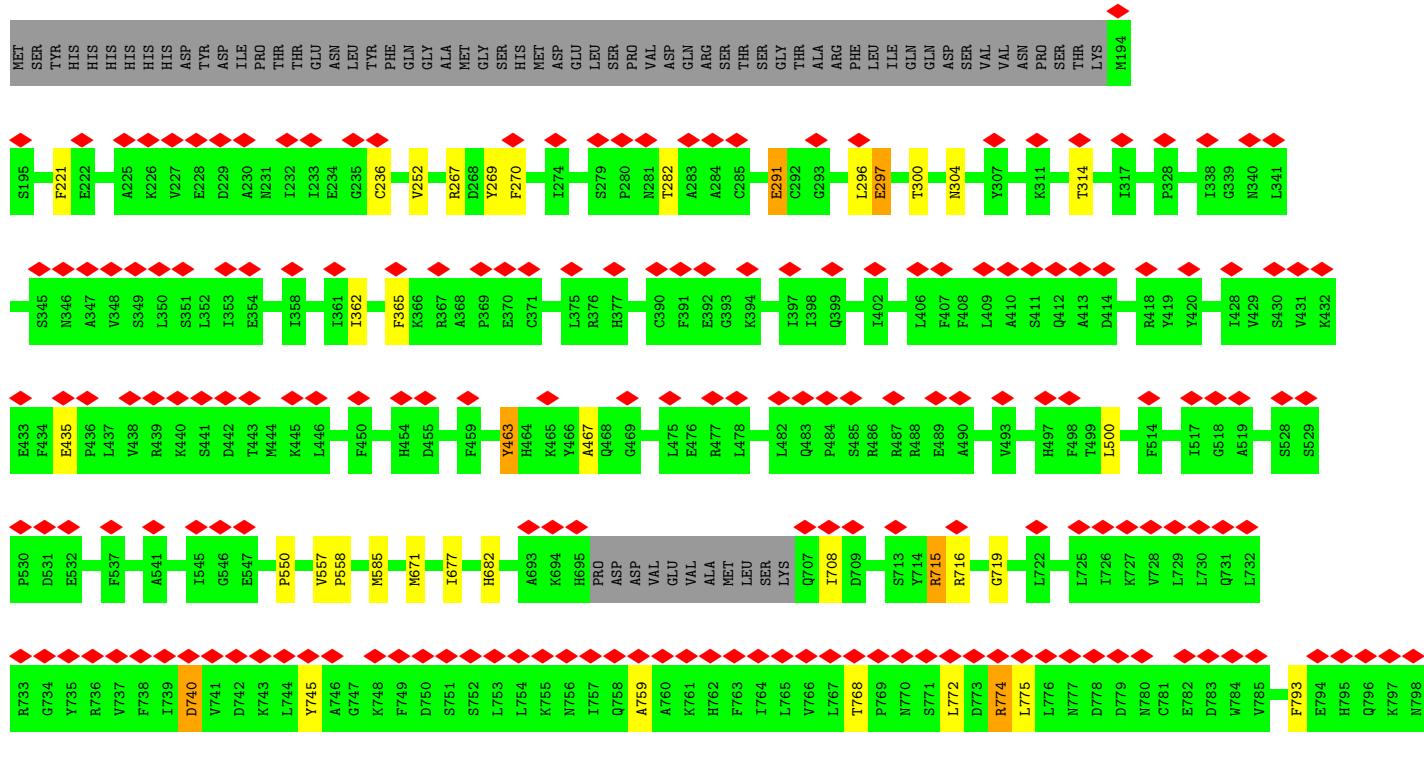
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: NAD(+) hydrolase tir-1



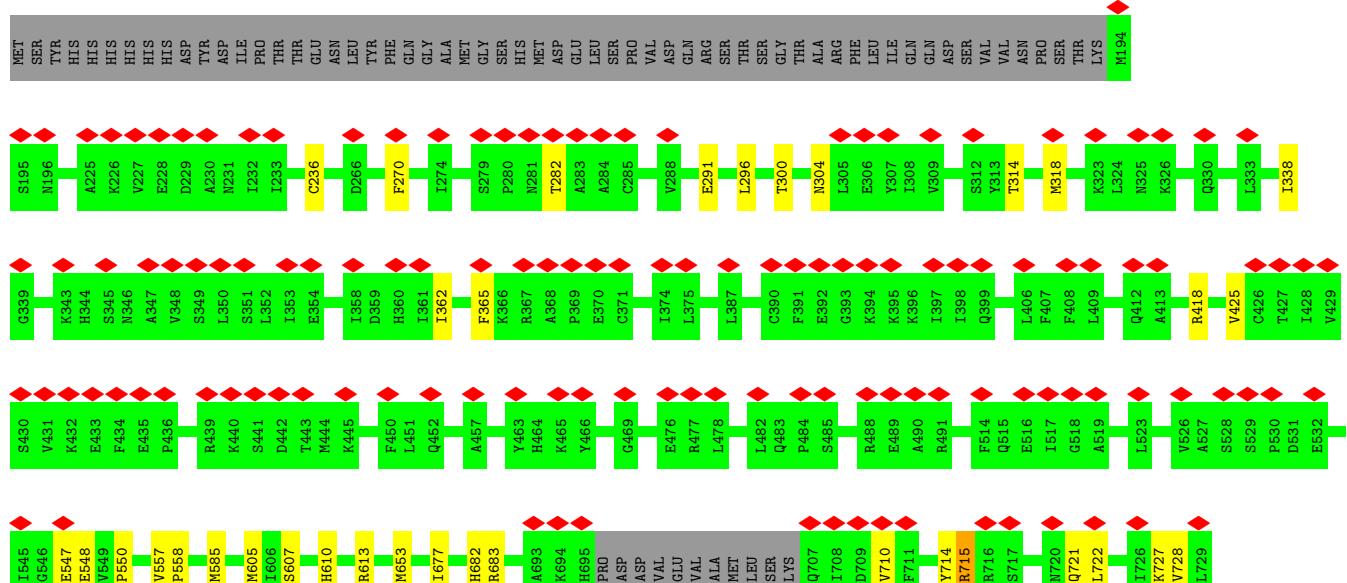
- Molecule 1: NAD(+) hydrolase tir-1

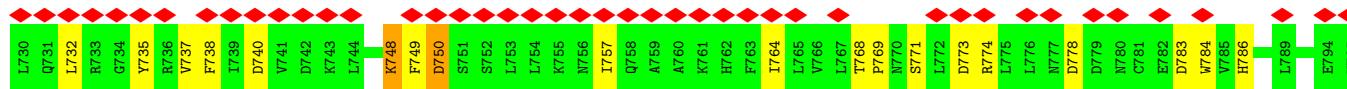




- Molecule 1: NAD(+) hydrolase tir-1

Chain C: 29% 78% 8% 13%

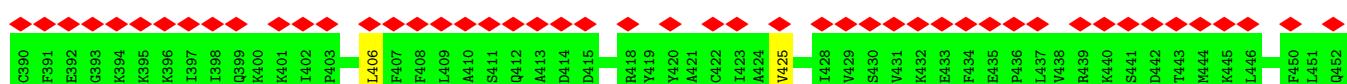
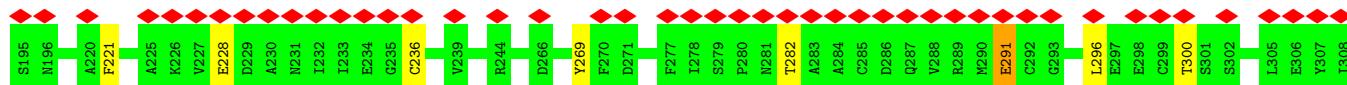




- Molecule 1: NAD(+) hydrolase tir-1

A horizontal bar chart titled "Chain D" showing its distribution across four categories. The total length of the bar is 100%.

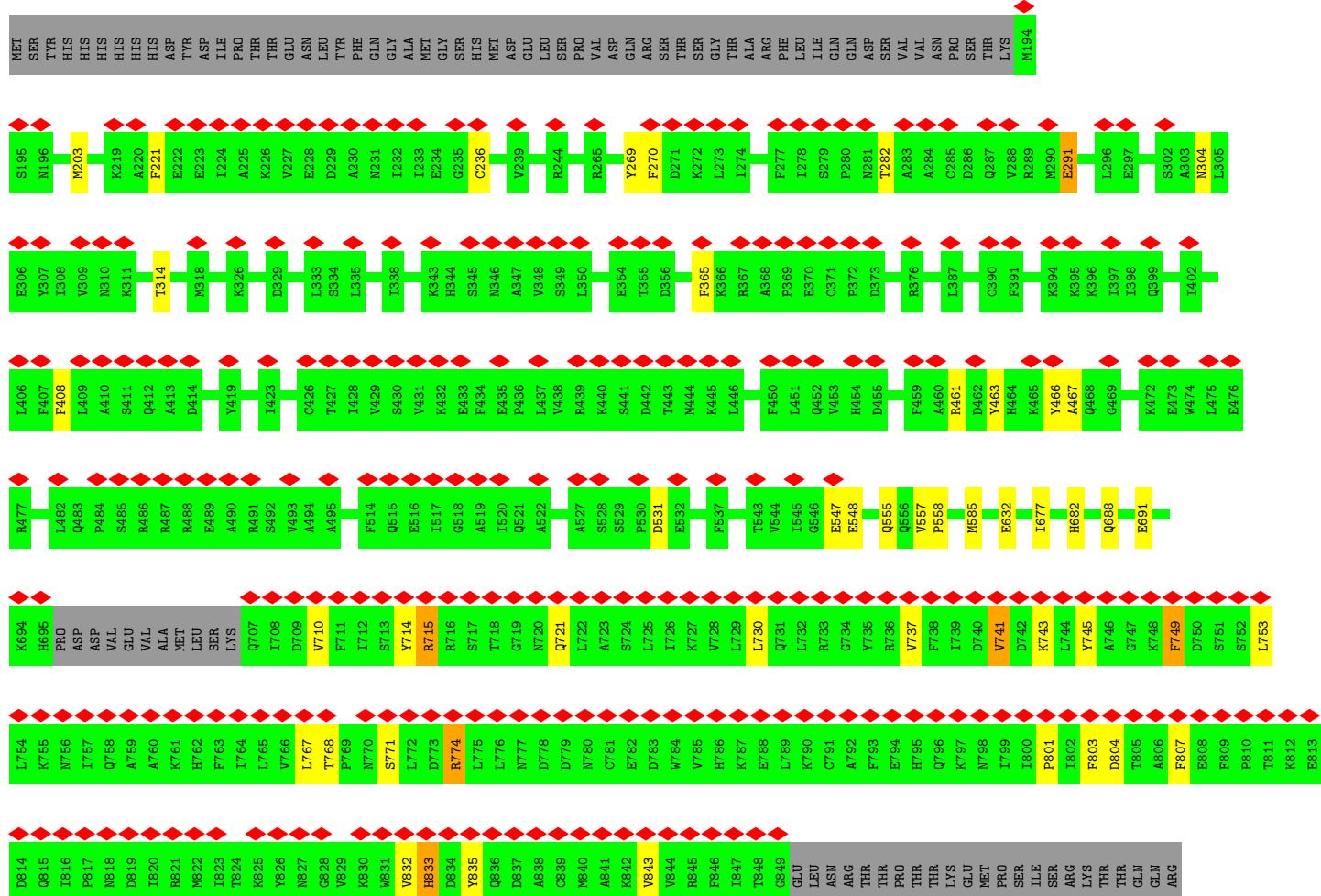
Category	Percentage
Red	45%
Green	81%
Yellow	6%
Grey	13%



- Molecule 1: NAD(+) hydrolase tir-1

A horizontal bar chart titled "Chain E" showing its distribution across four categories. The total length of the bar is 100%.

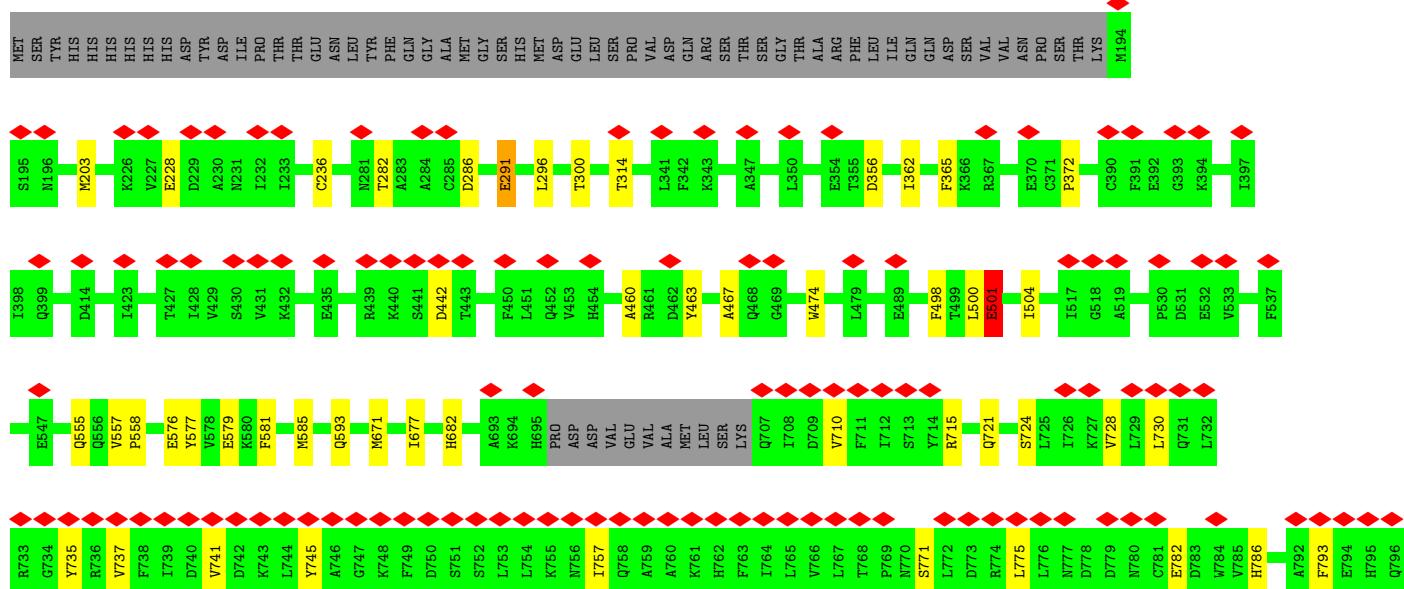
Category	Percentage
Red	40%
Green	81%
Yellow	6%
Blue	13%

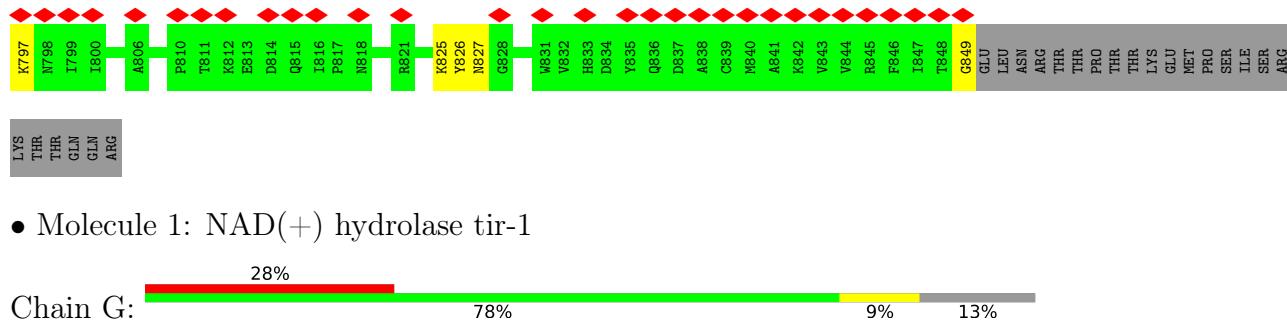


- Molecule 1: NAD(+) hydrolase tir-1

A horizontal bar chart titled "Chain F" showing its distribution across four categories. The categories are represented by colored segments: red (21%), green (80%), yellow (7%), and blue (13%).

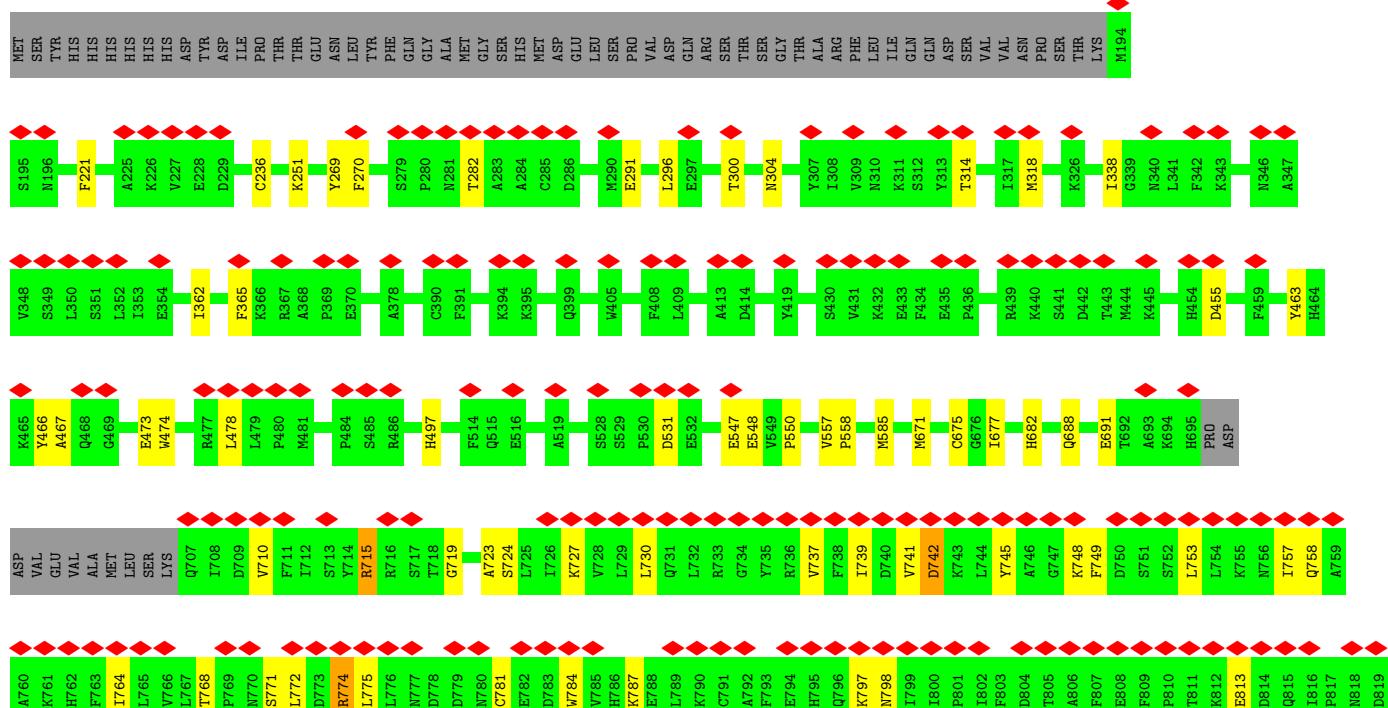
Category	Percentage
Red	21%
Green	80%
Yellow	7%
Blue	13%





- Molecule 1: NAD(+) hydrolase tir-1

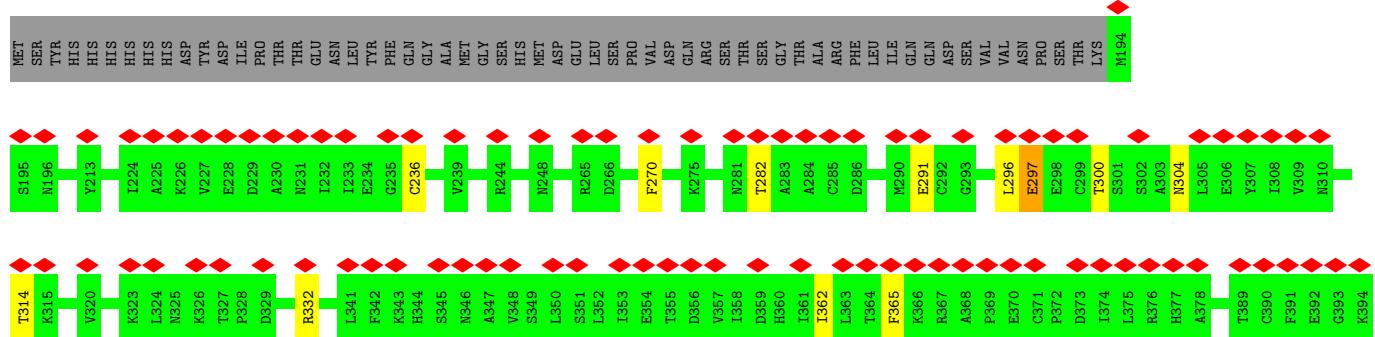
Chain G: 28% 78% 9% 13%

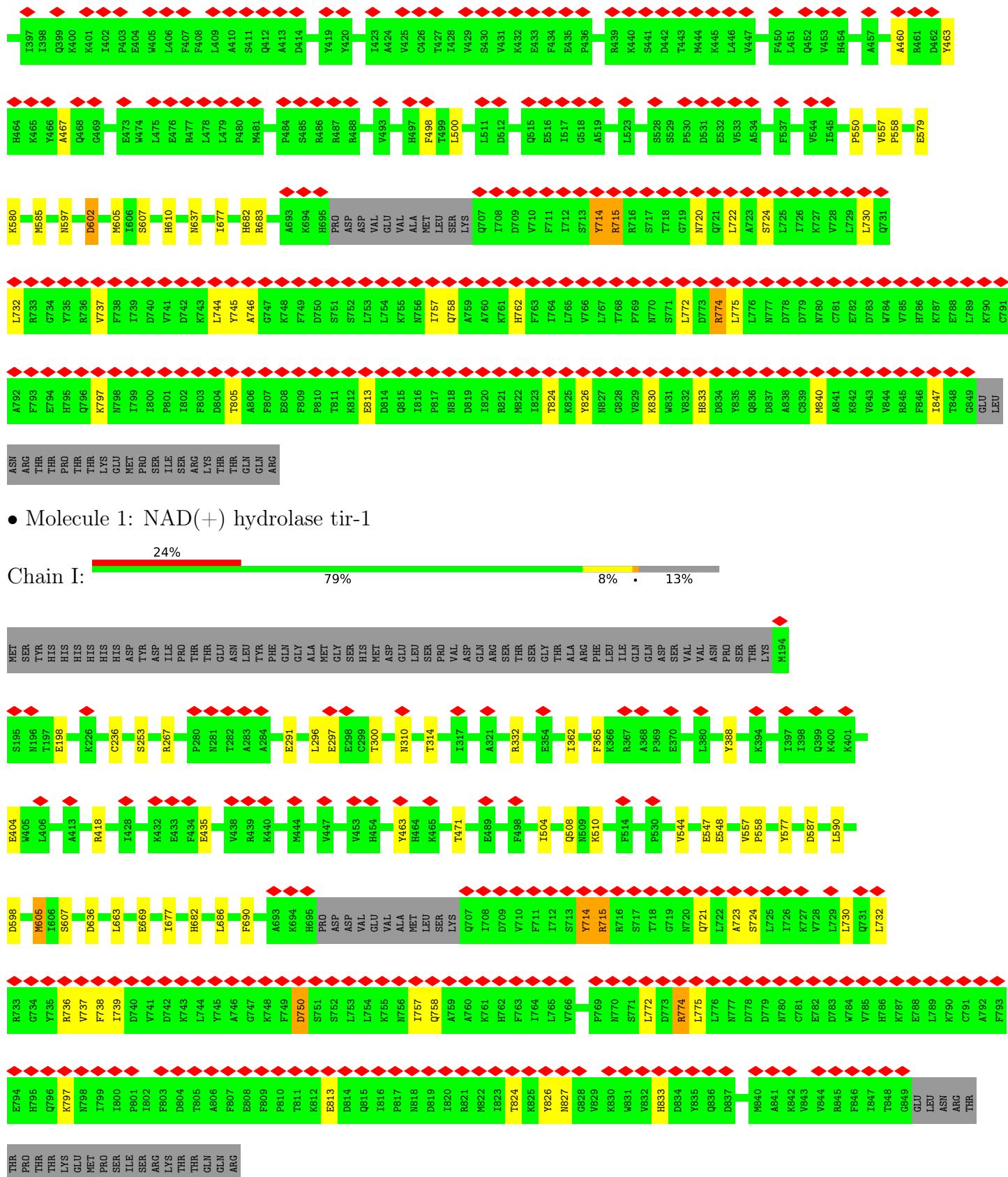


- Molecule 1: NAD(+) hydrolase tir-1

A horizontal bar chart illustrating the distribution of Chain H across four categories. The total length of the bar is 100%.

Category	Percentage
Red	43%
Green	80%
Yellow	7%
Grey	13%





4 Experimental information (i)

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 i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.63	4/5385 (0.1%)	1.04	26/7275 (0.4%)
1	B	0.50	3/5273 (0.1%)	0.90	11/7120 (0.2%)
1	C	0.54	0/5273	0.97	14/7120 (0.2%)
1	D	0.51	2/5273 (0.0%)	0.92	12/7120 (0.2%)
1	E	0.54	0/5273	0.92	13/7120 (0.2%)
1	F	0.59	5/5273 (0.1%)	1.05	17/7120 (0.2%)
1	G	0.50	1/5273 (0.0%)	0.88	9/7120 (0.1%)
1	H	0.52	1/5273 (0.0%)	0.90	12/7120 (0.2%)
1	I	0.56	4/5273 (0.1%)	0.93	16/7120 (0.2%)
All	All	0.55	20/47569 (0.0%)	0.95	130/64235 (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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	501	GLU	CD-OE2	-12.43	1.11	1.25
1	D	691	GLU	CD-OE1	8.80	1.35	1.25
1	I	669	GLU	CD-OE2	7.52	1.33	1.25
1	A	532	GLU	CD-OE1	7.43	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	435	GLU	CD-OE1	-7.01	1.18	1.25
1	F	576	GLU	CD-OE2	6.67	1.32	1.25
1	A	473	GLU	CD-OE1	6.29	1.32	1.25
1	F	579	GLU	CD-OE2	6.07	1.32	1.25
1	B	435	GLU	CD-OE1	5.73	1.31	1.25
1	F	228	GLU	CD-OE2	-5.56	1.19	1.25
1	G	473	GLU	CD-OE2	-5.53	1.19	1.25
1	A	532	GLU	CG-CD	5.50	1.60	1.51
1	A	679	ASN	CG-OD1	-5.41	1.12	1.24
1	B	297	GLU	CD-OE1	5.41	1.31	1.25
1	H	297	GLU	CD-OE2	5.34	1.31	1.25
1	I	404	GLU	CD-OE2	5.19	1.31	1.25
1	B	291	GLU	CD-OE2	5.15	1.31	1.25
1	F	501	GLU	CD-OE1	5.13	1.31	1.25
1	I	198	GLU	CD-OE2	-5.06	1.20	1.25
1	D	228	GLU	CD-OE2	-5.05	1.20	1.25

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	501	GLU	OE1-CD-OE2	-25.23	93.02	123.30
1	F	501	GLU	CG-CD-OE1	22.71	163.73	118.30
1	F	501	GLU	CG-CD-OE2	-16.77	84.75	118.30
1	H	714	TYR	CB-CG-CD2	-11.52	114.09	121.00
1	D	836	GLN	CB-CA-C	11.30	133.00	110.40
1	C	715	ARG	NE-CZ-NH1	-11.18	114.71	120.30
1	C	821	ARG	NE-CZ-NH1	-9.75	115.42	120.30
1	H	714	TYR	CB-CG-CD1	9.70	126.82	121.00
1	I	332	ARG	NE-CZ-NH1	-9.66	115.47	120.30
1	A	471	THR	CA-CB-CG2	8.70	124.58	112.40
1	I	714	TYR	CB-CG-CD2	8.42	126.05	121.00
1	A	783	ASP	CB-CG-OD1	8.38	125.84	118.30
1	A	388	TYR	CB-CG-CD2	8.15	125.89	121.00
1	F	498	PHE	CB-CG-CD1	8.10	126.47	120.80
1	A	779	ASP	CB-CG-OD1	7.53	125.08	118.30
1	B	716	ARG	NE-CZ-NH1	-7.40	116.60	120.30
1	E	715	ARG	NE-CZ-NH1	-7.38	116.61	120.30
1	D	461	ARG	CG-CD-NE	7.36	127.26	111.80
1	G	742	ASP	CB-CA-C	7.27	124.93	110.40
1	H	332	ARG	NE-CZ-NH1	-7.22	116.69	120.30
1	F	498	PHE	CB-CG-CD2	-7.09	115.84	120.80
1	F	442	ASP	CB-CG-OD1	6.78	124.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	773	ASP	CB-CG-OD1	-6.72	112.25	118.30
1	E	365	PHE	CB-CG-CD1	-6.70	116.11	120.80
1	D	550	PRO	N-CA-CB	6.67	111.31	103.30
1	F	849	GLY	CA-C-O	6.63	132.54	120.60
1	C	783	ASP	CB-CG-OD1	6.61	124.25	118.30
1	E	408	PHE	CB-CG-CD2	6.60	125.42	120.80
1	A	793	PHE	CB-CG-CD2	6.59	125.41	120.80
1	H	715	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	I	715	ARG	NE-CZ-NH1	-6.49	117.05	120.30
1	E	714	TYR	CB-CG-CD1	-6.45	117.13	121.00
1	E	461	ARG	CG-CD-NE	6.37	125.18	111.80
1	C	804	ASP	CB-CG-OD1	6.36	124.03	118.30
1	A	793	PHE	CB-CG-CD1	-6.33	116.37	120.80
1	G	269	TYR	CB-CG-CD1	6.29	124.78	121.00
1	A	565	VAL	CA-CB-CG1	6.28	120.31	110.90
1	I	714	TYR	CB-CG-CD1	-6.26	117.24	121.00
1	F	581	PHE	CB-CG-CD2	-6.24	116.43	120.80
1	A	486	ARG	NE-CZ-NH1	-6.10	117.25	120.30
1	F	356	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	774	ARG	CG-CD-NE	6.07	124.55	111.80
1	E	774	ARG	CG-CD-NE	6.07	124.54	111.80
1	H	774	ARG	CG-CD-NE	6.05	124.51	111.80
1	A	779	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	B	715	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	F	291	GLU	OE1-CD-OE2	-5.98	116.12	123.30
1	H	550	PRO	N-CA-CB	5.98	110.48	103.30
1	A	804	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	C	418	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	I	774	ARG	CG-CD-NE	5.96	124.31	111.80
1	I	750	ASP	CB-CA-C	5.95	122.31	110.40
1	A	598	ASP	CB-CG-OD1	5.92	123.62	118.30
1	B	803	PHE	CB-CG-CD2	5.91	124.94	120.80
1	D	463	TYR	CB-CG-CD2	-5.89	117.47	121.00
1	I	598	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	F	442	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	E	531	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	I	544	VAL	CA-CB-CG2	5.75	119.52	110.90
1	A	291	GLU	OE1-CD-OE2	5.75	130.19	123.30
1	C	653	MET	CG-SD-CE	5.74	109.38	100.20
1	A	388	TYR	CB-CG-CD1	-5.71	117.58	121.00
1	D	741	VAL	CG1-CB-CG2	-5.67	101.83	110.90
1	F	372	PRO	N-CA-CB	5.67	110.10	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	I	267	ARG	NE-CZ-NH2	5.67	123.13	120.30
1	G	455	ASP	CB-CG-OD1	-5.64	113.22	118.30
1	E	843	VAL	CA-CB-CG2	5.62	119.33	110.90
1	D	500	LEU	CB-CA-C	-5.61	99.55	110.20
1	B	291	GLU	OE1-CD-OE2	5.61	130.03	123.30
1	C	550	PRO	N-CA-CB	5.60	110.02	103.30
1	A	567	TYR	CB-CG-CD1	-5.59	117.64	121.00
1	A	442	ASP	CB-CG-OD1	-5.57	113.28	118.30
1	B	500	LEU	CB-CA-C	-5.54	99.67	110.20
1	I	605	MET	CG-SD-CE	-5.54	91.34	100.20
1	I	636	ASP	CB-CG-OD2	-5.52	113.34	118.30
1	A	595	THR	CA-CB-CG2	5.50	120.11	112.40
1	D	291	GLU	OE1-CD-OE2	-5.49	116.72	123.30
1	F	581	PHE	CB-CG-CD1	5.47	124.63	120.80
1	C	832	VAL	CA-CB-CG1	5.46	119.09	110.90
1	A	407	PHE	CB-CG-CD2	5.46	124.62	120.80
1	H	498	PHE	CB-CG-CD1	-5.44	116.99	120.80
1	A	814	ASP	CB-CG-OD1	-5.44	113.40	118.30
1	G	269	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	I	463	TYR	CB-CG-CD2	5.43	124.26	121.00
1	F	577	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	F	576	GLU	OE1-CD-OE2	5.41	129.79	123.30
1	G	531	ASP	CB-CG-OD2	-5.41	113.44	118.30
1	A	804	ASP	CB-CG-OD1	5.36	123.13	118.30
1	B	550	PRO	N-CA-CB	5.35	109.72	103.30
1	F	474	TRP	CA-CB-CG	5.34	123.86	113.70
1	E	741	VAL	CA-CB-CG1	5.34	118.92	110.90
1	A	365	PHE	CB-CG-CD1	5.33	124.53	120.80
1	G	474	TRP	CA-CB-CG	5.33	123.82	113.70
1	A	675	CYS	CA-CB-SG	-5.33	104.42	114.00
1	C	738	PHE	CB-CG-CD2	-5.31	117.08	120.80
1	G	550	PRO	N-CA-CB	5.30	109.66	103.30
1	B	740	ASP	CB-CA-C	5.26	120.92	110.40
1	F	286	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	267	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	H	597	ASN	CB-CG-OD1	5.23	132.07	121.60
1	I	738	PHE	CB-CA-C	5.23	120.86	110.40
1	C	613	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	H	683	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	E	291	GLU	OE1-CD-OE2	-5.21	117.05	123.30
1	E	833	HIS	CB-CA-C	5.21	120.81	110.40
1	B	500	LEU	CB-CG-CD2	-5.19	102.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	807	PHE	CB-CG-CD2	5.19	124.43	120.80
1	C	683	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	I	388	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	B	267	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	I	471	THR	OG1-CB-CG2	-5.17	98.11	110.00
1	B	252	VAL	CA-CB-CG1	5.14	118.61	110.90
1	D	500	LEU	CB-CG-CD2	-5.14	102.26	111.00
1	H	498	PHE	CB-CG-CD2	5.14	124.40	120.80
1	C	727	LYS	O-C-N	-5.13	114.50	122.70
1	D	683	ARG	NE-CZ-NH1	-5.13	117.74	120.30
1	I	418	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	H	840	MET	CG-SD-CE	5.12	108.39	100.20
1	H	585	MET	CA-CB-CG	5.11	121.98	113.30
1	D	774	ARG	CB-CA-C	-5.07	100.26	110.40
1	G	675	CYS	CA-CB-SG	-5.05	104.91	114.00
1	G	774	ARG	CG-CD-NE	5.04	122.39	111.80
1	E	714	TYR	CB-CG-CD2	5.04	124.02	121.00
1	A	834	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	488	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	D	498	PHE	CB-CG-CD1	-5.02	117.29	120.80
1	A	650	THR	OG1-CB-CG2	-5.01	98.48	110.00
1	C	738	PHE	CB-CG-CD1	5.01	124.31	120.80
1	A	733	ARG	NE-CZ-NH2	5.01	122.80	120.30
1	E	721	GLN	CB-CA-C	5.00	120.41	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
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

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Mol	Chain	Res	Type	Group
1	I	504	ILE	Mainchain
1	I	714	TYR	Sidechain

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5286	0	5365	15	0
1	B	5177	0	5253	28	0
1	C	5177	0	5253	30	0
1	D	5177	0	5253	19	0
1	E	5177	0	5253	27	0
1	F	5177	0	5253	26	0
1	G	5177	0	5253	39	0
1	H	5177	0	5253	37	0
1	I	5177	0	5253	35	0
All	All	46702	0	47389	218	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 (218) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:827:ASN:CG	1:H:744:LEU:HB3	2.22	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: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
1:G:781:CYS:SG	1:G:787:LYS:HG2	2.49	0.53
1:A:354:GLU:OE2	1:I:310:ASN:CG	2.48	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:758:GLN:O	1:G:797:LYS:NZ	2.42	0.51
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:H:758:GLN:O	1:H:797:LYS:NZ	2.40	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:I:758:GLN:O	1:I:797:LYS:NZ	2.42	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:547:GLU:HG2	1:E:548:GLU:N	2.33	0.44
1:E:715:ARG:NH1	1:E:774:ARG:CZ	2.80	0.44
1:I:236:CYS:HB2	1:I:291:GLU:HB3	1.98	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: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: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: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: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
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: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: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: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:G:798:ASN:CG	1:H:746:ALA:HB1	2.38	0.42
1:I:813:GLU:HG3	1:I:824:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:605:MET:HE3	1:C:605:MET:HB3	1.86	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:A:354:GLU:CD	1:I:310:ASN:HA	2.40	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	586/660 (89%)	579 (99%)	7 (1%)	71	84
1	B	572/660 (87%)	566 (99%)	6 (1%)	76	86
1	C	572/660 (87%)	556 (97%)	16 (3%)	43	67
1	D	572/660 (87%)	562 (98%)	10 (2%)	60	78
1	E	572/660 (87%)	565 (99%)	7 (1%)	71	84
1	F	572/660 (87%)	566 (99%)	6 (1%)	76	86
1	G	572/660 (87%)	562 (98%)	10 (2%)	60	78
1	H	572/660 (87%)	565 (99%)	7 (1%)	71	84
1	I	572/660 (87%)	565 (99%)	7 (1%)	71	84
All	All	5162/5940 (87%)	5086 (98%)	76 (2%)	66	80

All (76) 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	598	ASP
1	A	773	ASP
1	A	852	ASN
1	B	282	THR
1	B	297	GLU
1	B	314	THR
1	B	585	MET
1	B	740	ASP
1	B	826	TYR
1	C	282	THR
1	C	314	THR
1	C	425	VAL
1	C	585	MET
1	C	721	GLN
1	C	735	TYR
1	C	750	ASP
1	C	769	PRO
1	C	773	ASP
1	C	774	ARG
1	C	822	MET
1	C	826	TYR
1	C	833	HIS

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Mol	Chain	Res	Type
1	C	834	ASP
1	C	835	TYR
1	C	836	GLN
1	D	282	THR
1	D	314	THR
1	D	585	MET
1	D	605	MET
1	D	612	LYS
1	D	721	GLN
1	D	749	PHE
1	D	782	GLU
1	D	826	TYR
1	D	836	GLN
1	E	282	THR
1	E	314	THR
1	E	585	MET
1	E	632	GLU
1	E	745	TYR
1	E	749	PHE
1	E	832	VAL
1	F	282	THR
1	F	314	THR
1	F	501	GLU
1	F	585	MET
1	F	593	GLN
1	F	782	GLU
1	G	221	PHE
1	G	251	LYS
1	G	282	THR
1	G	314	THR
1	G	585	MET
1	G	715	ARG
1	G	724	SER
1	G	742	ASP
1	G	826	TYR
1	G	834	ASP
1	H	282	THR
1	H	297	GLU
1	H	314	THR
1	H	602	ASP
1	H	605	MET
1	H	637	ASN

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Mol	Chain	Res	Type
1	H	826	TYR
1	I	253	SER
1	I	297	GLU
1	I	314	THR
1	I	686	LEU
1	I	736	ARG
1	I	750	ASP
1	I	826	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	827	ASN
1	E	836	GLN
1	F	196	ASN
1	G	497	HIS
1	H	196	ASN
1	I	721	GLN
1	I	833	HIS

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

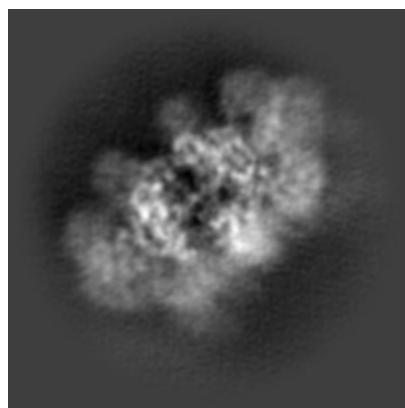
6 Map visualisation (i)

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

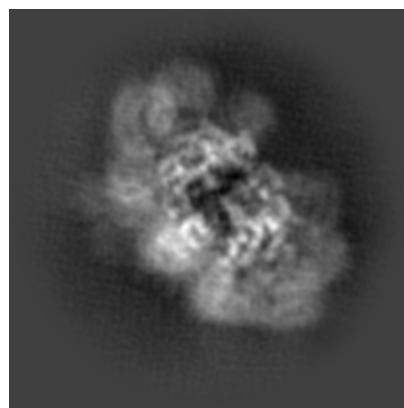
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

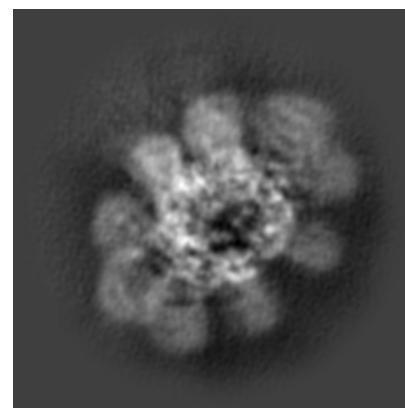
6.1.1 Primary map



X

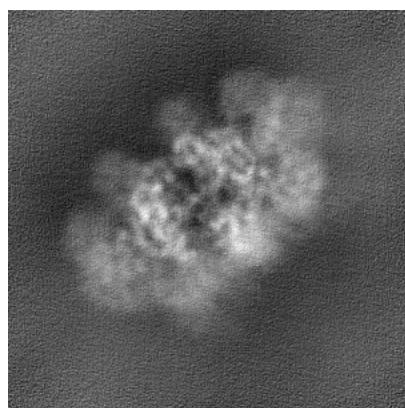


Y

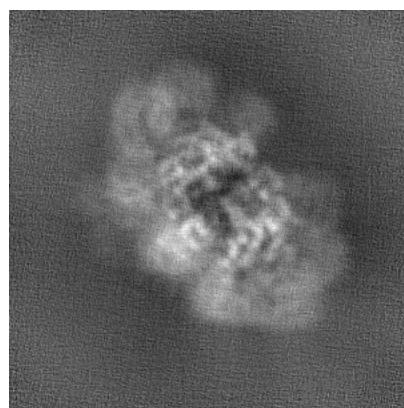


Z

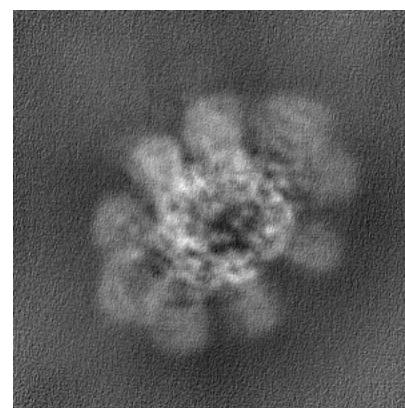
6.1.2 Raw map



X



Y

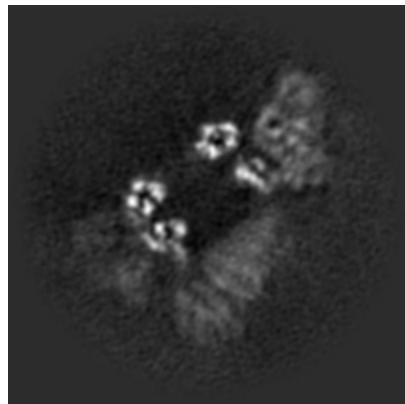


Z

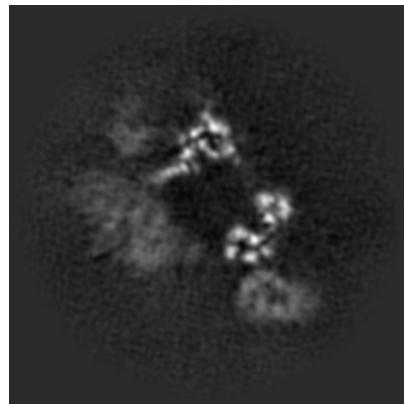
The images above show the map projected in three orthogonal directions.

6.2 Central slices [\(i\)](#)

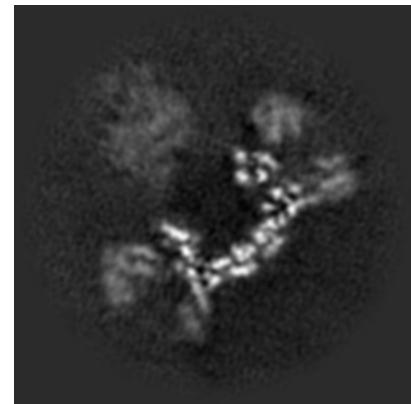
6.2.1 Primary map



X Index: 160



Y Index: 160

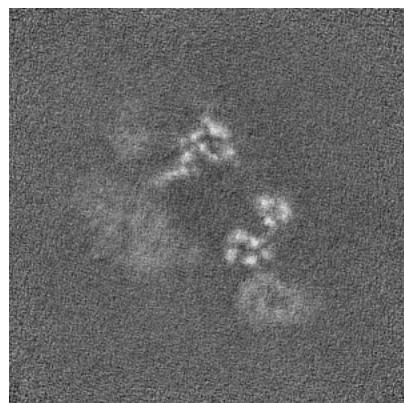


Z Index: 160

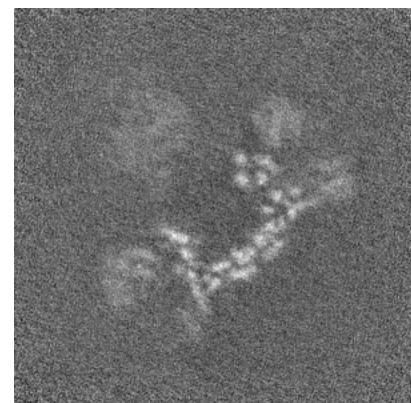
6.2.2 Raw map



X Index: 160



Y Index: 160

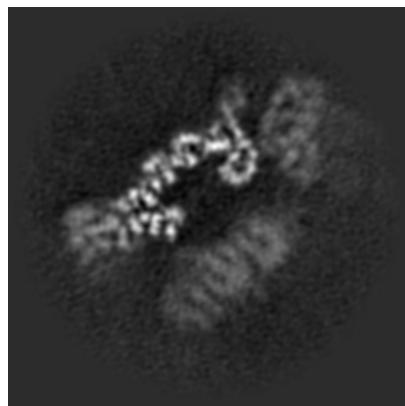


Z Index: 160

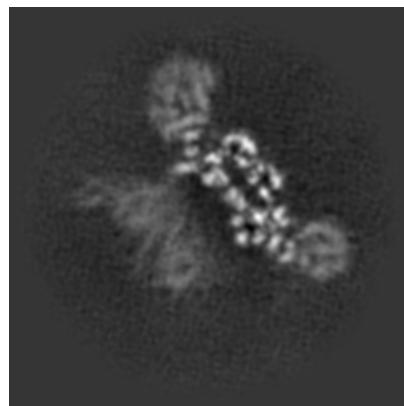
The images above show central slices of the map in three orthogonal directions.

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

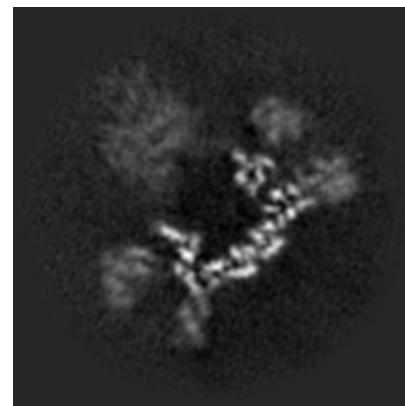
6.3.1 Primary map



X Index: 147

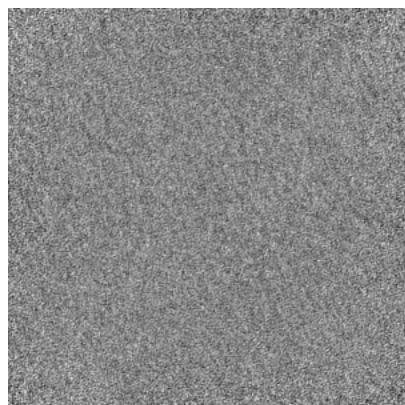


Y Index: 183

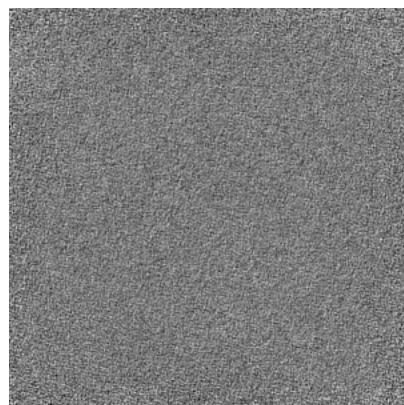


Z Index: 158

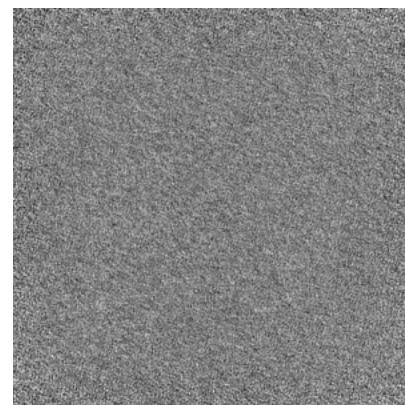
6.3.2 Raw map



X Index: 0



Y Index: 0

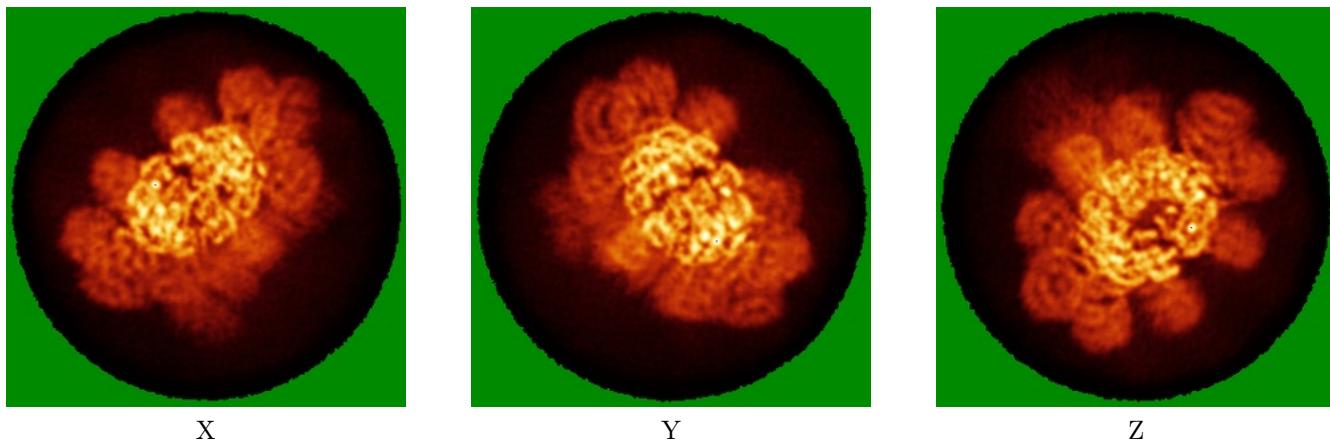


Z Index: 0

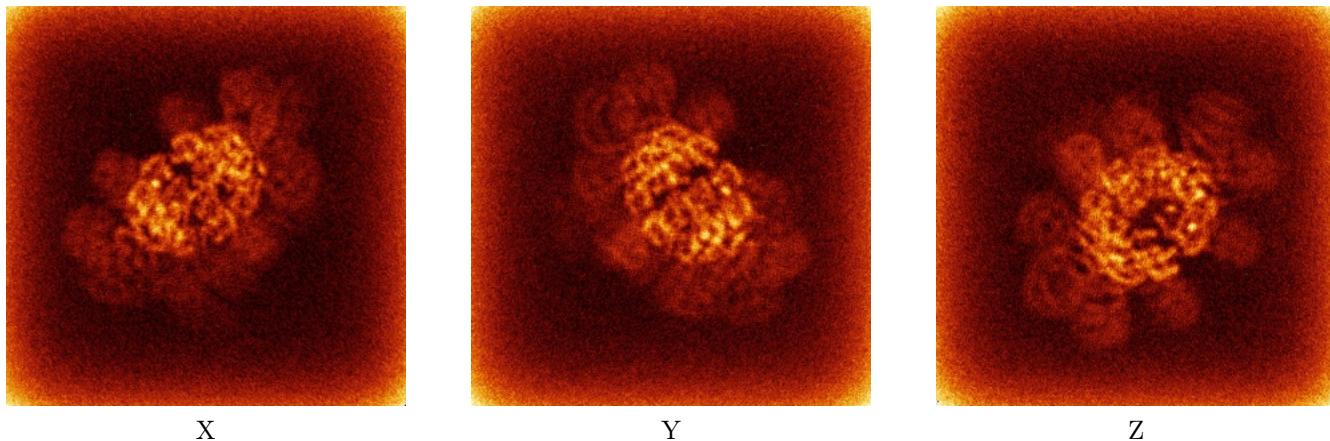
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



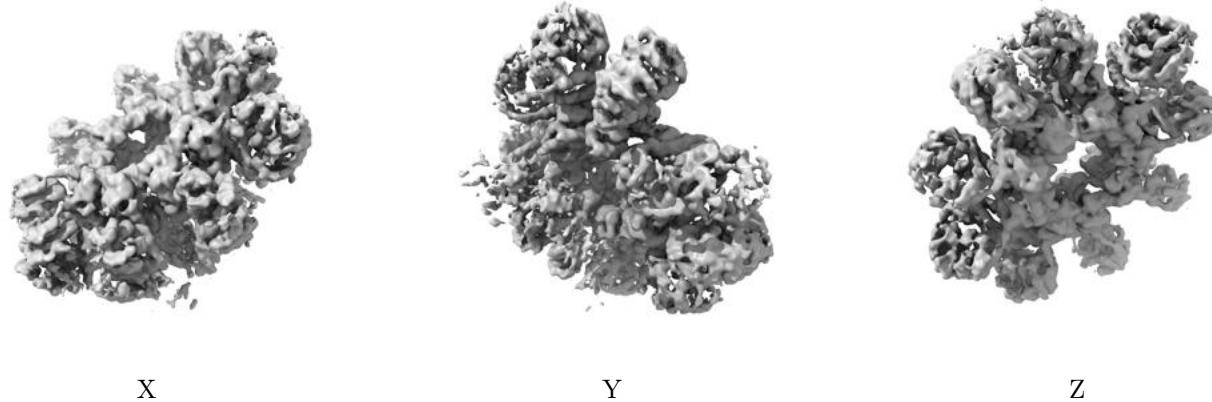
6.4.2 Raw map



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

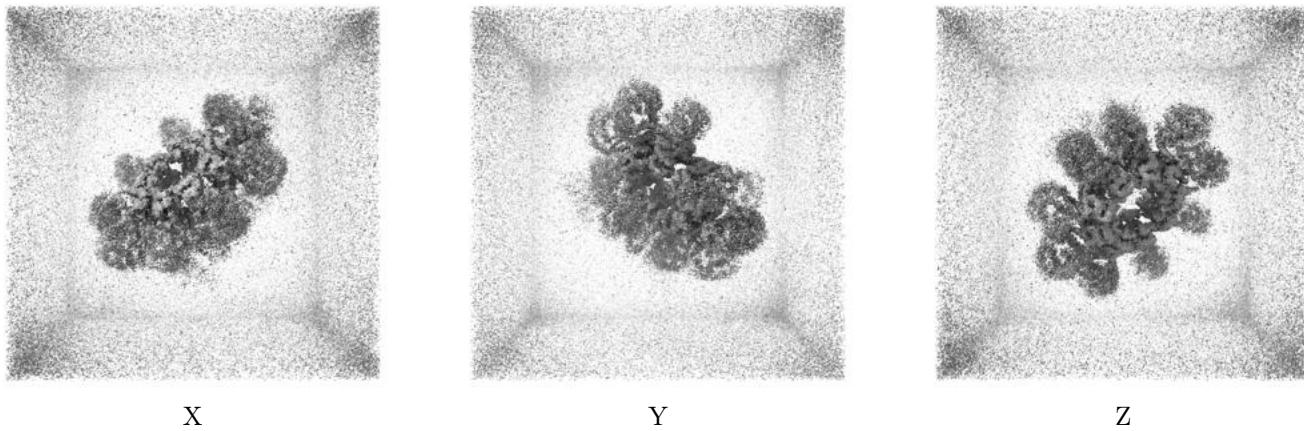
6.5 Orthogonal surface views [\(i\)](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. 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.

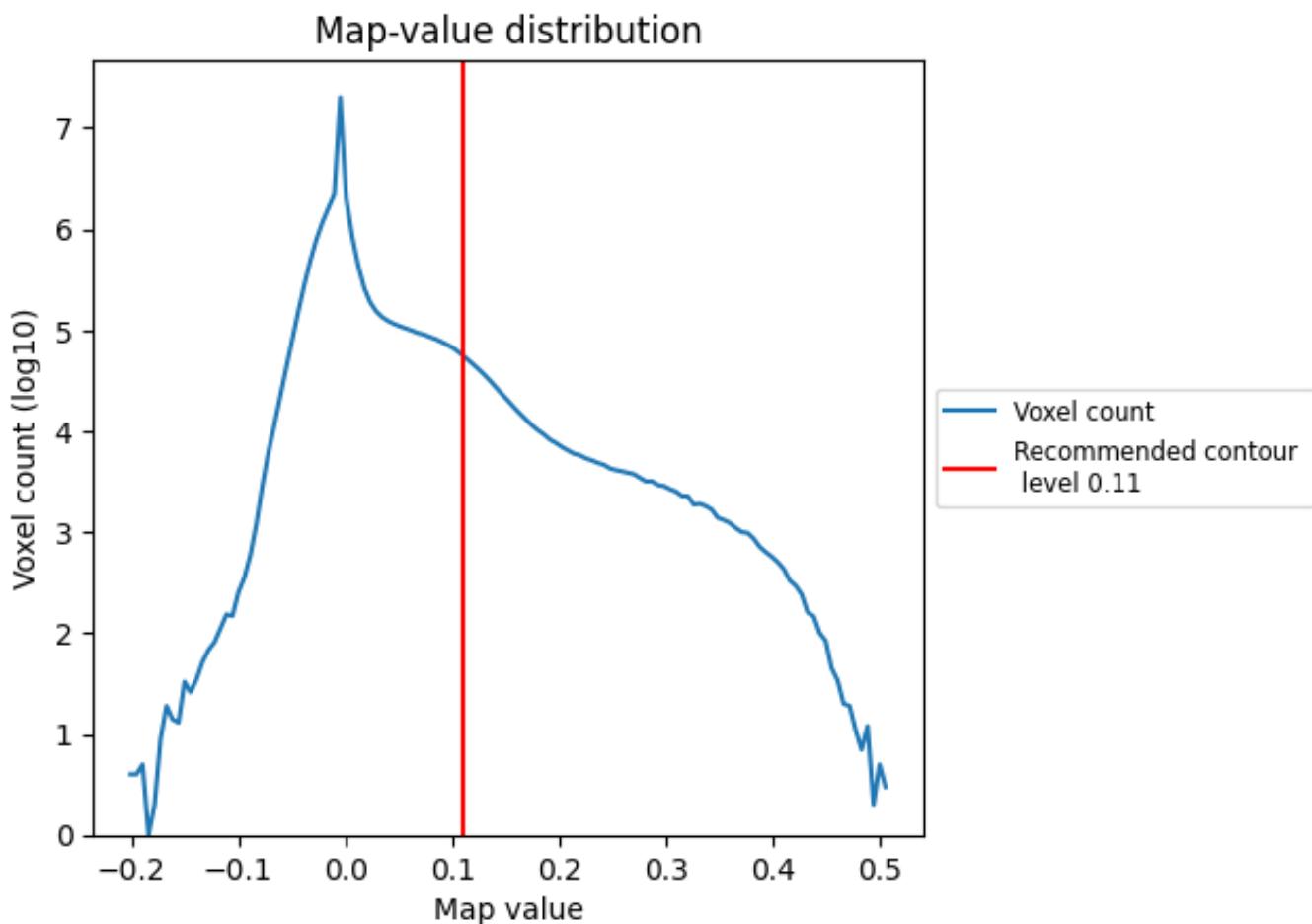
6.6 Mask visualisation [\(i\)](#)

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

7 Map analysis (i)

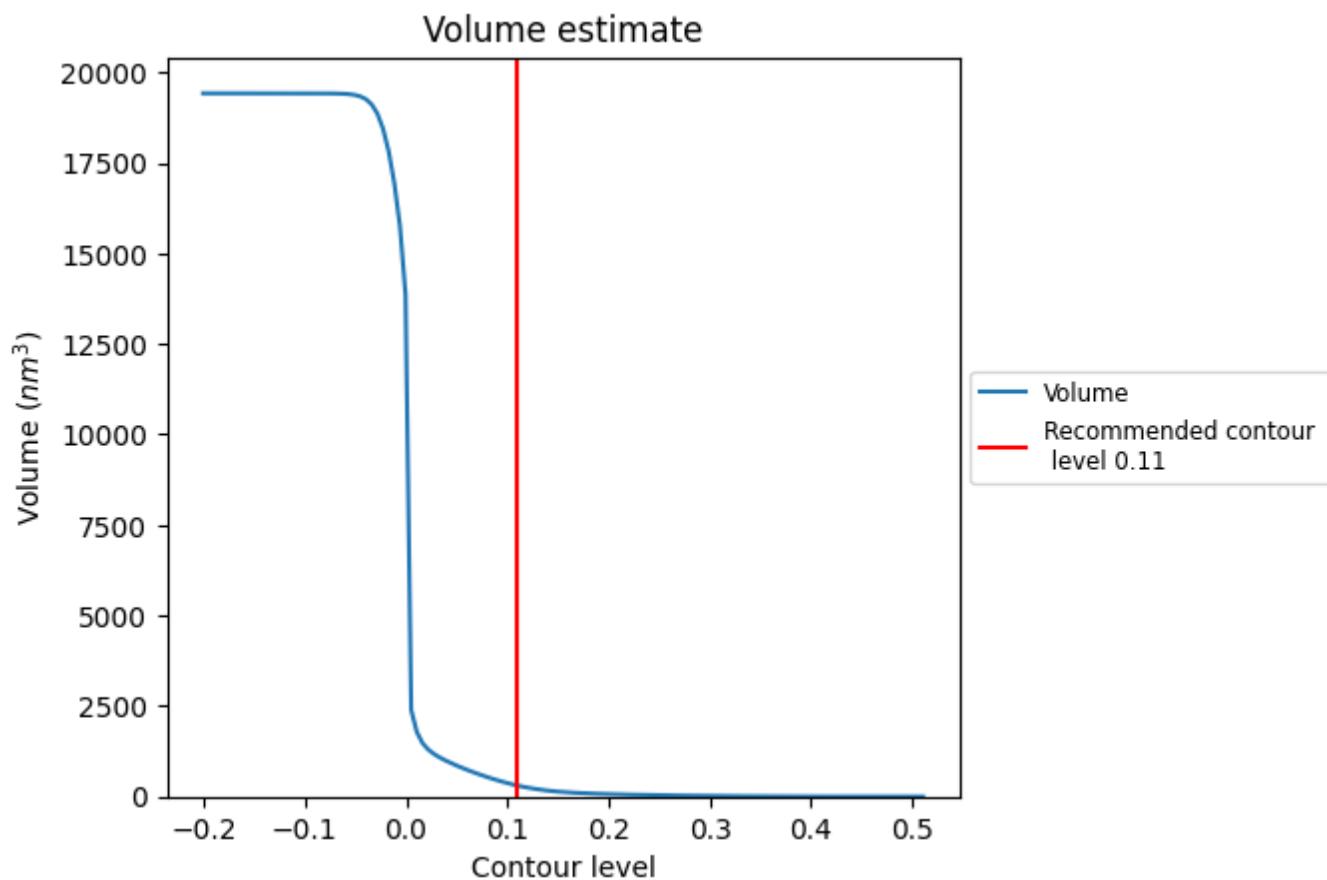
This section contains the results of statistical analysis of the map.

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.

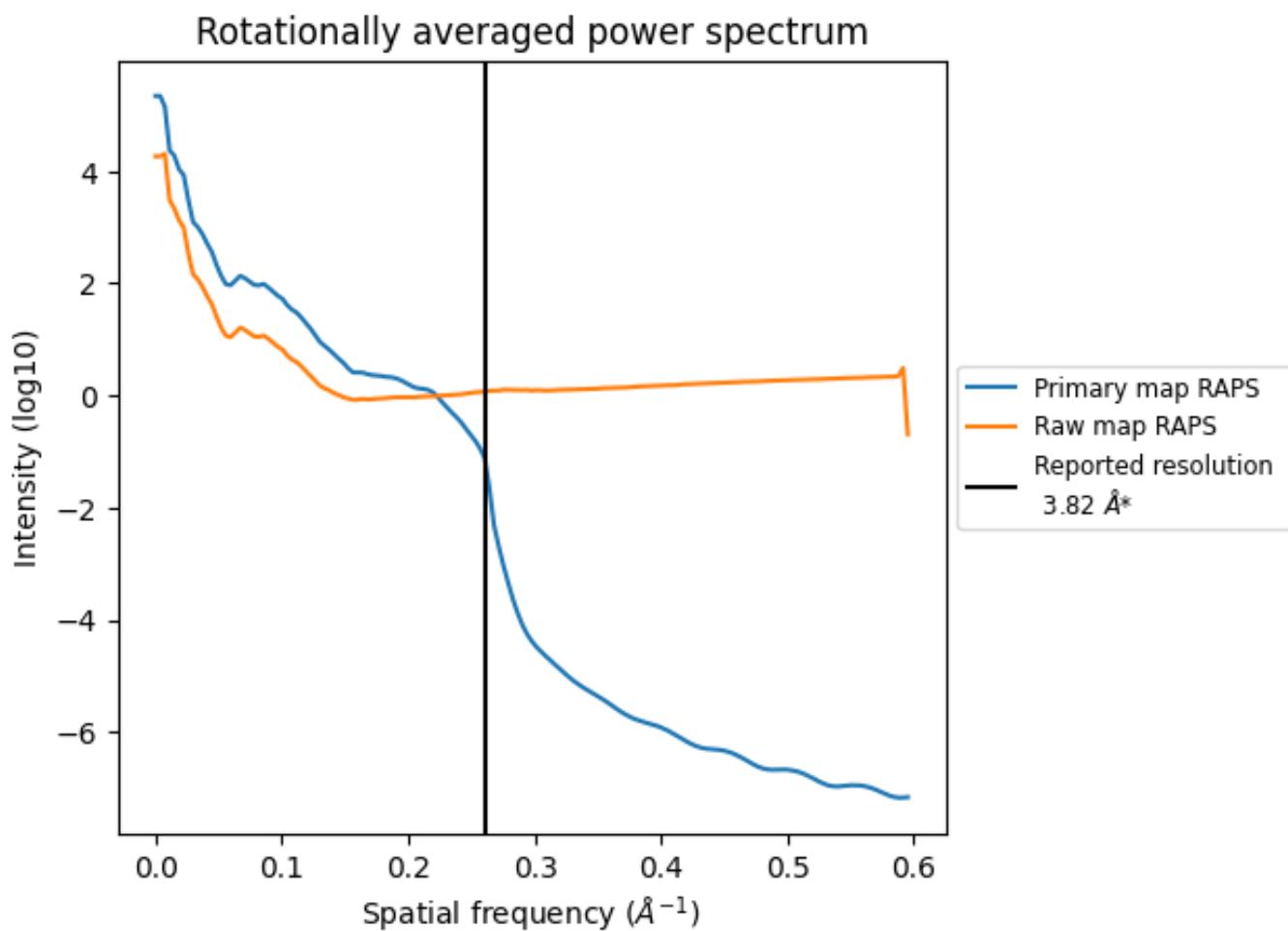
7.2 Volume estimate (i)



The volume at the recommended contour level is 304 nm^3 ; 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 [\(i\)](#)

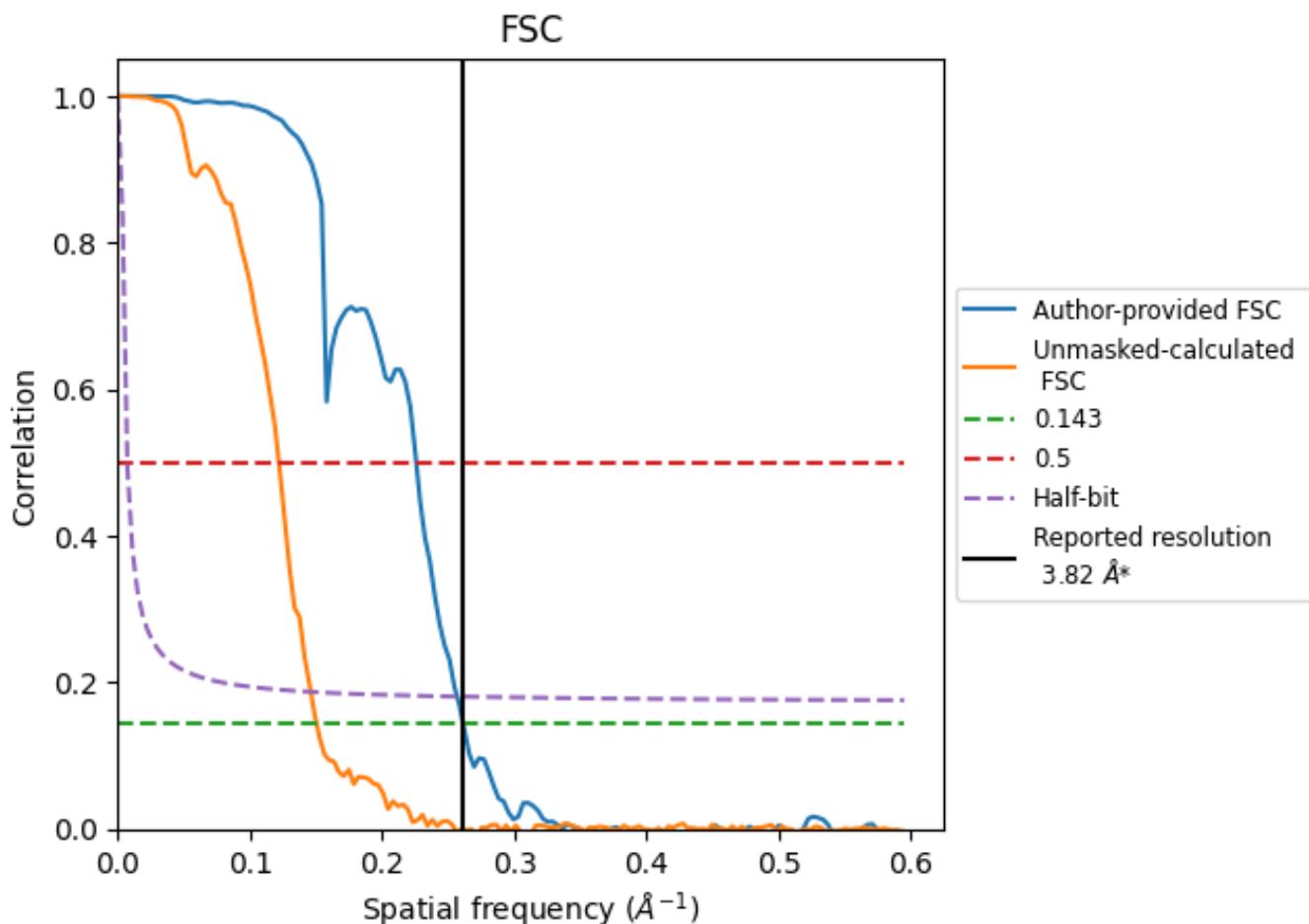


*Reported resolution corresponds to spatial frequency of 0.262 \AA^{-1}

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 \AA^{-1}

8.2 Resolution estimates [\(i\)](#)

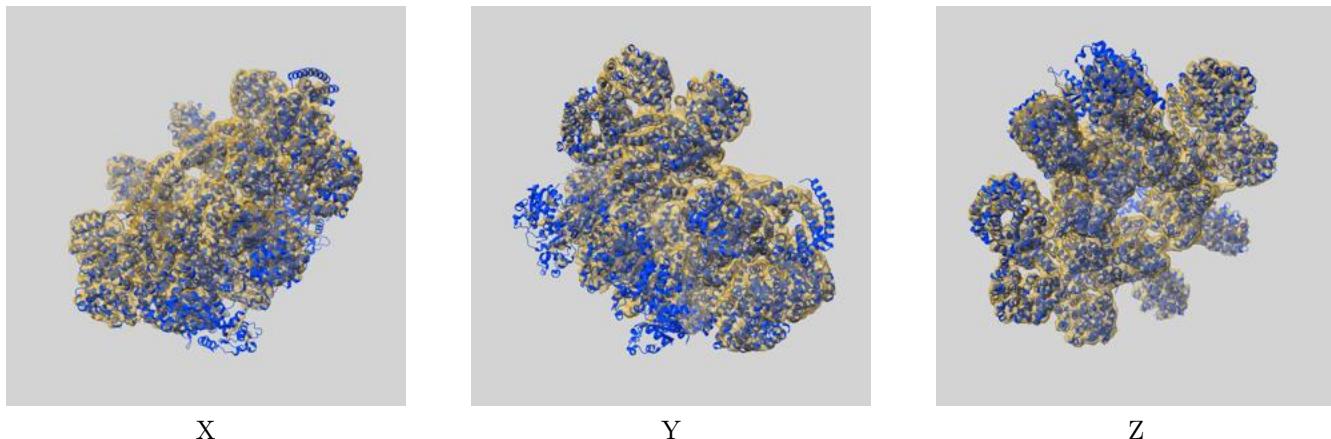
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.82	-	-
Author-provided FSC curve	3.83	4.43	3.89
Unmasked-calculated*	6.64	8.20	6.84

*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

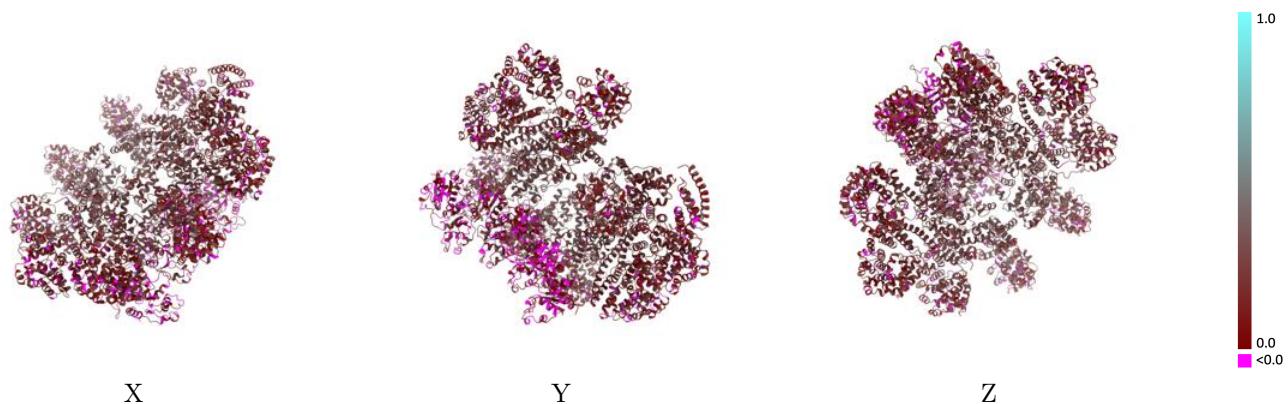
This section contains information regarding the fit between EMDB map EMD-17370 and PDB model 8P2M. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay i



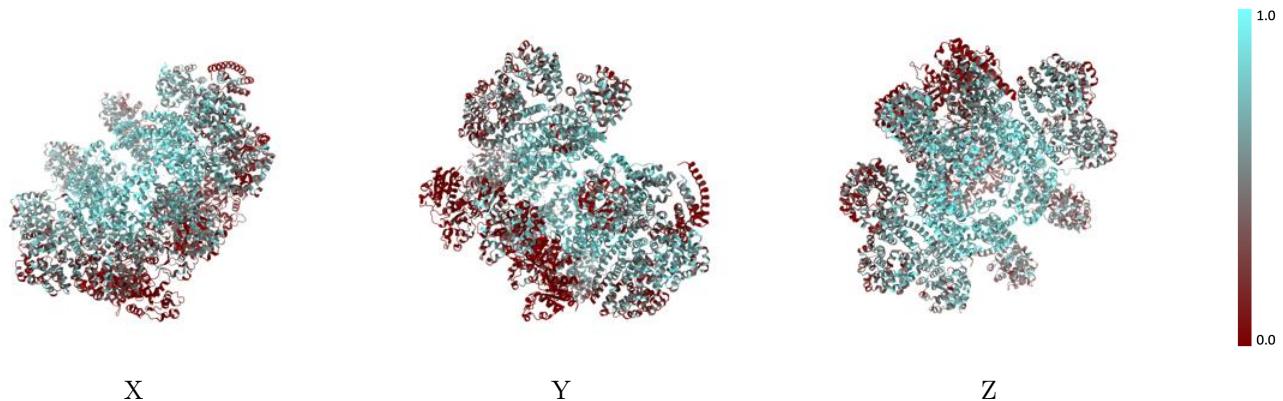
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



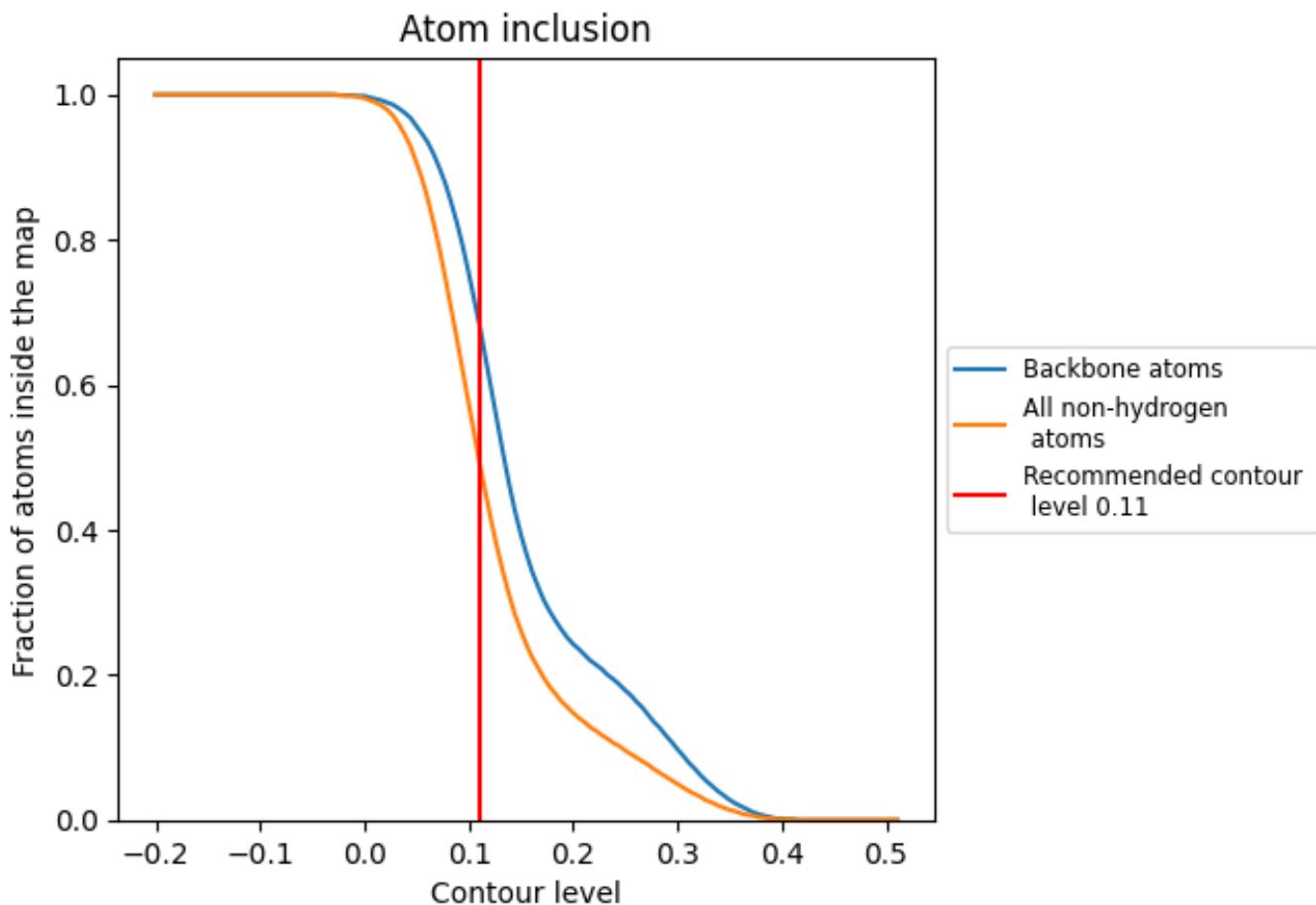
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

