



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:15 PM UTC

PDB ID : 9EK1 / pdb_00009ek1
EMDB ID : EMD-47842
Title : HIV-1 mature WT matrix protein p17 lattice
Authors : Rey, J.S.; Perilla, J.R.; Chen, L.; Zhang, P.
Deposited on : 2024-11-30
Resolution : 7.30 Å(reported)
Based on initial models : 7TBP, 2LYB

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
Mogul : 2022.3.0, CSD as543be (2022)
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

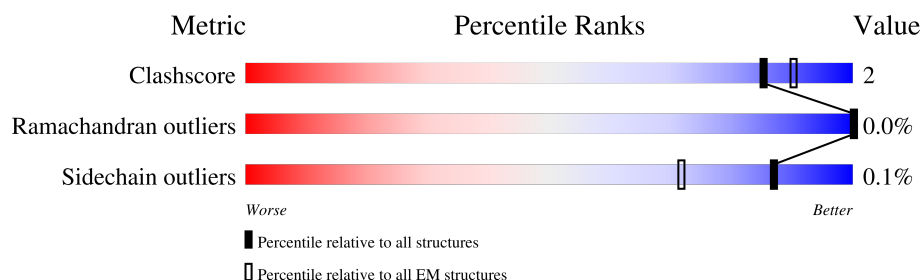
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	115	100% 87% 13%
1	B	115	100% 89% 11%
1	C	115	100% 89% 11%
1	D	115	100% 83% 17% .
1	E	115	100% 87% 13%
1	F	115	100% 88% 11% .
1	G	115	100% 82% 17% .
1	H	115	100% 87% 11% .

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Mol	Chain	Length	Quality of chain
1	I	115	100% 86%13%
1	J	115	100% 82%18%
1	K	115	100% 86%14%
1	L	115	100% 87%13%
1	M	115	99% 90%10%
1	N	115	99% 86%14%
1	O	115	100% 90%10%
1	P	115	100% 95%5%
1	Q	115	100% 80%20%
1	R	115	100% 86%12%
1	S	115	100% 93%6%
1	T	115	100% 95%5%
1	U	115	100% 89%11%
1	V	115	100% 95%5%
1	W	115	100% 92%8%
1	X	115	100% 88%12%
1	Y	115	100% 96%
1	Z	115	100% 85%15%
1	a	115	100% 84%16%
1	b	115	98% 89%11%
1	c	115	100% 88%12%
1	d	115	100% 97%
1	e	115	99% 90%10%
1	f	115	100% 90%10%
1	g	115	100% 96%

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Mol	Chain	Length	Quality of chain
1	h	115	100% 92% 8%
1	i	115	100% 93% 6% .
1	j	115	100% 96% .
1	k	115	100% 88% 12%
1	l	115	100% 90% 10%
1	m	115	100% 91% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 36387 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 Matrix protein p17.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	115	Total	C	N	O	S	0	0
			918	574	169	173	2		
1	B	115	Total	C	N	O	S	0	0
			918	574	169	173	2		
1	C	115	Total	C	N	O	S	0	0
			918	574	169	173	2		
1	D	115	Total	C	N	O	S	0	0
			918	574	169	173	2		
1	E	115	Total	C	N	O	S	0	0
			918	574	169	173	2		
1	F	115	Total	C	N	O	S	0	0
			918	574	169	173	2		
1	G	115	Total	C	N	O	S	0	0
			918	574	169	173	2		
1	H	115	Total	C	N	O	S	0	0
			918	574	169	173	2		
1	I	115	Total	C	N	O	S	0	0
			918	574	169	173	2		
1	J	115	Total	C	N	O	S	0	0
			918	574	169	173	2		
1	K	115	Total	C	N	O	S	0	0
			918	574	169	173	2		
1	L	115	Total	C	N	O	S	0	0
			918	574	169	173	2		
1	M	115	Total	C	N	O	S	0	0
			918	574	169	173	2		
1	N	115	Total	C	N	O	S	0	0
			918	574	169	173	2		
1	O	115	Total	C	N	O	S	0	0
			918	574	169	173	2		
1	P	115	Total	C	N	O	S	0	0
			918	574	169	173	2		
1	Q	115	Total	C	N	O	S	0	0
			918	574	169	173	2		

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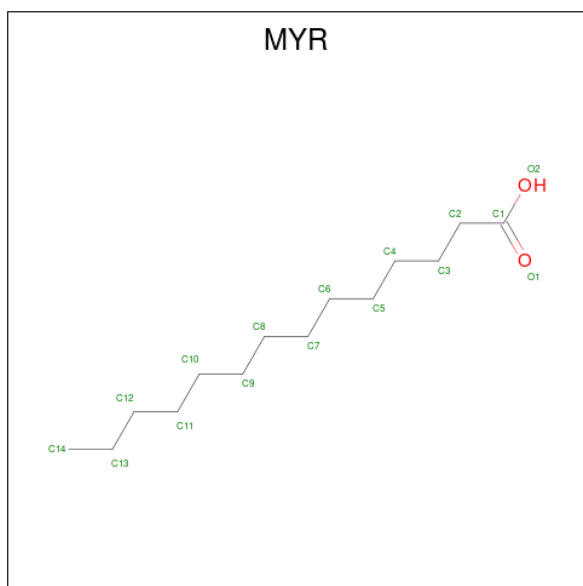
Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	115	Total 918	C 574	N 169	O 173	S 2	0	0
1	S	115	Total 918	C 574	N 169	O 173	S 2	0	0
1	T	115	Total 918	C 574	N 169	O 173	S 2	0	0
1	U	115	Total 918	C 574	N 169	O 173	S 2	0	0
1	V	115	Total 918	C 574	N 169	O 173	S 2	0	0
1	W	115	Total 918	C 574	N 169	O 173	S 2	0	0
1	X	115	Total 918	C 574	N 169	O 173	S 2	0	0
1	Y	115	Total 918	C 574	N 169	O 173	S 2	0	0
1	Z	115	Total 918	C 574	N 169	O 173	S 2	0	0
1	a	115	Total 918	C 574	N 169	O 173	S 2	0	0
1	b	115	Total 918	C 574	N 169	O 173	S 2	0	0
1	c	115	Total 918	C 574	N 169	O 173	S 2	0	0
1	d	115	Total 918	C 574	N 169	O 173	S 2	0	0
1	e	115	Total 918	C 574	N 169	O 173	S 2	0	0
1	f	115	Total 918	C 574	N 169	O 173	S 2	0	0
1	g	115	Total 918	C 574	N 169	O 173	S 2	0	0
1	h	115	Total 918	C 574	N 169	O 173	S 2	0	0
1	i	115	Total 918	C 574	N 169	O 173	S 2	0	0
1	j	115	Total 918	C 574	N 169	O 173	S 2	0	0
1	k	115	Total 918	C 574	N 169	O 173	S 2	0	0
1	l	115	Total 918	C 574	N 169	O 173	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	115	Total	C	N	O	S	0	0
			918	574	169	173	2		

- Molecule 2 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			15	14	1	
2	B	1	Total	C	O	0
			15	14	1	
2	C	1	Total	C	O	0
			15	14	1	
2	D	1	Total	C	O	0
			15	14	1	
2	E	1	Total	C	O	0
			15	14	1	
2	F	1	Total	C	O	0
			15	14	1	
2	G	1	Total	C	O	0
			15	14	1	
2	H	1	Total	C	O	0
			15	14	1	
2	I	1	Total	C	O	0
			15	14	1	
2	J	1	Total	C	O	0
			15	14	1	

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Mol	Chain	Residues	Atoms			AltConf
2	K	1	Total	C	O	0
			15	14	1	
2	L	1	Total	C	O	0
			15	14	1	
2	M	1	Total	C	O	0
			15	14	1	
2	N	1	Total	C	O	0
			15	14	1	
2	O	1	Total	C	O	0
			15	14	1	
2	P	1	Total	C	O	0
			15	14	1	
2	Q	1	Total	C	O	0
			15	14	1	
2	R	1	Total	C	O	0
			15	14	1	
2	S	1	Total	C	O	0
			15	14	1	
2	T	1	Total	C	O	0
			15	14	1	
2	U	1	Total	C	O	0
			15	14	1	
2	V	1	Total	C	O	0
			15	14	1	
2	W	1	Total	C	O	0
			15	14	1	
2	X	1	Total	C	O	0
			15	14	1	
2	Y	1	Total	C	O	0
			15	14	1	
2	Z	1	Total	C	O	0
			15	14	1	
2	a	1	Total	C	O	0
			15	14	1	
2	b	1	Total	C	O	0
			15	14	1	
2	c	1	Total	C	O	0
			15	14	1	
2	d	1	Total	C	O	0
			15	14	1	
2	e	1	Total	C	O	0
			15	14	1	

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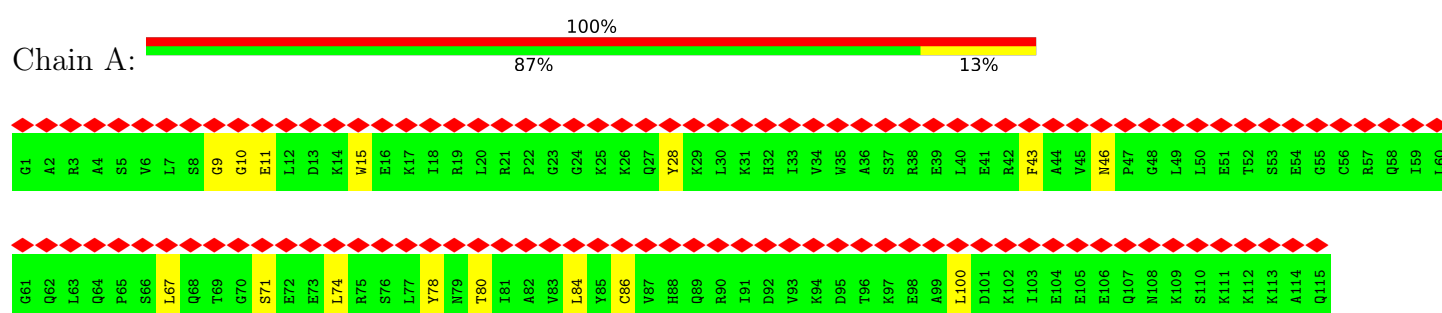
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Mol	Chain	Residues	Atoms			AltConf
2	f	1	Total	C	O	0
			15	14	1	
2	g	1	Total	C	O	0
			15	14	1	
2	h	1	Total	C	O	0
			15	14	1	
2	i	1	Total	C	O	0
			15	14	1	
2	j	1	Total	C	O	0
			15	14	1	
2	k	1	Total	C	O	0
			15	14	1	
2	l	1	Total	C	O	0
			15	14	1	
2	m	1	Total	C	O	0
			15	14	1	

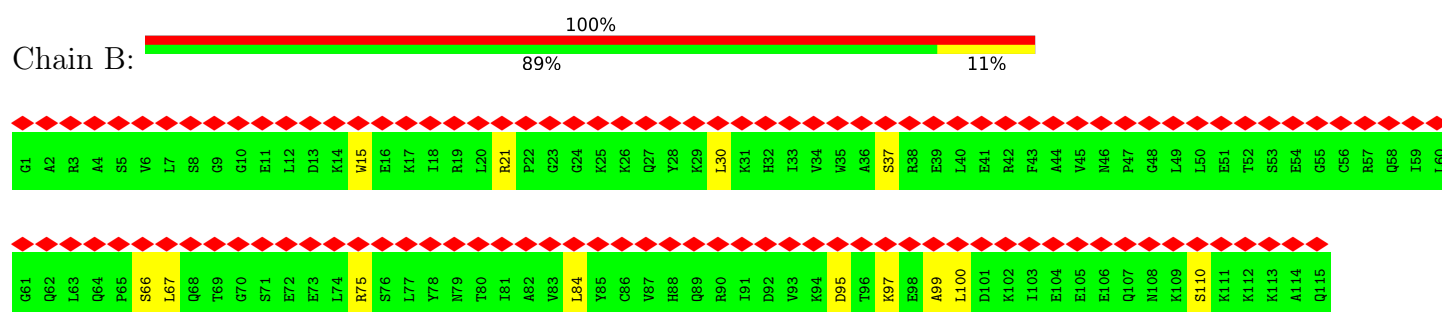
3 Residue-property plots

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

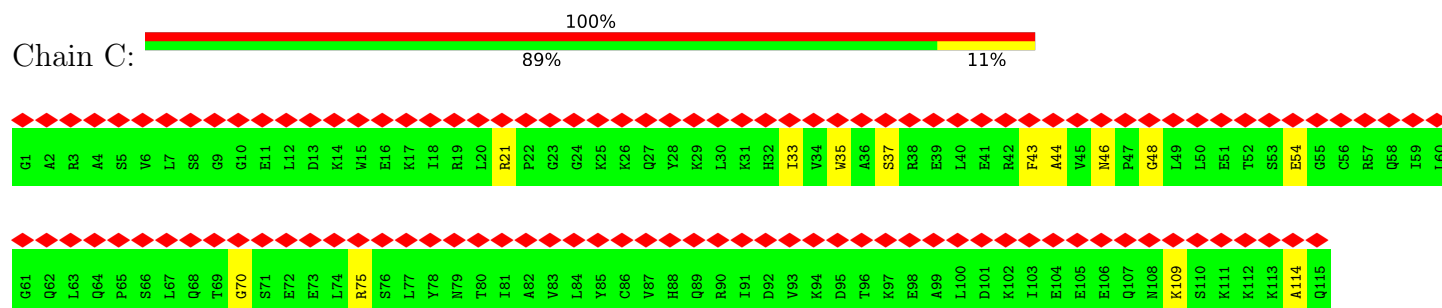
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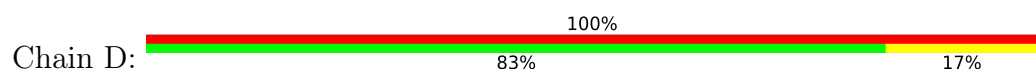
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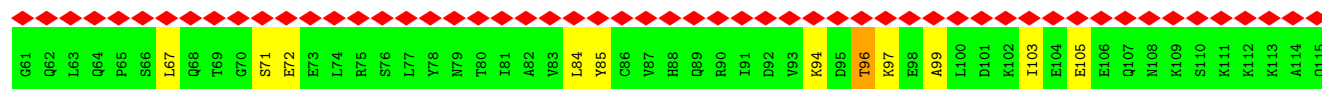
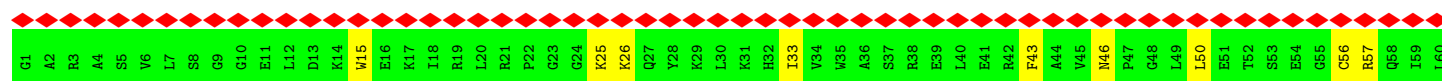


• Molecule 1: Matrix protein p17

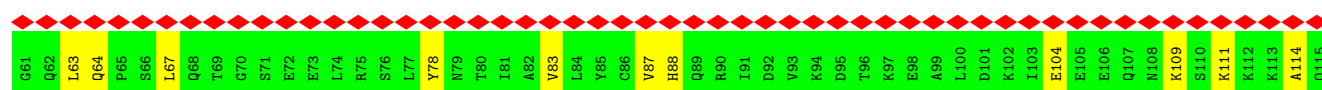
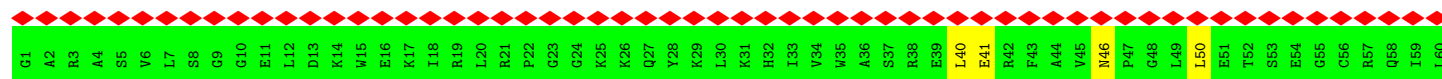
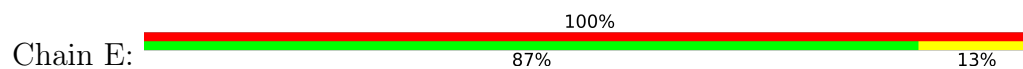


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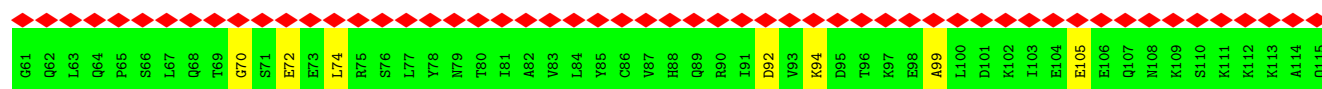
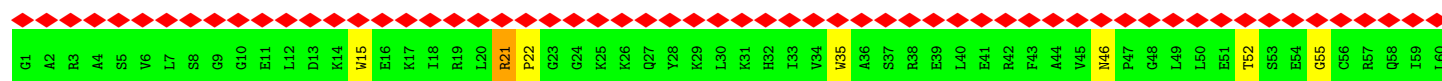
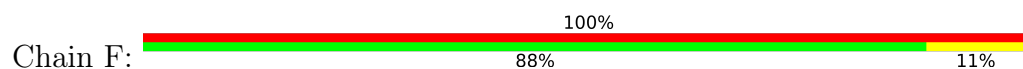




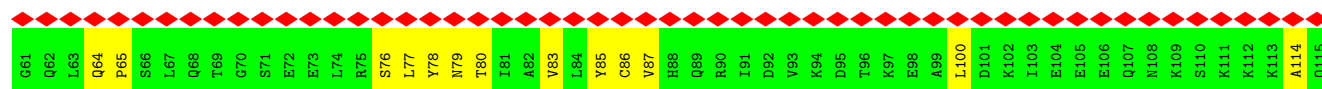
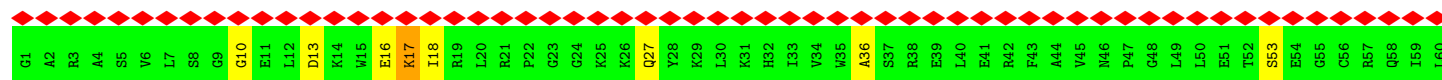
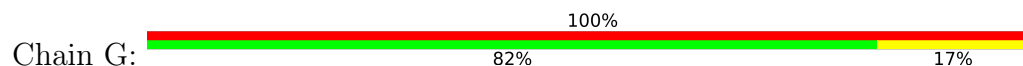
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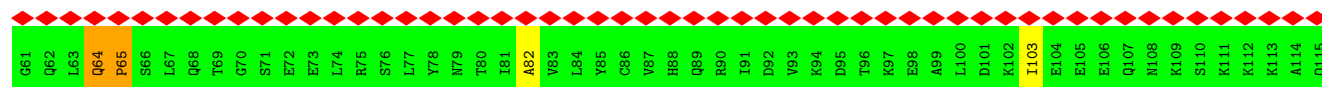
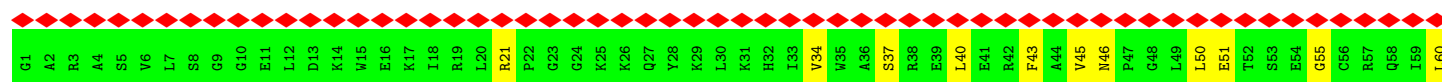
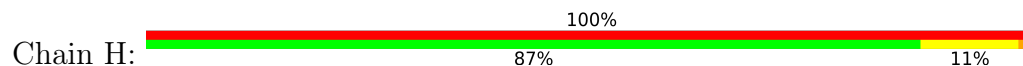
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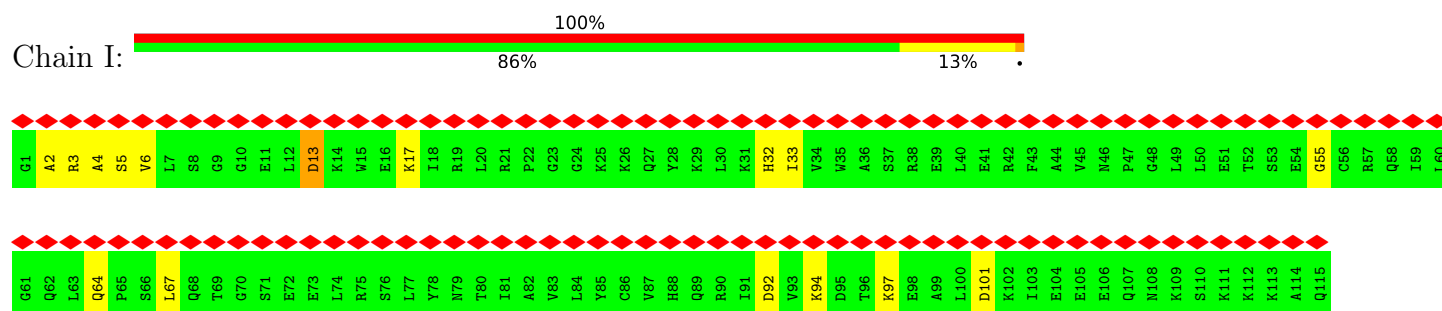
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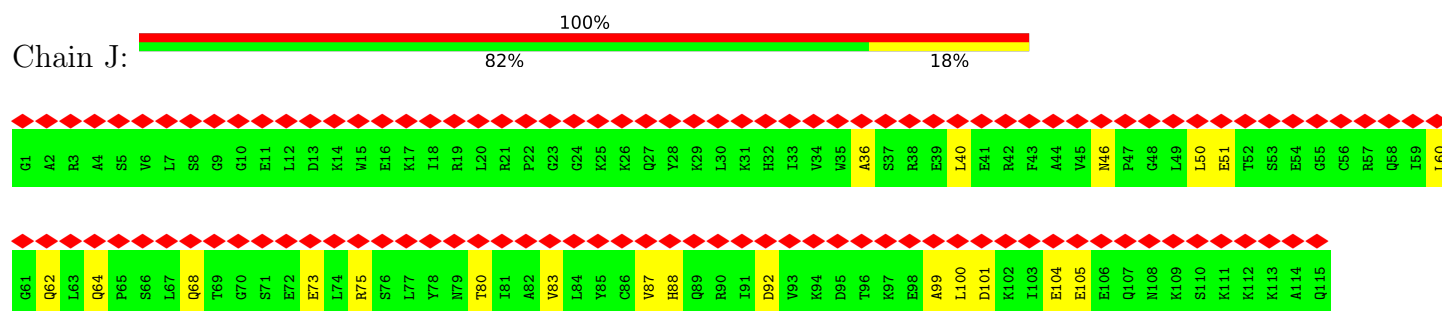
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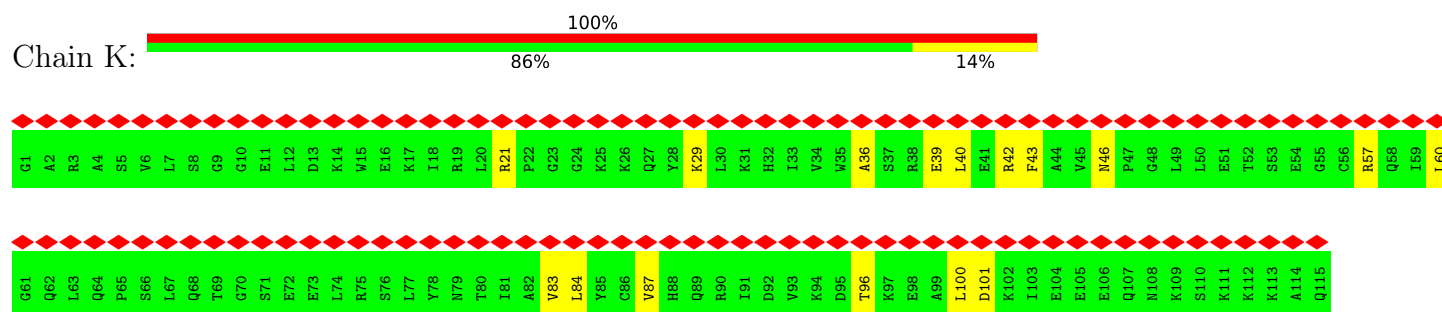
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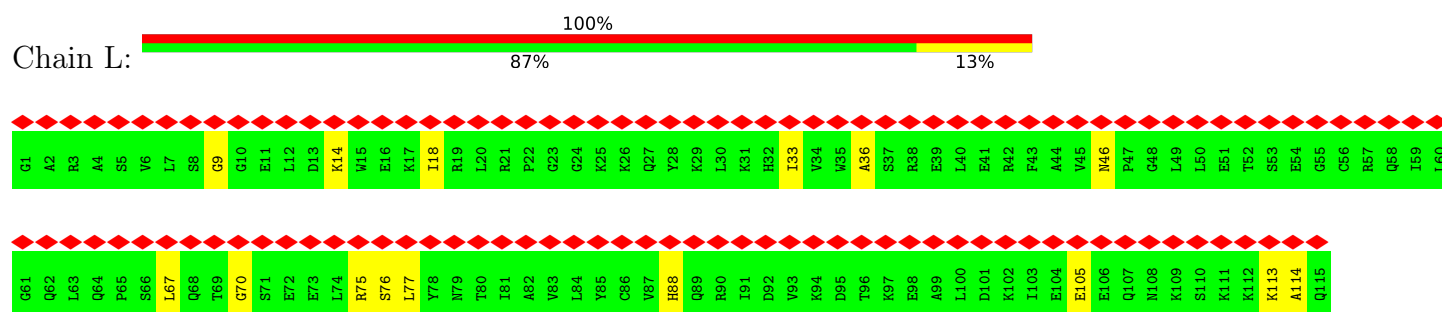
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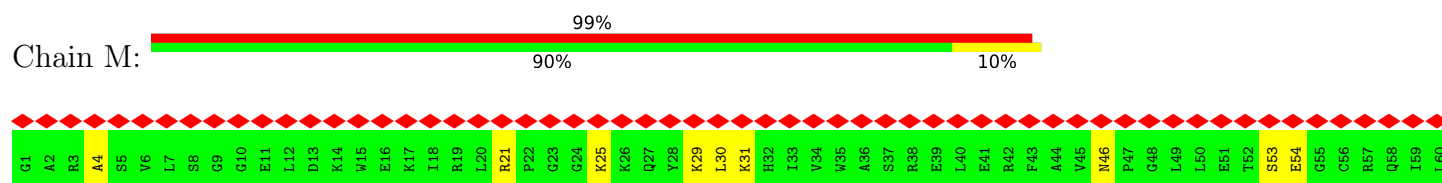
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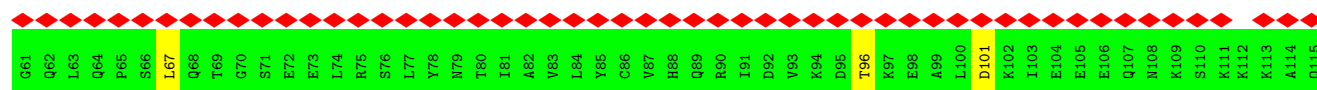


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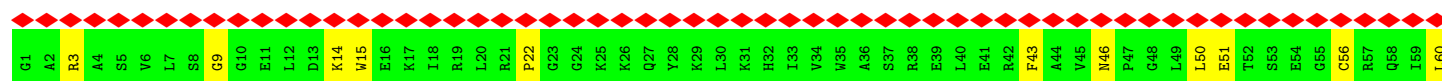
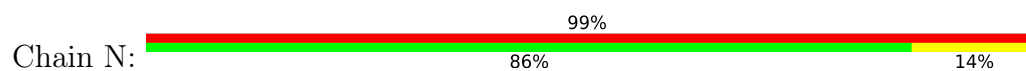


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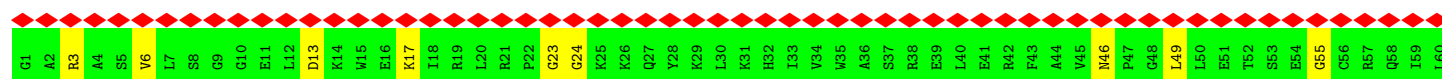
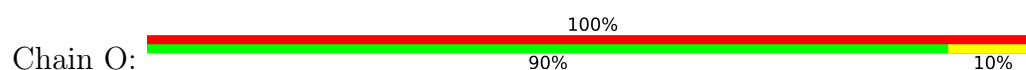




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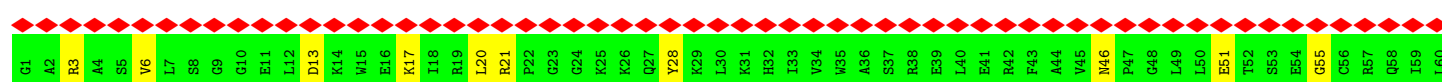
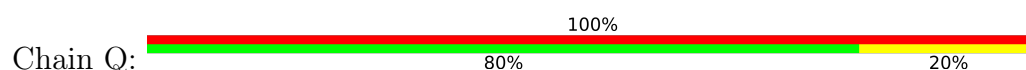
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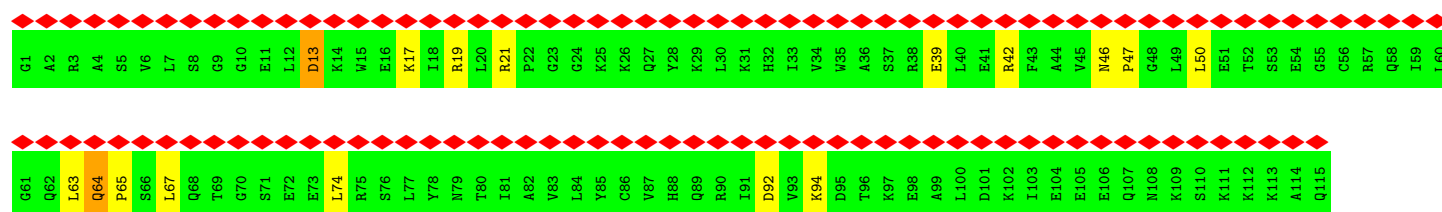
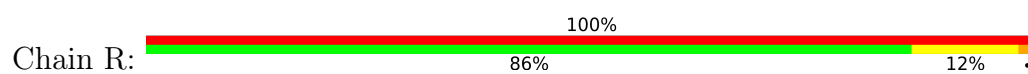
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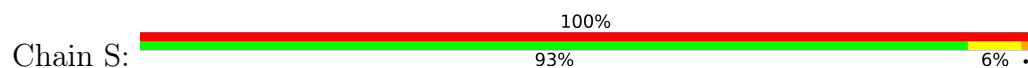
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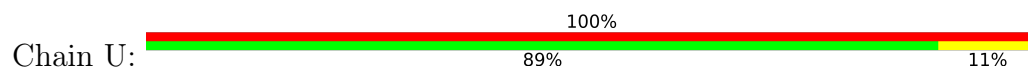
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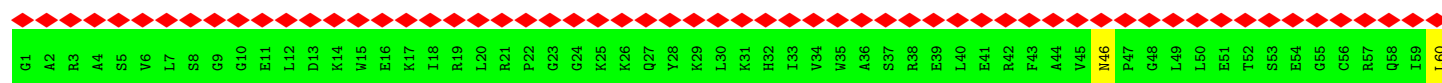
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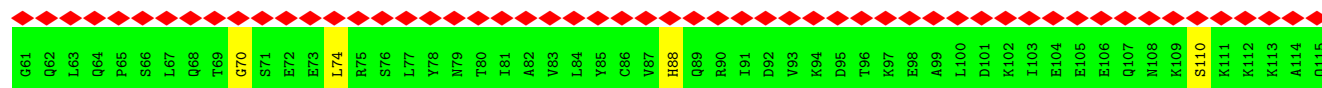


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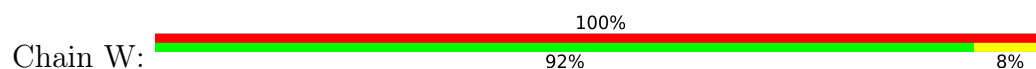


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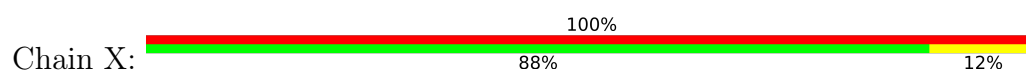




- Molecule 1: Matrix protein p17



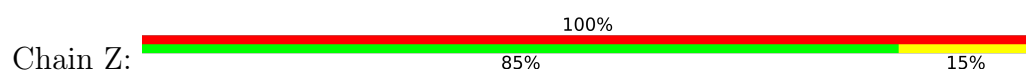
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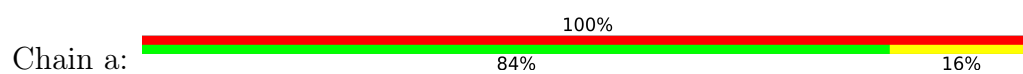
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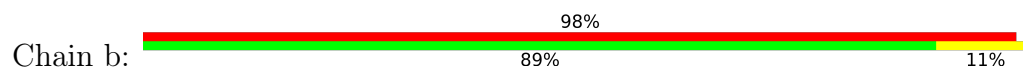
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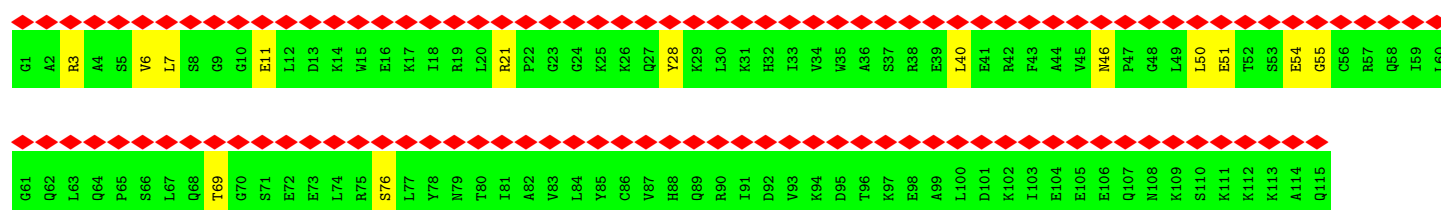
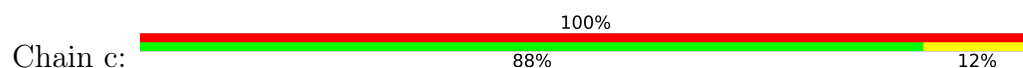
- Molecule 1: Matrix protein p17



- Molecule 1: Matrix protein p17



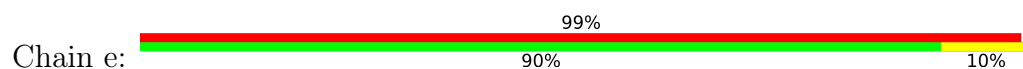
- Molecule 1: Matrix protein p17

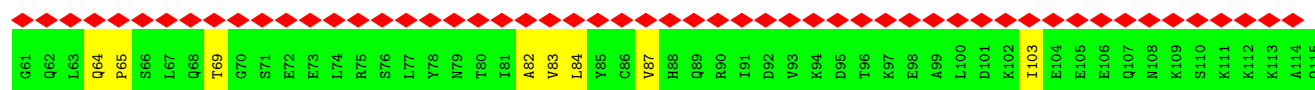


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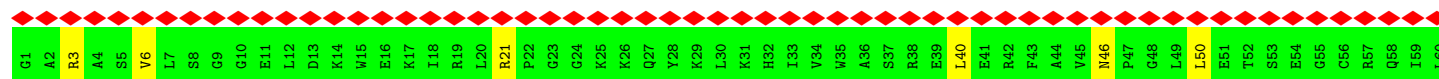
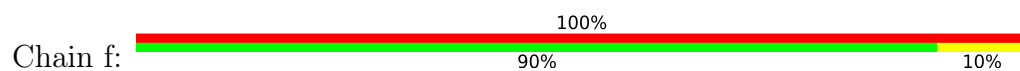


- Molecule 1: Matrix protein p17

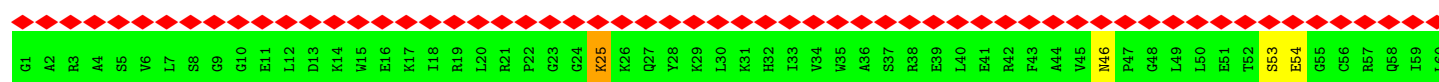




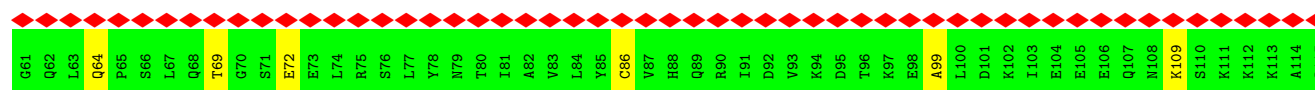
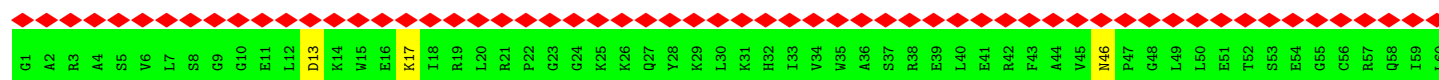
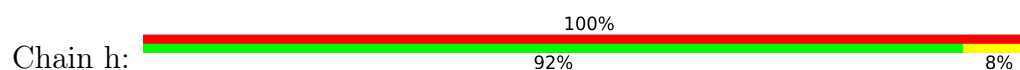
- Molecule 1: Matrix protein p17



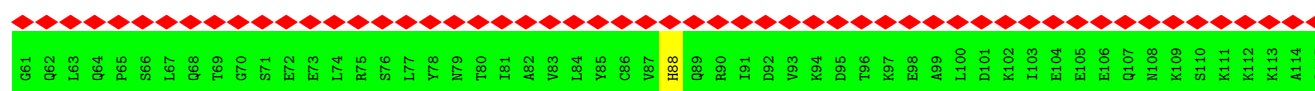
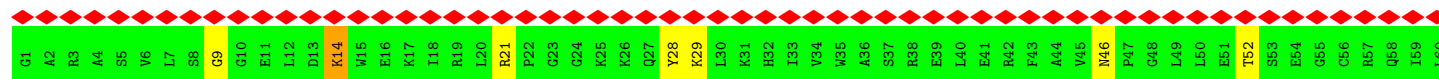
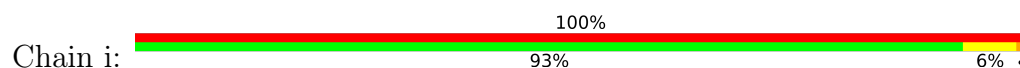
- Molecule 1: Matrix protein p17



- Molecule 1: Matrix protein p17



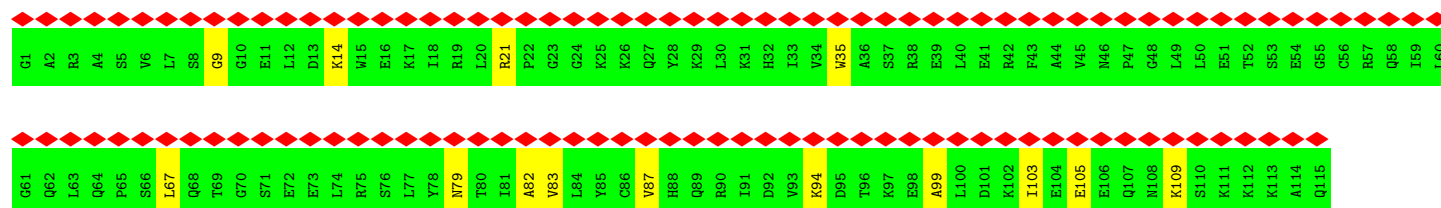
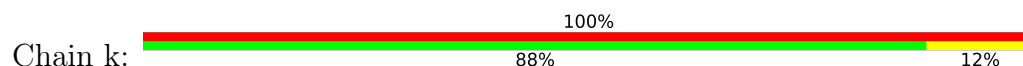
- Molecule 1: Matrix protein p17



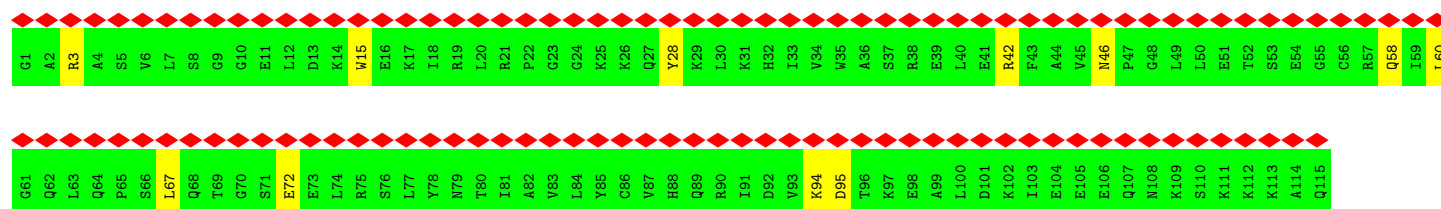
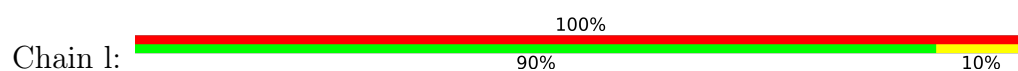
- Molecule 1: Matrix protein p17



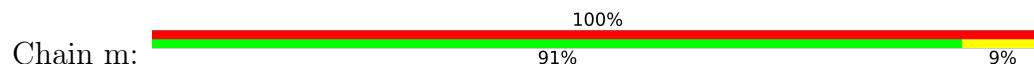
• Molecule 1: Matrix protein p17



• Molecule 1: Matrix protein p17



• Molecule 1: Matrix protein p17



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of subtomograms used	47770	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 ($e^-/\text{\AA}^2$)	123	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	85.202	Depositor
Minimum map value	-39.679	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	5.362	Depositor
Recommended contour level	20	Depositor
Map size (Å)	225.0, 225.0, 225.0	wwPDB
Map dimensions	150, 150, 150	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.5, 1.5, 1.5	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MYR

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	1.09	2/930 (0.2%)	1.31	9/1245 (0.7%)
1	B	1.17	7/930 (0.8%)	1.33	6/1245 (0.5%)
1	C	1.05	2/930 (0.2%)	1.28	8/1245 (0.6%)
1	D	1.15	4/930 (0.4%)	1.50	14/1245 (1.1%)
1	E	1.15	3/930 (0.3%)	1.29	9/1245 (0.7%)
1	F	1.14	3/930 (0.3%)	1.39	10/1245 (0.8%)
1	G	1.14	3/930 (0.3%)	1.32	5/1245 (0.4%)
1	H	1.13	3/930 (0.3%)	1.29	10/1245 (0.8%)
1	I	1.17	5/930 (0.5%)	1.36	9/1245 (0.7%)
1	J	1.36	10/930 (1.1%)	1.33	6/1245 (0.5%)
1	K	1.32	10/930 (1.1%)	1.35	11/1245 (0.9%)
1	L	1.03	3/930 (0.3%)	1.29	9/1245 (0.7%)
1	M	1.17	3/930 (0.3%)	1.39	14/1245 (1.1%)
1	N	1.06	2/930 (0.2%)	1.27	6/1245 (0.5%)
1	O	1.01	0/930	1.22	6/1245 (0.5%)
1	P	0.98	0/930	1.23	7/1245 (0.6%)
1	Q	1.23	2/930 (0.2%)	1.45	14/1245 (1.1%)
1	R	1.05	1/930 (0.1%)	1.20	6/1245 (0.5%)
1	S	1.01	1/930 (0.1%)	1.22	2/1245 (0.2%)
1	T	1.05	1/930 (0.1%)	1.27	3/1245 (0.2%)
1	U	1.12	2/930 (0.2%)	1.29	9/1245 (0.7%)
1	V	0.86	1/930 (0.1%)	1.26	6/1245 (0.5%)
1	W	0.94	0/930	1.22	4/1245 (0.3%)
1	X	1.22	2/930 (0.2%)	1.43	15/1245 (1.2%)
1	Y	0.95	1/930 (0.1%)	1.20	5/1245 (0.4%)
1	Z	1.24	6/930 (0.6%)	1.37	8/1245 (0.6%)
1	a	1.07	2/930 (0.2%)	1.35	8/1245 (0.6%)
1	b	0.87	0/930	1.22	4/1245 (0.3%)
1	c	1.11	0/930	1.33	16/1245 (1.3%)
1	d	0.87	1/930 (0.1%)	1.21	1/1245 (0.1%)
1	e	1.11	3/930 (0.3%)	1.28	7/1245 (0.6%)
1	f	0.90	0/930	1.19	4/1245 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	g	1.03	0/930	1.27	7/1245 (0.6%)
1	h	0.92	0/930	1.21	7/1245 (0.6%)
1	i	0.86	0/930	1.35	9/1245 (0.7%)
1	j	0.91	0/930	1.28	6/1245 (0.5%)
1	k	1.15	3/930 (0.3%)	1.33	5/1245 (0.4%)
1	l	1.12	3/930 (0.3%)	1.31	10/1245 (0.8%)
1	m	0.97	0/930	1.22	5/1245 (0.4%)
All	All	1.08	89/36270 (0.2%)	1.30	300/48555 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
1	J	0	1
All	All	0	3

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	LEU	CA-C	-9.36	1.40	1.52
1	K	29	LYS	CA-C	-9.28	1.41	1.52
1	K	101	ASP	CA-C	-8.65	1.41	1.52
1	l	58	GLN	CA-C	-8.35	1.41	1.52
1	I	101	ASP	CA-C	-8.34	1.42	1.52
1	B	97	LYS	N-CA	-7.70	1.36	1.46
1	A	86	CYS	CA-C	-7.60	1.42	1.52
1	G	86	CYS	CA-C	-7.58	1.43	1.52
1	Y	22	PRO	N-CD	-7.36	1.37	1.47
1	K	39	GLU	N-CA	-7.29	1.37	1.46
1	Q	100	LEU	CA-C	-7.29	1.43	1.52
1	G	10	GLY	CA-C	-7.22	1.39	1.52
1	D	105	GLU	N-CA	-7.17	1.37	1.46
1	L	105	GLU	N-CA	-7.01	1.37	1.46
1	e	58	GLN	CA-C	-7.01	1.43	1.52
1	N	74	LEU	CB-CG	7.00	1.67	1.53
1	K	39	GLU	CA-C	-6.92	1.43	1.52
1	G	100	LEU	CA-C	-6.89	1.43	1.52
1	D	105	GLU	CA-C	-6.84	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	101	ASP	N-CA	-6.82	1.38	1.46
1	B	100	LEU	CA-C	-6.81	1.44	1.52
1	X	103	ILE	CA-C	-6.77	1.44	1.52
1	Z	104	GLU	CA-C	-6.71	1.43	1.52
1	B	30	LEU	CA-C	-6.69	1.44	1.52
1	l	67	LEU	CB-CG	-6.64	1.40	1.53
1	U	100	LEU	CA-C	-6.64	1.44	1.52
1	B	37	SER	CA-C	-6.58	1.44	1.52
1	F	74	LEU	CA-C	-6.57	1.44	1.52
1	J	62	GLN	CA-C	-6.55	1.44	1.52
1	J	101	ASP	CA-C	-6.54	1.44	1.52
1	H	43	PHE	CA-C	-6.38	1.42	1.52
1	J	75	ARG	CA-C	-6.36	1.44	1.52
1	E	41	GLU	N-CA	-6.35	1.38	1.46
1	Z	101	ASP	CA-C	-6.26	1.44	1.52
1	I	32	HIS	CA-C	-6.22	1.44	1.52
1	K	36	ALA	CA-C	-6.09	1.44	1.52
1	L	67	LEU	N-CA	-6.04	1.39	1.46
1	J	104	GLU	CA-C	-6.00	1.44	1.52
1	J	64	GLN	N-CA	-5.98	1.41	1.46
1	e	58	GLN	N-CA	-5.98	1.39	1.46
1	U	64	GLN	N-CA	-5.96	1.41	1.46
1	B	30	LEU	N-CA	-5.94	1.39	1.46
1	k	105	GLU	N-CA	-5.94	1.39	1.46
1	I	101	ASP	N-CA	-5.89	1.39	1.46
1	E	104	GLU	N-CA	-5.84	1.38	1.46
1	a	104	GLU	CA-C	-5.84	1.44	1.52
1	I	33	ILE	N-CA	-5.80	1.39	1.46
1	I	64	GLN	N-CA	-5.77	1.41	1.46
1	F	99	ALA	CA-C	-5.74	1.45	1.52
1	F	105	GLU	CA-C	-5.67	1.45	1.52
1	J	104	GLU	N-CA	-5.63	1.39	1.46
1	K	42	ARG	N-CA	-5.60	1.39	1.46
1	Z	74	LEU	CB-CG	5.57	1.64	1.53
1	D	94	LYS	CA-C	-5.56	1.44	1.52
1	K	57	ARG	CA-C	-5.55	1.45	1.52
1	M	29	LYS	CA-C	-5.52	1.45	1.52
1	k	105	GLU	CA-C	-5.51	1.45	1.52
1	l	58	GLN	N-CA	-5.49	1.39	1.46
1	K	40	LEU	CA-C	-5.48	1.45	1.52
1	d	22	PRO	N-CD	-5.42	1.40	1.47
1	J	99	ALA	CA-C	-5.39	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	k	35	TRP	CZ3-CH2	-5.36	1.27	1.40
1	C	54	GLU	CA-C	-5.33	1.45	1.52
1	B	100	LEU	N-CA	-5.32	1.40	1.46
1	J	105	GLU	CA-C	-5.30	1.46	1.52
1	J	60	LEU	CB-CG	5.29	1.64	1.53
1	R	74	LEU	CB-CG	5.27	1.64	1.53
1	J	75	ARG	N-CA	-5.26	1.39	1.46
1	M	101	ASP	N-CA	-5.26	1.40	1.46
1	D	26	LYS	N-CA	-5.25	1.39	1.45
1	Q	102	LYS	CA-C	-5.23	1.46	1.52
1	C	44	ALA	CA-C	-5.22	1.46	1.53
1	S	60	LEU	CB-CG	5.20	1.63	1.53
1	X	12	LEU	CB-CG	5.19	1.63	1.53
1	M	101	ASP	CA-C	-5.19	1.46	1.52
1	V	60	LEU	CB-CG	5.18	1.63	1.53
1	H	60	LEU	CB-CG	5.17	1.63	1.53
1	E	104	GLU	CA-C	-5.13	1.45	1.52
1	T	74	LEU	CA-C	-5.13	1.46	1.52
1	Z	100	LEU	CA-C	-5.11	1.46	1.52
1	N	60	LEU	CB-CG	5.09	1.63	1.53
1	K	60	LEU	CB-CG	5.09	1.63	1.53
1	e	12	LEU	CB-CG	5.09	1.63	1.53
1	B	99	ALA	CA-C	-5.06	1.46	1.52
1	H	65	PRO	N-CD	-5.06	1.40	1.47
1	Z	104	GLU	N-CA	-5.05	1.39	1.46
1	L	105	GLU	CA-C	-5.03	1.46	1.52
1	Z	72	GLU	CA-C	-5.03	1.46	1.52
1	a	58	GLN	N-CA	-5.02	1.40	1.46

All (300) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	70	GLY	N-CA-C	13.88	122.84	110.21
1	D	96	THR	N-CA-C	11.68	124.01	111.28
1	Z	96	THR	N-CA-C	10.67	122.91	111.28
1	Q	21	ARG	N-CA-C	-9.37	96.38	110.07
1	B	67	LEU	CA-C-N	8.60	131.81	120.28
1	B	67	LEU	C-N-CA	8.60	131.81	120.28
1	A	10	GLY	N-CA-C	-8.54	98.83	112.66
1	F	46	ASN	CA-C-N	8.51	128.24	119.56
1	F	46	ASN	C-N-CA	8.51	128.24	119.56
1	K	96	THR	N-CA-C	8.41	120.44	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	67	LEU	CA-C-N	8.33	131.79	120.38
1	D	67	LEU	C-N-CA	8.33	131.79	120.38
1	Q	111	LYS	N-CA-C	8.29	121.25	111.71
1	M	4	ALA	N-CA-C	8.07	121.18	111.82
1	B	75	ARG	NE-CZ-NH2	-8.05	111.95	119.20
1	C	114	ALA	N-CA-C	-8.02	103.57	112.72
1	A	46	ASN	CA-C-N	8.01	127.73	119.56
1	A	46	ASN	C-N-CA	8.01	127.73	119.56
1	k	94	LYS	N-CA-C	-7.96	104.16	114.04
1	X	96	THR	N-CA-C	7.75	120.71	111.33
1	K	57	ARG	CA-C-O	7.68	128.69	120.55
1	E	114	ALA	N-CA-C	-7.61	103.97	112.57
1	a	94	LYS	N-CA-C	-7.45	104.34	113.50
1	J	51	GLU	N-CA-C	-7.40	103.85	113.17
1	Q	46	ASN	CA-C-N	7.39	127.10	119.56
1	Q	46	ASN	C-N-CA	7.39	127.10	119.56
1	L	33	ILE	N-CA-C	-7.39	103.75	111.58
1	m	46	ASN	CA-C-N	7.37	127.04	119.82
1	m	46	ASN	C-N-CA	7.37	127.04	119.82
1	N	46	ASN	CA-C-N	7.36	127.07	119.56
1	N	46	ASN	C-N-CA	7.36	127.07	119.56
1	P	59	ILE	CB-CA-C	-7.33	102.59	111.97
1	N	43	PHE	N-CA-C	7.16	121.62	113.02
1	k	109	LYS	N-CA-C	7.10	119.02	111.28
1	W	54	GLU	CA-C-N	7.06	127.64	119.94
1	W	54	GLU	C-N-CA	7.06	127.64	119.94
1	L	46	ASN	CA-C-N	7.03	126.71	119.82
1	L	46	ASN	C-N-CA	7.03	126.71	119.82
1	l	46	ASN	CA-C-N	6.96	126.66	119.56
1	l	46	ASN	C-N-CA	6.96	126.66	119.56
1	J	46	ASN	CA-C-N	6.91	126.61	119.56
1	J	46	ASN	C-N-CA	6.91	126.61	119.56
1	F	21	ARG	CA-C-N	6.88	126.57	119.82
1	F	21	ARG	C-N-CA	6.88	126.57	119.82
1	D	46	ASN	CA-C-N	6.87	126.56	119.56
1	D	46	ASN	C-N-CA	6.87	126.56	119.56
1	K	46	ASN	CA-C-N	6.84	126.54	119.56
1	K	46	ASN	C-N-CA	6.84	126.54	119.56
1	O	46	ASN	CA-C-N	6.83	126.53	119.56
1	O	46	ASN	C-N-CA	6.83	126.53	119.56
1	h	46	ASN	CA-C-N	6.82	126.52	119.56
1	h	46	ASN	C-N-CA	6.82	126.52	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	46	ASN	CA-C-N	6.80	126.49	119.56
1	c	46	ASN	C-N-CA	6.80	126.49	119.56
1	D	96	THR	CA-C-O	6.79	127.75	120.55
1	H	34	VAL	N-CA-C	6.78	116.93	110.42
1	M	54	GLU	CA-C-N	6.77	127.46	119.94
1	M	54	GLU	C-N-CA	6.77	127.46	119.94
1	I	97	LYS	N-CA-C	6.69	118.65	111.36
1	Y	46	ASN	CA-C-N	6.68	126.37	119.56
1	Y	46	ASN	C-N-CA	6.68	126.37	119.56
1	Z	46	ASN	CA-C-N	6.62	126.31	119.56
1	Z	46	ASN	C-N-CA	6.62	126.31	119.56
1	D	72	GLU	N-CA-C	6.60	119.47	111.82
1	U	97	LYS	CA-C-O	6.59	127.41	120.42
1	B	21	ARG	N-CA-C	-6.59	98.84	109.58
1	a	43	PHE	N-CA-C	6.59	120.92	113.02
1	E	109	LYS	N-CA-C	-6.57	104.20	111.36
1	a	46	ASN	CA-C-N	6.54	126.23	119.56
1	a	46	ASN	C-N-CA	6.54	126.23	119.56
1	a	55	GLY	N-CA-C	-6.54	104.91	112.50
1	C	46	ASN	CA-C-N	6.52	126.65	119.87
1	C	46	ASN	C-N-CA	6.52	126.65	119.87
1	I	6	VAL	N-CA-C	6.52	118.22	106.61
1	K	100	LEU	CA-C-N	6.49	128.97	120.28
1	K	100	LEU	C-N-CA	6.49	128.97	120.28
1	M	21	ARG	CA-C-N	6.47	126.16	119.56
1	M	21	ARG	C-N-CA	6.47	126.16	119.56
1	Q	96	THR	N-CA-C	6.44	118.30	111.28
1	G	114	ALA	N-CA-C	-6.43	104.59	112.88
1	i	21	ARG	O-C-N	-6.38	116.58	121.55
1	l	95	ASP	CA-C-N	6.32	128.75	120.28
1	l	95	ASP	C-N-CA	6.32	128.75	120.28
1	K	21	ARG	CA-C-N	6.32	127.73	119.84
1	K	21	ARG	C-N-CA	6.32	127.73	119.84
1	O	24	GLY	N-CA-C	6.32	120.62	112.54
1	b	46	ASN	CA-C-N	6.28	125.97	119.56
1	b	46	ASN	C-N-CA	6.28	125.97	119.56
1	E	46	ASN	CA-C-N	6.26	125.95	119.82
1	E	46	ASN	C-N-CA	6.26	125.95	119.82
1	l	72	GLU	N-CA-C	6.25	118.10	111.28
1	f	46	ASN	CA-C-N	6.17	125.85	119.56
1	f	46	ASN	C-N-CA	6.17	125.85	119.56
1	Y	13	ASP	N-CA-C	-6.16	104.65	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	91	ILE	N-CA-C	-6.16	100.77	108.89
1	X	109	LYS	N-CA-C	-6.13	104.60	111.28
1	K	43	PHE	CA-CB-CG	-6.10	107.70	113.80
1	Q	102	LYS	CA-C-O	6.10	127.22	120.82
1	H	51	GLU	N-CA-C	-6.08	104.21	111.69
1	J	100	LEU	N-CA-C	-6.07	104.78	111.82
1	U	112	LYS	N-CA-C	6.05	118.84	111.82
1	K	84	LEU	CB-CA-C	-6.05	101.13	110.81
1	b	70	GLY	N-CA-C	6.04	118.97	112.33
1	c	11	GLU	N-CA-C	6.04	117.66	111.14
1	D	43	PHE	CA-CB-CG	5.99	119.79	113.80
1	E	111	LYS	N-CA-C	5.99	117.81	111.28
1	C	109	LYS	N-CA-C	-5.97	104.71	112.23
1	N	51	GLU	N-CA-C	-5.96	105.19	112.88
1	l	94	LYS	N-CA-C	-5.95	106.07	113.38
1	D	71	SER	CA-C-N	5.95	129.35	120.31
1	D	71	SER	C-N-CA	5.95	129.35	120.31
1	I	13	ASP	CA-CB-CG	5.94	118.54	112.60
1	H	46	ASN	CA-C-N	5.93	126.35	119.47
1	H	46	ASN	C-N-CA	5.93	126.35	119.47
1	M	46	ASN	CA-C-N	5.91	125.59	119.56
1	M	46	ASN	C-N-CA	5.91	125.59	119.56
1	X	21	ARG	CA-C-N	5.90	126.05	119.32
1	X	21	ARG	C-N-CA	5.90	126.05	119.32
1	m	13	ASP	CA-CB-CG	5.90	118.50	112.60
1	i	46	ASN	CA-C-N	5.89	125.76	119.28
1	i	46	ASN	C-N-CA	5.89	125.76	119.28
1	F	72	GLU	O-C-N	5.88	128.36	122.12
1	U	46	ASN	CA-C-N	5.88	125.56	119.56
1	U	46	ASN	C-N-CA	5.88	125.56	119.56
1	Z	96	THR	CA-C-O	5.88	126.78	120.55
1	g	54	GLU	CA-C-N	5.87	126.49	119.98
1	g	54	GLU	C-N-CA	5.87	126.49	119.98
1	L	88	HIS	CA-CB-CG	5.85	119.65	113.80
1	X	7	LEU	N-CA-C	5.85	117.85	110.24
1	Q	72	GLU	CA-C-N	5.84	128.11	120.28
1	Q	72	GLU	C-N-CA	5.84	128.11	120.28
1	L	114	ALA	N-CA-C	-5.81	106.05	113.02
1	I	67	LEU	CA-C-N	5.80	128.63	120.28
1	I	67	LEU	C-N-CA	5.80	128.63	120.28
1	X	25	LYS	N-CA-C	-5.79	105.87	113.17
1	F	35	TRP	N-CA-C	-5.79	104.88	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	67	LEU	N-CA-C	5.78	119.59	112.54
1	P	21	ARG	CA-C-N	5.76	125.89	119.32
1	P	21	ARG	C-N-CA	5.76	125.89	119.32
1	M	30	LEU	N-CA-C	5.76	117.56	111.28
1	H	55	GLY	N-CA-C	-5.75	105.53	112.49
1	Z	52	THR	N-CA-C	5.74	118.46	108.76
1	M	31	LYS	CA-C-N	5.73	127.96	120.28
1	M	31	LYS	C-N-CA	5.73	127.96	120.28
1	X	46	ASN	CA-C-N	5.73	126.12	119.47
1	X	46	ASN	C-N-CA	5.73	126.12	119.47
1	c	69	THR	N-CA-C	-5.73	106.64	113.97
1	J	80	THR	N-CA-C	-5.72	105.12	111.36
1	c	28	TYR	CA-C-N	5.69	131.53	122.59
1	c	28	TYR	C-N-CA	5.69	131.53	122.59
1	W	46	ASN	CA-C-N	5.69	125.31	119.56
1	W	46	ASN	C-N-CA	5.69	125.31	119.56
1	R	46	ASN	CA-C-N	5.68	125.78	119.87
1	R	46	ASN	C-N-CA	5.68	125.78	119.87
1	B	66	SER	N-CA-C	5.68	120.33	113.17
1	l	42	ARG	N-CA-C	5.68	117.47	111.28
1	V	46	ASN	CA-C-N	5.67	125.35	119.56
1	V	46	ASN	C-N-CA	5.67	125.35	119.56
1	h	109	LYS	N-CA-C	-5.67	105.18	111.36
1	b	109	LYS	N-CA-C	5.66	117.92	111.02
1	e	69	THR	CA-C-N	5.65	125.47	120.10
1	e	69	THR	C-N-CA	5.65	125.47	120.10
1	C	21	ARG	N-CA-C	-5.64	100.39	109.58
1	i	14	LYS	CA-C-N	5.62	127.81	120.28
1	i	14	LYS	C-N-CA	5.62	127.81	120.28
1	J	88	HIS	CA-CB-CG	5.62	119.42	113.80
1	g	75	ARG	N-CA-C	-5.62	105.23	111.36
1	P	59	ILE	N-CA-CB	5.62	117.12	110.55
1	Q	51	GLU	N-CA-C	-5.62	106.01	112.92
1	c	7	LEU	CA-C-N	5.62	128.74	120.82
1	c	7	LEU	C-N-CA	5.62	128.74	120.82
1	V	110	SER	CA-C-N	5.62	127.81	120.28
1	V	110	SER	C-N-CA	5.62	127.81	120.28
1	U	9	GLY	N-CA-C	-5.61	107.90	115.36
1	O	23	GLY	CA-C-N	-5.61	114.19	120.53
1	O	23	GLY	C-N-CA	-5.61	114.19	120.53
1	A	11	GLU	CA-C-N	-5.60	112.33	120.29
1	A	11	GLU	C-N-CA	-5.60	112.33	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	54	GLU	CA-C-N	5.60	126.15	119.94
1	c	54	GLU	C-N-CA	5.60	126.15	119.94
1	g	25	LYS	N-CA-C	5.60	122.72	110.80
1	e	28	TYR	N-CA-C	5.54	117.84	110.53
1	R	13	ASP	N-CA-C	-5.52	105.26	111.28
1	j	21	ARG	CA-C-N	5.50	125.59	119.32
1	j	21	ARG	C-N-CA	5.50	125.59	119.32
1	c	55	GLY	N-CA-C	-5.50	106.12	112.50
1	M	53	SER	N-CA-C	5.50	117.35	111.36
1	Q	55	GLY	N-CA-C	-5.48	105.75	112.77
1	U	32	HIS	N-CA-C	-5.48	105.47	111.82
1	D	94	LYS	N-CA-C	-5.47	107.25	114.04
1	C	48	GLY	N-CA-C	-5.45	108.17	115.32
1	j	46	ASN	CA-C-N	5.45	125.12	119.56
1	j	46	ASN	C-N-CA	5.45	125.12	119.56
1	f	21	ARG	CA-C-N	5.45	125.53	119.32
1	f	21	ARG	C-N-CA	5.45	125.53	119.32
1	I	55	GLY	N-CA-C	-5.44	106.19	112.50
1	P	96	THR	N-CA-C	5.44	117.21	111.28
1	a	114	ALA	N-CA-C	-5.44	107.65	114.56
1	e	46	ASN	CA-C-N	5.44	125.11	119.56
1	e	46	ASN	C-N-CA	5.44	125.11	119.56
1	P	29	LYS	CA-C-N	5.43	128.10	120.28
1	P	29	LYS	C-N-CA	5.43	128.10	120.28
1	Q	95	ASP	CA-C-N	5.43	127.55	120.28
1	Q	95	ASP	C-N-CA	5.43	127.55	120.28
1	k	21	ARG	CA-C-N	5.41	125.74	119.47
1	k	21	ARG	C-N-CA	5.41	125.74	119.47
1	R	67	LEU	N-CA-C	5.40	116.85	111.07
1	c	21	ARG	CA-C-N	5.40	126.59	119.84
1	c	21	ARG	C-N-CA	5.40	126.59	119.84
1	h	69	THR	CA-C-N	5.40	126.32	120.44
1	h	69	THR	C-N-CA	5.40	126.32	120.44
1	B	110	SER	N-CA-C	-5.37	105.43	111.28
1	i	28	TYR	N-CA-C	5.37	117.65	110.35
1	F	72	GLU	CA-C-N	5.35	127.99	120.28
1	F	72	GLU	C-N-CA	5.35	127.99	120.28
1	E	40	LEU	CA-C-N	5.35	127.45	120.28
1	E	40	LEU	C-N-CA	5.35	127.45	120.28
1	k	67	LEU	N-CA-C	5.34	117.10	111.28
1	m	62	GLN	N-CA-C	5.34	117.10	111.28
1	j	54	GLU	CA-C-N	5.33	125.86	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	j	54	GLU	C-N-CA	5.33	125.86	119.94
1	g	53	SER	N-CA-C	5.33	118.00	111.82
1	Z	106	GLU	N-CA-C	-5.32	105.65	111.82
1	i	88	HIS	CA-CB-CG	5.32	119.12	113.80
1	K	42	ARG	N-CA-C	5.31	117.07	111.28
1	i	29	LYS	CA-C-N	5.31	127.39	120.28
1	i	29	LYS	C-N-CA	5.31	127.39	120.28
1	H	37	SER	CA-C-O	5.31	126.17	120.70
1	A	80	THR	N-CA-C	-5.30	105.42	111.14
1	a	44	ALA	CA-C-O	5.29	126.21	120.12
1	X	94	LYS	N-CA-C	-5.29	106.87	113.38
1	X	97	LYS	N-CA-C	5.29	117.12	111.36
1	e	84	LEU	CA-C-N	5.28	127.62	120.44
1	e	84	LEU	C-N-CA	5.28	127.62	120.44
1	Q	94	LYS	N-CA-C	-5.28	106.69	113.23
1	T	95	ASP	N-CA-C	5.27	115.49	108.38
1	S	64	GLN	CA-C-N	5.26	124.92	119.56
1	S	64	GLN	C-N-CA	5.26	124.92	119.56
1	X	51	GLU	N-CA-C	-5.25	106.46	112.92
1	V	88	HIS	CA-CB-CG	5.25	119.05	113.80
1	I	5	SER	CA-C-N	-5.25	116.45	123.17
1	I	5	SER	C-N-CA	-5.25	116.45	123.17
1	D	25	LYS	CA-C-O	5.25	125.41	119.27
1	D	33	ILE	N-CA-C	-5.24	105.28	111.00
1	L	9	GLY	N-CA-C	-5.24	108.39	115.21
1	X	113	LYS	N-CA-C	-5.24	105.34	112.26
1	l	60	LEU	CA-C-N	5.23	125.76	120.00
1	l	60	LEU	C-N-CA	5.23	125.76	120.00
1	I	4	ALA	CA-C-O	5.22	125.97	119.97
1	M	96	THR	CA-C-N	-5.22	112.37	120.31
1	M	96	THR	C-N-CA	-5.22	112.37	120.31
1	G	76	SER	N-CA-C	-5.22	105.59	111.28
1	A	9	GLY	N-CA-C	-5.22	108.42	115.36
1	c	51	GLU	N-CA-C	-5.20	106.61	113.17
1	Z	94	LYS	N-CA-C	-5.20	107.00	113.55
1	D	97	LYS	CA-C-O	5.19	125.92	120.42
1	G	78	TYR	N-CA-C	-5.19	105.52	111.07
1	A	71	SER	CA-C-N	5.18	128.19	120.31
1	A	71	SER	C-N-CA	5.18	128.19	120.31
1	C	35	TRP	N-CA-C	-5.18	105.52	111.07
1	X	97	LYS	CA-C-N	5.18	127.64	120.29
1	X	97	LYS	C-N-CA	5.18	127.64	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	96	THR	N-CA-C	5.17	116.91	111.28
1	Q	97	LYS	CA-C-O	5.16	126.02	120.55
1	Y	27	GLN	CB-CG-CD	5.15	121.35	112.60
1	C	43	PHE	CA-CB-CG	-5.14	108.66	113.80
1	F	15	TRP	CA-CB-CG	5.14	123.37	113.60
1	g	46	ASN	CA-C-N	5.14	126.27	119.84
1	g	46	ASN	C-N-CA	5.14	126.27	119.84
1	U	71	SER	CA-C-N	5.11	127.13	120.28
1	U	71	SER	C-N-CA	5.11	127.13	120.28
1	Z	92	ASP	CA-CB-CG	5.11	117.71	112.60
1	G	17	LYS	CA-C-N	-5.11	116.01	123.06
1	G	17	LYS	C-N-CA	-5.11	116.01	123.06
1	L	76	SER	CA-C-N	5.11	127.08	120.44
1	L	76	SER	C-N-CA	5.11	127.08	120.44
1	l	95	ASP	N-CA-C	5.11	115.79	108.74
1	m	103	ILE	CB-CA-C	-5.08	105.47	111.97
1	V	70	GLY	N-CA-C	5.08	117.92	112.33
1	d	28	TYR	N-CA-C	5.07	117.25	110.35
1	T	29	LYS	CA-C-N	5.06	127.56	120.28
1	T	29	LYS	C-N-CA	5.06	127.56	120.28
1	c	76	SER	CA-C-N	5.06	127.01	120.44
1	c	76	SER	C-N-CA	5.06	127.01	120.44
1	L	113	LYS	N-CA-C	-5.05	105.59	112.26
1	H	64	GLN	CA-C-N	5.05	124.71	119.56
1	H	64	GLN	C-N-CA	5.05	124.71	119.56
1	H	21	ARG	CA-C-N	5.05	126.15	119.84
1	H	21	ARG	C-N-CA	5.05	126.15	119.84
1	U	92	ASP	N-CA-C	5.04	116.83	108.20
1	Y	43	PHE	CA-CB-CG	5.04	118.84	113.80
1	N	22	PRO	N-CA-C	5.04	120.17	113.57
1	N	77	LEU	N-CA-C	5.02	116.44	111.07
1	E	67	LEU	CA-C-N	5.01	127.40	120.29
1	E	67	LEU	C-N-CA	5.01	127.40	120.29
1	X	92	ASP	N-CA-C	5.01	117.14	109.07
1	R	64	GLN	CA-C-N	5.01	124.67	119.56
1	R	64	GLN	C-N-CA	5.01	124.67	119.56
1	h	64	GLN	CA-C-N	5.01	124.67	119.56
1	h	64	GLN	C-N-CA	5.01	124.67	119.56

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	96	THR	Mainchain
1	E	78	TYR	Sidechain
1	J	92	ASP	Mainchain

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	918	0	948	6	0
1	B	918	0	947	2	0
1	C	918	0	947	2	0
1	D	918	0	947	5	0
1	E	918	0	948	4	0
1	F	918	0	947	3	0
1	G	918	0	948	11	0
1	H	918	0	947	8	0
1	I	918	0	948	5	0
1	J	918	0	948	6	0
1	K	918	0	948	1	0
1	L	918	0	948	4	0
1	M	918	0	948	1	0
1	N	918	0	948	6	0
1	O	918	0	948	7	0
1	P	918	0	948	1	0
1	Q	918	0	947	6	0
1	R	918	0	947	8	0
1	S	918	0	947	4	0
1	T	918	0	948	2	0
1	U	918	0	947	3	0
1	V	918	0	947	1	0
1	W	918	0	948	7	0
1	X	918	0	948	2	0
1	Y	918	0	948	0	0
1	Z	918	0	948	9	0
1	a	918	0	948	5	0
1	b	918	0	948	9	0
1	c	918	0	948	4	0
1	d	918	0	948	1	0
1	e	918	0	948	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	f	918	0	948	8	0
1	g	918	0	948	0	0
1	h	918	0	948	3	0
1	i	918	0	948	1	0
1	j	918	0	948	1	0
1	k	918	0	948	5	0
1	l	918	0	947	3	0
1	m	918	0	948	4	0
2	A	15	0	27	0	0
2	B	15	0	27	0	0
2	C	15	0	27	0	0
2	D	15	0	27	0	0
2	E	15	0	27	0	0
2	F	15	0	27	0	0
2	G	15	0	27	0	0
2	H	15	0	27	0	0
2	I	15	0	27	3	0
2	J	15	0	27	0	0
2	K	15	0	27	0	0
2	L	15	0	27	0	0
2	M	15	0	27	0	0
2	N	15	0	27	1	0
2	O	15	0	27	0	0
2	P	15	0	27	0	0
2	Q	15	0	27	0	0
2	R	15	0	27	0	0
2	S	15	0	27	0	0
2	T	15	0	27	0	0
2	U	15	0	27	0	0
2	V	15	0	27	0	0
2	W	15	0	27	0	0
2	X	15	0	27	2	0
2	Y	15	0	27	0	0
2	Z	15	0	27	2	0
2	a	15	0	27	0	0
2	b	15	0	27	0	0
2	c	15	0	27	2	0
2	d	15	0	27	0	0
2	e	15	0	27	0	0
2	f	15	0	27	0	0
2	g	15	0	27	0	0
2	h	15	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	i	15	0	27	0	0
2	j	15	0	27	0	0
2	k	15	0	27	0	0
2	l	15	0	27	2	0
2	m	15	0	27	0	0
All	All	36387	0	38014	161	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 (161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:49:LEU:HB2	1:b:59:ILE:HD11	1.53	0.89
1:W:49:LEU:HB2	1:W:59:ILE:HD11	1.62	0.80
1:b:49:LEU:CB	1:b:59:ILE:HD11	2.22	0.69
1:G:53:SER:HB2	1:G:85:TYR:CE1	2.28	0.68
1:O:13:ASP:OD1	1:O:17:LYS:NZ	2.26	0.68
1:H:82:ALA:HB1	1:H:103:ILE:CD1	2.25	0.66
1:O:49:LEU:HD12	1:O:55:GLY:CA	2.25	0.66
1:e:83:VAL:O	1:e:87:VAL:HG23	1.98	0.64
1:A:67:LEU:HD11	1:A:78:TYR:CD1	2.33	0.64
1:N:15:TRP:CH2	1:N:80:THR:HG23	2.32	0.63
1:i:9:GLY:O	1:i:14:LYS:NZ	2.33	0.62
1:Z:15:TRP:CZ2	1:Z:84:LEU:CD2	2.83	0.62
1:R:50:LEU:C	1:R:50:LEU:HD12	2.25	0.61
1:W:49:LEU:CB	1:W:59:ILE:HD11	2.31	0.61
1:Z:12:LEU:HA	1:Z:15:TRP:CE3	2.36	0.60
1:j:52:THR:HG23	1:j:55:GLY:H	1.68	0.59
1:f:40:LEU:CD1	1:f:50:LEU:HD11	2.34	0.58
1:e:82:ALA:HB1	1:e:103:ILE:HD11	1.86	0.58
1:b:59:ILE:HG21	1:b:81:ILE:HD13	1.85	0.58
1:R:64:GLN:N	1:R:65:PRO:HD2	2.19	0.57
1:R:47:PRO:O	1:R:50:LEU:HG	2.04	0.57
1:b:59:ILE:CG2	1:b:81:ILE:HD13	2.35	0.57
1:E:50:LEU:O	1:E:88:HIS:CD2	2.58	0.57
1:I:2:ALA:H	2:I:201:MYR:C1	2.17	0.57
1:b:67:LEU:HD11	1:b:78:TYR:CE1	2.39	0.56
1:G:53:SER:O	1:G:85:TYR:CE1	2.59	0.56
1:H:40:LEU:HD11	1:H:45:VAL:CG1	2.36	0.56
1:L:14:LYS:O	1:L:18:ILE:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:67:LEU:HD11	1:m:78:TYR:CD1	2.42	0.55
1:H:82:ALA:HB1	1:H:103:ILE:HD11	1.87	0.55
1:L:36:ALA:HB1	1:L:77:LEU:CD1	2.37	0.55
1:H:40:LEU:CD1	1:H:45:VAL:HB	2.36	0.54
1:h:13:ASP:OD1	1:h:17:LYS:NZ	2.40	0.54
1:O:49:LEU:HD12	1:O:55:GLY:HA2	1.89	0.54
1:W:15:TRP:CZ3	1:W:84:LEU:HD23	2.42	0.54
1:E:50:LEU:O	1:E:88:HIS:NE2	2.41	0.54
1:R:92:ASP:OD1	1:R:94:LYS:NZ	2.40	0.54
1:f:67:LEU:HD11	1:f:78:TYR:CD1	2.43	0.54
1:W:59:ILE:HG21	1:W:81:ILE:HD13	1.89	0.54
1:I:2:ALA:N	2:I:201:MYR:C1	2.71	0.54
1:U:50:LEU:HD22	1:U:84:LEU:CD1	2.38	0.54
1:J:40:LEU:HD12	1:J:50:LEU:HD11	1.90	0.53
1:G:53:SER:HB2	1:G:85:TYR:HE1	1.70	0.53
1:W:15:TRP:CZ3	1:W:84:LEU:CD2	2.91	0.53
1:k:99:ALA:O	1:k:103:ILE:HG12	2.09	0.53
1:f:40:LEU:HD12	1:f:50:LEU:HD11	1.90	0.53
1:f:3:ARG:O	1:f:6:VAL:HG22	2.09	0.52
1:m:59:ILE:HG21	1:m:81:ILE:HD13	1.90	0.52
1:D:57:ARG:HD3	1:D:85:TYR:OH	2.09	0.51
1:I:3:ARG:NH1	2:I:201:MYR:C1	2.73	0.51
1:a:40:LEU:HD21	1:a:81:ILE:HD11	1.93	0.51
1:c:3:ARG:HH11	2:c:201:MYR:C1	2.24	0.51
1:A:67:LEU:HD11	1:A:78:TYR:CE1	2.46	0.51
1:E:83:VAL:O	1:E:87:VAL:HG23	2.11	0.50
1:R:13:ASP:OD1	1:R:17:LYS:NZ	2.45	0.50
1:X:3:ARG:NH1	2:X:201:MYR:C1	2.75	0.50
1:e:82:ALA:HB1	1:e:103:ILE:CD1	2.40	0.50
1:m:67:LEU:HD11	1:m:78:TYR:CE1	2.47	0.50
1:Z:35:TRP:CH2	1:Z:73:GLU:HB3	2.46	0.50
1:a:3:ARG:O	1:a:6:VAL:HG22	2.12	0.50
1:f:67:LEU:HD11	1:f:78:TYR:CG	2.47	0.50
1:h:86:CYS:SG	1:h:99:ALA:HB1	2.51	0.50
1:I:13:ASP:OD1	1:I:17:LYS:NZ	2.45	0.49
1:N:64:GLN:N	1:N:65:PRO:HD2	2.27	0.49
1:U:40:LEU:HD12	1:U:50:LEU:HD11	1.93	0.49
1:b:105:GLU:OE2	1:b:112:LYS:NZ	2.41	0.49
1:H:64:GLN:HB3	1:H:65:PRO:HD3	1.93	0.49
1:J:83:VAL:O	1:J:87:VAL:HG23	2.11	0.49
1:k:82:ALA:HB1	1:k:103:ILE:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:40:LEU:HD22	1:H:50:LEU:CD1	2.42	0.49
1:Q:13:ASP:OD1	1:Q:17:LYS:NZ	2.46	0.49
1:Q:3:ARG:O	1:Q:6:VAL:HG22	2.13	0.49
1:A:15:TRP:HB3	1:A:28:TYR:HB2	1.95	0.49
1:O:49:LEU:CD1	1:O:55:GLY:CA	2.91	0.48
1:S:67:LEU:HD11	1:S:78:TYR:CE1	2.48	0.48
1:N:15:TRP:HH2	1:N:80:THR:HG23	1.75	0.48
1:Q:20:LEU:HG	1:Q:28:TYR:CE2	2.48	0.48
1:F:92:ASP:OD1	1:F:94:LYS:NZ	2.47	0.48
1:G:13:ASP:O	1:G:17:LYS:HG2	2.13	0.48
1:Z:35:TRP:CZ2	1:Z:73:GLU:HB3	2.49	0.48
1:a:64:GLN:HB3	1:a:65:PRO:HD3	1.96	0.47
1:D:57:ARG:HB2	1:D:85:TYR:CE1	2.49	0.47
1:D:50:LEU:HA	1:D:56:CYS:SG	2.54	0.47
1:J:36:ALA:O	1:J:40:LEU:HG	2.15	0.47
1:E:63:LEU:O	1:E:64:GLN:C	2.55	0.47
1:H:40:LEU:HD11	1:H:45:VAL:HG11	1.95	0.47
1:I:92:ASP:OD2	1:I:94:LYS:NZ	2.47	0.47
1:R:39:GLU:O	1:R:42:ARG:HB3	2.15	0.47
1:P:23:GLY:HA3	1:h:72:GLU:OE2	2.15	0.46
1:Z:3:ARG:NH1	2:Z:201:MYR:C1	2.77	0.46
1:l:3:ARG:HH11	2:l:201:MYR:C1	2.27	0.46
1:l:3:ARG:HG2	2:l:201:MYR:O1	2.16	0.46
1:T:77:LEU:C	1:T:77:LEU:HD23	2.40	0.46
1:e:82:ALA:CB	1:e:103:ILE:HD11	2.45	0.46
1:T:3:ARG:O	1:T:6:VAL:HG22	2.16	0.46
1:k:83:VAL:O	1:k:87:VAL:HG23	2.15	0.46
1:S:83:VAL:O	1:S:87:VAL:HG23	2.16	0.46
1:k:9:GLY:O	1:k:14:LYS:NZ	2.49	0.46
1:J:73:GLU:OE2	1:M:25:LYS:NZ	2.49	0.46
1:A:67:LEU:HD11	1:A:78:TYR:CG	2.51	0.46
1:Z:15:TRP:CZ2	1:Z:84:LEU:HD23	2.50	0.46
1:W:13:ASP:OD1	1:W:17:LYS:NZ	2.48	0.46
1:G:64:GLN:N	1:G:65:PRO:HD2	2.32	0.45
1:Q:83:VAL:O	1:Q:87:VAL:HG23	2.16	0.45
1:G:83:VAL:O	1:G:87:VAL:HG23	2.16	0.45
1:c:3:ARG:O	1:c:6:VAL:HG22	2.17	0.45
1:N:9:GLY:O	1:N:14:LYS:NZ	2.48	0.45
1:G:16:GLU:O	1:G:27:GLN:HG2	2.16	0.45
1:d:13:ASP:OD1	1:d:17:LYS:NZ	2.49	0.45
1:B:15:TRP:CZ2	1:B:84:LEU:HG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:19:ARG:HB3	1:R:21:ARG:O	2.16	0.45
1:G:79:ASN:O	1:G:83:VAL:HG23	2.17	0.45
1:f:98:GLU:O	1:f:102:LYS:HG2	2.17	0.45
1:k:79:ASN:O	1:k:83:VAL:HG23	2.17	0.44
1:Z:15:TRP:CZ2	1:Z:84:LEU:HD22	2.53	0.44
1:J:68:GLN:H	1:J:68:GLN:CD	2.25	0.44
1:S:64:GLN:HB3	1:S:65:PRO:HD3	1.99	0.44
1:Z:3:ARG:HH11	2:Z:201:MYR:C1	2.30	0.44
1:f:83:VAL:O	1:f:87:VAL:HG23	2.18	0.44
1:D:99:ALA:O	1:D:103:ILE:HG13	2.17	0.44
1:J:40:LEU:CD1	1:J:50:LEU:HD11	2.47	0.44
1:U:84:LEU:O	1:U:87:VAL:HG22	2.17	0.44
1:X:3:ARG:HH11	2:X:201:MYR:C1	2.31	0.44
1:Q:105:GLU:O	1:Q:109:LYS:N	2.50	0.44
1:b:27:GLN:N	1:b:27:GLN:CD	2.76	0.44
1:b:35:TRP:CZ2	1:b:39:GLU:HG3	2.53	0.43
1:G:18:ILE:HD11	1:G:83:VAL:CG1	2.49	0.43
1:F:21:ARG:HB3	1:F:22:PRO:HD2	1.99	0.43
1:O:49:LEU:CD1	1:O:55:GLY:HA3	2.49	0.43
1:l:15:TRP:CE2	1:l:28:TYR:HB3	2.53	0.43
1:V:74:LEU:C	1:V:74:LEU:HD23	2.43	0.43
1:c:40:LEU:HD12	1:c:50:LEU:HD11	2.01	0.43
1:C:70:GLY:O	1:C:75:ARG:NH1	2.52	0.43
1:a:92:ASP:OD1	1:a:92:ASP:C	2.61	0.42
1:L:70:GLY:O	1:L:75:ARG:NH1	2.53	0.42
1:c:3:ARG:NH1	2:c:201:MYR:C1	2.82	0.42
1:f:40:LEU:HD11	1:f:50:LEU:HD11	2.00	0.42
1:Z:12:LEU:HA	1:Z:15:TRP:HE3	1.81	0.42
1:A:43:PHE:CZ	1:A:74:LEU:HD13	2.55	0.42
1:e:64:GLN:N	1:e:65:PRO:HD2	2.34	0.42
1:D:15:TRP:CZ2	1:D:84:LEU:HG	2.55	0.42
1:O:82:ALA:CB	1:O:103:ILE:HD11	2.50	0.42
1:A:15:TRP:NE1	1:A:84:LEU:HD23	2.34	0.42
1:H:40:LEU:HD12	1:H:45:VAL:HB	1.99	0.42
1:W:59:ILE:CG2	1:W:81:ILE:HD13	2.50	0.41
1:F:52:THR:HG23	1:F:55:GLY:H	1.85	0.41
1:N:50:LEU:HA	1:N:56:CYS:SG	2.61	0.41
1:R:63:LEU:C	1:R:65:PRO:HD2	2.45	0.41
1:G:36:ALA:HB1	1:G:77:LEU:CD1	2.50	0.41
1:N:3:ARG:HH11	2:N:201:MYR:C1	2.34	0.41
1:C:33:ILE:O	1:C:37:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:67:LEU:HD11	1:S:78:TYR:CD1	2.56	0.41
1:L:36:ALA:HB1	1:L:77:LEU:HD13	2.02	0.41
1:a:15:TRP:CH2	1:a:80:THR:HG23	2.55	0.41
1:G:77:LEU:HD12	1:G:80:THR:HB	2.03	0.41
1:b:67:LEU:HD11	1:b:78:TYR:CZ	2.56	0.41
1:B:95:ASP:OD2	1:B:95:ASP:C	2.64	0.40
1:Q:79:ASN:O	1:Q:83:VAL:HG23	2.22	0.40
1:K:83:VAL:O	1:K:87:VAL:HG23	2.21	0.40
1:m:15:TRP:CH2	1:m:80:THR:HG23	2.57	0.40
1:O:3:ARG:O	1:O:6:VAL:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
1	B	113/115 (98%)	113 (100%)	0	0	100	100
1	C	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
1	D	113/115 (98%)	113 (100%)	0	0	100	100
1	E	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
1	F	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
1	G	113/115 (98%)	113 (100%)	0	0	100	100
1	H	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
1	I	113/115 (98%)	113 (100%)	0	0	100	100
1	J	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
1	K	113/115 (98%)	113 (100%)	0	0	100	100
1	L	113/115 (98%)	112 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	113/115 (98%)	113 (100%)	0	0	100	100
1	N	113/115 (98%)	113 (100%)	0	0	100	100
1	O	113/115 (98%)	113 (100%)	0	0	100	100
1	P	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
1	Q	113/115 (98%)	113 (100%)	0	0	100	100
1	R	113/115 (98%)	113 (100%)	0	0	100	100
1	S	113/115 (98%)	113 (100%)	0	0	100	100
1	T	113/115 (98%)	113 (100%)	0	0	100	100
1	U	113/115 (98%)	113 (100%)	0	0	100	100
1	V	113/115 (98%)	113 (100%)	0	0	100	100
1	W	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
1	X	113/115 (98%)	113 (100%)	0	0	100	100
1	Y	113/115 (98%)	113 (100%)	0	0	100	100
1	Z	113/115 (98%)	113 (100%)	0	0	100	100
1	a	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
1	b	113/115 (98%)	113 (100%)	0	0	100	100
1	c	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
1	d	113/115 (98%)	113 (100%)	0	0	100	100
1	e	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
1	f	113/115 (98%)	113 (100%)	0	0	100	100
1	g	113/115 (98%)	112 (99%)	0	1 (1%)	14	51
1	h	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
1	i	113/115 (98%)	113 (100%)	0	0	100	100
1	j	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
1	k	113/115 (98%)	113 (100%)	0	0	100	100
1	l	113/115 (98%)	113 (100%)	0	0	100	100
1	m	113/115 (98%)	113 (100%)	0	0	100	100
All	All	4407/4485 (98%)	4389 (100%)	17 (0%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	g	25	LYS

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	99/99 (100%)	99 (100%)	0	100	100
1	B	99/99 (100%)	99 (100%)	0	100	100
1	C	99/99 (100%)	99 (100%)	0	100	100
1	D	99/99 (100%)	99 (100%)	0	100	100
1	E	99/99 (100%)	99 (100%)	0	100	100
1	F	99/99 (100%)	99 (100%)	0	100	100
1	G	99/99 (100%)	99 (100%)	0	100	100
1	H	99/99 (100%)	99 (100%)	0	100	100
1	I	99/99 (100%)	99 (100%)	0	100	100
1	J	99/99 (100%)	99 (100%)	0	100	100
1	K	99/99 (100%)	99 (100%)	0	100	100
1	L	99/99 (100%)	99 (100%)	0	100	100
1	M	99/99 (100%)	99 (100%)	0	100	100
1	N	99/99 (100%)	99 (100%)	0	100	100
1	O	99/99 (100%)	99 (100%)	0	100	100
1	P	99/99 (100%)	98 (99%)	1 (1%)	68	78
1	Q	99/99 (100%)	99 (100%)	0	100	100
1	R	99/99 (100%)	99 (100%)	0	100	100
1	S	99/99 (100%)	98 (99%)	1 (1%)	68	78
1	T	99/99 (100%)	99 (100%)	0	100	100
1	U	99/99 (100%)	99 (100%)	0	100	100
1	V	99/99 (100%)	99 (100%)	0	100	100
1	W	99/99 (100%)	99 (100%)	0	100	100
1	X	99/99 (100%)	99 (100%)	0	100	100
1	Y	99/99 (100%)	99 (100%)	0	100	100
1	Z	99/99 (100%)	99 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	99/99 (100%)	99 (100%)	0	100	100
1	b	99/99 (100%)	99 (100%)	0	100	100
1	c	99/99 (100%)	99 (100%)	0	100	100
1	d	99/99 (100%)	99 (100%)	0	100	100
1	e	99/99 (100%)	99 (100%)	0	100	100
1	f	99/99 (100%)	99 (100%)	0	100	100
1	g	99/99 (100%)	99 (100%)	0	100	100
1	h	99/99 (100%)	99 (100%)	0	100	100
1	i	99/99 (100%)	98 (99%)	1 (1%)	68	78
1	j	99/99 (100%)	99 (100%)	0	100	100
1	k	99/99 (100%)	99 (100%)	0	100	100
1	l	99/99 (100%)	99 (100%)	0	100	100
1	m	99/99 (100%)	99 (100%)	0	100	100
All	All	3861/3861 (100%)	3858 (100%)	3 (0%)	87	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	52	THR
1	S	52	THR
1	i	52	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	115	GLN
1	D	89	GLN
1	E	88	HIS
1	F	32	HIS
1	H	89	GLN
1	I	89	GLN
1	K	68	GLN
1	L	89	GLN
1	Q	64	GLN
1	R	62	GLN
1	S	58	GLN

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Mol	Chain	Res	Type
1	T	64	GLN
1	U	32	HIS
1	Y	32	HIS
1	Y	79	ASN
1	c	32	HIS
1	d	32	HIS
1	e	89	GLN
1	f	27	GLN
1	f	62	GLN
1	k	58	GLN
1	m	64	GLN
1	m	107	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

39 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MYR	N	201	1	13,14,15	0.47	0	12,13,15	0.37	0
2	MYR	f	201	1	13,14,15	0.52	0	12,13,15	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MYR	A	201	1	13,14,15	0.51	0	12,13,15	0.31	0
2	MYR	X	201	1	13,14,15	0.49	0	12,13,15	0.35	0
2	MYR	c	201	1	13,14,15	0.51	0	12,13,15	0.39	0
2	MYR	P	201	1	13,14,15	0.53	0	12,13,15	0.25	0
2	MYR	R	201	1	13,14,15	0.51	0	12,13,15	0.31	0
2	MYR	F	201	1	13,14,15	0.51	0	12,13,15	0.33	0
2	MYR	M	201	1	13,14,15	0.51	0	12,13,15	0.31	0
2	MYR	D	201	1	13,14,15	0.52	0	12,13,15	0.31	0
2	MYR	C	201	1	13,14,15	0.53	0	12,13,15	0.32	0
2	MYR	K	201	1	13,14,15	0.51	0	12,13,15	0.32	0
2	MYR	j	201	1	13,14,15	0.52	0	12,13,15	0.31	0
2	MYR	a	201	1	13,14,15	0.51	0	12,13,15	0.37	0
2	MYR	H	201	1	13,14,15	0.48	0	12,13,15	0.33	0
2	MYR	I	201	1	13,14,15	0.53	0	12,13,15	0.45	0
2	MYR	m	201	1	13,14,15	0.51	0	12,13,15	0.30	0
2	MYR	i	201	1	13,14,15	0.52	0	12,13,15	0.35	0
2	MYR	d	201	1	13,14,15	0.51	0	12,13,15	0.35	0
2	MYR	W	201	1	13,14,15	0.53	0	12,13,15	0.37	0
2	MYR	Z	201	1	13,14,15	0.53	0	12,13,15	0.41	0
2	MYR	b	201	1	13,14,15	0.53	0	12,13,15	0.32	0
2	MYR	B	201	1	13,14,15	0.50	0	12,13,15	0.27	0
2	MYR	g	201	1	13,14,15	0.51	0	12,13,15	0.35	0
2	MYR	e	201	1	13,14,15	0.50	0	12,13,15	0.35	0
2	MYR	k	201	1	13,14,15	0.55	0	12,13,15	0.38	0
2	MYR	V	201	1	13,14,15	0.56	0	12,13,15	0.33	0
2	MYR	S	201	1	13,14,15	0.51	0	12,13,15	0.27	0
2	MYR	Q	201	1	13,14,15	0.51	0	12,13,15	0.34	0
2	MYR	L	201	1	13,14,15	0.51	0	12,13,15	0.32	0
2	MYR	O	201	1	13,14,15	0.52	0	12,13,15	0.32	0
2	MYR	h	201	1	13,14,15	0.51	0	12,13,15	0.32	0
2	MYR	l	201	1	13,14,15	0.49	0	12,13,15	0.35	0
2	MYR	J	201	1	13,14,15	0.54	0	12,13,15	0.28	0
2	MYR	U	201	1	13,14,15	0.54	0	12,13,15	0.34	0
2	MYR	T	201	1	13,14,15	0.52	0	12,13,15	0.35	0
2	MYR	E	201	1	13,14,15	0.55	0	12,13,15	0.30	0
2	MYR	G	201	1	13,14,15	0.52	0	12,13,15	0.30	0
2	MYR	Y	201	1	13,14,15	0.50	0	12,13,15	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MYR	N	201	1	-	0/12/12/13	-
2	MYR	f	201	1	-	2/12/12/13	-
2	MYR	A	201	1	-	0/12/12/13	-
2	MYR	X	201	1	-	1/12/12/13	-
2	MYR	c	201	1	-	0/12/12/13	-
2	MYR	P	201	1	-	2/12/12/13	-
2	MYR	R	201	1	-	2/12/12/13	-
2	MYR	F	201	1	-	1/12/12/13	-
2	MYR	M	201	1	-	1/12/12/13	-
2	MYR	D	201	1	-	0/12/12/13	-
2	MYR	C	201	1	-	5/12/12/13	-
2	MYR	K	201	1	-	0/12/12/13	-
2	MYR	j	201	1	-	0/12/12/13	-
2	MYR	a	201	1	-	2/12/12/13	-
2	MYR	H	201	1	-	1/12/12/13	-
2	MYR	I	201	1	-	0/12/12/13	-
2	MYR	m	201	1	-	1/12/12/13	-
2	MYR	i	201	1	-	1/12/12/13	-
2	MYR	d	201	1	-	1/12/12/13	-
2	MYR	W	201	1	-	3/12/12/13	-
2	MYR	Z	201	1	-	0/12/12/13	-
2	MYR	b	201	1	-	1/12/12/13	-
2	MYR	B	201	1	-	4/12/12/13	-
2	MYR	g	201	1	-	2/12/12/13	-
2	MYR	e	201	1	-	1/12/12/13	-
2	MYR	k	201	1	-	2/12/12/13	-
2	MYR	V	201	1	-	2/12/12/13	-
2	MYR	S	201	1	-	1/12/12/13	-
2	MYR	Q	201	1	-	1/12/12/13	-
2	MYR	L	201	1	-	0/12/12/13	-
2	MYR	O	201	1	-	1/12/12/13	-
2	MYR	h	201	1	-	1/12/12/13	-
2	MYR	l	201	1	-	0/12/12/13	-
2	MYR	J	201	1	-	0/12/12/13	-
2	MYR	U	201	1	-	3/12/12/13	-
2	MYR	T	201	1	-	0/12/12/13	-
2	MYR	E	201	1	-	1/12/12/13	-
2	MYR	G	201	1	-	0/12/12/13	-
2	MYR	Y	201	1	-	1/12/12/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	201	MYR	O1-C1-C2-C3
2	M	201	MYR	O1-C1-C2-C3
2	O	201	MYR	O1-C1-C2-C3
2	P	201	MYR	O1-C1-C2-C3
2	Q	201	MYR	O1-C1-C2-C3
2	R	201	MYR	O1-C1-C2-C3
2	S	201	MYR	O1-C1-C2-C3
2	U	201	MYR	O1-C1-C2-C3
2	W	201	MYR	O1-C1-C2-C3
2	Y	201	MYR	O1-C1-C2-C3
2	a	201	MYR	O1-C1-C2-C3
2	d	201	MYR	O1-C1-C2-C3
2	e	201	MYR	O1-C1-C2-C3
2	f	201	MYR	O1-C1-C2-C3
2	g	201	MYR	O1-C1-C2-C3
2	h	201	MYR	O1-C1-C2-C3
2	i	201	MYR	O1-C1-C2-C3
2	U	201	MYR	C9-C10-C11-C12
2	m	201	MYR	C11-C10-C9-C8
2	E	201	MYR	C7-C8-C9-C10
2	R	201	MYR	C5-C6-C7-C8
2	f	201	MYR	C6-C7-C8-C9
2	B	201	MYR	C9-C10-C11-C12
2	C	201	MYR	C6-C7-C8-C9
2	F	201	MYR	C5-C6-C7-C8
2	V	201	MYR	C3-C4-C5-C6
2	W	201	MYR	C3-C4-C5-C6
2	k	201	MYR	C2-C3-C4-C5
2	C	201	MYR	C11-C10-C9-C8
2	B	201	MYR	C7-C8-C9-C10
2	g	201	MYR	C4-C5-C6-C7
2	X	201	MYR	C7-C8-C9-C10
2	B	201	MYR	C3-C4-C5-C6
2	U	201	MYR	C10-C11-C12-C13
2	b	201	MYR	C10-C11-C12-C13
2	k	201	MYR	C4-C5-C6-C7
2	V	201	MYR	C10-C11-C12-C13
2	C	201	MYR	C1-C2-C3-C4
2	B	201	MYR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	a	201	MYR	C9-C10-C11-C12
2	W	201	MYR	C4-C5-C6-C7
2	C	201	MYR	C2-C3-C4-C5
2	H	201	MYR	C4-C5-C6-C7
2	P	201	MYR	C4-C5-C6-C7

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	201	MYR	1	0
2	X	201	MYR	2	0
2	c	201	MYR	2	0
2	I	201	MYR	3	0
2	Z	201	MYR	2	0
2	l	201	MYR	2	0

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.

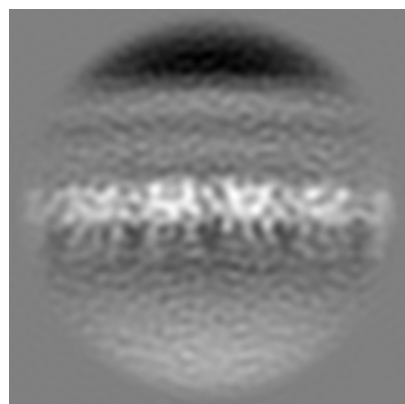
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47842. These allow visual inspection of the internal detail of the map and identification of artifacts.

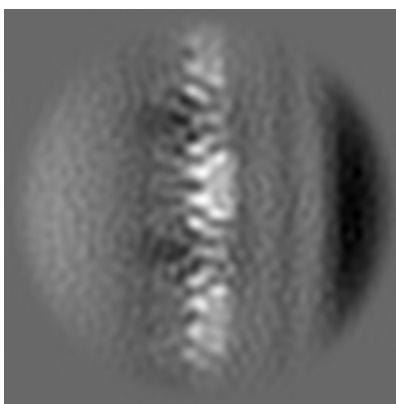
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

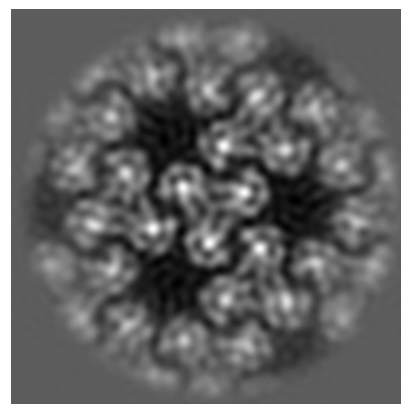
6.1.1 Primary map



X

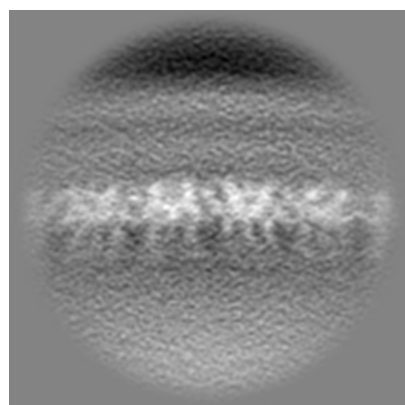


Y



Z

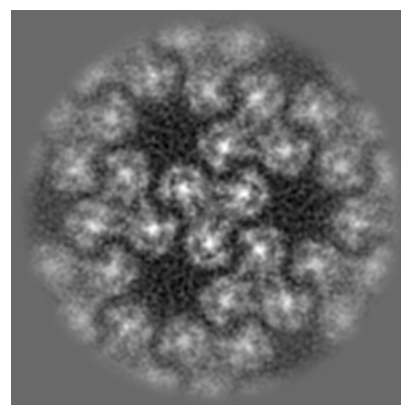
6.1.2 Raw map



X



Y

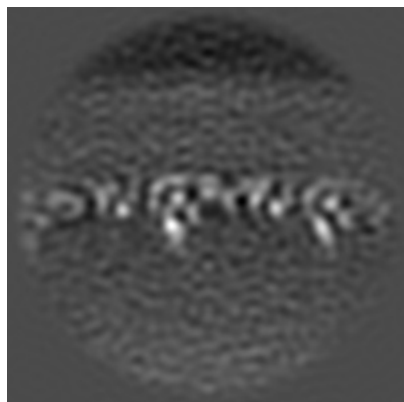


Z

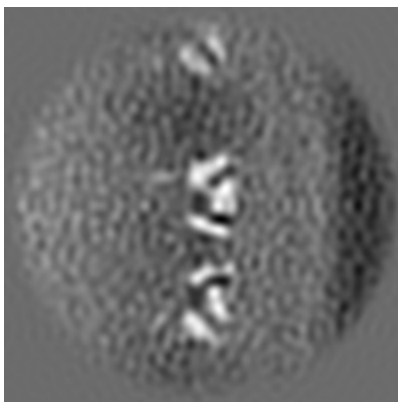
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

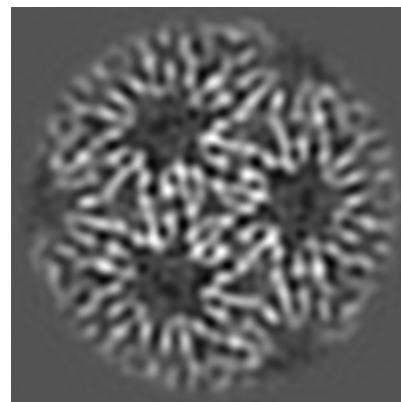
6.2.1 Primary map



X Index: 75

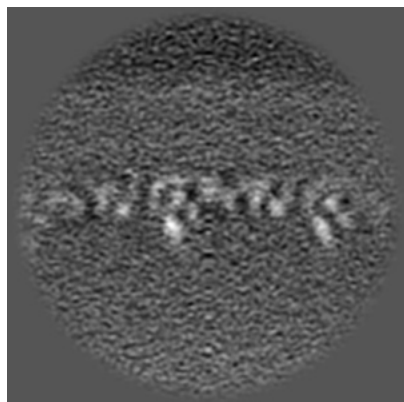


Y Index: 75

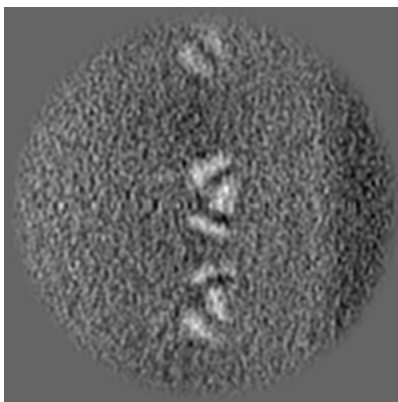


Z Index: 75

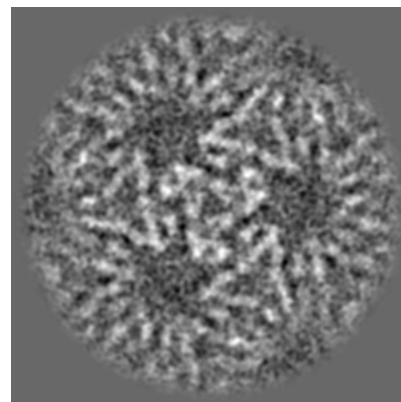
6.2.2 Raw map



X Index: 75



Y Index: 75

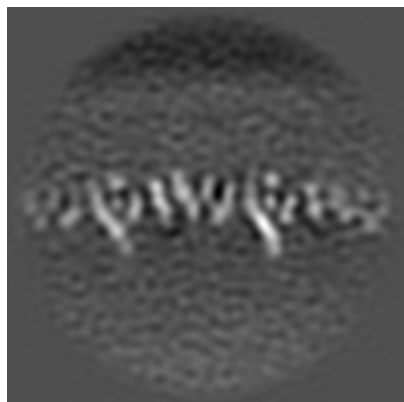


Z Index: 75

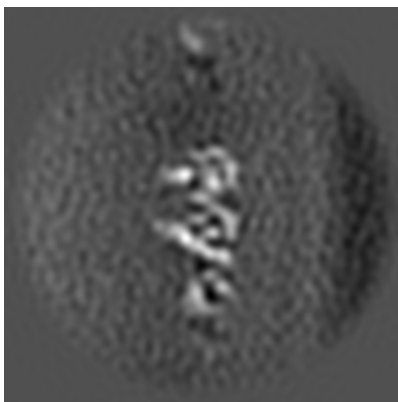
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

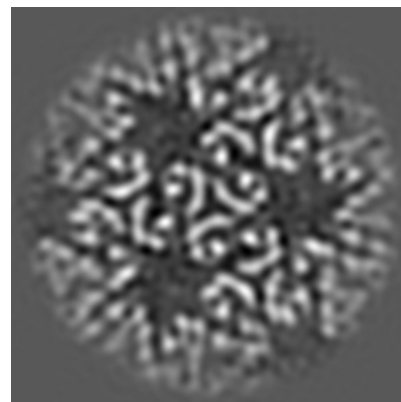
6.3.1 Primary map



X Index: 79

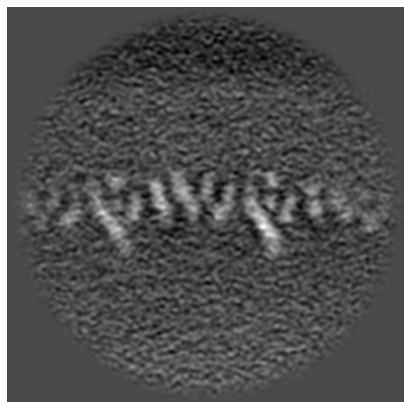


Y Index: 81

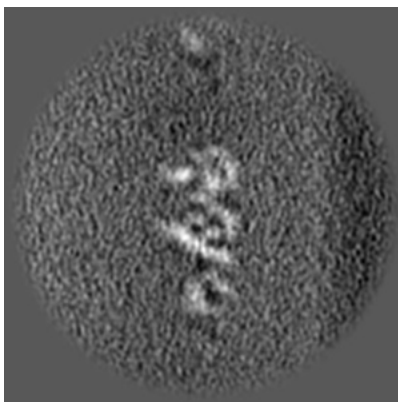


Z Index: 72

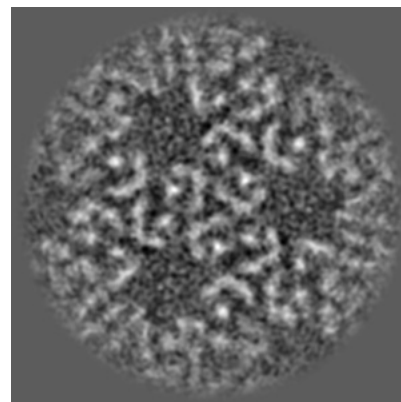
6.3.2 Raw map



X Index: 79



Y Index: 81

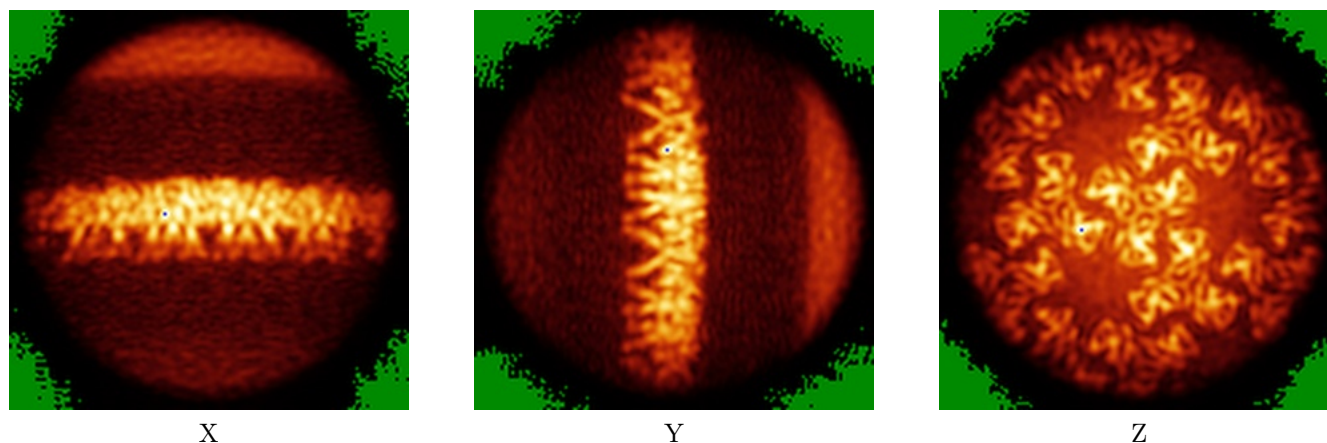


Z Index: 72

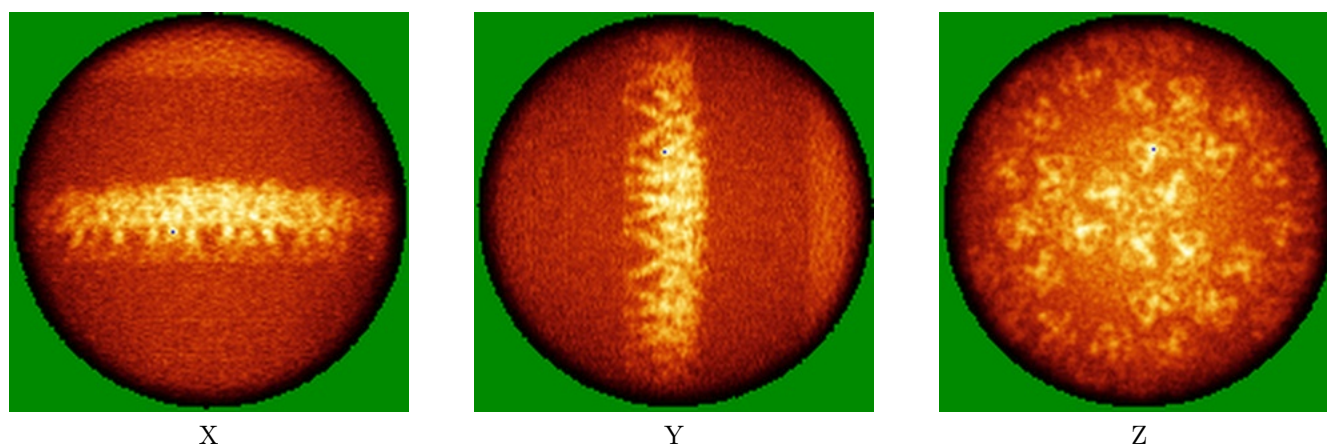
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

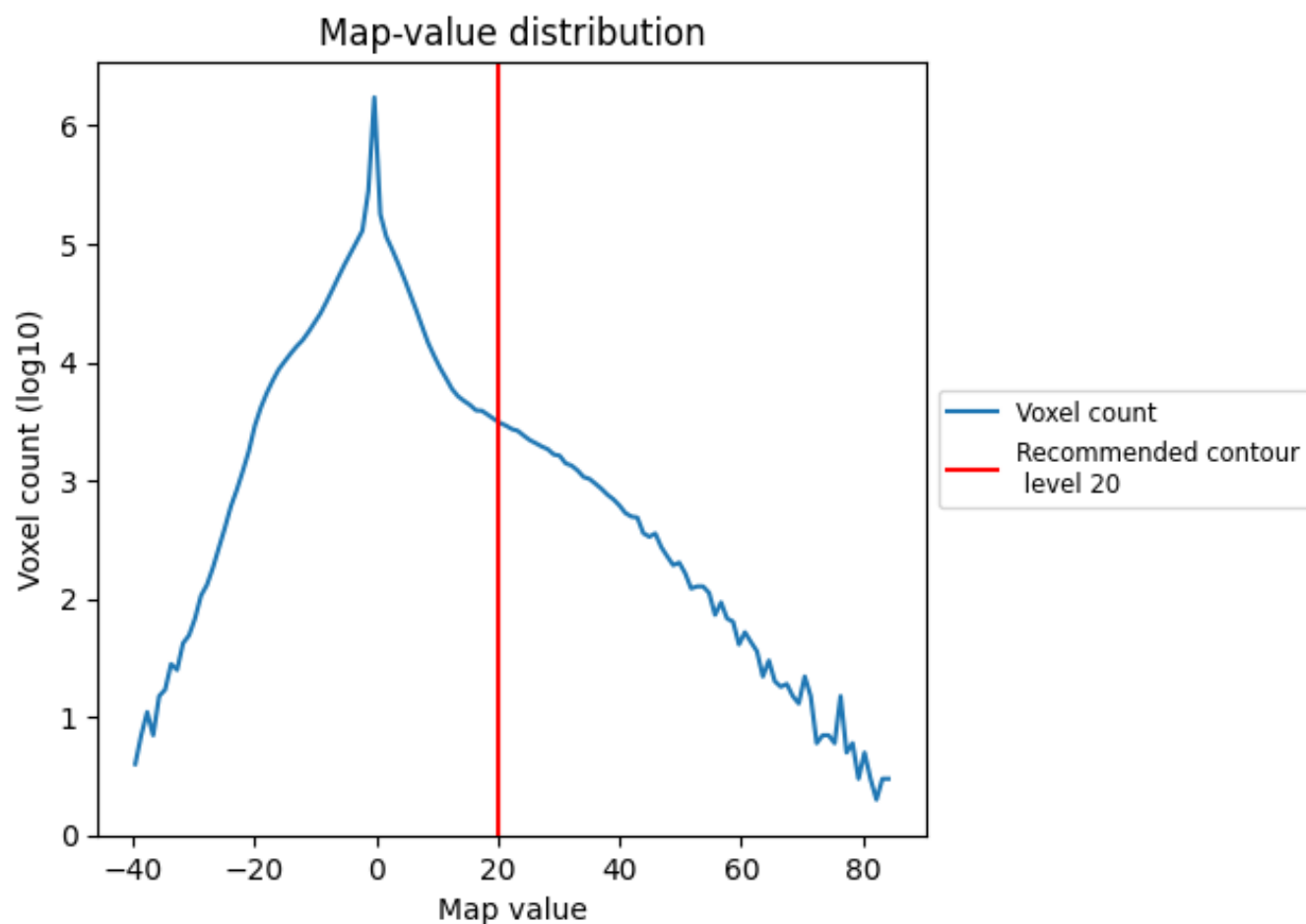
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

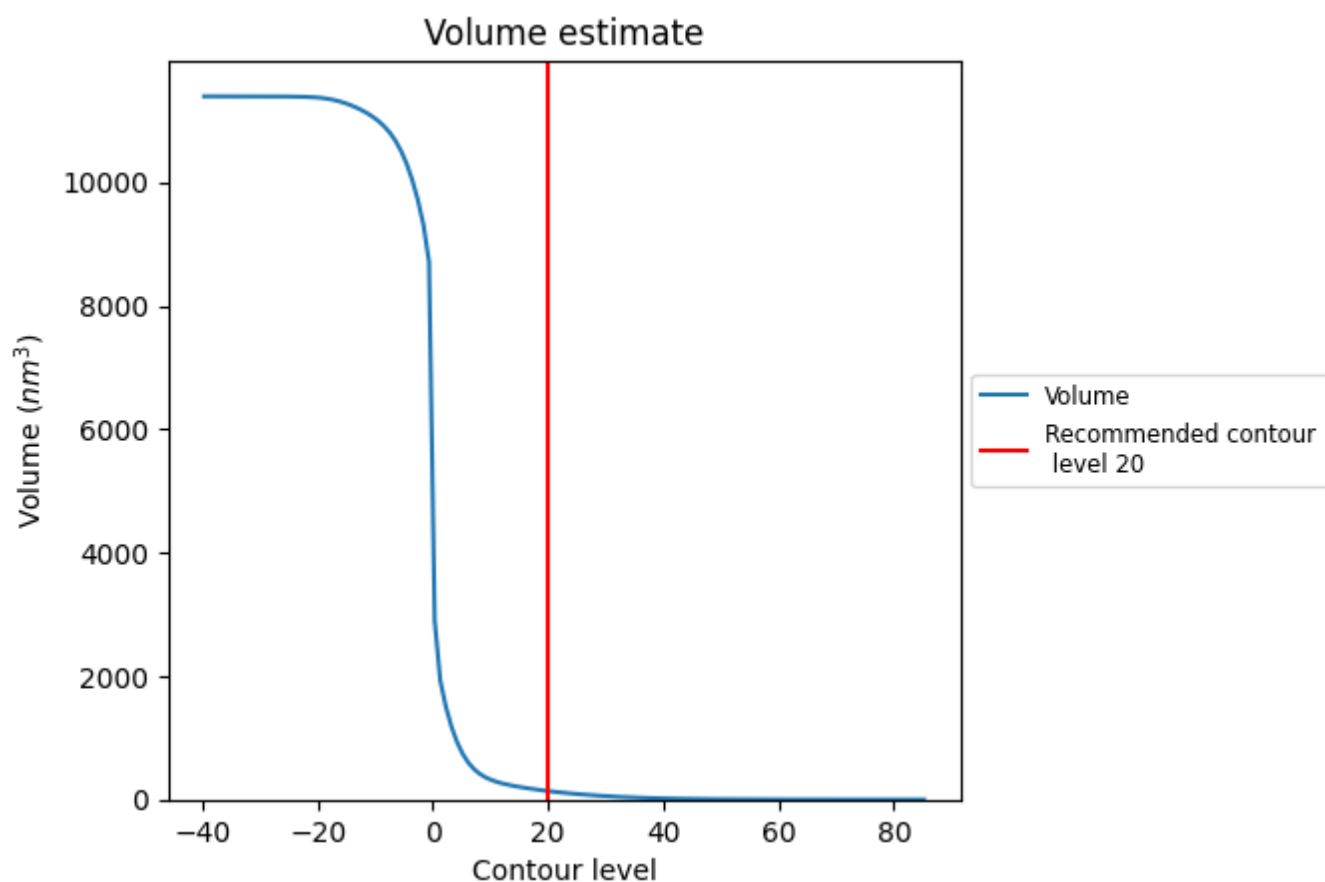
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

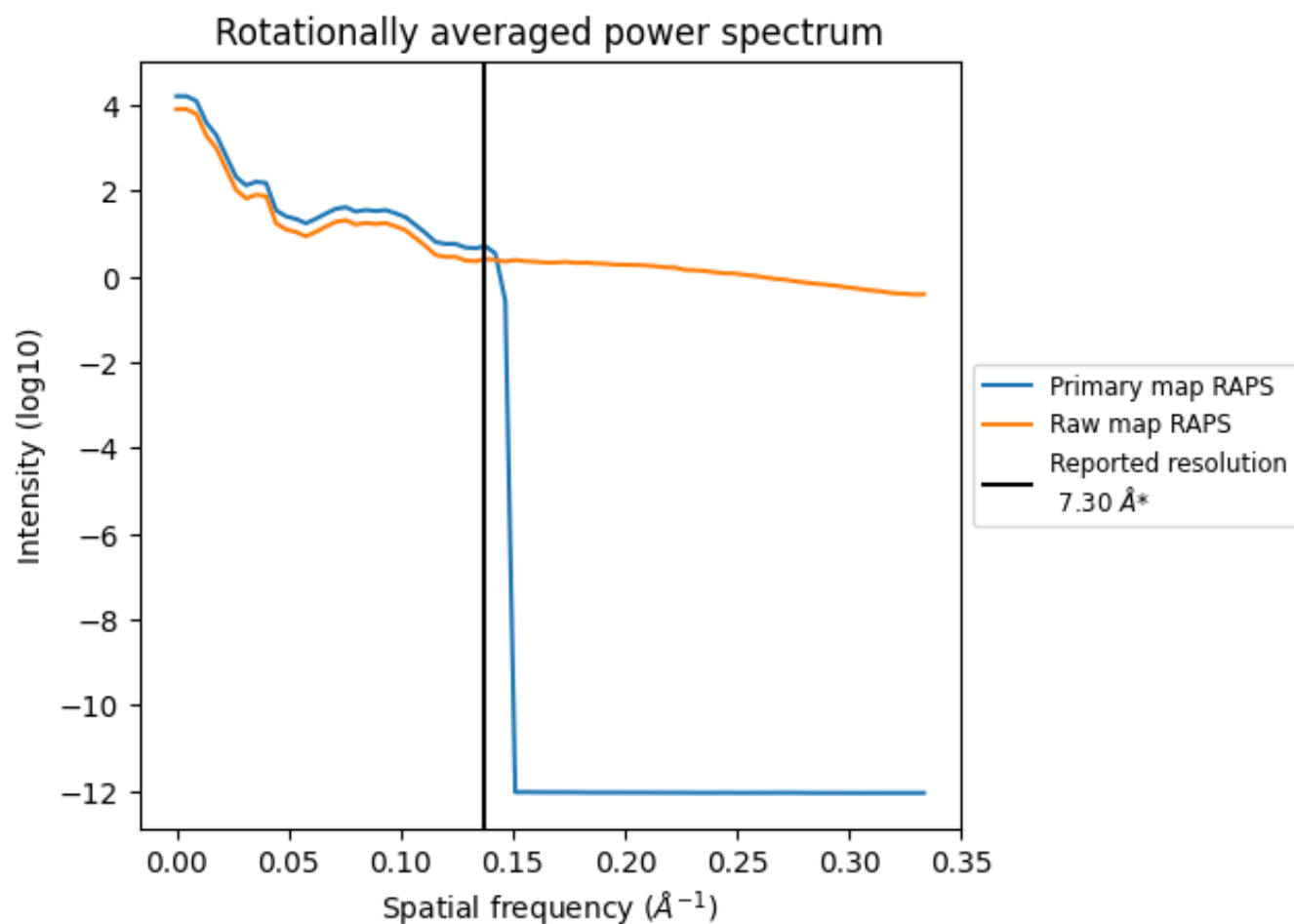
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 138 nm³; this corresponds to an approximate mass of 124 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 ⓘ

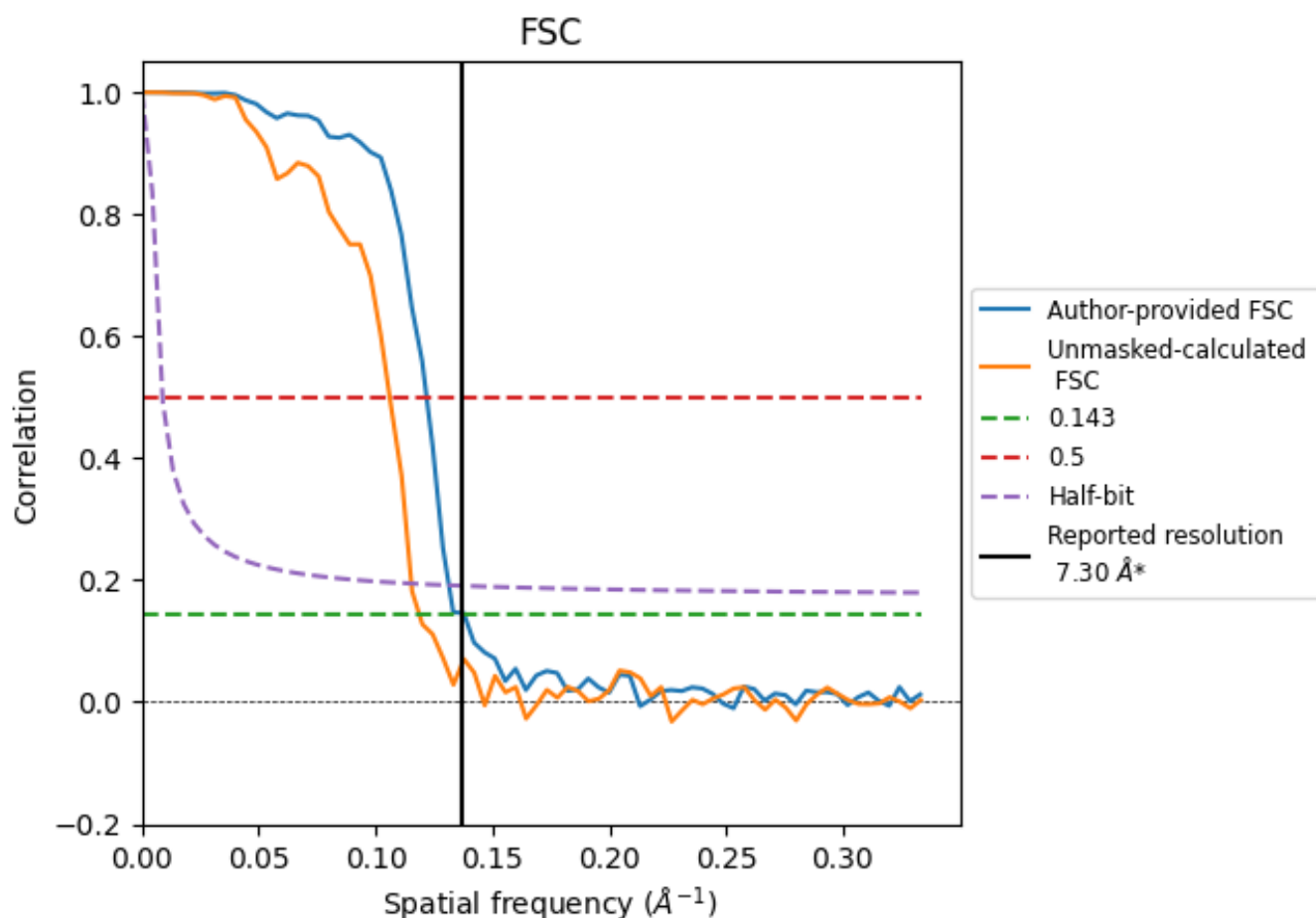


*Reported resolution corresponds to spatial frequency of 0.137 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.137 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

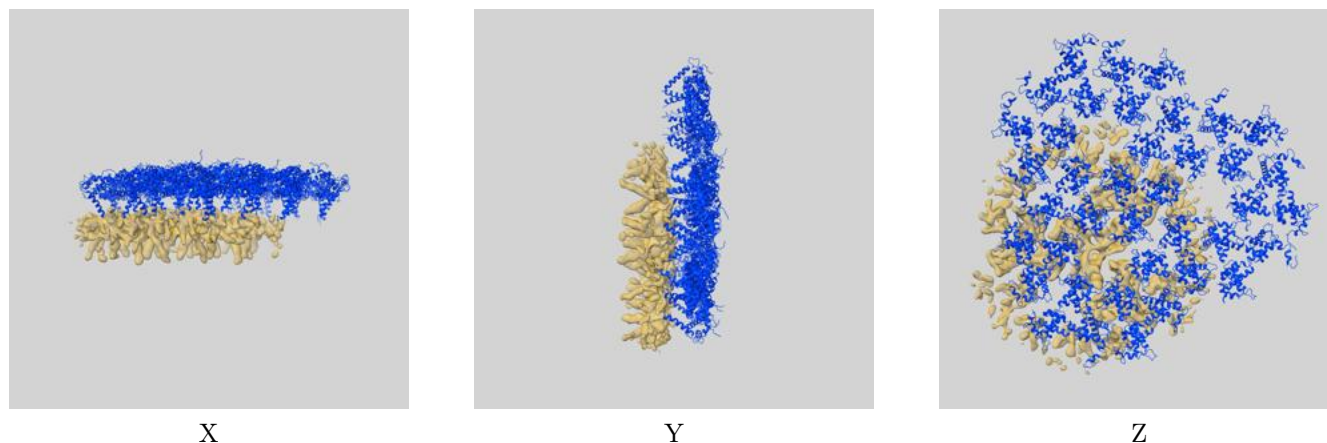
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.30	-	-
Author-provided FSC curve	7.25	8.21	7.61
Unmasked-calculated*	8.42	9.43	8.67

*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 8.42 differs from the reported value 7.3 by more than 10 %

9 Map-model fit [i](#)

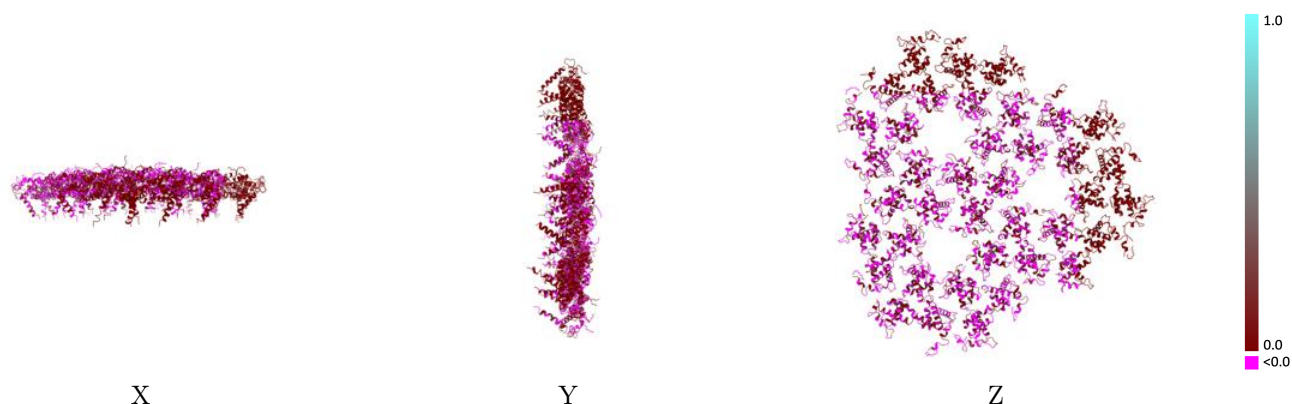
This section contains information regarding the fit between EMDB map EMD-47842 and PDB model 9EK1. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



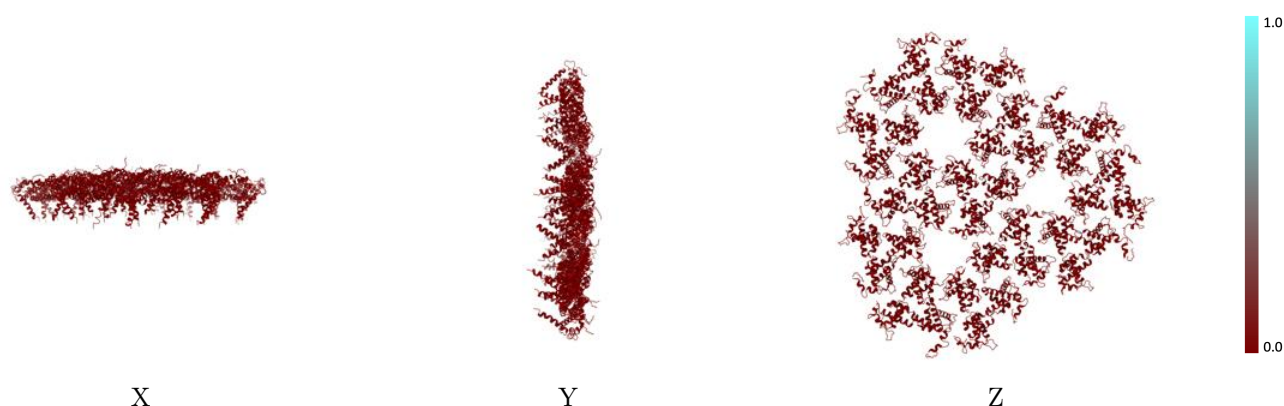
The images above show the 3D surface view of the map at the recommended contour level 20.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



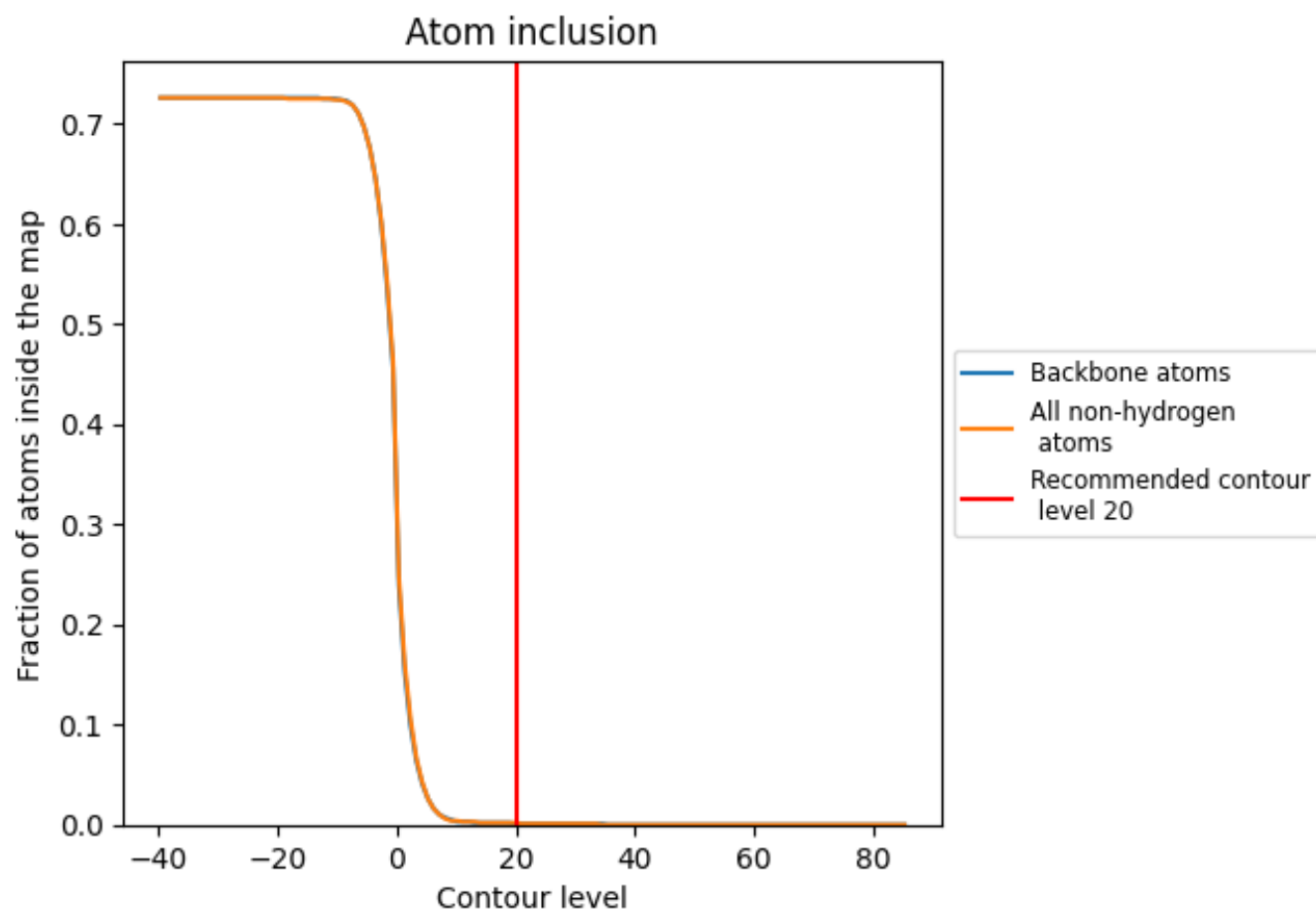
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (20).

9.4 Atom inclusion [i](#)



At the recommended contour level, 0% of all backbone atoms, 0% 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 (20) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0020	-0.0040
A	0.0000	0.0020
B	0.0000	-0.0170
C	0.0000	-0.0130
D	0.0000	-0.0060
E	0.0000	0.0020
F	0.0000	-0.0090
G	0.0000	-0.0210
H	0.0000	-0.0150
I	0.0000	-0.0100
J	0.0000	0.0250
K	0.0030	-0.0210
L	0.0000	0.0030
M	0.0090	-0.0090
N	0.0110	0.0010
O	0.0000	-0.0030
P	0.0000	0.0010
Q	0.0000	-0.0020
R	0.0000	0.0080
S	0.0000	0.0000
T	0.0000	0.0000
U	0.0000	-0.0040
V	0.0000	0.0000
W	0.0000	0.0120
X	0.0000	0.0050
Y	0.0000	0.0110
Z	0.0000	0.0150
a	0.0000	-0.0160
b	0.0140	-0.0200
c	0.0040	-0.0330
d	0.0000	-0.0030
e	0.0140	-0.0040
f	0.0030	-0.0090
g	0.0000	-0.0210
h	0.0000	0.0030



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Chain	Atom inclusion	Q-score
i	 0.0000	 0.0000
j	 0.0000	 0.0000
k	 0.0000	 0.0050
l	 0.0000	 -0.0020
m	 0.0000	 0.0010